Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Steric and electronic control regioselectivity in arylation of carbazoles using dual catalysis

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1. General Information:

All the vials (Borosil) used for carrying out the reactions were dried overnight on hot air oven at 120 ºC. All chemicals were obtained from commercial sources and were used as received unless otherwise noted. Carbazoles[31–33] and aryl diazonium salts[34,35] were synthesized according to literature reports. All the anhydrous solvents required were purchased from TCI, Sigma Aldrich and spectrochem and used without further purification. Reactions were monitored using precoated aluminum supported silica gel 60 F_{254} TLC (thin layer chromatography) plates (Merck) and are visualized by UV light at 254 nm. The final products were purified using column chromatography (100-200 mesh silica gel purchased from Merck). ^{1}H NMR (400 MHz), ^{19}F NMR (376 MHz), and ^{13}C NMR (101 MHz) spectra were recorded on the Bruker AVANCE NEO 400 MHz spectrometer. Deuterated chloroform was used as solvent for NMR, and Chemical shifts (δ) for ^{1}H and ^{13}C-NMR spectra are given in ppm relative to tetramethylsilane (TMS) [δ 7.27 for ^{1}H (chloroform-d), δ 77.0 for ^{13}C (chloroform-d), ^{19}F-NMR spectra are not externally calibrated and chemical shifts are given relative to CCl_3F as received from the automatic data processing. Abbreviations used in the NMR experiments: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; sep, septet; dd, doublet of doublet; m, multiplet. High resolution mass spectra (HRMS) was obtained from Orbitrap Elite HybridIon Trap-Orbitrap (Thermofischer scientific, Newington, NH, USA) Mass spectrometer in electrospray ionization mode (ESI^{+}). X-ray data for the compounds were collected on a Bruker D8 VENTURE diffractometer instrument with an IμS 3.0 Mo source (λ = 0.7107 Å) and a PHOTON-III C28 detector.

2. Optimization table and Experimental procedures

The following substrates containing the directing groups were synthesized using literature procedures.[11]

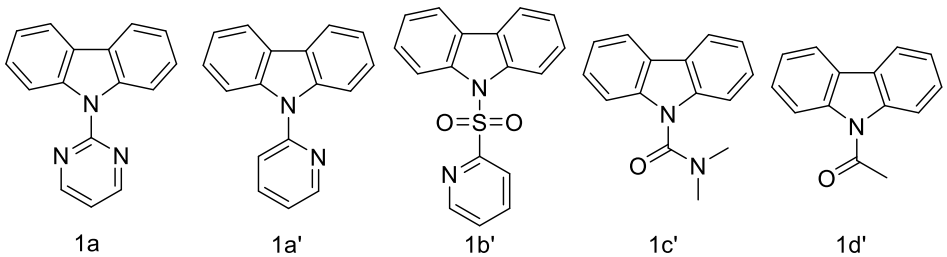


Table S1: Optimization of monoarylation

Sl NO	Photocatalyst	TM (10 mol%)	DG	Solvent	Yield
1	Eosin Y (5 mol %)	$Pd(OAc)_2$	1a	DMF	-
2	$Ru(bpy)_3Cl_2$ (5 mol %)	$Pd(OAc)_2$	1a	DMF	27%
3	**$Ru(bpy)_3Cl_2$ (2.5 mol %)**	**$Pd(OAc)_2$**	**1a**	**MeOH**	**82%**
4	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$	1a'	MeOH	54%
5	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$	1b'	MeOH	Trace
6	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$	1c'	MeOH	-
7	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$	1d'	MeOH	-
8	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$	1a	DMF	-
9		$Pd(OAc)_2$	1a	MeOH	-
10	$Ru(bpy)_3Cl_2$ (2.5 mol %)		1a	MeOH	
11 [b]	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$	1a	MeOH	Trace
12[c]	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$	1a	MeOH	62%
13	fac-$Ir(ppy)_3$ (2.5 mol %)	$Pd(OAc)_2$	1a	MeOH	44%
14	$Ru(phen)_3(PF_6)_2$ (2.5 mol %)	$Pd(OAc)_2$	1a	MeOH	68%

Reaction conditions: Carbazole **1** (1 equiv), aryldiazonium salt **2a** (4 equiv), $Pd(OAc)_2$ (10 mol%), $Ru(bpy)_3Cl_2$ (2.5 mol%), in methanol under argon at room temperature for 24 hours, 44 W Blue LED (Kessil). [b]without light, [c]without argon.

Table S2: Optimization of diarylation

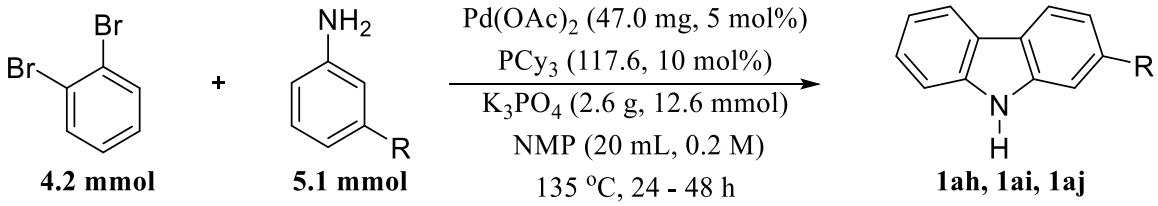
Sl NO	Photocatalyst	TM	Time (h)	ArN_2BF_4 (equiv)	Yield
1	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$ (10 mol %)	36	4	35%
2	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$ (10 mol %)	48	4	35%
3	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$ (10 mol %)	24	5	61%
4	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$ (10 mol %)	24	6	84%
5	$Ru(bpy)_3Cl_2$ (2.5 mo l%)	$Pd(OAc)_2$ (10 mol %)	24	8	79%
6	$Ru(bpy)_3Cl_2$ (5 mol %)	$Pd(OAc)_2$ (10 mol %)	24	6	78%
7	$Ru(bpy)_3Cl_2$ (2.5 mol %)	$Pd(OAc)_2$ (15 mol %)	24	6	76%

Reaction conditions: Carbazoles **1** (1 equiv), Aryl diazonium salt **2** (6 equiv), $Ru(bpy)_3Cl_2$ (2.5 mol %), $Pd(OAc)_2$ (10 mol %), in methanol under argon at room temperature for 24 h, 44 W Blue LED (Kessil).

2.1. General procedure for the synthesis of 9*H*-carbazoles (1ah, 1ai, 1aj)

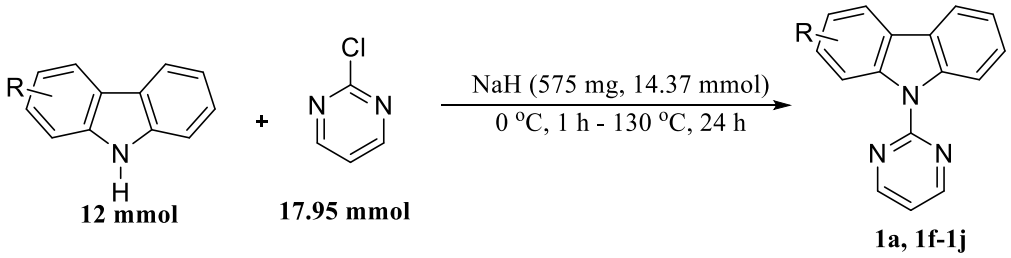
Compounds 1af and 1ag were obtained commercially

Carbazoles **1ah, 1ai, 1aj** were synthesised following the literature procedures.[32] Aniline derivative (4.8 mmol), 1,2-dichlorobenzene (588 mg, 4.0 mmol), K_3PO_4 (2.55 g, 12.0 mmol), $Pd(OAc)_2$ (45.0 mg, 5 mol %), tricyclohexylphospene (PCy_3) (112.0 mg, 10 mol%) and dry NMP (20 mL, 0.2 M) were added to a Schlenk tube with a magnetic stirring bar under argon atmosphere. The resulting mixture was heated at 135 °C for 18 h. The progress of the reaction was monitored by TLC. The mixture was cooled to room temperature and EtOAc was added to it. The resulting crude reaction mixture was filtered and washed several times with EtOAc. The filtrate was then washed twice with brine and then dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the desired 9*H*-carbazole was purified by silica gel column chromatography using hexane/ethyl acetate gradient as eluent.



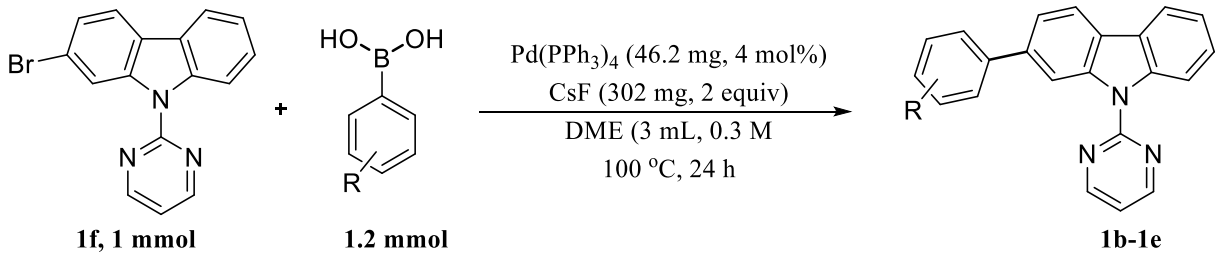
2.2. General procedure for synthesis of 9(pyrimidin-2-yl)-9H-carbazoles (1a, 1f-1j):

9(pyrimidin-2-yl)-9H-carbazoles (**1f-1j**) was synthesized using reported procedures.[36–38] To a stirred solution of carbazole (11.97 mmol) in DMF (57 mL, 0.21 M), NaH (60% dispersion in mineral oil, 575 mg, (14.37 mmol) was added in portions at 0 °C. After stirring for 30 min at that temperature, 2-chloropyrimidine (2.046 g, 17.95 mmol) was added and the mixture was stirred at 130 °C for 24 h. The, reaction mixture was then cooled to room temperature, poured over H_2O (400 mL) and extracted with EtOAc (4 × 75 mL). The combined organic phase was dried over Na_2SO_4. After filtration and evaporation of the solvents under reduced pressure, the crude product was purified by column chromatography on silica gel (n-hexane/EtOAc = 10/0.11) to afford the corresponding 9(pyrimidin-2-yl)-9H-carbazoles.



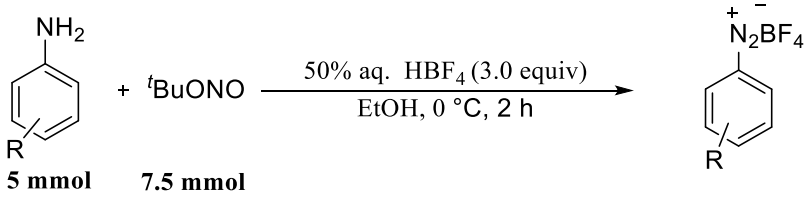
2.3. General procedure for the synthesis of 9(pyrimidin-2-yl)-9*H*-carbazoles derivatives (1b-1e):

To a solution of 2-bromo-9-(pyrimidin-2-yl)-9H-carbazole (**1f)** (323 mg, 1 equiv)**,** arylboronic acid (1.2 equiv) in DME (3 mL) was added CsF (302 mg, 2 equiv) and $Pd(PPh_3)_4$ (46.2 mg, 4 mol%) under argon atmosphere in a sealed tube. Heat the reaction mixture to 100 ºC for 24 h followed by cooling the mixture to room temperature, then add ice cooled water to it. The reaction mixture was then extracted with EtOAc and dried over Na_2SO_4. The crude mixture was finally purified by column chromatography using hexane/EtOAc as eluent.



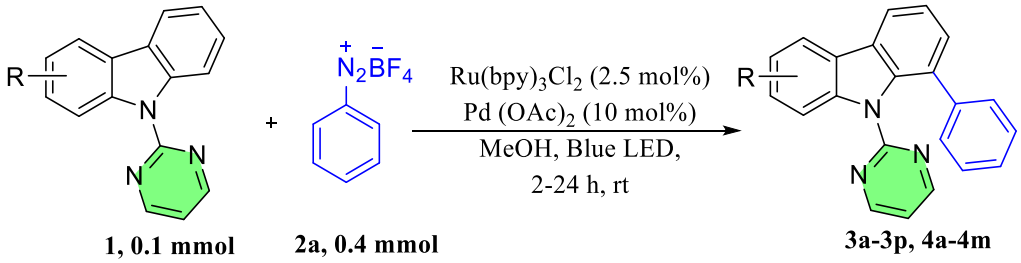
2.4. General procedure for the preparation of aryldiazonium tetrafluoroborates

In a 50 mL round-bottom flask, the aniline (10 mmol) was dissolved in a mixture of absolute ethanol (3 mL) and an aqueous solution of HBF4 (50%, 5.4 mL, 3 equiv). The tert-butyl nitrite (1.7 mL, 1.5 equiv) was added drop wise to the solution at 0 °C. The mixture was stirred at room temperature for 1 h and diethyl ether (20 mL) was added to precipitate the arenediazonium tetrafluoroborate. The solid was filtered off and washed with diethyl ether (3 × 10 mL). The aryldiazonium tetrafluoroborate was dried in vacuo (10-3 mbar) for 10 minutes and was then directly used without further purification. Spectral data are agreement with the data available in the literature.[9,10]



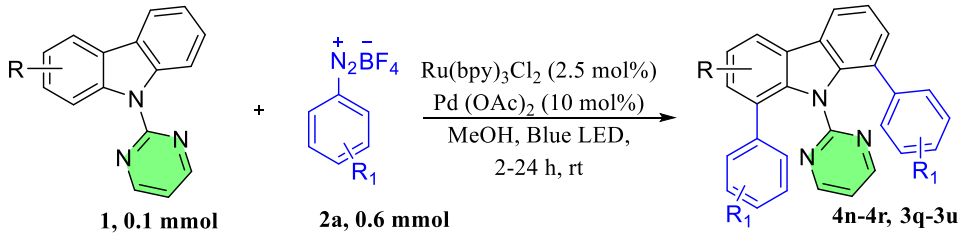
2.5. General procedure for *ortho* arylation of 9(pyrimidin-2-yl)-9H-carbazoles:

To an oven dried 4 mL vial, the corresponding carbazole derivative (0.1 mmol) aryldiazonium salt (0.4 mmol, 4 equiv), $Ru(bpy)_3Cl_2$ (1.6 mg, 2.5 mol%) and $Pd(OAc)_2$ (2.24mg,10 mol%) was added. Anhydrous MeOH (1 mL, 0.1 M) was then added to this reaction mixture and sealed with a Teflon screw cap. This mixture was then subjected to freeze pump thaw cycle using liquid nitrogen and high vacuum for three times in order to remove oxygen and maintain inert atmosphere (Argon). The mixture was irradiated with blue LED light for 2-24 h and the reaction mixture was monitored using TLC. Upon completion, the solvent was evaporated under reduced pressure. The reaction mixture was then subjected to column chromatography on silica gel (n-hexane/EtOAc) to get the pure product.



2.6. General procedure for diarylation of 9(pyrimidin-2-yl)-9H-carbazoles:

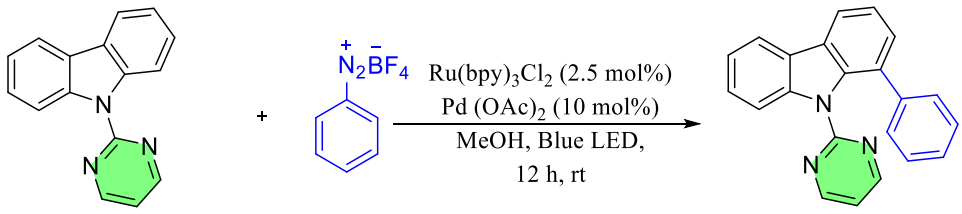
To an oven dried 4 mL vial containing the carbazole (0.1 mmol), was added aryldiazonium salt (0.6 mmol, 6 equiv), $Ru(bpy)_3Cl_2$ (1.6 mg, 2.5 mol%) and $Pd(OAc)_2$ (2.24mg, 10 mol%). Anhydrous MeOH (1 mL, 0.1 M) was then added to this reaction mixture and then sealed with a Teflon screw cap. This mixture was then subjected to freeze pump thaw cycle using liquid nitrogen and high vacuum three times in order to remove oxygen and maintain inert atmosphere (Argon). The mixture was then irradiated with blue LED light for 2-24 h and the reaction mixture was monitored using TLC. Upon completion, the solvent was evaporated under reduced pressure. The reaction mixture was then subjected to column chromatography on silica gel (n-hexane/EtOAc) to get the pure product.



1, 0.1 mmol **2a, 0.6 mmol** **4n-4r, 3q-3u**

2.7. Gram scale procedure for monoarylation of 9(Pyrimidin-2-yl)-9H-carbazoles, (3a):

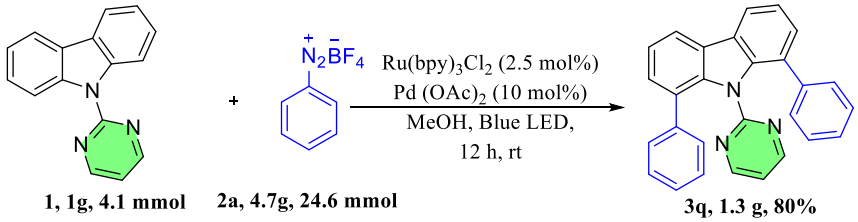
To an oven dried 50 mL RB, carbazole, **1a** (1 g, 4.1 mmol) aryladiazonium salt, **2a** (2.74 g, 4 equiv, 14.35 mmol), $Ru(bpy)_3Cl_2$ (65.6 mg, 2.5 mol%) and $Pd(OAc)_2$ (91.8 mg, 10 mol%) was added. Anhydrous MeCN (41 mL, 0.2 M) was added to this reaction mixture and sealed with a rubber septum. This mixture was then subjected to freeze pump thaw cycle using liquid nitrogen and high vacuum three times in order to remove oxygen and maintain inert atmosphere (Argon). The mixture was irradiated with blue LED light for 12 h and the reaction mixture was monitored using TLC. Upon completion, the solvent was evaporated under reduced pressure. The reaction mixture was then subjected to column chromatography on silica gel (n-hexane/EtOAc) to get the pure product, **3a** (947.52 mg, 72 %).



1, 1g, 4.1 mmol **2a, 2.74g, 14.35 mmol** **3a, 647.52 mg, 72%**

2.8. Gram scale procedure for diarylation of 9(Pyrimidin-2-yl)-9H-carbazoles, (3q):

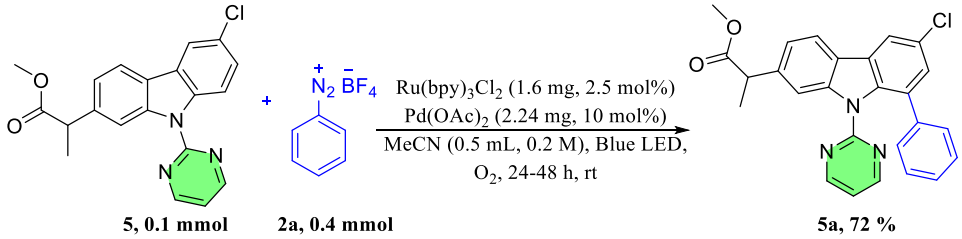
To an oven dried 50 mL RB, carbazole, **1a** (1 g, 4.1 mmol) aryladiazonium salt, **2a** (4.7 g, 6 equiv, 14.35 mmol), $Ru(bpy)_3Cl_2$ (65.6 mg, 2.5 mol%) and $Pd(OAc)_2$ (91.8 mg, 10 mol%) was added. Anhydrous MeCN (41 mL, 0.2 M) was then added to this reaction mixture and sealed with a rubber septum. This mixture was then subjected to freeze pump thaw cycle using liquid nitrogen and high vacuum three times in order to remove oxygen and maintain inert atmosphere (Argon). The mixture was irradiated with blue LED light for 12 h and the reaction mixture was monitored using TLC. Upon completion, the solvent was evaporated under reduced pressure. The reaction mixture was then subjected to column chromatography on silica gel (n-hexane/EtOAc) to get the pure product, **3q** (1.3g, 80 %).



1, 1g, 4.1 mmol **2a, 4.7g, 24.6 mmol** **3q, 1.3 g, 80%**

2.9. *Ortho* arylation of carprofen derivative, 5:

To an oven dried 4 mL vial, methyl 2-(6-chloro-9-(pyrimidin-2-yl)-9H-carbazol-2-yl) propanoate (36.5 mg, 0.1 mmol), aryldiazonium salt (76.4 mg, 0.4 mmol), $Ru(bpy)_3Cl_2$ (1.6 mg, 2.5 mol%) and $Pd(OAc)_2$ (2.24 mg, 10 mol%) was added. Dry MeOH (1.0 mL, 0.1 M) was added to this reaction mixture and the vial was sealed with a Teflon screw cap. The mixture was then subjected to blue light irradiation for 12 h under O_2 atmosphere. The solvent was evaporated under reduced pressure. The reaction mixture was then subjected to column chromatography on silica gel (n-hexane/EtOAc) to afford product, **5a** in 30.4 mg (72%).

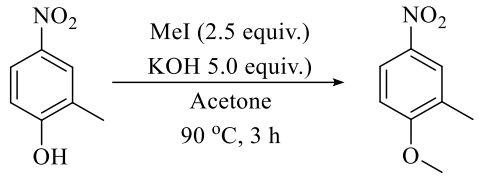


5, 0.1 mmol **2a, 0.4 mmol** **5a, 72 %**

2.10. Procedure for the synthesis of hyellazole derivatives

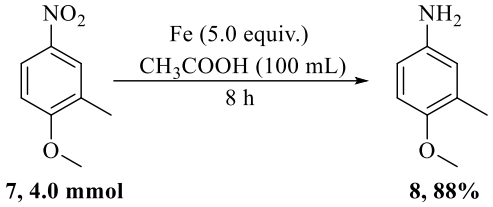
2.10.1 Synthesis of 2-methoxy-1-methyl-4-nitrobenzene, 7:

To an oven dried 60 ml pressure tube, 4-nitro-*o*-cresol, **6** (765 mg, 5 mmol) was added along with KOH (1.4 g, 25 mmol) and acetone (17 mL, 0.3 M). Upon stirring, MeI (1.76 g, 12.5 mmol) was slowly added to this mixture and sealed in a pressure tube. The reaction mixture was heated at 90 °C for 3 hours. The solvent was evaporated under reduced pressure and the reaction mixture was then subjected to column chromatography on silica gel (n-hexane/EtOAc) to afford the pure product, **7** in 793 mg (95%).



2.10.2 Synthesis of 3-methoxy-4-methylaniline, 8:

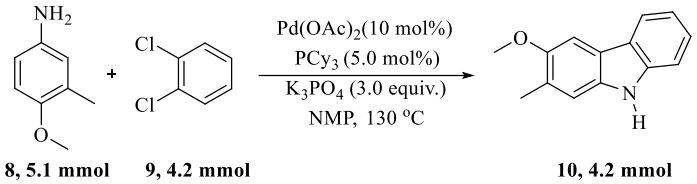
To an oven dried 100 mL round bottom flask charged with a magnetic stir bar, compound **7** (668 mg, 4 mmol) was added along with Fe (1.1 g, 20 mmol) and acetic acid (100 mL). The reaction mixture was stirred at room temperature for 8 hours. The reaction mixture was passed through celite and the filtrate was neutralized with saturated sodium bicarbonate solution and extracted with EtOAc (4 × 75 mL). The combined organic phase was dried over Na_2SO_4. The reaction mixture was then subjected to column chromatography on silica gel (n-hexane/EtOAc) to afford the pure product, **8** in 482 mg (88%).



2.10.3 Synthesis of 2-methoxy-3-methyl-9H-carbazole, 10:

Compound **8** (699 mg, 5.1. mmol), 1,2-dichlorobenzene (617 mg, 4.2 mmol), K_3PO_4 (2.6 g, 12.2 mmol), $Pd(OAc)_2$ (47.0 mg, 5 mol %), tricyclohexylphospene (PCy_3) (117.6 mg, 10 mol%) and dry NMP (20 mL, 0.2 M) were added to a Schlenk tube with a magnetic stirring bar under argon atmosphere. The resulting mixture was heated at 135 °C for 18 h. The mixture was cooled to room temperature and EtOAc was added to it. The resulting crude reaction mixture was filtered and washed several times with the EtOAc. The filtrate was then washed twice with brine and then dried

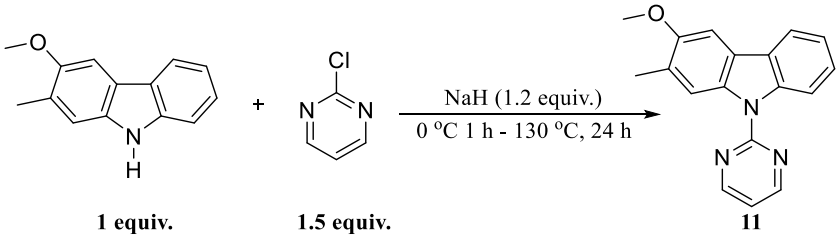
over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the reaction mixture was subjected to column chromatography on silica gel (n-hexane/EtOAc) to afford the pure product, **10** in 580 mg (70 %).



8, 5.1 mmol **9, 4.2 mmol** **10, 4.2 mmol**

2.10.4 Synthesis of 3-methoxy-2-methyl-9-(pyrimidin-2-yl)-9H-carbazole, 11

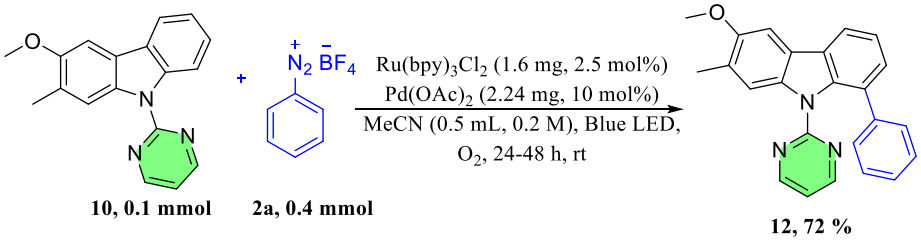
3-methoxy-2-methyl-9-(pyrimidin-2-yl)-9H-carbazole, **10** was prepared using the general procedure **2.2.**



1 equiv. **1.5 equiv.** **11**

2.10.5 Synthesis of hyellazole regioisomer, 12

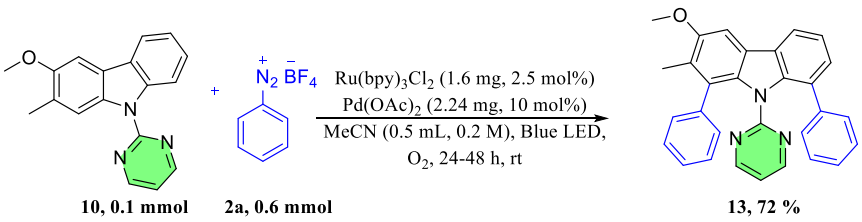
Hyellazole regioisomer (**12)** was prepared using the general procedure **2.4.**



10, 0.1 mmol **2a, 0.4 mmol** **12, 72 %**

2.10.6 Synthesis of functionalized hyellazole, 13:

Functionalized Hyellazole (**13)** was prepared using the general procedure **2.5.**

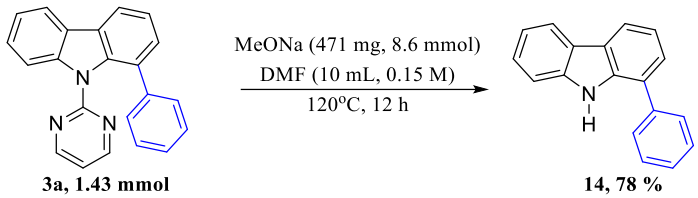


10, 0.1 mmol **2a, 0.6 mmol** **13, 72 %**

2.11. Deprotection of pyrimidine, 3a to form free carbazole, 14:

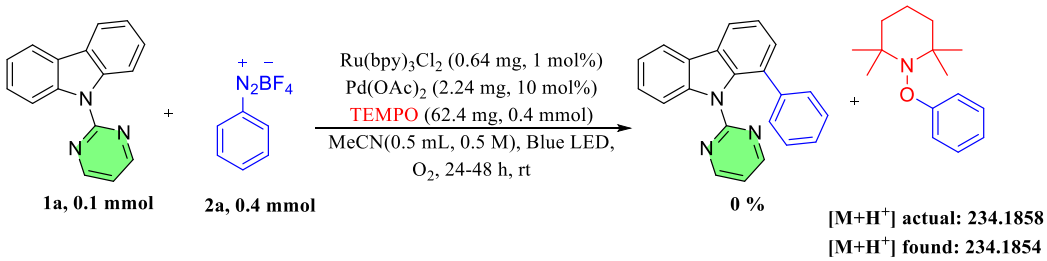
To an oven dried 10 mL RB, 1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (500 mg, 1.43 mmol) was added along with sodium methoxide (471 mg, 8.6 mmol) in dry DMF (10 mL, 0.15 M). The

reaction mixture was heated to 120 °C for 12 h and brought to room temperature. Ice-cooled water was then added to the reaction mixture and the aqueous layer was extracted with ethyl acetate (3 × 20 mL). Dry the combined organic layers over Na_2SO_4 followed by purification using column chromatography on silica gel (n-hexane/EtOAc) to afford product **14** in 302 mg (78%).



2.12. Procedure for trapping aryl radical using TEMPO:

To an oven dried 4 mL vial, carbazole, **1a** (24.5mg, 0.1 mmol) was added along with aryldiazonium salt, **2a** (76.4 mg, 0.4 mmol), $Ru(bpy)_3Cl_2$ (1.64 mg, 2.5 mol%), $Pd(OAc)_2$ (2.24 mg, 10 mol%) and TEMPO (62.4 mg, 0.4 mmol). To this dry MeCN (0.5 mL, 0.2 M) was added, and the reaction mixture was sealed with a teflon screw cap. The reaction mixture was then irradiated with blue light for 48 h under oxygen atmosphere (balloon). The reaction was monitored by TLC and upon completion the solvent was evaporated under reduced pressure. The crude mixture was then subjected to HRMS analysis.



3.0 Crystallographic data

General data collection and structure solution details:

X-ray data for the compound was collected at room temperature on a Bruker D8 VENTURE diffractometer instrument with an IμS 3.0 Mo source (λ = 0.7107 Å) and a PHOTON-III C28 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 4 software suite programs.1 The structure was refined with the SHELXL2 program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. CCDC contains the supplementary crystallographic data for this paper which can be obtained free of charge at https://www.ccdc.cam.ac.uk/structures/

3.1 Crystallographic data 4g

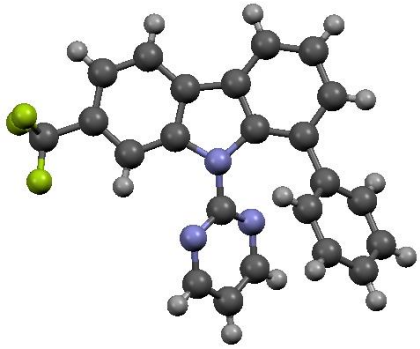


Figure S1. Crystal structure of 4g

Table S2 Crystal data and structure refinement of 4g

CCDC number	2267782
Crystal data Crystal	
Chemical formula	$2(C_{23}H_{14}F_3N_3)$
M_r	778.74
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	19.4774 (17), 12.0444 (11), 16.5411 (15)
β (°)	106.097 (3)
V (Å^3)	3728.3 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	× ×
Data collection	
Diffractometer	Bruker D8 venture
Absorption correction	-
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25773, 7429, 4971
R_{int}	0.101
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.159, 1.05
No. of reflections	7429
No. of parameters	579
No. of restraints	360
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.27

3.2 Crystallographic Data 4i

Figure S2. Crystal structure of 4i

Table S3 Crystal data and structure refinement of 4i

CCDC number	2267784
Crystal data	
Chemical formula	$C_{2.71}H_2N_{0.35}O_{0.12}$
M_r	41.34
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	149
a, *b*, *c* (Å)	12.1412 (11), 12.7990 (9), 12.1671 (7)
β (°)	115.924 (3)
V (Å^3)	1700.5 (2)
Z	34
Radiation type	Mo *K*α
μ (mm−1)	0.09
Crystal size (mm)	× ×
Data collection	
Diffractometer	Bruker D8 venture
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6831, 3166, 2667
R_{int}	0.051
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.607
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.121, 1.07
No. of reflections	3166
No. of parameters	245
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.27

3.3 Crystallographic Data 4k

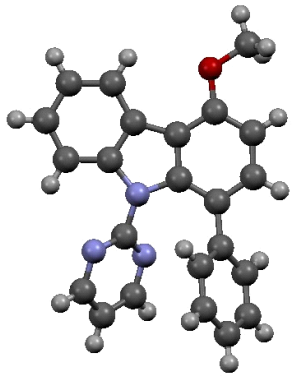


Figure S3. Crystal structure of 4k

Table S4 Crystal data and structure refinement of 4k

CCDC number	2267783
Crystal data	
Chemical formula	$C_{23}H_{17}N_3O$
M_r	351.39
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	7.3575 (5), 19.3150 (15), 12.3105 (9)
β (°)	97.192 (2)
V (Å^3)	1735.7 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	× ×
Data collection	
Diffractometer	Bruker D8 venture
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	95588, 3073, 2476
R_{int}	0.079
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.101, 1.02
No. of reflections	3073
No. of parameters	245
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.16

3.4 Crystallographic Data 4m

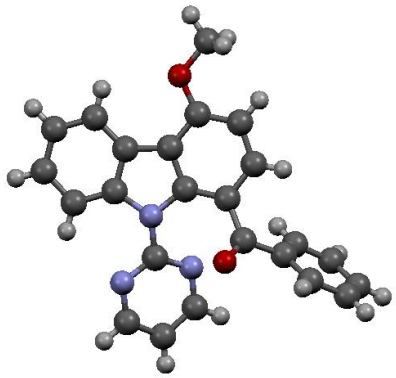


Figure S4. Crystal structure of 4m

Table S5 Crystal data and structure refinement of 4m

CCDC number	
Crystel data	
Chemical formula	$C_{24}H_{17}N_3O_2$
M_r	379.40
Crystel system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	12.7425 (10), 13.5862 (11), 10.3411 (7)
β (°)	97.302 (2)
V (Å^3)	1775.8 (2)
Z	4
Radiation type	Mo $K\alpha$
M (mm^{-1})	0.09
Crystal size (mm)	0.20 × 0.1 × 0.05
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0966 before and 0.0769 after correction. The Ratio of minimum to maximum transmission is 0.9522. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.702, 0.737
No of measured, independent and observed [$I > 2\sigma(I)$] reflections	42328, 3158, 2421
R_{int}	0.087
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.596

refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.091, 1.06
No. of reflections	3158
No. of parameters	263
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.22

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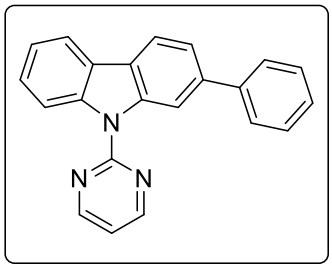
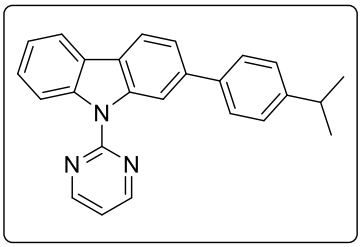
5.0. Analytical data of compounds

2-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (1b)



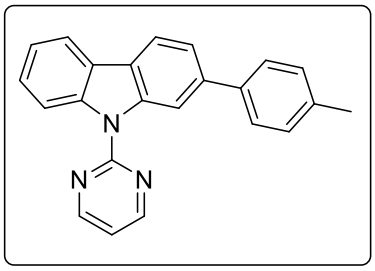
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.14 (dd, *J* = 1.5, 0.5 Hz, 1H), 8.91 – 8.82 (m, 3H), 8.16 – 8.08 (m, 2H), 7.79 – 7.74 (m, 2H), 7.64 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.56 – 7.49 (m, 3H), 7.43 – 7.37 (m, 2H), 7.13 (t, *J* = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.17 (s), 157.93 (s), 142.28 (s), 140.02 (s), 139.71 (s), 139.63 (s), 128.74 (s), 127.73 (s), 127.07 (s), 126.64 (s), 125.56 (s), 125.01 (s), 122.43 (s), 121.89 (s), 119.71 (s) 119.59 (s), 116.29 (s), 116.07 (s), 115.09 (s). **HR-MS** (ESI) m/z calcd for $C_{25}H_{16}N_3^+$[M+H$^+$] 322.1344, found 322.1339.

2-(4-methoxyphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (1c)



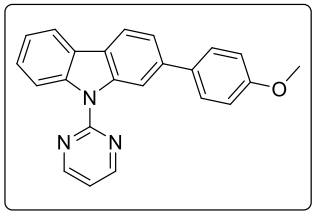
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.02 (dd, *J* = 1.5, 0.5 Hz, 1H), 8.78 – 8.68 (m, 3H), 7.97 (ddd, *J* = 4.7, 1.9, 0.6 Hz, 2H), 7.63 – 7.54 (m, 2H), 7.50 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.40 (ddd, *J* = 8.5, 7.2, 1.4 Hz, 1H), 7.27 (ddd, *J* = 8.1, 5.3, 1.4 Hz, 3H), 6.96 (t, *J* = 4.8 Hz, 1H), 2.89 (dt, *J* = 13.8, 6.9 Hz, 1H), 1.23 (d, *J* = 6.9 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.22 (s), 157.90 (s), 147.83 (s), 140.05 (s), 139.85 (s), 139.76 (s), 139.63 (s), 127.68 (s), 126.86 (s), 126.56 (s), 125.67 (s), 124.82 (s), 122.42 (s), 121.83 (s), 119.65 (s), 119.54 (s), 116.34 (s), 116.01 (s), 115.02 (s), 33.88 (s), 24.12 (s). **HR-MS** (ESI) m/z calcd for $C_{25}H_{22}N_3^+$[M+H$^+$] 364.1814, found 364.1832

9-(pyrimidin-2-yl)-2-(p-tolyl)-9H-carbazole (1d)



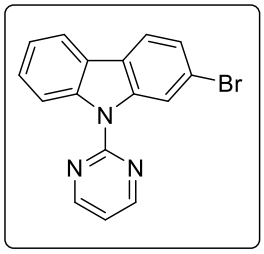
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.15 (dd, *J* = 1.5, 0.4 Hz, 1H), 8.91 – 8.87 (m, 1H), 8.83 (d, *J* = 4.8 Hz, 2H), 8.14 – 8.09 (m, 2H), 7.66 (ddd, *J* = 9.6, 7.2, 1.7 Hz, 3H), 7.54 (ddd, *J* = 8.5, 7.2, 1.3 Hz, 1H), 7.41 (td, *J* = 7.7, 1.0 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 2H), 7.09 (t, *J* = 4.8 Hz, 1H), 2.47 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.18 (s), 157.97 (s), 140.00 (s), 139.72 (s), 139.58 (s), 139.41 (s), 136.81 (s), 129.46 (s), 127.56 (s), 126.54 (s), 125.62 (s), 124.78 (s), 122.40 (s), 121.75 (s), 119.65 (s), 119.53 (s), 116.26 (s), 116.06 (s), 114.87 (s), 21.16 (s). **HR-MS** (ESI) m/z calcd for $C_{23}H_{18}N_3^+$[M+H$^+$] 336.1501, found 336.1492.

2-(4-methoxyphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (1e)

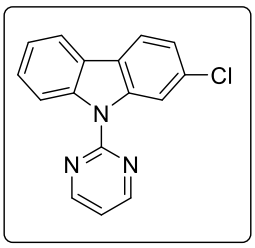


Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.02 (d, *J* = 1.0 Hz, 1H), 8.84 (dd, *J* = 15.4, 6.6 Hz, 3H), 8.10 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.58 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.55 – 7.46 (m, 2H), 7.41 – 7.35 (m, 2H), 7.13 – 7.08 (m, 2H), 7.06 (dd, *J* = 8.3, 0.8 Hz, 1H), 3.85 (s, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.17 (s), 158.38 (s), 157.76 (s), 140.41 (s), 119.70 (s), 119.09 (s), 115.87 (s), 109.82 (s), 101.94 (s), 55.79 (s). **HR-MS** (ESI) m/z calcd for $C_{23}H_{18}N_3O^+$[M+H$^+$] 352.1450, found 352.1442.

2-bromo-9-(pyrimidin-2-yl)-9H-carbazole (1f)



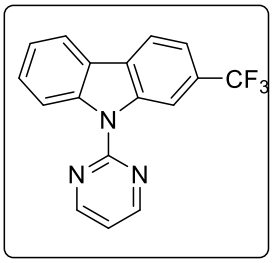
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.10 (d, *J* = 1.6 Hz, 1H), 8.86 (dd, *J* = 5.0, 2.8 Hz, 3H), 8.04 (ddd, *J* = 7.7, 1.2, 0.6 Hz, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.56 – 7.48 (m, 2H), 7.41 – 7.36 (m, 1H), 7.16 (t, *J* = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.88 (s), 157.96 (s), 139.77 (s), 139.23 (s), 127.03 (s), 125.43 (s), 125.05 (s), 124.73 (s), 122.64 (s), 120.53 (s), 120.16 (s), 119.51 (s), 119.45 (s), 116.50 (s), 116.34 (s). **HR-MS** (ESI) m/z calcd for $C_{16}H_{11}BrN_3^+$[M+H$^+$] 324.0136, found 324.0127.



2-chloro-9-(pyrimidin-2-yl)-9H-carbazole (1g)

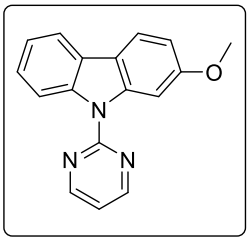
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.96 – 8.92 (m, 1H), 8.88 – 8.83 (m, 3H), 8.03 (ddd, *J* = 7.7, 1.3, 0.7 Hz, 1H), 7.99 – 7.94 (m, 1H), 7.52 (ddd, *J* = 8.5, 7.2, 1.3 Hz, 1H), 7.41 – 7.34 (m, 2H), 7.14 (t, *J* = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.89 (s), 157.92 (s), 139.54 (s), 139.39 (s), 132.17 (s), 126.87 (s), 125.06 (s), 124.36 (s), 122.69 (s), 122.62 (s), 120.16 (s), 119.47 (s), 116.65 (s), 116.53 (s), 116.30 (s).**HR-MS** (ESI) m/z calcd for $C_{16}H_{11}ClN_3$ $^+$[M+H$^+$] 280.7350, found 280.7337.

2-trifluromethyl-9-(pyrimidin-2-yl)-9H-carbazole (1h)



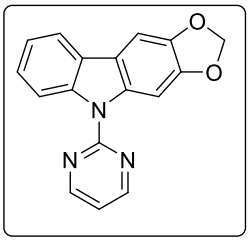
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 9.11 (s, 1H), 8.78 (dd, J = 13.4, 6.6 Hz, 3H), 8.02 (dd, J = 13.1, 7.9 Hz, 2H), 7.55 – 7.44 (m, 2H), 7.31 (t, J = 7.4 Hz, 1H), 7.06 (t, J = 4.7 Hz, 1H). **^{13}C NMR** (101 MHz, CDCl3) δ 158.89 (s), 157.99 (s), 140.04 (s), 138.41 (s), 128.42 (s), 128.10 (s), 127.84 (s), 126.28 (s), 124.62 (s), 123.57 (s), 122.71 (s), 120.10 (s), 119.69 (s), 119.01 (d, J = 3.7 Hz), 116.56 (d, J = 19.0 Hz), 113.98 (d, J = 4.3 Hz). **HR-MS** (ESI) m/z calcd for $C_{17}H_{11}F_3N_3$ O^+[M+H$^+$] 314.0905, found 314.0893.

2-methoxy-9-(pyrimidin-2-yl)-9H-carbazole (1i)



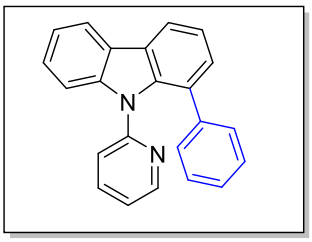
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.86 – 8.81 (m, 3H), 8.50 (d, J = 2.3 Hz, 1H), 8.00 – 7.94 (m, 2H), 7.44 (ddd, J = 8.5, 7.2, 1.4 Hz, 1H), 7.35 (td, J = 7.5, 1.0 Hz, 1H), 7.12 (t, J = 4.8 Hz, 1H), 7.00 (dd, J = 8.5, 2.4 Hz, 1H), 3.97 (s, 3H).**^{13}C NMR** (101 MHz, CDCl3) δ 159.28 (s), 159.19 (s), 157.85 (s), 140.39 (s), 139.24 (s), 125.91 (s), 125.35 (s), 122.38 (s), 120.00 (s), 119.54 (s), 118.73 (s), 116.17 (s), 115.95 (s), 110.08 (s), 101.45 (s), 55.77 (s).**HR-MS** (ESI) m/z calcd for $C_{17}H_{14}ClN_3\ O^+[M+H^+]$ 276.1137, found 276.1142.

5-(pyrimidin-2-yl)-5H-[1,3]dioxolo[4,5-b]carbazole (1j)



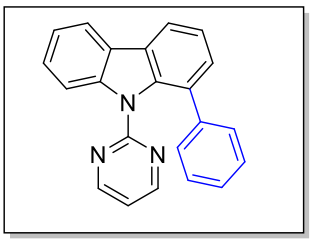
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.83 (t, *J* = 5.7 Hz, 3H), 8.41 (d, *J* = 8.7 Hz, 1H), 8.07 (d, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.11 (t, *J* = 4.1 Hz, 1H), 7.03 (d, *J* = 8.7 Hz, 1H), 6.20 (s, 2H). **^{13}C NMR** (101 MHz, CDCl3) δ 159.16 (s), 157.82 (s), 142.84 (s), 140.56 (s), 139.66 (s), 135.60 (s), 126.68 (s), 122.98 (s), 122.43 (s), 121.99 (s), 116.17 (s), 115.83 (s), 110.66 (s), 108.19 (s), 106.78 (s), 101.87 (s). **HR-MS** (ESI) m/z calcd for $C_{17}H_{12}N_3\ O_2^+[M+H^+]$ 290.0930, found 290.0932.

1-phenyl-9-(pyridin-2-yl)-9H-carbazole (3a')



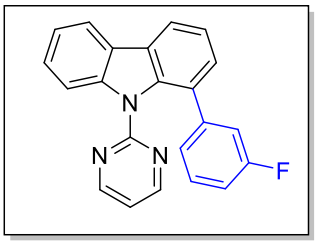
Yield (0.1 mmol scale, 26 mg, 82 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (dd, *J* = 4.7, 1.3 Hz, 1H), 8.20 – 8.13 (m, 2H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.44 – 7.39 (m, 3H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.23 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.16 (dd, *J* = 6.3, 2.9 Hz, 2H), 7.06 – 7.00 (m, 3H), 6.96 (dd, *J* = 7.0, 5.0 Hz, 1H), 6.74 (d, *J* = 8.0 Hz, 1H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.5, 148.3, 141.6, 139.7, 137.1, 136.7, 128.6, 128.5, 127.7, 126.9, 126.5, 126.2, 125.8, 123.9, 121.6, 121.2, 121.0, 120.9, 120.1, 119.4, 111.0. **HR-MS** (ESI) m/z calcd for $C_{23}H_{17}N_2^+[M+H^+]$ 321.1393, found 321.1394.

1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (3a)



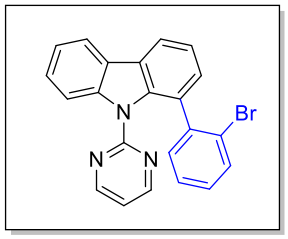
Yield (0.1 mmol scale, 26 mg, 82 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 4.8 Hz, 2H), 8.48 (d, *J* = 2.3 Hz, 2H), 7.88 – 7.76 (m, 2H), 7.07 (t, *J* = 4.8 Hz, 1H), 6.96 (dd, *J* = 8.5, 2.4 Hz, 2H), 3.95 (s, 6H).**^{13}C NMR** (101 MHz, CDCl3) δ 157.6, 157.3, 141.45, 141.0, 137.1, 128.7, 128.5, 128.1, 127.7, 126.9, 126.8, 126.2, 125.2, 122.4, 122.1, 120.2, 119.3, 117.1, 112.3. **HR-MS** (ESI) m/z calcd for $C_{22}H_{16}N_3^+[M+H^+]$ 322.1344, found 322.1339.

1-(3-fluorphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3b)



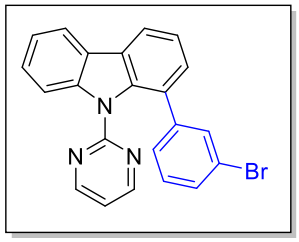
Yield (0.1 mmol scale, 27 mg, 80%); white solid (petroleum ether/ethyl acetate = 9.1:1.0, V/V).**^{1}H NMR** (400 MHz, Chloroform-d) δ 8.38 (d, *J* = 4.8 Hz, 2H), 8.21 – 8.06 (m, 3H), 7.51 – 7.41 (m, 3H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.08 – 7.00 (m, 3H), 6.88 (t, *J* = 4.8 Hz, 1H), 6.79 (m, 1H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ161.4 (d, J_{C-F} = 246.6 Hz), 157.5, 157.3, 143.5 (d, J_{C-F} = 8.0 Hz), 140.7, 136.8, 129.2 (d, J_{C-F} = 8.3 Hz), 128.4, 127.1, 126.9, 126.8, 124.9, 123.3, 122.3, 122.1, 120.1, 119.6, 117.1, 114.5(d, J_{C-F} = 21.8 Hz), 112.7 (d, J_{C-F} = 21.2 Hz), 112.1. **HR-MS** (ESI) m/z calcd for $C_{22}H_{15}F_3N_3^+$[M+H$^+$] 340.1250, found 340.1234.

1-(2-bromophenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3c)



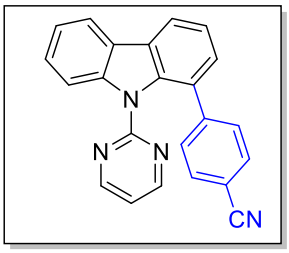
Yield (0.1 mmol scale, 28 mg, 69 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V)**^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.35 (d, J = 4.9 Hz, 2H), 8.20 – 8.09 (m, 3H), 7.49 – 7.40 (m, 4H), 7.36 (t, J = 7.2 Hz, 1H), 7.20 (dd, J = 7.6, 1.7 Hz, 1H), 7.08 (m, 1H), 6.96 (m, 1H), 6.82 (t, J = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, Chloroform-d) δ 157.34, 157.18, 142.22, 140.56, 136.92, 132.61, 131.05, 129.58, 128.04, 127.05, 126.94, 126.88, 126.71, 125.02, 123.17, 122.07, 121.69, 120.06, 119.91, 116.87, 112.35. **HR-MS** (ESI) m/z calcd for $C_{22}H_{15}BrN_3^+$[M+H$^+$] 400.0449, found 400.0430.

1-(3-Bromophenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3d)



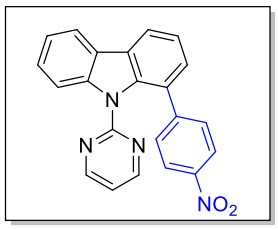
Yield (0.1 mmol scale, 31 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 (d, J = 4.8 Hz, 2H), 8.18 – 8.06 (m, 3H), 7.49 – 7.43 (m, 3H), 7.41 – 7.34 (m, 2H), 7.23 (m, 2H), 7.00 (t, J = 7.8 Hz, 1H), 6.91 (t, J = 4.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.58, 143.42, 140.86, 136.91, 130.89, 129.62, 129.24, 128.48, 126.99, 126.82, 126.39, 124.97, 122.34, 122.19, 122.16, 120.23, 119.89, 117.44, 112.24. HR-MS (ESI) m/z calcd for $C_{22}H_{15}BrN_3^+$[M+H$^+$] 400.0449, found 400.0435.

4-(9-(pyrimidin-2-yl)-9H-carbazol-1-yl)benzonitrile (3e)



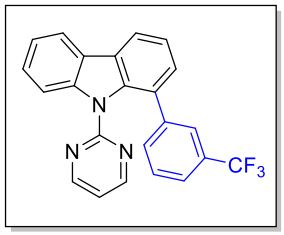
Yield (0.1 mmol scale, 24.5 mg, 70 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 (d, *J* = 4.8 Hz, 2H), 8.23(m, 3H), 7.52 (m, 8H), 6.91 (t, *J* = 4.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.60, 146.55, 140.89, 136.75, 131.83, 128.40, 128.24, 127.30, 127.23, 126.65, 125.04, 122.61, 122.51, 120.47, 120.25, 119.03, 117.40, 112.60, 109.71. HR-MS (ESI) m/z calcd for $C_{23}H_{15}N_4^+$[M+H$^+$] 347.1297, found 347.1294.

1-(4-Nitrophenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3f)



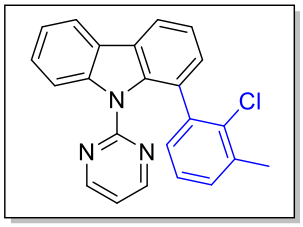
Yield (0.1 mmol scale, 28 mg, 75 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.36 (d, J = 4.8 Hz, 2H), 8.22 – 8.12 (m, 3H), 7.99 (d, J = 8.7 Hz, 2H), 7.53 – 7.45 (m, 5H), 7.40 (m, 1H), 6.86 (t, J = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.67, 148.66, 146.10, 140.92, 136.81, 128.48, 128.26, 127.38, 127.31, 126.28, 125.05, 123.35, 122.64, 122.60, 120.72, 120.29, 117.49, 112.68. **HR-MS** (ESI) m/z calcd for $C_{22}H_{15}N_4O_2^+$[M+H$^+$] 367.1195, found 367.1178.

9-(pyrimidin-2-yl)-1-(3-(trifluoromethyl)phenyl)-9H-carbazole (3g)



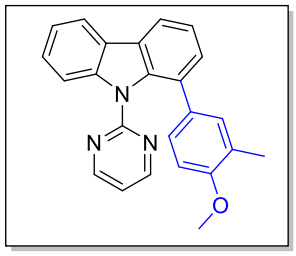
Yield (0.1 mmol scale, 31 mg, 81 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.32 (d, J = 4.8 Hz, 4H), 8.15 (t, J = 8.2 Hz, 6H), 7.56 – 7.42 (m, 10H), 7.38 (dd, J = 14.8, 7.7 Hz, 4H), 7.32 – 7.22 (m, 3H), 6.84 (t, J = 4.8 Hz, 2H). **^{13}C NMR** (101 MHz, CDCl3) δ 157.5, 157.4, 142.4, 140.9, 136.9, 131.0, 128.6, 128.6, 127.1, 127.1, 126.9, 125.0, 124.5 (d, J = 3.7 Hz), 122.9 (d, J = 3.9 Hz), 122.5, 122.3, 120.2, 120.0, 117.2, 112.4. HR-MS (ESI) m/z calcd for C23H15F3N3+[M+H+] 390.1218, found 390.1199.

1-(2-chloro-3-methylphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3h)



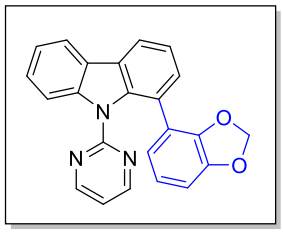
Yield (0.1 mmol scale, 30 mg, 80 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 4.8 Hz, 2H), 8.17 – 8.11 (m, 2H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.44 (ddd, *J* = 7.6, 3.7, 1.7 Hz, 2H), 7.35 (ddd, *J* = 8.5, 7.7, 0.9 Hz, 2H), 7.14 – 7.04 (m, 2H), 6.93 (t, *J* = 7.8 Hz, 1H), 6.86 (t, *J* = 4.8 Hz, 1H), 2.11 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.23, 157.1, 143.0, 140.7, 137.3, 134.8, 134.0, 128.9, 128.1, 127.6, 127.0, 126.9, 126.4, 126.2, 124.8, 122.0, 121.8, 120.2, 119.6, 117.3, 112.0, 17.8. HR-MS (ESI) m/z calcd for $C_{23}H_{17}ClN_3^+$[M+H$^+$] 370.1111, found 370.1101.

1-(4-methoxy-3-methylphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3i)



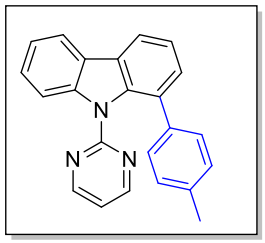
Yield (0.1 mmol scale, 28 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). ^{1}H NMR (400 MHz, CDCl3) δ 8.26 (d, J = 4.8 Hz, 2H), 8.05 (ddd, J = 8.9, 4.4, 1.0 Hz, 2H), 7.93 – 7.88 (m, 1H), 7.39 – 7.30 (m, 2H), 7.30 – 7.23 (m, 2H), 6.95 (d, J = 8.3 Hz, 1H), 6.76 (t, J = 4.8 Hz, 1H), 6.50 – 6.41 (m, 2H), 3.66 (s, 3H), 1.98 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 158.5, 157.4, 157.1, 140.8, 137.7, 137.0, 133.6, 130.6, 129.4, 127.5, 126.7, 126.3, 125.0, 121.8, 121.8, 120.1, 119.0, 117.0, 115.1, 111.9, 110.9, 55.4, 20.4. HR-MS (ESI) m/z calcd for $C_{24}H_{20}N_3O^+$[M+H$^+$] 366.1606, found 366.1671.

1-(benzo[d][1,3]dioxol-4-yl)-9-(pyrimidin-2-yl)-9H-carbazole (3j)



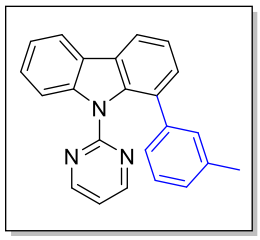
Yield (0.1 mmol scale, 27 mg, 27 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.43 (d, *J* = 4.8 Hz, 2H), 8.13 – 8.04 (m, 3H), 7.49 – 7.33 (m, 4H), 6.93 (t, *J* = 4.8 Hz, 1H), 6.80 – 6.71 (m, 2H), 6.56 (d, *J* = 8.0 Hz, 1H), 5.87 (s, 2H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.82, 157.40, 147.49, 146.11, 140.97, 137.15, 135.48, 128.50, 128.09, 126.95, 126.84, 125.15, 122.36, 122.09, 121.32, 120.19, 119.15, 117.11, 112.20, 108.35, 108.02, 100.95. HR-MS (ESI) m/z calcd for $C_{23}H_{15}N_3O_2$+[M+H$^+$] 366.1243, found 366.1237.

1-(4-methoxy-3-methylphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3k)



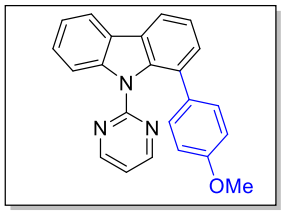
Yield (0.1 mmol scale, 23 mg, 69 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 4.8 Hz, 2H), 8.16 – 8.10 (m, 3H), 7.50 – 7.45 (m, 3H), 7.38 (s, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 7.8 Hz, 2H), 6.84 (t, *J* = 4.8 Hz, 1H), 2.28 (s, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.21, 156.83, 140.47, 137.97, 136.75, 135.33, 128.26, 128.15, 128.06, 127.00, 126.41, 126.28, 124.73, 121.88, 121.54, 119.69, 118.57, 116.38, 111.72, 20.67. **HR-MS** (ESI) m/z calcd for $C_{23}H_{18}N_3$+[M+H$^+$] 336.1501, found 336.1492.

1-(4-methoxy-3-methylphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3l)



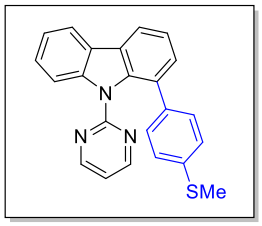
Yield (0.1 mmol scale, 23 mg, 69 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** 1H NMR (400 MHz, CDCl3) δ 8.25 (d, J = 4.8 Hz, 2H), 8.04 (ddd, J = 14.4, 4.8, 3.8 Hz, 3H), 7.42 – 7.36 (m, 3H), 7.31 – 7.27 (m, 1H), 7.05 (d, J = 7.6 Hz, 1H), 6.96 (dd, J = 12.2, 4.4 Hz, 2H), 6.83 – 6.80 (m, 1H), 6.76 (t, J = 4.8 Hz, 1H), 2.07 (s, 3H). **^{13}C NMR** (101 MHz, CDCl3) δ 157.52 (s), 157.15 (s), 141.05 (s), 140.72 (s), 137.45 (s), 136.97 (s), 128.49 (s), 128.35 (s), 128.28 (s), 128.02 (s), 126.85 (s), 126.66 (s), 125.43 (s), 124.99 (s), 124.74 (s), 122.20 (s), 121.89 (s), 120.08 (s), 119.10 (s), 116.99 (s), 111.91 (s), 21.08 (s).**HR-MS** (ESI) m/z calcd for $C_{23}H_{18}N_3$+[M+H$^+$] 336.1501, found 336.1492.

1-(4-Methoxyphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3m)



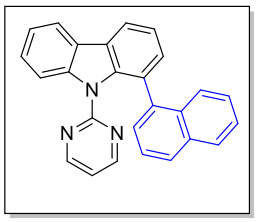
Yield (0.1 mmol scale, 30 mg, 85 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.36 (d, *J* = 4.8 Hz, 2H), 8.14 (m, 2H), 8.09 (dd, *J* = 6.1, 2.8 Hz, 1H), 7.49 (m, 3H), 7.40(m, 1H), 7.18 (d, *J* = 8.8 Hz, 2H), 6.87 (t, *J* = 4.8 Hz, 1H), 6.65 (d, *J* = 8.8 Hz, 2H), 3.76 (s, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 158.26, 157.68, 157.32, 141.02, 137.23, 133.99, 128.68, 128.63, 128.24, 126.96, 126.78, 125.24, 122.40, 122.06, 120.18, 118.92, 117.01, 113.62, 112.25, 55.51. **HR-MS** (ESI) m/z calcd for $C_{23}H_{18}N_3O^+$[M+H$^+$] 352.1450, found 352.1442.

1-(4-(Methylthio)phenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3n)



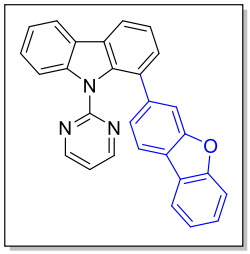
Yield (0.1 mmol scale, 30 mg, 82 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.36 (d, J = 4.8 Hz, 2H), 8.18 – 8.01 (m, 3H), 7.50 – 7.40 (m, 3H), 7.36 (m,1H), 7.20 – 7.15 (m, 2H), 6.87 (t, J = 4.8 Hz, 1H), 6.68 – 6.61 (m, 2H), 3.76 (s, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 158.26, 157.68, 157.32, 141.02, 137.23, 133.99, 128.68, 128.63, 128.24, 126.96, 126.78, 125.24, 122.40, 122.06, 120.18, 118.92, 117.02, 113.62, 112.24, 55.51. **HR-MS** (ESI) m/z calcd for $C_{22}H_{15}N_4O_2^+$[M+H$^+$] 368.1221, found 368.1223.

1-(naphthalen-1-yl)-9-(pyrimidin-2-yl)-9H-carbazole (3o)



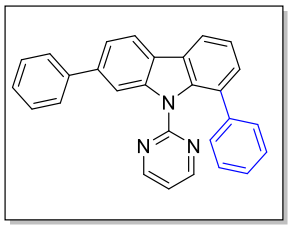
Yield (0.1 mmol scale, 26 mg, 70 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.22 (dd, J = 7.6, 1.4 Hz, 1H), 8.20 – 8.15 (m, 1H), 7.95 – 7.88 (m, 1H), 7.84 (d, J = 4.8 Hz, 2H), 7.70 (dd, J = 13.7, 7.9 Hz, 2H), 7.62 (d, J = 8.0 Hz, 1H), 7.57 (dd, J = 7.4, 1.4 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.45 – 7.28 (m, 7H), 6.50 (t, J = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.09, 156.39, 140.62, 139.26, 137.97, 133.45, 130.97, 129.94, 127.67, 127.12, 126.80, 126.65, 126.51, 126.37, 126.21, 126.13, 125.77, 125.43, 124.83, 121.86, 120.13, 119.63, 116.74, 111.98. **HR-MS** (ESI) m/z calcd for $C_{26}H_{18}N_3^+$[M+H$^+$] 372.1501, found 372.1497.

1-(dibenzo[b,d]furan-3-yl)-9-(pyrimidin-2-yl)-9H-carbazole (3q)



Yield (0.1 mmol scale, 26 mg, 70 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 9.4, 3.9 Hz, 4H), 8.08 (d, *J* = 8.2 Hz, 1H), 7.85 (dd, *J* = 11.0, 4.6 Hz, 2H), 7.57 (dd, *J* = 12.4, 4.8 Hz, 2H), 7.50 – 7.44 (m, 3H), 7.42 – 7.38 (m, 2H), 7.32 (dd, *J* = 7.8, 4.7 Hz, 2H), 6.54 (t, *J* = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.5, 157.1, 156.4, 154.7, 140.8, 137.2, 136.0, 128.8, 128.0, 127.2, 127.0, 126.8, 126.7, 124.9, 123.9, 13.8, 122.8, 122.2, 121.9, 120.7, 120.1, 119.6, 119.1, 116.93, 111.9, 111.6, 111.0. **HR-MS** (ESI) m/z calcd for $C_{28}H_{18}N_3O^+$[M+H$^+$] 412.1450, found 412.1453.

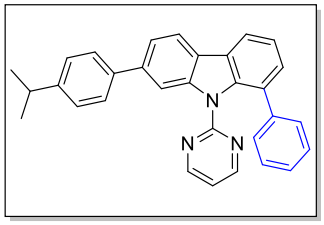
7-methyl-1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (4a)



Yield (0.1 mmol scale, 30 mg, 75 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.36 – 8.35 (m, 1H), 8.33 (d, J = 4.8 Hz, 2H), 8.18 (dd, J = 8.1, 0.5 Hz, 1H), 8.13 (dd, J = 6.9, 2.1 Hz, 1H), 7.72 – 7.69 (m, 2H), 7.61 (dd, J = 8.1, 1.6 Hz, 1H), 7.49 – 7.44 (m, 4H), 7.38 – 7.34 (m, 1H), 7.29 (ddd, J = 5.6, 4.9, 2.9 Hz, 2H), 7.13 – 7.08 (m, 3H), 6.83 (t, J = 4.8 Hz, 1H).**^{13}C NMR** (101 MHz, CDCl3) δ 157.5, 157.3, 142.0, 141.4, 141.2, 140.2, 137.5, 128.7, 128.6, 128.4, 128.0, 127.6, 127.5, 127.1,

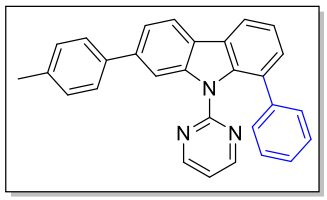
126.6, 126.1, 124.3, 122.4, 121.6, 120.3, 119.2, 117.0, 110.8. **HR-MS** (ESI) m/z calcd for $C_{28}H_{20}N_3^+[M+H^+]$ 398.1657, found 398.1665.

7-(4-isopropylphenyl)-1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (4b)



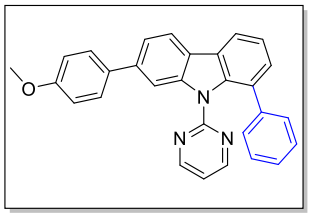
Yield (0.1 mmol scale, 35 mg, 79 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.37 – 8.30 (m, 3H), 8.15 (ddd, J = 15.6, 7.4, 1.3 Hz, 2H), 7.66 – 7.59 (m, 3H), 7.49 (td, J = 7.1, 4.2 Hz, 2H), 7.36 – 7.28 (m, 4H), 7.14 – 7.05 (m, 3H), 6.82 (t, J = 4.8 Hz, 1H), 2.96 (dq, J = 13.8, 6.9 Hz, 1H), 1.31 (d, J = 6.9 Hz, 6H).**^{13}C NMR** (101 MHz, CDCl3) δ 157.5, 157.3, 147.9, 141.4, 141.3, 140.2, 139.6, 137.5, 128.9, 128.5, 128.4, 128.0, 127.5, 126.8, 126.7, 126.1, 124.1, 122.4, 121.6, 120.2, 119.2, 116.9, 110.7, 33.8, 24.1. **HR-MS** (ESI) m/z calcd for $C_{31}H_{26}N_3^+[M+H^+]$ 440.5700, found 440.5704.

1-phenyl-9-(pyrimidin-2-yl)-7-(p-tolyl)-9H-carbazole (4c)



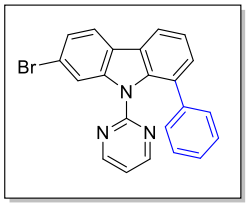
Yield (0.1 mmol scale, 33 mg, 80 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.35 – 8.31 (m, 3H), 8.17 – 8.11 (m, 2H), 7.62 – 7.58 (m, 3H), 7.50 – 7.45 (m, 2H), 7.32 – 7.26 (m, 4H), 7.13 – 7.07 (m, 3H), 6.82 (t, J = 4.8 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.5, 157.3, 141.4, 141.3, 140.2, 139.2, 137.5, 136.9, 129.4, 128.5, 128.4, 128.0, 127.5, 127.4, 126.7, 126.1, 124.1, 122.4, 121.5, 120.2, 119.1, 117.0, 110.6, 21.1. HR-MS (ESI) m/z calcd for $C_{29}H_{22}N_3$+[M+H+] 411.1735, found 412.1724.

7-(4-methoxyphenyl)-1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (4d)



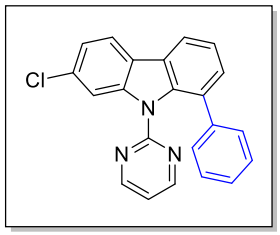
Yield (0.1 mmol scale, 30 mg, 71 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.31 – 8.23 (m, 3H), 8.16 – 8.08 (m, 2H), 7.56 (dd, J = 8.0, 1.5 Hz, 1H), 7.49 – 7.42 (m, 3H), 7.35 – 7.27 (m, 3H), 7.12 – 6.97 (m, 5H), 6.76 (t, J = 4.8 Hz, 1H), 3.79 (s, 3H).**^{13}C NMR** (101 MHz, CDCl3) δ 157.5, 157.2, 156.7, 141.4, 141.0, 137.4, 131.6, 131.4, 128.5, 128.5, 128.0, 127.5, 126.8, 126.0, 124.0, 123.9, 122.3, 120.8, 119.3, 119.1, 116.8, 113.1, 111.4, 55.7. **HR-MS** (ESI) m/z calcd for $C_{29}H_{22}N_3O^+[M+H^+]$ 428.1763, found 428.1751.

6-phenyl-5-(pyrimidin-2-yl)-5H-[1,3]dioxolo[4,5-b]carbazole (4e)



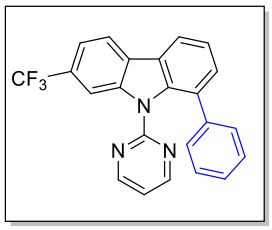
Yield (0.1 mmol scale, 30 mg, 75%); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.24 (t, J = 3.3 Hz, 3H), 8.00 (dd, J = 7.4, 1.5 Hz, 1H), 7.90 (d, J = 8.3 Hz, 1H), 7.41 (ddd, J = 7.4, 6.3, 4.8 Hz, 3H), 7.17 – 7.13 (m, 2H), 7.04 – 6.99 (m, 3H), 6.77 (t, J = 4.8 Hz, 1H)..**^{13}C NMR** (101 MHz, CDCl3) δ 157.3, 157.1, 141.4, 141.0, 137.0, 129.0, 128.6, 128.0, 127.5, 126.2, 126.1, 125.1, 124.0, 122.6, 121.2, 120.2, 119.1, 117.3, 115.4. HR-MS (ESI) m/z calcd for $C_{22}H_{15}BrN_3$+[M+H+] 399.0460, found 400.0471

7-chloro-1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (4f)



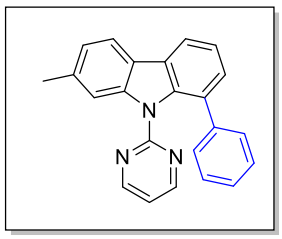
Yield (0.1 mmol scale, 25 mg, 71 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.32 (d, *J* = 4.8 Hz, 2H), 8.15 (d, *J* = 1.8 Hz, 1H), 8.07 (dd, *J* = 7.2, 1.8 Hz, 1H), 8.03 (d, *J* = 8.3 Hz, 1H), 7.53 – 7.43 (m, 2H), 7.34 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.24 (dd, *J* = 7.7, 1.9 Hz, 2H), 7.14 – 7.05 (m, 3H), 6.86 (t, *J* = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.46, 157.22, 141.38, 141.15, 137.32, 132.50, 129.01, 128.72, 128.16, 127.63, 126.33, 126.21, 122.76, 122.56, 120.98, 119.25, 117.37, 112.67. **HR-MS** (ESI) m/z calcd for $C_{22}H_{15}ClN_3^+$[M+H$^+$] 356.0955, found 356.0949.

7-methoxy-1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (4g)



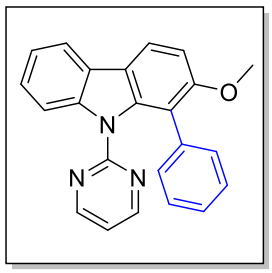
Yield (0.1 mmol scale, 31 mg, 80 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.33 (s, 1H), 8.22 (d, J = 4.8 Hz, 2H), 8.13 – 8.02 (m, 2H), 7.53 (dd, J = 8.1, 0.7 Hz, 1H), 7.47 – 7.36 (m, 2H), 7.17 – 7.11 (m, 2H), 7.04 – 6.96 (m, 3H), 6.75 (t, J = 4.8 Hz, 1H).**^{13}C NMR** (101 MHz, CD2Cl2) δ 155.50 (s), 155.1, 138.9, 138.1, 136.0, 127.9, 126.8, 126.7, 126.4, 126.2, 125.8, 125.6, 124.4, 123.7, 120.8, 118.46, 117.8, 116.8 (d, J = 3.6 Hz), 115.5 (s), 107.8 (d, J = 4.2 Hz). **HR-MS** (ESI) m/z calcd for $C_{23}H_{15}F_3N_3^+$[M+H$^+$] 390.1218, found 390.1204.

7-methyl-1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (4h)



Yield (0.1 mmol scale, 20 mg, 61 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.32 (d, J = 4.8 Hz, 2H), 8.06 (dd, J = 6.2, 2.7 Hz, 1H), 8.00 (d, J = 7.9 Hz, 1H), 7.95 – 7.90 (m, 1H), 7.46 – 7.41 (m, 2H), 7.27 (dd, J = 2.8, 0.9 Hz, 1H), 7.26 – 7.24 (m, 1H), 7.19 (ddd, J = 7.9, 1.3, 0.5 Hz, 1H), 7.13 – 7.03 (m, 3H), 6.82 (t, J = 4.8 Hz, 1H), 2.52 (s, 3H).**^{13}C NMR** (101 MHz, CDCl3) δ 157.5, 157.2, 141.4, 141.2, 136.98, 137.0, 128.9, 128.3, 128.1, 127.5, 126.9, 126.0, 123.3, 122.7, 122.2, 119.7, 118.9, 116.9, 112.2, 22.2. **HR-MS** (ESI) m/z calcd for $C_{22}H_{18}N_3^+$[M+H$^+$] 336.1501, found 336.1504.

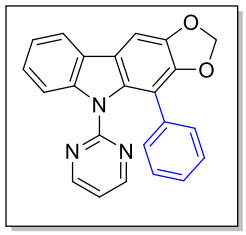
7-methoxy-1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (4i)



Yield (0.1 mmol scale, 25 mg, 72 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.29 (t, J = 4.9 Hz, 2H), 8.08 – 8.01 (m, 2H), 7.96 (dd, J = 7.3, 1.1 Hz, 1H), 7.39 – 7.31 (m, 2H), 7.27 (d, J = 1.6 Hz, 1H), 7.25 (q, J = 2.0 Hz, 1H), 7.13 – 7.01 (m, 4H), 6.79 (t, J = 4.8 Hz, 1H), 3.87 (s, 3H). **^{13}C NMR** (101 MHz, CDCl3) δ 157.4, 157.3, 156.2, 141.2, 139.0, 136.3, 130.0, 127.6, 126.2, 125.6, 125.0, 122.0, 120.9,

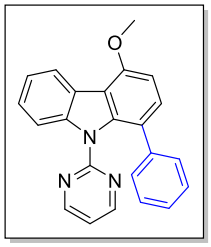
119.9, 119.3, 117.0, 116.2, 111.8, 107.0, 56.8. **HR-MS** (ESI) m/z calcd for $C_{23}H_{18}N_3O^+$[M+H$^+$] 352.1450, found 352.1465.

6-phenyl-5-(pyrimidin-2-yl)-5H-[1,3]dioxolo[4,5-b]carbazole (4j)



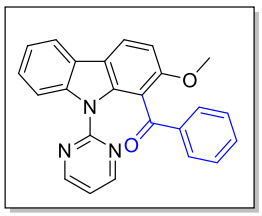
Yield (0.1 mmol scale, 27 mg, 75 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.29 (d, J = 4.8 Hz, 2H), 8.10 (t, J = 7.7 Hz, 2H), 7.46 – 7.41 (m, 1H), 7.34 (td, J = 7.4, 1.0 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.11 – 6.99 (m, 4H), 6.80 (t, J = 4.8 Hz, 1H), 6.23 (d, J = 5.7 Hz, 2H).**^{13}C NMR** (101 MHz, CDCl3) δ 157.6, 157.2, 143.3, 141.5, 141.2, 140.4, 133.5, 128.0, 127.6, 126.8, 125.82, 122.4, 122.3, 122.1, 120.8, 116.8, 111.9, 111.3, 109.2, 102.0. HR-MS (ESI) m/z calcd for $C_{23}H_{16}N_3O_2$+[M+H+] 366.1243, found 366.1237.

7-methoxy-1-phenyl-9-(pyrimidin-2-yl)-9H-carbazole (4k)



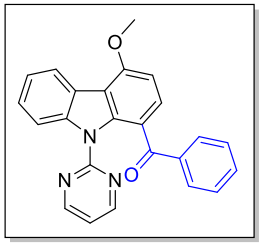
Yield (0.1 mmol scale, 25 mg, 72 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.44 (dd, *J* = 7.6, 0.7 Hz, 1H), 8.33 (d, *J* = 4.8 Hz, 2H), 8.08 (d, *J* = 8.1 Hz, 1H), 7.45 – 7.35 (m, 3H), 7.23 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.11 – 7.02 (m, 3H), 6.94 (d, *J* = 8.3 Hz, 1H), 6.83 (t, *J* = 4.8 Hz, 1H), 4.16 (s, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.49, 157.27, 155.55, 141.22, 140.04, 138.10, 129.23, 127.93, 127.54, 125.74, 125.55, 124.30, 123.19, 122.03, 121.27, 117.06, 115.62, 111.30, 103.45, 55.68. **HR-MS** (ESI) m/z calcd for $C_{23}H_{18}N_3O^+$[M+H$^+$] 352.1450, found 352.1449.

(2-methoxy-9-(pyrimidin-2-yl)-9H-carbazol-1-yl)(phenyl)methanone (4l)



Yield (0.1 mmol scale, 25 mg, 72 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.2 Hz, 1H), 8.16 (d, *J* = 4.8 Hz, 2H), 8.12 (d, *J* = 8.6 Hz, 1H), 8.01 (d, *J* = 7.2 Hz, 1H), 7.97 – 7.90 (m, 2H), 7.52 (ddd, *J* = 6.6, 3.8, 1.2 Hz, 1H), 7.42 (dt, *J* = 8.2, 4.5 Hz, 3H), 7.35 (td, *J* = 7.5, 0.9 Hz, 1H), 7.06 (d, *J* = 8.6 Hz, 1H), 6.88 (t, *J* = 4.8 Hz, 1H), 3.73 (s, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 194.3, 157.2, 157.1, 157.0, 139.9, 139.3, 137.0, 131.8, 129.0, 127.9, 126.0, 125.2, 122.4, 121.6, 121.0, 118.8, 117.1, 115.8, 114.6, 107.1, 56.7. **HR-MS** (ESI) m/z calcd for $C_{24}H_{18}N_3O_2^+$[M+H$^+$] 380.1399, found 380.1389.

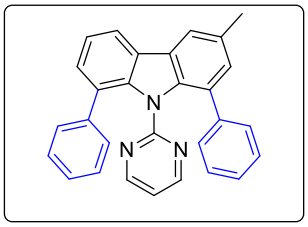
(4-methoxy-9-(pyrimidin-2-yl)-9H-carbazol-1-yl)(phenyl)methanone (4m)



Yield (0.1 mmol scale, 25 mg, 72 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.45 (d, J = 4.8 Hz, 2H), 8.40 (dd, J = 14.5, 7.9 Hz, 2H), 7.80 – 7.69 (m, 2H), 7.55 (d, J = 8.4 Hz, 1H), 7.48 – 7.33 (m, 5H), 6.94 (t, J = 4.8 Hz, 1H), 6.85 (d, J = 8.4 Hz, 1H), 4.16 (s, 3H).**^{13}C NMR** (101 MHz, CDCl3) δ 195.0, 158.5, 158.2, 157.7, 139.4, 138.3, 138.0, 132.1, 129.8, 129.7, 128.1, 126.2, 124.2, 123.0, 122.5, 119.7,

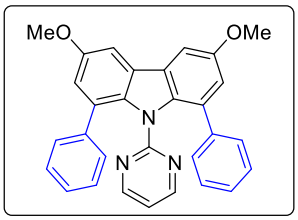
117.5, 115.5, 113.1, 102.5, 55.8. **HR-MS** (ESI) m/z calcd for $C_{24}H_{18}N_3O_2^+$[M+H$^+$] 380.1399, found 380.1401.

3-methyl-1,8-diphenyl-9-(pyrimidin-2-yl)-9H-carbazole (4n)



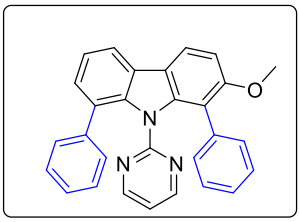
Yield (0.1 mmol scale, 34 mg, 84 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.17 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.02 – 7.94 (m, 1H), 7.76 (d, *J* = 4.8 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.29 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.15 – 7.12 (m, 1H), 6.94 (d, *J* = 2.1 Hz, 10H), 6.51 (t, *J* = 4.9 Hz, 1H), 2.57 (s, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.66, 156.45, 140.54, 137.62, 135.78, 130.81, 130.09, 129.33, 128.44, 128.42, 127.67, 127.66, 126.92, 126.64, 125.71, 125.20, 124.95, 120.56, 119.42, 119.35, 118.01, 21.36. **HR-MS** (ESI) m/z calcd for $C_{29}H_{22}N_3^+$[M+H$^+$] 412.1814, found 412.1819.

3,6-dimethoxy-1,8-diphenyl-9-(pyrimidin-2-yl)-9H-carbazole (4o)



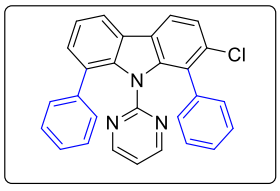
Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 8.5 Hz, 2H), 7.74 (d, *J* = 4.9 Hz, 2H), 7.01 (d, *J* = 8.6 Hz, 2H), 6.94 – 6.87 (m, 10H), 6.43 (t, *J* = 4.9 Hz, 1H), 3.75 (s, 6H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.71, 156.75, 155.94, 139.77, 135.09, 130.47, 127.44, 125.81, 119.21, 118.92, 118.19, 115.34, 105.94, 56.97. **HR-MS** (ESI) m/z calcd for $C_{30}H_{24}N_3O_2^+$[M+H$^+$] 458.1869, found 458.1851.

3-methoxy-1,8-diphenyl-9-(pyrimidin-2-yl)-9H-carbazole (4p)



Yield (0.1 mmol scale, 36 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** δ 8.20 – 8.06 (m, 2H), 7.76 (d, *J* = 4.8 Hz, 2H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.22 (dd, *J* = 7.4, 1.2 Hz, 1H), 7.07 (d, *J* = 8.6 Hz, 1H), 6.99 – 6.90 (m, 10H), 6.48 (t, *J* = 4.8 Hz, 1H), 3.80 (s, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.0, 156.1, 156.1, 139.8, 138.6, 137.5, 134.7, 129.8, 128.0, 128.0, 127.1, 127.0, 126.3, 125.4, 125.2, 124.5, 120.3, 119.4, 118.7, 118.1, 117.6, 114.6, 105.5, 56.4. **HR-MS** (ESI) m/z calcd for $C_{30}H_{24}N_3O_2^+$[M+H$^+$] 428.1763, found 428.1751.

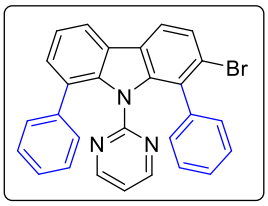
2-chloro-1,8-diphenyl-9-(pyrimidin-2-yl)-9H-carbazole (4q)



Yield (0.1 mmol scale, 31 mg, 72 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.16 (dd, *J* = 7.8, 1.3 Hz, 1H), 8.12 (d, *J* = 8.3 Hz, 1H), 7.79 (d, *J* = 4.9 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.28 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.05 – 6.88 (m, 10H), 6.49 (t, *J* = 4.9 Hz, 1H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.36, 156.81, 139.79, 138.84, 138.23, 136.36, 132.46, 130.20, 129.70, 128.67,

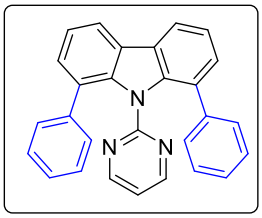
127.68, 127.62, 127.19, 126.68, 125.90, 125.04, 124.25, 123.65, 122.31, 121.14, 120.13, 119.32, 118.47. **HR-MS** (ESI) m/z calcd for $C_{28}H_{19}ClN_3^+$[M+H$^+$] 432.1268, found 432.1256.

2-bromo-1,8-diphenyl-9-(pyrimidin-2-yl)-9H-carbazole (4r)



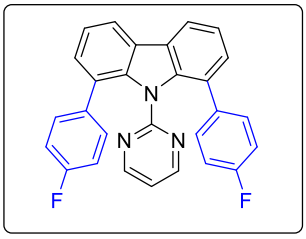
Yield (0.1 mmol scale, 40 mg, 86 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 7.8, 1.3 Hz, 1H), 8.06 (d, *J* = 8.3 Hz, 1H), 7.79 (d, *J* = 4.9 Hz, 2H), 7.66 (d, *J* = 8.3 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.28 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.04 – 6.89 (m, 10H), 6.49 (t, *J* = 4.9 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.3, 156.7, 139.6, 138.8, 138.1, 138.0, 130.1, 129.7, 128.6, 127.5, 127.5, 127.1, 126.7, 126.6, 125.8, 125.2, 124.1, 124.1, 123.1, 121.0, 120.4, 119.2, 118.4. **HR-MS** (ESI) m/z calcd for $C_{30}H_{22}Cl_2N_3^+$[M+H$^+$] 494.1191, found 494.1183.

1,8-diphenyl-9-(pyrimidin-2-yl)-9H-carbazole (3s)



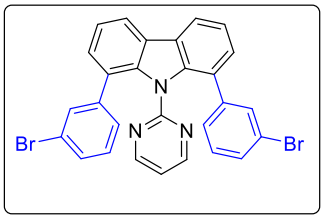
Yield (0.1 mmol scale, 32 mg, 80 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.21 (dd, *J* = 7.7, 1.3 Hz, 2H), 7.78 (d, *J* = 4.8 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.31 (dd, *J* = 7.4, 1.4 Hz, 2H), 7.01 – 6.92 (m, 10H), 6.52 (t, *J* = 4.9 Hz, 1H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 156.33, 140.31, 137.23, 129.36, 128.31, 127.53, 126.83, 125.59, 124.84, 120.57, 119.28, 118.00. **HR-MS** (ESI) m/z calcd for $C_{28}H_{20}N_3^+$[M+H$^+$] 398.1657, found 398.1652.

1,8-bis(4-fluorophenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3t)



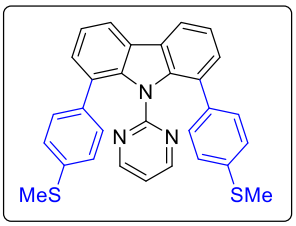
Yield (0.1 mmol scale, 34 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.23 – 8.15 (m, 2H), 7.90 (d, *J* = 4.8 Hz, 2H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 5.7 Hz, 2H), 6.89 (m, 4H), 6.72 – 6.58 (m, 5H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.47, 160.03, 157.86, 156.78, 137.60, 136.34, 136.31, 130.11, 130.03, 129.59, 125.86, 124.99, 120.86, 119.69, 118.31, 114.60, 114.39. **HR-MS** (ESI) m/z calcd for $C_{28}H_{18}F_2N_3^+$[M+H$^+$] 434.1469, found 434.1462.

1,8-bis(3-bromophenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3u)



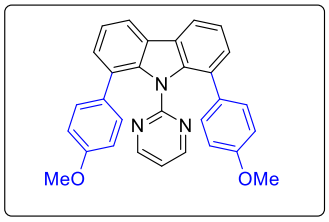
Yield (0.1 mmol scale, 42 mg, 76 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.22 (dd, *J* = 7.7, 1.2 Hz, 2H), 8.00 (d, *J* = 4.9 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.29 (dd, *J* = 7.4, 1.2 Hz, 2H), 7.14 (m, 3H), 7.06 – 6.81 (m, 5H), 6.68 (t, *J* = 4.8 Hz, 1H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.52, 156.87, 142.25, 137.10, 131.80, 129.43, 129.38, 129.20, 127.34, 125.35, 124.93, 121.79, 120.90, 120.08, 119.07. **HR-MS** (ESI) m/z calcd for $C_{28}H_{18}Br_2N_3^+$[M+H$^+$] 553.9867, found 553.9840.

1,8-bis(4-(methylthio)phenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3v)



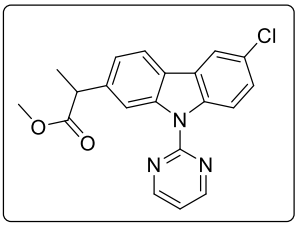
Yield (0.1 mmol scale, 43 mg, 88 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.18 (d, *J* = 7.6 Hz, 2H), 7.87 (d, *J* = 4.8 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.27 (d, *J* = 7.3 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 4H), 6.61 (t, *J* = 4.8 Hz, 1H), 6.50 (d, *J* = 8.5 Hz, 4H), 3.72 (s, 6H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.95, 157.78, 156.48, 137.72, 132.96, 129.58, 129.52, 126.63, 124.99, 120.70, 119.21, 117.95, 113.25, 55.46. **HR-MS** (ESI) m/z calcd for $C_{30}H_{24}S_2N_3^+$[M+H$^+$] 490.1412, found 490.1417.

1,8-bis(4-methoxyphenyl)-9-(pyrimidin-2-yl)-9H-carbazole (3w)



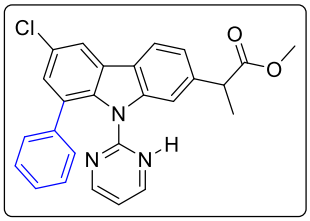
Yield (0.1 mmol scale, 38 mg, 83 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.18 (dd, *J* = 7.7, 1.3 Hz, 2H), 7.87 (d, *J* = 4.8 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.28 (dd, *J* = 7.3, 1.3 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 4H), 6.61 (t, *J* = 4.8 Hz, 1H), 6.54 – 6.47 (m, 4H), 3.72 (s, 6H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 157.77, 157.60, 156.29, 137.54, 132.78, 129.40, 129.34, 126.45, 124.81, 120.52, 119.03, 117.77, 113.07, 55.28. **HR-MS** (ESI) m/z calcd for $C_{30}H_{24}N_3O_2^+$[M+H$^+$] 458.1869, found 458.1862.

Methyl 2-(6-chloro-9-(pyrimidin-2-yl)-9H-carbazol-2-yl)propanoate (5)



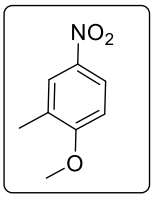
The title compound was prepared according to procedure **2.3,** White solid, Yield (2.0 mmol scale, 446 mg, 61 %); (hexane/ethyl acetate = 8.2:1.8, V/V).**m.p:** 148-152 ^{o}C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 4.8 Hz, 3H), 8.79 (d, *J* = 8.9 Hz, 1H), 7.99 (d, *J* = 2.1 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.43 (dd, *J* = 9.0, 2.2 Hz, 1H), 7.35 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.15 (t, *J* = 4.8 Hz, 1H), 3.97 (q, *J* = 7.1 Hz, 1H), 3.69 (s, 3H), 1.64 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** 13C NMR (101 MHz, CDCl3) δ 175.2, 158.9, 157.9, 140.1, 139.8, 137.7, 127.8, 126.9, 126.4, 123.9, 122.0, 119.8, 119.2, 117.6, 116.3, 115.8, 52.1, 46.2, 19.1. **HR-MS** (ESI) m/z calcd for $C_{20}H_{17}N_3O2^+$[M+H$^+$] 366.1009, found 366.1017.

Caprofen derivatives (5a)



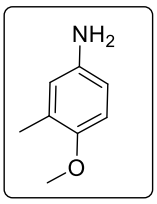
Yield (0.1 mmol scale, 33 mg, 72 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 4.8 Hz, 2H), 8.03 (dd, *J* = 12.6, 10.5 Hz, 3H), 7.44 (d, *J* = 2.0 Hz, 1H), 7.33 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.22 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.12 – 7.06 (m, 3H), 6.84 (t, *J* = 4.8 Hz, 1H), 3.89 (q, *J* = 7.1 Hz, 1H), 3.65 (s, 3H), 1.58 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, CDCl3) δ 175.0, 157.3, 157.1, 141.5, 140.2, 140.0, 135.7, 129.7, 128.2, 128.1, 127.8, 127.7, 127.4,126.6, 123.2, 121.8, 120.4, 118.7, 117.2, 111.5, 52.1, 46.1, 19.0. **HR-MS** (ESI) m/z calcd for $C_{26}H_{21}N_3O_2^+$[M+H$^+$] 442.1322, found 442.1334.

1-methoxy-2-methyl-4-nitrobenzene (7)



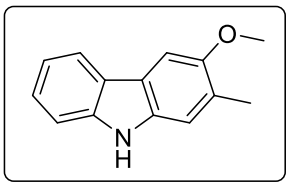
Yield (0.1 mmol scale, 27 mg, 76 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 9.0, 2.7 Hz, 1H), 8.03 (dd, *J* = 2.8, 0.7 Hz, 1H), 6.86 (d, *J* = 9.0 Hz, 1H), 3.94 (s, 3H), 2.27 (s, 3H).**^{13}C NMR** (101 MHz, CDCl3) δ 162.8, 140.9, 127.8, 125.9, 123.6, 109.2, 55.9, 16.2. **HR-MS** (ESI) m/z calcd for $C_8H_{10}NO_3^+$[M+H$^+$] 168.0661, found 168.0662.

4-methoxy-3-methylaniline (8)



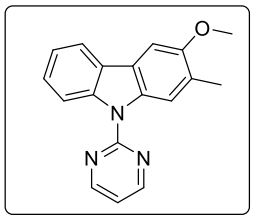
Yield (0.1 mmol scale, 27 mg, 76 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 6.64 (d, J = 8.4 Hz, 1H), 6.49 (ddd, J = 8.4, 5.8, 1.5 Hz, 2H), 3.73 (s, 3H), 3.35 (s, 2H), 2.15 (s, 3H).**^{13}C NMR** (101 MHz, CDCl3) δ 150.7, 139.0, 127.2, 118.2, 112.7, 111.1, 55.5, 15.79. **HR-MS** (ESI) m/z calcd for $C_8H_{12}NO^+$[M+H$^+$] 138.0919, found 138.0910.

Hyellazole isomer (10)



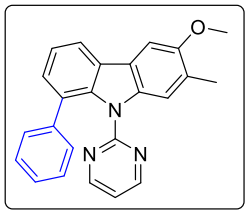
Yield (0.1 mmol scale, 27 mg, 76 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.37 (d, J = 4.8 Hz, 2H), 7.38 (dd, J = 8.7, 2.7 Hz, 1H), 7.31 – 7.24 (m, 1H), 7.16 (s, 1H), 6.82 (d, J = 8.7 Hz, 1H), 6.65 (t, J = 4.8 Hz, 1H), 3.83 (s, 3H), 2.24 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 152.75, 140.04, 134.36, 126.72, 125.33, 123.88, 121.59, 120.06, 119.18, 112.62, 110.96, 101.25, 56.25, 17.61. **HR-MS** (ESI) m/z calcd for $C_{14}H_{14}NO^+$[M+H$^+$] 212.1075, found 212.1075.

Hyellazole isomer (11)



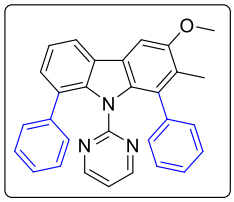
Yield (0.1 mmol scale, 27 mg, 76 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.79 – 8.70 (m, 3H), 8.58 (s, 1H), 7.91 (dd, J = 7.7, 0.5 Hz, 1H), 7.40 – 7.35 (m, 2H), 7.28 – 7.23 (m, 1H), 6.97 (t, J = 4.8 Hz, 1H), 3.90 (s, 3H), 2.36 (s, 3H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.16, 157.83, 154.15, 139.18, 133.39, 126.41, 126.10, 125.98, 124.26, 122.01, 118.99, 118.17, 116.42, 115.55, 100.07, 55.77, 17.54. **HR-MS** (ESI) m/z calcd for $C_{18}H_{16}N_3O^+$[M+H$^+$] 290.1293, found 290.1295.

Hyellazole isomer (12)



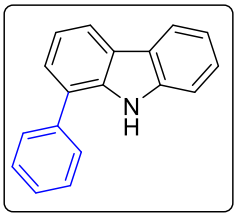
Yield (0.1 mmol scale, 27 mg, 76 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 4.8 Hz, 2H), 7.96 (dd, *J* = 6.5, 2.4 Hz, 1H), 7.87 (d, *J* = 0.4 Hz, 1H), 7.43 (s, 1H), 7.36 (dd, *J* = 4.5, 2.7 Hz, 2H), 7.23 – 7.19 (m, 2H), 7.05 – 6.99 (m, 3H), 6.72 (t, *J* = 4.8 Hz, 1H), 3.92 (s, 3H), 2.31 (s, 3H). **^{13}C NMR** (101 MHz, CDCl3) δ 157.53, 157.1, 154.1, 141.5, 137.0, 136.9, 135.1, 128.5, 127.9, 127.4, 127.2, 126.8, 126.0, 123.3, 122.0, 118.6, 116.6, 114.0, 100.6, 55.9, 17.4. **HR-MS** (ESI) m/z calcd for $C_{24}H_{20}N_3O^+$[M+H$^+$] 366.1606, found 366.1603.

Hyellazole derivative (13)



Yield (0.1 mmol scale, 36 mg, 82 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.05 (dd, J = 7.8, 1.2 Hz, 1H), 7.69 (d, J = 4.8 Hz, 2H), 7.57 (s, 1H), 7.25 (t, J = 7.5 Hz, 1H), 7.14 (dd, J = 7.3, 1.3 Hz, 1H), 6.92 – 6.84 (m, 8H), 6.79 (dt, J = 4.6, 3.5 Hz, 2H), 6.37 (t, J = 4.8 Hz, 1H), 3.97 (s, 3H), 1.94 (s, 3H).**^{13}C NMR** (101 MHz, CDCl3) δ 157.9, 156.5, 153.0, 140.1, 138.3, 138.2, 133.4, 129.9, 128.7, 128.6, 127.6, 127.4, 127.0, 126.9, 125.9, 125.6, 125.6, 125.5, 122.4, 120.1, 118.7, 117.8, 100.1, 56.1, 13.9. **HR-MS** (ESI) m/z calcd for $C_{30}H_{24}N_3O^+$[M+H$^+$] 442.1919, found 442.1927.

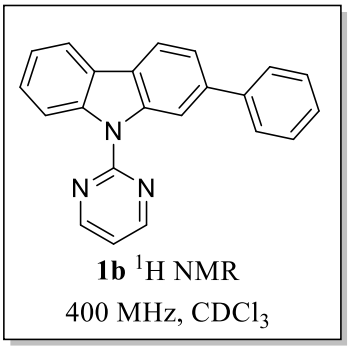
1-phenyl-9H-carbazole (14)



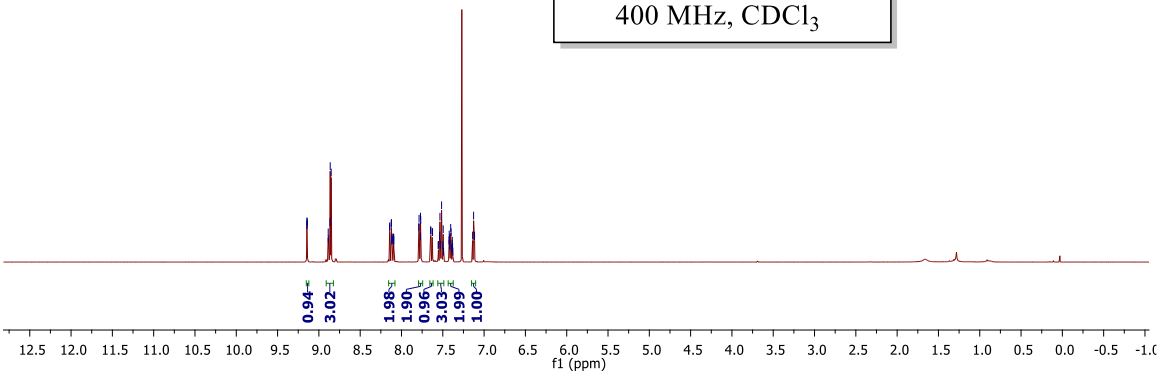
Yield (0.1 mmol scale, 18.72 mg, 78 %); white solid (hexane/ethyl acetate = 9.1:1.0, V/V). **^{1}H NMR** (400 MHz, CDCl3) δ 8.32 (s, 1H), 8.11 (ddd, J = 13.3, 7.7, 0.7 Hz, 2H), 7.71 (dt, J = 8.0, 1.6 Hz, 2H), 7.59 – 7.54 (m, 2H), 7.47 – 7.41 (m, 4H), 7.33 (t, J = 7.6 Hz, 1H), 7.28 – 7.23 (m, 1H).**^{13}C NMR** (101 MHz, CDCl3) δ 139.5, 139.1, 137.3, 129.3, 128.4, 127.6, 126.0, 125.7, 125.0, 123.7, 123.5, 120.5, 119.9, 119.6, 119.5, 110.7.**HR-MS** (ESI) m/z calcd for $C_{18}H_{14}N^+$[M+H$^+$] 244.1121, found 244.1117.

6.0 ^{1}H and ^{13}C NMR spectra

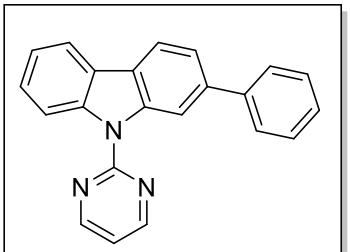
GP-SS-6.10.1.1r



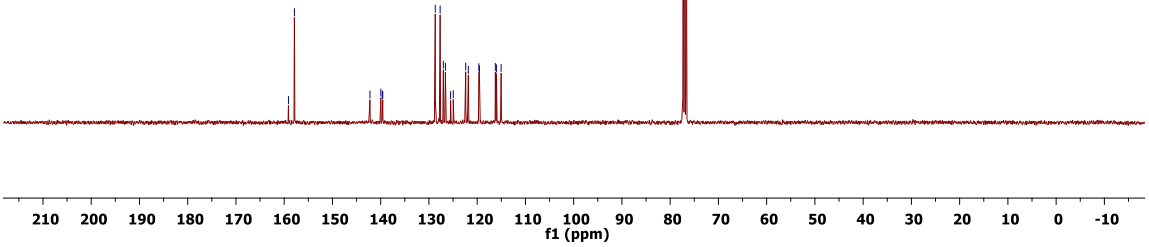
1b ^{1}H NMR
400 MHz, $CDCl_3$



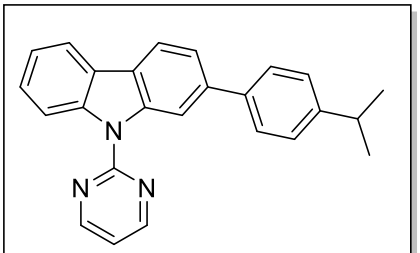
GP-SS-6.11.1.1r



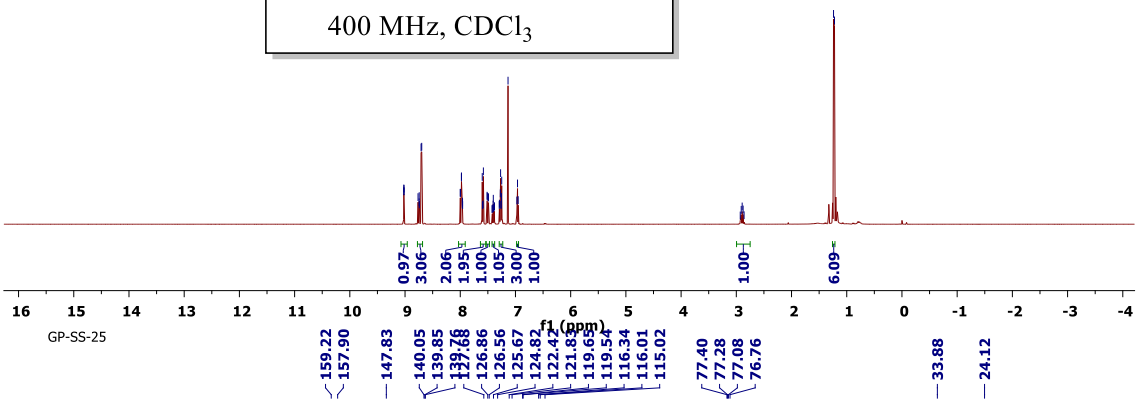
1b ^{13}C NMR
101 MHz, $CDCl_3$



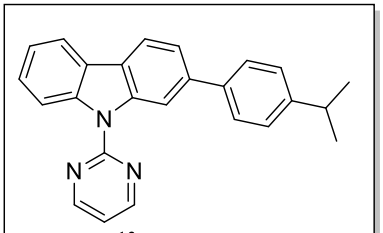
GP-SS-25



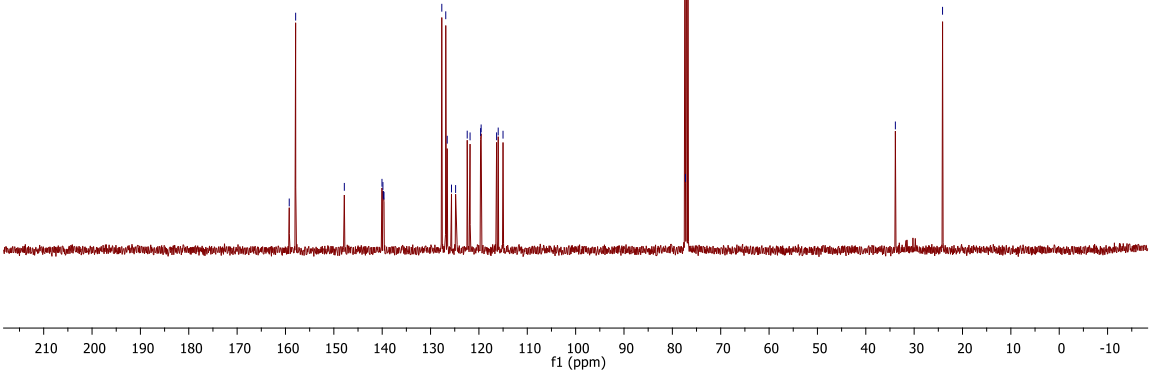
1c ^{1}H NMR
400 MHz, $CDCl_3$



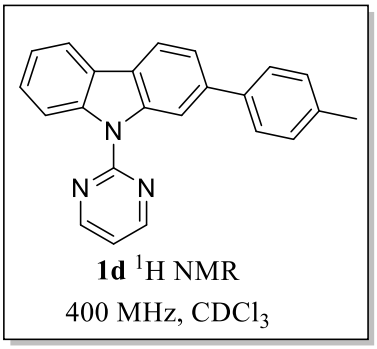
GP-SS-25



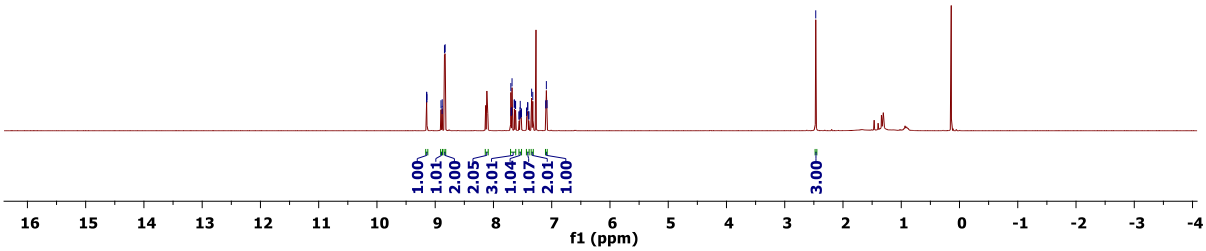
1c ^{13}C NMR
101 MHz, $CDCl_3$



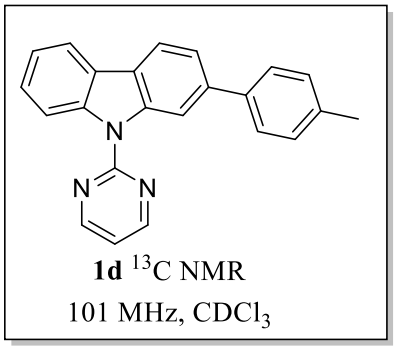
GP-SS-26



1d ^{1}H NMR
400 MHz, $CDCl_3$

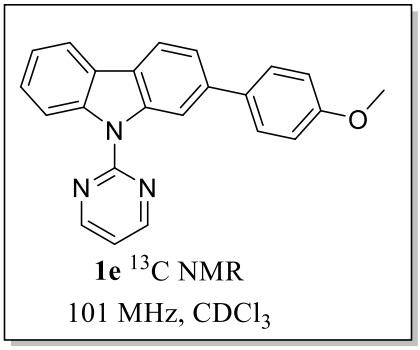


GP-SS-11.43.1.1r



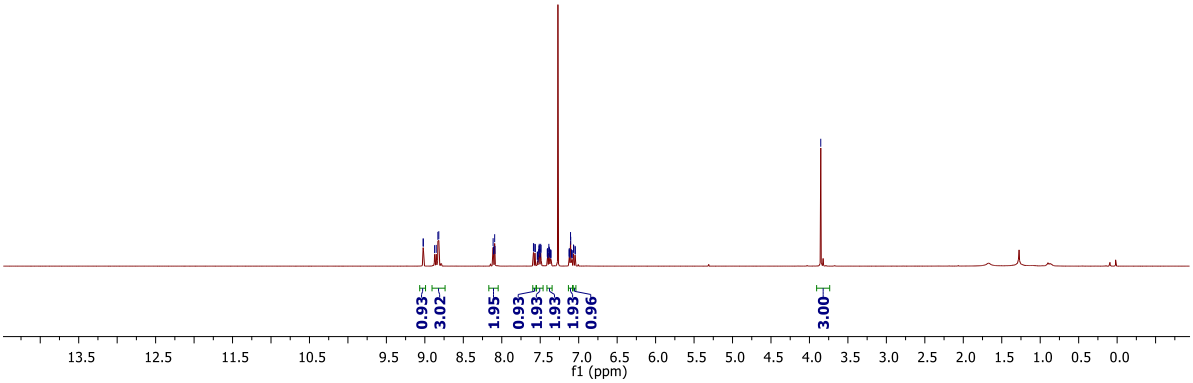
1d ^{13}C NMR
101 MHz, $CDCl_3$

GP-SS-12.52.1.1r

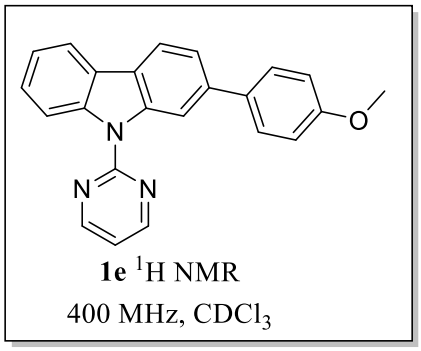


1e ^{13}C NMR

101 MHz, $CDCl_3$

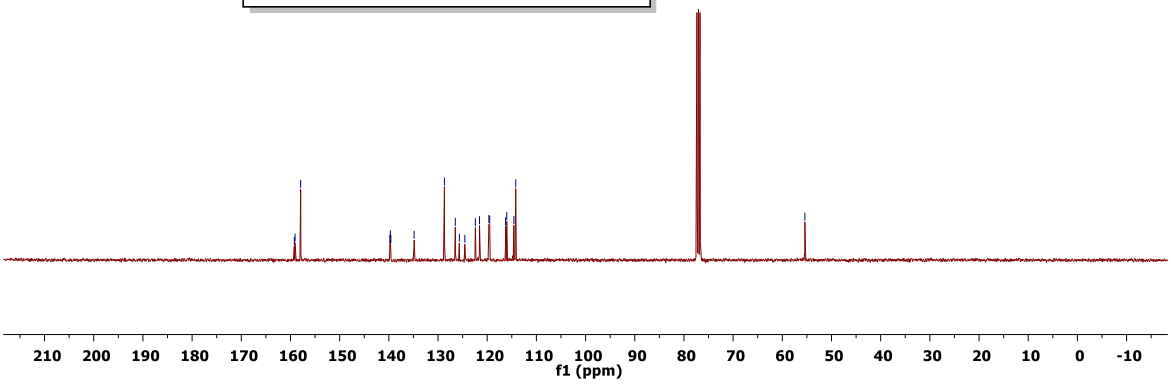


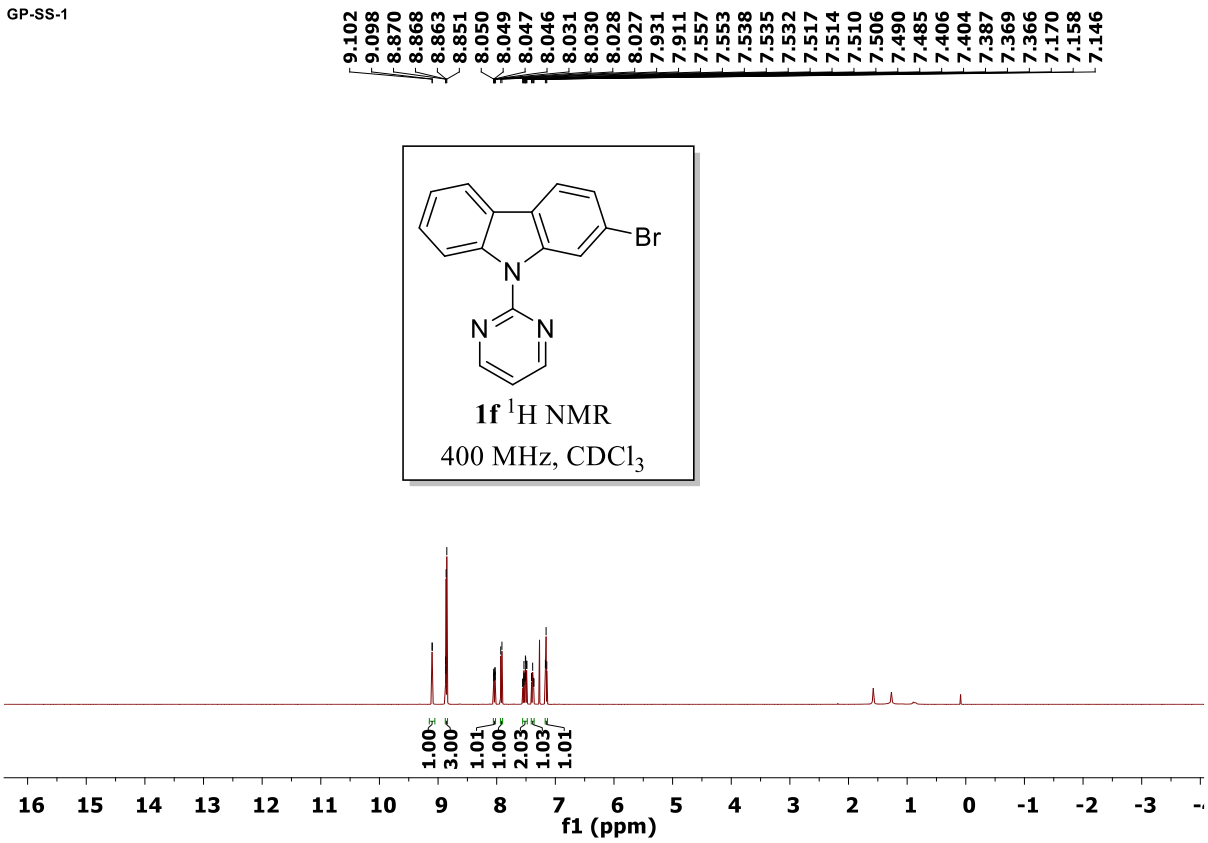
GP-SM-09-122

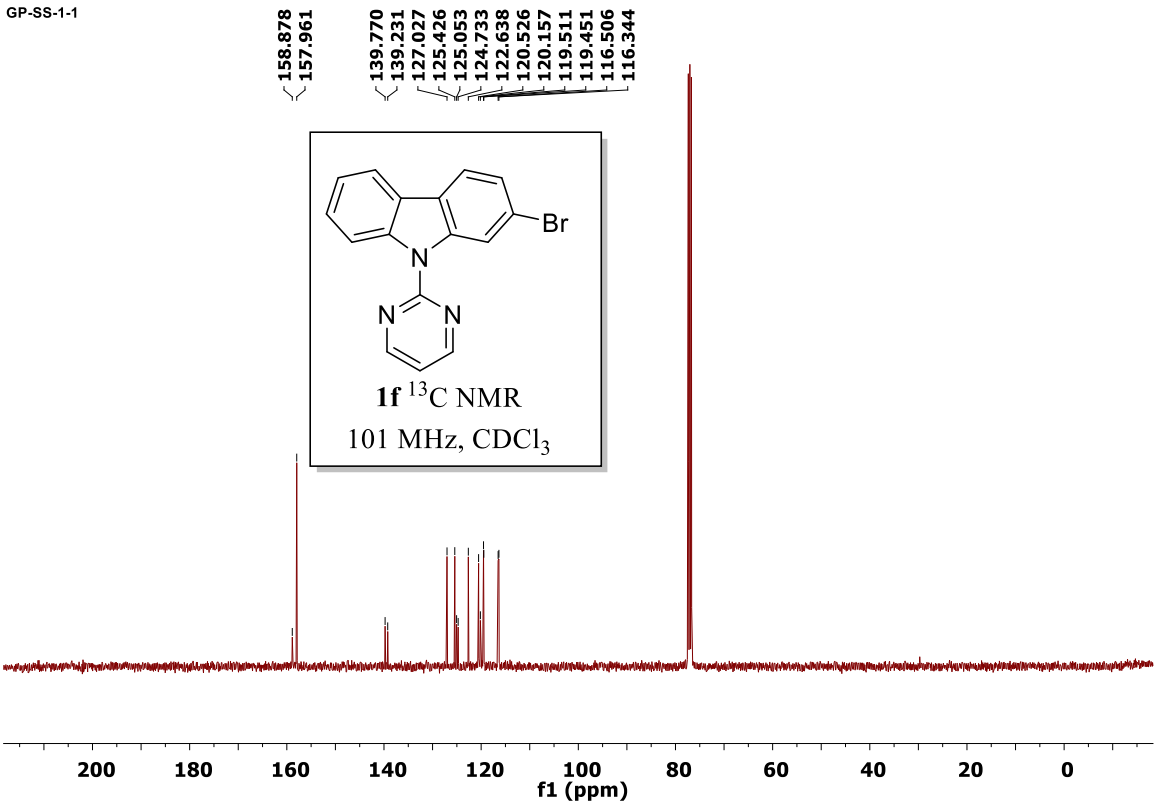


1e ^{1}H NMR

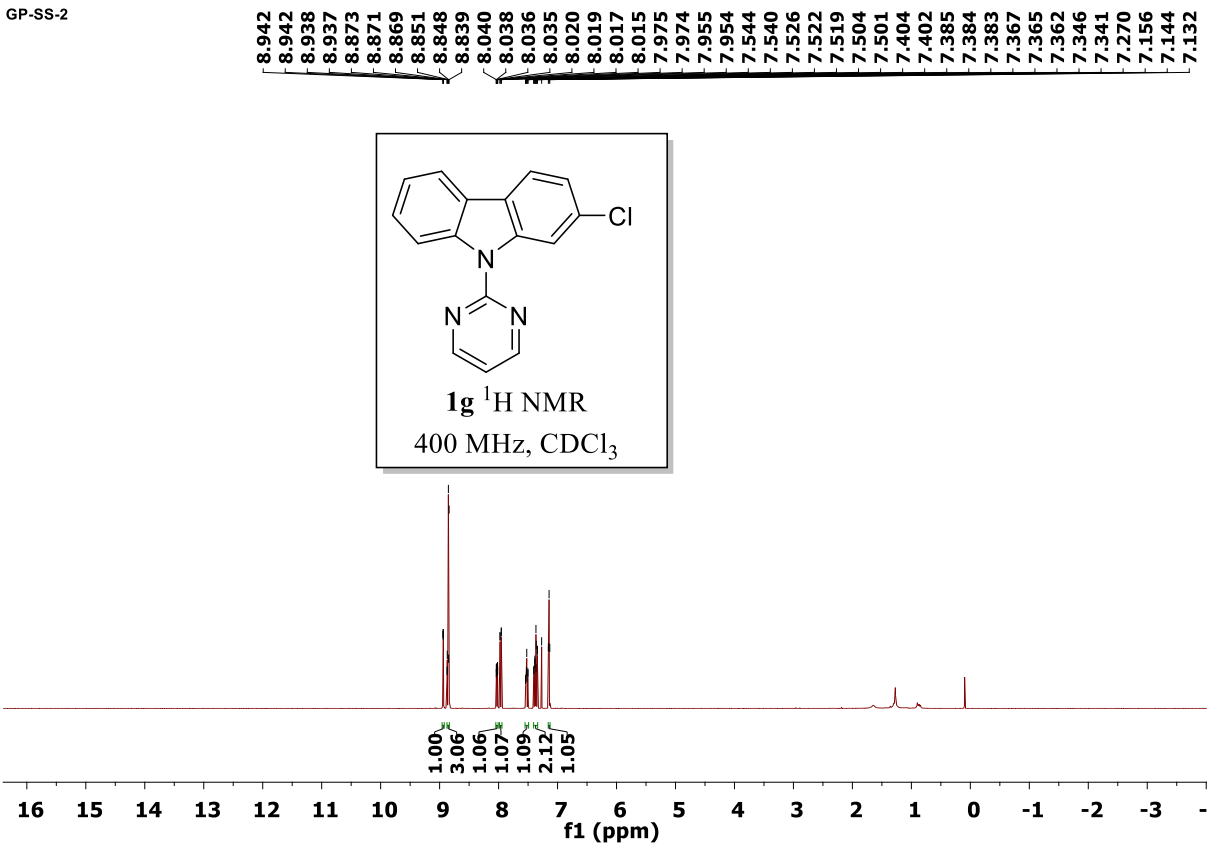
400 MHz, $CDCl_3$



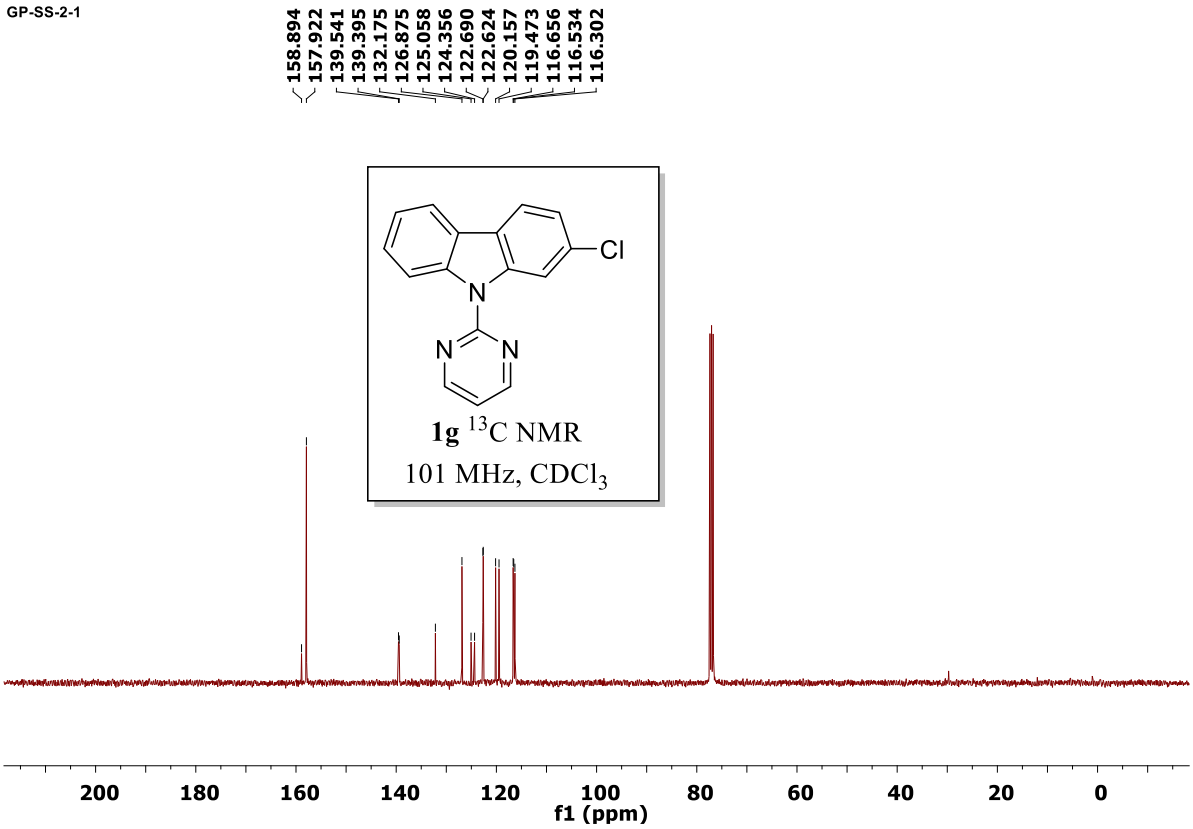

GP-SS-1
9.102
9.098
8.870
8.868
8.863
8.851
8.050
8.049
8.047
8.046
8.031
8.030
8.028
8.027
7.931
7.911
7.557
7.553
7.538
7.535
7.532
7.517
7.514
7.510
7.506
7.490
7.485
7.406
7.404
7.387
7.369
7.366
7.170
7.158
7.146
Br
N
N
N
1f 1H NMR
400 MHz, CDCl3
1.00
3.00
1.01
1.00
2.03
1.03
1.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


GP-SS-1-1
158.878
157.961
139.770
139.231
127.027
125.426
125.053
124.733
122.638
120.526
120.157
119.511
119.451
116.506
116.344
Br
N
N
N
1f 13C NMR
101 MHz, CDCl3
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

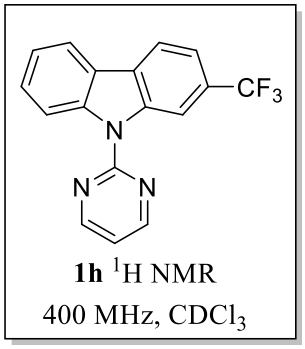
GP-SS-2



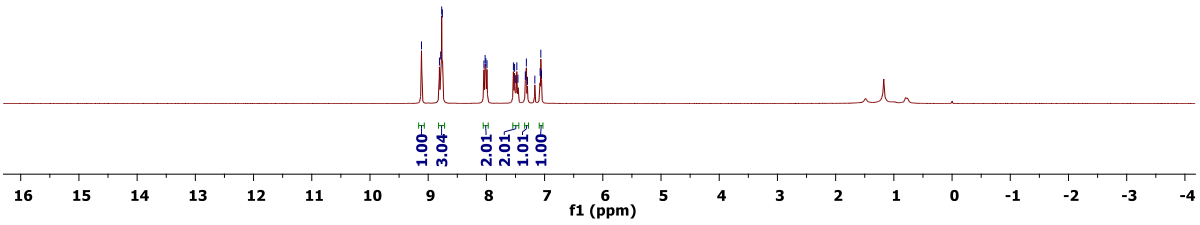
GP-SS-2-1



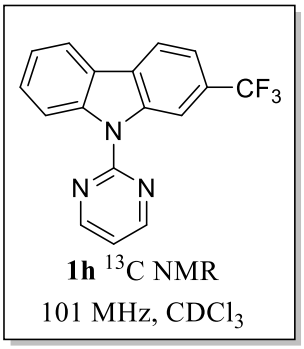
GP-SS-4.10.1.1r



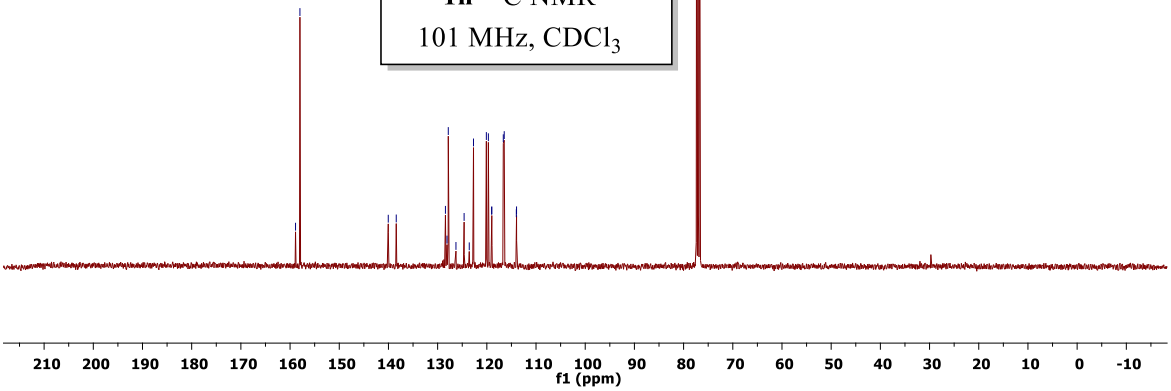
1h ^{1}H NMR
400 MHz, $CDCl_3$



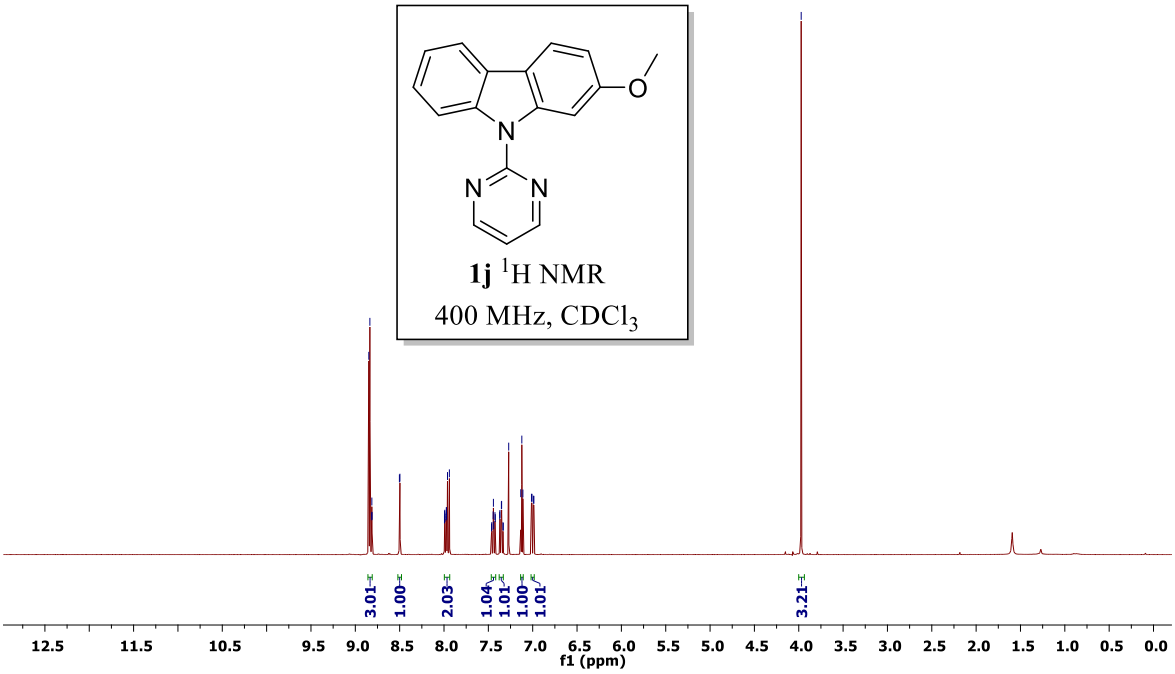
pdata/1



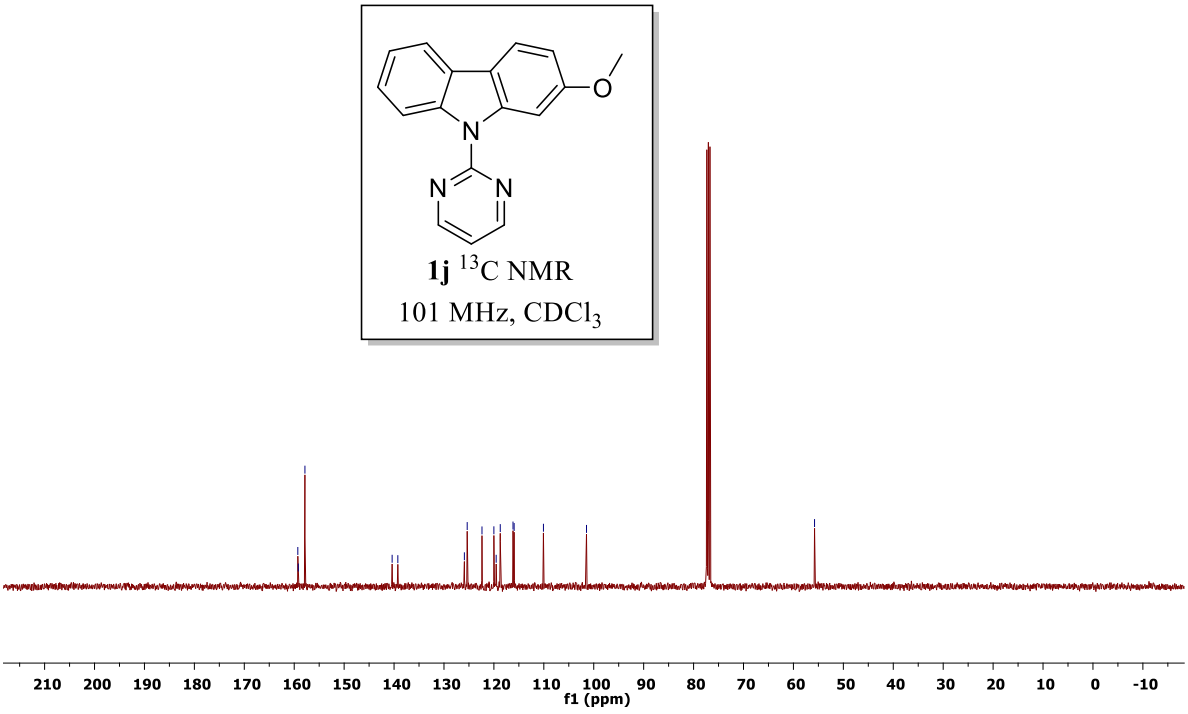
1h ^{13}C NMR
101 MHz, $CDCl_3$



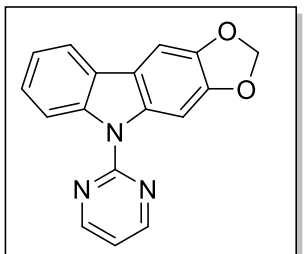
GP-5S-5.10.1.1r



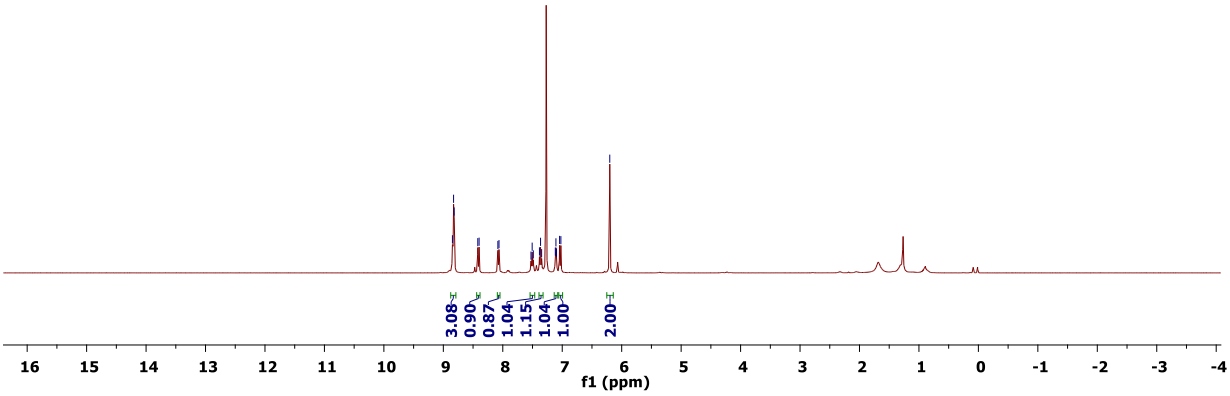
GP-5S-5.11.1.1r



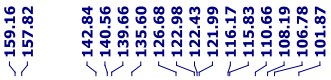
GP-SS-10.32.1.1r

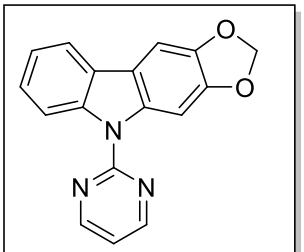


1k ^{1}H NMR
400 MHz, $CDCl_3$

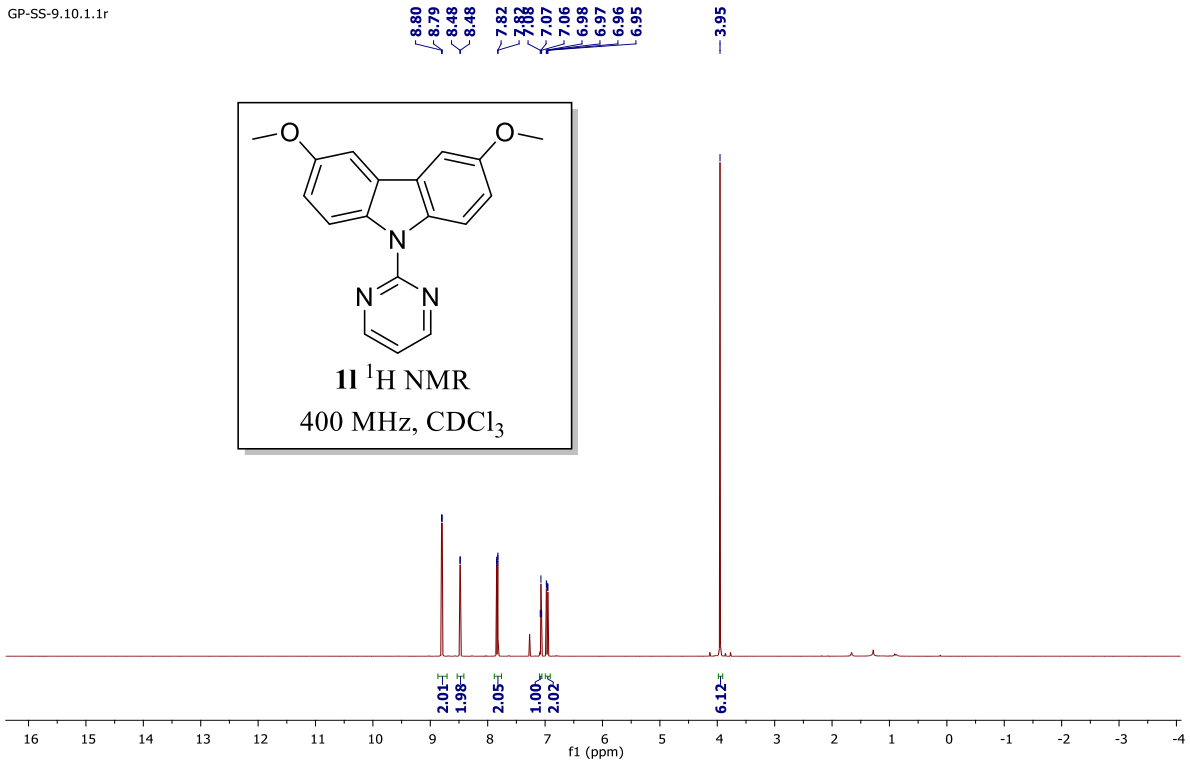


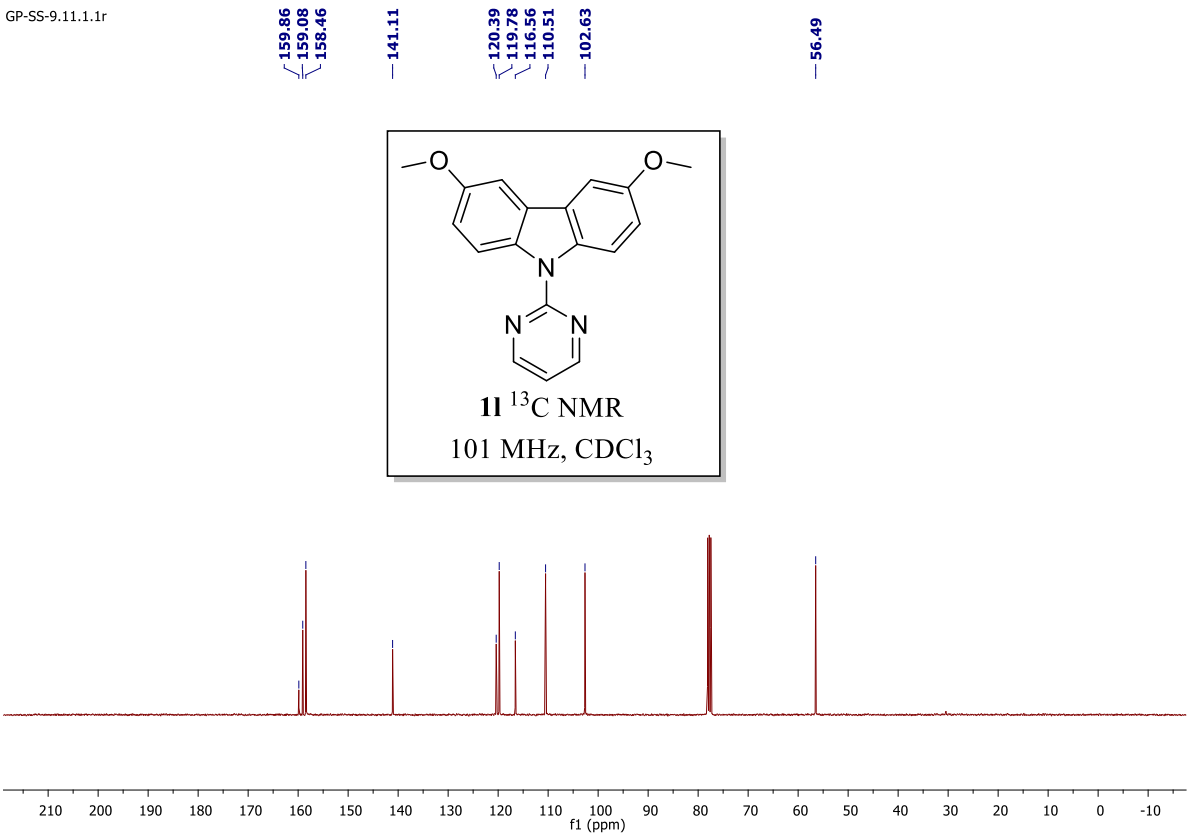
GP-SS-10.33.1.1r



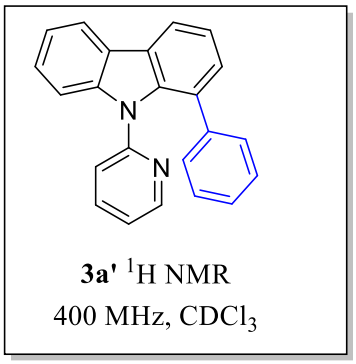


1k ^{13}C NMR
101 MHz, $CDCl_3$

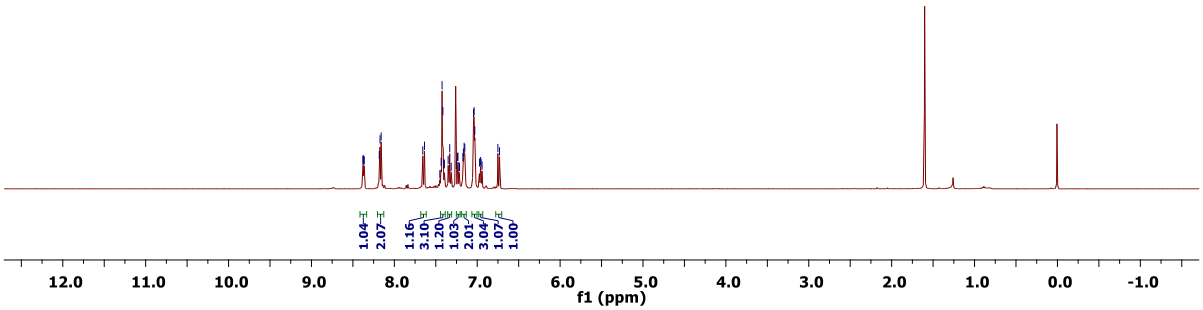

GP-SS-9.10.1.1r
8.80
8.79
8.48
8.48
7.82
7.82
7.08
7.07
7.06
6.98
6.97
6.96
6.95
3.95
O
O
N
N
N
11 1H NMR
400 MHz, CDCl3
2.01
1.98
2.05
1.00
2.02
6.12
f1 (ppm)


GP-SS-9.11.1.1r
159.86
159.08
158.46
141.11
120.39
119.78
116.56
110.51
102.63
56.49
O
O
N
N
N
11 13C NMR
101 MHz, CDCl3
f1 (ppm)

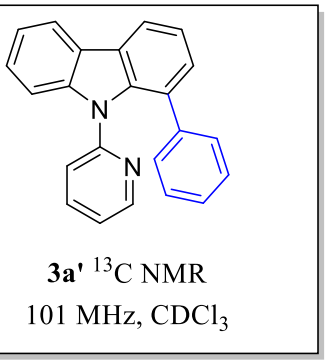
GP-SM-10-105



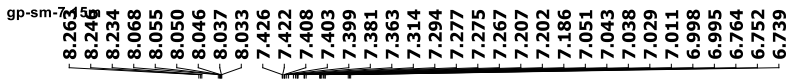
3a' ^{1}H NMR
400 MHz, $CDCl_3$

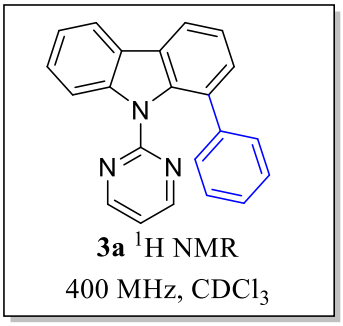


GP-SM-10-105

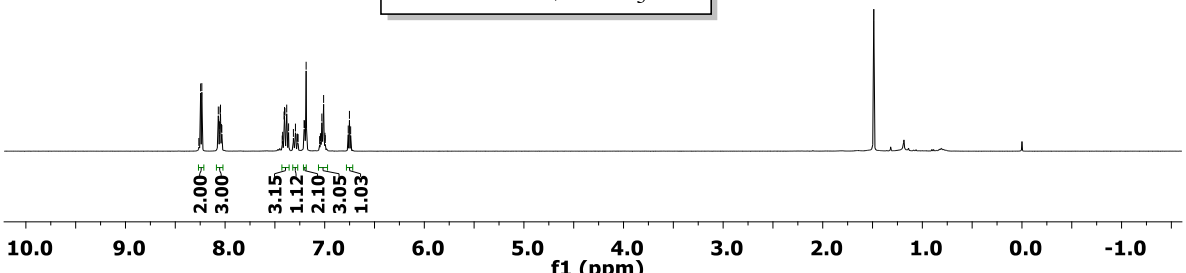


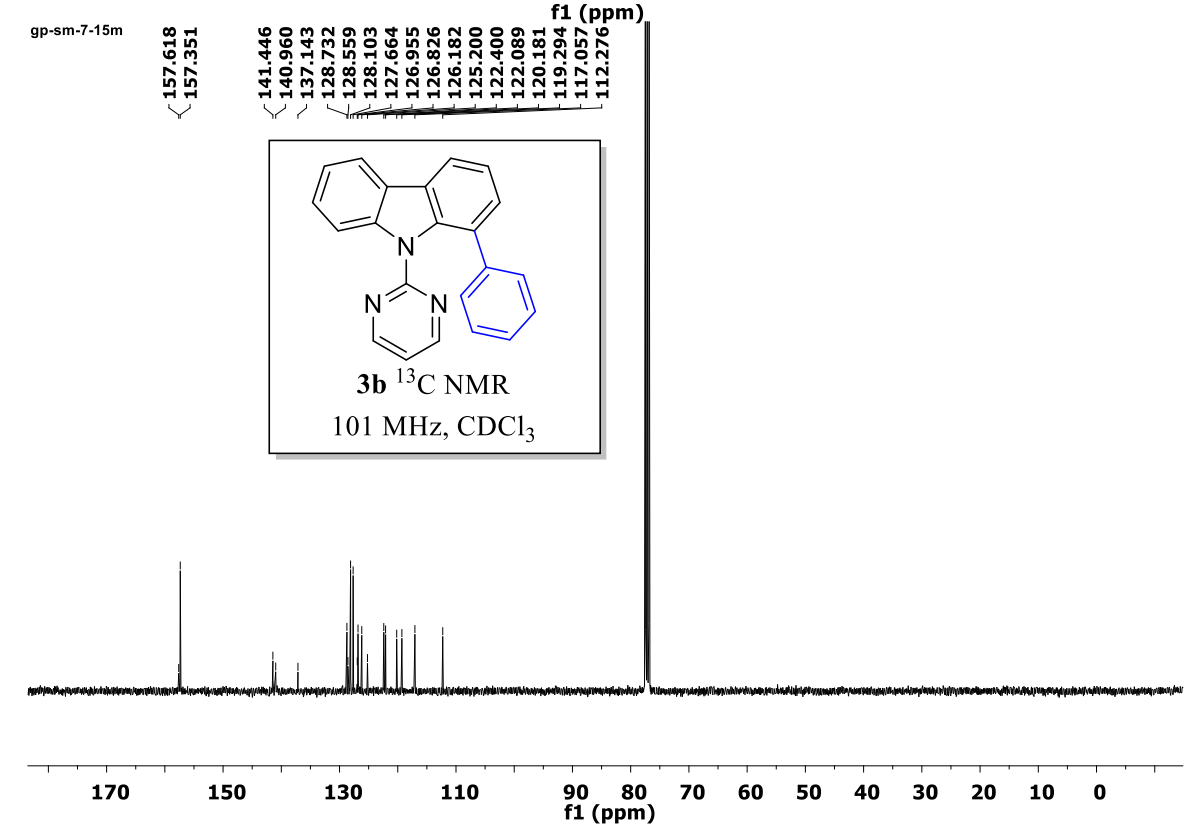
3a' ^{13}C NMR
101 MHz, $CDCl_3$





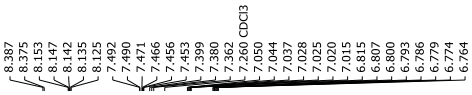
3a ^{1}H NMR
400 MHz, $CDCl_3$

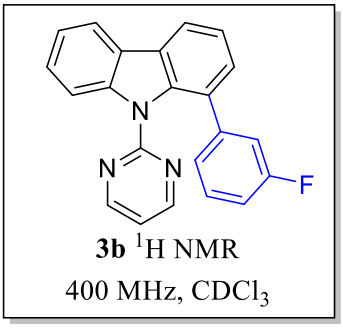




3b ^{13}C NMR
101 MHz, $CDCl_3$

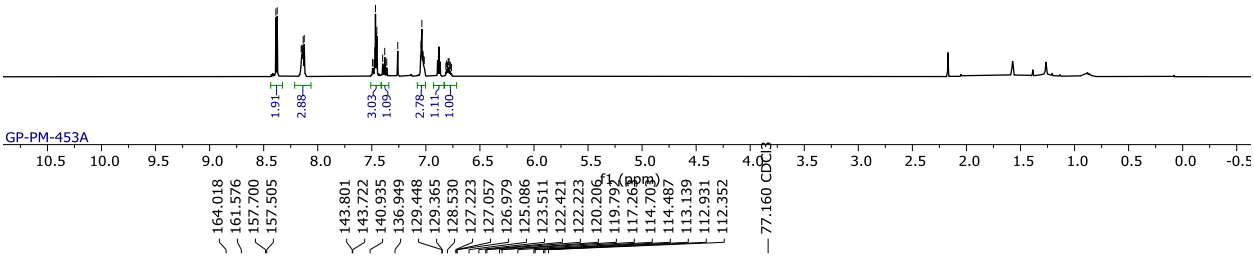
GP-PM-453A



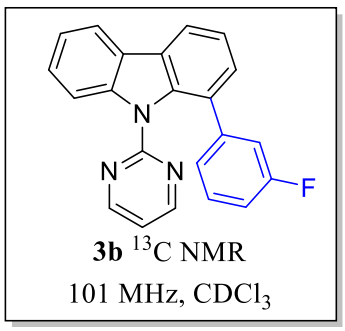


3b ^{1}H NMR

400 MHz, $CDCl_3$

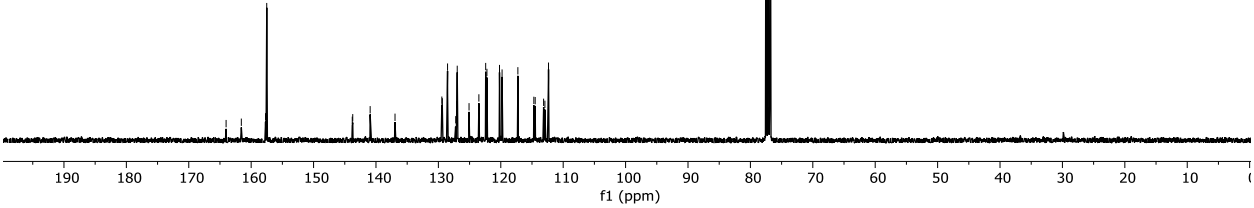


GP-PM-453A

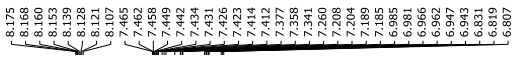


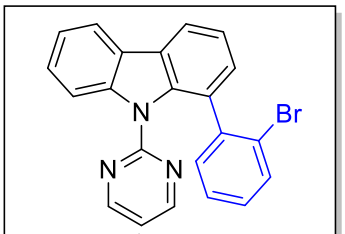
3b ^{13}C NMR

101 MHz, $CDCl_3$



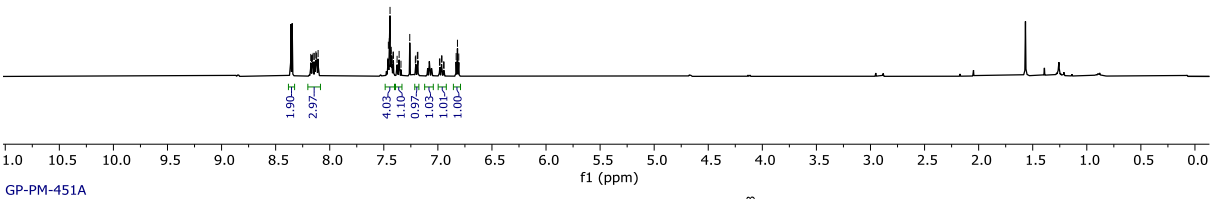
GP-PM-451A



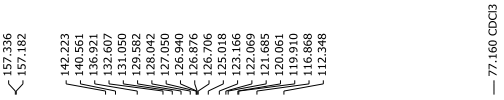


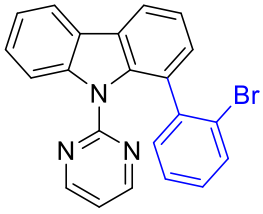
3c ^{1}H NMR

400 MHz, $CDCl_3$



GP-PM-451A



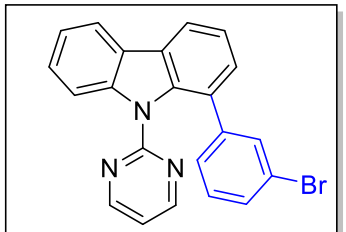


3c ^{13}C NMR

101 MHz, $CDCl_3$

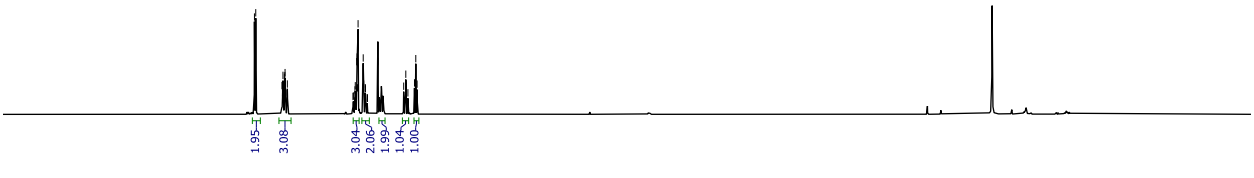
GP-SM-7-118

8.403 8.391 8.148 8.144 8.142 8.141 8.139 8.136 8.126 8.123 8.121 8.120 8.101 8.098 8.097 7.490 7.487 7.475 7.472 7.469 7.467 7.457 7.453 7.448 7.443 7.400 7.396 7.391 7.377 7.375 7.359 7.356 7.260 CDCl3 7.021 7.002 6.982 6.921 6.909 6.897



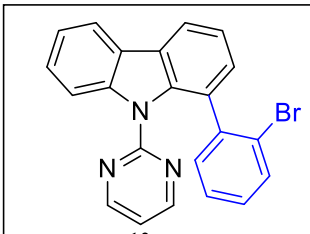
3d ^{1}H NMR

400 MHz, $CDCl_3$



GP-SM-7-118

157.579 143.420 140.864 136.914 130.885 129.624 129.241 128.481 126.988 126.821 126.394 124.972 122.345 122.192 122.157 120.229 119.890 117.436 112.236 77.160 CDCl3



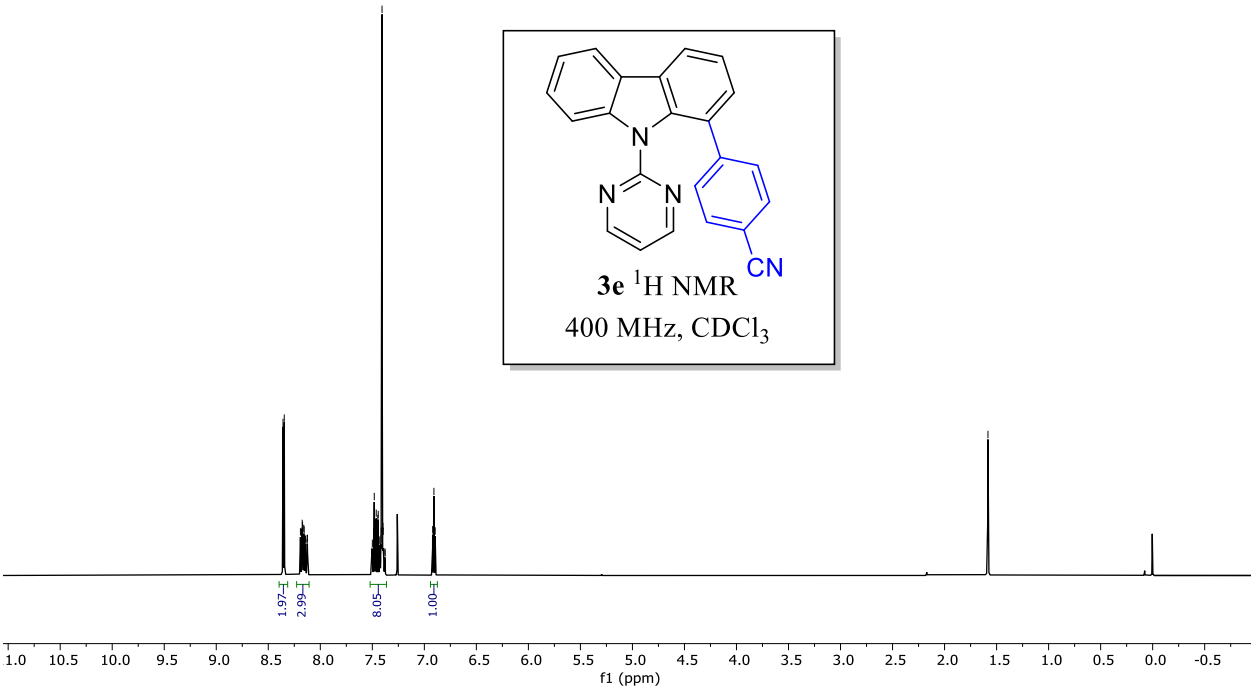
3d ^{13}C NMR

101 MHz, $CDCl_3$

GP-SM-7-156-B

8.358
8.346
8.191
8.178
8.174
8.170
8.159
8.155
8.147
8.145
8.144
8.127
8.126
8.124
7.507
7.504
7.500
7.489
7.486
7.483
7.481
7.469
7.465
7.463
7.447
7.443
7.428
7.425
7.420
7.417
7.414
7.407
7.398
7.395
7.379
7.377
6.920
6.908
6.896

1.583



3e ^{1}H NMR

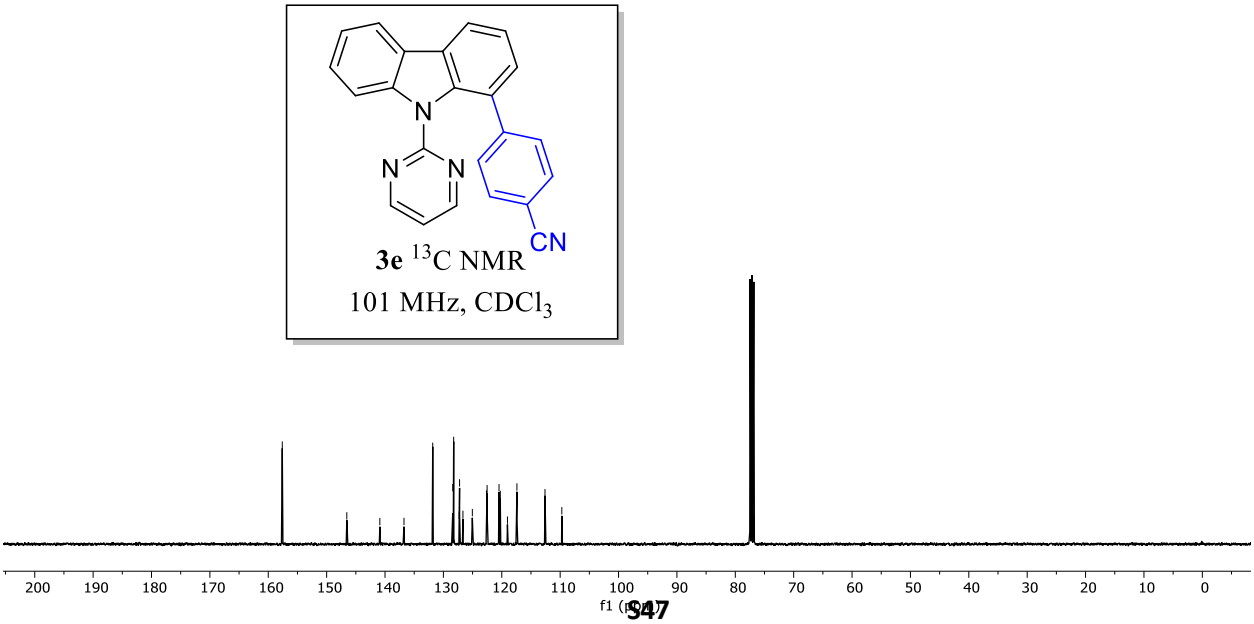
400 MHz, $CDCl_3$

GP-SM-7-156-B

157.600

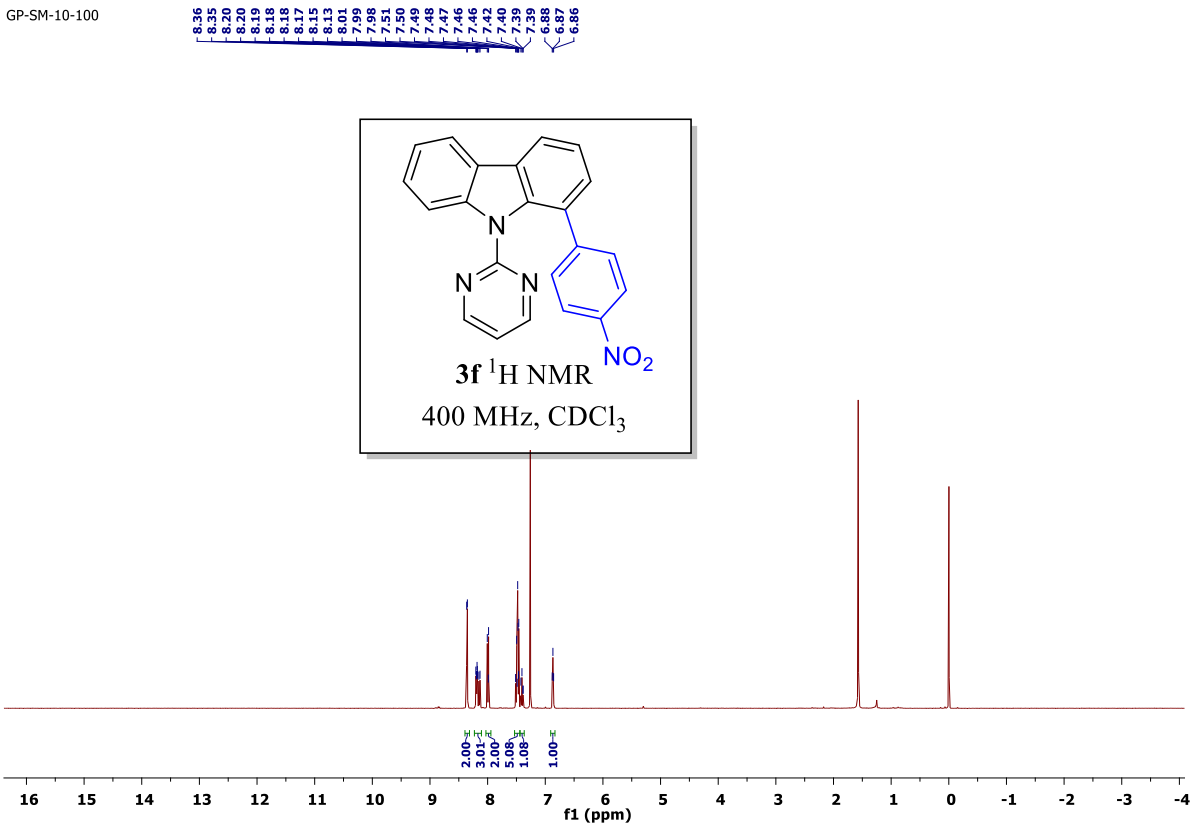
146.545
140.886
136.753
131.831
128.400
128.242
127.296
127.230
126.653
125.042
122.605
122.515
120.472
120.253
119.027
117.404
112.597
109.714

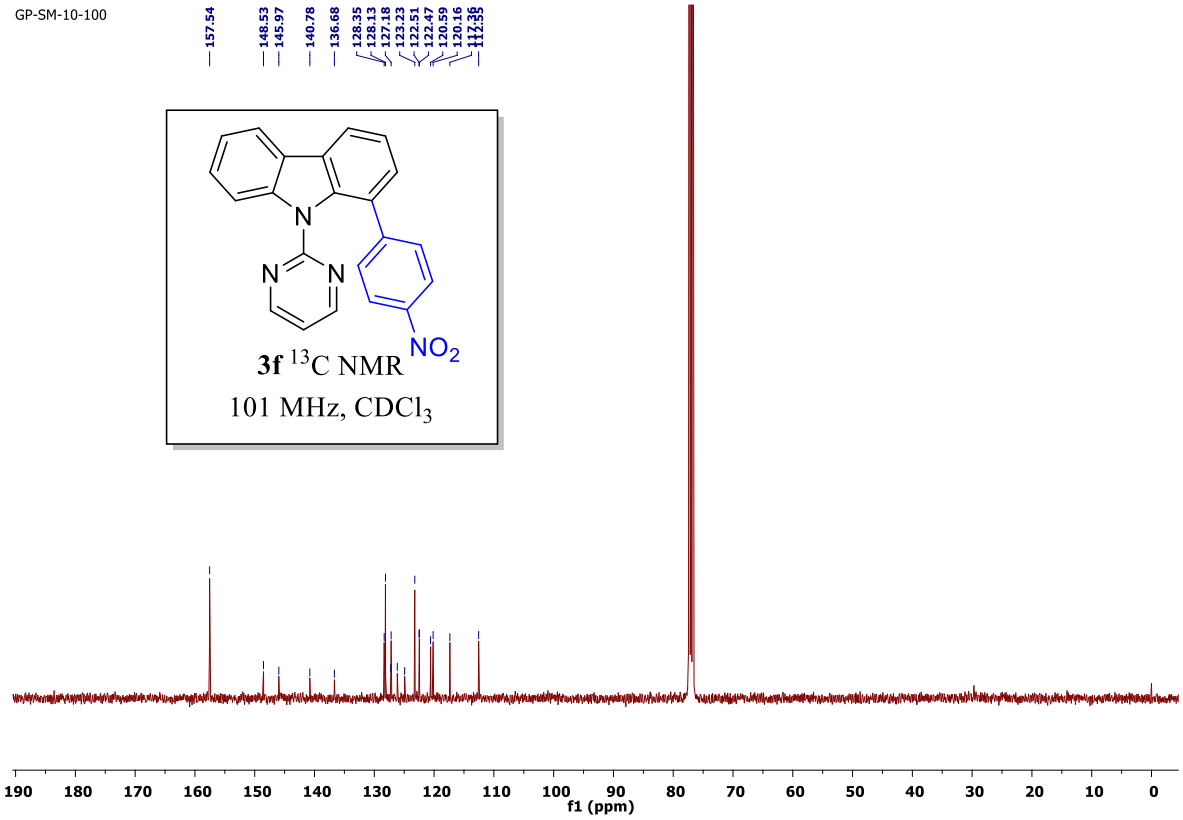
77.160 CDCl3

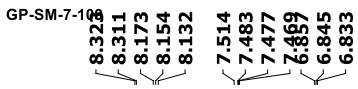


3e ^{13}C NMR

101 MHz, $CDCl_3$


GP-SM-10-100
8.36
8.35
8.20
8.20
8.19
8.18
8.18
8.17
8.15
8.13
8.01
7.99
7.98
7.51
7.50
7.49
7.48
7.47
7.46
7.46
7.42
7.40
7.39
7.39
6.88
6.87
6.86
N
N
N
NO2
3f 1H NMR
400 MHz, CDCl3
2.00
3.01
2.00
5.08
1.08
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


GP-SM-10-100
157.54
148.53
145.97
140.78
136.68
128.35
128.13
127.18
123.23
122.51
122.47
120.59
120.16
N
N
N
NO2
3f 13C NMR
101 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


GP-SM-7-109
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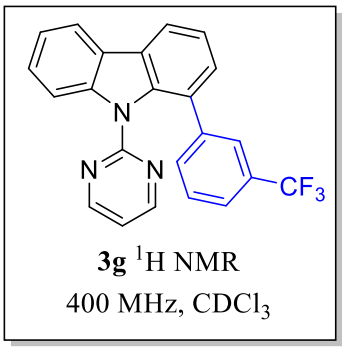
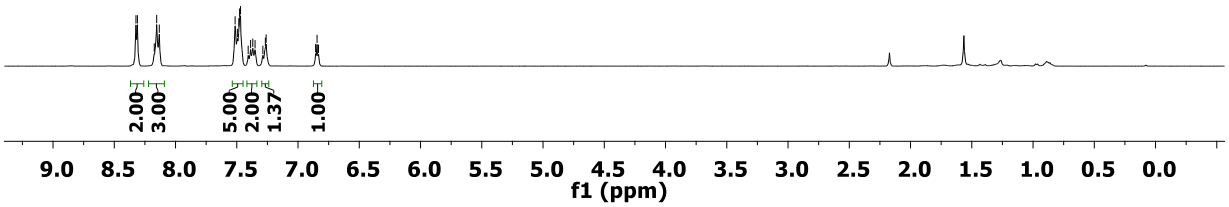
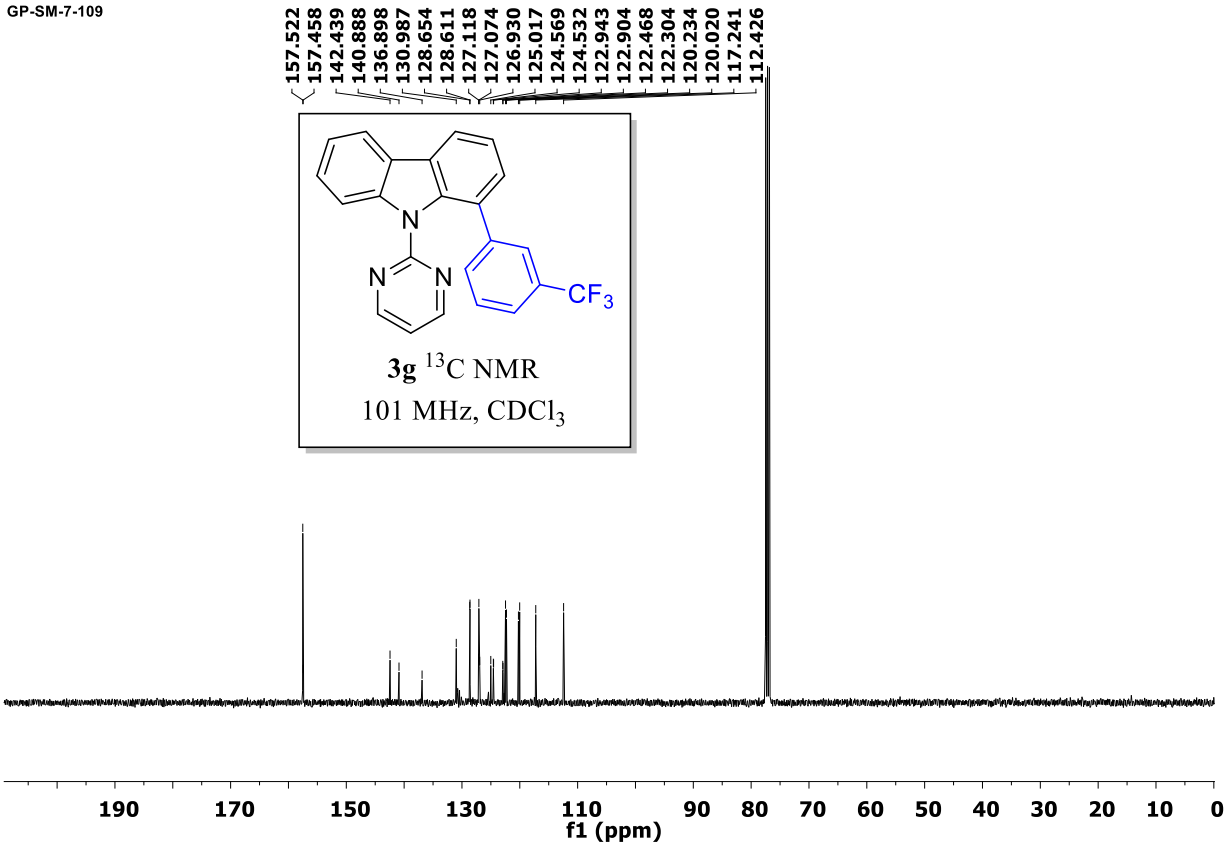
8.311
8.173
8.154
8.132
7.514
7.483
7.477
7.469
6.857
6.845
6.833


N
N
N
CF3
3g 1H NMR
400 MHz, CDCl3


2.00
3.00
5.00
2.00
1.37
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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140.888
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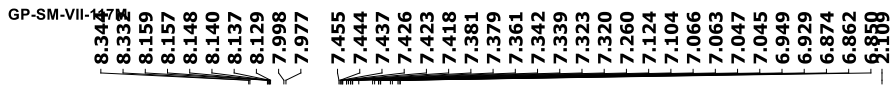
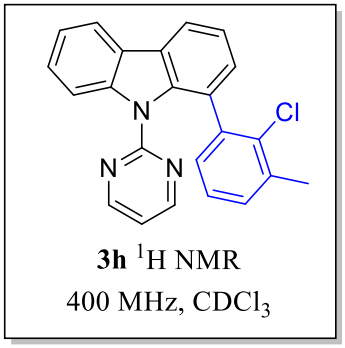
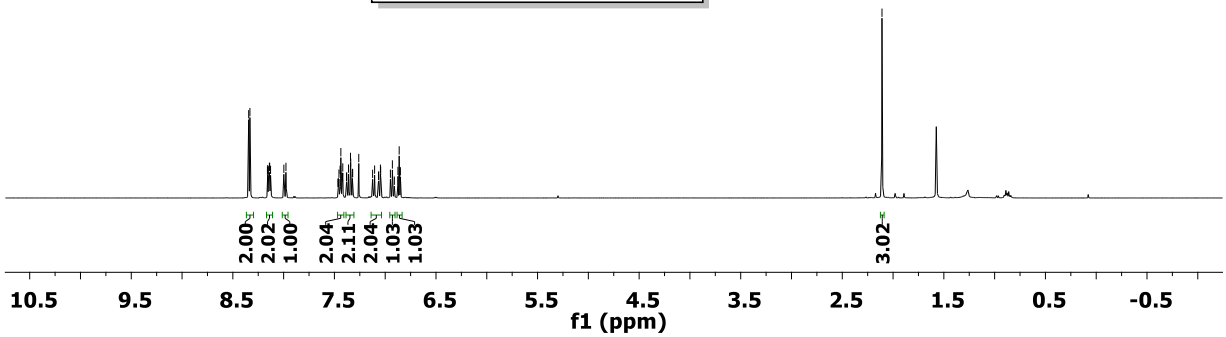
130.987
128.654
128.611
127.118
127.074
126.930
125.017
124.569
124.532
122.943
122.904
122.468
122.304
120.234
120.020
117.241
112.426
N
N
N
CF3
3g 13C NMR
101 MHz, CDCl3
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

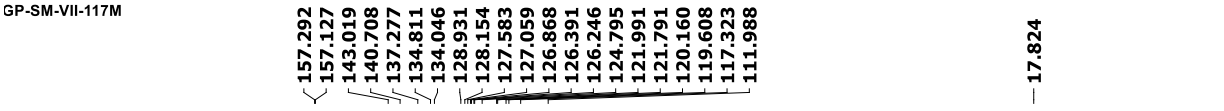


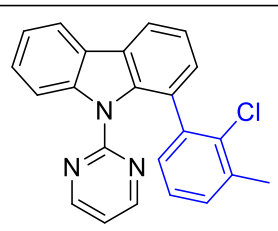


3h ^{1}H NMR

400 MHz, $CDCl_3$

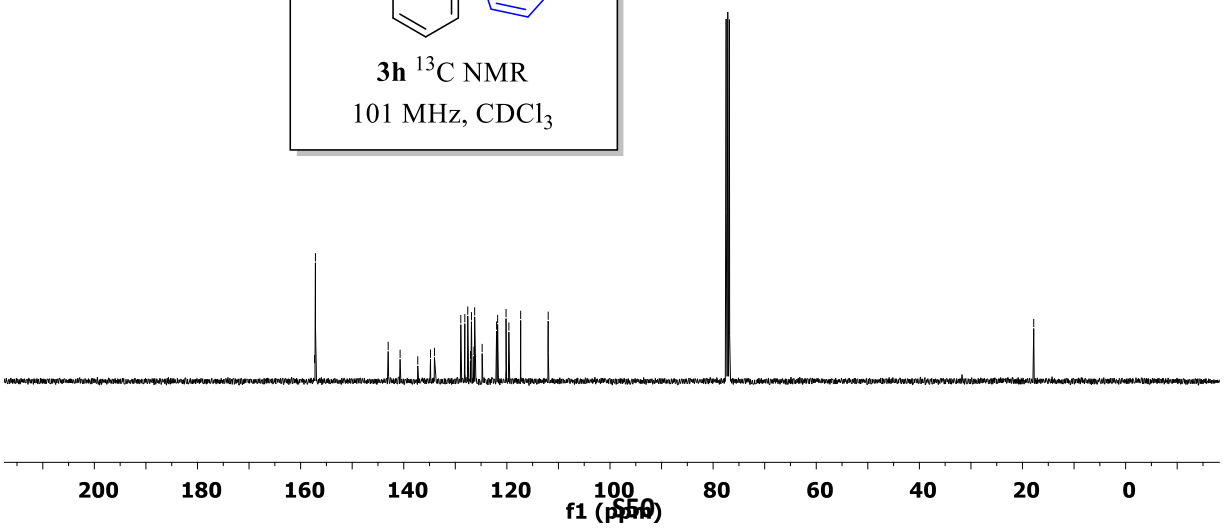






3h ^{13}C NMR

101 MHz, $CDCl_3$




GP-SM-7-126
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8.140
8.138
8.136
8.121
8.118
8.102
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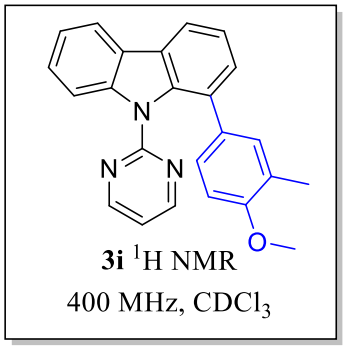
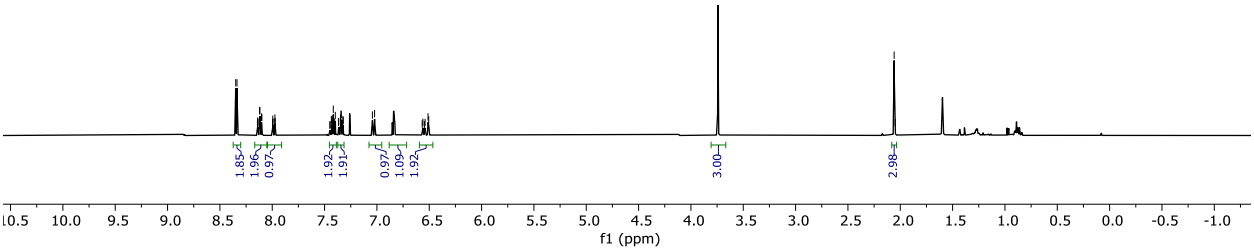
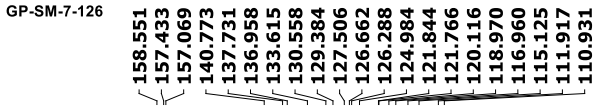
7.996
7.994
7.993
7.976
7.974
7.972
7.450
7.446
7.435
7.432
7.429
7.426
7.417
7.411
7.408
7.398
7.367
7.365
7.348
7.346
7.343
7.340
7.330
7.327
7.325
7.322
7.043
7.022
6.567
6.561
6.546
6.540
6.512
6.505
2.058
2.049


N
N
N
O
3i 1H NMR
400 MHz, CDCl3


1.85
1.96
0.97
1.92
1.91
0.97
1.09
1.92
3.00
2.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


GP-SM-7-126
158.551
157.433
157.069
140.773
137.731
136.958
133.615
130.558
129.384
127.506
126.662
126.288
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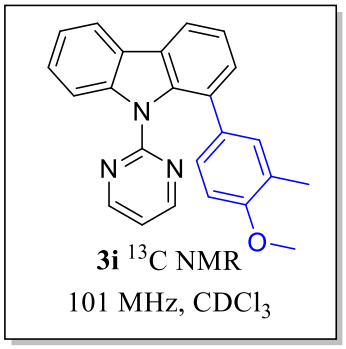
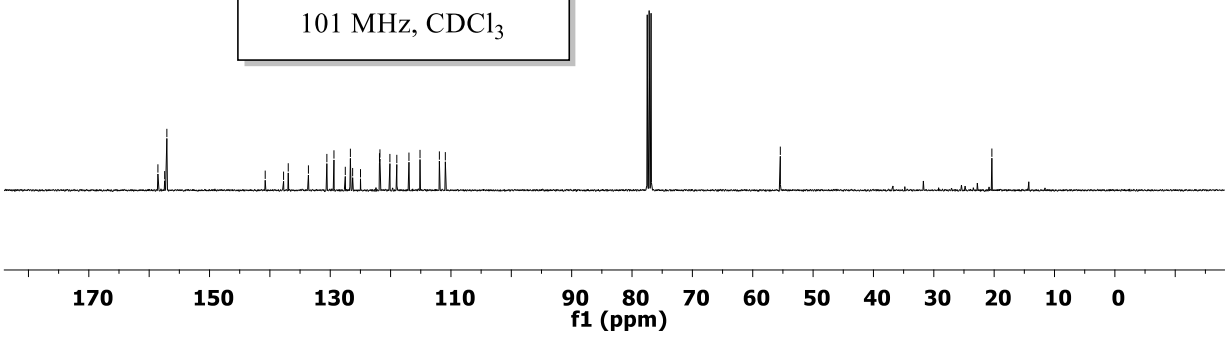
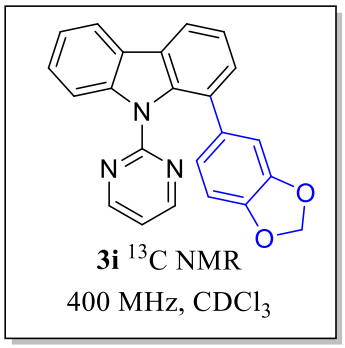
115.125
111.917
110.931
55.430
20.377


N
N
N
O
3i 13C NMR
101 MHz, CDCl3

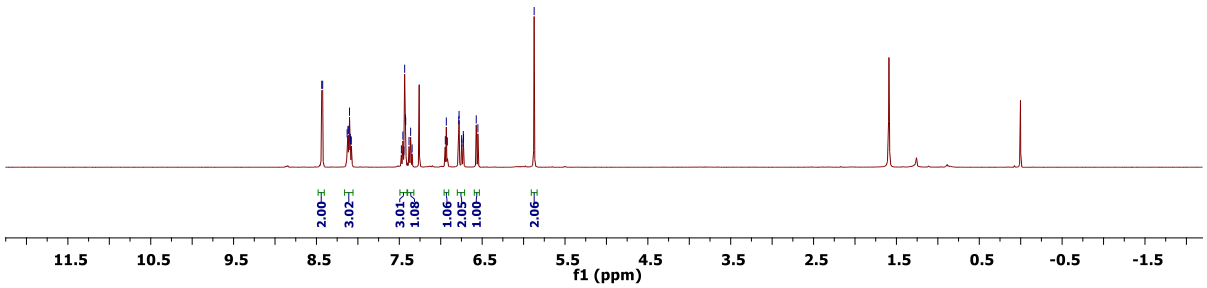

170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

GP-SM-10-96

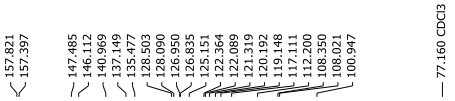


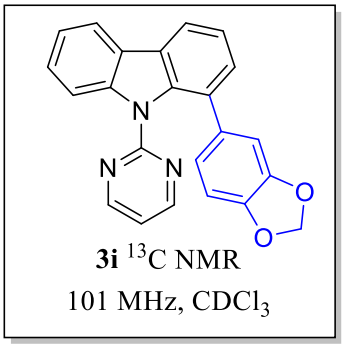
3i ^{13}C NMR

400 MHz, $CDCl_3$



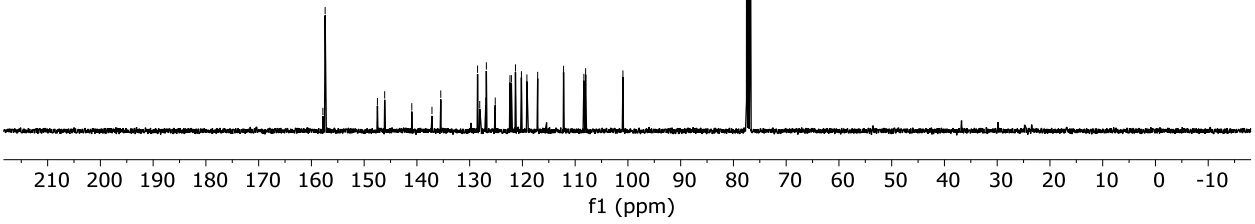
GP-SM-7-139



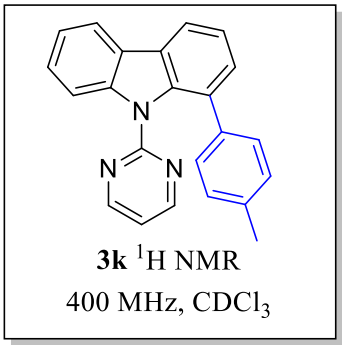


3i ^{13}C NMR

101 MHz, $CDCl_3$

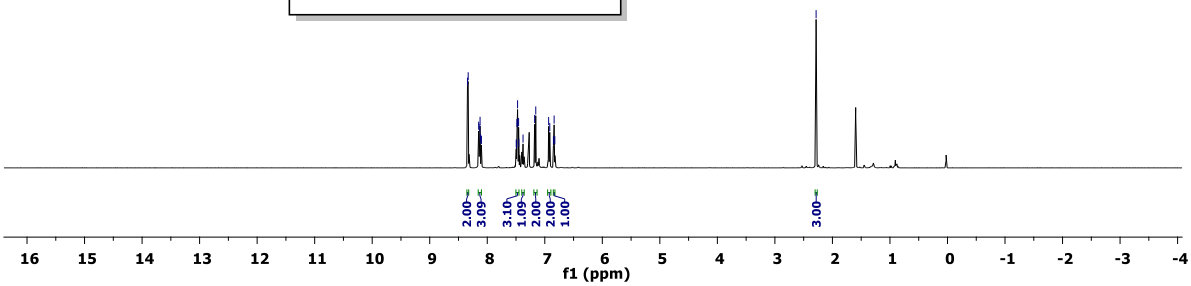


GP-SM-81-149-P

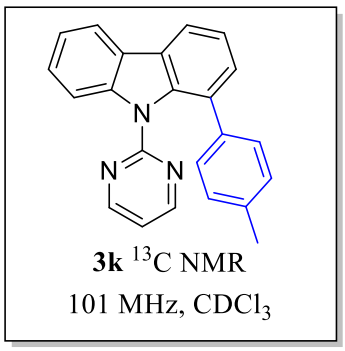


3k ^{1}H NMR

400 MHz, $CDCl_3$

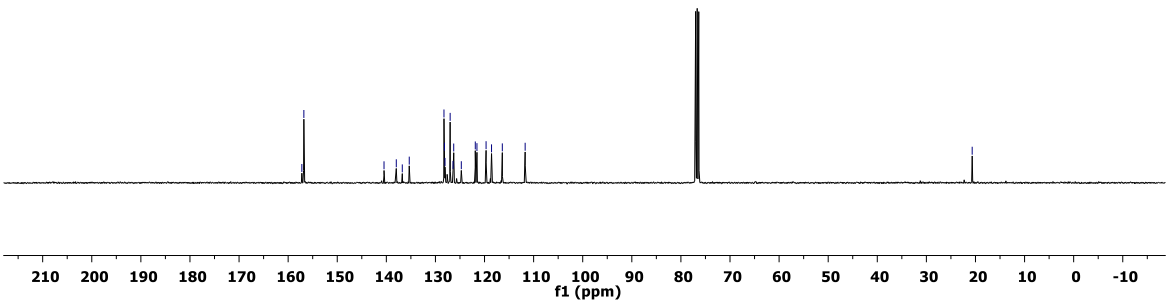


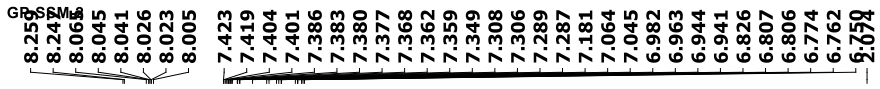
GP-SM-81-149-P

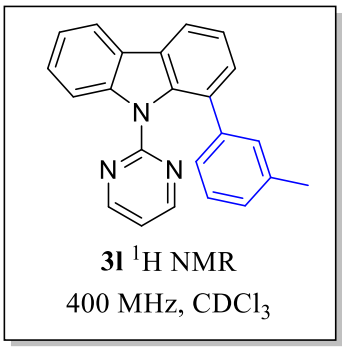


3k ^{13}C NMR

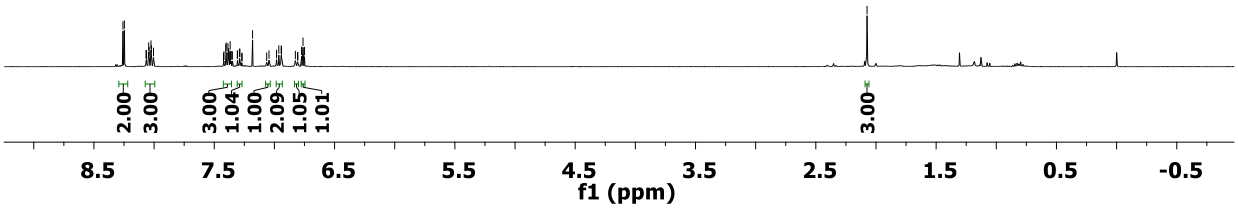
101 MHz, $CDCl_3$

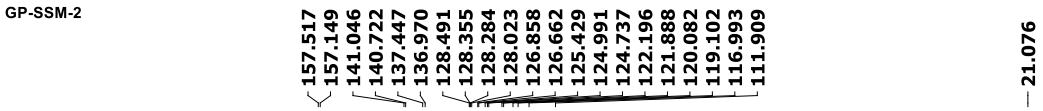


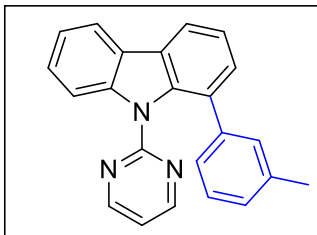




3l ^{1}H NMR
400 MHz, $CDCl_3$

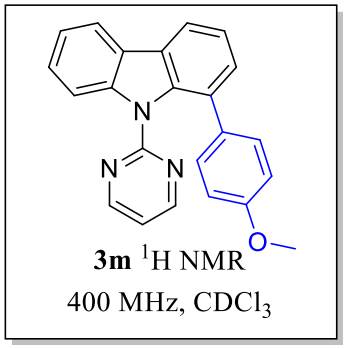






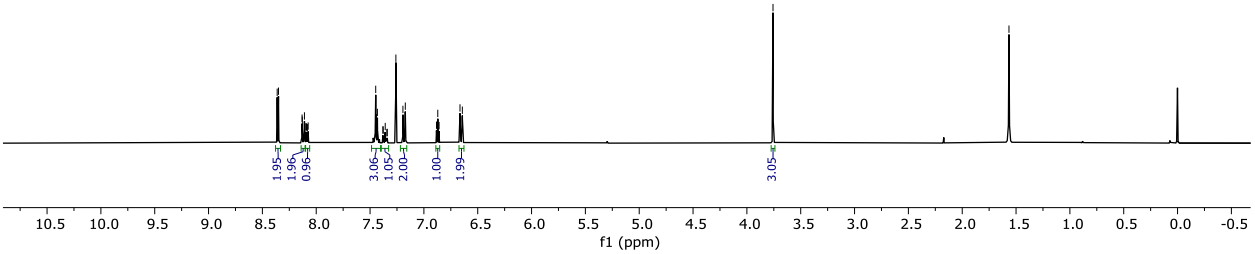
3l ^{13}C NMR
101 MHz, $CDCl_3$

GP-SM-7-160

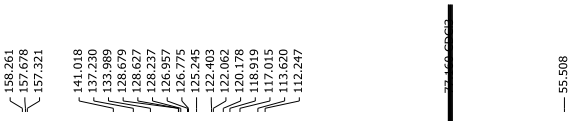


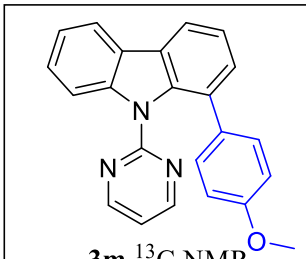
3m ^{1}H NMR

400 MHz, $CDCl_3$



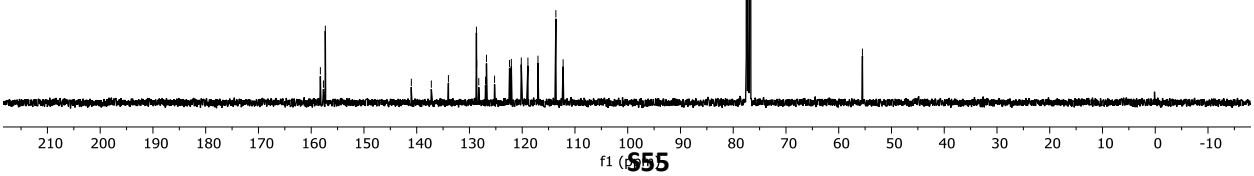
GP-SM-7-160



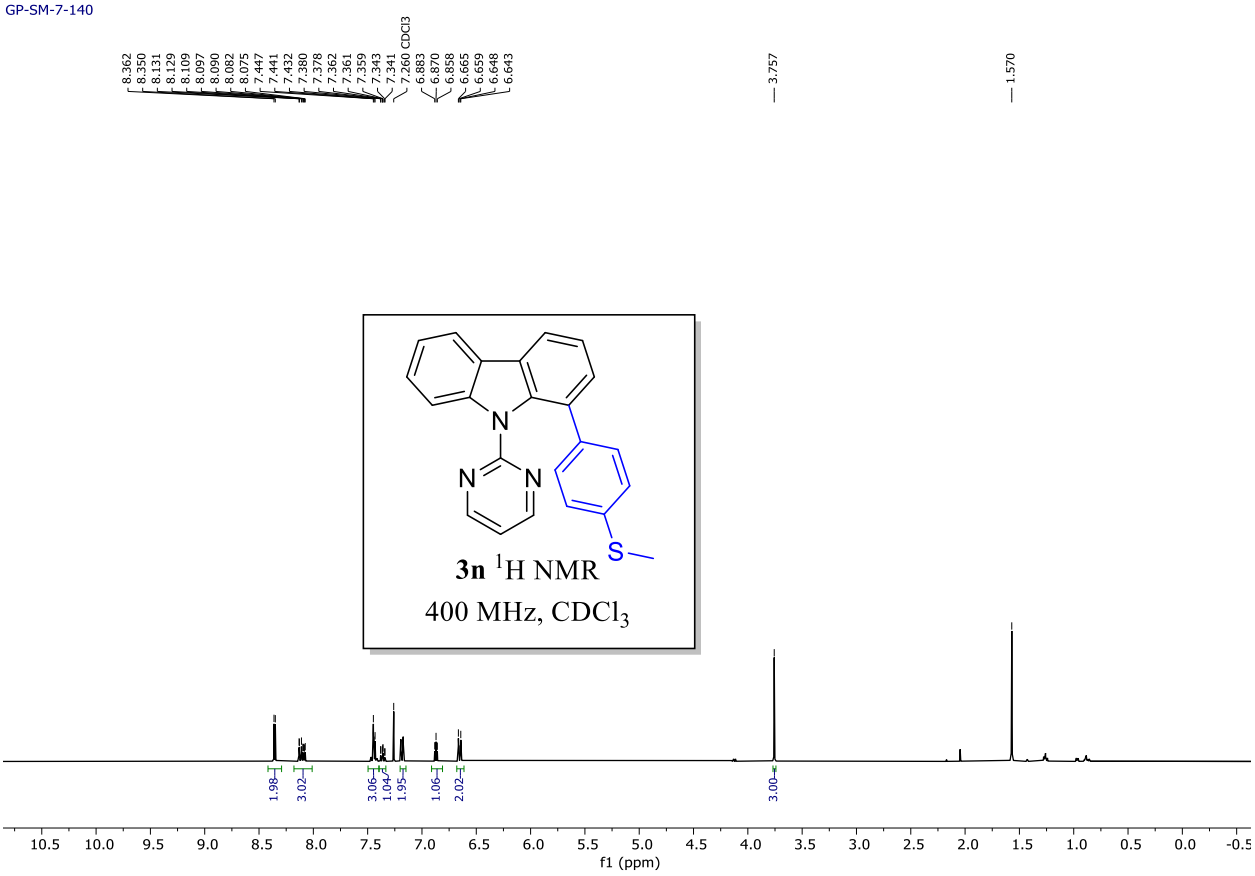


3m ^{13}C NMR

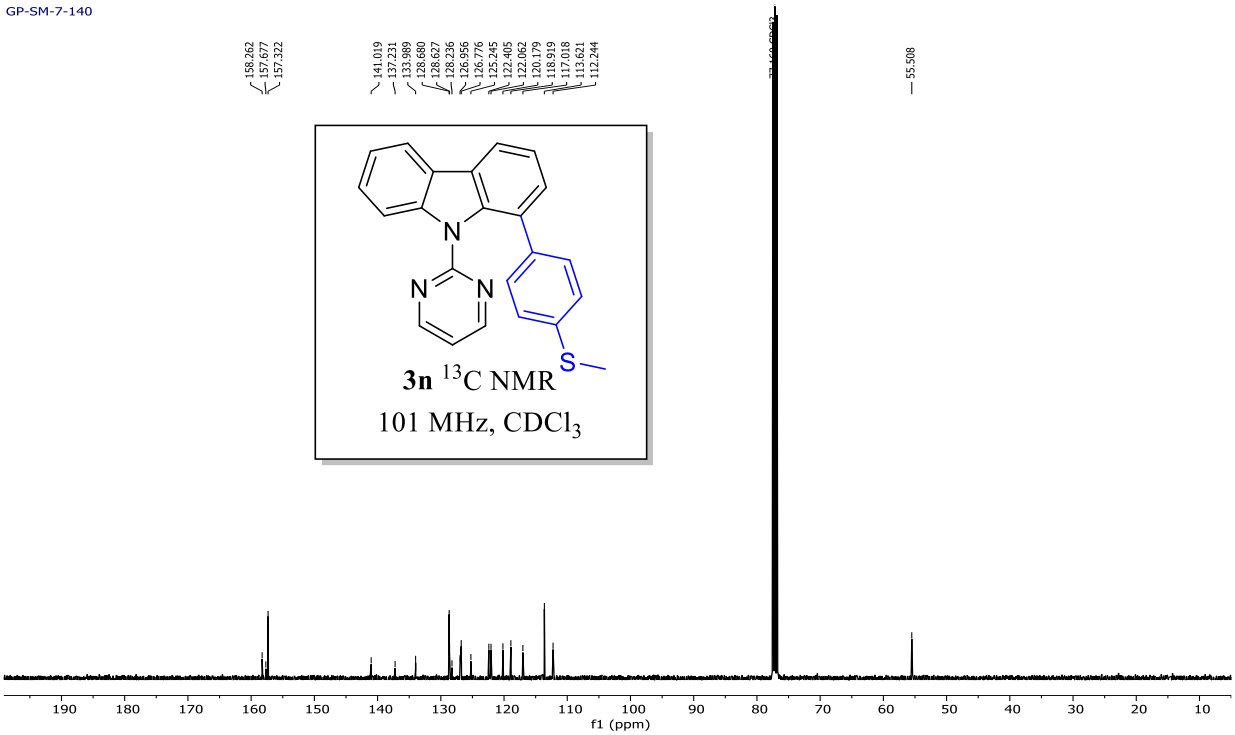
101 MHz, $CDCl_3$



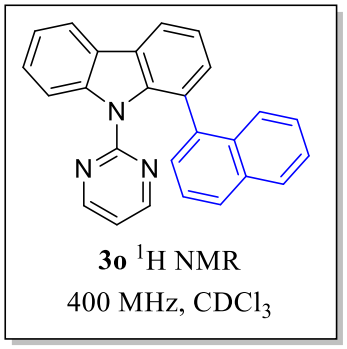
GP-SM-7-140



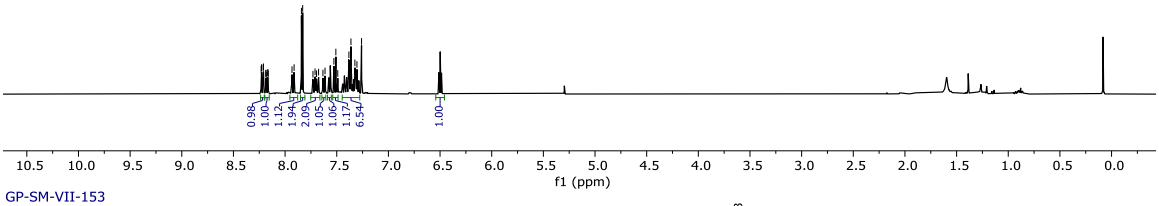
GP-SM-7-140



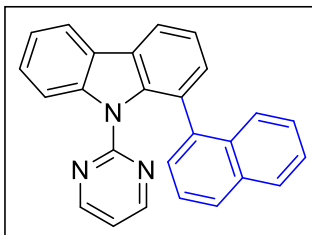
GP-SM-VII-153



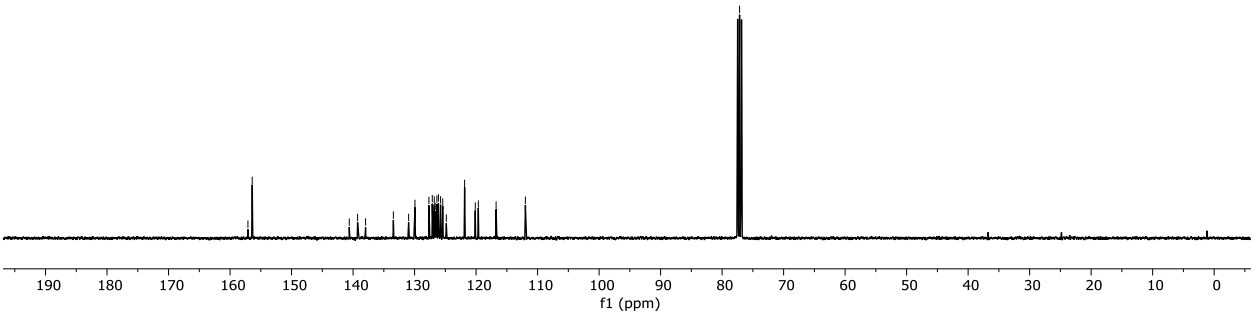
3o ^{1}H NMR
400 MHz, $CDCl_3$



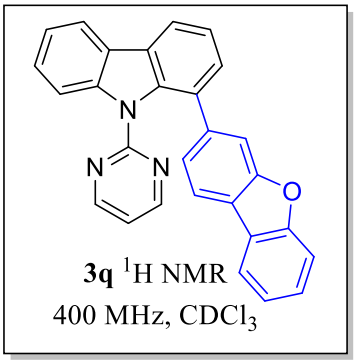
GP-SM-VII-153

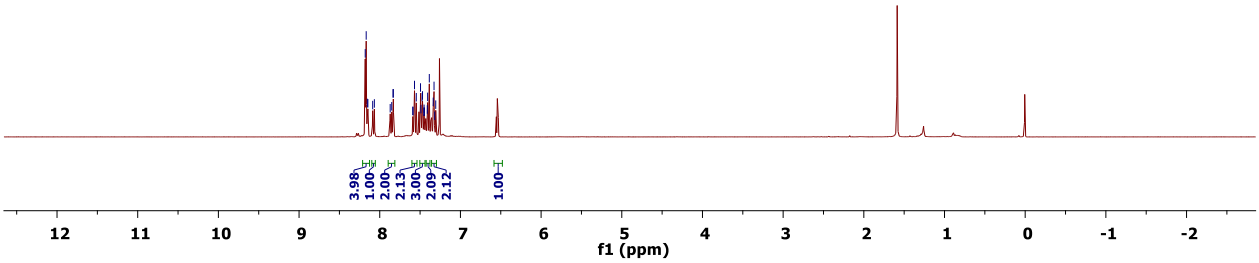


3o ^{13}C NMR
101 MHz, $CDCl_3$

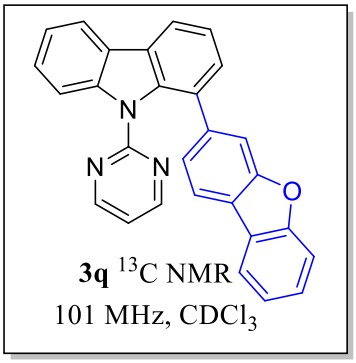


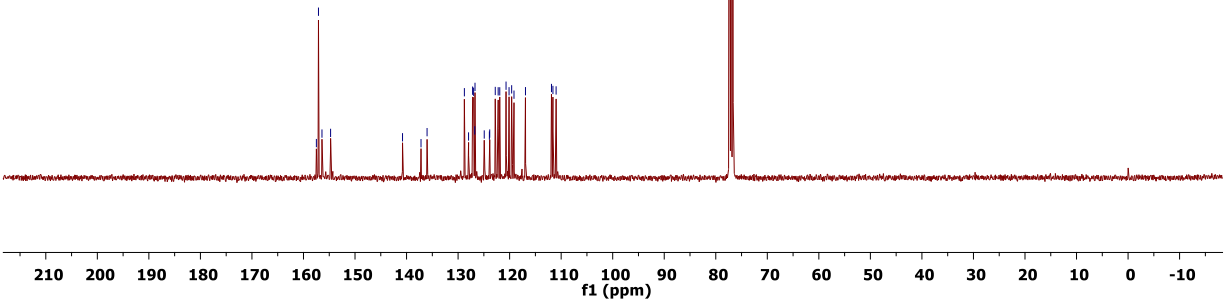
GP-SM-10-106

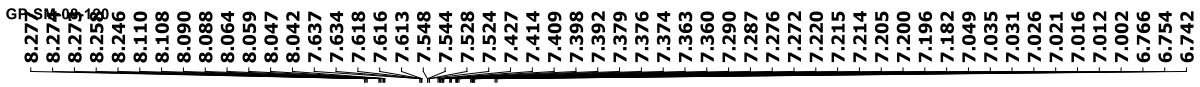


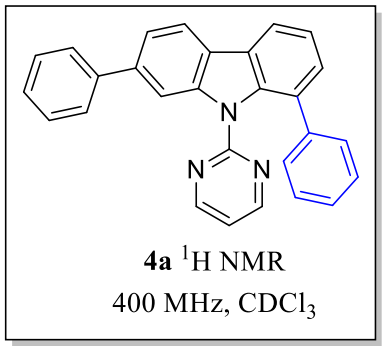


GP-SM-10-106

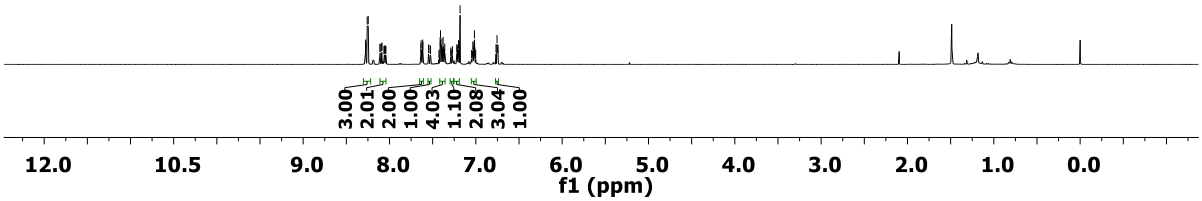


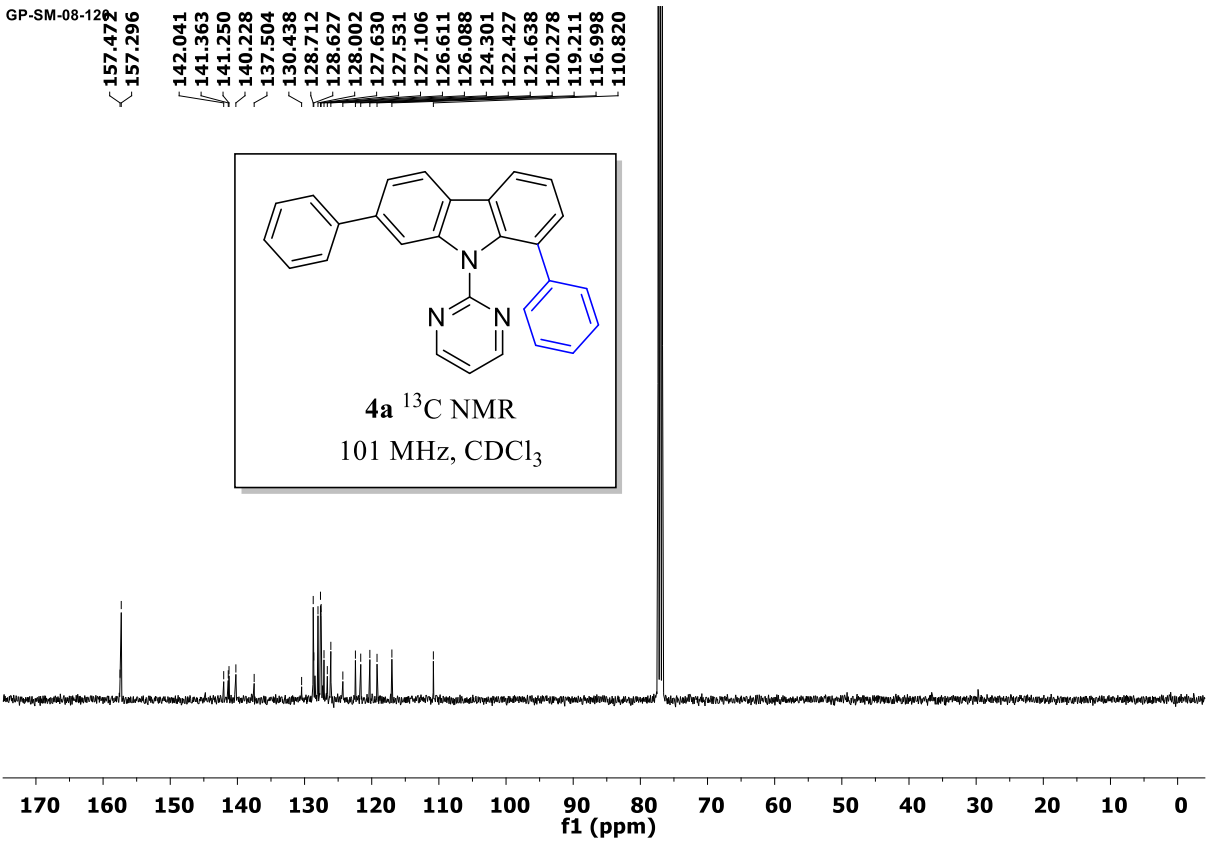




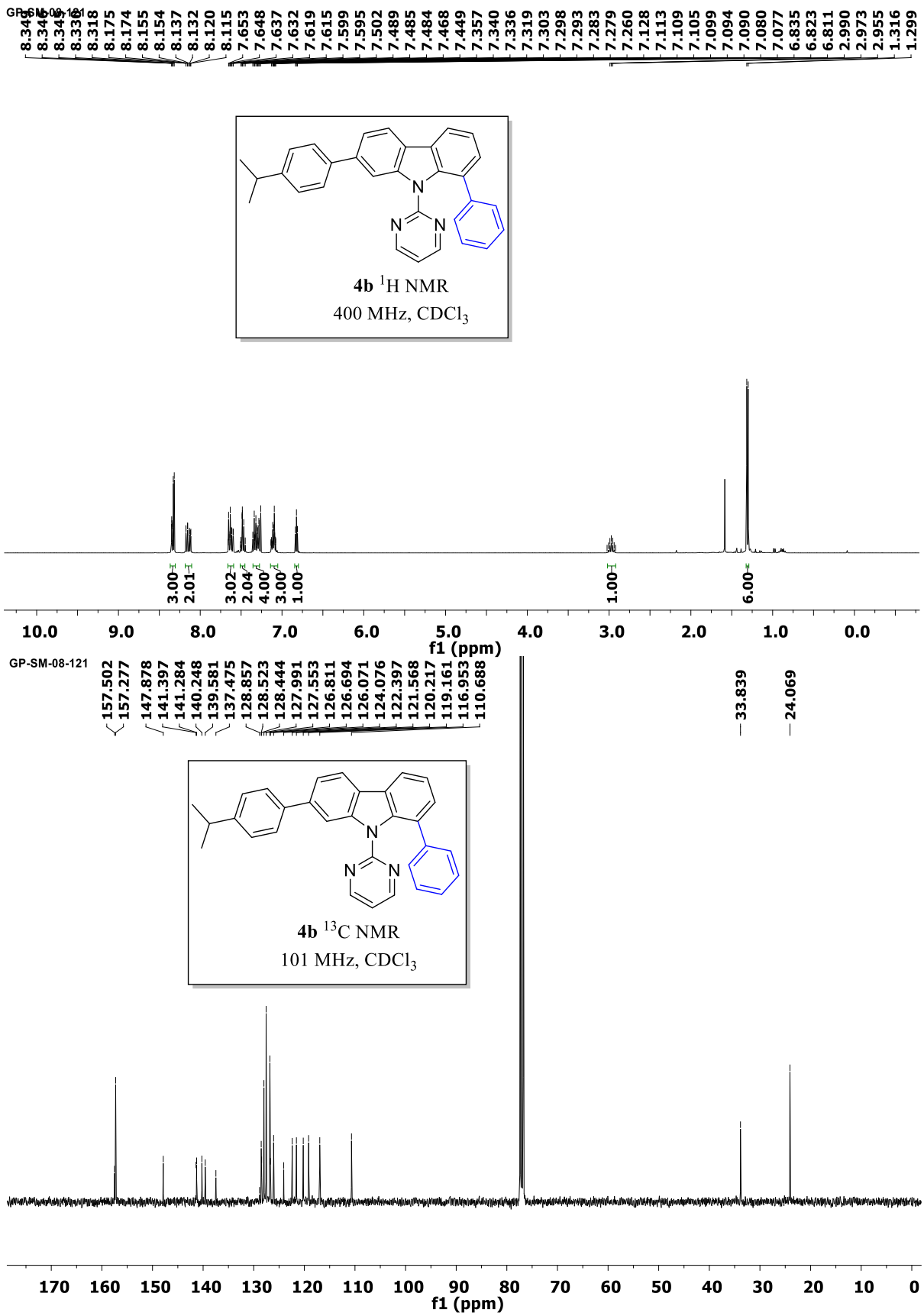


4a ^{1}H NMR
400 MHz, $CDCl_3$





4a ^{13}C NMR
101 MHz, $CDCl_3$


GP-SM-08-121
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8.347
8.336
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8.154
8.137
8.132
8.120
8.115
7.653
7.648
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7.615
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7.595
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7.293
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7.279
7.260
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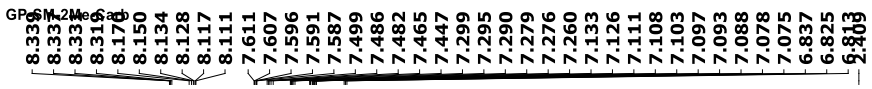
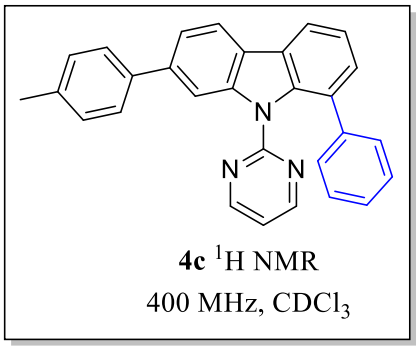
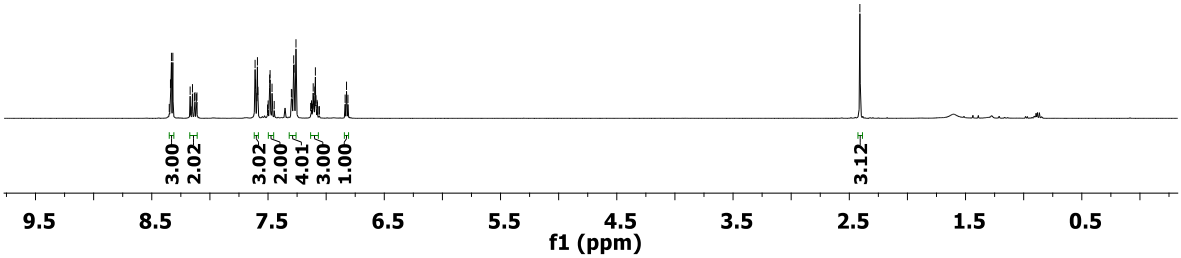
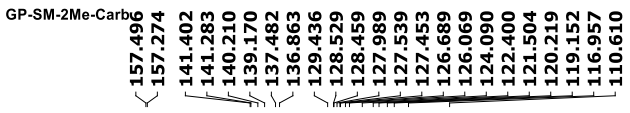
7.113
7.109
7.105
7.099
7.094
7.090
7.080
7.077
6.835
6.823
6.811
2.990
2.973
2.955
1.316
1.299
4b 1H NMR
400 MHz, CDCl3
3.00
2.01
3.02
2.04
4.00
3.00
1.00
1.00
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
GP-SM-08-121
157.502
157.277
147.878
141.397
141.284
140.248
139.581
137.475
128.857
128.523
128.444
127.991
127.553
126.811
126.694
126.071
124.076
122.397
121.568
120.217
119.161
116.953
110.688
33.839
24.069
4b 13C NMR
101 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

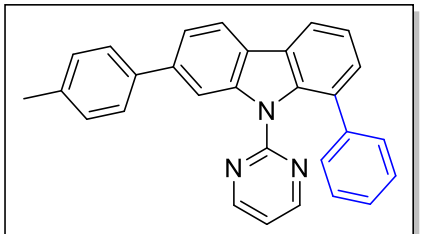




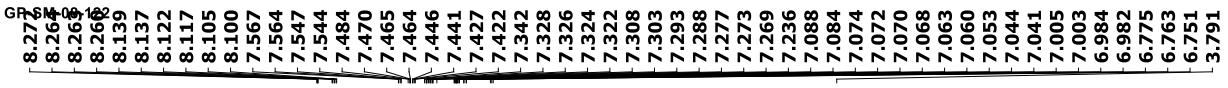
4c ^{1}H NMR
400 MHz, $CDCl_3$

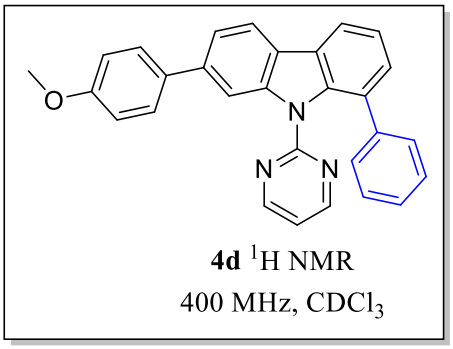




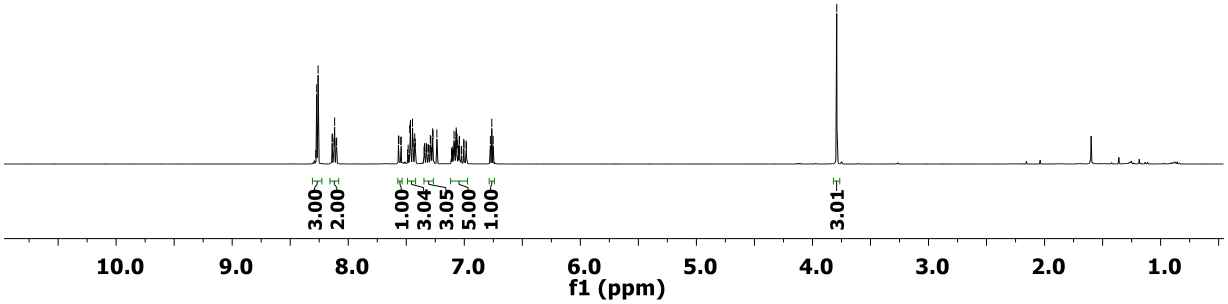


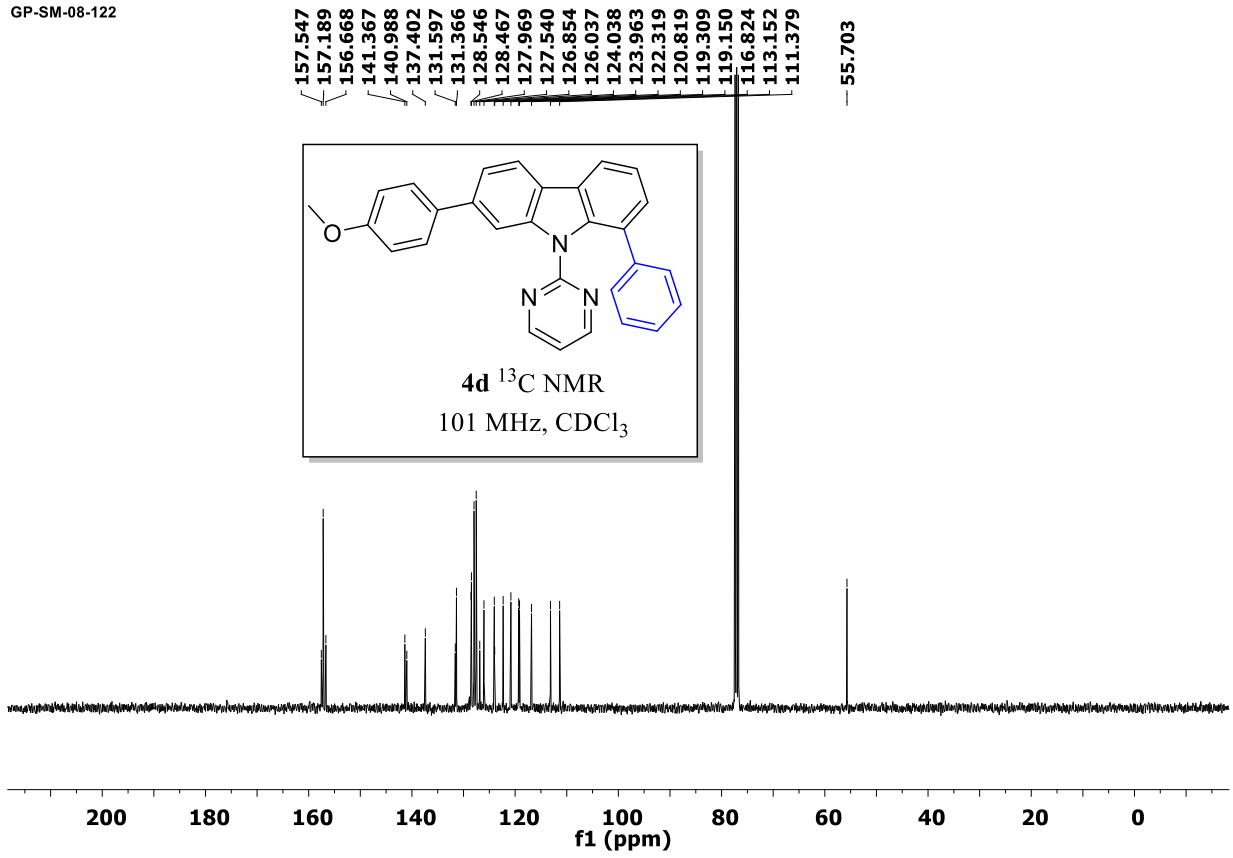
4c ^{13}C NMR
101 MHz, $CDCl_3$



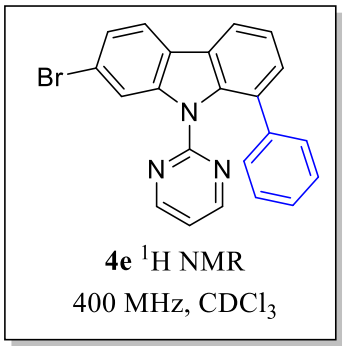


4d ^{1}H NMR
400 MHz, $CDCl_3$

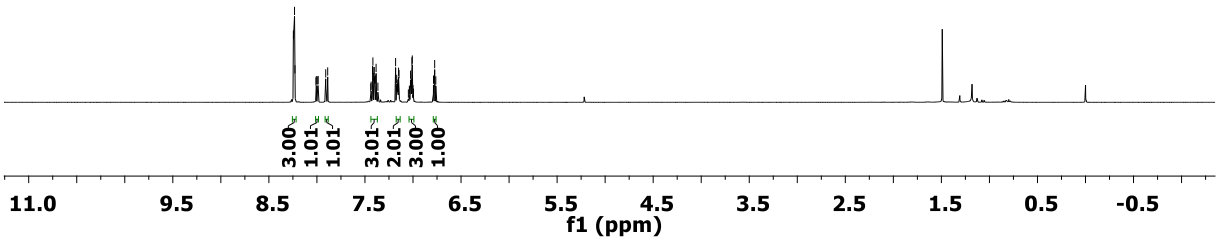


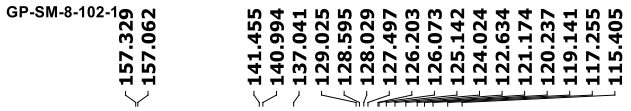


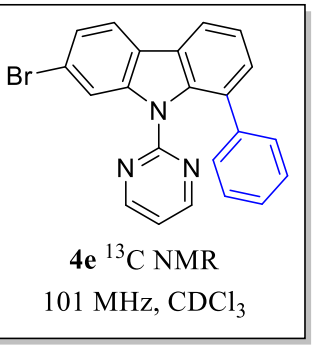
4d ^{13}C NMR
101 MHz, $CDCl_3$



4e ^{1}H NMR
400 MHz, $CDCl_3$

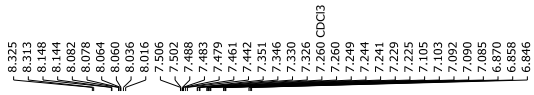


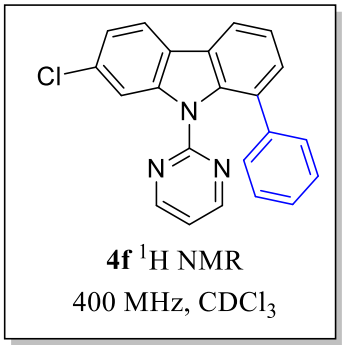




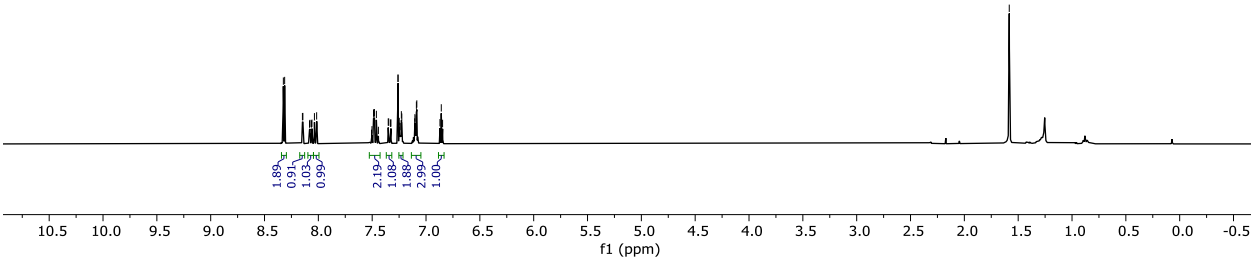
4e ^{13}C NMR
101 MHz, $CDCl_3$

GP-PM-458-A

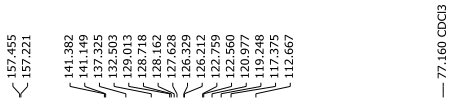


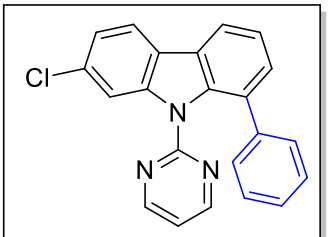


4f ^{1}H NMR
400 MHz, $CDCl_3$



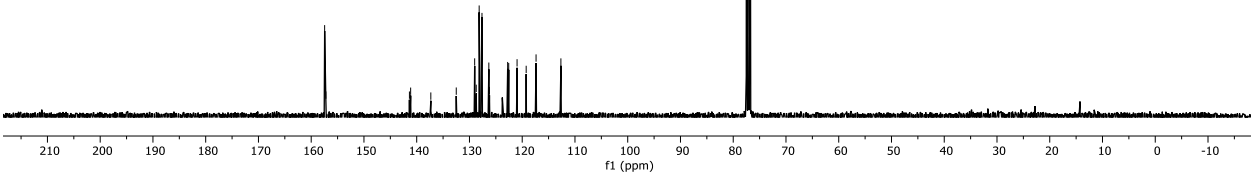
GP-PM-458-A



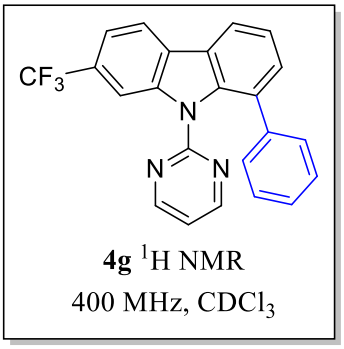


4f ^{13}C NMR
101 MHz, $CDCl_3$

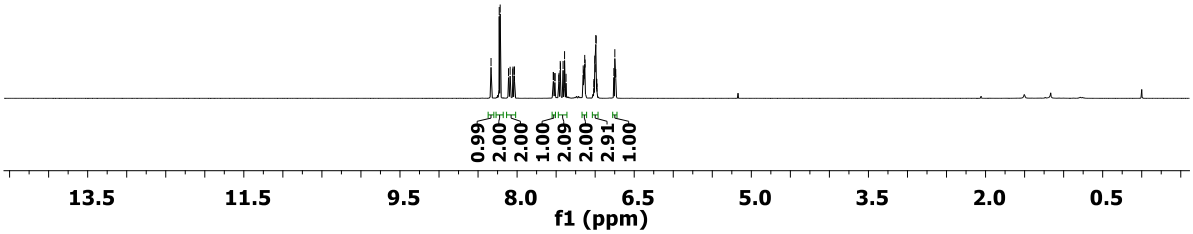
\



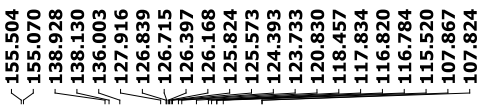
GP-SM-08-92

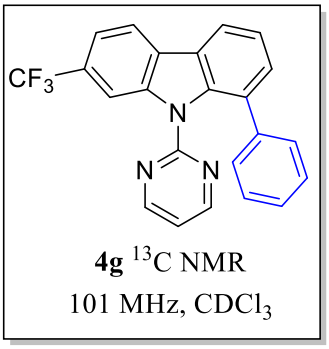


4g ^{1}H NMR
400 MHz, $CDCl_3$

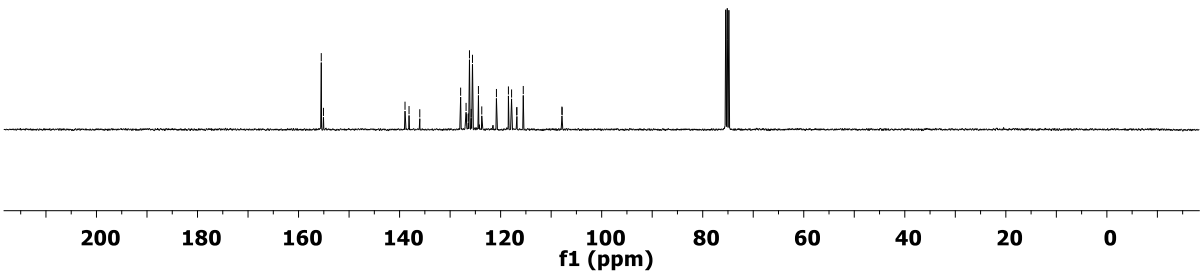


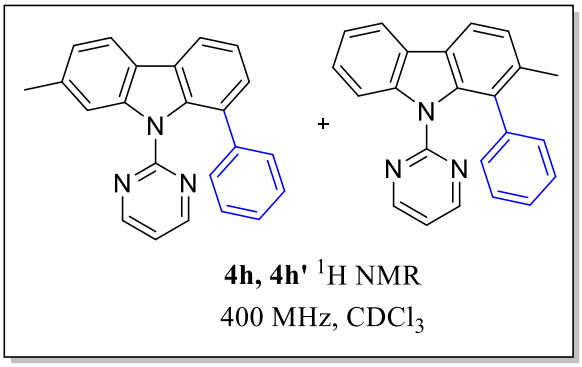
GP-SM-08-92

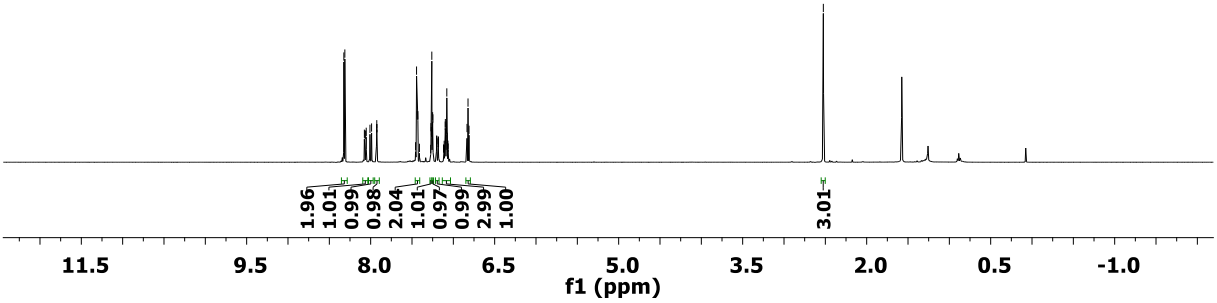


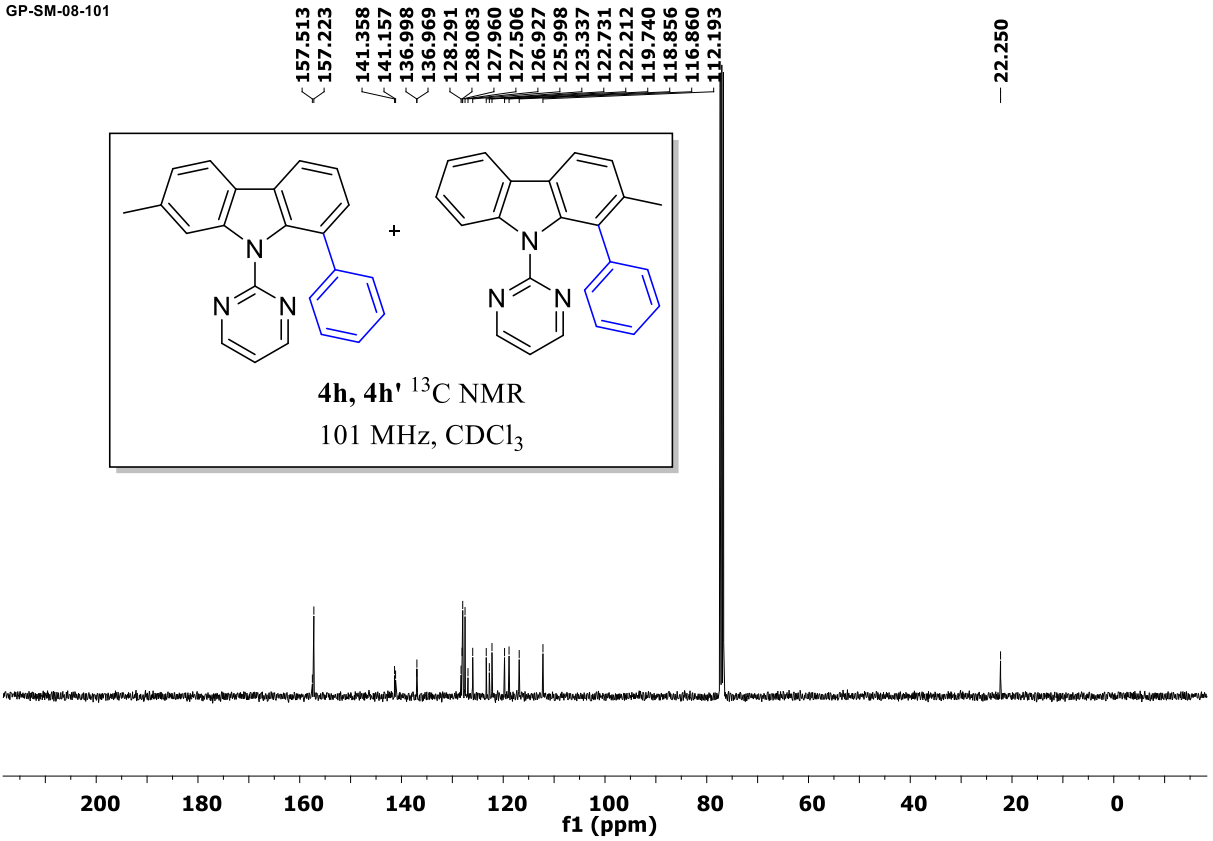


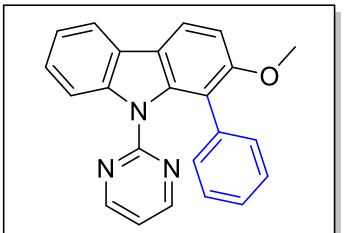
4g ^{13}C NMR
101 MHz, $CDCl_3$




4h, 4h' ^{1}H NMR
400 MHz, $CDCl_3$

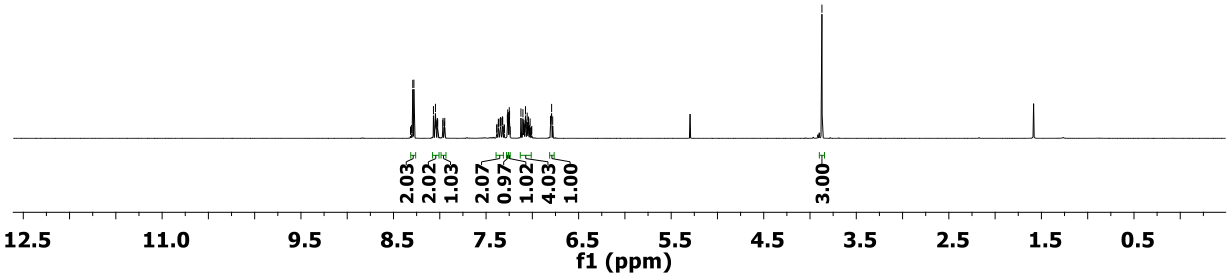

1.96
1.01
0.99
0.98
2.04
1.01
0.97
0.99
2.99
1.00
3.01
11.5
9.5
8.0
6.5
5.0
3.5
2.0
0.5
-1.0
f1 (ppm)

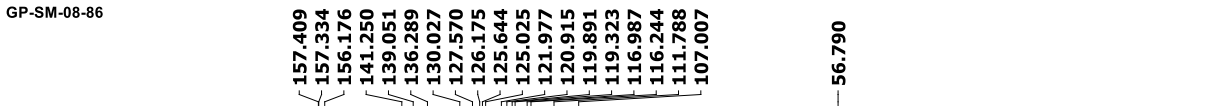

GP-SM-08-101
157.513
157.223
141.358
141.157
136.998
136.969
128.291
128.083
127.960
127.506
126.927
125.998
123.337
122.731
122.212
119.740
118.856
116.860
112.193
22.250
4h, 4h' ^{13}C NMR
101 MHz, $CDCl_3$
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

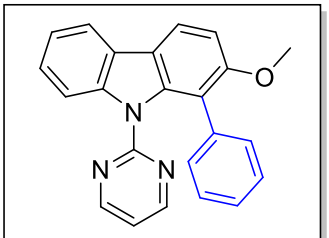


4i ^{1}H NMR

400 MHz, $CDCl_3$





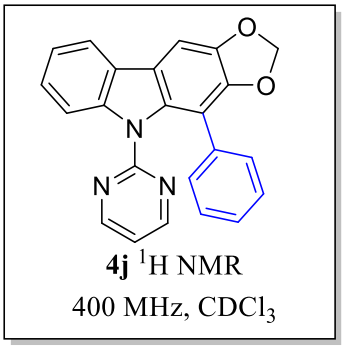


4i ^{13}C NMR

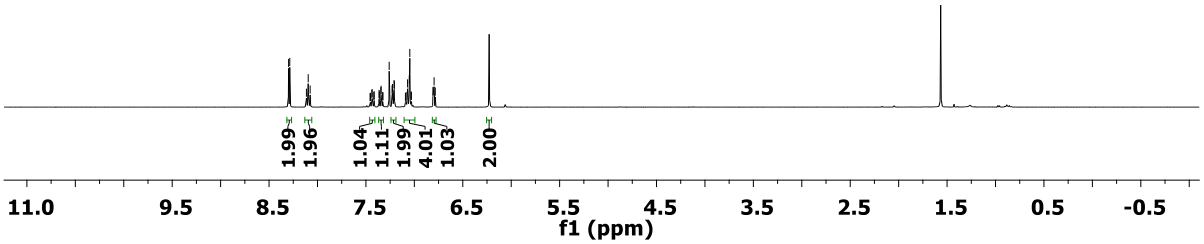
101 MHz, $CDCl_3$

GP-SM-7-27

8.298 8.286 8.114 8.096 8.076 7.457 7.454 7.438 7.436 7.418 7.415 7.364 7.362 7.346 7.343 7.327 7.325 7.260 7.230 7.226 7.221 7.210 7.206 7.092 7.085 7.070 7.052 7.047 7.033 7.031 6.808 6.796 6.784

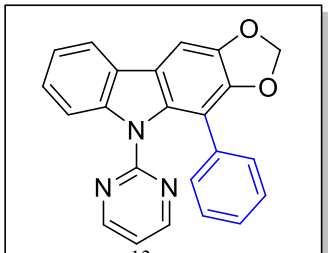


4j ^{1}H NMR
400 MHz, $CDCl_3$



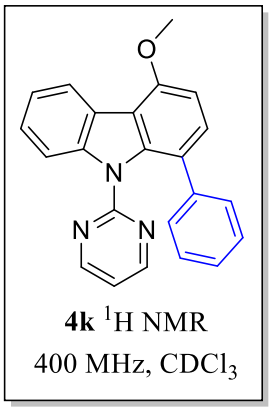
GP-SM-7-27

157.582 157.214 143.259 141.523 141.156 140.414 128.003 127.575 126.796 125.816 122.319 122.111 116.770 111.937 109.231 102.040

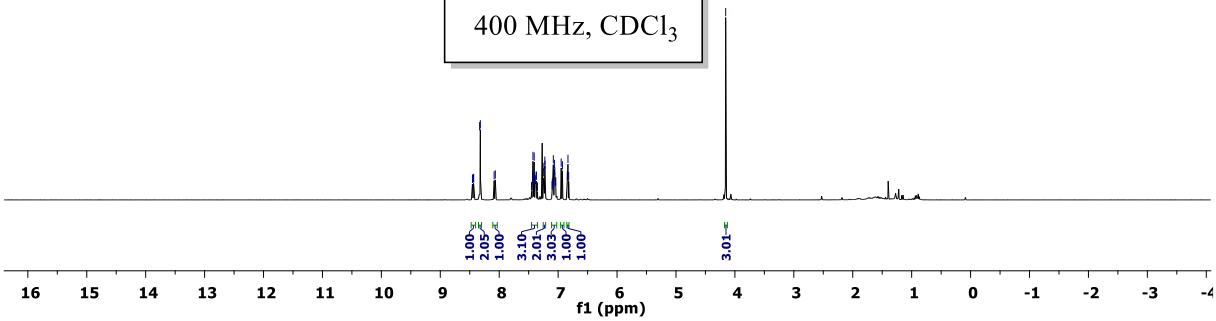


4j ^{13}C NMR
101 MHz, $CDCl_3$

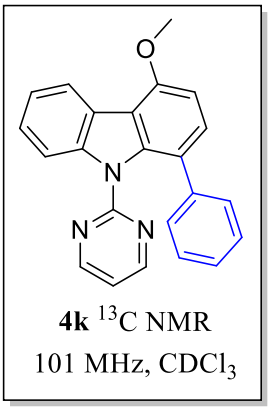
GP-SM-09-III-I



4k ^{1}H NMR
400 MHz, $CDCl_3$

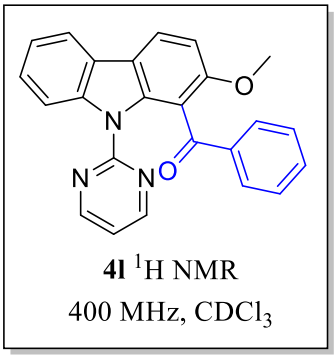


GP-SM-09-III-I

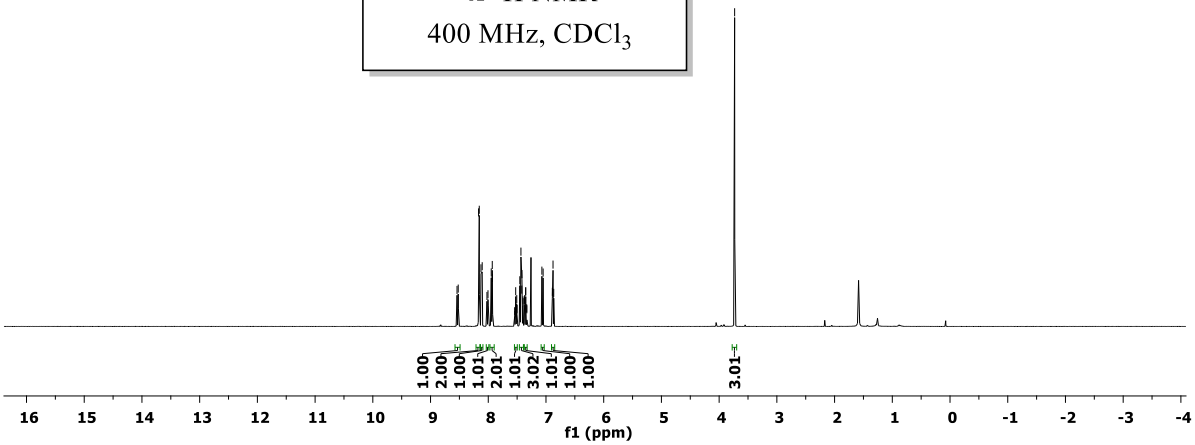


4k ^{13}C NMR
101 MHz, $CDCl_3$

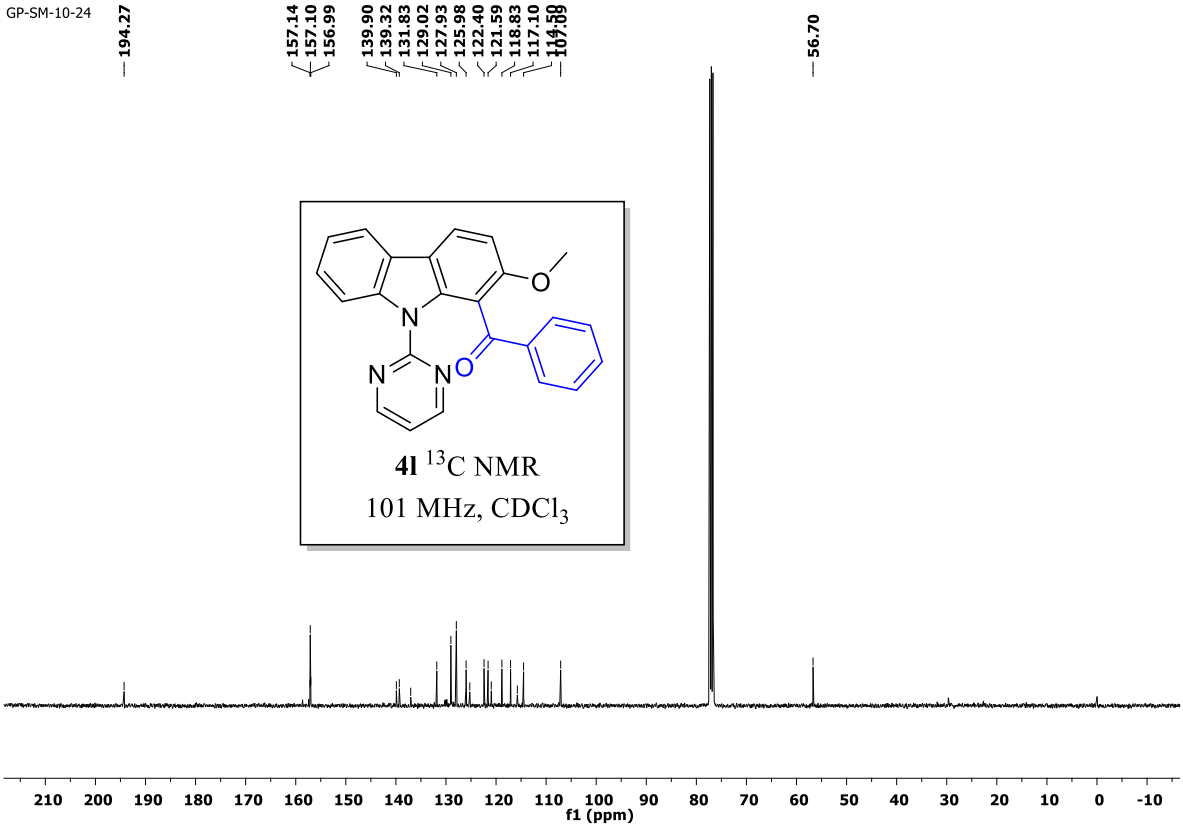
GP-SS-2-46



4l ^{1}H NMR
400 MHz, $CDCl_3$

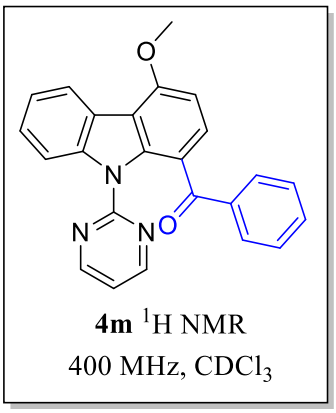


GP-SM-10-24

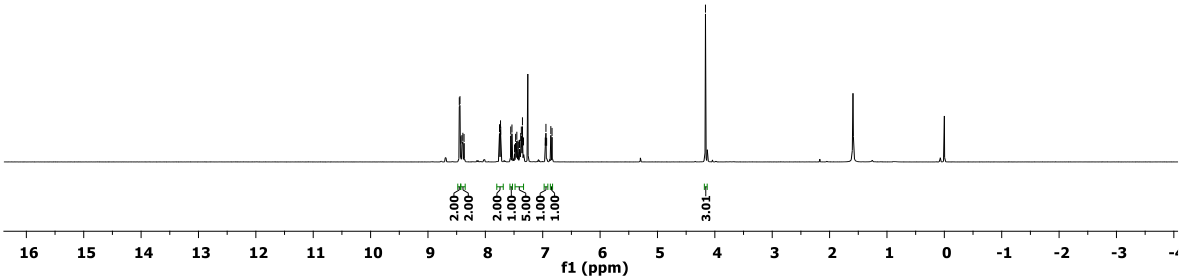


4l ^{13}C NMR
101 MHz, $CDCl_3$

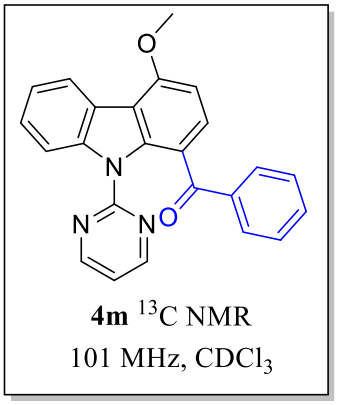
GP-SM-08-212-1



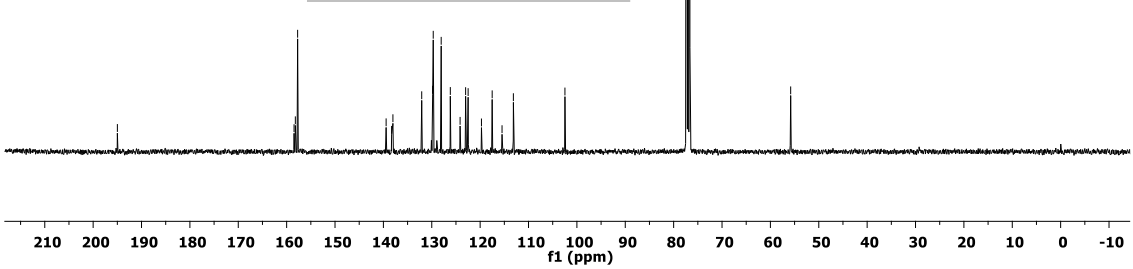
4m ^{1}H NMR
400 MHz, $CDCl_3$



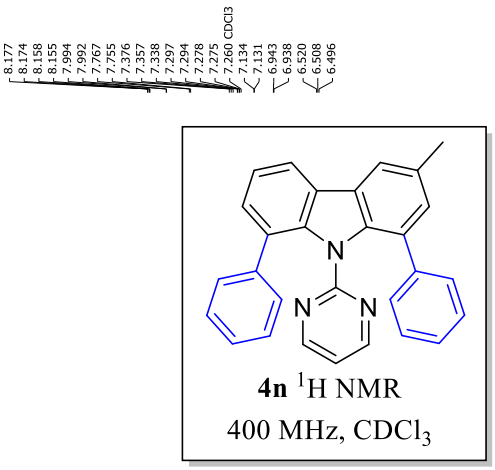
GP-SM-08-212-1

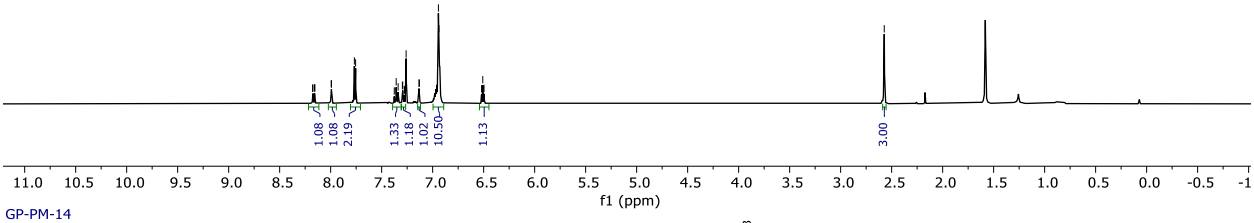


4m ^{13}C NMR
101 MHz, $CDCl_3$

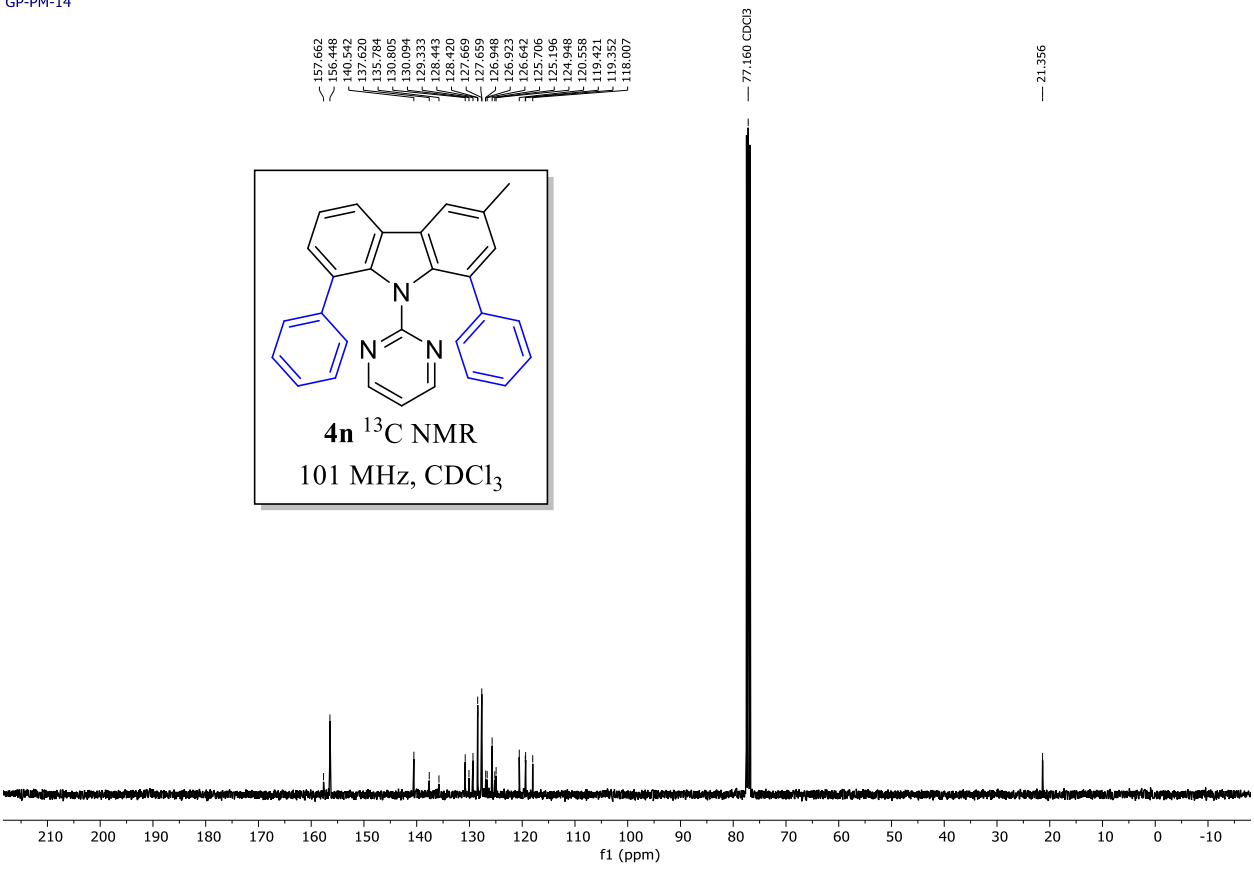


GP-PM-14

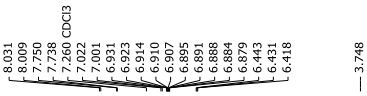


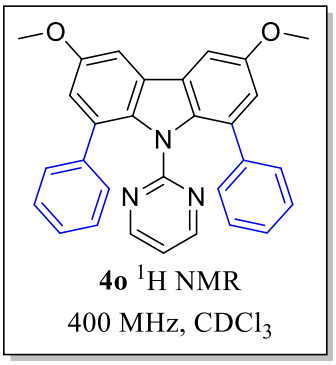


GP-PM-14



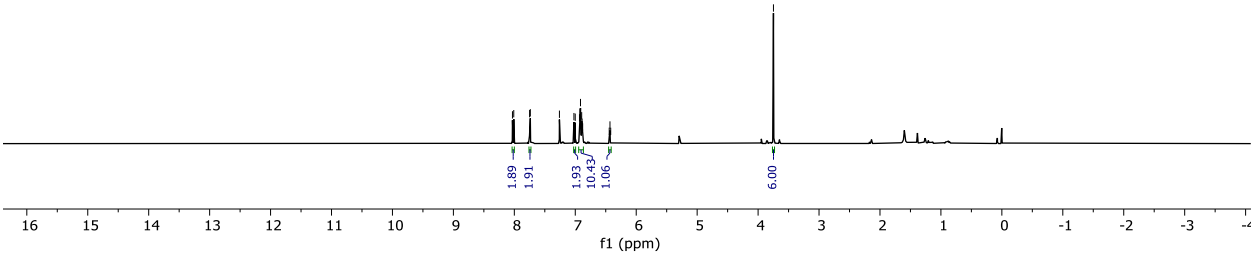
GP-PM-465A



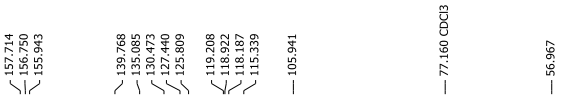


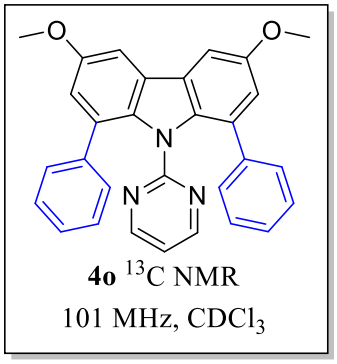
4o ^{1}H NMR

400 MHz, $CDCl_3$



GP-PM-465A



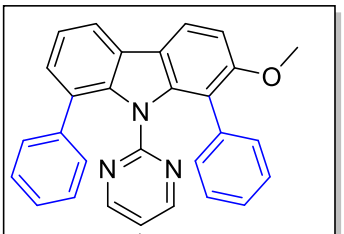


4o ^{13}C NMR

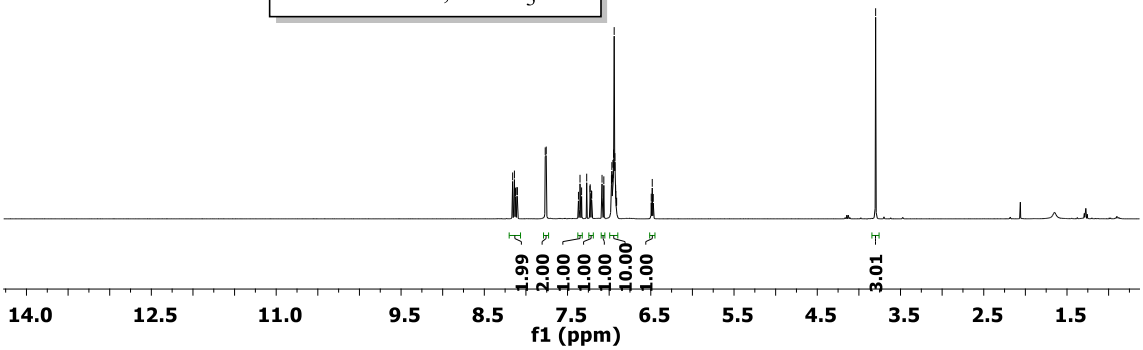
101 MHz, $CDCl_3$

GP-SM-09-14

8.160 8.138 8.126 8.123 8.107 8.104 7.768 7.756 7.369 7.350 7.331 7.270 7.231 7.228 7.213 7.210 7.086 7.064 6.973 6.968 6.960 6.955 6.950 6.946 6.940 6.931 6.922 6.920 6.914 6.910 6.494 6.482 6.470 3.799

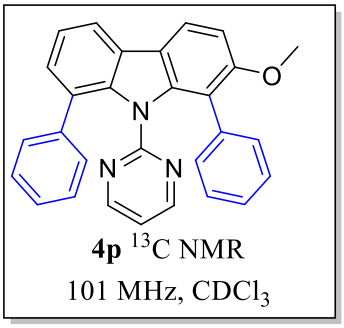


4p ^{1}H NMR
400 MHz, $CDCl_3$

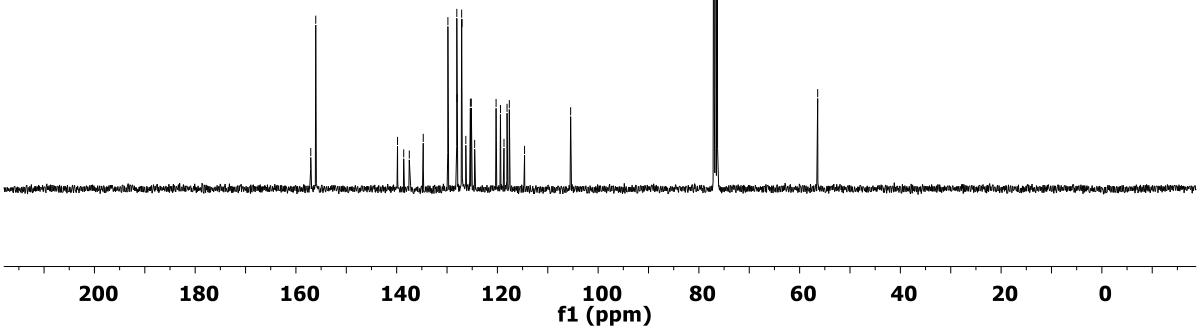


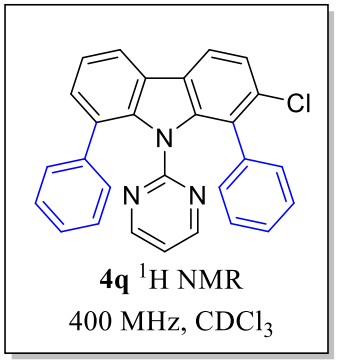
GP-SM-09-14

157.053 156.100 156.065 129.828 128.059 127.994 127.099 127.031 125.367 125.180 120.262 117.635 105.459 56.418

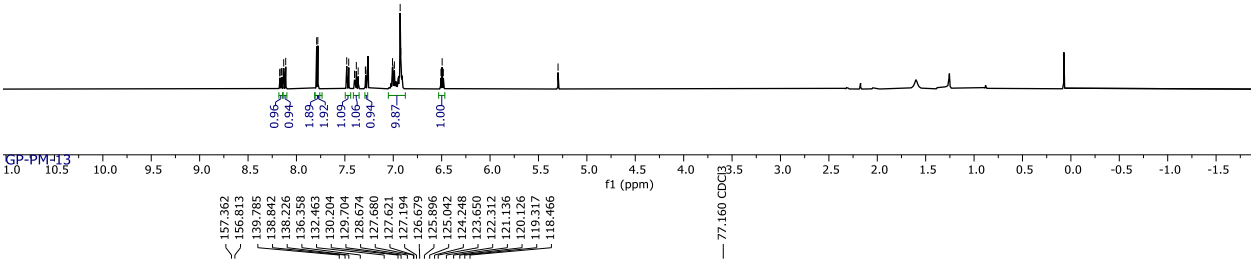


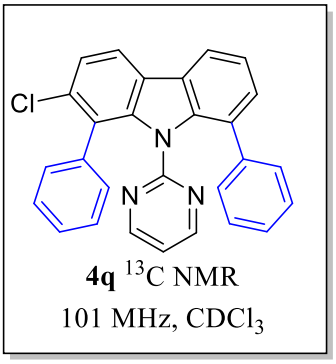
4p ^{13}C NMR
101 MHz, $CDCl_3$



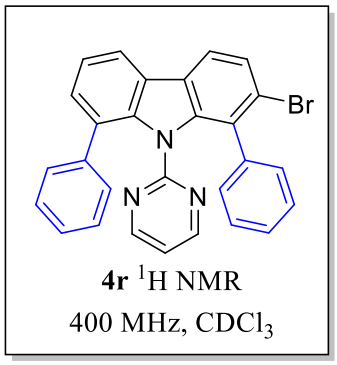


4q ^{1}H NMR
400 MHz, $CDCl_3$



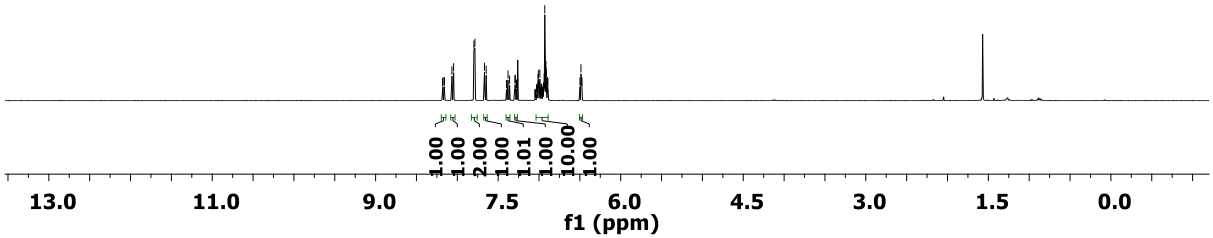


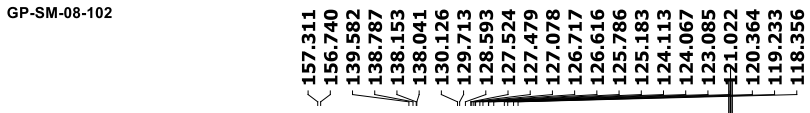
4q ^{13}C NMR
101 MHz, $CDCl_3$

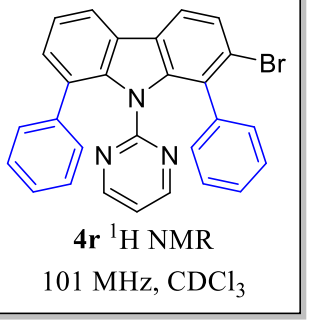


4r ^{1}H NMR

400 MHz, $CDCl_3$

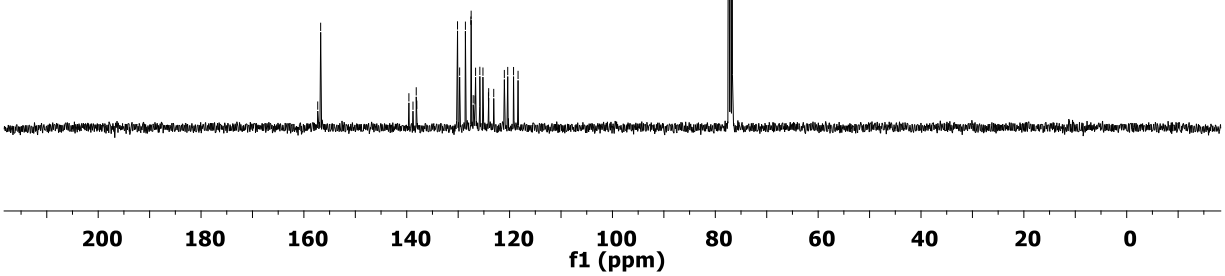




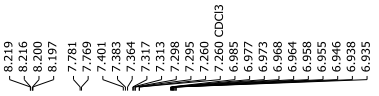


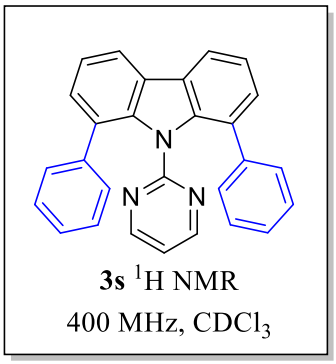
4r ^{1}H NMR

101 MHz, $CDCl_3$



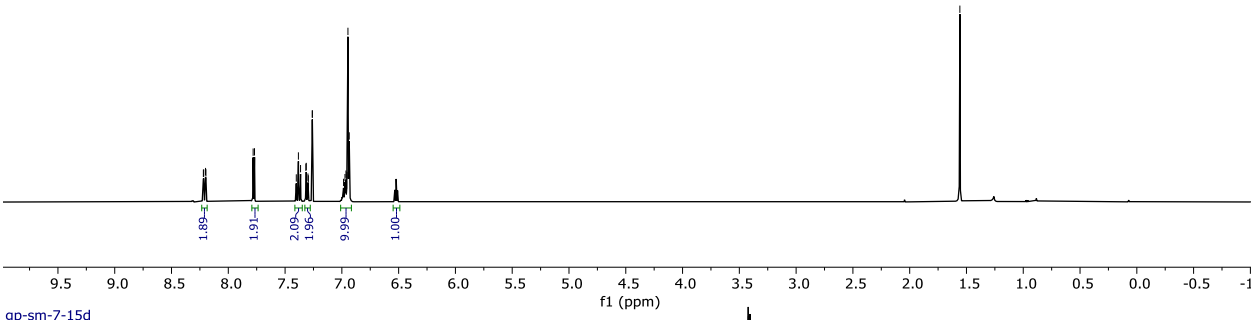
gp-sm-7-15d



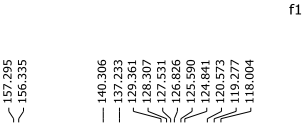


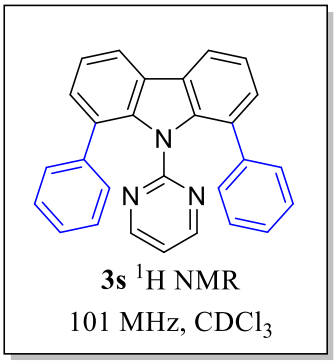
3s ^{1}H NMR

400 MHz, $CDCl_3$



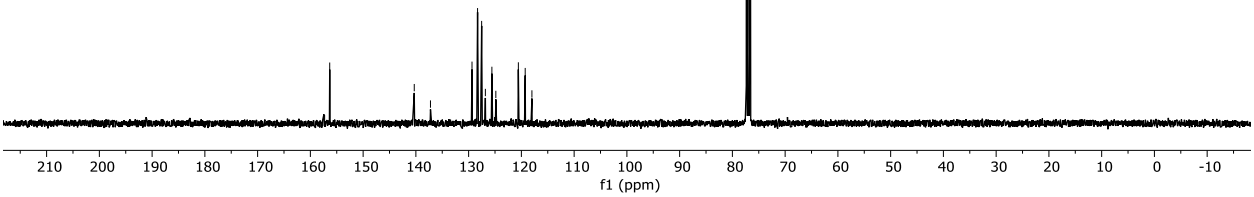
gp-sm-7-15d



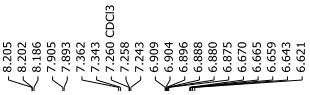


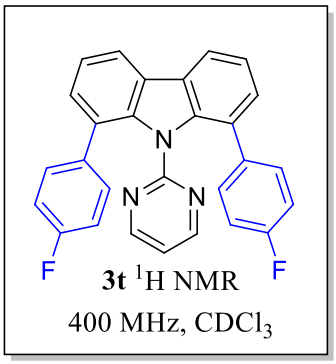
3s ^{1}H NMR

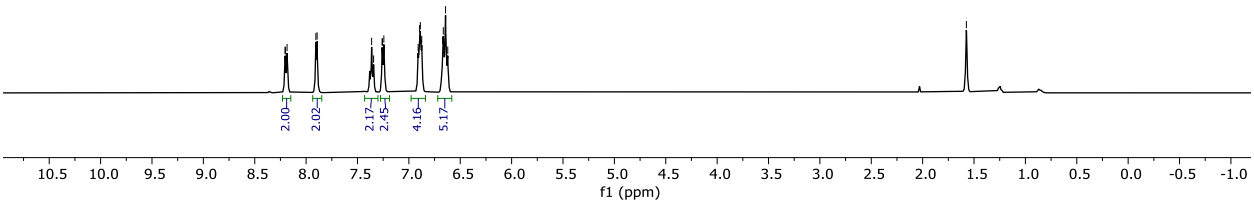
101 MHz, $CDCl_3$



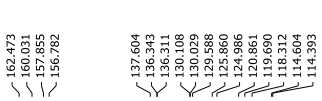
GP-SM-7-56

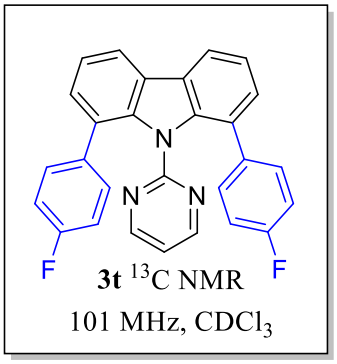


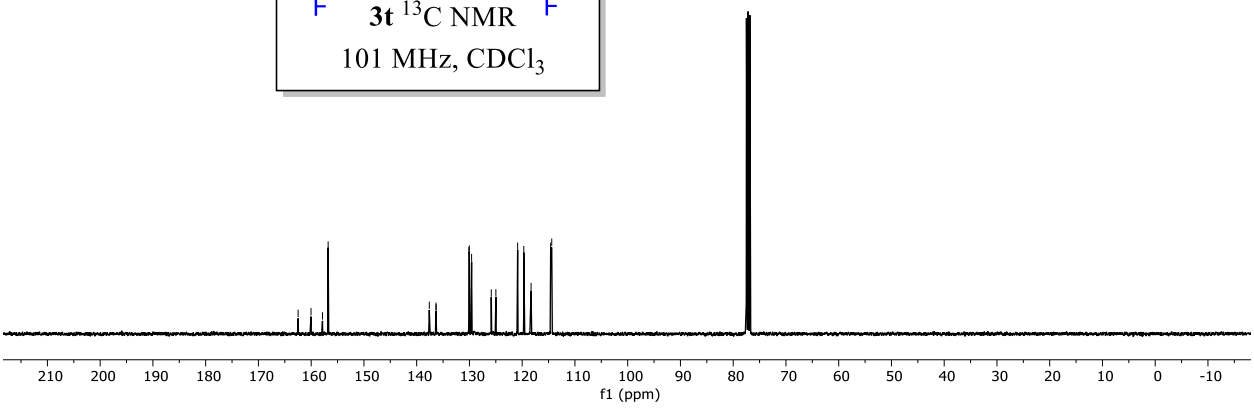




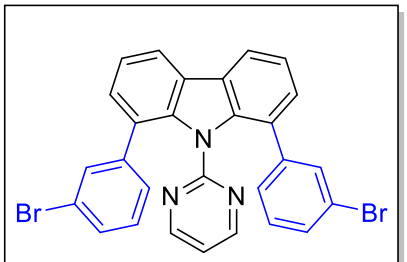
GP-SM-7-56





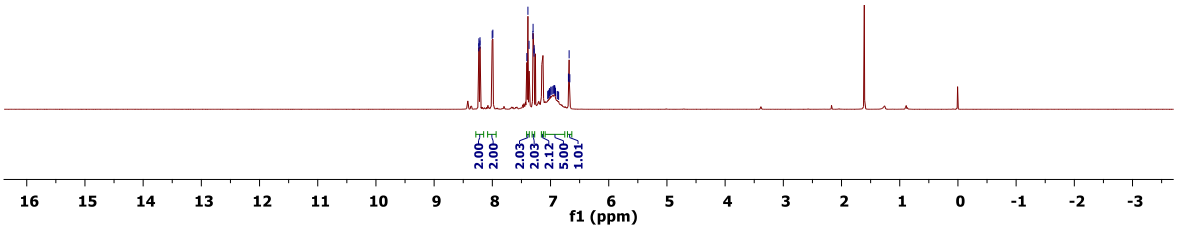


GP-SM-10-10

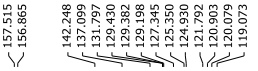


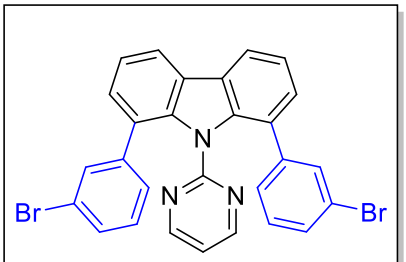
3u ^{1}H NMR

400 MHz, $CDCl_3$



GP-PM-480

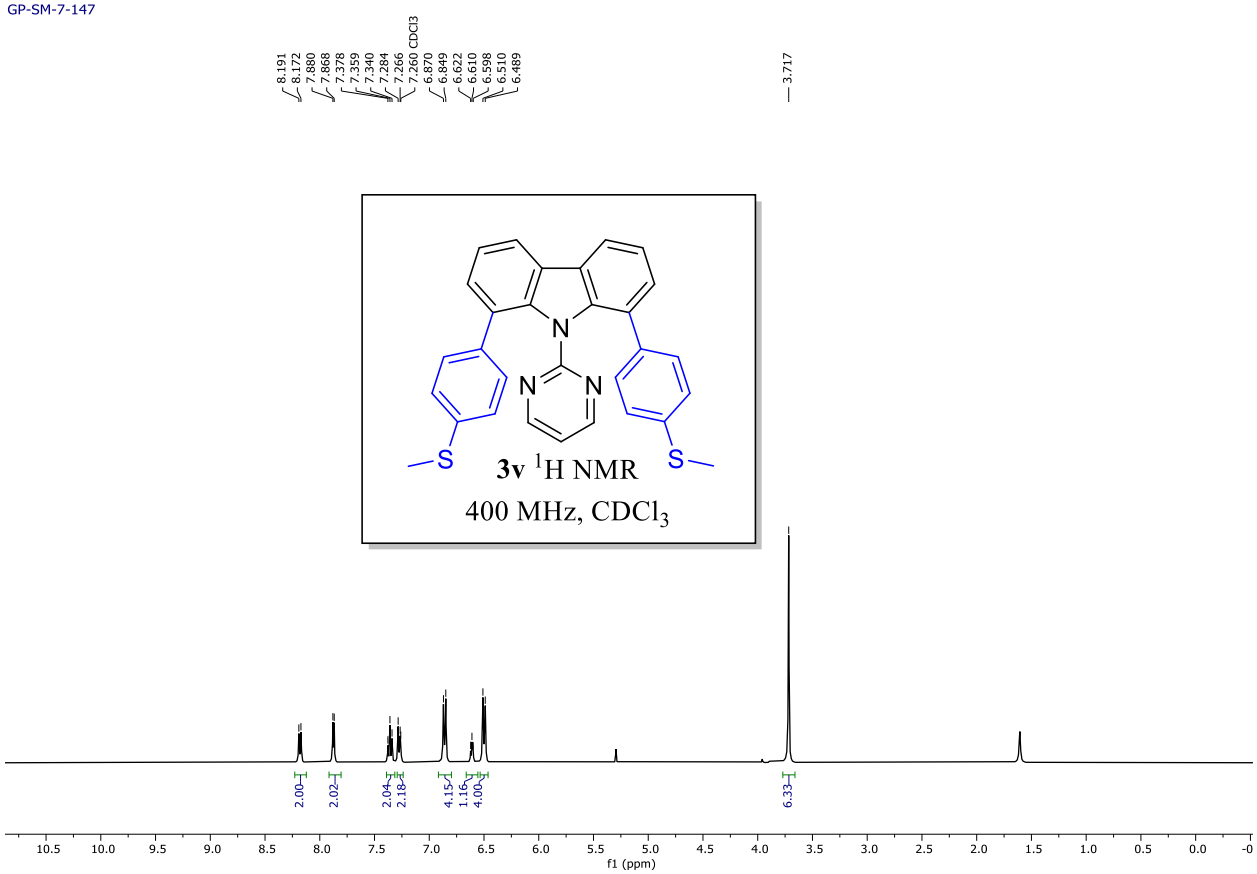




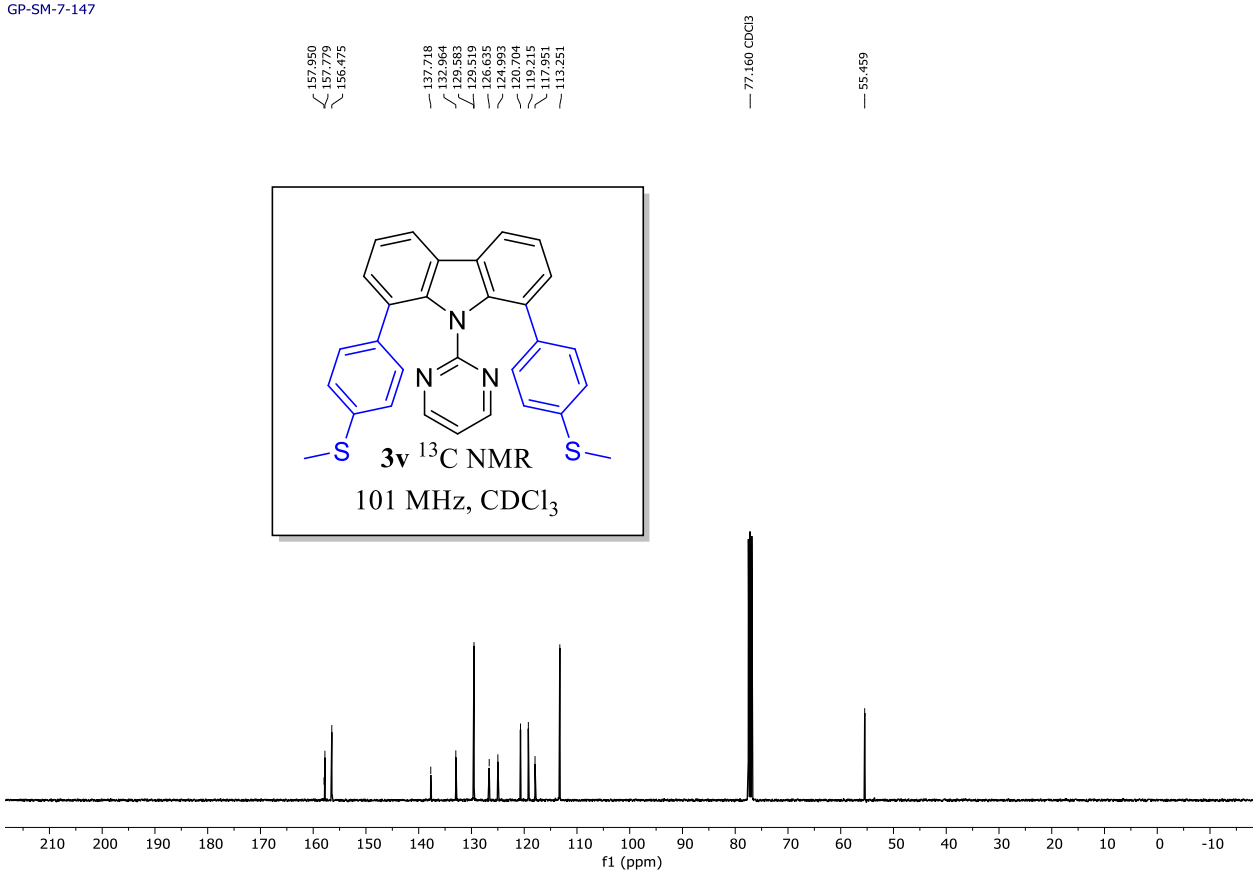
3u ^{13}C NMR

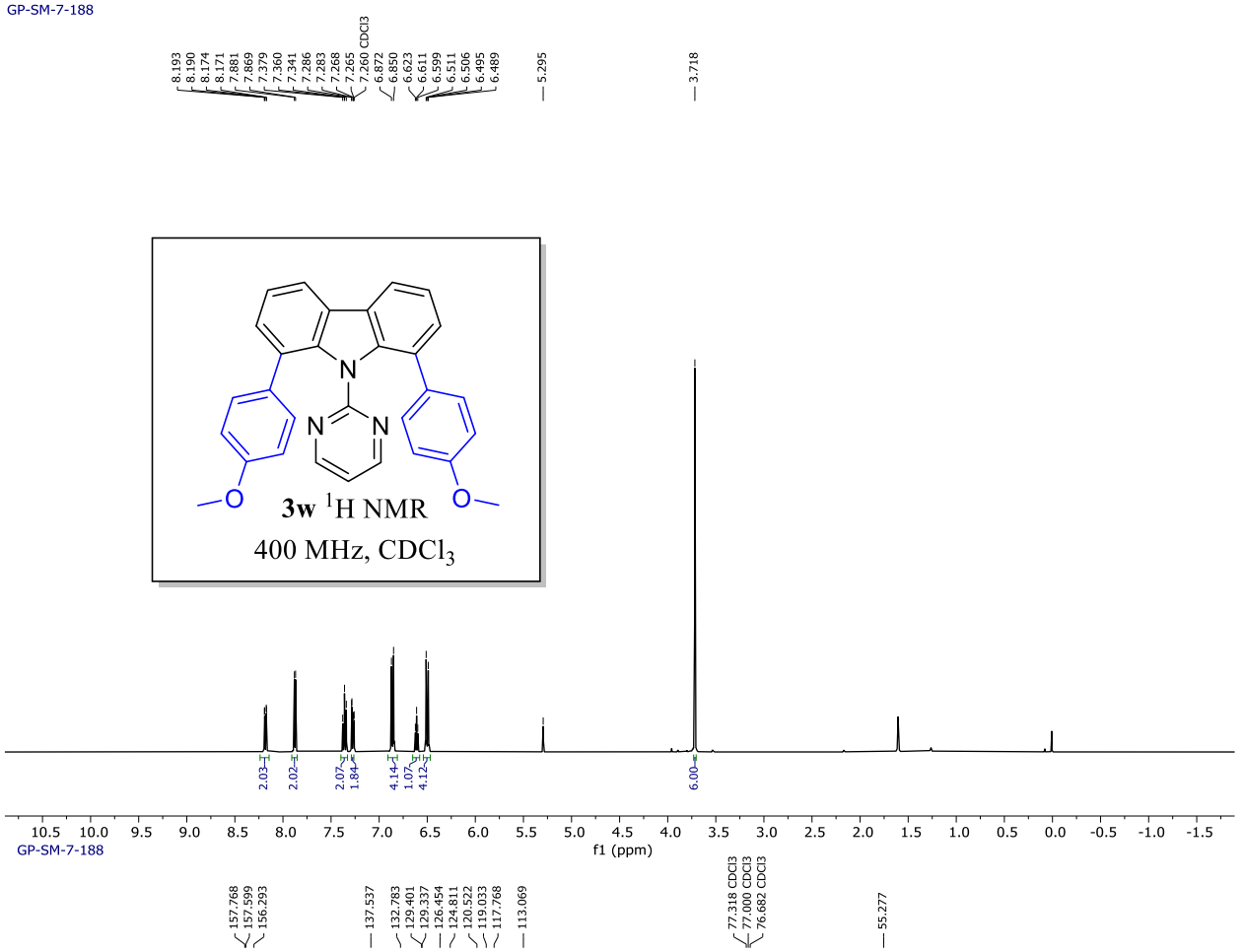
101 MHz, $CDCl_3$

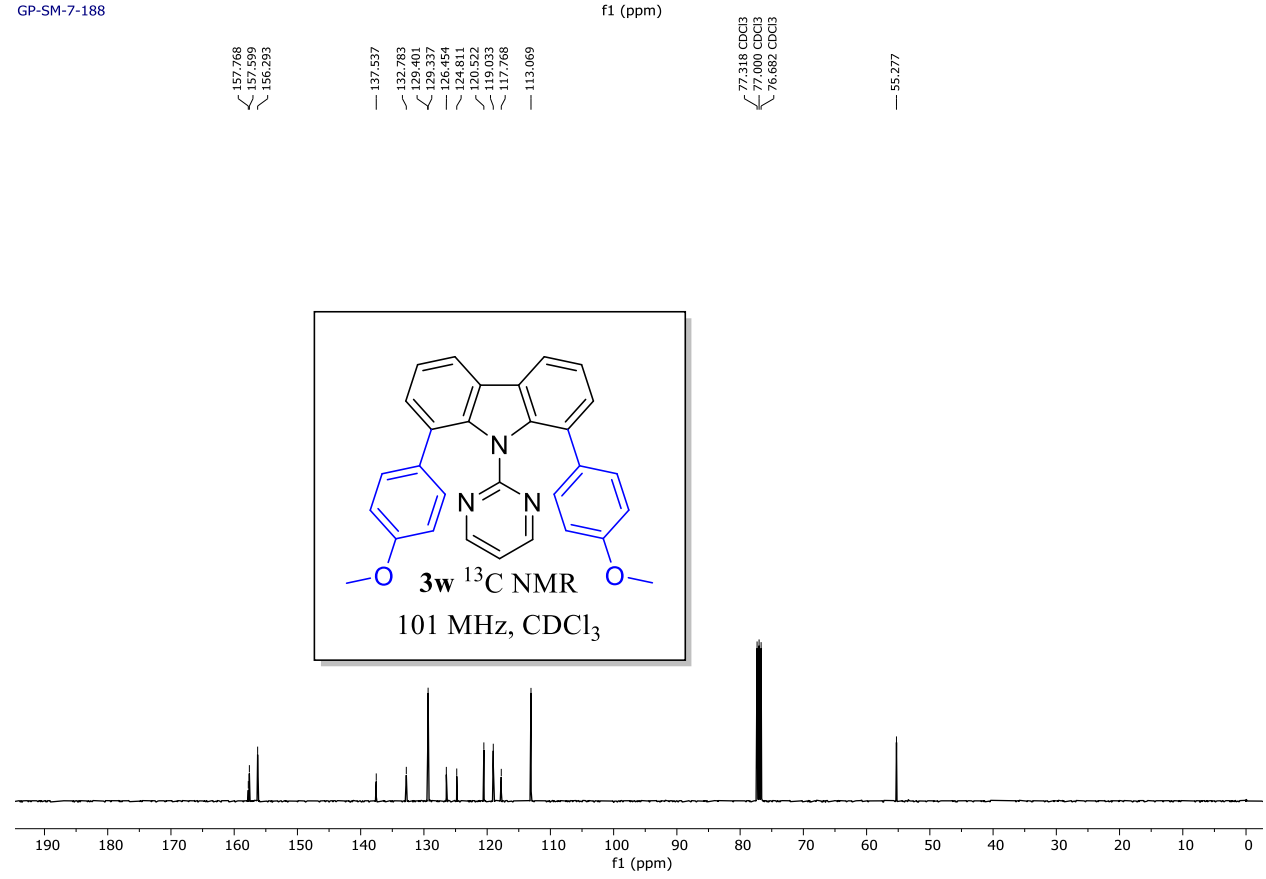
GP-SM-7-147

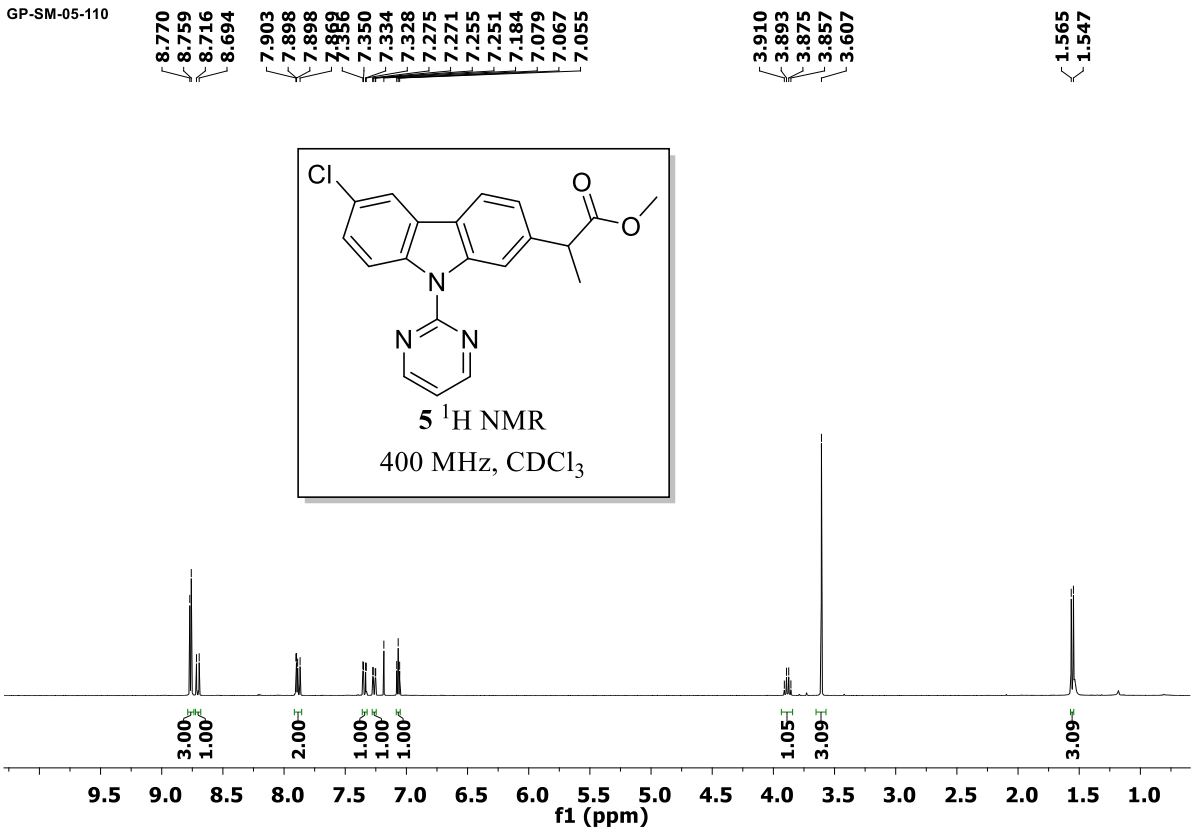


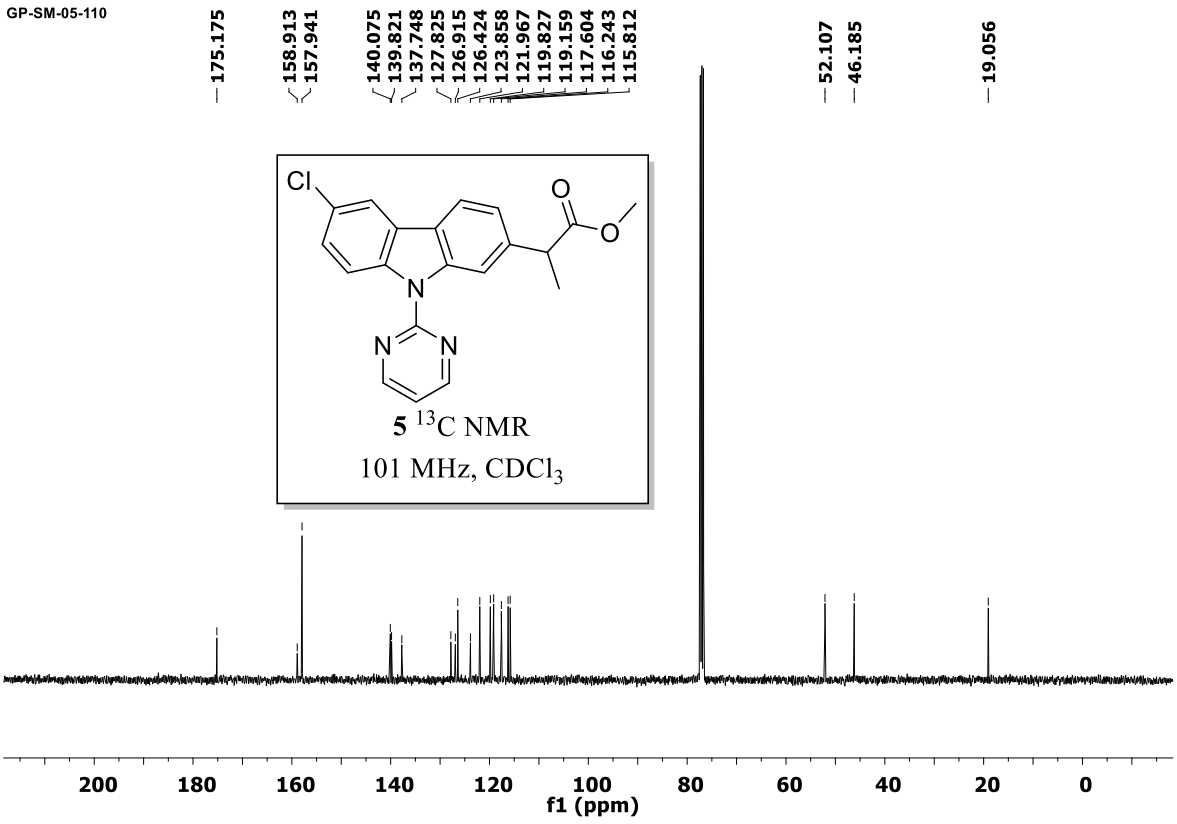
GP-SM-7-147




GP-SM-7-188
8.193
8.190
8.174
8.171
7.881
7.869
7.379
7.360
7.341
7.286
7.283
7.268
7.265
7.260 CDCl3
6.872
6.850
6.623
6.611
6.599
6.511
6.506
6.495
6.489
5.295
3.718
3w 1H NMR
400 MHz, CDCl3
2.03
2.02
2.07
1.84
4.14
1.07
4.12
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)
GP-SM-7-188

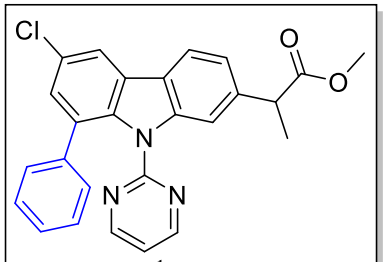

157.768
157.599
156.293
137.537
132.783
129.401
129.337
126.454
124.811
120.522
119.033
117.768
113.069
77.318 CDCl3
77.000 CDCl3
76.682 CDCl3
55.277
3w 13C NMR
101 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


GP-SM-05-110
8.770
8.759
8.716
8.694
7.903
7.898
7.898
7.869
7.350
7.334
7.328
7.275
7.271
7.255
7.251
7.184
7.079
7.067
7.055
3.910
3.893
3.875
3.857
3.607
1.565
1.547
Cl
O
O
N
N
N
5 1H NMR
400 MHz, CDCl3
3.00
1.00
2.00
1.00
1.00
1.00
1.05
3.09
3.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

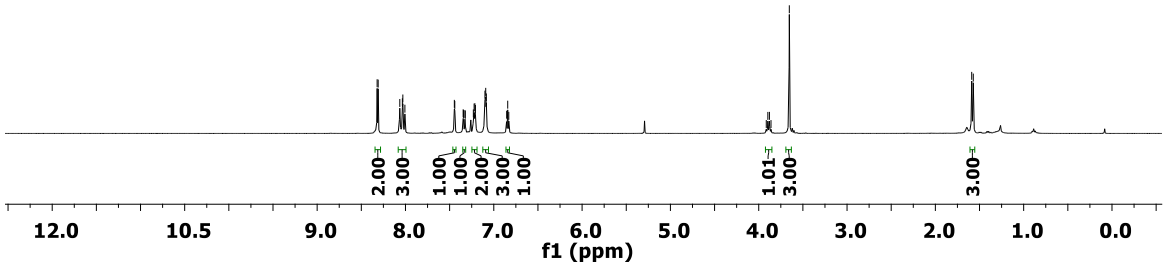

GP-SM-05-110
175.175
158.913
157.941
140.075
139.821
137.748
127.825
126.915
126.424
123.858
121.967
119.827
119.159
117.604
116.243
115.812
52.107
46.185
19.056
Cl
O
O
N
N
N
5 13C NMR
101 MHz, CDCl3
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

GP-SM-08-11

8.321 8.309 8.064 8.035 8.030 8.006 7.447 7.442 7.346 7.344 7.326 7.231 7.223 7.214 7.208 7.100 7.091 7.084 6.842 3.914 3.897 3.879 3.861 3.654 1.588 1.571

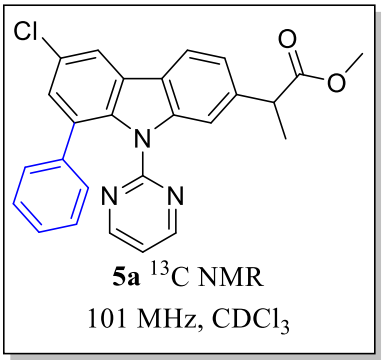


5a ^{1}H NMR
400 MHz, $CDCl_3$

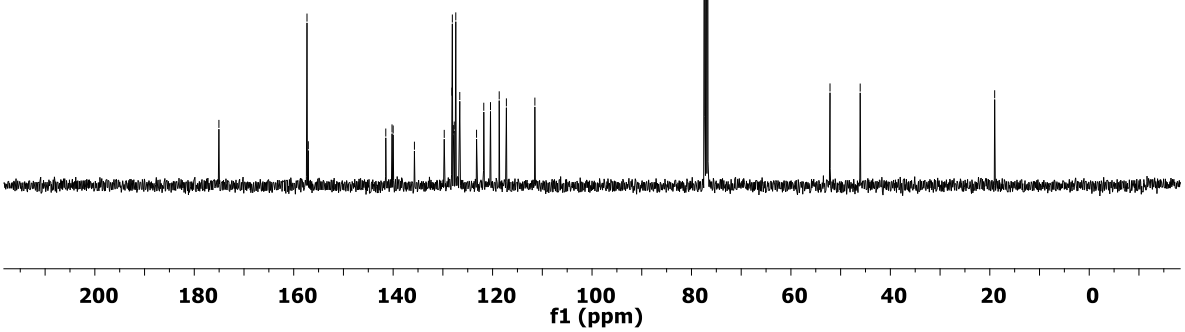


GP-SM-08-11

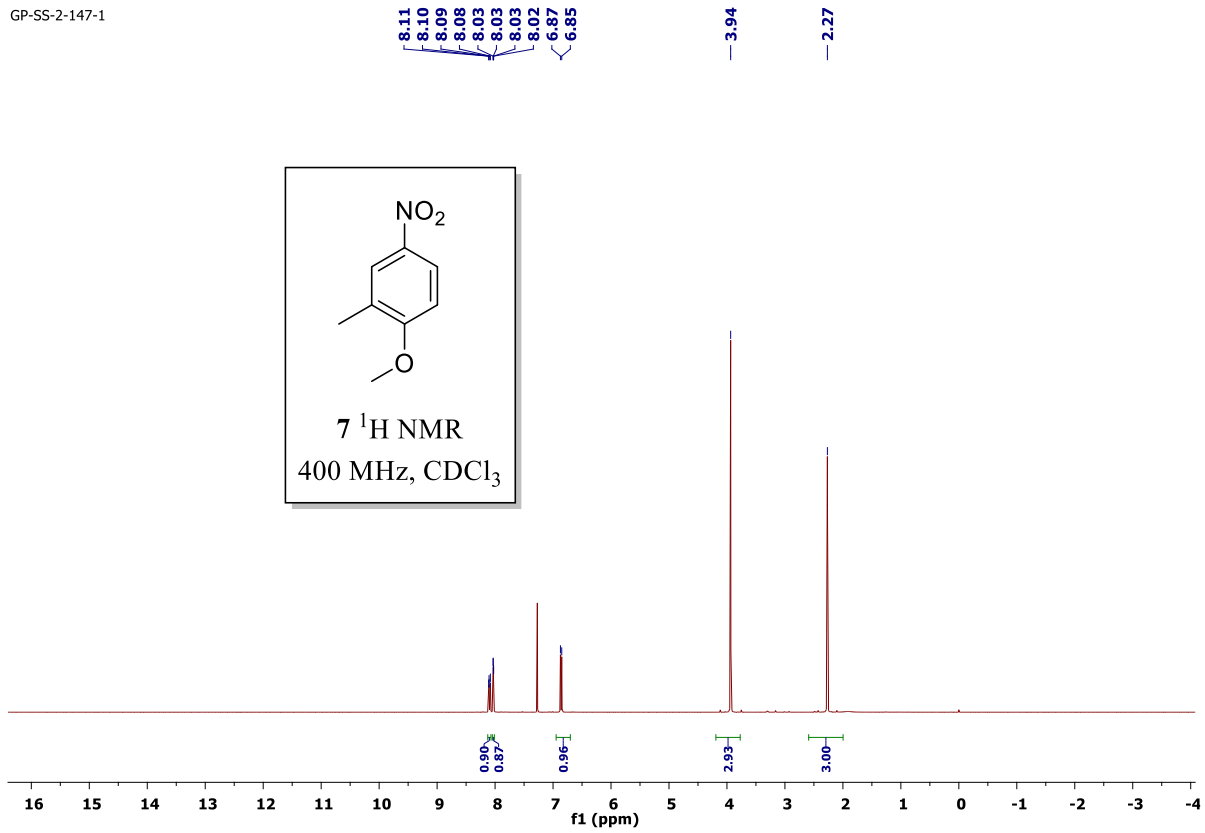
175.044 157.329 157.063 141.481 140.228 139.999 135.721 129.724 128.176 128.094 127.835 127.712 127.404 126.600 123.225 121.774 120.425 118.667 117.224 111.495 52.137 46.065 19.018



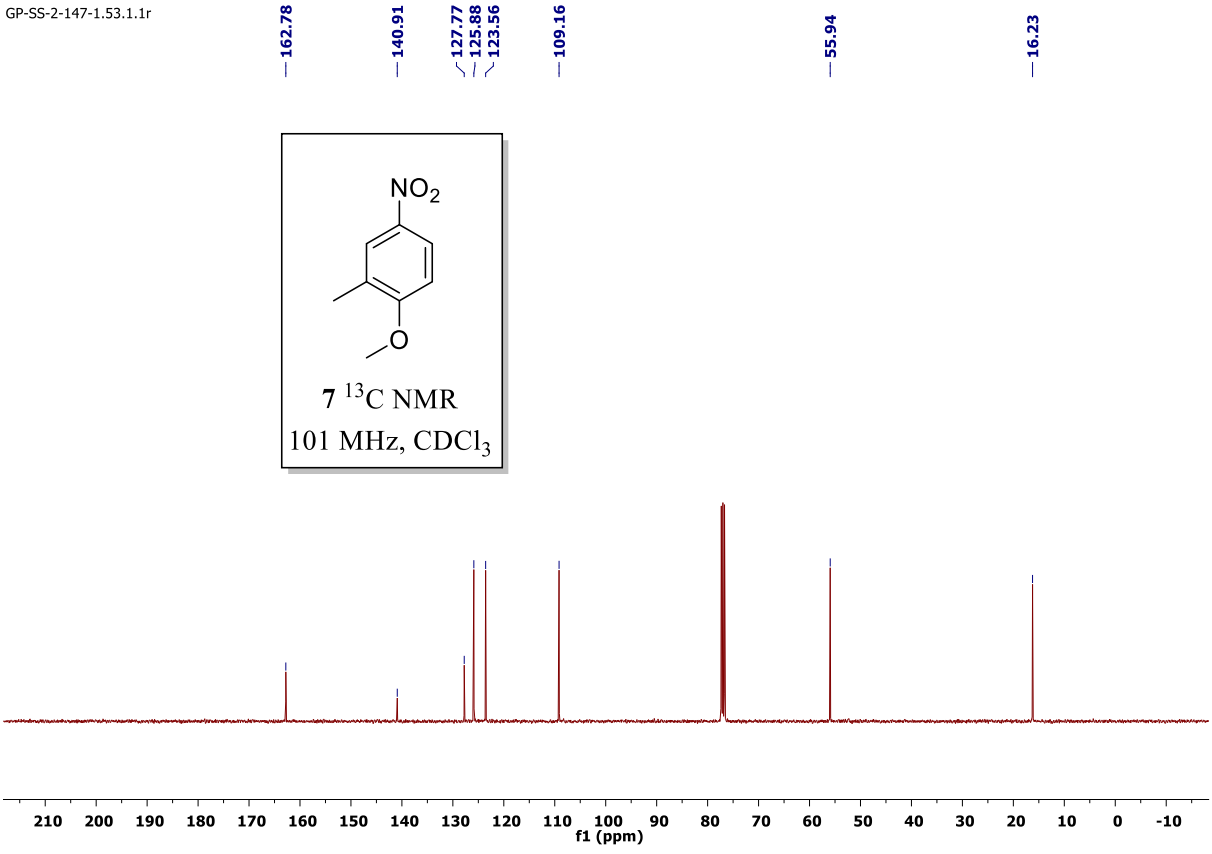
5a ^{13}C NMR
101 MHz, $CDCl_3$



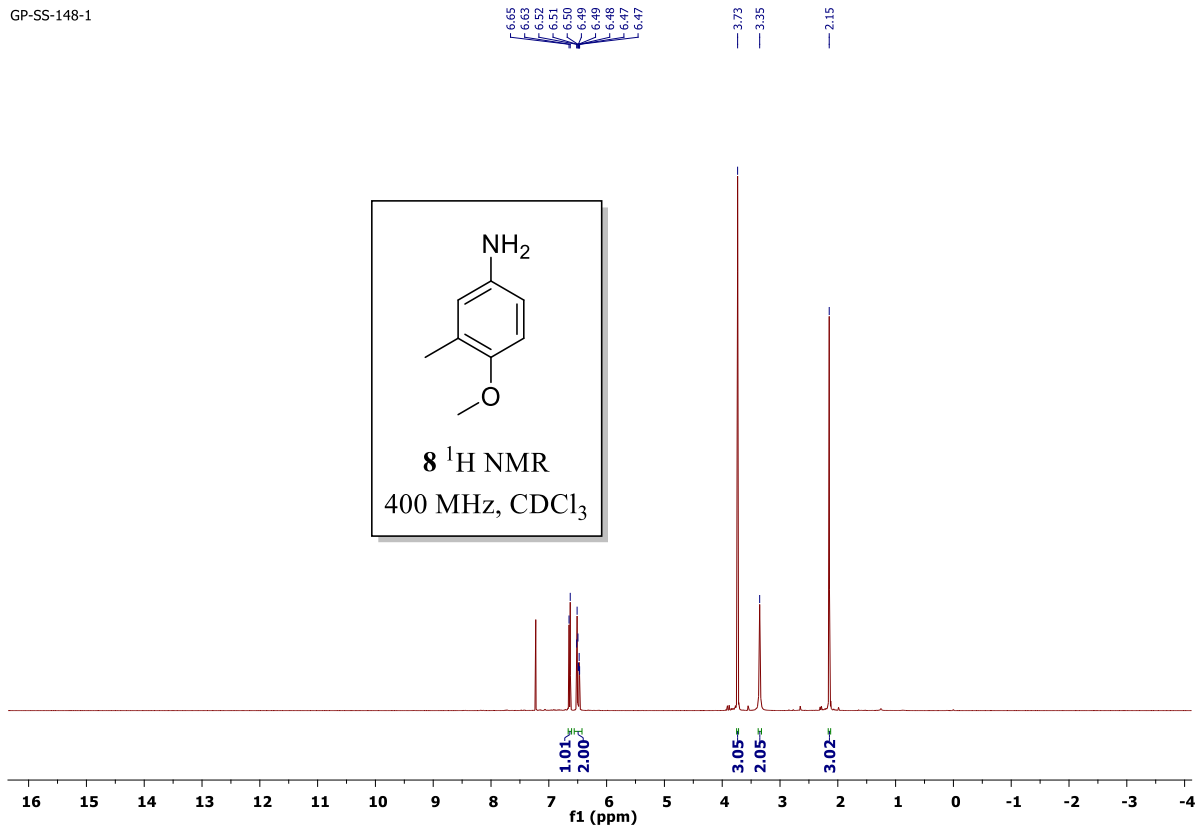
GP-SS-2-147-1



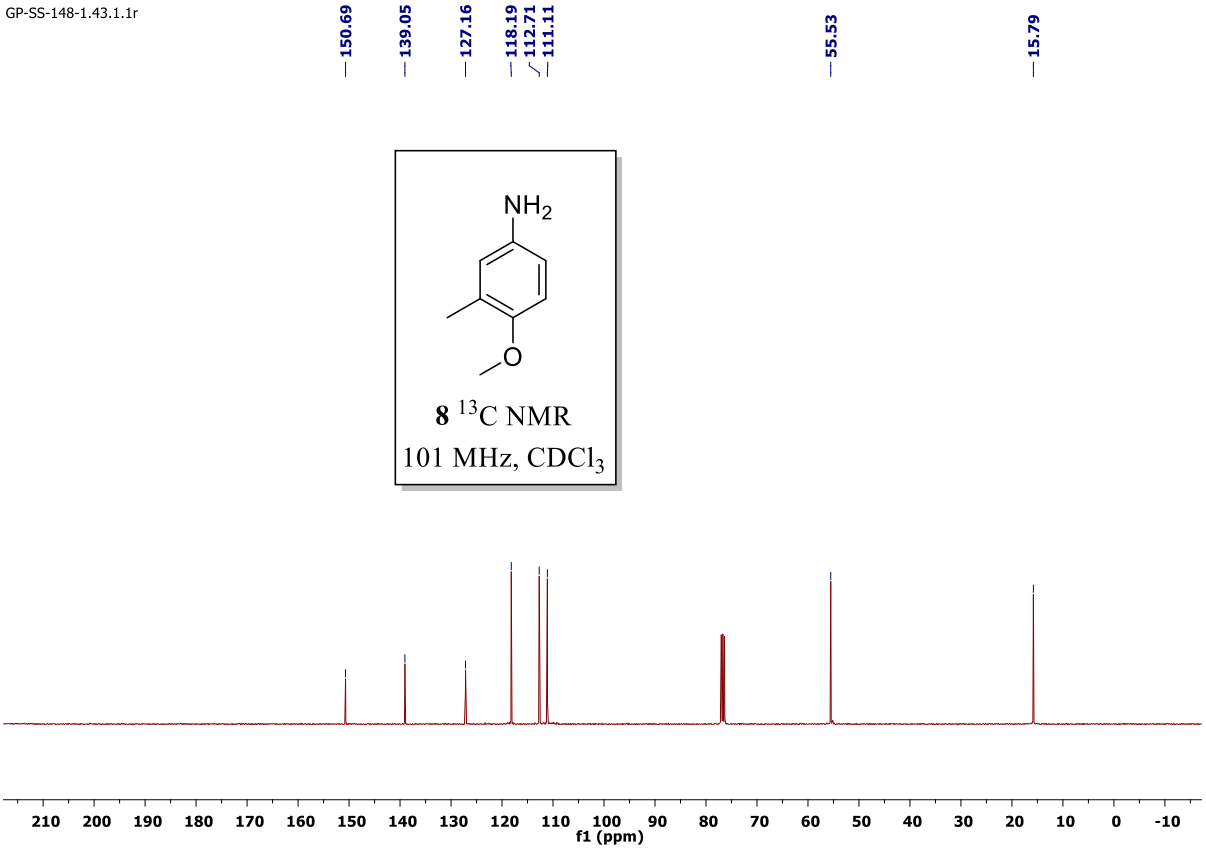
GP-SS-2-147-1.53.1.1r



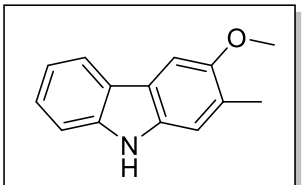
GP-SS-148-1



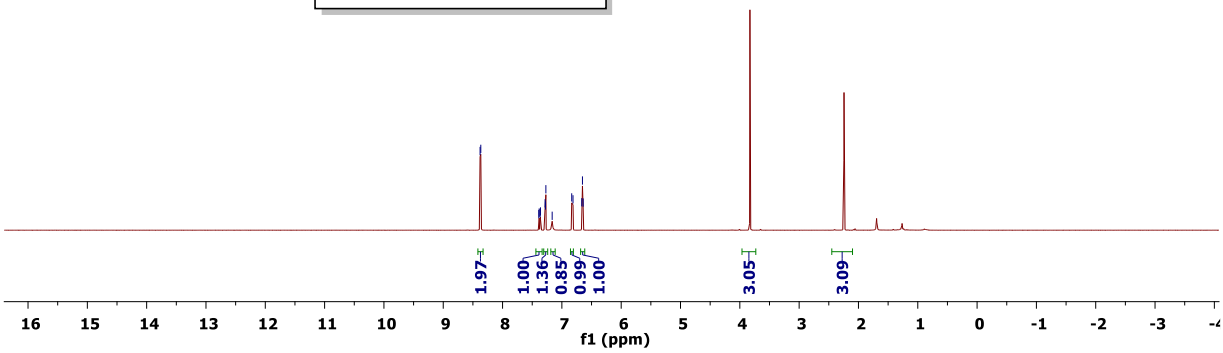
GP-SS-148-1.43.1.1r



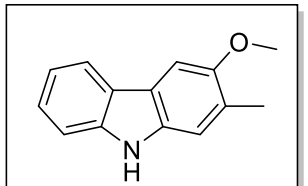
GP-SM-08-89



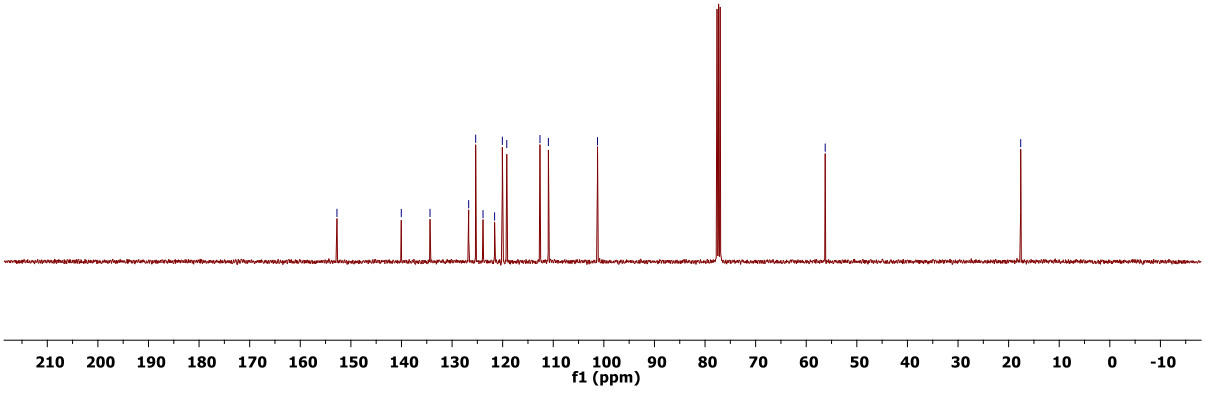
10 ^{1}H NMR
400 MHz, $CDCl_3$



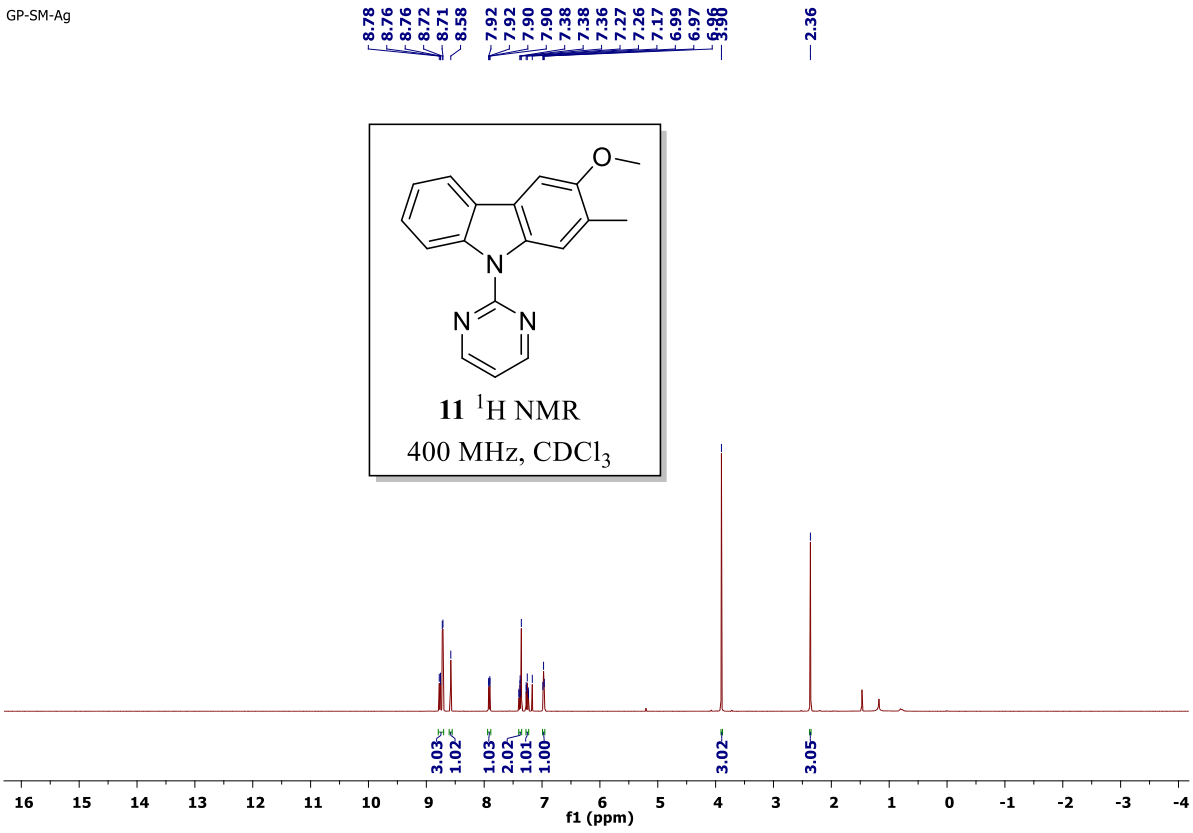
GP-SH-1-A



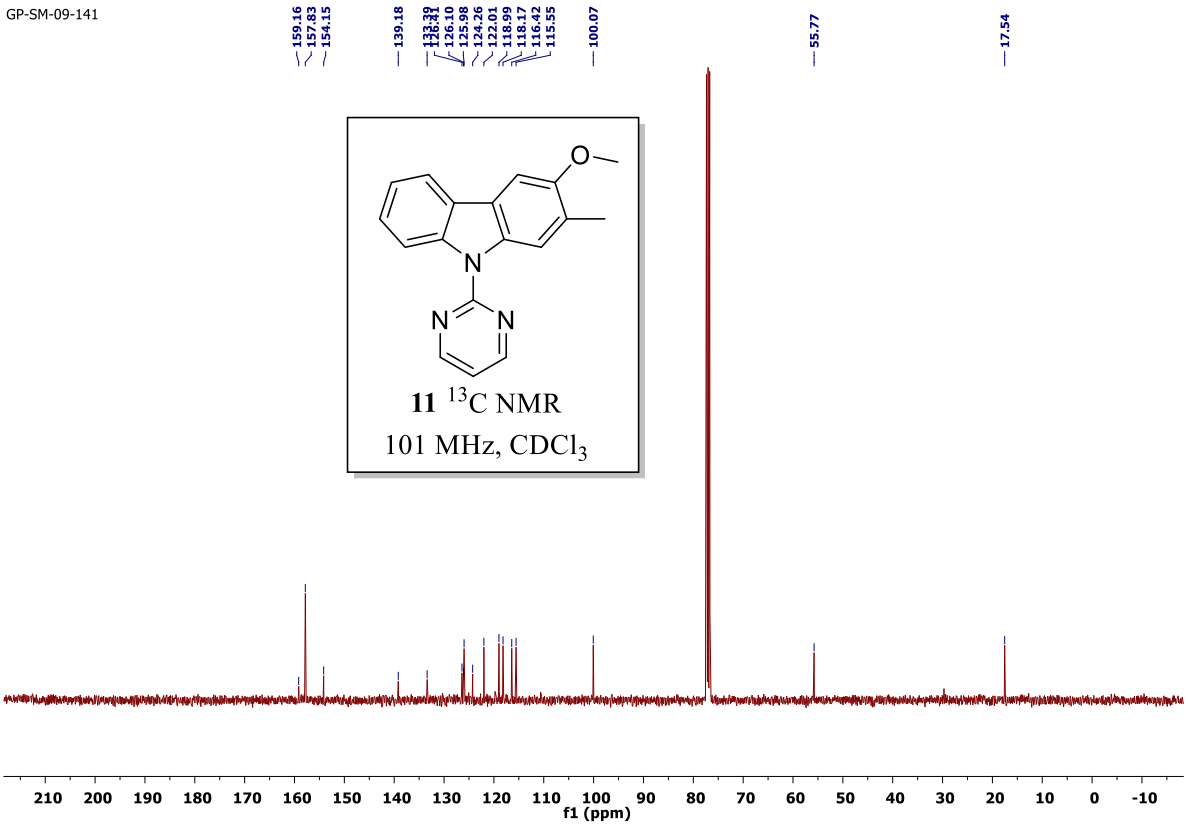
10 ^{13}C NMR
101 MHz, $CDCl_3$

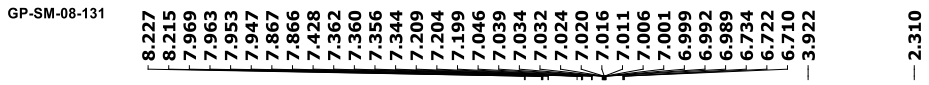


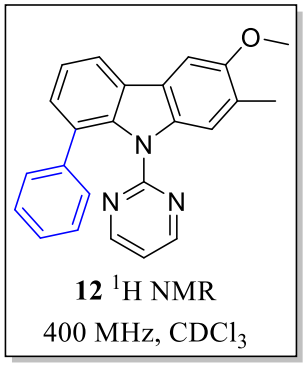
GP-SM-Ag



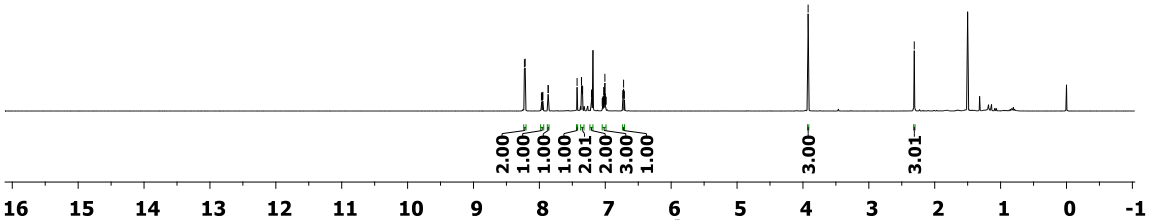
GP-SM-09-141

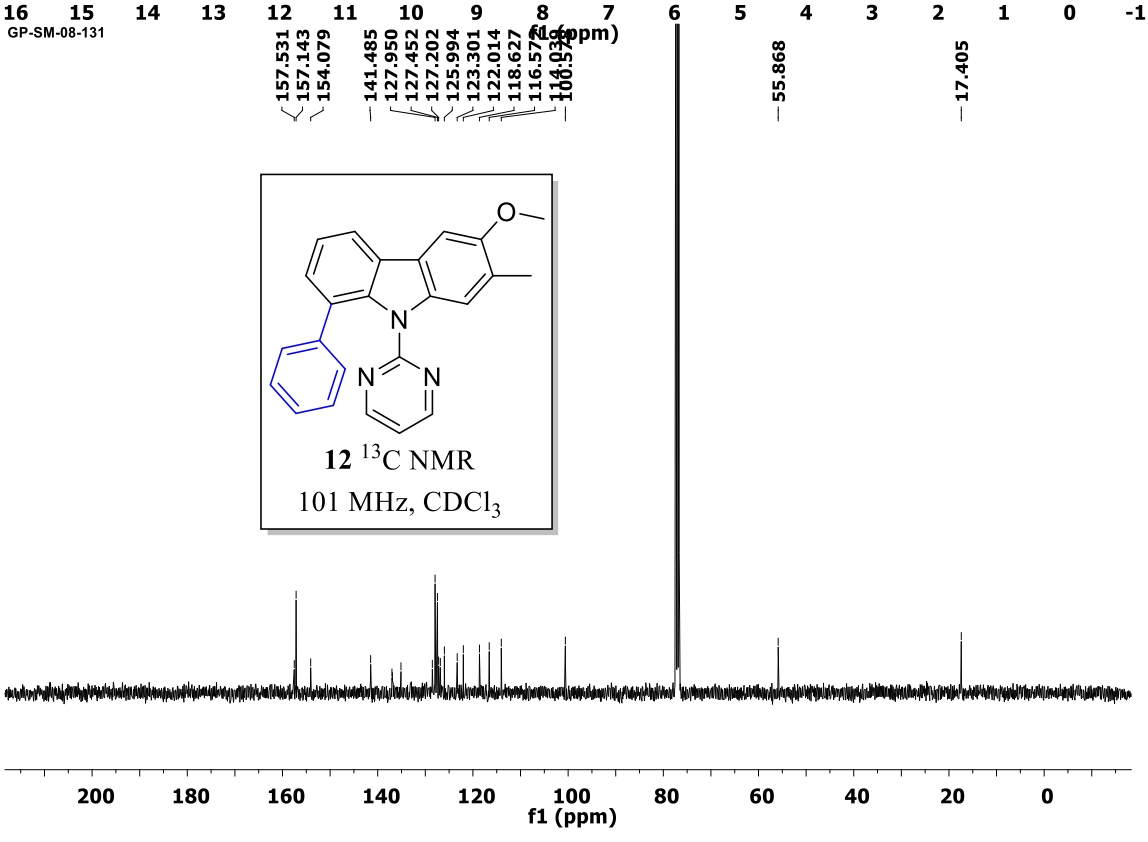




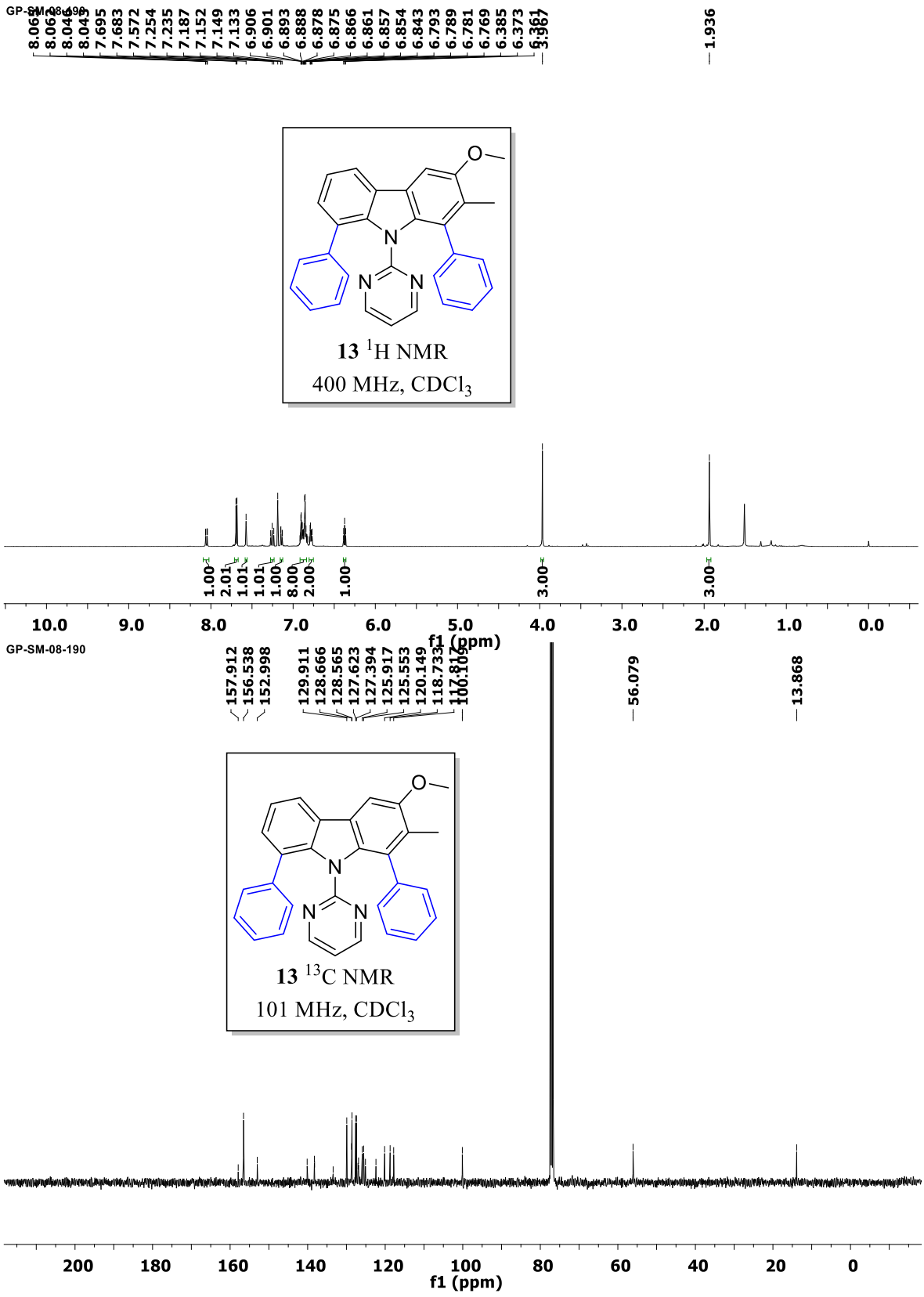


12 ^{1}H NMR
400 MHz, $CDCl_3$

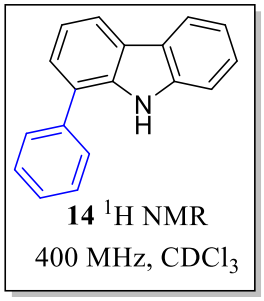


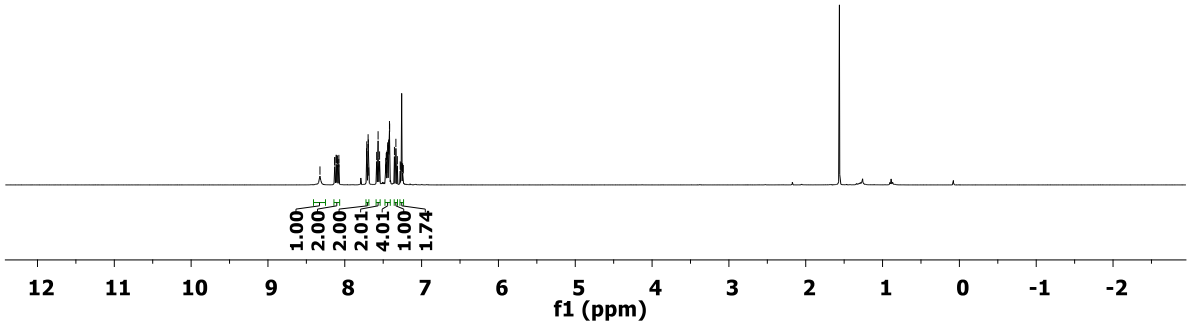


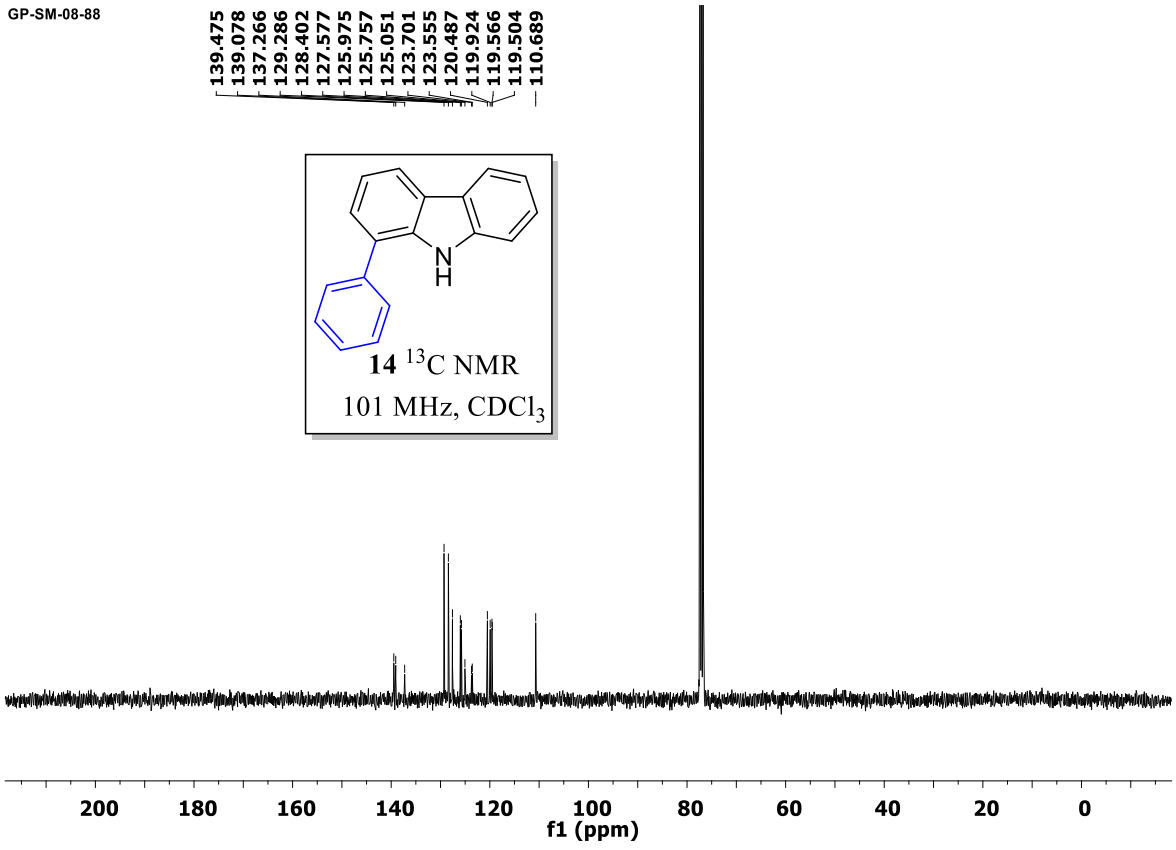
12 ^{13}C NMR
101 MHz, $CDCl_3$


GP-SM-08-190
8.064
8.062
8.046
8.043
7.695
7.683
7.572
7.254
7.235
7.187
7.152
7.149
7.133
6.906
6.901
6.893
6.888
6.878
6.875
6.866
6.861
6.857
6.854
6.843
6.793
6.789
6.781
6.769
6.385
6.373
3.967
1.936
O
N
N
N
13 1H NMR
400 MHz, CDCl3
1.00
2.01
1.01
1.01
1.00
8.00
2.00
1.00
3.00
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
GP-SM-08-190
157.912
156.538
152.998
129.911
128.666
128.565
127.623
127.394
125.917
125.553
120.149
118.733
117.816
100.105
56.079
13.868
O
N
N
N
13 13C NMR
101 MHz, CDCl3
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


GP-SM-08-88
8.323
8.131
8.130
8.117
8.110
8.098
8.096
8.079
8.077
7.717
7.714
7.709
7.696
7.693
7.689
7.585
7.580
7.566
7.551
7.547
7.470
7.467
7.463
7.460
7.457
7.453
7.448
7.442
7.439
7.430
7.428
7.427
7.424
7.418
7.416
7.354
7.335
7.316
7.278
7.270
7.266
7.250
7.247
7.238


N
H
14 ^{1}H NMR
400 MHz, $CDCl_3$


1.00
2.00
2.00
2.01
4.01
1.00
1.74
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


GP-SM-08-88
139.475
139.078
137.266
129.286
128.402
127.577
125.975
125.757
125.051
123.701
123.555
120.487
119.924
119.566
119.504
110.689
N
H
14 ^{13}C NMR
101 MHz, $CDCl_3$
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)