

Supporting Information

Cobalt Catalyzed Multisubstituted Allylation of Chelation Assisted C-H bond of (Hetero)arenes with Cyclopropenes

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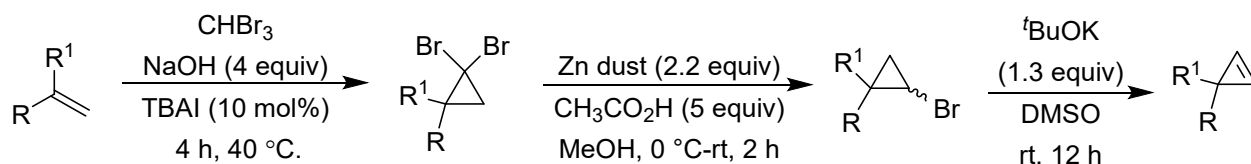
1. General Comments:

All reactions were carried out under nitrogen atmosphere using oven dried reaction tubes. Dry toluene was prepared by distilling over calcium hydride and stored over molecular sieves 4Å under nitrogen atmosphere. All the 1-(pyridin-2-yl)indole derivatives were synthesized from corresponding indoles employing literature procedure.¹ [Cp*CoI₂CO], and [Cp*Co(CH₃CN)₃](SbF₆)₂ were synthesized from Co₂CO₈ according to the literature procedure.² Column chromatography was performed using RankemSilica gel (100-200 mesh) and the solvent system used unless otherwise specified, was ethyl acetate-hexanes with various percentage of polarity depending on the nature of the substrate.

2. Analytical Methods:

NMR data were recorded on 400 and 500 MHz spectrometers. ¹H and ¹³C NMR spectra were referenced to signals of either deuterated solvents or residual protonated solvents. Infrared spectra were recorded on a Jasco ATR IR spectrometer. HRMS were recorded by electron spray ionization (ESI) method on a Q-TOF Micro with lock spray source.

3.1 Synthesis of cyclopropene derivatives:



Substituted alkene (1.0 equiv) was taken into the round bottom flask followed by bromoform (1.5 equiv) was added slowly through a syringe. The mixture was allowed to stir for 5 min, then 4 equivalents of 50% of aqueous NaOH solution was added to the reaction. Finally, TBAI (10 mol%) was added and the reaction mixture was kept in 40 °C preheated oil bath. TLC was checked during the reaction, after the completion of reaction, the reaction mixture was quenched with water followed by extracted with DCM and wash with water. The extracted organic layer was dried over Na₂SO₄, filtered, and concentrated to give a crude product. The obtained crude was further purified by column chromatography with silica gel using ethyl acetate/hexane as an eluent to give the product in excellent yield as yellow oil. R_f = 0.60 in 1:9 ethyl acetate/hexane. Dibromocyclopropane (1.0 equiv) and MeOH (30 mL) as taken into the round bottom flask with a stir bar. The reaction mixture was kept at 0 °C followed by 5 equivalents of CH₃CO₂H and 2.2 equivalents of Zn dust were added into the reaction mixture slowly. The reaction was monitored

¹Ackermann, L.; Lygin, A. V. *Org. Lett.* **2011**, *13*, 3332.

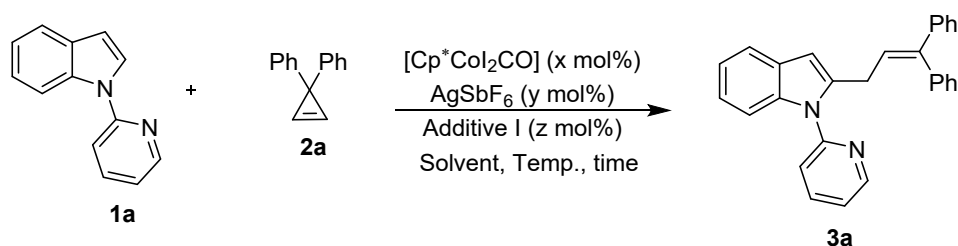
²B. Sun, T. Yoshino, S. Matsunaga, M. Kanai, *Adv. Synth. Catal.* **2014**, *356*, 1491 - 1495.

by TLC. Once the reaction was completed, the solvent was evaporated in a high vacuum then the crude was extracted with Et₂O and washed with water. The extracted organic layer was dried over Na₂SO₄, filtered, and concentrated in vacuo to obtained crude product, which was purified with silica gel column chromatography using ethyl acetate/hexane as an eluent to afford the product in good yield as yellow oil. R_f = 0.60 in 1:9 ethyl acetate/hexane.

Bromocyclopropane (1.0 equiv) was taken into two-neck round bottom flask with dry DMSO (20 mL) under argon atmosphere. Then, ^tBuOK was added into the reaction flask at ambient temperature and stirred overnight. After the completion of reaction, the reaction mixture was quenched with distilled water. Subsequently, the reaction mixture was extracted with ethyl acetate, washed with water, and brine solution. The extracted organic layer was dried over Na₂SO₄, filtered, concentrated under vacuum and the resultant crude product was purified using column chromatography. The substituted cyclopropenes were obtained with good yield.

4.1 Cobalt catalyzed allylation of arenes: Optimization

In an oven-dried reaction tube, 1-(pyridin-2-yl)-1*H*-indole **1a** (50 mg, 0.26 mmol) and 3,3-diphenylcyclopropene **2a** (100 mg, 0.52 mmol), was added into the reaction tube. Subsequently, catalyst and additive (mol% as mentioned in the table) were added and 2 mL of dry solvent was added to the reaction tube and sealed with septa. It was kept in a preheated oil bath at the temperature mentioned in the table and stirred at same temperature for the time mentioned in the table below. Next, the reaction mixture was cooled to room temperature and dissolved in 5 mL of DCM, and filtered through a small pad of Celite. The solvent was evaporated to get the crude product, which was further purified by column chromatography to afford product 2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1*H*-indole **3a**.

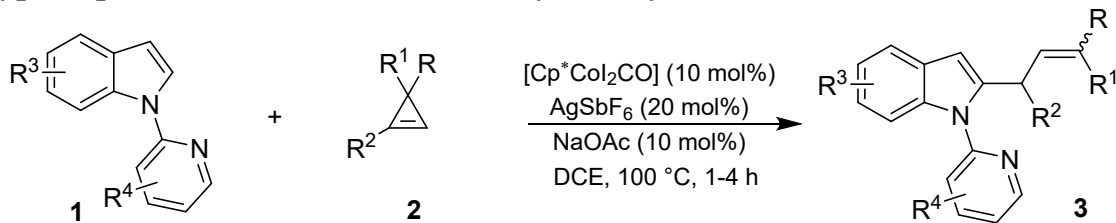


Entry	[Cp*CoI ₂ CO] (x mol%)	AgSbF ₆ (y mol%)	Additive I (z mol%)	Solvent	Temp. (°C)	Time (h)	Yield (%)
1 ^a	[10]	20	K ₂ CO ₃ [10]	PhCl	100	24	-
2 ^a	[10]	20	K ₂ CO ₃ [10]	DCE	100	24	5
3	[10]	20	K ₂ CO ₃ [10]	DCE	100	24	24
4	[10]	20	K ₂ CO ₃ [10]	DCE	120	24	48
5	[5]	10	K ₂ CO ₃ [10]	DCE	100	24	14
6	[5]	10	K ₂ CO ₃ [10]	DCE	120	36	10

7	[10]	20	KOAc [10]	DCE	100	24	60
8	[10]	20	AgOAc [10]	DCE	100	24	50
9	[10]	20	AgOTf [10]	DCE	100	24	25
10	[10]	20	Ag ₂ CO ₃ [10]	DCE	100	24	trace
11	[10]	20	AgOAc [20]	DCE	100	24	trace
12	[10]	20	KOAc [30]	DCE	100	24	42
13	[10]	20	KOAc [50]	DCE	100	24	39
14	[10]	20	KOAc [100]	DCE	100	24	20
15	[10]	20	NaOPiv [10]	DCE	100	24	56
16	[10]	20	KOPiv [10]	DCE	100	24	72
17	[10]	20	Cs ₂ CO ₃ [10]	DCE	100	24	20
18	[10]	20	KOAc [10]	DMF	100	24	-
19	[10]	20	KOAc [10]	DMSO	100	24	-
20	[10]	20	KOAc [10]	CH ₃ CN	100	24	-
21	[10]	20	KOAc [10]	DCM	100	24	36
22	[10]	20	NaOAc [10]	toluene	100	4	28
23	[10]	20	NaOAc [10]	DCE	100	1.5	91
24	[10]	20	NaOAc [10]	DCE	rt	2	-
25	-	20	NaOAc [10]	DCE	100	2	-
26	[10]	-	NaOAc [10]	DCE	100	2	trace
27	[10]	20	-	DCE	100	2	5
28	[Cp*RhCl ₂] ₂ [5]	10	NaOAc [10]	DCE	100	4	trace
29	[Cp*Co(CH ₃ CN) ₃ (SbF ₆) ₂] [10]	-	NaOAc [10]	DCE	100	4	47
30	[Cp*CoCl ₂] ₂ [10]	10	NaOAc [10]	DCE	100	4	5

Reaction conditions: 1-(pyridin-2-yl)-1*H*-indole **1a** (1.0 equiv), Cycloprop-2-ene-1,1-diylidibenzene **2a** (2 equiv), Catalyst [Cp*CoI₂CO] (5-10 mol %), Temperature, Time; 4 h, (1-2)^a 1-Phenyl-1*H*-pyrazole (1.0 equiv).

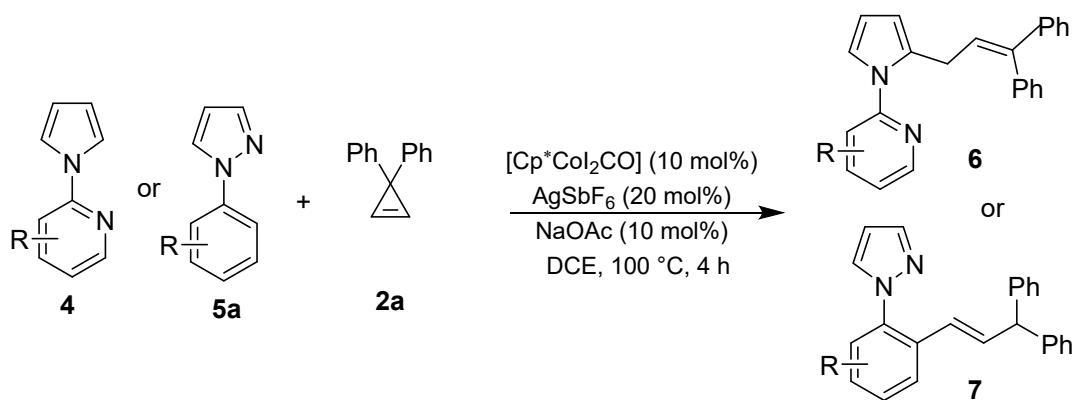
5. Typical procedure for the cobalt catalyzed allylation of 1 with 2:



Oven-dried Schlenk tube was charged with substituted indole **1** (0.26 mmol, 1.0 equiv), NaOAc (10 mol%), AgSbF₆ (20 mol%) and [Cp*CoI₂CO] (10 mol%). The charged schlenk tube inner atmosphere was made inert through repeated (thrice) evacuation and refilled with nitrogen. Subsequently, 1 mL of dry DCE solvent was added to Schlenk tube. Cyclopropene **2** (0.52 mmol%, 2.0 equiv) was taken in (5 mL) dried vial, followed by 1 mL of dry DCE solvent was added. The charged schlenk tube was kept in preheated oil-bath at 100 °C and DCE solution of **2** was slowly added to reaction mixture about 1.5 h. The reaction mixture was stirred at same temperature throughout the mentioned period. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and passes through a pad of celite and concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the expected product **3** in good to excellent yield.

5.2 Typical procedure for the cobalt catalyzed reaction of **4** and **5** with **2a**:

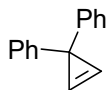
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Oven-dried Schlenk tube was charged with substrate **4** or **5** (0.28 mmol, 1.0 equiv), **2a** (0.56 mmol%, 2.0 equiv), NaOAc (10 mol%), AgSbF₆ (20 mol%) and [Cp*CoI₂CO] (10 mol%). The charged Schlenk tube's inner atmosphere was made inert through repeated (thrice) evacuation and refilled with nitrogen. Subsequently, 2 mL of dry DCE solvent was added and it was kept in preheated oil bath at 100 °C. The reaction mixture was stirred at same temperature throughout the mentioned period. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and passes through a pad of celite, and concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the product **6** and **7** 82% isolated yield. This same reaction procedure was followed for other pyrazole derivatives.

6. Properties and spectral data of synthesized compounds:

3,3-Diphenylcyclopropene (2a):



Yield: 60%; colourless liquid; R_f = 0.60 in 100% Hexane.

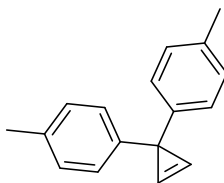
IR ($\nu_{\max}$, cm^{-1}): 3060, 1964, 1727, 1659, 1390, 1267, 1044.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.46 (s, 2H), 7.30-7.24 (m, 4H), 7.20-7.15 (m, 6H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 147.2, 128.8, 128.2, 125.8, 113.3,

HRMS: (ESI) m/z calcd for $\text{C}_{15}\text{H}_{12}$, 193.1012 $[\text{M}+\text{H}]^+$; found 193.1014.

3,3-Bis(4-methylphenyl)cyclopropene (2t):



Yield: 34%; white solid; R_f = 0.5 in 100% Hexane.

IR ($\nu_{\max}$, cm^{-1}): 2998, 2867, 1726, 1510, 1470, 1275, 1176.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.45 (s, 2H), 7.10-7.05 (m, 8H), 2.31 (s, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 144.4, 135.2, 128.8, 128.1, 113.1, 31.3, 21.1

HRMS: (ESI) m/z calcd for $\text{C}_{17}\text{H}_{16}$, 221.1325 $[\text{M}+\text{H}]^+$; found 221.1323.

3-Methyl-3-phenylcyclopropene (2v):



Yield: 58%; colourless liquid; R_f = 0.60 in 100% Hexane.

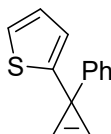
IR ($\nu_{\max}$, cm^{-1}): 2972, 1743, 1589, 1467, 1273, 755.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.32–7.19 (m, 6H), 7.13 (t, J = 8.0 Hz, 1H), 1.62 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 150.0, 129.3, 127.9, 126.8, 126.1, 125.1, 115.6, 28.0.

HRMS: (ESI) m/z calcd for $\text{C}_{10}\text{H}_{10}$, 131.0855 $[\text{M}+\text{H}]^+$; found 131.0855.

3-Phenyl-3-thiophene-2-ylcyclopropene (2y):



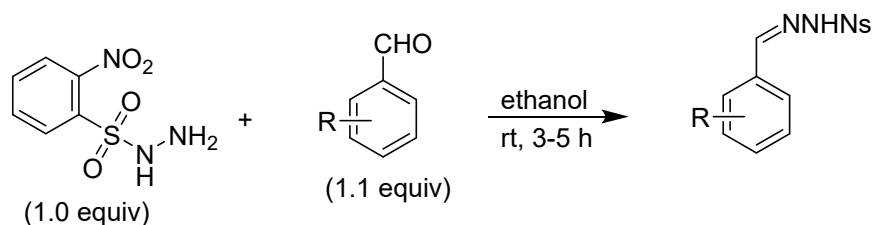
Yield: 25%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 2972, 1738, 1587, 1470, 1141, 753.

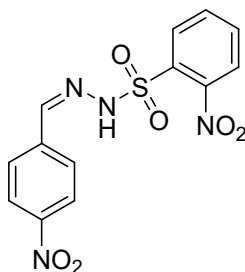
^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.49 (s, 2H), 7.36-7.29 (m, 5H), 7.11 (dd, J = 5.1, 1.1 Hz, 1H), 6.92 (dd, J = 5.1, 3.5 Hz, 1H), 6.71 (dd, J = 3.4, 1.2 Hz, 1H),
 $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 155.3, 145.8, 128.8, 128.4, 128.3, 127.9, 127.2, 126.4, 124.5, 123.2, 113.6
 HRMS: (ESI) m/z calcd for $\text{C}_{13}\text{H}_{10}\text{S}$, 199.0576 $[\text{M}+\text{H}]^+$; found 199.0575.

General synthesis method for *N*-nosylhydrazones:

To a stirred solution of NsNHNH_2 (3.3 mmol, 1 equiv) in ethanol (10 mL) carbonyl compounds (3.6 mmol, 1.1 equiv) were added and the mixture was stirred for 3-5 h at room temperature. After completion of the reaction, the mixture was evaporated under high vacuum and the resulting solid *N*-nosylhydrazones was separated using flash column chromatography with 75-90% yields. Similar procedure was followed for *N*-tosylhydrazones.



2-Nitro-*N'*-(4-nitrobenzylidene)benzenesulfonohydrazide:



Yield: 78%; yellow solid; R_f = 0.50 1:1 in Hexane/Ethylacetate.

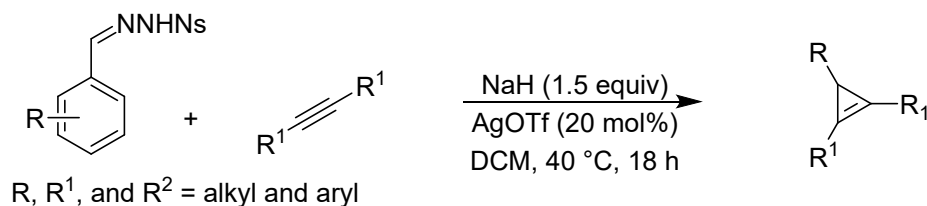
IR (ν_{max} , cm^{-1}): 3024, 2435, 1570, 1376, 959, 750.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.24-8.15 (m, 3H), 8.12-8.00 (m, 2H), 7.96-7.55 (m, 4H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 148.4, 145.6, 133.2, 131.1, 130.9, 129.4, 128.3, 127.5, 125.1, 124.7, 124.5, 123.9, 123.7.

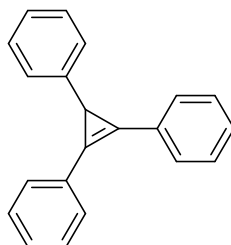
HRMS: (ESI) m/z calcd for $\text{C}_{13}\text{H}_{10}\text{N}_4\text{O}_6\text{S}$, 350.0321 $[\text{M}+\text{H}]^+$; found 351.0392.

General procedure for the cyclopropenation of internal alkynes:



A two neck round bottom flask was charged with *N*-nosylhydrazone of *p*-nitrobenzaldehyde (0.71 mmol, 1.0 equiv) and 60% NaH (0.73 mmol, 1.5 equiv) and was evacuated and filled with N₂ for three times, followed by addition of dry DCM (8.0 mL) via syringe. The resulting mixture was stirred at room temperature for 1 h. Then, diphenylacetylene (1.4 mmol, 2.0 equiv) and AgOTf (0.428 mmol, 20 mol %) were added and the system was stirred at 40 °C for 18 h. The progress of the reaction was monitored by TLC. When the reaction was completed, the crude reaction mixture was allowed to room temperature, and filtered through a short pad of silica gel with EtOAc as an eluent. The filtrate was evaporated under reduced pressure below 35 °C to leave a crude mixture, which was purified by column chromatography on silica gel (eluting with petroleum ether) to afford cyclopropene as a colorless oil with 20-30% yield. Other cyclopropenes also prepared using same procedure.

1,2,3-Triphenylcyclopropene (2ae):



Yield: 25%; yellow semi solid; *R*_f = 0.4 in 100% Hexane.

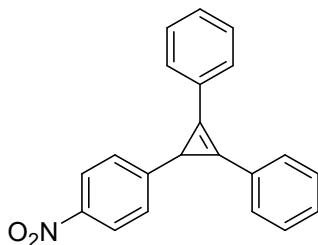
IR (ν_{max} , cm⁻¹): 3032, 1950, 1720, 1640, 1245, 1070.

¹H NMR (400 MHz, CDCl₃, 24 °C): δ 7.66 (d, *J* = 7.6 Hz, 4H), 7.39 (t, *J* = 8.4 Hz, 4H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.25-7.17 (m, 4H), 7.14-7.10 (m, 1H), 3.35 (s, 1H).

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C): δ 144.6, 130.0, 128.9, 128.7, 128.6, 128.3, 125.9, 125.5, 112.6, 24.5

HRMS: (ESI) *m/z* calcd for C₂₁H₁₆, 269.1325 [M+H]⁺; found 269.1321.

(3-(4-Nitrophenyl)cycloprop-1-ene-1,2-diyl)dibenzene (2ag):



Yield: 30%; yellow liquid; R_f = 0.20 in Hexane.

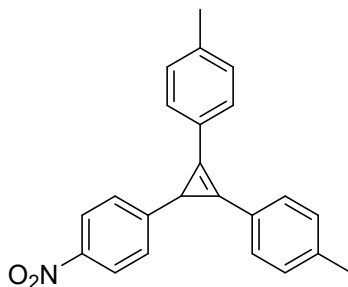
IR ($\nu_{\max}$, cm^{-1}): 3034, 2445, 1571, 1370, 870, 768.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.34 (d, J = 8.2 Hz, 2H), 7.64 (d, J = 7.3 Hz, 4H), 7.45 (t, J = 7.6 Hz, 4H), 7.41-7.34 (m, 4H), 3.34 (s, 1H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 153.5, 146.2, 130.0, 129.4, 129.1, 127.6, 126.4, 123.8, 111.3, 24.7.

HRMS: (ESI) m/z calcd for $\text{C}_{21}\text{H}_{15}\text{F}_4\text{NO}_2$, 313.1103 $[\text{M}+\text{H}]^+$; found 314.1169.

4,4'-(3-(4-Nitrophenyl)cycloprop-1-ene-1,2-diyl)bis(methylbenzene) (2ah):



Yield: 22%; yellow liquid; R_f = 0.20 in Hexane.

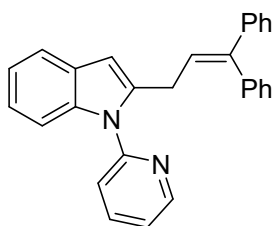
IR ($\nu_{\max}$, cm^{-1}): 3006, 2345, 1450, 1230, 900, 750.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.13 (d, J = 8.6 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 7.41 (d, J = 7.8 Hz, 2H), 7.36 (d, J = 8.6 Hz, 2H), 7.23 (d, J = 7.8 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 3.37 (s, 1H), 2.39 (s, 3H), 2.37 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.1, 140.6, 139.7, 131.9, 130.1, 129.9, 129.4, 126.8, 123.8, 115.9, 28.1, 21.8, 21.7.

HRMS: (ESI) m/z calcd for $\text{C}_{22}\text{H}_{14}\text{F}_4\text{NO}$, 384.1012 $[\text{M}+\text{H}]^+$; found 384.0992.

2-(3,3-Diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3a):



Yield: 91%; pale yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

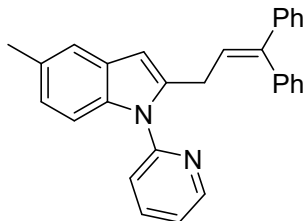
IR ($\nu_{\max}$, cm^{-1}): 3060, 2930, 1738, 1589, 1478, 1138, 766.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.53 (s, 1H), 7.77 (t, J = 8.7, Hz, 1H), 7.57 (d, J = 4.6, Hz, 1H), 7.35–7.27 (m, 5H), 7.25–7.20 (m, 4H), 7.16–7.10 (m, 6H), 6.53 (s, 1H), 6.15 (t, J = 8.1 Hz, 1H), 3.70 (d, J = 7.2 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 151.3, 149.7, 143.2, 142.6, 139.9, 139.5, 138.3, 137.5, 129.9, 128.6, 128.2, 128.1, 127.6, 127.3, 127.2, 125.5, 122.0, 121.9, 121.0, 120.8, 120.1, 110.3, 103.2, 28.8.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{22}\text{N}_2$, 387.1856 $[\text{M}+\text{H}]^+$; found 387.1857.

4-Bromo-2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3b):



Yield: 72%; Yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

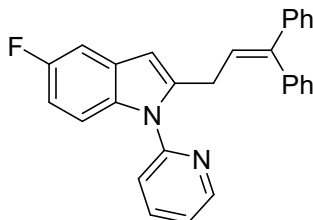
IR (ν_{max} , cm^{-1}): 3006, 2212, 1734, 1441, 1267, 753.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.52 (dd, J = 4.5, 2.1 Hz, 1H), 7.76 (dt, J = 8.6, 1.9 Hz, 1H), 7.35 (s, 1H), 7.32–7.28 (m, 4H), 7.25 (s, 1H), 7.24–7.20 (m, 4H), 6.95 (dd, J = 6.9, 1.3 Hz, 1H), 6.45 (s, 1H), 6.15 (t, J = 7.0 Hz, 1H), 3.69 (d, J = 7.3 Hz, 2H), 3.17 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 151.5, 149.6, 143.0, 142.6, 139.9, 139.5, 138.2, 135.7, 130.0, 129.9, 128.8, 128.2, 128.1, 127.5, 127.2, 127.1, 125.6, 123.3, 121.7, 120.7, 119.8, 109.9, 102.8, 28.7, 21.4

HRMS: (ESI) m/z calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2$, 401.2012 $[\text{M}+\text{H}]^+$; found 401.1999.

2-(3,3-Diphenylallyl)-5-fluoro-1-(pyridin-2-yl)-1H-indole (3c):



Yield: 73%; Yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

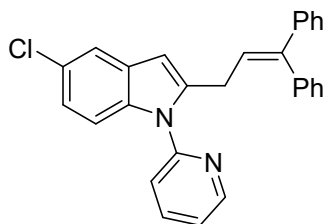
IR (ν_{max} , cm^{-1}): 2987, 1733, 1587, 1446, 1264, 756.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.54 (dd, J = 4.8, 1.2 Hz, 1H), 7.78 (dt, J = 7.9, 1.8 Hz, 1H), 7.36–7.20 (m, 11H), 7.18–7.10 (m, 4H), 6.86 (dt, J = 9.1, 2.6 Hz, 1H), 6.48 (s, 1H), 6.14 (t, J = 7.2 Hz, 1H), 3.67 (d, J = 7.5 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 151.2, 149.8, 143.5, 142.4, 141.5, 139.4, 138.5, 134.1, 129.9, 128.3, 128.2, 128.2, 127.5, 127.3, 127.2, 120.9, 111.2, 110.1, 109.7, 105.2, 105.0, 103.5, 103.1, 28.7.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{N}_2$, 405.1762 $[\text{M}+\text{H}]^+$; found 405.1759.

5-Chloro-2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3d):



Yield: 81 %; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

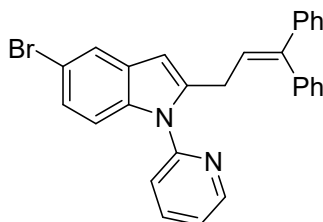
IR ($\nu_{\max}$, cm^{-1}): 3059, 2889, 1955, 1655, 1443, 1274, 701.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.54 (d, J = 2.1 Hz, 1H), 7.78 (t, J = 8.8 Hz, 1H), 7.52 (s, 1H), 7.34-7.21 (m, 10H), 7.17–7.06 (m, 5H), 6.40 (s, 1H), 6.13 (t, J = 9.2 Hz, 1H), 3.67 (d, J = 7.1 Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 151.0, 149.9, 143.6, 142.5, 141.4, 139.4, 138.5, 135.9, 129.9, 129.7, 128.7, 128.3, 128.2, 127.6, 127.4, 127.3, 126.4, 124.9, 122.4, 122.1, 120.9, 119.5, 111.5, 102.7, 28.7.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{ClN}_2$, 421.1466 $[\text{M}+\text{H}]^+$; found 421.1443.

5-Bromo-2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3e):



Yield: 90%; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

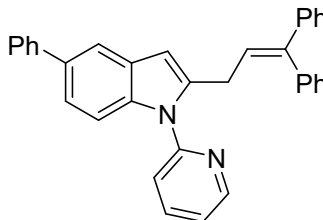
IR ($\nu_{\max}$, cm^{-1}): 3012, 2902, 1588, 1474, 1444, 1264, 749.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.53 (dd, J = 4.6, 0.9 Hz, 1H), 7.77 (dt, J = 7.9, 1.9 Hz, 1H), 7.68 (d, J = 3.0 Hz, 1H), 7.33-7.18 (m, 14H), 7.15–7.12 (m, 2H), 7.11–7.09 (m, 2H), 6.45 (s, 1H), 6.12 (dt, J = 7.5, 1.4 Hz, 1H), 3.66 (d, J = 7.3 Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 150.9, 149.8, 143.5, 141.2, 139.3, 138.5, 136.1, 130.3, 129.9, 128.3, 128.2, 127.8, 128.2, 127.6, 127.4, 127.3, 126.2, 124.9, 124.6, 122.6, 122.4, 120.9, 113.9, 111.8, 102.5, 28.6.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{BrN}_2$, 465.0961 $[\text{M}+\text{H}]^+$; found 467.0943.

2-(3,3-Diphenylallyl)-1-(pyrimidin-2-yl)-1H-indole (3f):

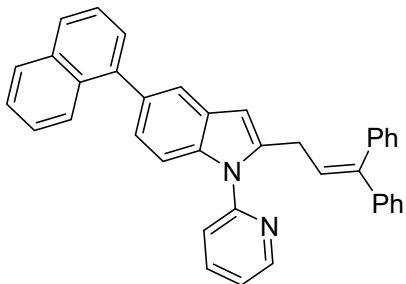


Yield: 78%; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 2988, 1653, 1470, 1262, 754.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.56 (dd, J = 4.8, 1.2 Hz, 1H), 7.25–7.78 (m, 2H), 7.64 (d, J = 7.6 Hz, 2H), 7.45–7.39 (m, 5H), 7.36–7.29 (m, 6H), 7.27–7.25 (m, 1H), 7.24–7.21 (m, 2H), 7.17–7.12 (m, 4H), 6.55 (s, 1H), 6.17 (t, J = 7.6 Hz, 1H), 3.72 (d, J = 7.4 Hz, 2H),
 $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 °C): δ 151.4, 149.8, 143.4, 140.7, 139.5, 138.4, 137.0, 134.4, 129.2, 128.8, 128.3, 128.2, 127.6, 127.4, 127.3, 127.2, 126.5, 125.4, 122.1, 121.8, 120.9, 118.7, 110.6, 103.6, 28.8.
 HRMS: (ESI) m/z calcd for $\text{C}_{34}\text{H}_{26}\text{N}_2$, 463.2169 $[\text{M}+\text{H}]^+$; found 463.2159.

2-(3,3-Diphenylallyl)-5-(naphthalen-1-yl)-1-(pyridin-2-yl)-1H-indole (3g):



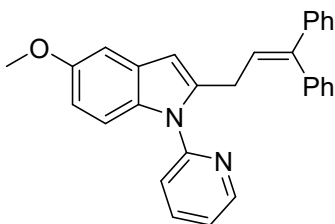
Yield: 65%; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

IR (ν_{max} , cm^{-1}): 3007, 2691, 1733, 1442, 1262, 758.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.50 (d, J = 4.1 Hz, 1H), 7.92 (d, J = 8.3 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.78–7.72 (m, 2H), 7.61 (s, 1H), 7.46–7.38 (m, 4H), 7.33–7.14 (m, 12H), 7.10–7.06 (m, 4H), 6.52 (s, 1H), 6.12 (dt, J = 8.1, 2.1 Hz, 1H), 3.67 (d, J = 6.6 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 151.4, 149.8, 143.3, 142.6, 141.4, 140.6, 139.5, 138.4, 136.8, 133.9, 133.5, 132.2, 130.0, 128.7, 128.6, 128.4, 128.3, 128.2, 127.6, 127.4, 127.3, 127.1, 126.7, 125.8, 125.7, 125.5, 125.4, 124.5, 122.1, 121.5, 121.0, 110.1, 110.0, 103.3, 28.8.
 HRMS: (ESI) m/z calcd for $\text{C}_{38}\text{H}_{28}\text{N}_2$, 513.2325 $[\text{M}+\text{H}]^+$; found 513.2311.

2-(3,3-diphenylallyl)-5-methoxy-1-(pyridin-2-yl)-1H-indole (3h):



Yield: 82%; white semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

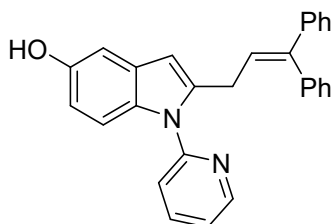
IR (ν_{max} , cm^{-1}): 2989, 1733, 1633, 1652, 1447, 1265, 754.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.52 (dd, J = 4.9, 1.9 Hz, 1H), 7.77 (t, J = 8.1 Hz, 1H), 7.35–7.20 (m, 10H), 7.19–7.10 (m, 4H), 7.05 (d, J = 2.4 Hz, 1H), 6.78 (dd, J = 8.8, 2.6 Hz, 1H), 6.47 (s, 1H), 6.15 (t, J = 7.5 Hz, 1H), 3.85 (s, 3H), 3.69 (d, J = 7.3 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 154.9, 151.4, 149.6, 143.1, 142.6, 140.4, 139.4, 138.3, 132.5, 129.6, 129.2, 128.2, 127.6, 127.3, 127.2, 125.5, 121.8, 120.6, 111.5, 111.2, 103.1, 102.2, 55.9, 28.8.

HRMS: (ESI) m/z calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2\text{O}$, 417.1961 $[\text{M}+\text{H}]^+$; found 417.1952

2-(3,3-Diphenylallyl)-1-(pyridin-2-yl)-1H-indol-5-ol (3i):



Yield: 32%; yellow semi solid; R_f = 0.5 in 2:8 EtOAc/Hexane.

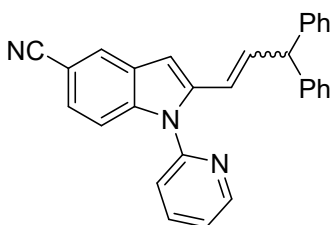
IR ($\nu_{\max}$, cm^{-1}): 3220, 2998, 2475, 1668, 1497, 756.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.54 (d, J = 4.8 Hz, 1H), 8.19 (d, J = 3.6 Hz, 1H), 7.79 (dt, J = 7.9, 1.8 Hz, 1H), 7.62 (t, J = 8.6 Hz, 1H), 7.36–7.30 (m, 6H), 7.27–7.20 (m, 7H), 7.16–7.10 (m, 4H), 6.95–6.91 (m, 3H), 6.84 (d, J = 8.4 Hz, 1H), 6.86 (s, 1H), 6.14 (t, J = 6.7 Hz, 1H), 3.69 (d, J = 7.2 Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 165.1, 151.3, 149.8, 147.9, 143.4, 142.6, 141.1, 139.2, 138.4, 135.0, 129.9, 129.4, 128.3, 128.2, 127.6, 127.3, 127.2, 125.3, 122.1, 120.9, 117.9, 116.2, 112.3, 111.2, 4, 28.8.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{23}\text{N}_2\text{O}$, 403.1805 $[\text{M}+\text{H}]^+$; found 403.1802.

(E) and (Z)-2-(3,3-Diphenylprop-1-en-1-yl)-1-(pyridin-2-yl)-1H-indole-5-carbonitrile (3j):



Yield: 48% E/Z isomer (1.2 : 1) ratio pale pink semi solid; R_f = 0.5 in 2:8 EtOAc/Hexane.

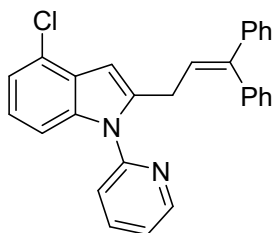
IR ($\nu_{\max}$, cm^{-1}): 3046, 2652, 1743, 1476, 1287, 790.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.11 (d, J = 4.8 Hz, 1H), 7.82 (d, J = 4.8 Hz, 0.8H), 7.79 (s, 1H), 7.64 (s, 0.8H), 7.31–7.21 (m, 6H), 7.20–7.11 (m, 10H), 7.08–6.94 (m, 10H), 6.92–6.87 (m, 2.7H), 6.65 (d, J = 7.3 Hz, 2H), 6.34 (s, 1H), 6.32 (s, 0.6H), 6.17 (s, 0.8H), 6.14 (d, J = 8.5 Hz, 1.6H), 6.03 (d, J = 10 Hz, 0.8H), 4.48–4.41 (m, 1.8H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 149.7, 149.5, 149.4, 149.2, 143.7, 143.6, 142.9, 142.6, 142.3, 142.2, 139.5, 139.2, 138.7, 138.4, 137.9, 137.8, 130.1, 129.9, 128.4, 128.3, 128.2, 128.1, 128.0, 127.6, 127.5, 127.4, 127.3, 127.0, 125.5, 125.4, 125.1, 124.9, 122.5, 12.4, 120.9, 120.6, 111.8, 111.6, 104.0, 103.9, 103.7, 103.7, 103.4, 43.3, 42.4.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{23}\text{N}_2\text{O}$, 403.1808 $[\text{M}+\text{H}]^+$; found 403.1800.

4-Chloro-2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3k):



Yield: 71%; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

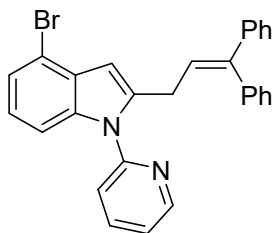
IR ($\nu_{\max}$, cm^{-1}): 2922, 1749, 1589, 1478, 1451, 1138, 742.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.54 (s, 1H), 7.79 (d, J = 3.9 Hz, 1H), 7.61-7.40 (m, 2H), 7.33-7.26 (m, 5H), 7.24-7.20 (m, 3H), 7.16-7.08 (m, 5H), 6.95 (s, 1H), 6.48 (s, 1H), 6.13 (d, J = 7.0 Hz, 2H), 3.65 (s, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 149.9, 143.6, 142.5, 140.8, 139.5, 138.6, 137.9, 129.9, 129.8, 128.3, 128.7, 128.2, 127.9, 127.6, 127.4, 127.3, 127.1, 125.1, 122.5, 121.4, 121.4, 121.0, 120.9, 110.6, 103.1, 28.7.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{ClN}_2$, 421.1466 $[\text{M}+\text{H}]^+$; found 421.1442.

4-Bromo-2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3l):



Yield: 80%; Yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

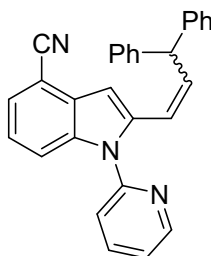
IR ($\nu_{\max}$, cm^{-1}): 2988, 1733, 1589, 1441, 1276, 752.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.49 (dd, J = 4.8, 1.5 Hz, 1H), 7.73 (dt, J = 9.2, 3.3 Hz, 1H), 7.41 (s, 1H), 7.36 (dd, J = 8.0, 1.8 Hz, 1H), 7.28-7.20 (m, 6H), 7.19-7.14 (m, 5H), 7.09-7.02 (m, 4H), 6.43 (s, 1H), 6.05 (dt, J = 8.8, 1.8 Hz, 1H), 3.58 (d, J = 7.0, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 150.8, 149.9, 143.6, 142.5, 140.7, 139.4, 138.7, 138.3, 129.9, 128.3, 128.2, 127.6, 127.4, 127.3, 124.9, 124.0, 122.5, 121.3, 121.0, 115.5, 113.4, 121.4, 103.1, 28.6.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{BrN}_2$, 465.0961 $[\text{M}+\text{H}]^+$; found 467.0932.

(E) and (Z)-2-(3,3-diphenylprop-1-en-1-yl)-1-(pyridin-2-yl)-1H-indole-4-carbonitrile (3m):



Yield: 71%; Mixture of E/Z (2:1) ratio, Yellow semi solid; R_f = 0.5 in 3:7 EtOAc/Hexane.

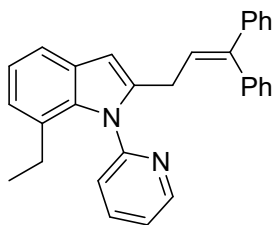
Spectra Z-isomer: IR ($\nu_{\max}$, cm^{-1}): 2988, 1733, 1589, 1441, 1276, 752.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.49 (s, 1H), 7.36-7.29 (m, 4H) 7.21-6.97 (m, 13H), 6.19-6.06 (m, 2H), 6.06 (d, J = 5.0 Hz, 1H), 4.52 (d, J = 6.5 Hz, 1H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 149.1, 148.9, 144.6, 142.8, 142.1, 139.5, 137.7, 136.6, 130.2, 129.9, 128.7, 128.5, 128.3, 127.6, 127.5, 125.7, 122.5, 121.5, 120.7, 118.7, 115.9, 102.1, 100.9, 44.0.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{N}_3$, 412.1808 $[\text{M}+\text{H}]^+$; found 412.1798.

2-(3,3-Diphenylallyl)-7-ethyl-1-(pyridin-2-yl)-1H-indole (3n):



Yield: 66%; white semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

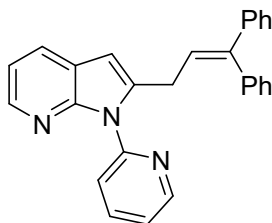
IR ($\nu_{\max}$, cm^{-1}): 3055, 2984, 1730, 1655, 1468, 1265, 753.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.47 (dd, J = 4.8, 1.3 Hz, 1H), 7.63 (dt, J = 8.2, 1.9 Hz, 1H), 7.36 (d, J = 7.7 Hz, 1H), 7.24-7.18 (m, 5H), 7.17-7.12 (m, 4H), 7.11-7.09 (m, 2H), 7.01-6.98 (m, 3H), 6.87 (d, J = 7.2 Hz, 1H), 6.42 (s, 1H), 6.08 (t, J = 6.9, 1H), 3.25 (d, J = 7.3 Hz, 2H), 2.09-2.04 (m, 2H), 0.84 (t, J = 8.6 Hz, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 153.3, 149.3, 143.1, 142.5, 140.8, 139.3, 137.8, 136.2, 129.9, 128.2, 127.6, 127.8, 127.2, 125.2, 124.0, 123.3, 122.3, 120.7, 118.0, 102.5, 28.4, 24.9, 14.6.

HRMS: (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2$, 415.2169 $[\text{M}+\text{H}]^+$; found 415.2170.

2-(3,3-Diphenylallyl)-1-(pyridin-2-yl)-1H-pyrrolo[2,3-b]pyridine(3o):



Yield: 81%; yellow semi solid; R_f = 0.5 in 2:8 EtOAc/Hexane.

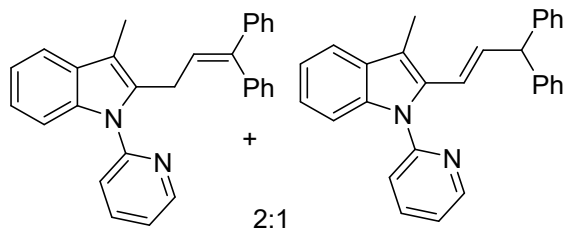
IR ($\nu_{\max}$, cm^{-1}): 2987, 1734, 1470, 1262, 752.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.53 (dd, J = 5.6, 1.8 Hz, 1H), 7.78 (dt, J = 8.5, 2.0 Hz, 1H), 7.68 (t, J = 1.4 Hz, 1H), 7.35-7.31 (m, 2H), 7.31-7.29 (m, 2H), 7.28-7.23 (m, 5H), 7.23-7.21 (m, 2H), 7.20-7.19 (m, 2H), 6.46 (s, 1H), 6.12 (t, J = 6.1, 1H), 3.66 (dd, J = 7.4, 0.6 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 150.9, 149.8, 142.4, 141.3, 139.4, 138.6, 136.2, 129.9, 128.6, 128.3, 128.2, 127.8, 127.8, 127.6, 122.6, 122.4, 120.9, 116.4, 113.9, 111.8, 102.6, 28.6.

HRMS: (ESI) m/z calcd for $C_{27}H_{21}N_3$, 388.1808 $[M+H]^+$; found 388.1805.

Mixture of 2-(3,3-Diphenylallyl)-3-methyl-1-(pyridin-2-yl)-1H-indole and (E)-2-(3,3-Diphenylprop-1-en-1-yl)-3-methyl-1-(pyridin-2-yl)-1H-indole (3p):



Yield: 52%; 2 : 1 ratio of allylated and vinylate products; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

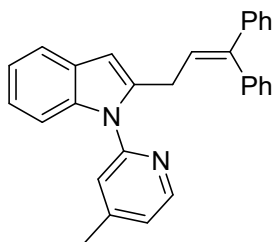
IR ($\nu_{\max}$, cm^{-1}): 2985, 1730, 1486, 1269, 750.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.58 (dd, J = 5.2, 1.8 Hz, 1H), 8.40 (dd, J = 4.7, 1.8 Hz, 0.3H), 7.69 (dt, J = 7.7, 1.9 Hz, 1H), 7.59–7.46 (m, 3H), 7.35–7.25 (m, 6H), 7.23–7.14 (m, 14H), 7.11–7.00 (m, 3H), 6.95–6.89 (m, 1H), 6.34 (d, J = 16.1 Hz, 1H), 6.24–6.20 (m, 1H), 6.18 (d, J = 7.7 Hz, 0.3H), 5.96 (t, J = 7.9 Hz, 0.3H), 4.85 (d, J = 7.3 Hz, 1H), 4.08–3.97 (m, 0.3H), 2.42 (s, 3H), 2.22 (s, 1H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.1, 151.8, 149.5, 149.4, 138.0, 137.9, 137.3, 137.2, 136.5, 133.1, 130.0, 129.8, 129.6, 128.7, 128.5, 128.3, 128.1, 127.4, 127.3, 127.2, 127.1, 127.0, 126.9, 126.5, 123.2, 122.2, 122.1, 121.6, 121.5, 121.4, 120.7, 120.1, 118.8, 118.1, 112.9, 110.8, 110.2, 54.9, 35.8, 10.1.

HRMS: (ESI) m/z calcd for $C_{29}H_{25}N_2$, 401.1012 $[M+H]^+$; found 401.2010.

2-(3,3-Diphenylallyl)-1-(4-methylpyridin-2-yl)-1H-indole (3q):



Yield: 64%; yellow semi liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

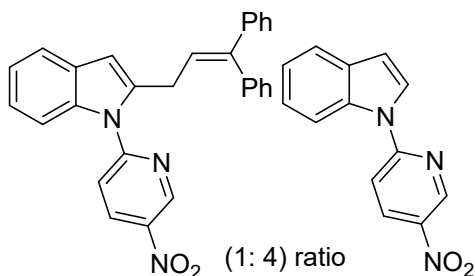
IR ($\nu_{\max}$, cm^{-1}): 3056, 1695, 1654, 1276, 1177, 702.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.38 (d, J = 5.0 Hz, 1H), 7.56 (dt, J = 5.0, 3.1 Hz, 1H), 7.38–7.27 (m, 4H), 7.24–7.20 (m, 3H), 7.16–7.10 (m, 7H), 7.05 (d, J = 5.0, 1H), 6.51 (s, 1H), 6.15 (t, J = 7.7 Hz, 1H), 3.68 (d, J = 7.4 Hz, 2H), 2.36 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 151.4, 149.8, 149.3, 143.1, 142.6, 139.9, 139.5, 137.6, 129.9, 128.6, 128.2, 128.1, 127.6, 127.2, 125.6, 123.3, 121.9, 121.8, 120.6, 120.1, 110.3, 102.9, 28.6, 21.1

HRMS: (ESI) m/z calcd for $C_{29}H_{24}N_2$, 401.2012 $[M+H]^+$; found 401.2001.

2-(3,3-Diphenylallyl)-1-(5-nitropyridin-2-yl)-1*H*-indole and 1-(5-Nitropyridin-2-yl)-1*H*-indole (3r):



Yield: 30%; Mixture of compounds (1:3) ratio; yellow solid; R_f = 0.5 in 3:7 EtOAc/Hexane.

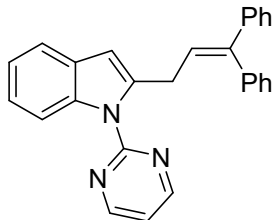
IR ($\nu_{\max}$, cm^{-1}): 3020, 1753, 1456, 1492, 760.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 9.37 (d, J = 2.7 Hz, 1H), 9.19 (d, J = 2.7 Hz, 0.3H), 8.54 (dt, J = 9.0, 2.9 Hz, 0.3H), 8.49 (dd, J = 8.8, 2.7 Hz, 0.3H), 7.74 (d, J = 7.7 Hz, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.59 (dd, J = 6.6, 1.0 Hz, 2H), 7.55 (d, J = 9.0 Hz, 0.3H), 7.51–7.48 (m, 0.8H), 7.39–7.31 (m, 4H), 7.28 (dt, J = 6.6, 1.0 Hz, 2H), 7.24–7.19 (m, 2H), 7.13–7.08 (m, 1.4H), 6.80 (d, J = 3.5 Hz, 1H), 6.62 (s, 1H), 6.10 (t, J = 7.1 Hz, 0.3H), 3.83 (d, J = 7.3 Hz, 0.6H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 155.9, 155.4, 145.6, 143.6, 142.4, 141.5, 140.3, 140.1, 139.2, 136.9, 135.4, 133.8, 133.5, 131.2, 129.9, 128.8, 128.7, 128.3, 128.2, 127.7, 127.6, 127.5, 125.3, 125.1, 124.5, 123.1, 123.0, 122.2, 121.6, 120.7, 119.1, 114.8, 112.2, 110.5, 109.1, 106.1, 110.2, 29.1.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{22}\text{N}_3\text{O}_2$, 432.1702 $[\text{M}+\text{H}]^+$; found 432.1704.

2-(3,3-Diphenylallyl)-1-(pyrimidin-2-yl)-1*H*-indole (3s):



Yield: 90%; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

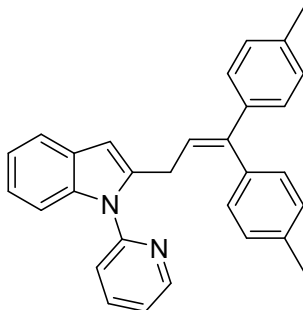
IR ($\nu_{\max}$, cm^{-1}): 3020, 2987, 1563, 1427, 1208, 755.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.65 (d, J = 4.8 Hz, 2H), 8.25 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 7.5 Hz, 1H), 7.36–7.32 (m, 2H), 7.30–7.29 (m, 1H), 7.24–7.21 (m, 4H), 7.20–7.17 (m, 5H), 7.04 (t, J = 5.0 Hz, 1H), 6.55 (s, 1H), 6.24 (t, J = 7.5 Hz, 1H), 4.03 (d, J = 7.0 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 158.2, 143.1, 142.9, 140.6, 139.8, 137.2, 130.0, 129.4, 128.3, 128.2, 127.7, 127.3, 127.2, 126.3, 122.8, 121.2, 117.1, 113.3, 106.5, 53.6, 30.7

HRMS: (ESI) m/z calcd for $\text{C}_{27}\text{H}_{21}\text{N}_3$, 388.1808 $[\text{M}+\text{H}]^+$; found 388.1811.

2-(3,3-Di-*p*-tolylallyl)-1-(pyridin-2-yl)-1*H*-indole (3t):



Yield: 95%; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

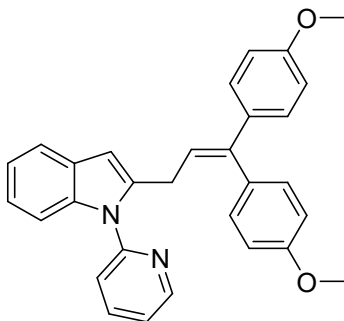
IR ($\nu_{\max}$, cm^{-1}): 2988, 2921, 1733, 1587, 1468, 1266, 755.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.54 (dd, J = 4.5, 1.0 Hz, 1H), 7.75 (dt, J = 8.4, 1.6 Hz, 1H), 7.57 (d, J = 7.6 Hz, 1H), 7.38–7.20 (m, 4H), 7.16–7.09 (m, 4H), 7.06–6.99 (m, 4H), 6.52 (s, 1H), 6.07 (t, J = 7.3 Hz, 1H), 3.69 (d, J = 7.3 Hz, 2H), 2.35 (s, 3H), 2.30 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 151.4, 149.7, 142.9, 140.2, 140.0, 138.3, 137.5, 136.9, 136.8, 136.6, 129.8, 128.9, 128.8, 127.8, 127.5, 124.4, 121.9, 121.9, 120.9, 120.7, 120.1, 116.4, 110.3, 103.1, 28.7, 21.3, 21.1

HRMS: (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2$, 415.2169 $[\text{M}+\text{H}]^+$; found 415.2165.

2-(3,3-Bis(4-methoxyphenyl)allyl)-1-(pyridin-2-yl)-1H-indole (3u):



Yield: 80%; yellow semi solid; R_f = 0.5 in 2:8 EtOAc/Hexane.

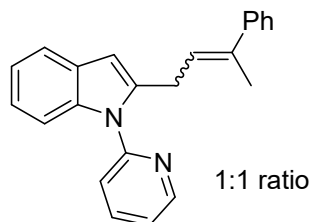
IR ($\nu_{\max}$, cm^{-1}): 3007, 2681, 1691, 1464, 1272, 756.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.57 (d, J = 4.8, Hz, 0.3H), 8.54 (dd, J = 4.9, 1.0 Hz, 1H), 8.21 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.0 Hz, 0.3H), 7.80–7.76 (m, 1.7H), 7.55–7.53 (m, 2H), 7.47–7.45 (m, 1.3H), 7.30–7.10 (m, 12H), 7.25 (d, J = 8.3 Hz, 0.5H), 6.91 (d, J = 8.0 Hz, 2.3H), 6.82–6.77 (m, 3.6H), 6.26 (t, J = 7.5 Hz, 1H), 3.88 (s, 0.7H), 3.83 (s, 3H), 3.78 (s, 3H), 3.76 (s, 1.5H), 3.61 (d, J = 7.0 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.7, 149.2, 149.0, 143.6, 141.7, 140.7, 138.4, 138.3, 135.8, 135.6, 132.5, 132.3, 131.2, 131.1, 130.6, 130.3, 129.4, 128.9, 128.7, 128.2, 125.2, 123.4, 123.1, 121.3, 121.0, 120.3, 119.7, 119.4, 119.0, 116.4, 114.3, 113.7, 113.5, 113.4, 113.3, 113.2, 112.8, 55.6, 55.5, 55.4, 55.3, 47.8, 27.7, 26.1

HRMS: (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2\text{O}_2$, 447.2067 $[\text{M}+\text{H}]^+$; found 447.2067.

(Z)-2-(3-Phenylbut-2-en-1-yl)-1-(pyridin-2-yl)-1H-indole and (E)-2-(3-Phenylbut-2-en-1-yl)-1-(pyridin-2-yl)-1H-indole(3v):



Yield: 96%; (1:1) ratio; yellow semi solid; R_f = 0.4 in 1:9 EtOAc/Hexane.

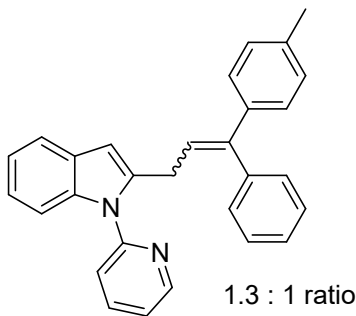
IR ($\nu_{\max}$, cm^{-1}): 2994, 2350, 1458, 1268, 775, 735.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.66 (dd, J = 8.3, 1.6 Hz, 1H), 8.52 (dd, J = 4.3, 1.8 Hz, 0.8H), 7.86 (dt, J = 7.8, 2 Hz, 1H), 7.76 (dt, J = 7.8, 2 Hz, 1H), 7.60-7.55 (m, 1.9H), 7.46 (d, J = 7.9 Hz, 1H), 7.36-7.18 (m, 14H), 7.17-7.09 (m, 6H), 6.52-6.47 (m, 1.9H), 5.83 (t, J = 7.8 Hz, 1H), 5.61 (t, J = 7.9 Hz, 1H), 3.79 (d, J = 7.1 Hz, 2H), 3.52 (d, J = 7.5 Hz, 2H), 2.03 (s, 2.5H), 1.97 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 151.6, 149.8, 149.6, 143.6, 141.3, 140.5, 139.9, 138.3, 138.2, 137.5, 137.4, 136.7, 128.6, 128.3, 128.2, 128.2, 127.9, 126.9, 125.8, 124.3, 123.3, 121.1, 121.9, 121.8, 121.2, 121.1, 120.8, 120.7, 120.1, 120.0, 110.3, 110.1, 102.9, 102.8, 27.9, 27.6, 25.5, 16.0

HRMS: (ESI) m/z calcd for $\text{C}_{23}\text{H}_{20}\text{N}_2$, 325.1699 $[\text{M}+\text{H}]^+$; found 325.1704.

(E)-2-(3-phenyl-3-(p-tolyl)allyl)-1-(pyridin-2-yl)-1H-indole and (Z)-2-(3-phenyl-3-(p-tolyl)allyl)-1-(pyridin-2-yl)-1H-indole (3w):



Yield: 78%; mixture of (E/Z) isomers (1.3:1) ratio; white semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

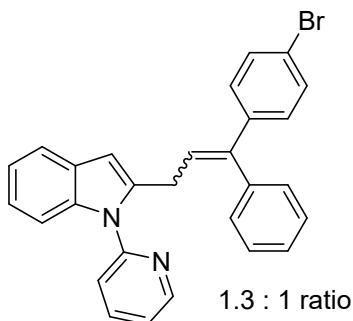
IR ($\nu_{\max}$, cm^{-1}): 2988, 2694, 1696, 1469, 1264, 756.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.47-8.44 (m, 1.4H), 7.75-7.68 (m, 2H), 7.53-7.48 (m, 1.5H), 7.32-7.10 (m, 14H), 7.09-7.02 (m, 9H), 6.97-6.93 (m, 4H), 6.45 (s, 1.5H), 6.04 (dt, J = 7.0, 1.3 Hz, 1.5H), 3.64-3.60 (m, 3H), 2.28 (s, 2H), 2.23 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 149.8, 143.2, 143.0, 142.9, 140.1, 139.7, 138.4, 138.3, 137.5, 136.5, 129.9, 129.8, 128.9, 128.6, 128.2, 127.9, 127.8, 127.6, 127.5, 127.2, 127.1, 125.2, 124.6, 122.0, 121.9, 121.8, 121.2, 121.0, 120.8, 120.3, 120.1, 119.5, 110.3, 103.2, 103.1, 28.7, 28.6, 21.3, 21.1

HRMS: (ESI) m/z calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2$, 401.1939 $[\text{M}+\text{H}]^+$; found 401.2012.

(E)-2-(3-(4-bromophenyl)-3-phenylallyl)-1-(pyridin-2-yl)-1H-indole and (Z)-2-(3-(4-bromophenyl)-3-phenylallyl)-1-(pyridin-2-yl)-1H-indole(3x):



Yield: 73%; mixture of (E/Z) isomers (1.3:1) ratio; white semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

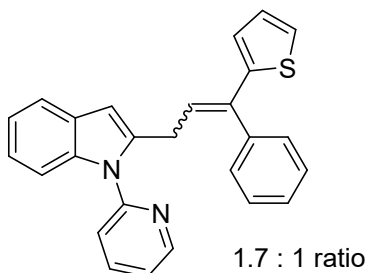
IR ($\nu_{\max}$, cm^{-1}): 3057, 2956, 1736, 1557, 1469, 1368, 1141, 698.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.54-8.51 (m, 1.3H), 7.83-7.76 (m, 1.5H), 7.61-7.55 (m, 1.5H), 7.46-7.42 (d, J = 7.6 Hz, 1.5H), 7.37-7.29 (m, 6H), 7.28-7.21 (m, 5H), 7.16-7.07 (m, 7H), 7.02-6.97 (m, 2.5H), 6.55-6.51 (m, 1.3H), 6.21-6.11 (m, 1.5H), 3.70-3.67 (m, 2.5H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 151.3, 149.8, 142.2, 142.0, 141.6, 139.6, 138.9, 138.4, 137.5, 131.7, 131.5, 131.3, 130.1, 129.9, 128.6, 128.4, 128.3, 128.2, 127.6, 127.5, 127.4, 127.3, 127.2, 126.2, 126.0, 122.1, 121.4, 121.1, 120.9, 120.2, 110.3, 103.3, 29.8, 28.7

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{BrN}_2$, 401.1939 $[\text{M}+\text{H}]^+$; found 467.0940.

(E)-2-(3-(4-bromophenyl)-3-phenylallyl)-1-(pyridin-2-yl)-1H-indole and (Z)-2-(3-(4-bromophenyl)-3-phenylallyl)-1-(pyridin-2-yl)-1H-indole(3y):



Yield: 51%; mixture of (E/Z) isomers (1.7:1) ratio; white semi solid; R_f = 0.5 in 2:8 EtOAc/Hexane.

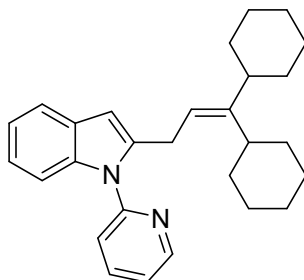
IR ($\nu_{\max}$, cm^{-1}): 3057, 2956, 1736, 1557, 1469, 1368, 1141, 698.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.56 (dd, J = 4.8, 1.9 Hz, 0.5H), 8.54 (dd, J = 4.9, 1.9 Hz, 1H), 7.81 (dt, J = 7.7, 1.6 Hz, 1.5H), 7.58 (dt, J = 4.4, 1.6 Hz, 1.6H), 7.39 (d, J = 7.9 Hz, 0.7H), 7.37-7.29 (m, 7H), 7.29-7.25 (m, 2H), 7.23-7.18 (m, 3.5H), 7.00 (dd, J = 5.1, 3.5 Hz, 0.5H), 6.91 (dd, J = 4.0, 1.1 Hz, 0.5H), 6.87 (dd, J = 4.7, 3.5 Hz, 1H), 6.57 (dd, J = 3.5, 1.2 Hz, 1H), 6.54 (s, 0.7H), 6.52 (d, J = 0.8 Hz, 1H), 6.23 (t, J = 7.3 Hz, 1H), 6.03 (t, J = 6.5 Hz, 0.5H), 3.91 (d, J = 7.4 Hz, 0.5H), 3.60 (d, J = 7.3 Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 138.4, 137.5, 137.2, 136.3, 129.7, 129.6, 128.7, 128.6, 128.4, 128.3, 128.2, 128.1, 128.0, 129.9, 127.8, 127.7, 127.6, 127.5, 127.3, 126.8, 126.4, 125.9, 125.5, 124.4, 124.2, 123.7, 122.1, 122.0, 121.9, 121.1, 120.9, 120.8, 120.7, 120.4, 120.1, 110.3, 103.3, 103.2, 29.0, 28.2.

HRMS: (ESI) m/z calcd for $C_{26}H_{20}SN_2$, 393.1420 $[M+H]^+$; found 393.1419.

2-(3,3-Dicyclohexylallyl)-1-(pyridin-2-yl)-1H-indole (3z):



Yield: 74%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane.

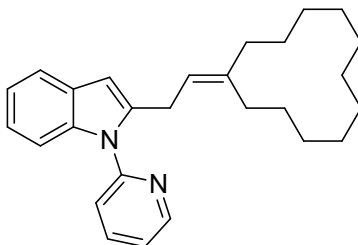
IR ($\nu_{\max}$, cm^{-1}): 3020, 2945, 1550, 1455, 1280, 750.

1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.55 (d, J = 4.7 Hz, 1H), 7.64 (t, J = 7.8 Hz, 1H), 7.49 (d, J = 8.4 Hz, 2H), 7.13-7.10 (m, 2H), 7.05 (t, J = 4.4 Hz, 2H), 6.46 (s, 1H), 5.44 (t, J = 7.7 Hz, 1H), 2.06-1.97 (m, 5H), 1.32-1.09 (m, 12H), 0.84-0.75 (m, 5H), 0.75-0.69 (m, 4H),

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 152.8, 149.1, 142.7, 137.8, 133.7, 132.2, 128.6, 127.5, 122.5, 121.5, 121.4, 121.0, 120.2, 111.3, 104.4, 31.7, 31.0, 30.3, 27.9, 22.7, 22.4, 14.0, 13.9,

HRMS: (ESI) m/z calcd for $C_{28}H_{34}N_2$, 399.2795 $[M+H]^+$; found 399.2802.

2-(2-Cyclododecylideneethyl)-1-(pyridin-2-yl)-1H-indole (3aa):



Yield: 40%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane.

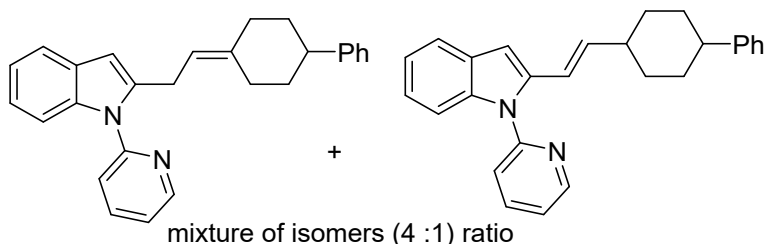
IR ($\nu_{\max}$, cm^{-1}): 3020, 2945, 1550, 1455, 1280, 750.

1H NMR (400 MHz, $CDCl_3$, 24 °C): δ 8.54 (d, J = 4.6 Hz, 1H), 8.22 (d, J = 8.2 Hz, 2H), 7.78 (t, J = 8.4 Hz, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.48 (s, 1H), 7.45 (d, J = 8.1 Hz, 1H), 7.30 (d, J = 6.9 Hz, 1H), 7.20 (t, J = 8.1 Hz, 1H), 7.11 (t, J = 6.6 Hz, 1H), 5.55 (t, J = 7.8 Hz, 1H), 3.54 (d, J = 6.9 Hz, 2H), 2.23 (t, J = 7.1 Hz, 2H), 2.12 (t, J = 6.6 Hz, 2H), 1.40-1.36 (m, 9H), 1.35-1.33 (m, 6H),

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 24 °C): δ 152.6, 149.1, 138.5, 135.2, 130.5, 126.1, 123.2, 121.3, 121.2, 120.2, 119.5, 114.7, 113.1, 105.6, 32.0, 28.8, 25.1, 24.8, 24.5, 24.4, 24.3, 24.2, 23.9, 23.6, 23.3, 22.4.

HRMS: (ESI) m/z calcd for $C_{27}H_{34}N_2$, 387.2795 $[M+H]^+$; found 387.2808.

2-(2-(4-Phenylcyclohexylidene)ethyl)-1-(pyridin-2-yl)-1*H*-indole and (E)-2-(2-(4-Phenylcyclohexyl)vinyl)-1-(pyridin-2-yl)-1*H*-indole (3ab):



Yield: 64%; yellow liquid; R_f = 0.50 in 1:9 EtOAc/Hexane.

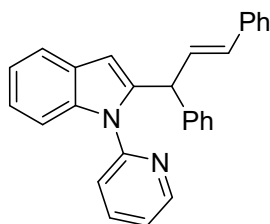
IR ($\nu_{\max}$, cm^{-1}): 3020, 2945, 1550, 1455, 1280, 750.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.59 (d, J = 4.4 Hz, 0.25H), 8.56 (d, J = 4.7 Hz, 1H), 7.76 (t, J = 7.5 Hz, 1H), 7.48 (d, J = 4.9 Hz, 1.3H), 7.40-7.33 (m, 1.5H), 7.29-7.16 (m, 5.5H), 7.15-7.01 (m, 8H), 6.75 (d, J = 14.5 Hz, 0.25H), 6.74 (d, J = 16.0 Hz, 0.25H), 6.38 (s, 1H), 6.31 (s, 0.25H), 5.18 (t, J = 8.0 Hz, 1H), 3.61-3.44 (m, 2H), 2.55 (t, J = 15 Hz, 2H), 2.22-2.00 (m, 2.5H), 1.89-1.65 (m, 4H), 1.40-1.17 (m, 2.4H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 151.6, 151.5, 149.7, 149.6, 149.1, 146.9, 146.7, 140.8, 140.2, 138.3, 137.5, 137.2, 135.7, 134.1, 130.6, 128.7, 128.5, 128.4, 127.0, 126.9, 126.2, 126.0, 125.9, 122.6, 122.0, 121.7, 121.6, 121.3, 120.7, 120.3, 120.1, 119.7, 118.2, 115.2, 110.8, 102.7, 101.5, 44.7, 40.2, 36.8, 35.8, 35.0, 34.4, 33.9, 30.7, 29.6, 29.4, 28.4, 26.1, 24.9.

HRMS: (ESI) m/z calcd for $\text{C}_{27}\text{H}_{26}\text{N}_2$, 378.5190 $[\text{M}+\text{H}]^+$; found 376.2175.

(E)-3-(1,3-diphenylallyl)-1-(pyridin-2-yl)-1*H*-indole (3ac):



Yield: 92%; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

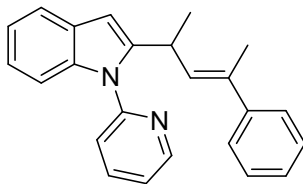
IR ($\nu_{\max}$, cm^{-1}): 3045, 2656, 1656, 1445, 1254, 756.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.44 (d, J = 4.6 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.67 (t, J = 8.0 Hz, 1H), 7.40-7.33 (m, 3H), 7.31-7.28 (m, 3H), 7.25-7.11 (m, 8H), 7.02 (t, J = 7.6 Hz, 2H), 6.67 (dd, J = 15.8, 7.4 Hz, 1H), 6.39 (d, J = 15.8 Hz, 1H), 5.07 (d, J = 7.2 Hz, 1H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 152.5, 149.0, 142.8, 138.4, 137.4, 135.9, 132.0, 131.1, 129.6, 128.7, 128.6, 128.6, 127.4, 126.6, 124.4, 123.4, 121.5, 121.1, 120.3, 119.9, 114.6, 113.1, 46.2

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{23}\text{N}_2$, 387.1856 $[\text{M}+\text{H}]^+$; found 387.1858.

(E)-2-(4-phenylpent-3-en-2-yl)-1-(pyridin-2-yl)-1*H*-indole (3ad):



Yield: 30%; yellow semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

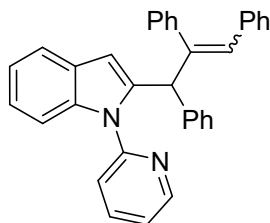
IR ($\nu_{\max}$, cm^{-1}): 2988, 2921, 1733, 1587, 1468, 1266, 755.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.54 (dd, J = 4.4, 1.0 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 7.79 (dt, J = 8.1, 2.0 Hz, 1H), 7.67 (d, J = 7.8 Hz, 1H), 7.56 (s, 1H), 7.48 (d, J = 7.8 Hz, 1H), 7.41 (d, J = 7.2 Hz, 2H), 7.31-7.26 (m, 4H), 7.22-7.17 (m, 2H), 7.12 (dt, J = 7.1, 0.7 Hz, 1H), 6.00 (d, J = 5.9 Hz, 1H), 4.18-4.12 (m, 1H), 2.21 (d, J = 1.2 Hz, 3H), 1.56 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.6, 149.0, 143.8, 138.3, 135.8, 132.8, 133.2, 129.8, 128.2, 126.8, 125.9, 124.3, 123.2, 121.9, 120.9, 119.9, 119.7, 114.5, 113.1, 30.7, 21.1, 16.1.

HRMS: (ESI) m/z calcd for $\text{C}_{24}\text{H}_{22}\text{N}_2$, 339.1856 $[\text{M}+\text{H}]^+$; found 339.1863.

1-(Pyridin-2-yl)-2-(1,2,3-triphenylallyl)-1H-indole (3ae):



Yield: 51%; yellow semi solid; R_f = 0.5 in 2:8 EtOAc/Hexane.

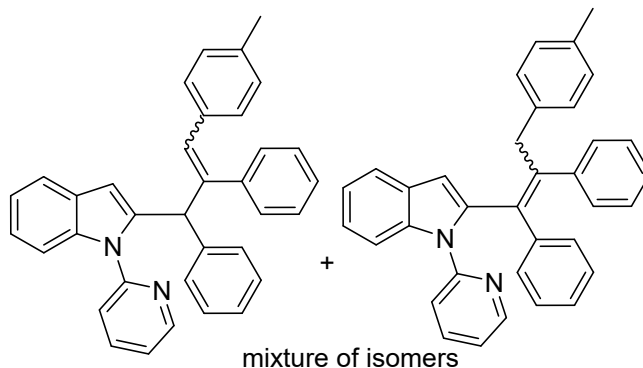
IR ($\nu_{\max}$, cm^{-1}): 3020, 2642, 1750, 1446, 1354, 690.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.20 (d, J = 2.6 Hz, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.27 (d, J = 5.6 Hz, 2H), 7.18-7.08 (m, 6H), 7.03-7.01 (m, 15H), 6.84 (d, J = 7.7 Hz, 1H), 5.10 (s, 1H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 150.6, 150.3, 148.7, 141.7, 139.2, 137.1, 129.3, 129.2, 128.6, 128.3, 128.1, 128.0, 127.8, 127.9, 126.9, 126.6, 126.5, 124.3, 121.8, 121.4, 121.3, 120.9, 118.1, 111.9, 52.3

HRMS: (ESI) m/z calcd for $\text{C}_{34}\text{H}_{27}\text{N}_2$, 463.2169 $[\text{M}+\text{H}]^+$; found 463.2165.

2-(1,2-Diphenyl-3-(p-tolyl)allyl)-1-(pyridin-2-yl)-1H-indole and 2-(2,3-Diphenyl-1-(p-tolyl)allyl)-1-(pyridin-2-yl)-1H-indole (3af):



Yield: 26%; 2 (1:1) : 1 (2:1) ratio; yellow semi liquid; R_f = 0.50 in 2:8 EtOAc/Hexane.

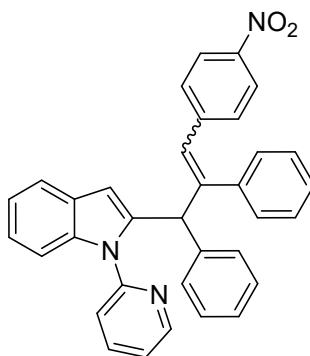
IR ($\nu_{\max}$, cm^{-1}): 3010, 2940, 1450, 1355, 1258, 754.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.62 (d, J = 4.9 Hz, 0.6H), 8.49 (d, J = 4.4 Hz, 1H), 8.43 (d, J = 3.8 Hz, 0.3H), 8.28 (d, J = 4.4 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.76 (d, J = 8.3 Hz, 1H), 7.66-7.57 (m, 3H), 7.56-7.49 (m, 3H), 7.46-7.39 (m, 2H), 7.38-7.30 (m, 5H), 7.18-6.87 (m, 38H), 6.80 (d, J = 7.8 Hz, 2H), 6.63 (d, J = 7.7 Hz, 1.3H), 6.58 (d, J = 7.6 Hz, 1H), 6.14 (s, 1.3H), 5.78 (s, 0.6H), 5.28 (s, 0.3H), 5.14 (s, 1H), 2.42 (s, 3H), 2.32 (s, 0.6H), 2.27 (s, 0.6H), 2.22 (s, 3H), 2.18 (s, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.0, 151.3, 150.6, .5, 150.4, 149.8, 149.1, 148.7, 145.7, 142.7, 141.8, 141.1, 140.6, 139.8, 138.4, 138.1, 137.4, 137.3, 137.2, 137.1, 136.5, 136.4, 135.9, 135.2, 134.2, 133.9, 133.5, 131.7, 130.7, 130.3, 130.0, 129.6, 129.2, 129.1, 128.8, 128.6, 128.5, 128.2, 127.8, 127.0, 126.9, 126.5, 126.4, 125.9, 124.3, 123.3, 122.3, 122.2, 122.1, 121.8, 121.4, 121.3, 121.2, 121.0, 120.8, 120.6, 120.7, 120.6, 119.9, 118.1, 117.1, 112.4, 111.8, 110.0, 106.6, 54.5, 52.8, 51.9, 21.5, 21.2, 21.1.

HRMS: (ESI) m/z calcd for $\text{C}_{35}\text{H}_{18}\text{N}_2$, 476.2252 $[\text{M}+\text{H}]^+$; found 476.2255.

2-(3-(4-Nitrophenyl)-1,2-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3ag):



Yield: 30%; (5:3) ratio; yellow liquid; R_f = 0.50 in 9:1 Hexane/Ethyl acetate.

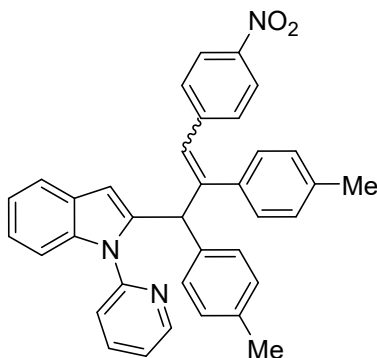
IR ($\nu_{\max}$, cm^{-1}): 3006, 2345, 1450, 1230, 900, 750.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.49 (dd, J = 4.8, 1.9 Hz, 1H), 8.27 (d, J = 9.0 Hz, 2H), 7.83 (d, J = 7.1 Hz, 1H), 7.76 (d, J = 8.5 Hz, 2H), 7.65 (dt, J = 8.5, 2.2 Hz, 2H), 7.51 (d, J = 9.0 Hz, 2H), 7.21-7.17 (m, 3H), 7.12-7.07 (m, 8H), 7.00-6.98 (m, 2H), 6.97 (m, 4H), 5.48 (s, 1H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 °C): δ 151.0, 150.7, 149.2, 144.2, 143.7, 139.8, 136.2, 135.5, 130.5, 129.4, 129.3, 128.6, 128.4, 128.3, 126.9, 126.8, 123.9, 122.6, 121.6, 121.2, 119.5, 117.1, 112.1, 111.2, 108.6, 55.1.

HRMS: (ESI) m/z calcd for $\text{C}_{34}\text{H}_{25}\text{N}_3\text{O}_2$, 507.2437 $[\text{M}+\text{H}]^+$; found 507.2437.

2-(3-(4-Nitrophenyl)-1,2-di-p-tolylallyl)-1-(pyridin-2-yl)-1H-indole (3ah):



Yield: 28%; yellow liquid; R_f = 0.50 in 9:1 Hexane/Ethyl acetate.

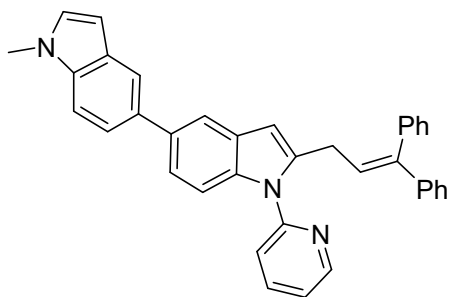
IR (ν_{max} , cm^{-1}): 3006, 2345, 1450, 1230, 900, 750.

^1H NMR (500 MHz, CDCl_3 , 24 °C): δ 8.51 (dd, J = 4.8, 1.8 Hz, 1H), 7.84 (d, J = 8.6 Hz, 2H), 7.70 (t, J = 7.9 Hz, 2H), 7.61 (dt, J = 8.1, 1.7 Hz, 1H), 7.19–7.15 (m, 2H), 7.06–7.02 (m, 8H), 6.93 (s, 1H), 6.88 (s, 1H), 6.63 (d, J = 8.6 Hz, 2H), 2.96 (s, 1H), 2.35 (s, 3H), 2.32 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 °C): δ 152.8, 151.8, 149.1, 145.7, 139.7, 139.6, 138.2, 137.8, 137.7, 137.2, 132.9, 130.6, 129.7, 128.3, 126.1, 124.3, 123.4, 123.1, 121.5, 121.1, 120.9, 120.0, 112.9, 111.5, 110.2, 107.0, 27.6, 21.5, 21.3.

HRMS: (ESI) m/z calcd for $\text{C}_{36}\text{H}_{29}\text{N}_3\text{O}_2$, 535.2260 $[\text{M}+\text{H}]^+$; found 535.257.

2-(3,3-Diphenylallyl)-1'-methyl-1-(pyridin-2-yl)-1H,1'H-5,5'-biindole (3ai):



Yield: 92%; white solid; R_f = 0.5 in 2:8 EtOAc/Hexane.

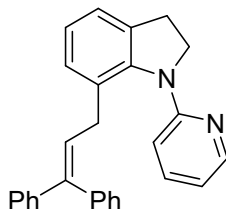
IR (ν_{max} , cm^{-1}): 3009, 2694, 1794, 1732, 1586, 1466, 1272, 753.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.54 (d, J = 4.5 Hz, 1H), 7.85 (d, J = 15.6 Hz, 2H), 7.78 (t, J = 8.2 Hz, 1H), 7.53 (d, J = 8.5 Hz, 1H), 7.48–7.40 (m, 2H), 7.39–7.28 (m, 5H), 7.28–7.20 (m, 5H), 7.19–7.12 (m, 4H), 7.05 (d, J = 2.8 Hz, 1H), 6.58 (s, 1H), 6.52 (d, J = 2.3 Hz, 1H), 6.18 (t, J = 7.7 Hz, 1H), 3.80 (s, 3H), 3.73 (d, J = 7.3 Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 151.4, 149.7, 143.2, 142.6, 140.4, 139.5, 138.3, 136.5, 136.0, 135.8, 135.8, 134.2, 130.0, 129.3, 129.2, 129.0, 128.2, 127.6, 127.3, 127.2, 125.6, 122.2, 121.9, 120.8, 119.5, 118.7, 110.4, 109.3, 103.5, 101.2, 33.0, 28.8.

HRMS: (ESI) m/z calcd for $\text{C}_{37}\text{H}_{29}\text{N}_{32}$, 516.2434 $[\text{M}+\text{H}]^+$; found 516.2437.

7-(3,3-Diphenylallyl)-1-(pyridin-2-yl)indoline (3aj):



Yield: 33%; yellow liquid; R_f = 0.52 in 1:9 EtOAc/Hexane.

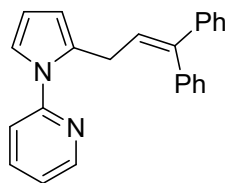
IR (ν_{max} , cm^{-1}): 3010, 2940, 1490, 1355, 1267, 740.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.24 (d, J = 5.1 Hz, 1H), 8.01 (d, J = 8.2 Hz, 1H), 7.48 (t, J = 8.0 Hz, 1H), 7.31 (t, J = 7.5 Hz, 2H), 7.25 (d, J = 7.0 Hz, 1H), 7.21-7.12 (m, 8H), 6.93 (d, J = 4.6 Hz, 1H), 6.66 (t, J = 7.8 Hz, 2H), 6.18 (t, J = 7.3 Hz, 1H), 3.94 (t, J = 8.6 Hz, 2H), 3.34 (d, J = 7.7 Hz, 2H), 3.09 (t, J = 8.5 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 148.1, 142.7, 142.0, 140.1, 137.3, 133.1, 131.9, 130.1, 130.0, 128.6, 128.4, 128.3, 128.2, 127.5, 127.4, 127.2, 127.0, 124.7, 114.2, 113.3, 108.6, 49.6, 35.5, 27.8.

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{24}\text{N}_2$, 388.1939 $[\text{M}]^+$; found 387.1854.

2-(2-(3,3-Diphenylallyl)-1H-pyrrol-1-yl)pyridine (6a):



Yield: 82%; yellow liquid; R_f = 0.5 in 2:8 EtOAc/Hexane.

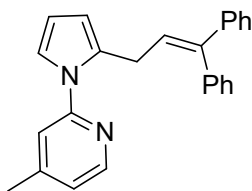
IR (ν_{max} , cm^{-1}): 2988, 2701, 1700, 1470, 1272, 705.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 8.41 (d, J = 3.4 Hz, 1H), 8.24 (d, J = 4.2 Hz, 0.2H), 7.68 (t, J = 7.3 Hz, 1H), 7.59 (t, J = 7.3 Hz, 0.3H), 7.37-7.26 (m, 5H), 7.23-7.10 (m, 14H), 7.08-6.99 (m, 3H), 6.25 (s, 1H), 6.19-6.13 (m, 1.5H), 6.10-5.99 (m, 1.4H), 3.68 (d, J = 6.8 Hz, 2H), 3.34 (d, J = 6.8 Hz, 0.4H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 148.9, 142.8, 139.8, 130.0, 128.3, 128.2, 128.1, 127.6, 127.5, 127.4, 127.2, 127.1, 126.8, 121.2, 120.9, 117.4, 109.9, 109.3, 28.8.

HRMS: (ESI) m/z calcd for $\text{C}_{24}\text{H}_{21}\text{N}_2$, 337.1699 $[\text{M}+\text{H}]^+$; found 337.1695.

2-(2-(3,3-Diphenylallyl)-1H-pyrrol-1-yl)-4-methylpyridine (6b):



Yield: 66%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

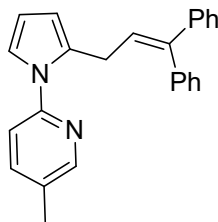
IR ($\nu_{\max}$, cm^{-1}): 3009, 2690, 1774, 1462, 1254, 756.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.27 (d, J = 5.1 Hz, 1H), 7.34–7.28 (m, 3H), 7.23–7.19 (m, 3H), 7.16–7.13 (m, 4H), 7.01–6.99 (m, 2H), 6.97 (d, J = 4.5 Hz, 1H), 6.23 (t, J = 3.4 Hz, 1H), 6.16–6.13 (m, 2H), 3.67 (d, J = 7.1 Hz, 2H), 2.33 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.9, 149.7, 148.6, 142.3, 139.0, 132.5, 130.1, 128.1, 127.7, 127.2, 127.3, 127.1, 127.0, 122.5, 121.0, 118.5, 109.7, 109.2, 28.7, 21.2.

HRMS: (ESI) m/z calcd for $\text{C}_{25}\text{H}_{22}\text{N}_2$, 351.1856 $[\text{M}+\text{H}]^+$; found 351.1853.

2-(2-(3,3-Diphenylallyl)-1H-pyrrol-1-yl)-5-methylpyridine (6c):



Yield: 54%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

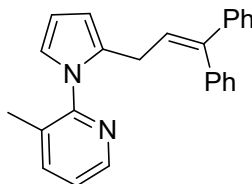
IR ($\nu_{\max}$, cm^{-1}): 3007, 2685, 1732, 1518, 1262, 1045, 755.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.27 (d, J = 4.8 Hz, 1H), 7.35–7.26 (m, 4H), 7.24–7.19 (m, 4H), 7.18–7.13 (m, 4H), 7.01–6.99 (m, 2H), 6.97 (d, J = 4.7 Hz, 1H), 6.23 (t, J = 3.4 Hz, 1H), 6.16–6.13 (m, 2H), 3.67 (d, J = 7.2 Hz, 2H), 2.33 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.9, 149.7, 148.6, 142.9, 142.3, 139.8, 132.4, 130.0, 128.2, 128.1, 127.6, 127.2, 127.2, 127.1, 122.5, 121.1, 118.4, 109.7, 109.1, 28.7, 21.3.

HRMS: (ESI) m/z calcd for $\text{C}_{25}\text{H}_{22}\text{N}_2$, 351.1856 $[\text{M}+\text{H}]^+$; found 351.1860.

2-(2-(3,3-Diphenylallyl)-1H-pyrrol-1-yl)-3-methylpyridine (6d):



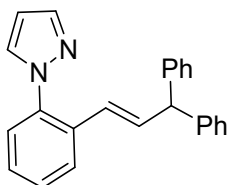
Yield: 48%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 3006, 1596, 1489, 1360, 1275, 756.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.22 (d, J = 1.6 Hz, 1H), 7.48 (dd, J = 7.9, 2.3 Hz, 1H), 7.35–7.28 (m, 4H), 7.23–7.20 (m, 3H), 7.17–7.13 (m, 5H), 7.17–7.13 (m, 5H), 7.07 (d, J = 8.2 Hz, 1H), 7.00 (t, J = 2.6 Hz, 1H), 6.23 (t, J = 3.4 Hz, 1H), 6.16–6.13 (m, 2H), 3.65 (d, J = 7.4 Hz, 2H), 2.32 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 150.6, 149.1, 142.3, 139.8, 138.8, 132.3, 130.9, 130.0, 128.2, 128.1, 127.6, 127.1, 126.9, 120.9, 117.3, 109.4, 109.0, 28.8, 17.9.
HRMS: (ESI) m/z calcd for $\text{C}_{25}\text{H}_{22}\text{N}_2$, 351.1856 $[\text{M}+\text{H}]^+$; found 351.351860.

(E)-1-(2-(3,3-Diphenylprop-1-en-1-yl)phenyl)-1H-pyrazole (7a):



Yield: 67%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

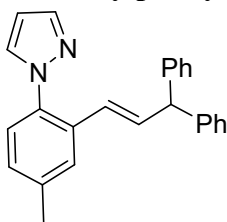
IR (ν_{max} , cm^{-1}): 2942, 2680, 1750, 1575, 1268, 1297, 754.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.66 (d, J = 1.8 Hz, 1H), 7.63 (dd, J = 7.5, 1.8 Hz, 1H), 7.51 (d, J = 2.4 Hz, 1H), 7.39 (dd, J = 7.4, 1.8 Hz, 1H), 7.35–7.31 (m, 2H), 7.30–7.26 (m, 4H), 7.24–7.16 (m, 6H), 6.59 (dd, J = 16.5, 7.8 Hz, 1H), 6.35 (t, J = 2.4 Hz, 1H), 6.18 (d, J = 15.6 Hz, 1H), 4.82 (d, J = 7.8 Hz, 1H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 143.2, 140.6, 138.5, 135.4, 133.0, 131.4, 128.7, 128.4, 128.1, 127.2, 127.0, 126.6, 126.3, 106.4, 54.4.

HRMS: (ESI) m/z calcd for $\text{C}_{24}\text{H}_{20}\text{N}_2$, 337.1699 $[\text{M}+\text{H}]^+$; found 337.1694.

(E)-1-(2-(3,3-Diphenylprop-1-en-1-yl)-4-methylphenyl)-1H-pyrazole (7b):



Yield: 47%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

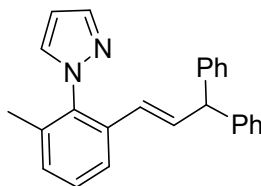
IR (ν_{max} , cm^{-1}): 2988, 2685, 1732, 1518, 1262, 1045, 755.

^1H NMR (400 MHz, CDCl_3 , 24 °C): δ 7.64 (d, J = 1.6 Hz, 1H), 7.47 (d, J = 2.3 Hz, 1H), 7.30–7.25 (m, 5H), 7.22–7.17 (m, 6H), 7.12 (d, J = 7.9 Hz, 1H), 6.56 (dd, J = 15.9, 7.7 Hz, 1H), 6.34 (t, J = 2.3 Hz, 1H), 6.14 (d, J = 15.7 Hz, 1H), 4.80 (d, J = 7.8 Hz, 1H), 2.38 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C): δ 143.3, 140.4, 138.3, 136.3, 135.0, 132.7, 131.5, 128.8, 128.7, 128.6, 127.3, 127.1, 126.6, 126.3, 106.3, 54.4, 21.3.

HRMS: (ESI) m/z calcd for $\text{C}_{25}\text{H}_{22}\text{N}_2$, 337.1699 $[\text{M}+\text{H}]^+$; found 337.1862.

(E)-1-(2-(3,3-Diphenylprop-1-en-1-yl)-6-methylphenyl)-1H-pyrazole (7c):



Yield: 61%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

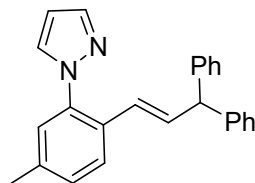
IR ($\nu_{\max}$, cm^{-1}): 3007, 2699, 1732, 1456, 1272, 756.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 7.64 (d, J = 1.8 Hz, 1H), 7.47 (dd, J = 2.4, 0.7 Hz, 1H), 7.43 (d, J = 1.4 Hz, 1H), 7.30–7.26 (m, 5H), 7.21–7.16 (m, 6H), 7.12 (dd, J = 7.9, 1.7 Hz, 1H), 6.56 (dd, J = 16.4, 7.7 Hz, 1H), 6.34 (t, J = 2.4 Hz, 1H), 6.14 (d, J = 15.9 Hz, 1H), 4.80 (d, J = 7.7 Hz, 1H), 2.38 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 143.4, 140.4, 138.3, 136.3, 135.1, 132.7, 131.5, 128.8, 128.5, 128.7, 127.3, 126.6, 126.3, 106.3, 54.4, 21.3.

HRMS: (ESI) m/z calcd for $\text{C}_{25}\text{H}_{22}\text{N}_2$, 351.1856 $[\text{M}+\text{H}]^+$; found 351.1859.

(E)-1-(2-(3,3-Diphenylprop-1-en-1-yl)-5-methylphenyl)-1H-pyrazole (7d):



Yield: 46%; yellow liquid; R_f = 0.5 in 1:9 EtOAc/Hexane.

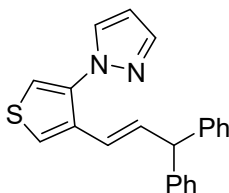
IR ($\nu_{\max}$, cm^{-1}): 3005, 2886, 1756, 1245, 1091, 755.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 7.65 (d, J = 1.6 Hz, 1H), 7.52 (d, J = 8.1 Hz, 1H), 7.49 (d, J = 2.5 Hz, 1H), 7.30–7.26 (m, 4H), 7.23–7.20 (m, 3H), 7.19–7.15 (m, 6H), 6.54 (dd, J = 15.6, 7.5 Hz, 1H), 6.34 (t, J = 2.5 Hz, 1H), 6.15 (d, J = 15.9 Hz, 1H), 4.80 (d, J = 7.7 Hz, 1H), 2.36 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 143.4, 140.5, 138.4, 138.3, 134.5, 131.4, 130.1, 129.9, 129.2, 128.7, 128.6, 128.1, 127.4, 127.0, 126.9, 126.8, 126.6, 106.3, 54.4, 21.1

HRMS: (ESI) m/z calcd for $\text{C}_{25}\text{H}_{22}\text{N}_2$, 351.1856 $[\text{M}+\text{H}]^+$; found 351.1853.

(E)-1-(4-(3,3-Diphenylprop-1-en-1-yl)thiophen-3-yl)-1H-pyrazole (7e):



Yield: 75%; yellow liquid; R_f = 0.52 in 1:9 EtOAc/Hexane.

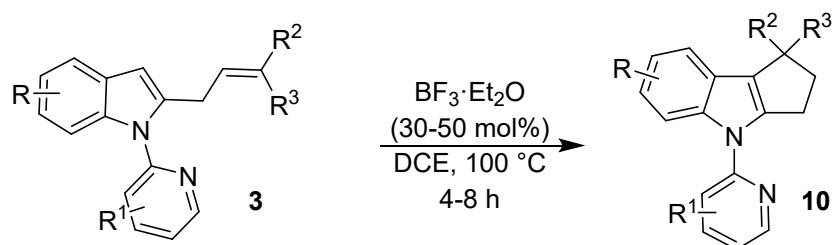
IR ($\nu_{\max}$, cm^{-1}): 3016, 2950, 1560, 1459, 1270, 680.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 7.64 (d, J = 2.4 Hz, 1H), 7.54 (d, J = 1.6 Hz, 1H), 7.39 (d, J = 7.1 Hz, 1H), 7.20–7.19 (m, 4H), 7.16–7.13 (m, 2H), 7.05 (t, J = 7.7 Hz, 2H), 6.94 (dd, J = 8.1, 0.8 Hz, 2H), 6.78 (d, J = 3.7 Hz, 1H), 6.55 (dd, J = 3.7, 1.5 Hz, 1H), 6.38 (d, J = 10.3 Hz, 1H), 6.31 (t, J = 2.4 Hz, 1H), 5.06 (dd, J = 10.5 Hz, 1H), 3.64 (d, J = 11.7 Hz, 1H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 145.5, 143.8, 143.2, 142.8, 142.2, 141.1, 140.8, 138.7, 129.5, 128.8, 128.6, 128.3, 127.9, 127.8, 127.7, 127.5, 127.4, 126.5, 125.1, 123.9, 122.6, 120.5, 114.1, 107.6, 37.6.

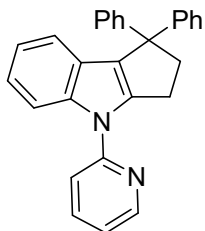
HRMS: (ESI) m/z calcd for $\text{C}_{22}\text{H}_{18}\text{N}_2\text{S}$, 342.1191 $[\text{M}+\text{H}]^+$; found 343.1261.

6. Synthesis of 10:



Reaction tube (15 mL) was charged with allylated indole **3** (0.13 mmol, 1.0 equiv) and dry DCE (2 mL). Subsequently, $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (30 mol%) was added and kept in preheated oil bath at 100°C . After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and quenched with NaHCO_3 solution, then extracted DCM and washed with water. The collected organic layer was concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the expected product **10** in good yield.

1,1-Diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (**10a**):



Yield: 81%; white solid; $R_f = 0.5$ in 1:9 EtOAc/Hexane.

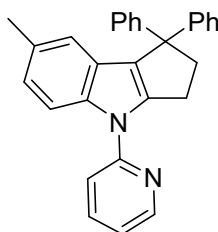
IR (ν_{max} , cm^{-1}): 3050, 2964, 1652, 1475, 1297, 1038, 736.

^1H NMR (400 MHz, CDCl_3 , 24°C): δ 8.47 (d, $J = 4.8$ Hz, 1H), 7.85 (d, $J = 8.2$ Hz, 1H), 7.67 (t, $J = 8.5$ Hz, 1H), 7.34 (d, $J = 7.3$ Hz, 1H), 7.32–7.27 (m, 4H), 7.24 (d, $J = 7.9$ Hz, 1H), 7.21–7.13 (m, 4H), 7.12–6.94 (m, 6H), 3.18 (t, $J = 7.2$ Hz, 2H), 3.09 (t, $J = 7.8$ Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24°C): δ 152.1, 149.3, 148.3, 143.8, 140.3, 138.3, 128.9, 127.6, 126.0, 125.6, 121.8, 121.3, 120.4, 119.5, 116.5, 112.8, 57.4, 47.4, 27.0

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{22}\text{N}_2$, 387.1856 $[\text{M}+\text{H}]^+$; found 387.1853.

1,1-Diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (**10b**):



Yield: 55%; white solid; $R_f = 0.5$ in 1:9 EtOAc/Hexane.

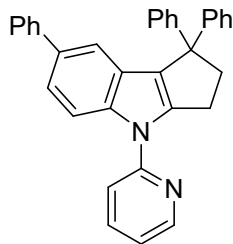
IR (ν_{max} , cm^{-1}): 3007, 1589, 1473, 1284, 1294, 752.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.59 (dd, J = 4.8, 1.2 Hz, 1H), 7.87-7.82 (m, 2H), 7.48 (d, J = 7.5 Hz, 1H), 7.43 (d, J = 8.1 Hz, 4H), 7.33–7.29 (m, 5H), 7.24-7.18 (m, 3H), 7.14 (s, 1H), 7.02 (d, J = 8.9 Hz, 1H), 3.31 (t, J = 7.7 Hz, 2H), 3.20 (t, J = 7.2 Hz, 2H), 2.40 (s, 3H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.3, 149.2, 148.4, 143.9, 138.5, 138.2, 130.6, 128.2, 128.7, 128.2, 128.1, 128.0, 127.2, 125.9, 125.8, 123.2, 120.1, 119.4, 116.2, 112.5, 57.4, 47.5, 27.9, 21.6.

HRMS: (ESI) m/z calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2$, 401.2012 $[\text{M}+\text{H}]^+$; found 401.2015.

1,1,7-Triphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10c):



Yield: 61%; white solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

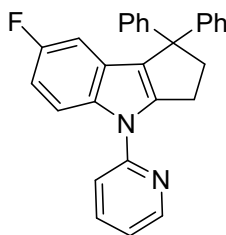
IR (ν_{max} , cm^{-1}): 2924, 1737, 1588, 1452, 701.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.59 (dd, J = 5.0, 1.6 Hz, 1H), 8.00 (d, J = 8.6 Hz, 1H), 7.83 (dt, J = 8.6, 1.8 Hz, 1H), 7.83 (dt, J = 8.2, 1.8 Hz, 1H), 7.43–7.38 (m, 7H), 7.28–7.25 (m, 4H), 7.21–7.17 (m, 3H), 3.31 (t, J = 7.3 Hz, 2H), 3.20 (t, J = 7.3 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.1, 149.3, 148.3, 144.5, 142.4, 139.8, 138.4, 134.7, 129.1, 128.9, 128.7, 128.3, 127.9, 127.8, 127.5, 126.6, 126.1, 122.2, 121.6, 120.7, 120.5, 117.9, 116.3, 113.2, 57.5, 47.4, 27.9

HRMS: (ESI) m/z calcd for $\text{C}_{34}\text{H}_{26}\text{N}_2$, 463.2169 $[\text{M}+\text{H}]^+$; found 463.2167.

7-Fluoro-1,1-diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10d):



Yield: 73%; white semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

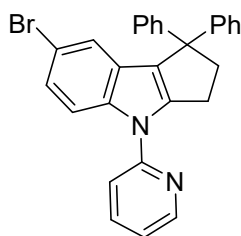
IR (ν_{max} , cm^{-1}): 3020, 2844, 1589, 1470, 1263, 1062, 702.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.55 (dd, J = 4.9, 1.5 Hz, 1H), 7.93 (dd, J = 8.9, 4.6 Hz, 1H), 7.79 (dt, J = 7.8, 1.8 Hz, 1H), 7.39 (d, J = 8.4 Hz, 1H), 7.39-7.32 (m, 4H), 7.29-7.24 (m, 4H), 7.20–7.16 (m, 3H), 6.94 (dd, J = 9.3, 2.6 Hz, 1H), 6.88 (dt, J = 9.5, 2.6 Hz, 1H), 3.26 (t, J = 7.3 Hz, 2H), 3.17 (t, J = 7.3 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 159.5, 157.6, 152.0, 149.2, 147.9, 145.3, 138.4, 136.7, 128.2, 127.8, 126.1, 120.5, 116.1, 113.9, 109.7, 104.6, 57.2, 47.2, 28.0, 27.9

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{FN}_2$, 405.1762 $[\text{M}+\text{H}]^+$; found 405.1764.

7-Bromo-1,1-diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10e):



Yield: 59%; brown solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

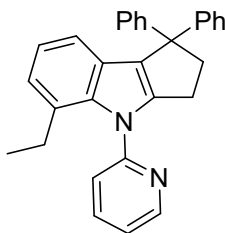
IR ($\nu_{\max}$, cm^{-1}): 3012, 2907, 1588, 1474, 1444, 1264, 749.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.57 (dd, J = 4.8, 1.5 Hz, 1H), 7.85 (d, J = 8.9 Hz, 1H), 7.81 (dt, J = 7.8, 2.0 Hz, 1H), 7.42 (d, J = 7.3 Hz, 1H), 7.32–7.27 (m, 4H), 7.24 (d, J = 7.9 Hz, 1H), 7.21–7.13 (m, 4H), 7.12–6.94 (m, 6H), 3.18 (t, J = 2.0 Hz, 1H), 7.40 (d, J = 8.3 Hz, 1H), 7.35–7.32 (m, 4H), 7.29–7.23 (m, 5H), 7.22–7.18 (m, 3H), 3.26 (t, J = 7.3 Hz, 2H), 3.17 (t, J = 7.3 Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 151.8, 149.3, 147.9, 145.1, 139.0, 138.5, 128.3, 127.8, 127.2, 127.0, 126.2, 124.7, 121.8, 120.8, 116.4, 114.7, 114.6, 57.4, 47.4, 27.8

HRMS: (ESI) m/z calcd for $\text{C}_{28}\text{H}_{21}\text{BrN}_2$, 465.0961 $[\text{M}+\text{H}]^+$; found 465.0949.

5-Ethyl-1,1-diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10f):



Yield: 72%; white semi solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

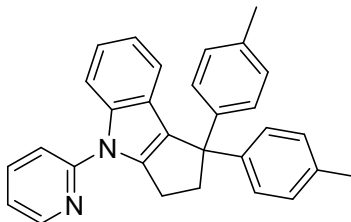
IR ($\nu_{\max}$, cm^{-1}): 2968, 2873, 1694, 1586, 1438, 1262, 1033, 750.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.58 (dd, J = 4.8, 1.7 Hz, 1H), 7.79 (dt, J = 8.2, 1.8 Hz, 1H), 7.39–7.35 (m, 4H), 7.30–7.20 (m, 8H), 7.19–7.13 (m, 3H), 7.03 (t, J = 7.6 Hz, 1H), 6.98 (d, J = 6.8 Hz, 1H), 7.12–6.94 (m, 6H), 3.18 (t, J = 2.0 Hz, 1H), 7.40 (d, J = 8.3 Hz, 1H), 7.35–7.32 (m, 4H), 3.12 (t, J = 7.0 Hz, 2H), 2.93 (t, J = 6.8 Hz, 2H), 2.42 (m, 2H), 0.97 (t, J = 7.8 Hz, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 153.2, 148.9, 148.5, 145.9, 139.6, 137.9, 129.1, 128.1, 127.9, 126.4, 126.2, 125.9, 122.3, 122.1, 121.2, 121.0, 117.4, 58.0, 47.2, 26.4, 25.8, 14.1

HRMS: (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2$, 415.2169 $[\text{M}+\text{H}]^+$; found 415.2151.

4-(Pyridin-2-yl)-1,1-di-p-tolyl-1,2,3,4-tetrahydrocyclopenta[b]indole (10g):



Yield: 70%; white solid; R_f = 0.5 in 1:9 EtOAc/Hexane.

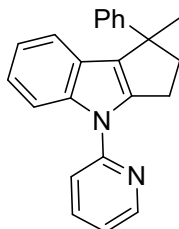
IR ($\nu_{\max}$, cm^{-1}): 2950, 2861, 1903, 1694, 1470, 1442, 812, 739.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.56 (dd, $J = 4.8, 1.3$ Hz, 1H), 7.94 (d, $J = 8.3$ Hz, 1H), 7.79 (dt, $J = 8.5, 1.9$ Hz, 1H), 7.43 (d, $J = 8.2$ Hz, 1H), 7.33 (d, $J = 7.7$ Hz, 1H), 7.30–7.24 (m, 4H), 7.18–7.12 (m, 2H), 7.11–7.00 (m, 5H), 3.26 (t, $J = 7.3$ Hz, 2H), 3.13 (t, $J = 7.3$ Hz, 2H), 2.29 (s, 6H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.2, 149.2, 145.5, 143.7, 140.3, 138.3, 135.4, 129.1, 128.4, 127.8, 125.6, 121.8, 121.2, 120.3, 119.5, 116.4, 112.8, 56.7, 47.4, 21.1

HRMS: (ESI) m/z calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2$, 415.2169 $[\text{M}+\text{H}]^+$; found 415.2170.

1-Methyl-1-phenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10h):



Yield: 80%; white semi solid; $R_f = 0.5$ in 1:9 EtOAc/Hexane.

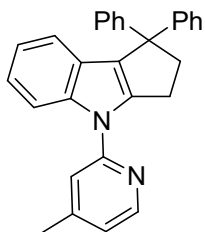
IR ($\nu_{\max}$, cm^{-1}): 2964, 1692, 1473, 1262, 1062, 729.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.58 (dd, $J = 4.9, 0.8$ Hz, 1H), 8.01 (d, $J = 8.3$ Hz, 1H), 7.81 (dt, $J = 8.1, 2.0$ Hz, 1H), 7.47 (d, $J = 8.3$ Hz, 1H), 7.41 (d, $J = 8.3$, 2H), 7.33 (d, $J = 7.7$ Hz, 1H), 7.27 (t, $J = 7.7$ Hz, 2H), 7.22–7.15 (m, 3H), 7.10 (t, $J = 7.6$ Hz, 1H), 3.17–3.12 (m, 2H), 2.76–2.64 (m, 2H), 1.81 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.4, 152.0, 149.3, 149.2, 143.6, 140.4, 138.3, 128.6, 128.3, 126.4, 125.5, 121.1, 120.2, 119.0, 116.2, 113.0, 47.8, 47.6, 27.9, 27.1

HRMS: (ESI) m/z calcd for $\text{C}_{23}\text{H}_{20}\text{N}_2$, 325.1699 $[\text{M}+\text{H}]^+$; found 325.1700.

4-(4-Methylpyridin-2-yl)-1,1-diphenyl-1,2,3,4-tetrahydrocyclopenta[b]indole (10i):



Yield: 54%; white semi solid; $R_f = 0.5$ in 1:9 EtOAc/Hexane.

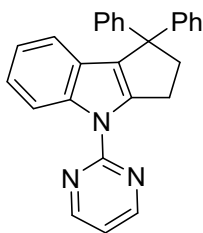
IR ($\nu_{\max}$, cm^{-1}): 2924, 1731, 1599, 1431, 1361, 702.

^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.58 (dd, $J = 4.8, 1.0$ Hz, 1H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.82 (dd, $J = 8.4, 2.0$ Hz, 1H), 7.47 (d, $J = 8.1$ Hz, 1H), 7.40 (d, $J = 8.2$ Hz, 2H), 7.33 (d, $J = 7.7$ Hz, 1H), 7.30–7.25 (m, 2H), 7.21–7.16 (m, 3H), 7.10 (dt, $J = 7.2, 1.2$ Hz, 1H), 3.17–3.12 (m, 2H), 2.75–2.63 (m, 2H), 2H), 1.81 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 152.4, 152.0, 149.3, 149.2, 143.6, 140.4, 138.3, 128.6, 128.3, 126.4, 125.5, 121.1, 120.2, 119.0, 116.2, 113.0, 47.8, 47.6, 27.9, 27.1

HRMS: (ESI) m/z calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2$, 401.2012 $[\text{M}+\text{H}]^+$; found 401.2013.

1,1-Diphenyl-4-(pyrimidin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10j):



Yield: 71%; white solid; R_f = 0.5 in 2:8 EtOAc/Hexane.

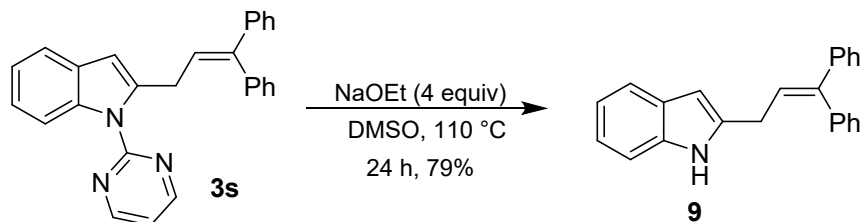
IR ($\nu_{\max}$, cm^{-1}): 3020, 2345, 1745, 1422, 1237, 752.

^1H NMR (500 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 8.82 (d, J = 8.4 Hz, 1H), 8.73 (d, J = 4.6 Hz, 2H), 7.33 (d, J = 7.7 Hz, 4H), 7.34-7.26 (m, 7H), 7.22 (t, J = 7.9 Hz, 2H), 7.17 (t, J = 7.9 Hz, 1H), 7.06 (t, J = 7.9 Hz, 1H), 3.62 (t, J = 6.8 Hz, 2H), 3.22 (t, J = 6.6 Hz, 2H),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 158.6, 158.0, 148.4, 144.3, 140.4, 1129.2, 128.1, 128.0, 126.6, 126.0, 122.5, 122.2, 119.2, 116.8, 115.9, 57.1, 47.5, 30.6.

HRMS: (ESI) m/z calcd for $\text{C}_{27}\text{H}_{21}\text{N}_3$, 388.1808 $[\text{M}+\text{H}]^+$; found 388.1810.

7. Removal of directing group: Synthesis of 9:



Compound **3s** (100 mg, 0.28 mmol) and NaOEt (76.6 mg, 1.12 mmol) were stirred in dry DMSO (3.0 ml) at 110 $^\circ\text{C}$ under N_2 for 24 h. Progress of the reaction was monitored by TLC. Once it completed, the reaction mixture was cooled to room temperature, the solvent was removed through reduced pressure and the residue was purified by silica gel chromatography using EA/Hexane (2: 8) as an eluent to afford compound **9** (68 mg, 79%).

Yield: 79%; Yellow semi liquid; R_f = 0.5 in 2:8 EtOAc/Hexane.

IR ($\nu_{\max}$, cm^{-1}): 3046, 2652, 1740, 1475, 1280, 752.

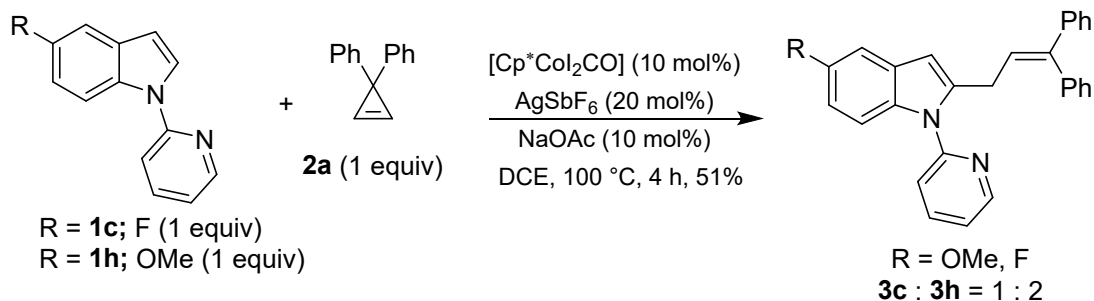
^1H NMR (400 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 7.50 (d, J = 7.9 Hz, 1H), 7.35-7.28 (m, 3H), 7.26-7.16 (m, 10H), 7.13 (t, J = 7.3 Hz, 1H), 6.39 (s, 1H), 6.28 (t, J = 8.2 Hz, 1H), 3.61 (d, J = 6.8 Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 $^\circ\text{C}$): δ 154.2, 143.9, 142.4, 139.5, 139.4, 135.7, 129.9, 128.3, 128.2, 127.5, 127.4, 127.3, 124.5, 122.5, 121.2, 120.4, 111.0, 103.7, 28.2.

HRMS: (ESI) m/z calcd for $\text{C}_{23}\text{H}_{19}\text{N}$, 332.1410 $[\text{M}+\text{Na}]^+$; found 332.2013.

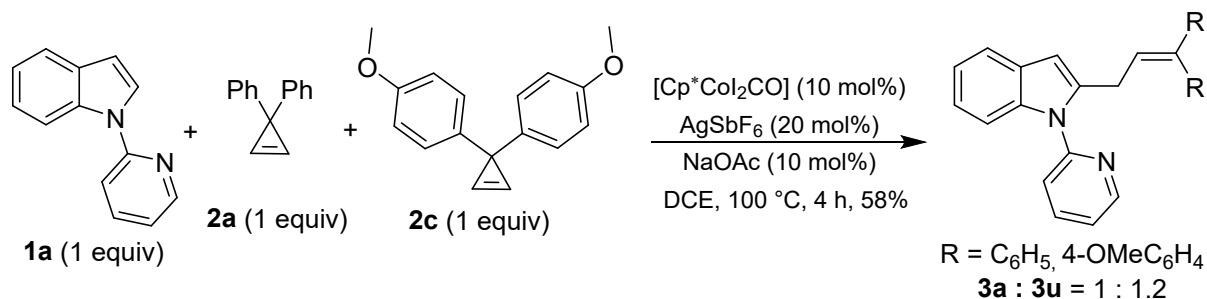
8. Control Experiments:

8.1 Intermolecular competitive experiment with 1:



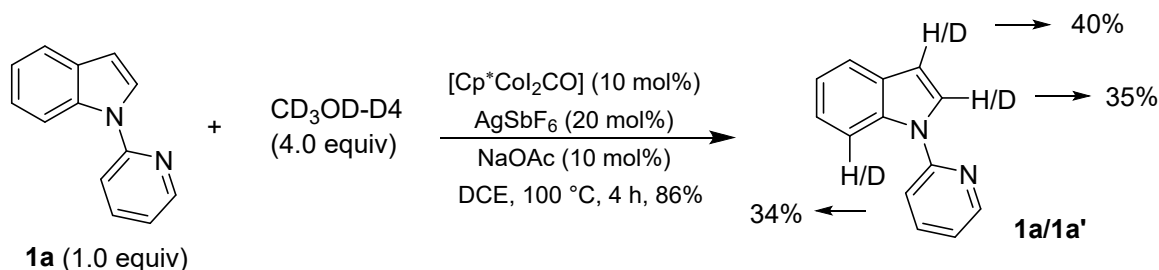
Following the general procedure, expected products **3c** and **3h** were isolated in 51% yield in 1: 2 ratio.

8.2 Intermolecular competitive experiment with 2:



Following the general procedure, expected products **3a** and **3u** were isolated in 58% yield in 1: 1.2 ratio.

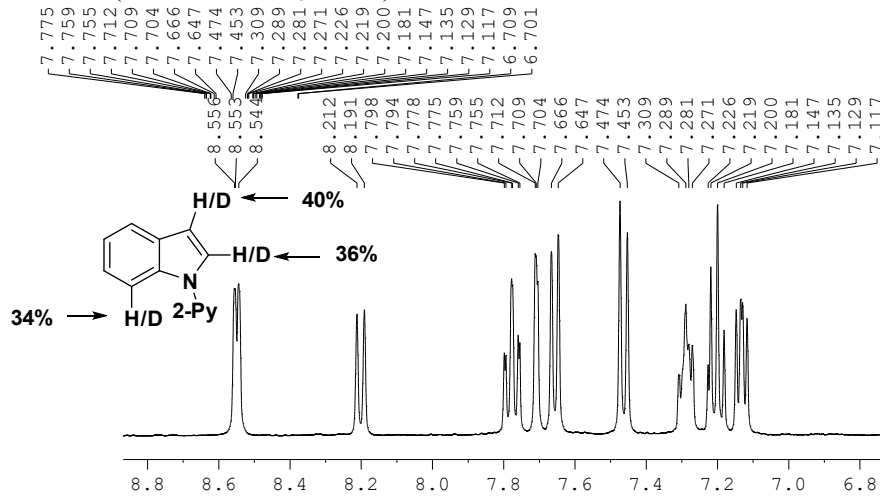
8.3 Deuterium exchange experiment:



1-(Pyridin-2-yl)-1*H*-indole **1a** (50 mg) (1 equiv), $[\text{Cp}^*\text{CoI}_2\text{CO}]$, (10 mol %), NaOAc (10 mol %) and AgSbF₆ (20 mol%) were taken in a 15 mL Schlenk tube. DCE (2 mL) was added to the reaction mixture, followed by methanol-*d*₄ (4.0 equiv) was added to the reaction tube. The reaction was allowed to stir at ambient temperature for 4 hours. After 4 hours, the reaction was diluted with DCM, filtered through celite, and the filtrate was concentrated. The crude residue was purified by column chromatography using hexane: ethylacetate (1: 9). The recovered **1a** (86%) had deuterium incorporation at C2, C3, and C7 in 35%, 40%, and 34%, respectively.

Deuterium NMR of 1a'

¹H NMR (400 MHz, CDCl₃, 24 °C):

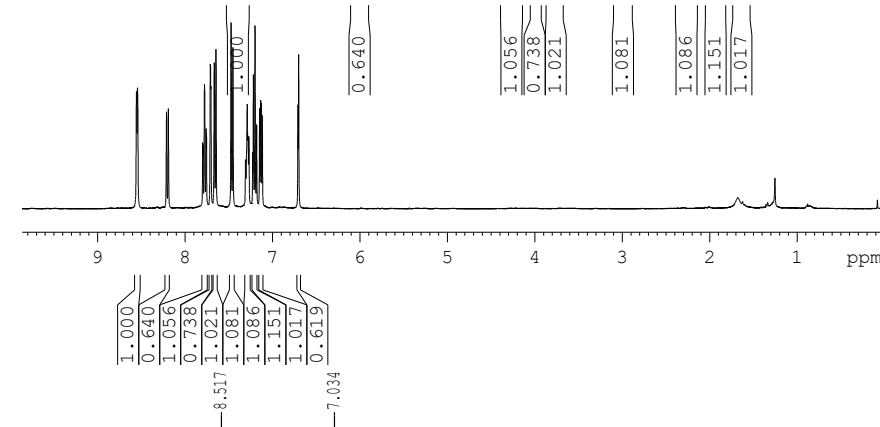


Current Data Parameters
NAME ksr deut ind
EXPNO 379
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190622
Time 9.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300232 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

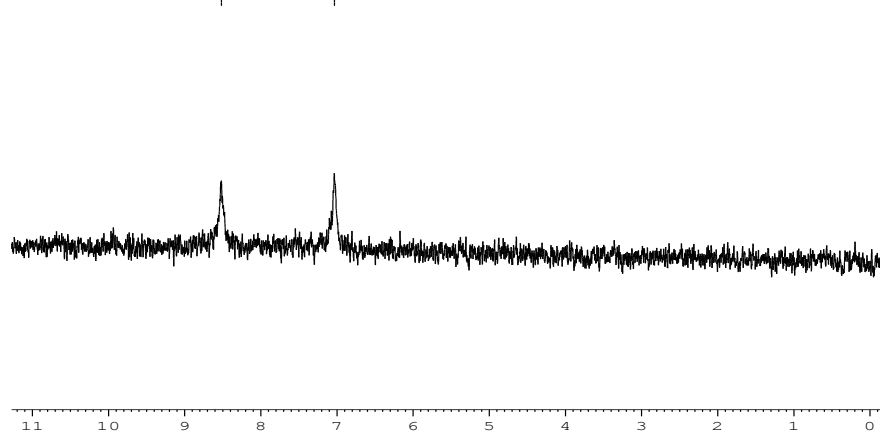


Current Data Parameters
NAME spa
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210611
Time 11.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg2h
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 921.376 Hz
FIDRES 0.014059 Hz
AQ 35.5642014 sec
RG 5.06
DW 542.667 usec
DE 6.50 usec
TE 302.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

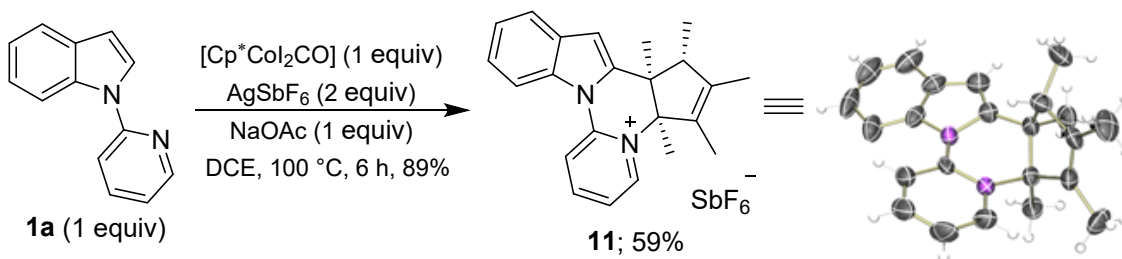
===== CHANNEL f1 =====
SFO1 76.7764539 MHz
NUC1 2H
P1 530.00 usec
PLW1 1.79999995 W

F2 - Processing parameters
SI 65536
SF 76.7760491 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



9. Stoichiometric experiments:

9.1 Synthesis of pyridinium salt **11**:



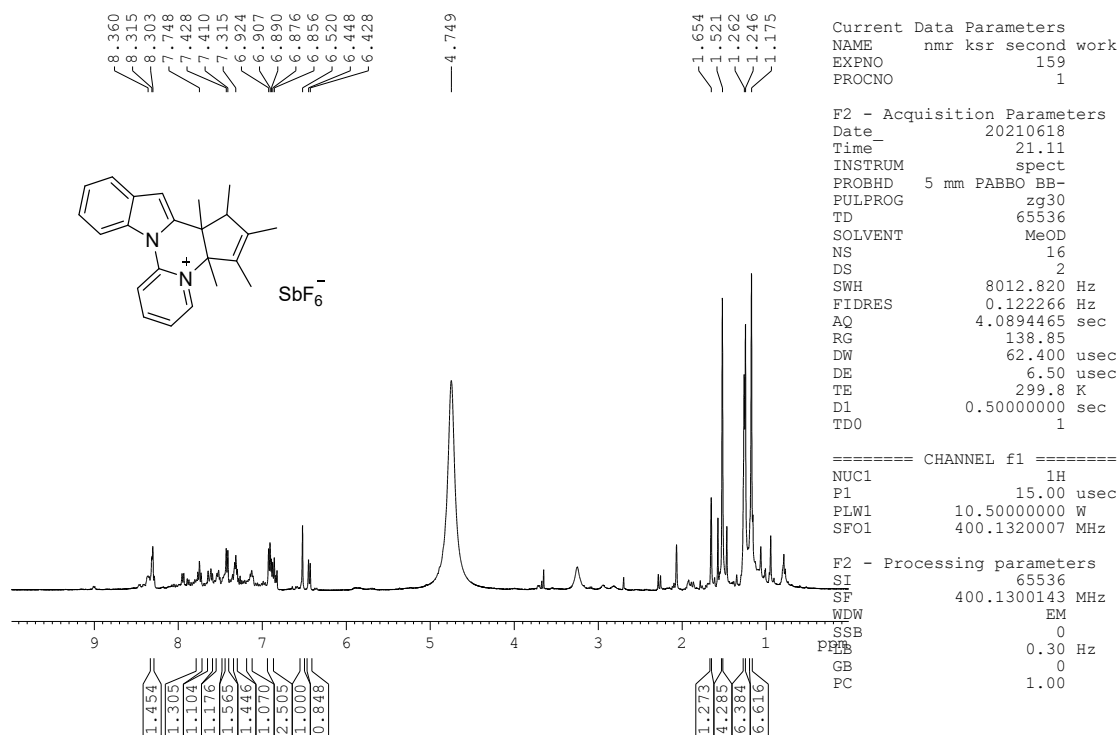
Oven-dried Schlenk tube was charged with **1a** (1 equiv, 0.26 mmol), NaOAc (1 equiv), AgSbF_6 (2 equiv) and $[\text{Cp}^*\text{CoI}_2\text{CO}]$ (1 equiv), then 4 mL of dry DCE was added. The charged schlenk tube's inner atmosphere was made inert through repeated (thrice) evacuation and refilling with nitrogen. The reaction tube stirs at $100\text{ }^\circ\text{C}$ in preheated oil-bath for 6 hours. After 6 h, the reaction was cooled to room temperature and solvent was removed under vacuum. The remaining residue was washed with dry hexane ($2 \times 10\text{ mL}$) under an inert atmosphere. The remaining residue was dissolved in dry DCM (25 mL) and the resulting reaction solution was filtered under argon atmosphere using sintered filter stick setup. The solvent was removed under vacuum to yield (98 mg, 59%) as a dark brown solid. Furthermore, compound **11** was confirmed by single crystal XRD.

Chemical formula of complex: $(\text{C}_{23}\text{H}_{25}\text{F}_6\text{N}_2\text{Sb}) [\text{M}^+]$

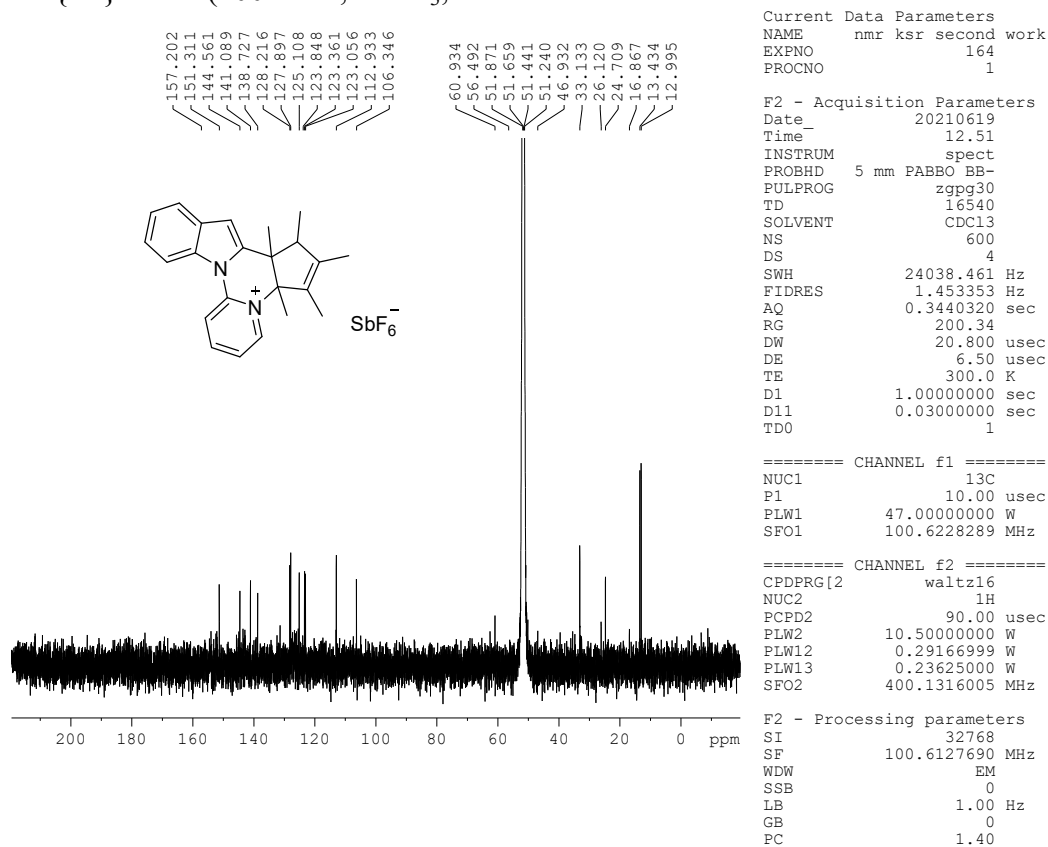
Calculated m/z: 564.0960

Found: 564.0957

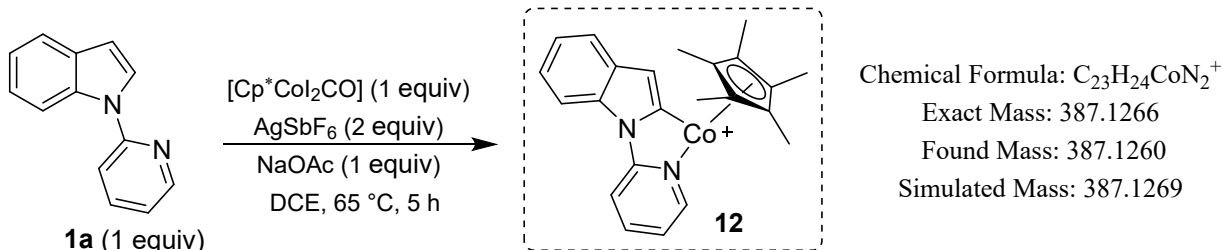
^1H NMR (400 MHz, MeOH- d_4 , 24 °C):



$^{13}\text{C}\{^1\text{H}\}$ NMR (400 MHz, CDCl_3 , 24 °C):

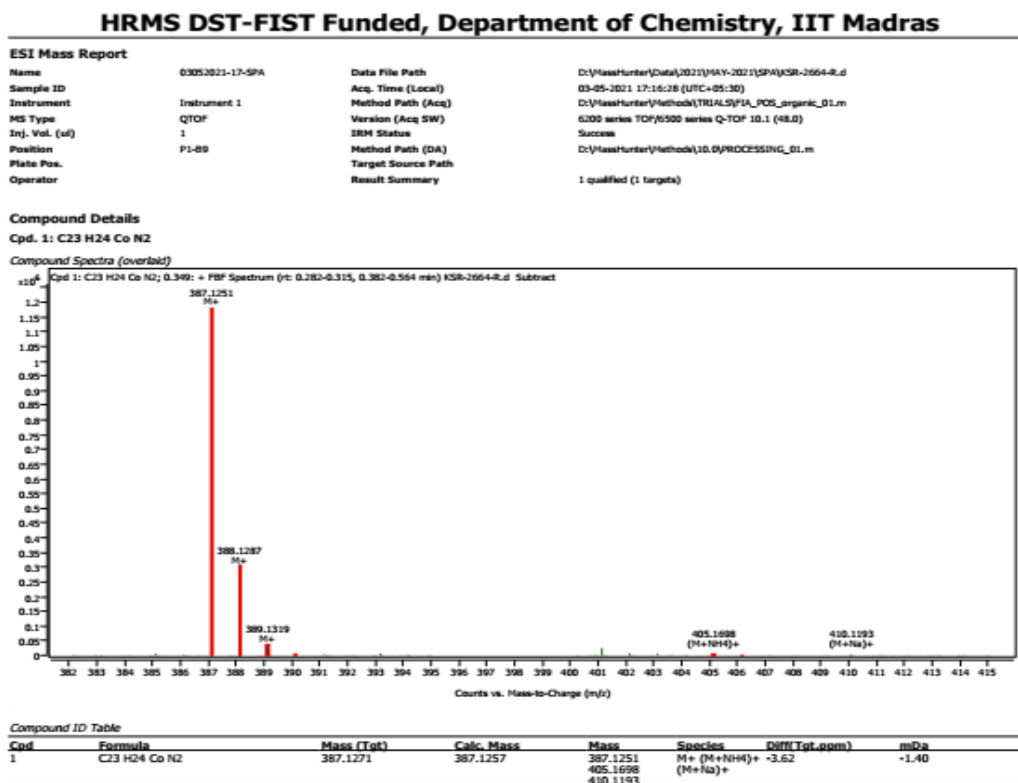


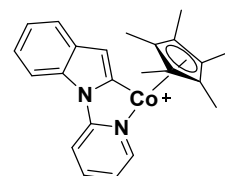
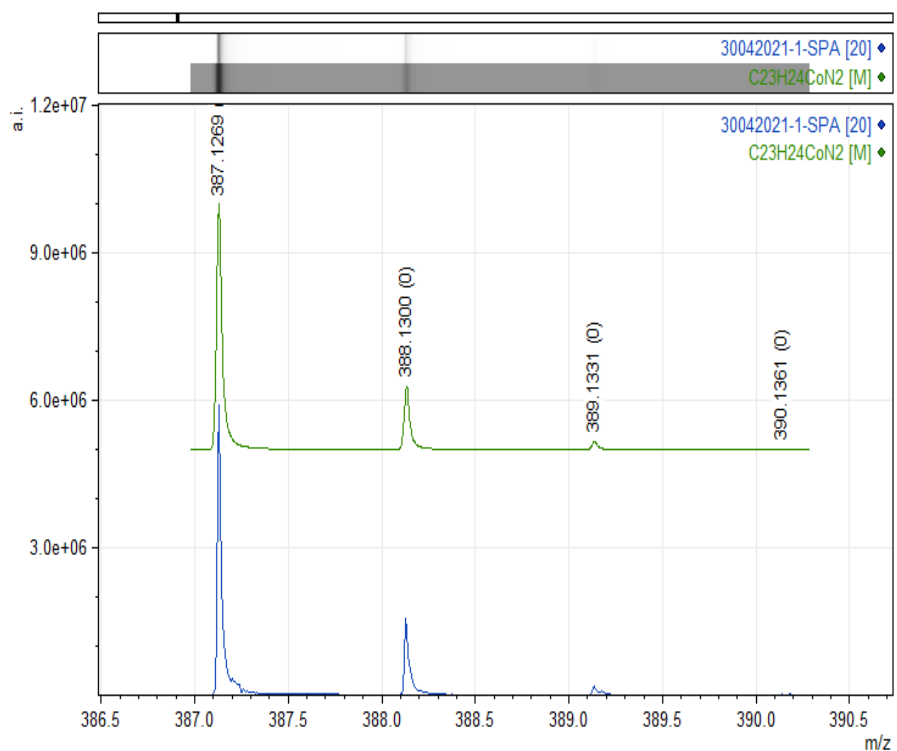
9.3 Preparation of complex 12:



Oven-dried Schlenk tube was charged with **1a** (1 equiv, 0.26 mmol), NaOAc (1 equiv), AgSbF₆ (2 equiv) and [Cp*CoI₂CO] (1 equiv), then 4 mL of dry DCE was added. The charged schlenk tube's inner atmosphere was made inert through repeated (thrice) evacuation and refilling with nitrogen. The reaction tube stirs at 100 °C in preheated oil-bath for 6 hours. Then, the reaction was cooled to room temperature and solvent was removed under vacuum. The remaining residue was washed with dry hexane (2×10 mL) under an inert atmosphere. The remaining residue was dissolved in dry DCM (25 mL) and the resulting solution was filtered under argon atmosphere using sintered filter stick setup. The solvent was removed under vacuum and the resultant compound was analyzed by HRMS, which was in complete agreement with simulated mass spectra.

HRMS and simulated isotopic pattern of 12:

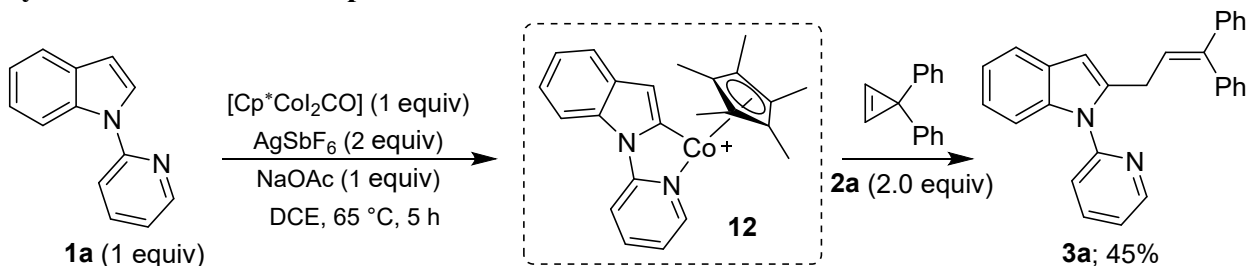




Chemical Formula: $C_{23}H_{24}CoN_2^+$
 Exact Mass: 387.1266
 Found Mass: 387.1251
 Simulated Mass: 387.1269

Simulated Isotopic pattern of 12

9.4 Synthesis of 3a from complex 12:

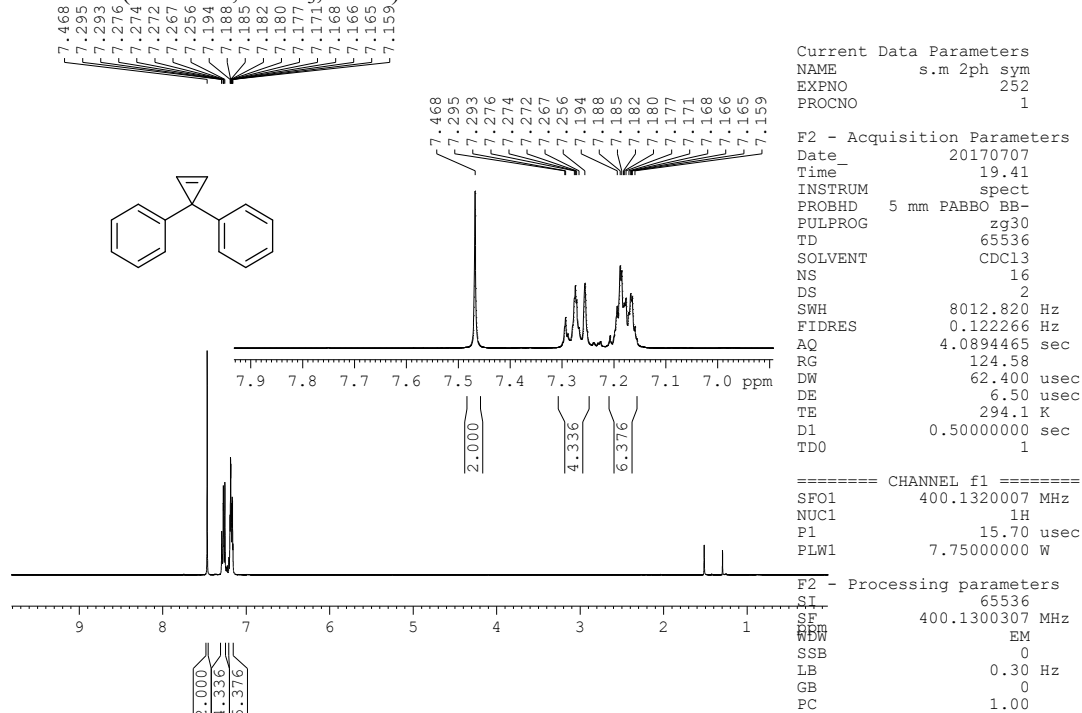


Oven-dried Schlenk tube was charged with **1a** (1 equiv, 0.26 mmol), NaOAc (1 equiv), AgSbF₆ (2 equiv) and [Cp*CoI₂CO] (1 equiv), then 4 mL of dry DCE was added. The charged schlenk tube's inner atmosphere was made inert through repeated (thrice) evacuation and refilling with nitrogen. The reaction tube stirs at 100 °C in preheated oil-bath for 6 hours (complex **13** identified with HRMS). After 6 h, **2a** was added to the reaction slowly through a syringe pump for one hour. Then, the reaction was brought into room temperature and passes through a pad of celite and concentrated to get the crude product. The crude product was purified by column chromatography through silica gel to afford the expected product **3a** in 45% yield.

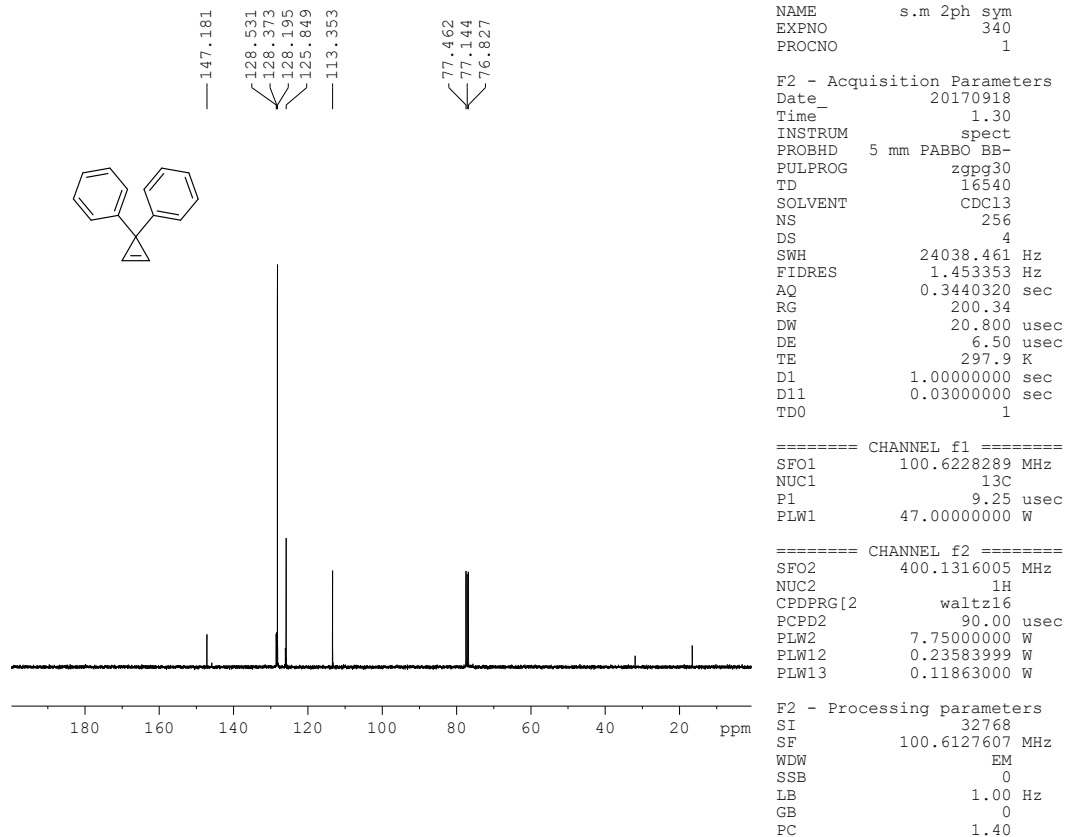
10. Spectral data:

3,3-Diphenylcyclopropene (2a):

^1H NMR (400 MHz, CDCl_3 , 24 °C):

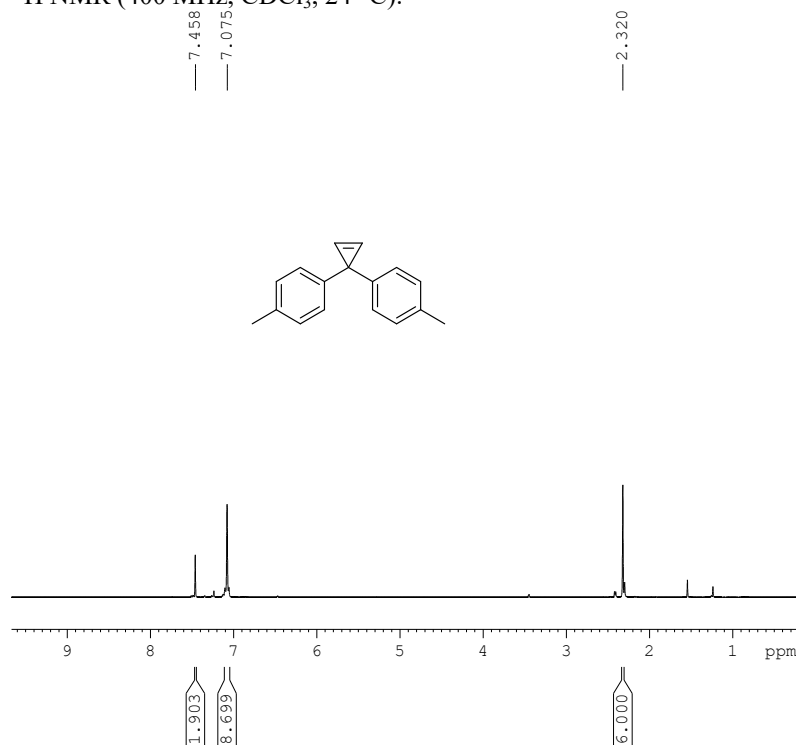


$^{13}\text{C}\{^1\text{H}\}$ NMR (400 MHz, CDCl_3 , 24 °C):



3,3-Bis(4-methylphenyl)cyclopropene (2t):

¹H NMR (400 MHz, CDCl₃, 24 °C):



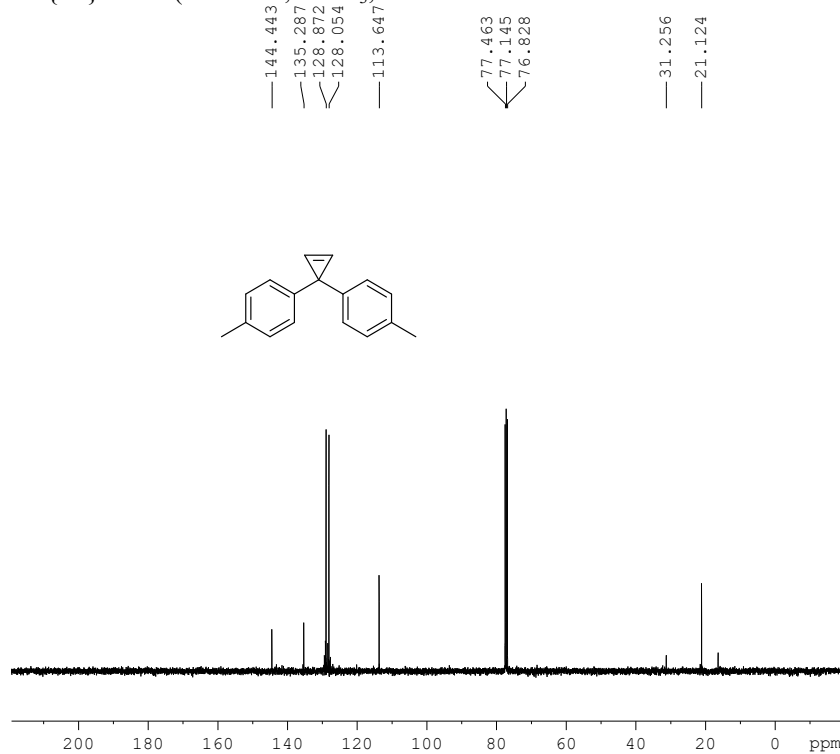
Current Data Parameters
NAME s.m 2 me ph sym
EXPNO 531
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171226
Time 16.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300205 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME s.m 2 me ph sym
EXPNO 532
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171226
Time 16.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

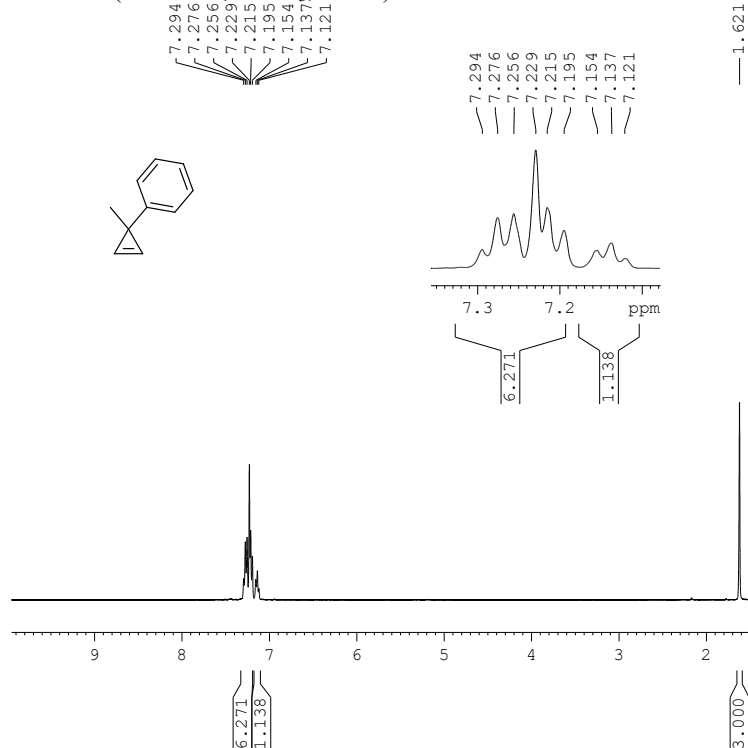
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127602 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-Methyl-3phenylcyclopropene (2v):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



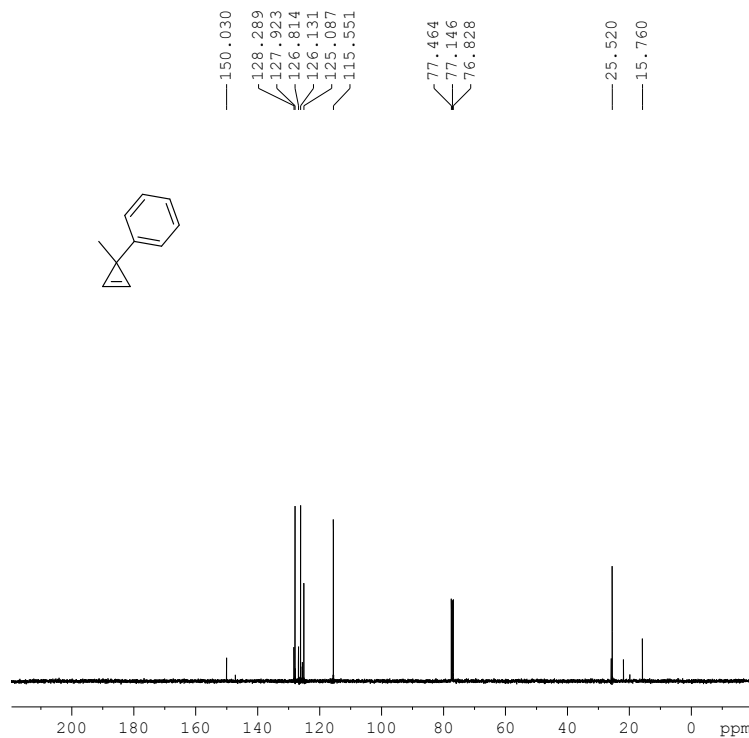
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Current Data Parameters
NAME      s.m ph and me
EXPNO     720
PROCNO    1

F2 - Acquisition Parameters
Date_     20170330
Time      21.57
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894465 sec
RG         88.51
DW         62.400 usec
DE         6.50 usec
TE         294.4 K
D1         0.50000000 sec
TD0        1
```

```
===== CHANNEL f1 =====
SFO1      400.1320007 MHz
NUC1       1H
P1         15.70 usec
PLW1       7.75000000 W
```

```
F2 - Processing parameters
SI         65536
SF         400.1300369 MHz
WDW        EM
SSB        0
GB         0
PC         1.00
```

$^{13}\text{C}\{^1\text{H}\}$ NMR (400 MHz, CDCl_3 , 24 °C):



```
Current Data Parameters
NAME      s.m ph and me
EXPNO     721
PROCNO    1
```

```
F2 - Acquisition Parameters
Date_     20170330
Time      21.59
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        16540
SOLVENT   CDCl3
NS         144
DS         4
SWH        24038.461 Hz
FIDRES     1.453353 Hz
AQ         0.3440320 sec
RG         200.34
DW         20.800 usec
DE         6.50 usec
TE         294.6 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1
```

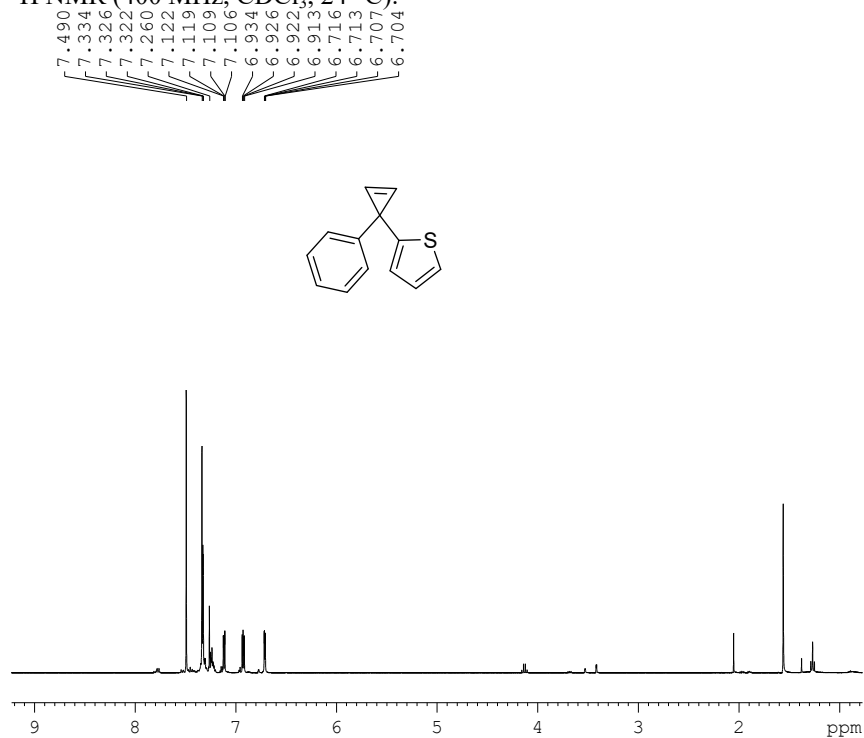
```
===== CHANNEL f1 =====
SFO1      100.6228289 MHz
NUC1       13C
P1         9.25 usec
PLW1       47.00000000 W
```

```
===== CHANNEL f2 =====
SFO2      400.1316005 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2       7.75000000 W
PLW12      0.23583999 W
PLW13      0.11863000 W
```

```
F2 - Processing parameters
SI         32768
SF         100.6127634 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

3-Phenyl-3-thiophene-2-ylcyclopropene (2y):

^1H NMR (400 MHz, CDCl_3 , 24 °C):



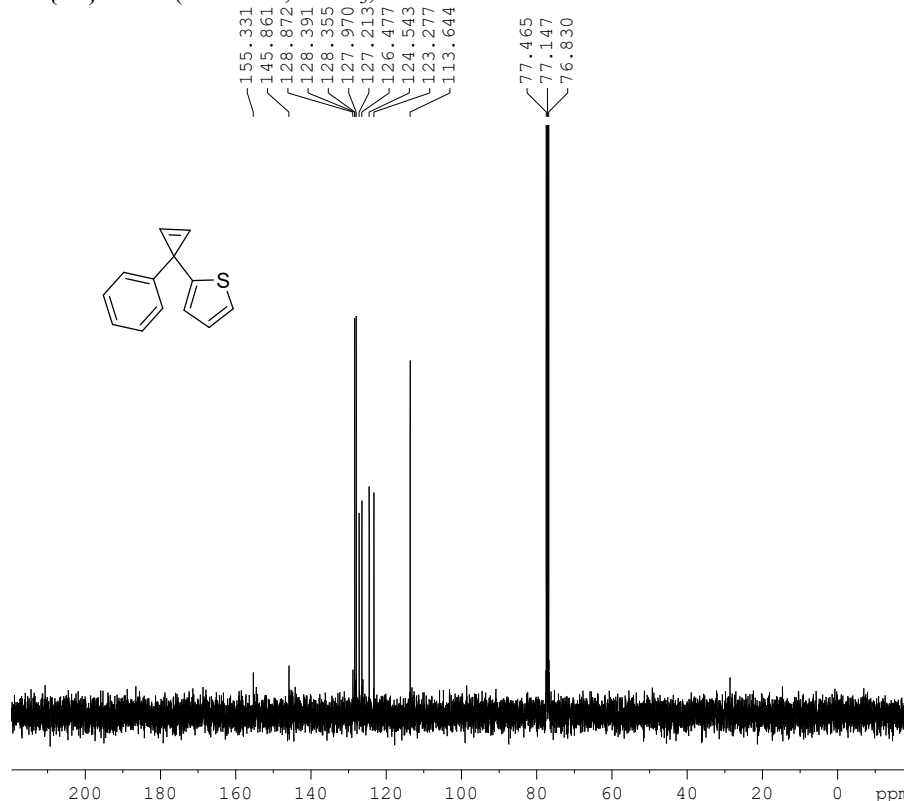
Current Data Parameters
NAME spa40218
EXPNO 593
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180225
Time_ 5.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 298.9 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 ^1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 24 °C):



Current Data Paramete
NAME spa402
EXPNO 5
PROCNO

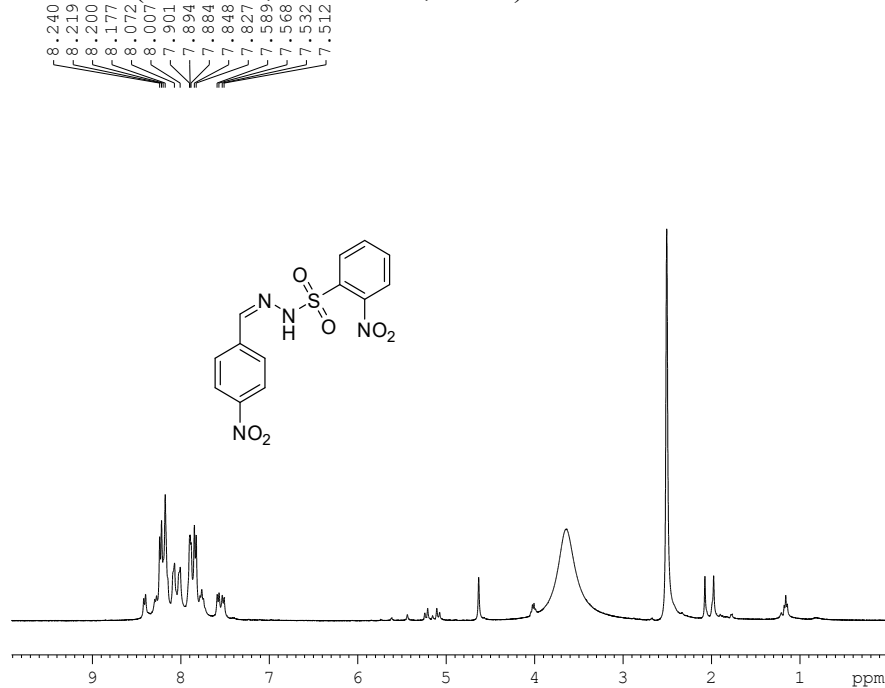
F2 - Acquisition Para
Date_ 201802
Time_ 5.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDCl_3
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 299
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 ^{13}C
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2 ^1H
CPDPRG[2 waltz
PCPD2 90.
PTW2 7.750000

2-Nitro-*N'*-(4-Nitrobenzylidene)benzenesulfonohydrazide:

¹H NMR (500 MHz, DMSO-D₆, 24 °C):

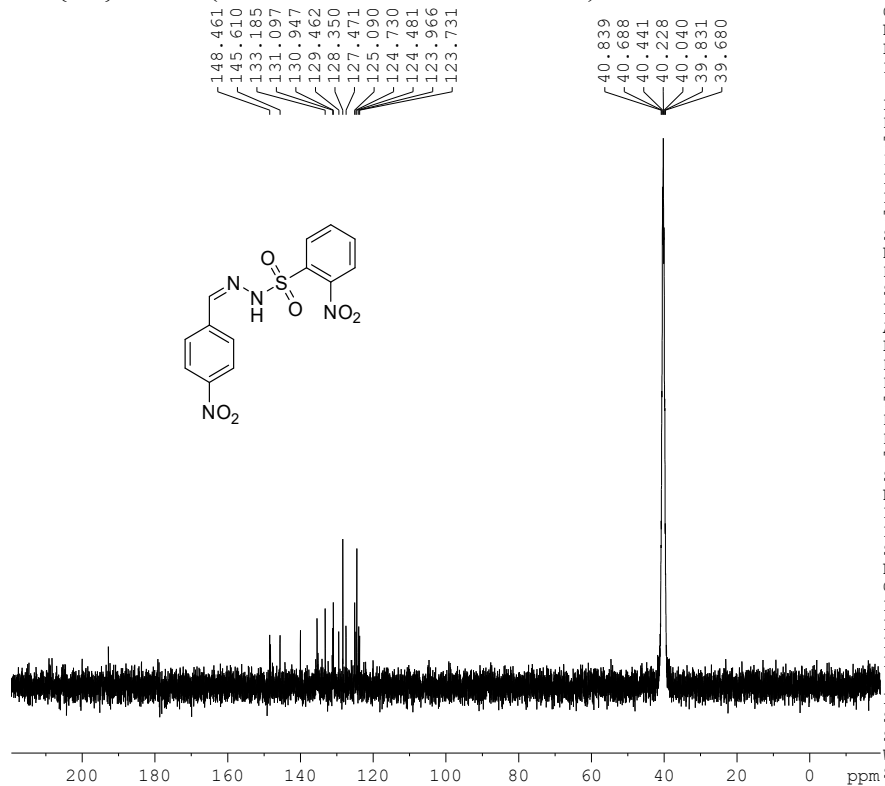


Current Data Parameters
NAME 2727 II
EXPNO 480
PROCNO 1

F2 - Acquisition Paramet
Date_ 20210822
Time_ 13.10
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820
FIDRES 0.244532
AQ 4.0894465
RG 153.13
DW 62.400
DE 6.50
TE 297.6
D1 0.50000000
TD0 1
SFO1 400.1320007
NUC1 1H
P1 15.00
PLW1 10.50000000

F2 - Processing paramet
SI 65536
SF 400.1300000
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, DMSO-D₆, 24 °C):



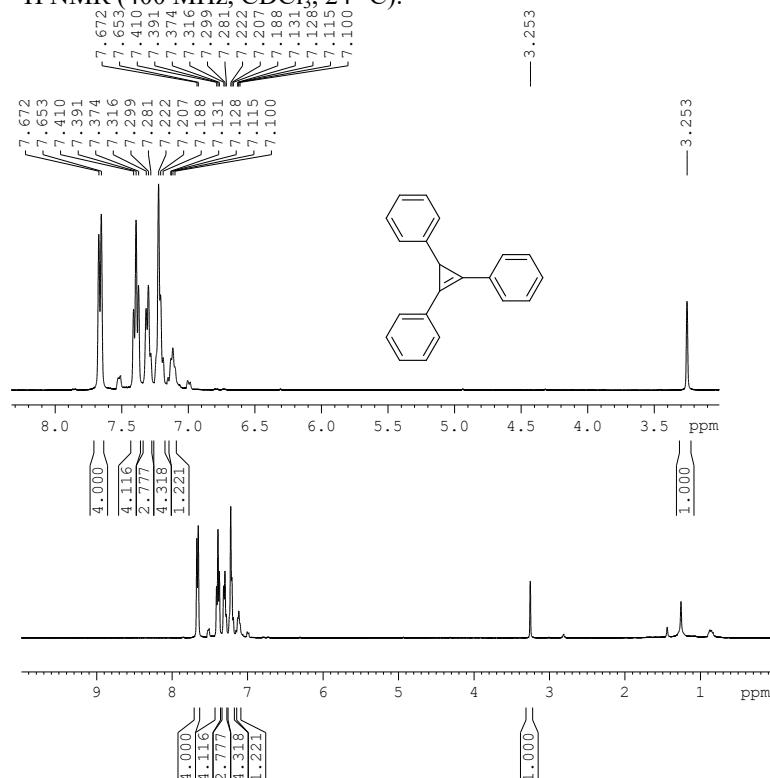
Current Data Parameters
NAME 2727 II
EXPNO 481
PROCNO 1

F2 - Acquisition Paramet
Date_ 20210822
Time_ 13.16
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 16540
SOLVENT DMSO
NS 256
DS 4
SWH 24038.461
FIDRES 2.906706
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 297.7
D1 1.00000000
D11 0.03000000
TD0 1
SFO1 100.6228289
NUC1 13C
P1 10.00
PLW1 47.00000000
SFO2 400.1316005
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00
PLW2 10.50000000
PLW12 0.29166999
PLW13 0.14670999

F2 - Processing paramete
SI 32768
SF 100.6127690
WDW EM
SSB 0
PC 1.00

1,2,3-Triphenylcyclopropene (2ae):

¹H NMR (400 MHz, CDCl₃, 24 °C):



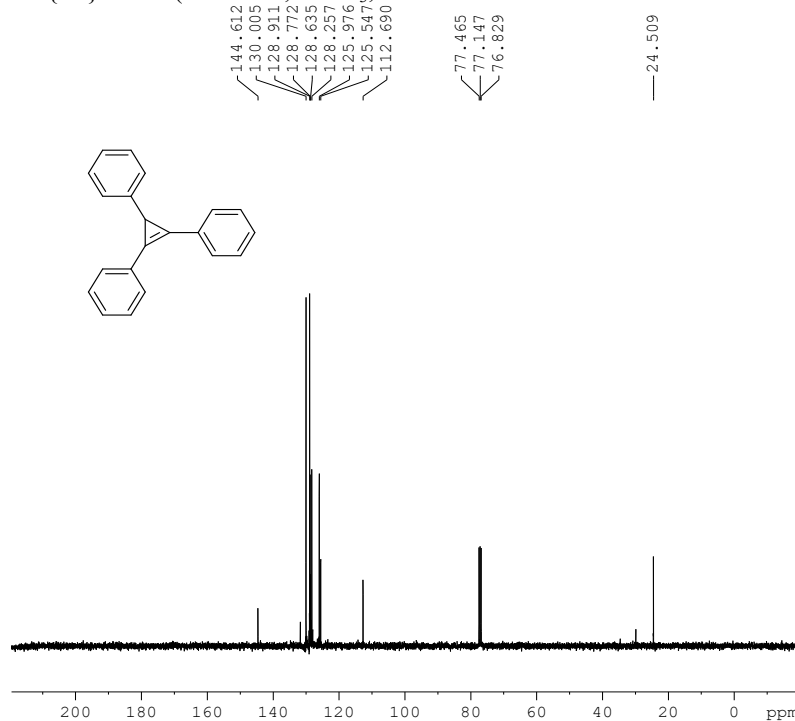
```
Current Data Parameters
NAME      nmr_2085%2f2087
EXPNO     32
PROCNO    1

F2 - Acquisition Parameters
Date_     20200507
Time      16.59
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS         7
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894465 sec
RG         79.8
DW         62.400 usec
DE         6.50 usec
TE         297.3 K
D1         0.50000000 sec
TD0        1
```

```
===== CHANNEL f1 =====
SFO1      400.1320007 MHz
NUC1       1H
P1         15.70 usec
PLW1       7.75000000 W
```

```
F2 - Processing parameters
SI         65536
SF         400.1300525 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



```
Current Data Parameters
NAME      nmr_2085%2f2087
EXPNO     33
PROCNO    1
```

```
F2 - Acquisition Parameters
Date_     20200507
Time      17.00
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        16540
SOLVENT   CDCl3
NS         27
DS         4
SWH        24038.461 Hz
FIDRES     1.453353 Hz
AQ         0.3440320 sec
RG         200.34
DW         20.800 usec
DE         6.50 usec
TE         297.4 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1
```

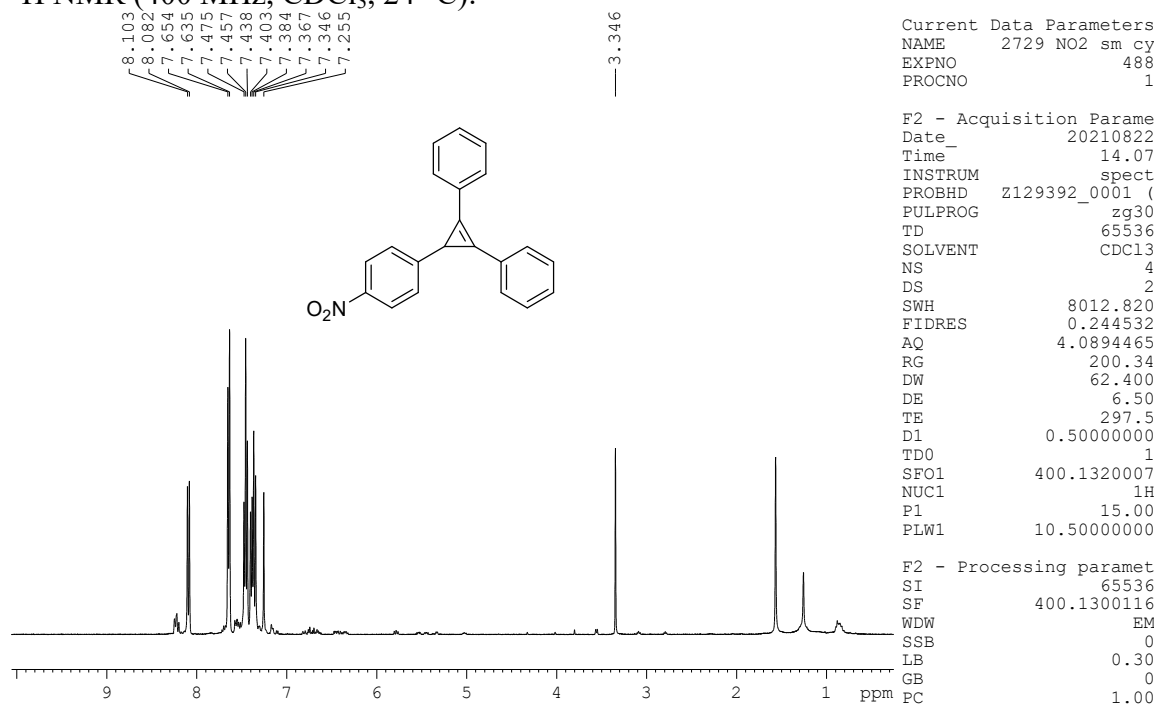
```
===== CHANNEL f1 =====
SFO1      100.6228289 MHz
NUC1       13C
P1         9.25 usec
PLW1       47.00000000 W
```

```
===== CHANNEL f2 =====
SFO2      400.1316005 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2      7.75000000 W
PLW12     0.23583999 W
PLW13     0.11863000 W
```

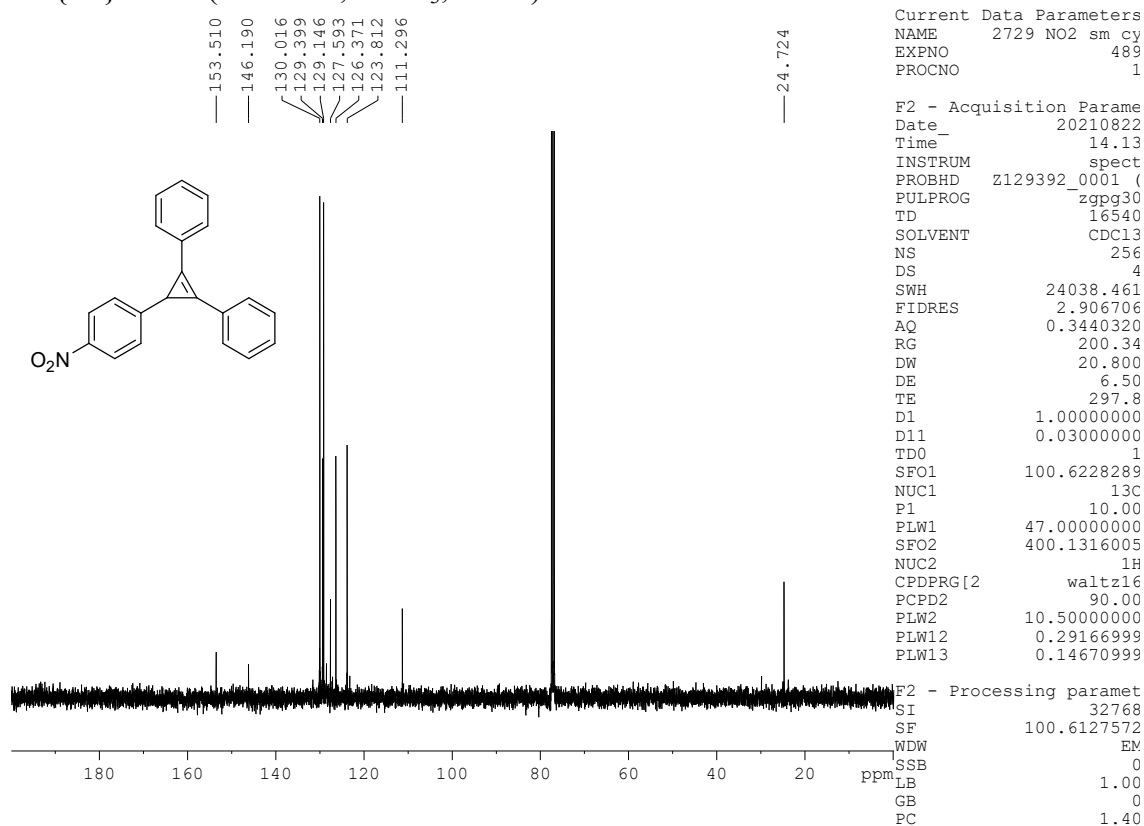
```
F2 - Processing parameters
SI         32768
SF         100.6127684 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

(3-(4-Nitrophenyl)cycloprop-1-ene-1,2-diyl)dibenzene (2ag):

¹H NMR (400 MHz, CDCl₃, 24 °C):

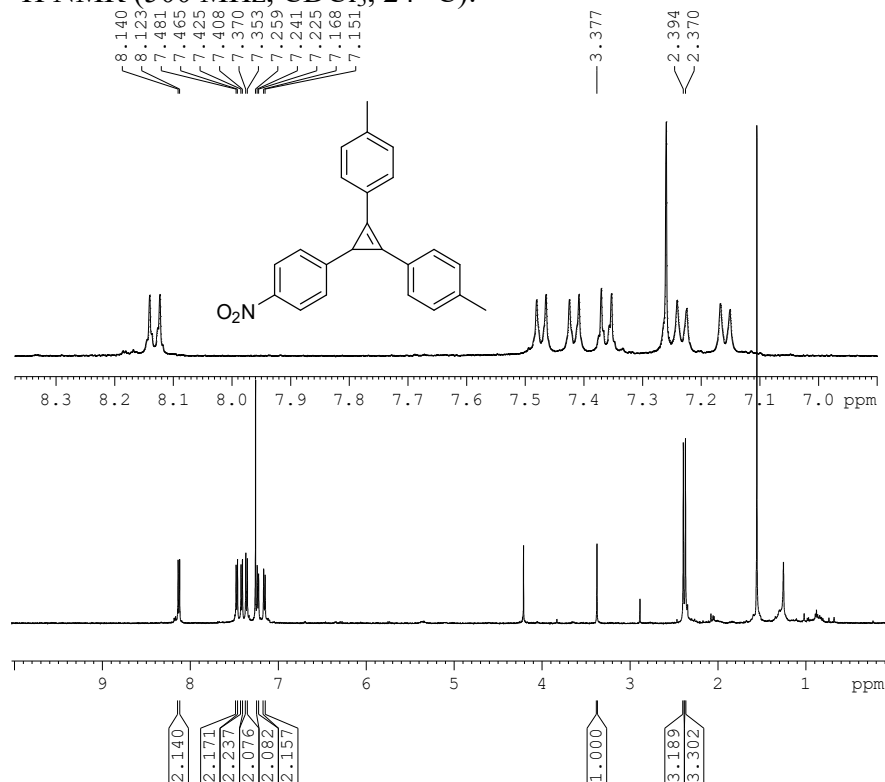


¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



4,4'-(3-(4-Nitrophenyl)cycloprop-1-ene-1,2-diyl)bis(methylbenzene) (2ah):

¹H NMR (500 MHz, CDCl₃, 24 °C):



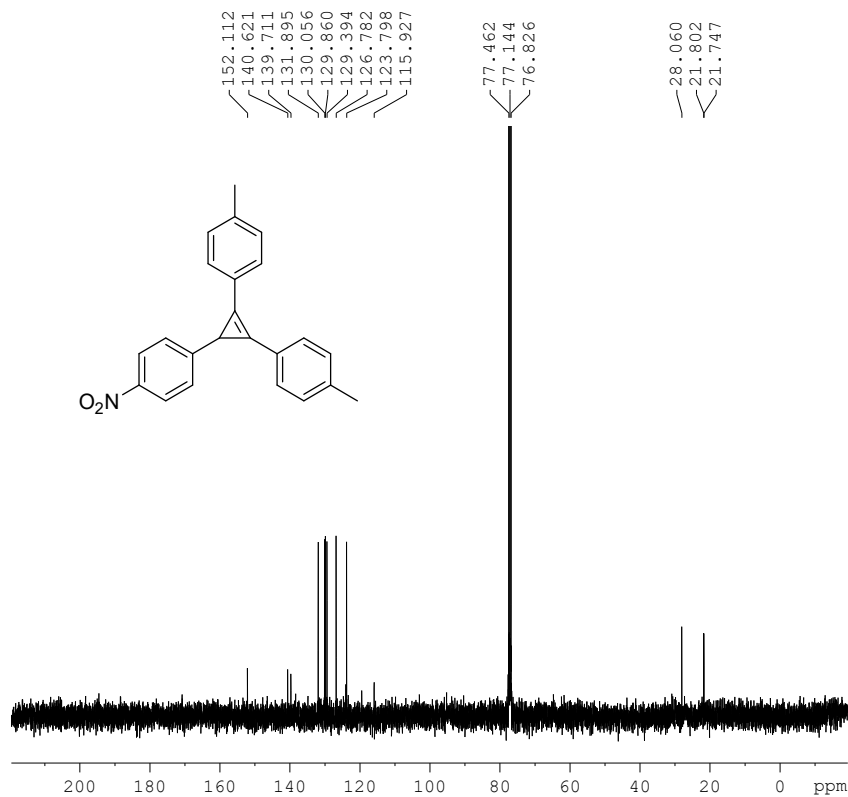
Current Data Parameters
NAME 2733 sm
EXPNO 67
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210825
Time_ 15.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 10000.000
FIDRES 0.305176
AQ 1.6384000
RG 202.34
DW 50.000
DE 6.50
TE 299.7
D1 0.50000000
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008
NUC1 1H
P1 11.75
PLW1 15.30000019

F2 - Processing parameters
SI 65536
SF 500.1500122
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



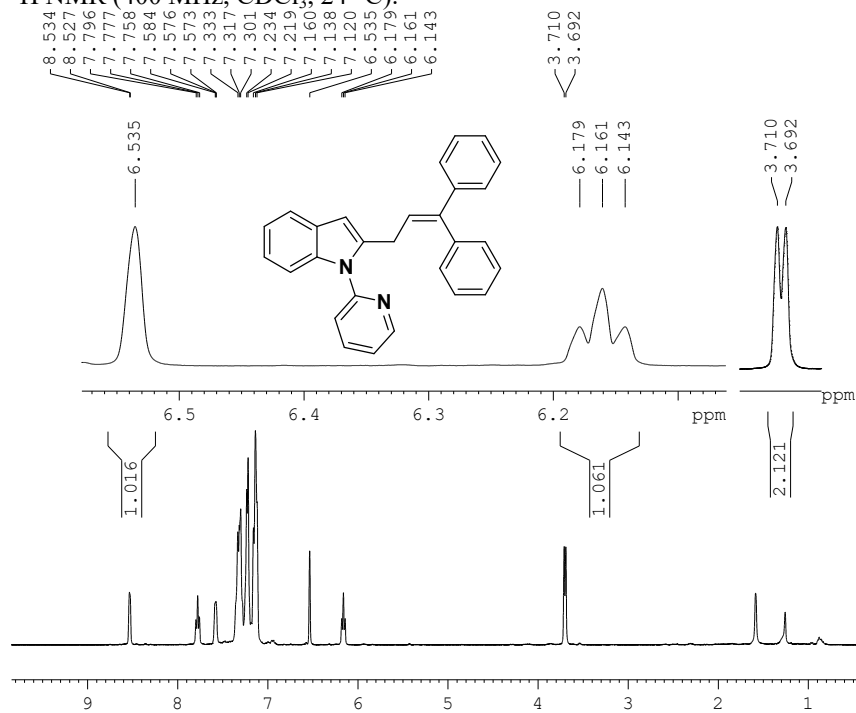
Current Data Parameters
NAME 2733 sm
EXPNO 129
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210825
Time_ 16.13
INSTRUM spect
PROBHD Z129392_0001 (zpgpg30)
PULPROG zgpg30
TD 16540
SOLVENT CDCl₃
NS 1095
DS 4
SWH 24038.461
FIDRES 2.906706
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 297.8
D1 1.00000000
D11 0.03000000
TD0 1
SFO1 100.6228289
NUC1 13C
P1 10.00
PLW1 47.00000000
SFO2 400.1316005
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00
PLW2 10.50000000
PLW12 0.29166999
PLW13 0.14670999

F2 - Processing parameters
SI 32768
SF 100.6127561
WDW EM
SSB 0
LB 1.00
GB 0

2-(3,3-Diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3a)

¹H NMR (400 MHz, CDCl₃, 24 °C):



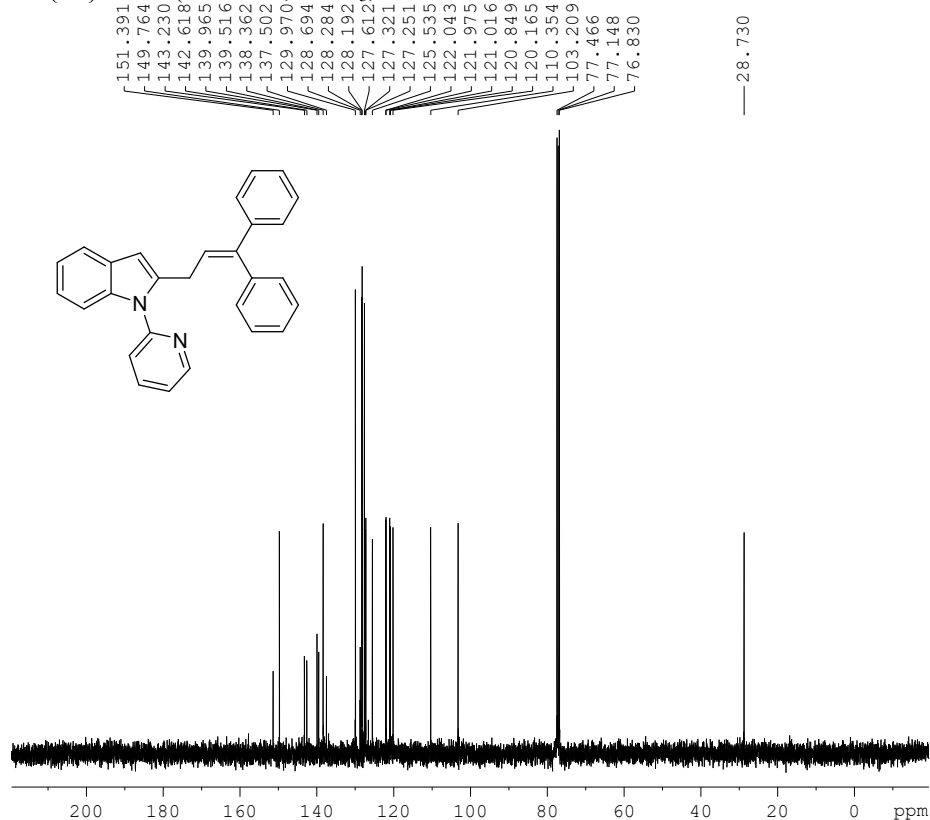
Current Data Parameters
NAME ksr 945
EXPNO 191
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200526
Time_ 17.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 297.5 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300197 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME ex. no. 945
EXPNO 4
PROCNO

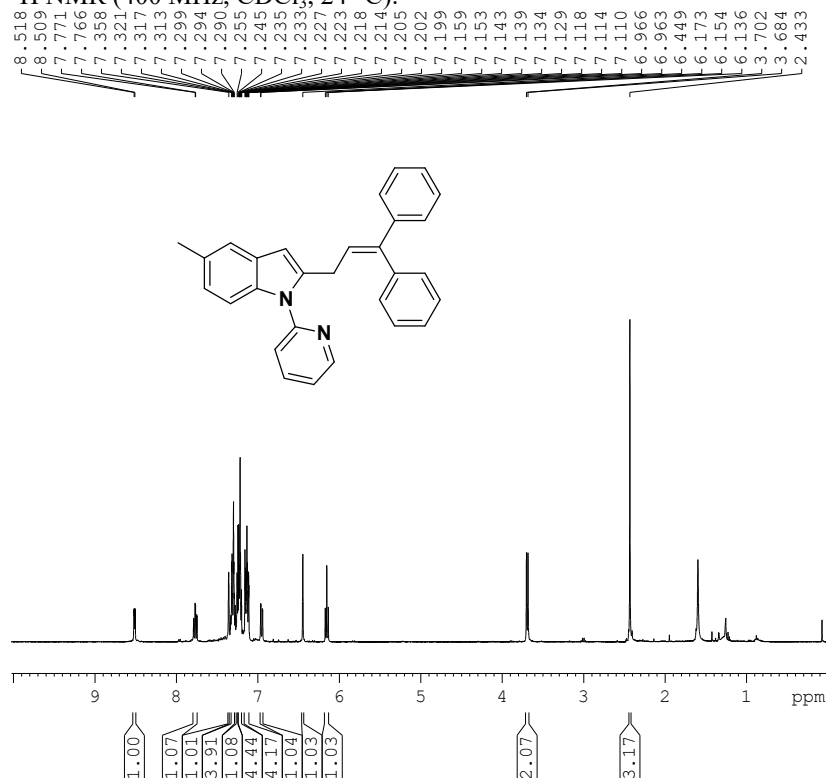
F2 - Acquisition Para
Date_ 201908
Time_ 9.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 298
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 13
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2 waltz
PCPD2 90.
D11 7.750000

2-(3,3-Diphenylallyl)-5-methyl-1-(pyridin-2-yl)-1H-indole (3b):

¹H NMR (400 MHz, CDCl₃, 24 °C):



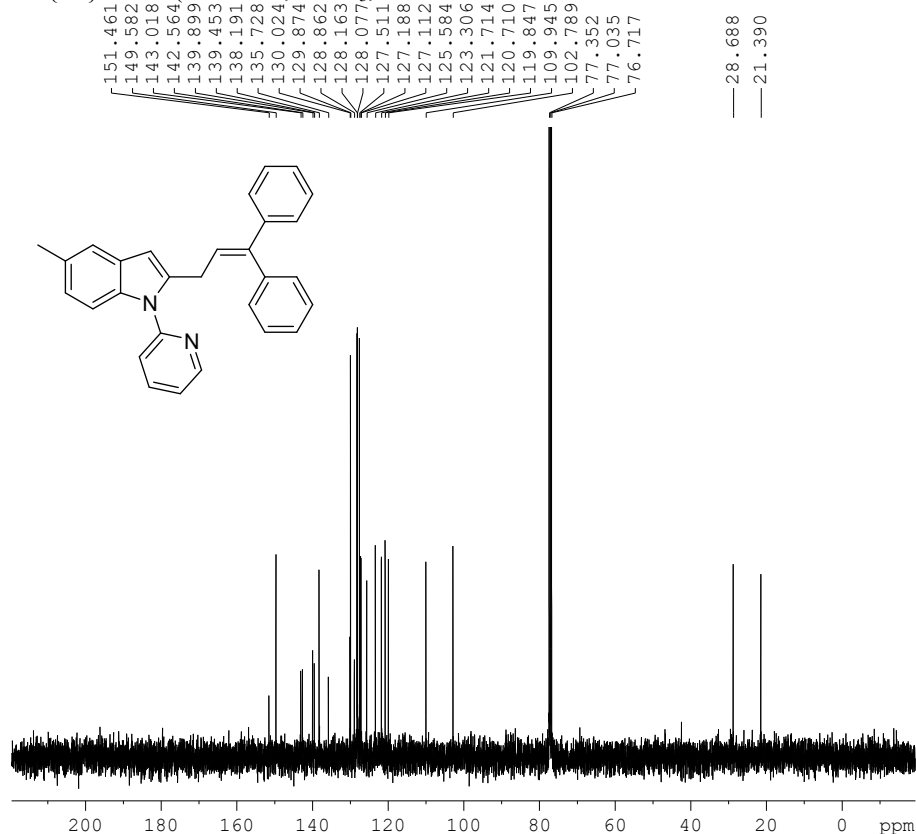
Current Data Parameters
NAME 1121 5me
EXPNO 311
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171117
Time_ 23.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.77
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300158 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1121 5me
EXPNO 312
PROCNO 1

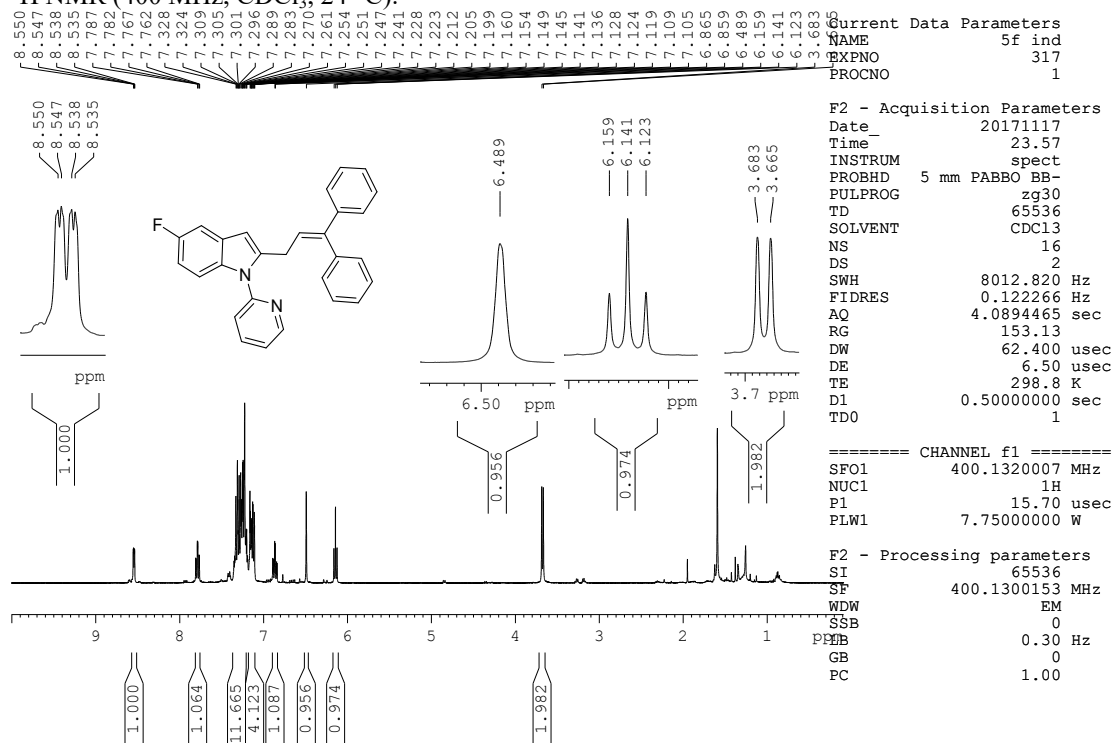
F2 - Acquisition Parameters
Date_ 20171117
Time_ 23.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 MHz
FIDRES 1.453353 MHz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

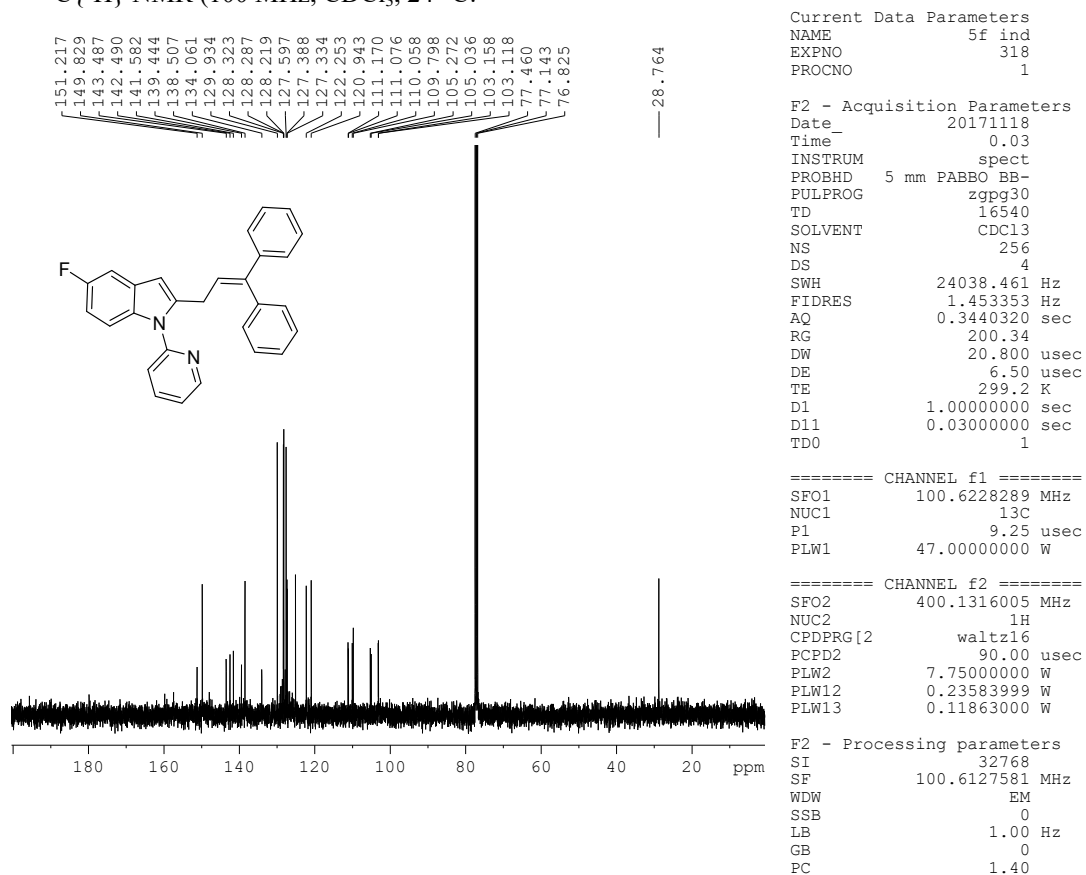
===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W

2-(3,3-Diphenylallyl)-5-fluoro-1-(pyridin-2-yl)-1H-indole (3c):

¹H NMR (400 MHz, CDCl₃, 24 °C):

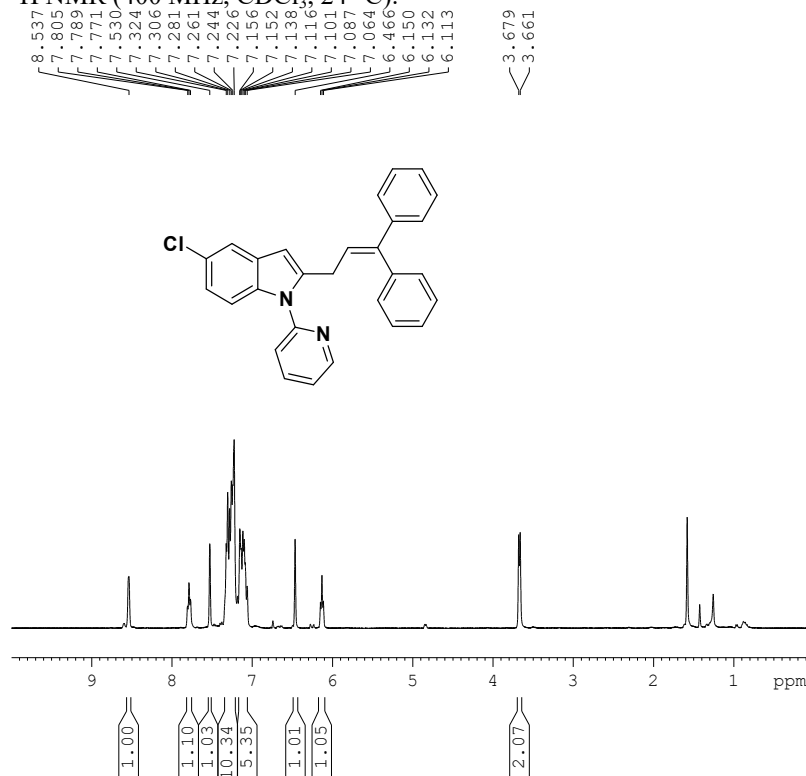


¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



5-Chloro-2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3d):

¹H NMR (400 MHz, CDCl₃, 24 °C):



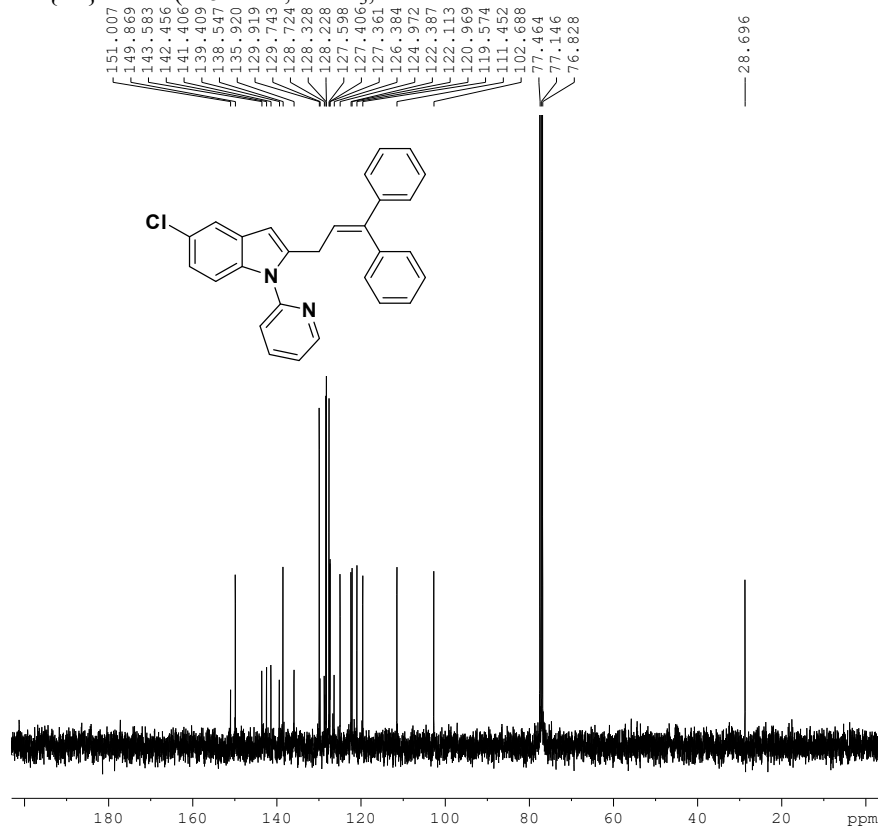
Current Data Parameters
NAME 1066 5 c1
EXPNO 342
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170918
Time 1.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.77
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300161 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1066 5 c1
EXPNO 343
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170918
Time 1.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 19.43
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

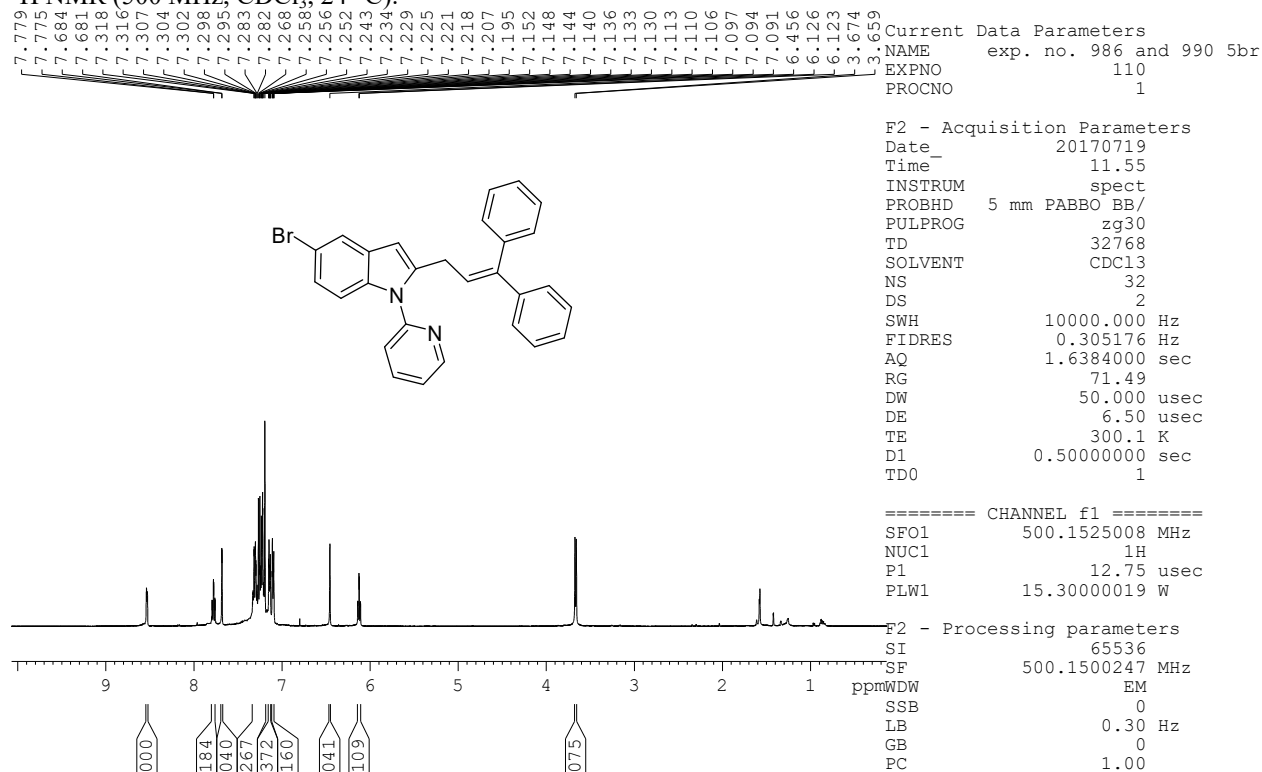
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

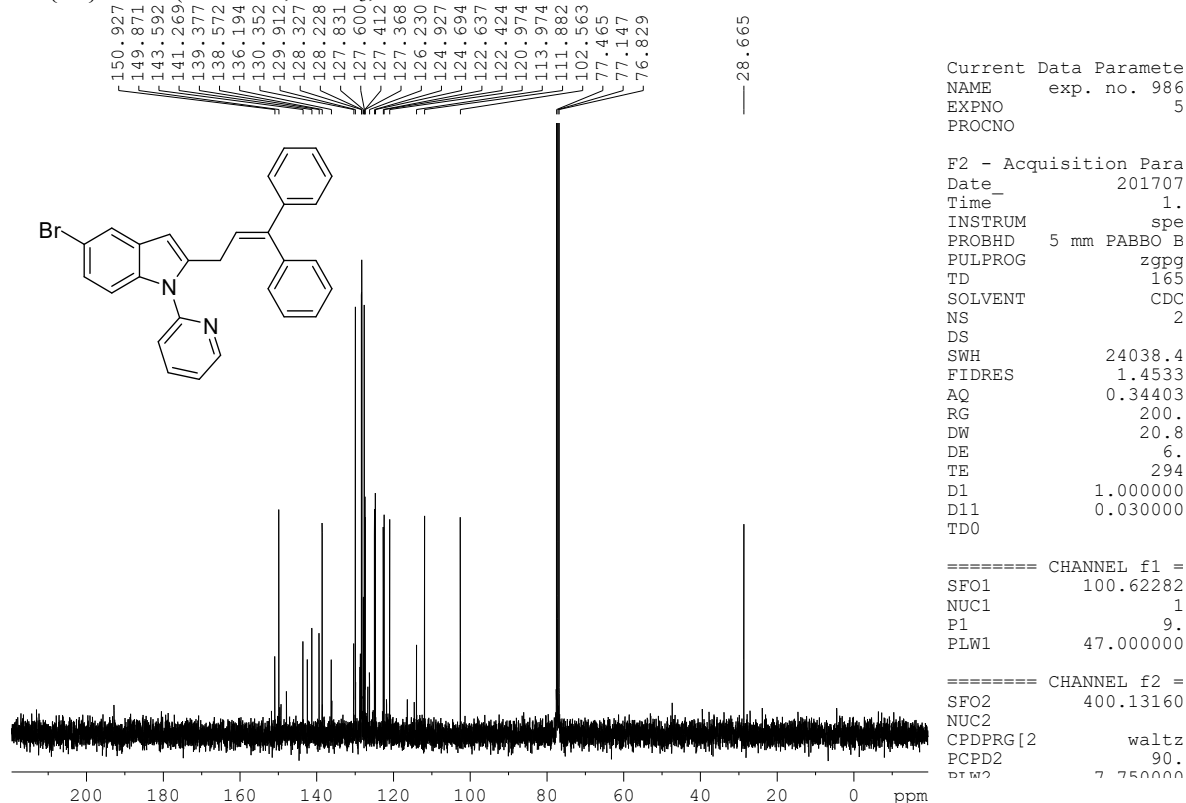
F2 - Processing parameters
SI 32768
SF 100.6127587 MHz
WDW EM

5-Bromo-2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3e):

¹H NMR (500 MHz, CDCl₃, 24 °C):

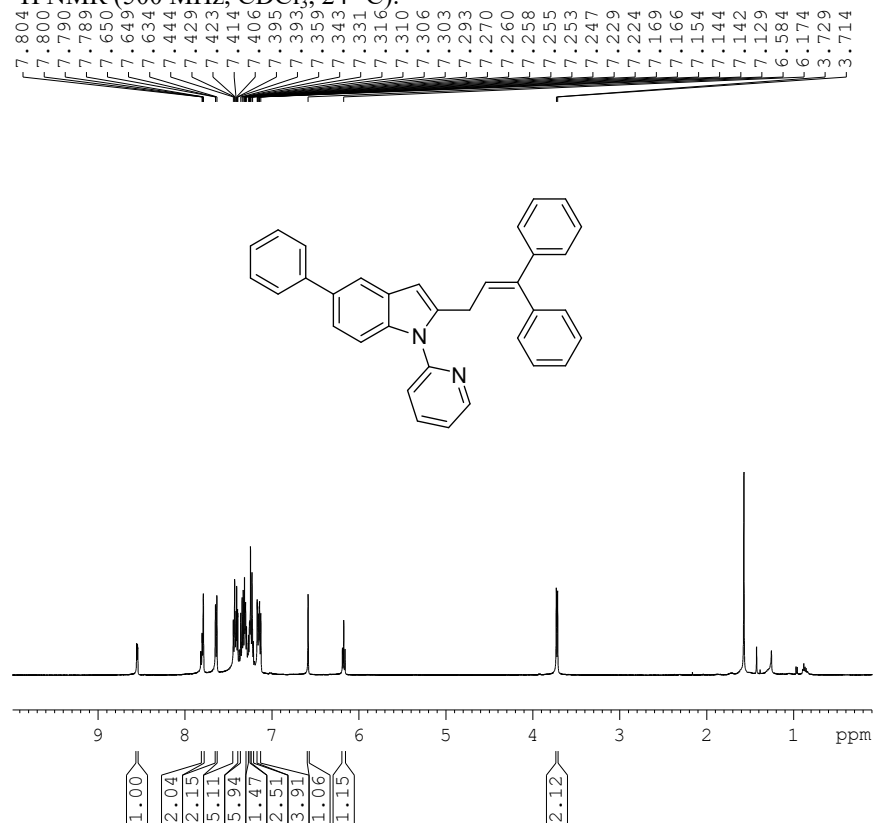


¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



2-(3,3-Diphenylallyl)-5-phenyl-1-(pyridin-2-yl)-1H-indole (3f):

¹H NMR (500 MHz, CDCl₃, 24 °C):



¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):

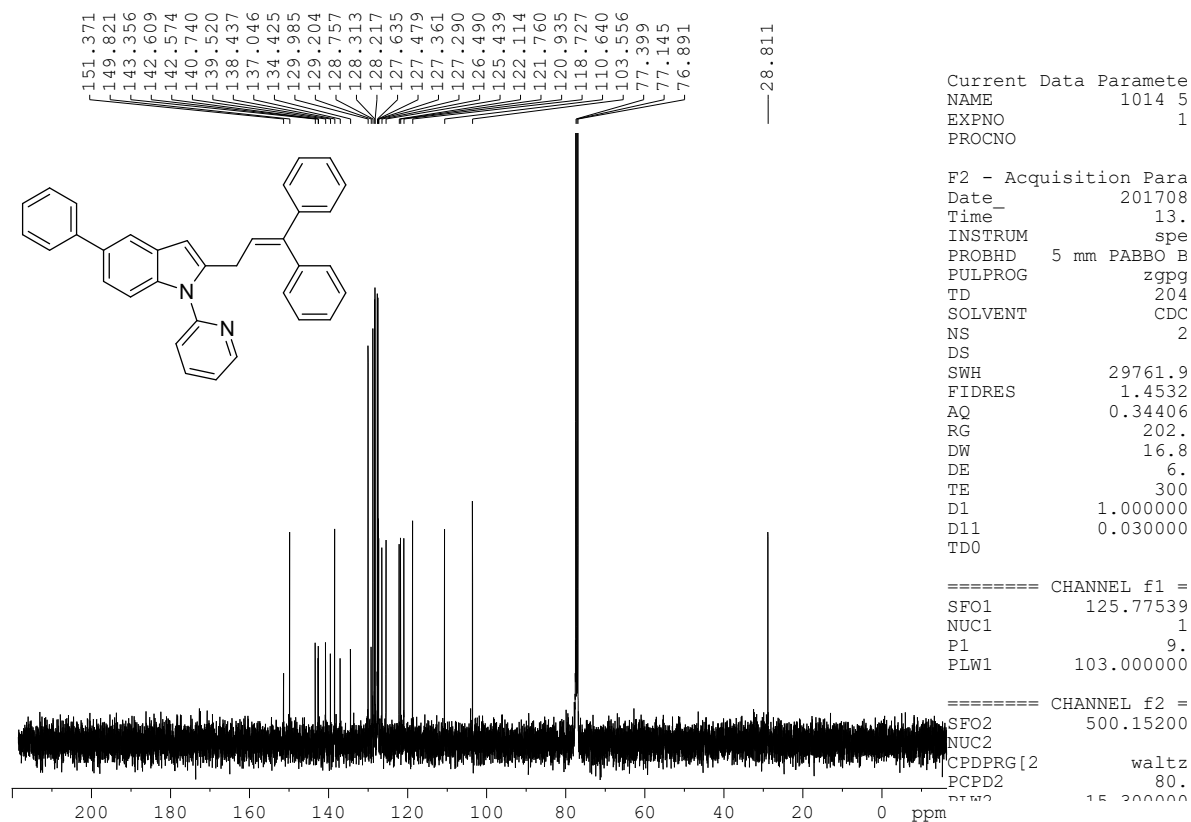
Current Data Parameters
NAME 1014 5ph
EXPNO 140
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170816
Time_ 13.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 114.76
DW 50.000 usec
DE 6.50 usec
TE 300.1 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

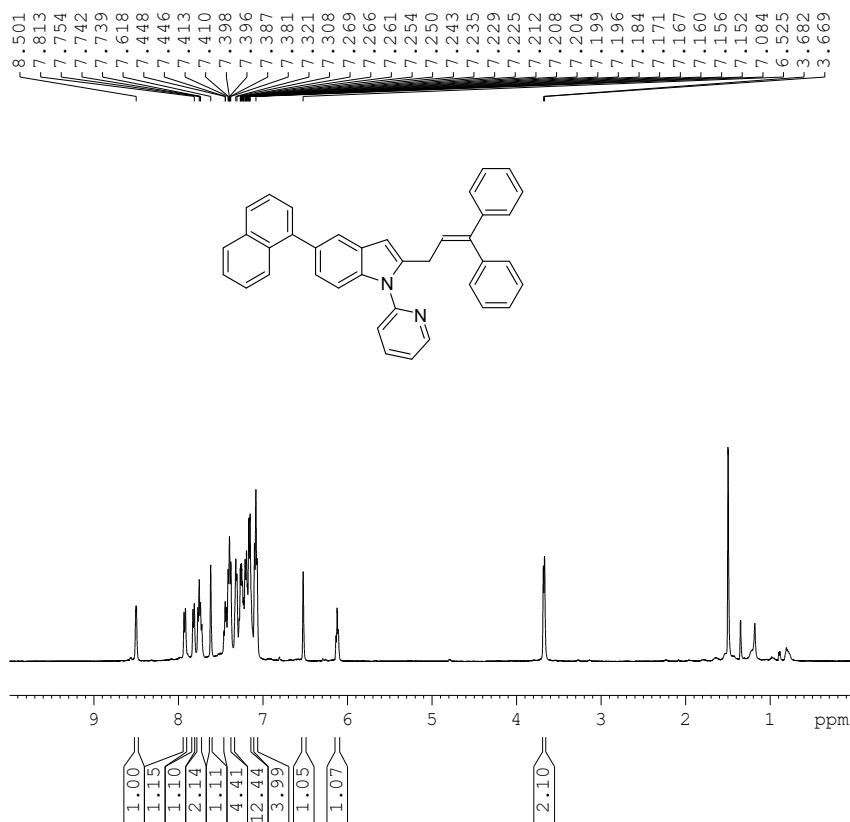
F2 - Processing parameters
SI 65536
SF 500.1500188 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13



2-(3,3-Diphenylallyl)-5-(naphthalen-1-yl)-1-(pyridin-2-yl)-1H-indole (3g):

¹H NMR (500 MHz, CDCl₃, 24 °C):



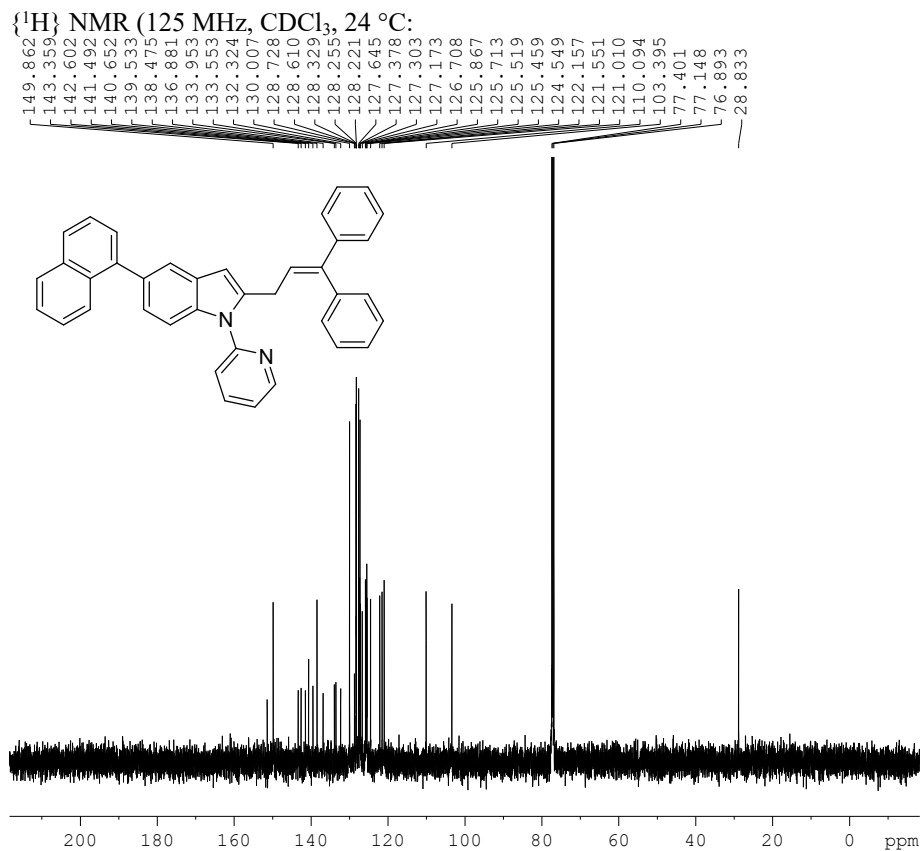
Current Data Parameters
NAME 500 nmr data pure
EXPNO 143
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170816
Time_ 13.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 101.5
DW 50.000 usec
DE 6.50 usec
TE 299.8 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500589 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C



Current Data Paramete
NAME 500 nmr data
EXPNO 1
PROCNO

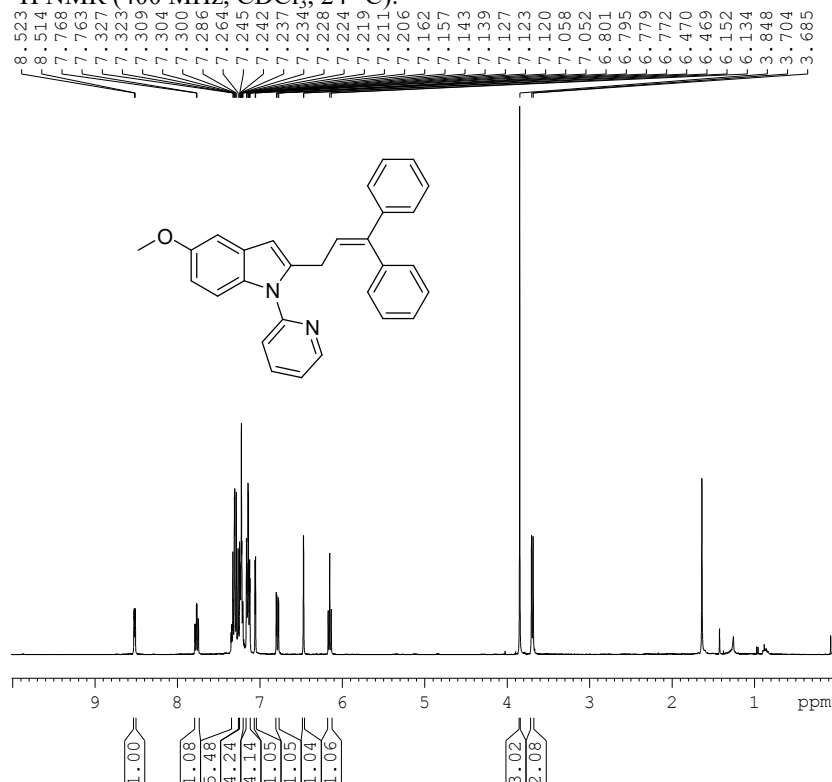
F2 - Acquisition Para
Date_ 201708
Time_ 14.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 204
SOLVENT CDC
NS 2
DS
SWH 29761.9
FIDRES 1.4532
AQ 0.34406
RG 202.
DW 16.8
DE 6.
TE 300
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 125.77539
NUC1 1
P1 9.
PLW1 103.000000

===== CHANNEL f2 =
SFO2 500.15200
NUC2
CPDPRG[2 waltz
PCPD2 80.
PLW2 15.300000

2-(3,3-Diphenylallyl)-5-methoxy-1-(pyridin-2-yl)-1H-indole (3h):

¹H NMR (400 MHz, CDCl₃, 24 °C):



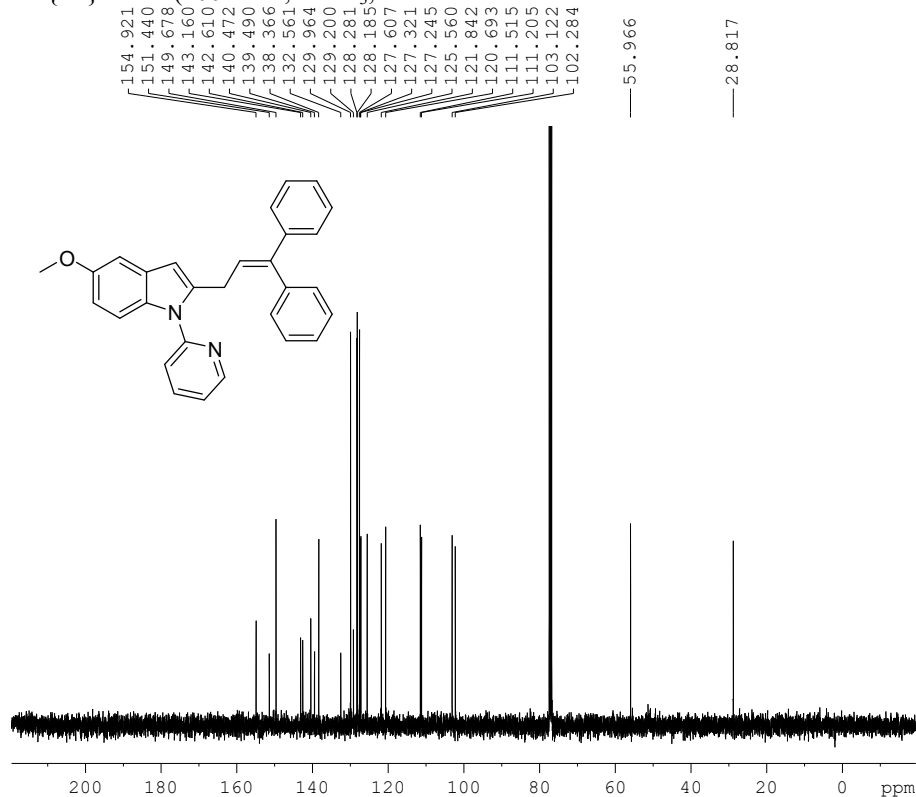
Current Data Parameters
NAME ex. no. 966 and 1104
EXPNO 518
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171028
Time 10.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 292.2 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300157 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME ex. no. 966 ar
EXPNO 519
PROCNO 1

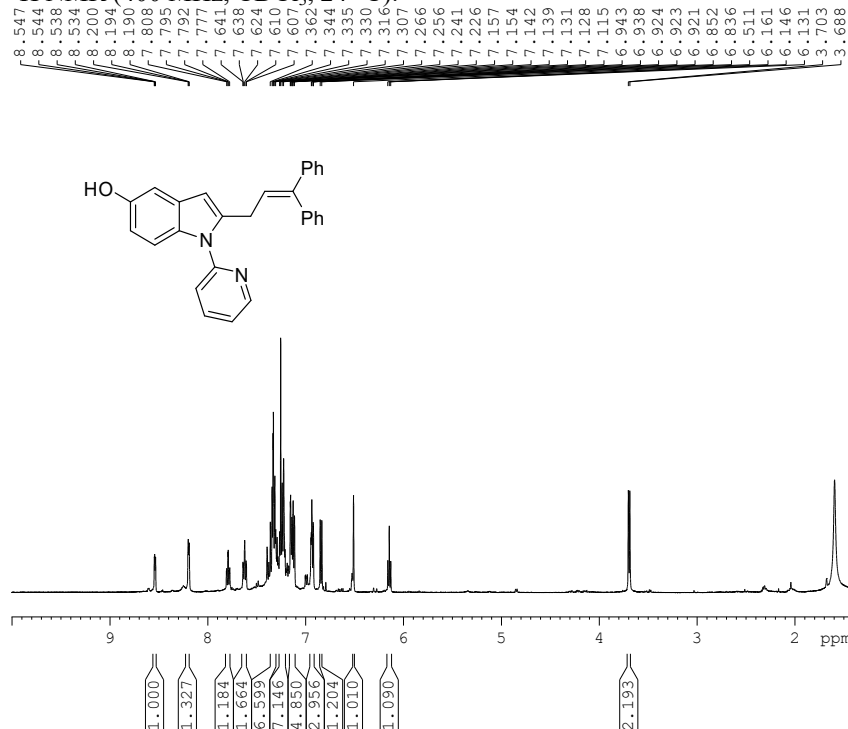
F2 - Acquisition Paramete
Date_ 20171028
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461
FIDRES 1.453353
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 292.2
D1 1.00000000
D11 0.03000000
TD0 1

===== CHANNEL f1 ===
SFO1 100.6228289
NUC1 13C
P1 9.25
PLW1 47.00000000

===== CHANNEL f2 ===
SFO2 400.1316009
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00
P1 7.75000000

2-(3,3-Diphenylallyl)-1-(pyridin-2-yl)-1*H*-indol-5-ol (3i):

¹H NMR (400 MHz, CDCl₃, 24 °C):



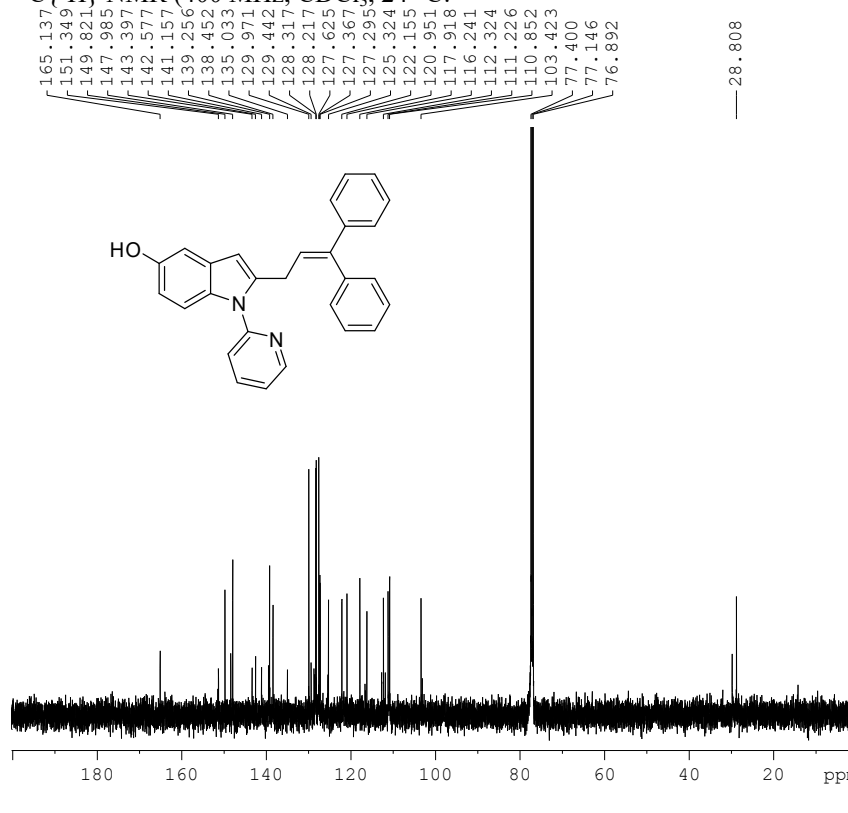
Current Data Parameters
NAME pure
EXPNO 108
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180217
Time_ 3.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 124.08
DW 50.000 usec
DE 6.50 usec
TE 301.1 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500144 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME pu
EXPNO 1
PROCNO

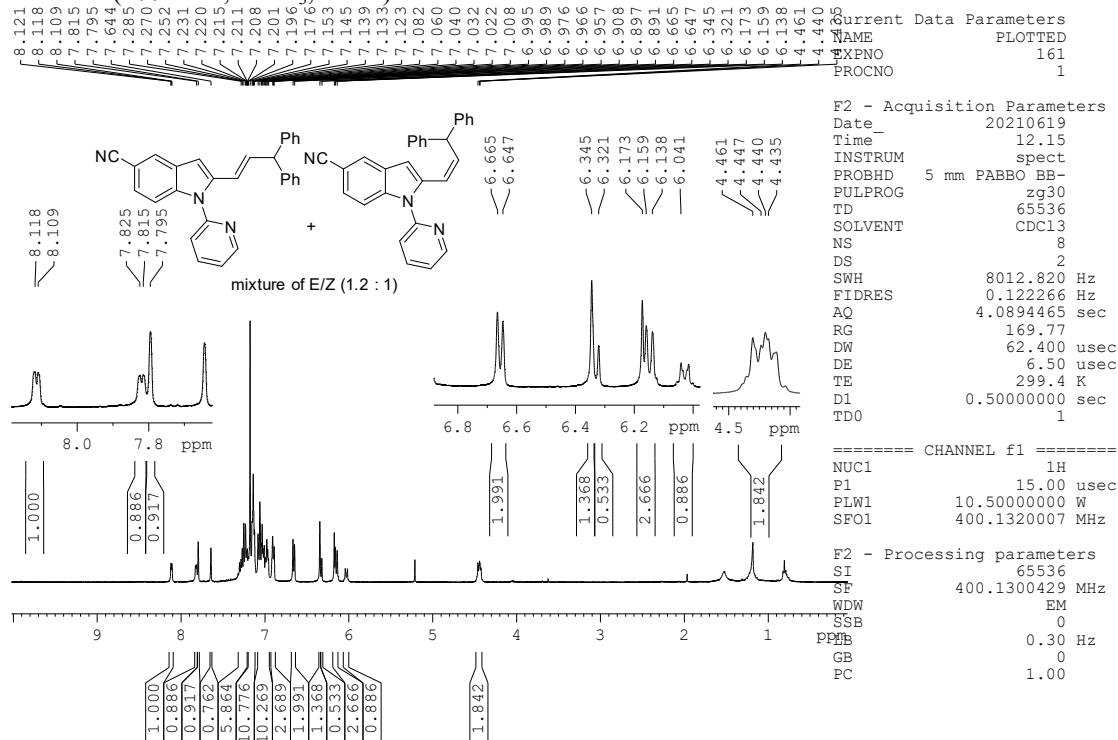
F2 - Acquisition Para
Date_ 201802
Time_ 4.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 204
SOLVENT CDC
NS 5
DS
SWH 29761.9
FIDRES 1.4532
AQ 0.34406
RG 202.
DW 16.8
DE 6.
TE 301
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 125.77539
NUC1 1
P1 9.
PLW1 103.000000

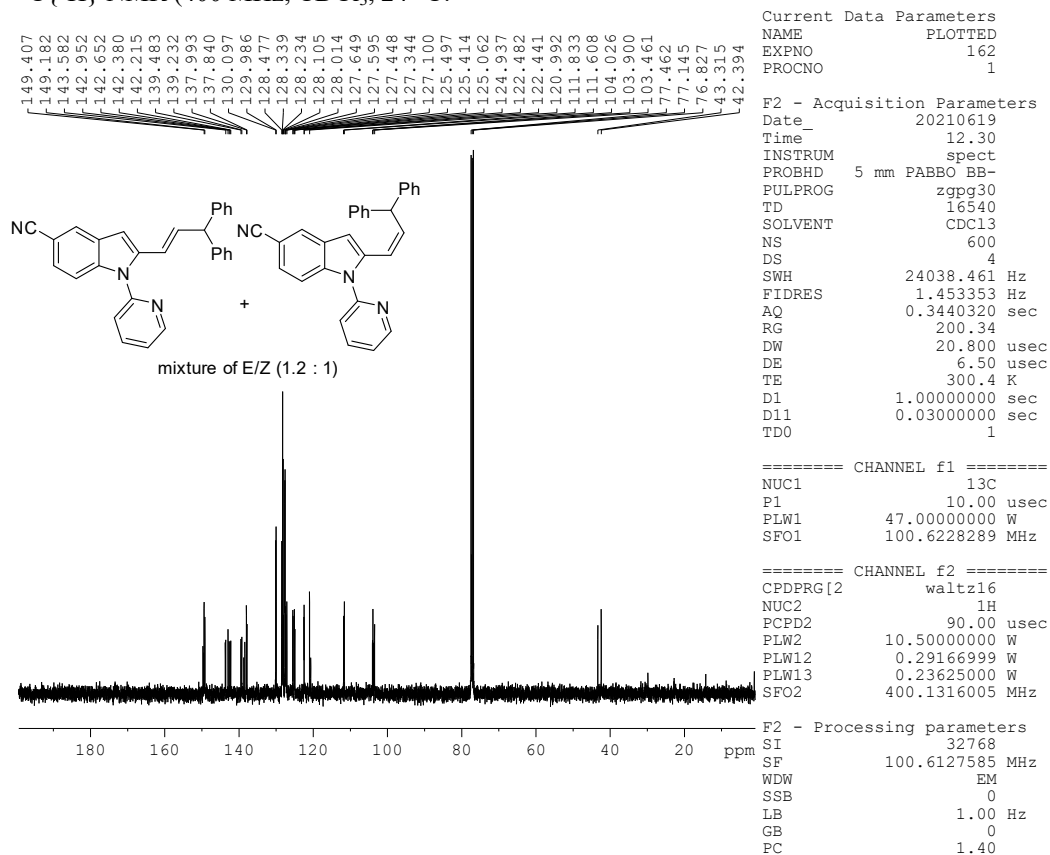
===== CHANNEL f2 =
SFO2 500.15200
NUC2
CPDPRG[2] waltz
PCPD2 80.
PLW2 15.300000

Mixture of (E)-2-(3,3-Diphenylprop-1-en-1-yl)-1-(pyridin-2-yl)-1H-indole-5-carbonitrile (xx) and (Z)-2-(3,3-Diphenylprop-1-en-1-yl)-1-(pyridin-2-yl)-1H-indole-5-carbonitrile (3j):

¹H NMR (400 MHz, CDCl₃, 24 °C):

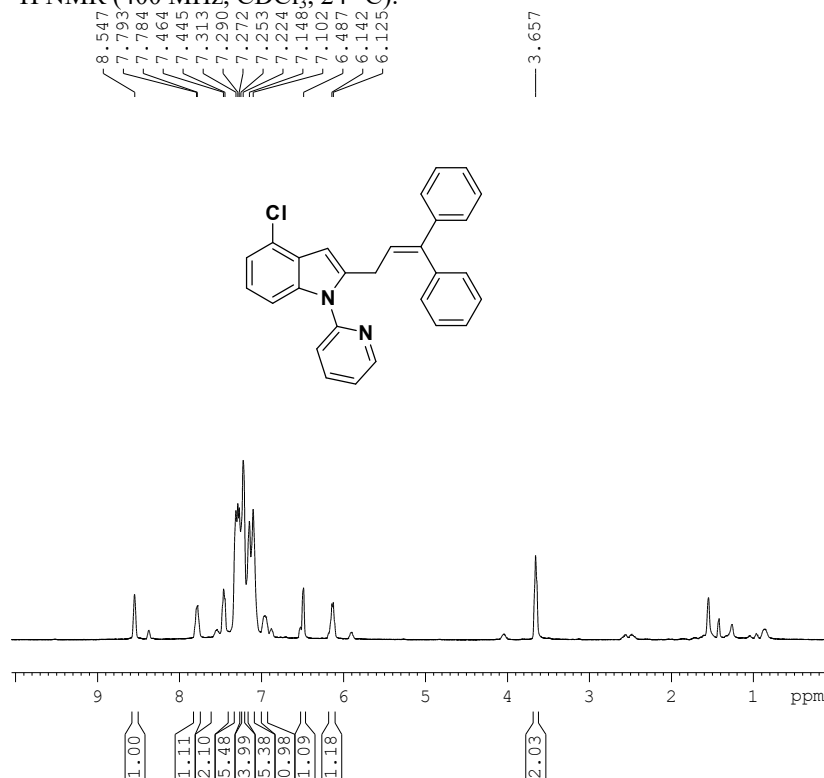


¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



4-Chloro-2-(3,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3k):

¹H NMR (400 MHz, CDCl₃, 24 °C):



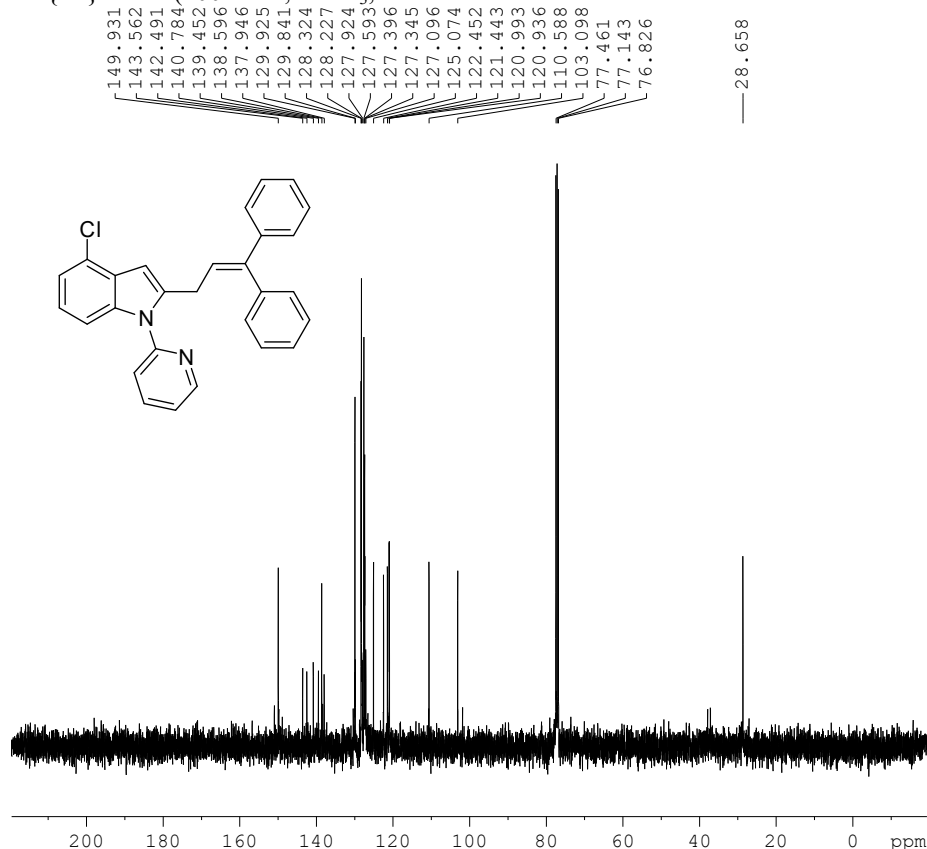
Current Data Parameters
NAME exp. no. 1067 and
EXPNO 448
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170924
Time_ 17.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 304.2 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300217 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):

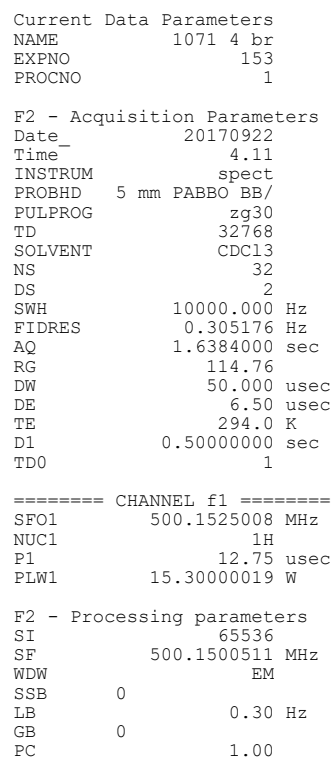


Current Data Paramete
NAME exp. no. 106
EXPNO 4
PROCNO

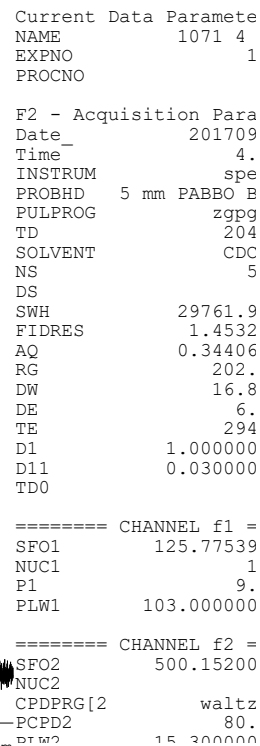
F2 - Acquisition Para
Date_ 201709
Time_ 17.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 305
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 1
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2] waltz
PCPD2 90.
PLW2 7.750000

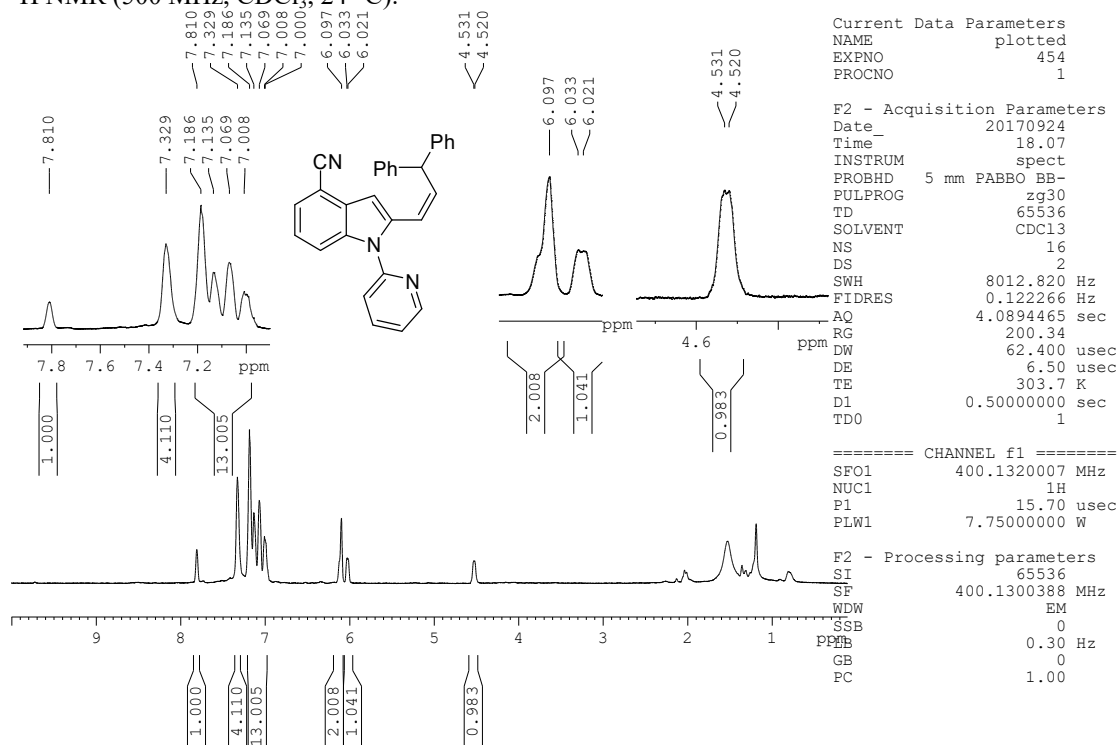
¹H NMR (500 MHz, CDCl₃, 24 °C):

H} NMR (125 MHz, CDCl₃, 24 °C:

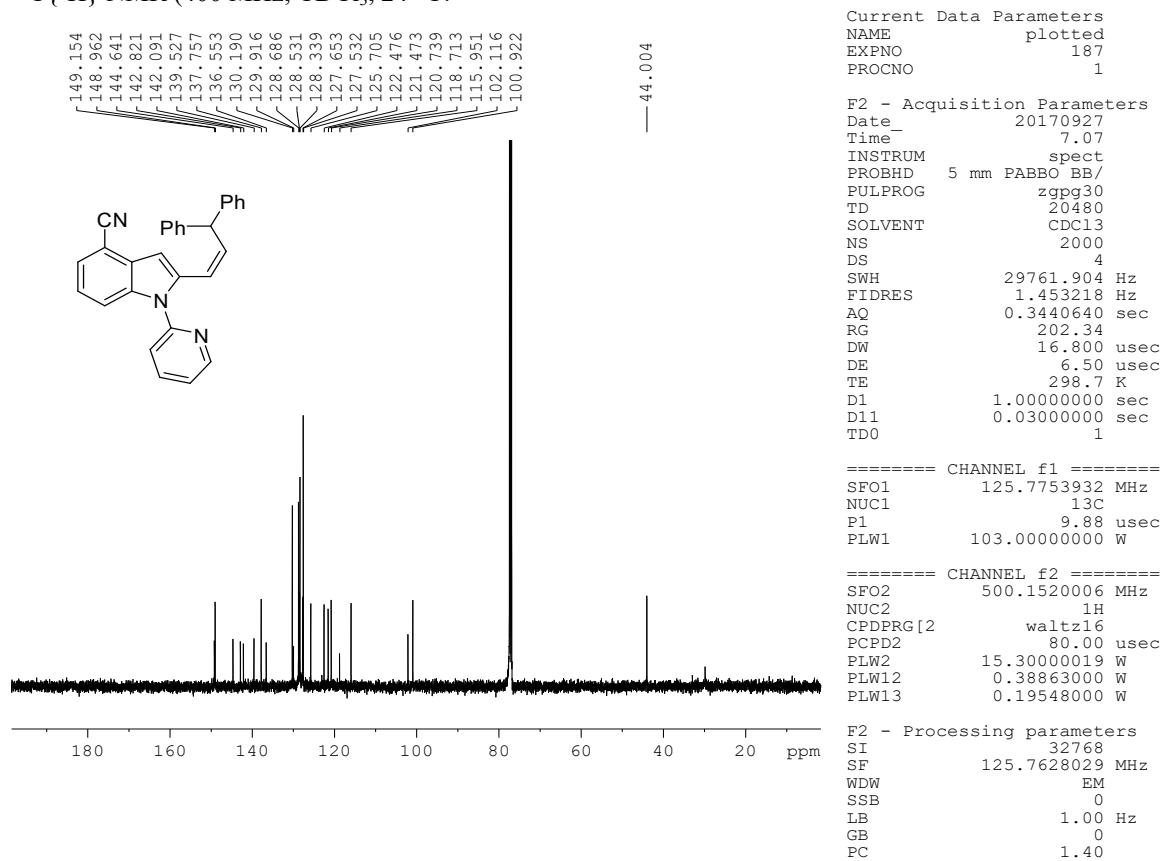


(E)-2-(3,3-Diphenylprop-1-en-1-yl)-1-(pyridin-2-yl)-1H-indole-4-carbonitrile(3m):

¹H NMR (500 MHz, CDCl₃, 24 °C):

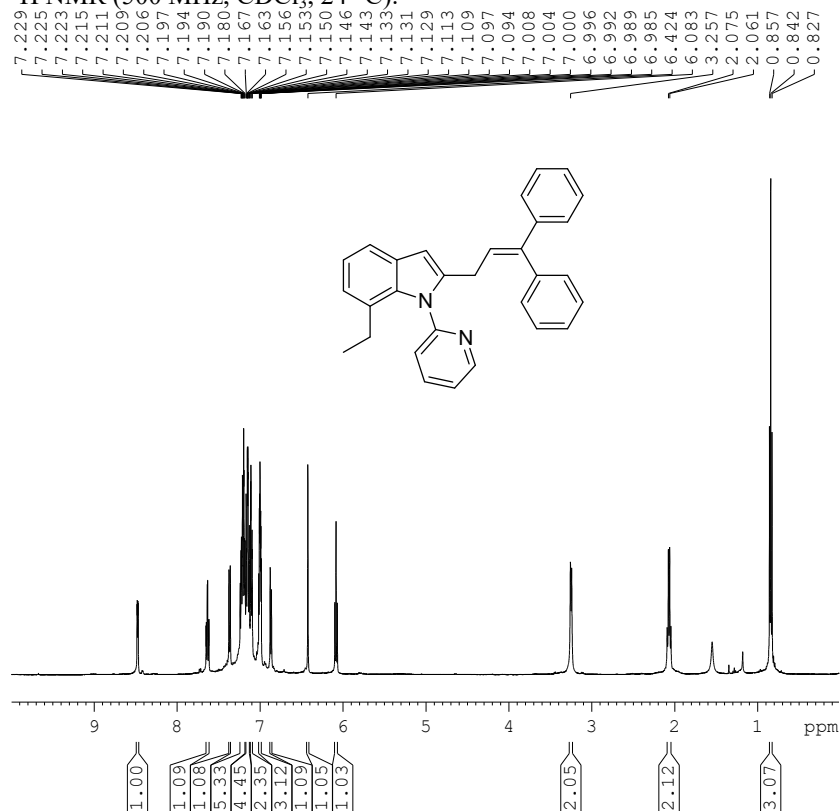


¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



2-(3,3-Diphenylallyl)-7-ethyl-1-(pyridin-2-yl)-1H-indole (3n):

¹H NMR (500 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME ex. no. 1059 7et
EXPNO 43
PROCNO 1

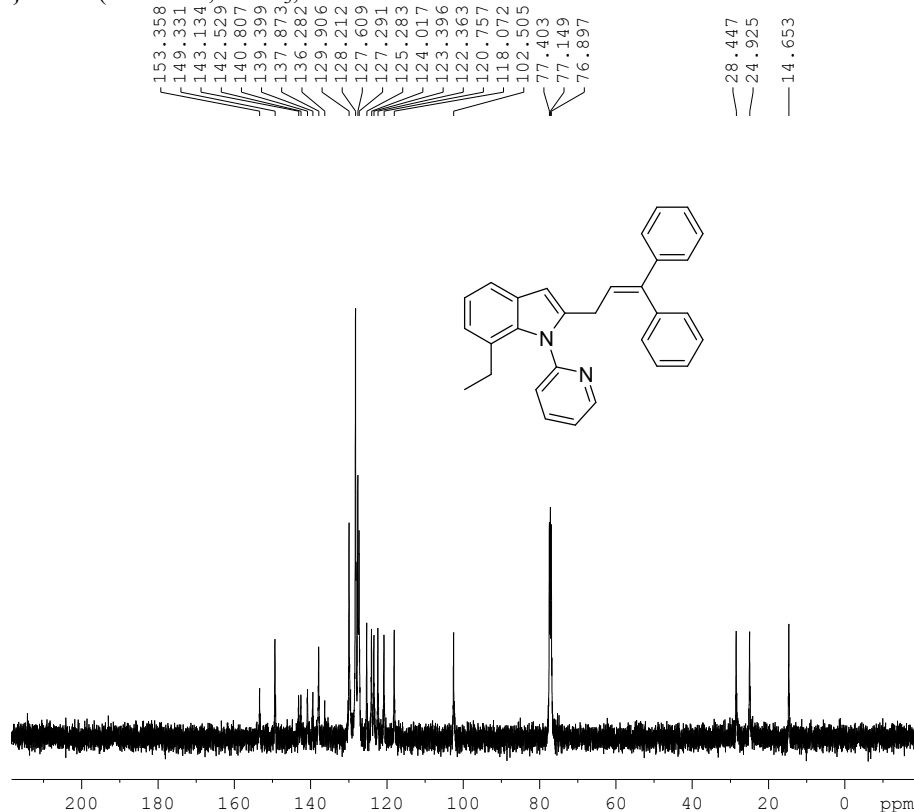
F2 - Acquisition Parameters
Date_ 20170911
Time 15.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 64
DW 50.000 usec
DE 6.50 usec
TE 299.8 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500679 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H

} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME ex. no. 1059
EXPNO
PROCNO

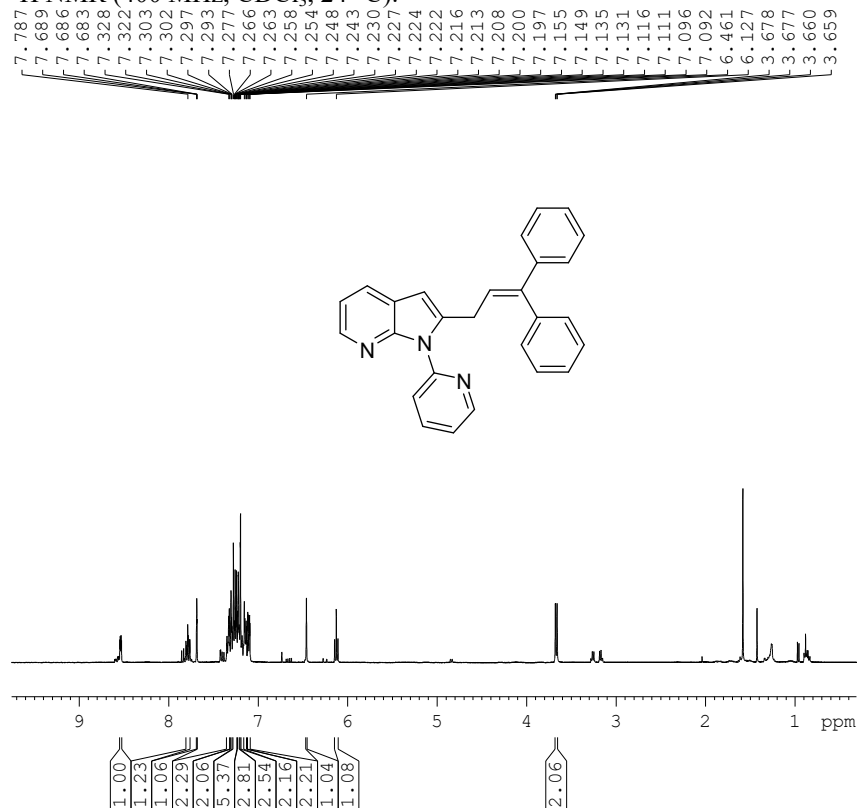
F2 - Acquisition Para
Date_ 201709
Time 7.
INSTRUM spe
PROBHD 5 mm PABBO E
PULPROG zgpg
TD 204
SOLVENT CDC
NS 5
DS
SWH 29761.9
FIDRES 1.4532
AQ 0.34406
RG 202.
DW 16.8
DE 6.
TE 300
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 125.77539
NUC1 1
P1 9.
PLW1 103.000000

===== CHANNEL f2 =
SFO2 500.15200
NUC2
CPDPRG[2] waltz
PCPD2 80.
D1W2 15.300000

2-(3,3-Diphenylallyl)-1-(pyridin-2-yl)-1H-pyrrolo[2,3-b]pyridine (3o):

¹H NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1035 7n prd
EXPNO 583
PROCNO 1

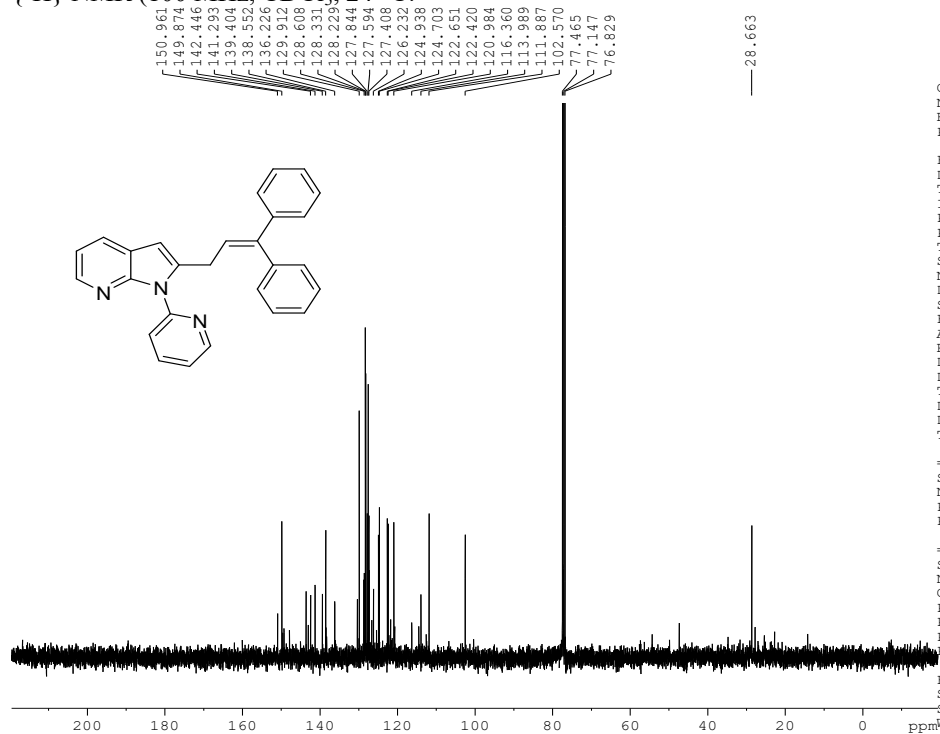
F2 - Acquisition Parameters
Date_ 20170827
Time_ 22.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300165 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C

{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1035 7n prd
EXPNO 584
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170827
Time_ 22.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 MHz
FIDRES 1.453353 MHz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

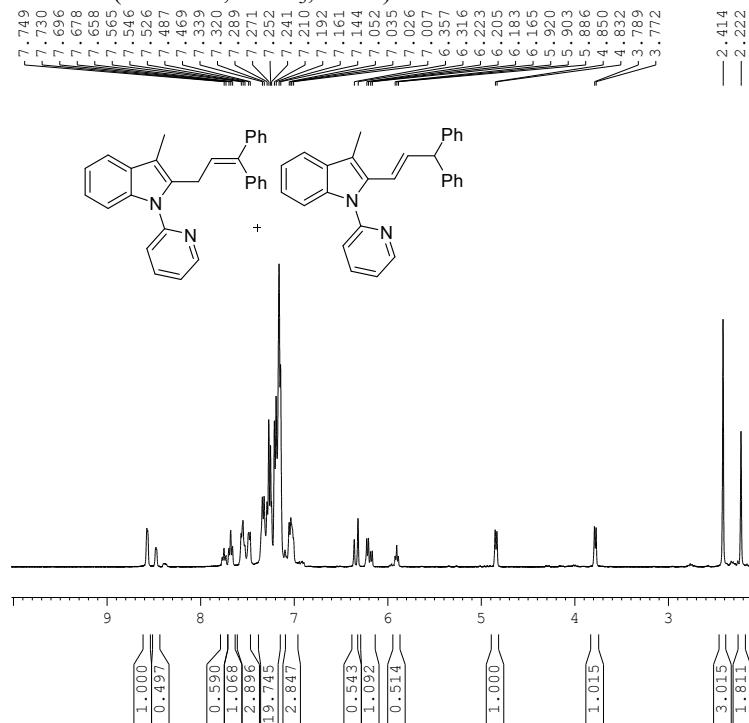
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 ¹³C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127586 MHz
WDW EM

2-(3,3-Diphenylallyl)-3-methyl-1-(pyridin-2-yl)-1H-indole and (E)-2-(3,3-Diphenylprop-1-en-1-yl)-3-methyl-1-(pyridin-2-yl)-1H-indole (3p):

¹H NMR (400 MHz, CDCl₃, 24 °C):

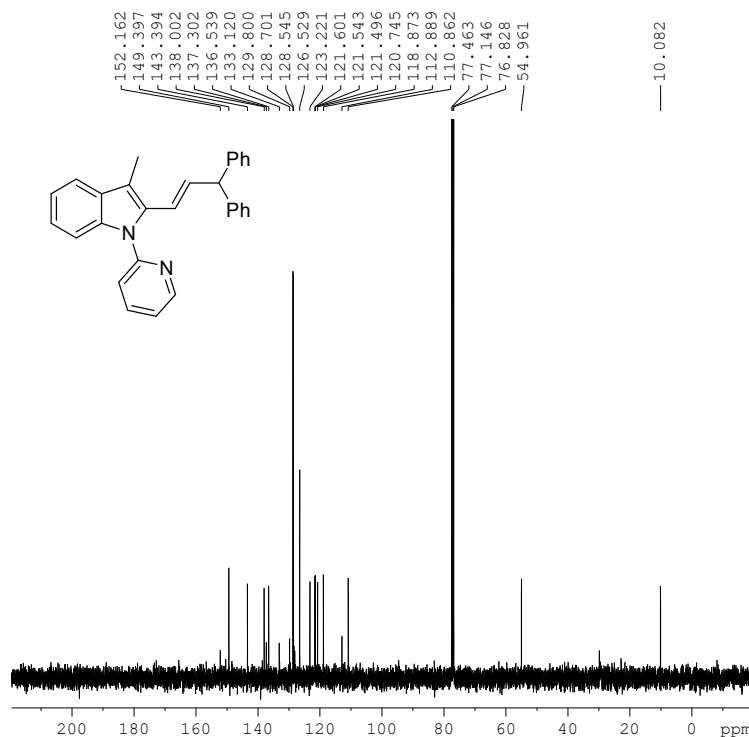


Current Data Parameters
NAME 1077 indole 3 methyl prd
EXPNO 27
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171003
Time 23.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 124.58
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.132007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300185 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 1077 indole 3 methyl prd
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171003
Time 23.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

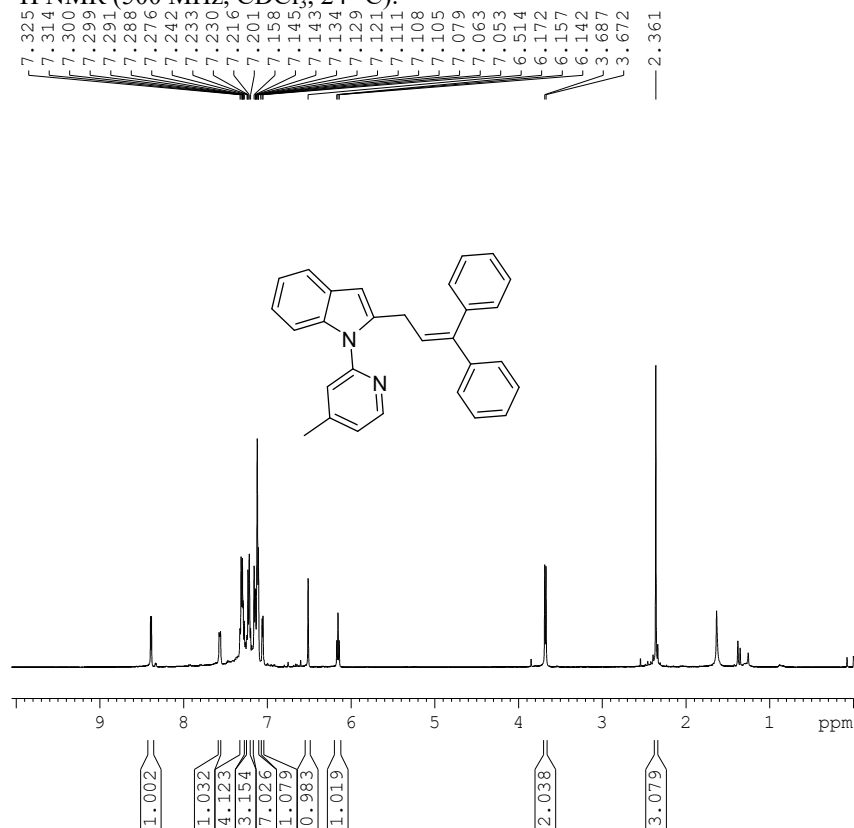
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127579 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-(3,3-Diphenylallyl)-1-(4-methylpyridin-2-yl)-1H-indole (3q):

¹H NMR (500 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME exp. no. 1020 3me py
EXPNO 118
PROCNO 1

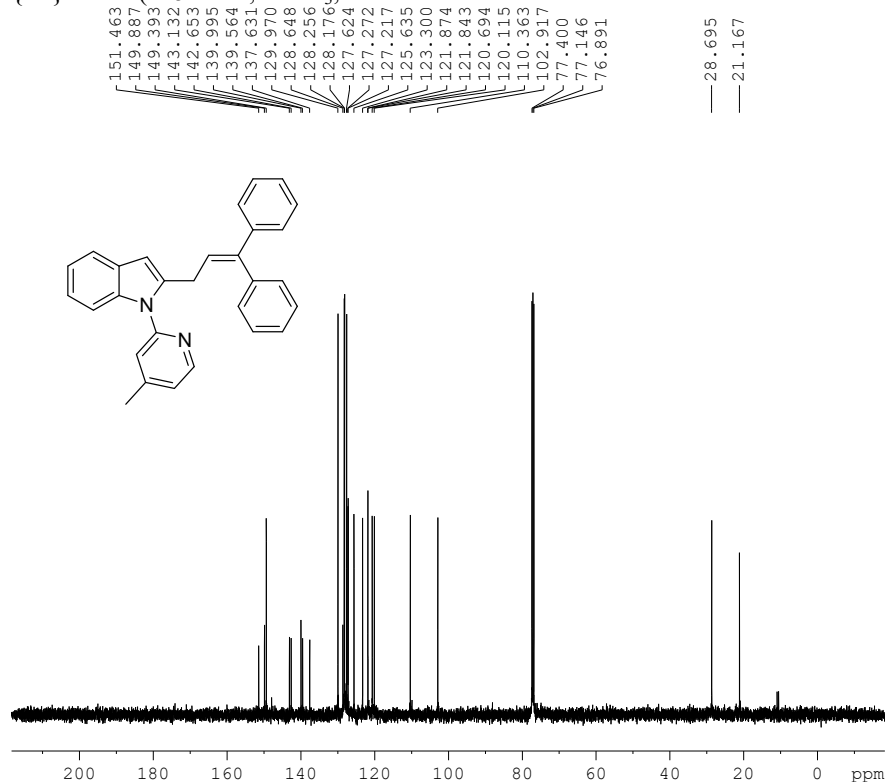
F2 - Acquisition Parameters
Date_ 20170814
Time_ 15.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 71.49
DW 50.000 usec
DE 6.50 usec
TE 300.9 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500269 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C

{¹H} NMR (125 MHz, CDCl₃, 24 °C):



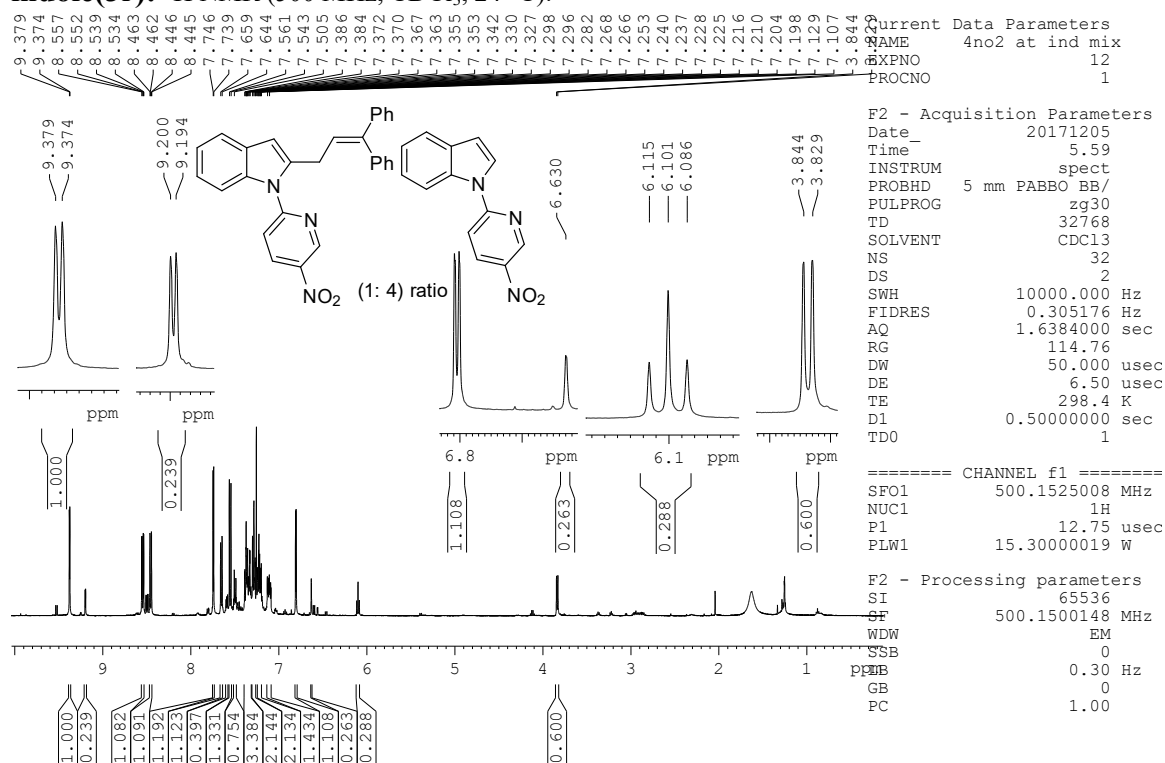
Current Data Paramete
NAME exp. no. 10
EXPNO 1
PROCNO

F2 - Acquisition Para
Date_ 201708
Time_ 15.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 204
SOLVENT CDC
NS 2
DS
SWH 29761.9
FIDRES 1.4532
AQ 0.34406
RG 202.
DW 16.8
DE 6.
TE 301
D1 1.000000
D11 0.030000
TD0

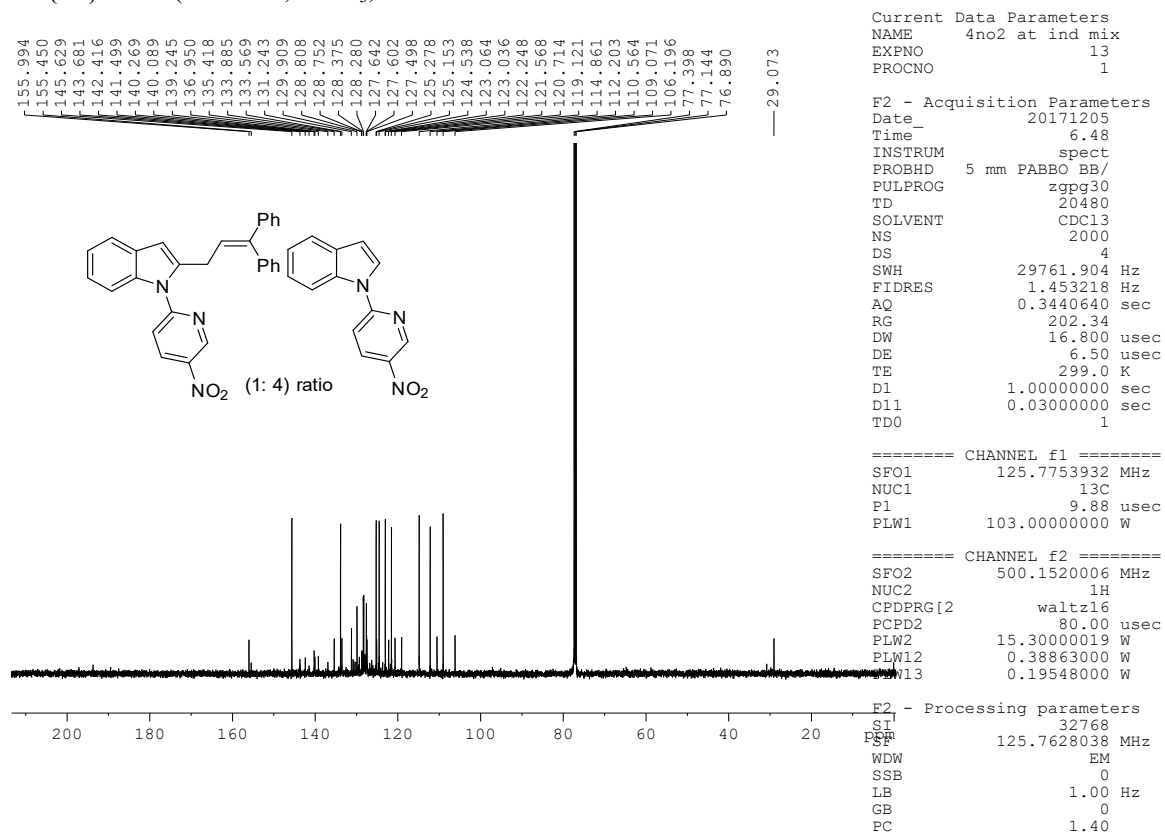
===== CHANNEL f1 =
SFO1 125.77539
NUC1 1
P1 9.
PLW1 103.000000

===== CHANNEL f2 =
SFO2 500.15200
NUC2
CPDPRG[2] waltz
PCPD2 80.
D11 15.300000

2-(3,3-Diphenylallyl)-1-(5-nitropyridin-2-yl)-1H-indole and 1-(5-nitropyridin-2-yl)-1H-indole(3r): ¹H NMR (500 MHz, CDCl₃, 24 °C):

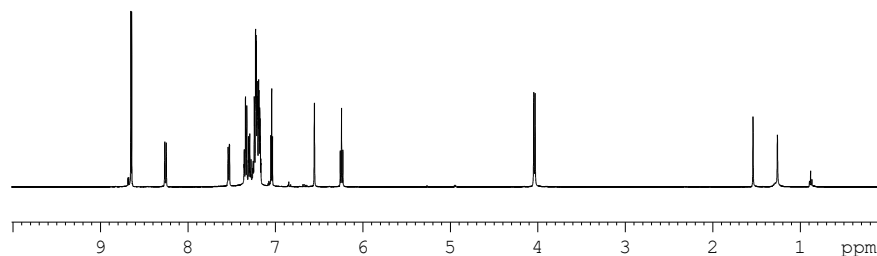
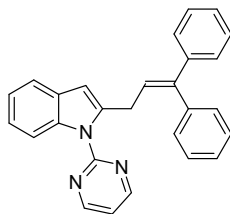


¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):

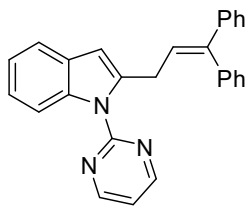
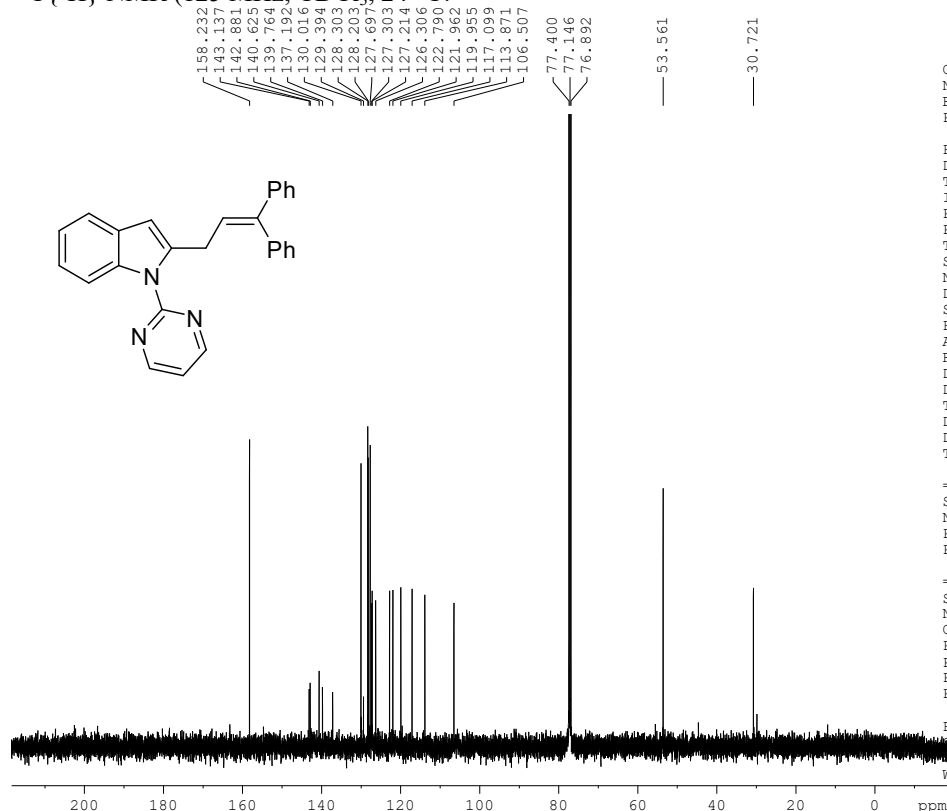


2-(3,3-diphenylallyl)-1-(pyrimidin-2-yl)-1H-indole (3s):

¹H NMR (500 MHz, CDCl₃, 24 °C):



¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 994 pym direct allyl
EXPNO 150
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170720
Time 18.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 71.49
DW 50.000 usec
DE 6.50 usec
TE 302.0 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500286 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME spa50617
EXPNO 99
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170623
Time 7.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 256
DS 4
SWH 29761.904 F
FIDRES 1.453218 F
AQ 0.3440640 s
RG 202.34
DW 16.800 u
DE 6.50 u
TE 296.4 F
D1 1.00000000 s
D11 0.03000000 s
TD0 1

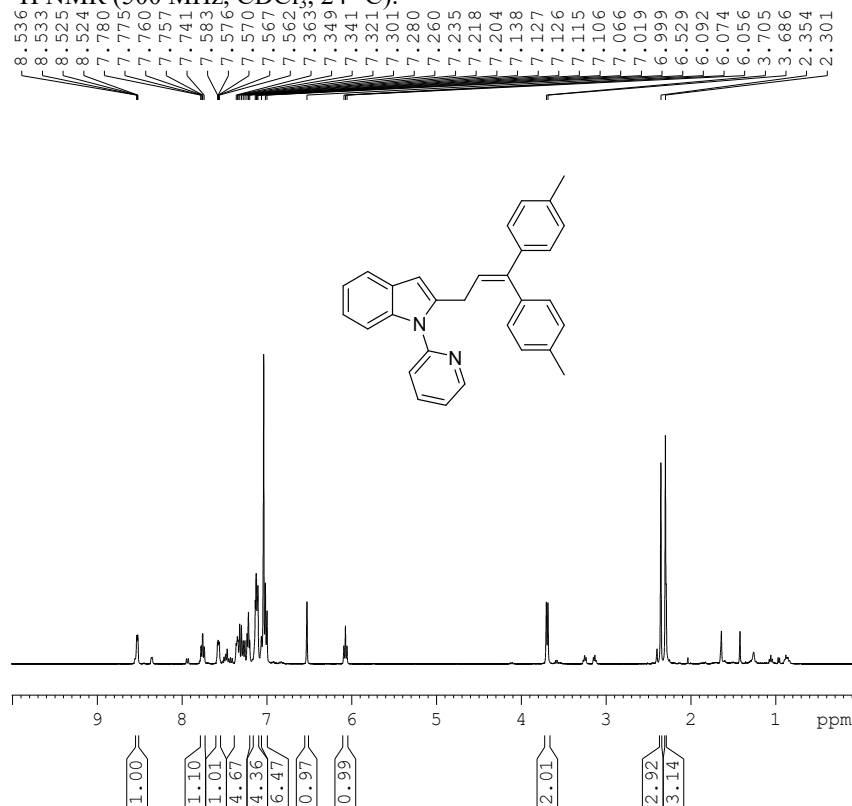
===== CHANNEL f1 =====
SFO1 125.7753932 M
NUC1 13C
P1 9.88 u
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 M
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 u
PLW2 15.30000019 W
PLW12 0.38863000 W
PLW13 0.19548000 W

F2 - Processing parameter
SI 32768
SF 125.7628049 M
WDW EM

2-(3,3-Di-p-tolylallyl)-1-(pyridin-2-yl)-1H-indole (3t):

¹H NMR (500 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1171 ph me symmetric
EXPNO 540
PROCNO 1

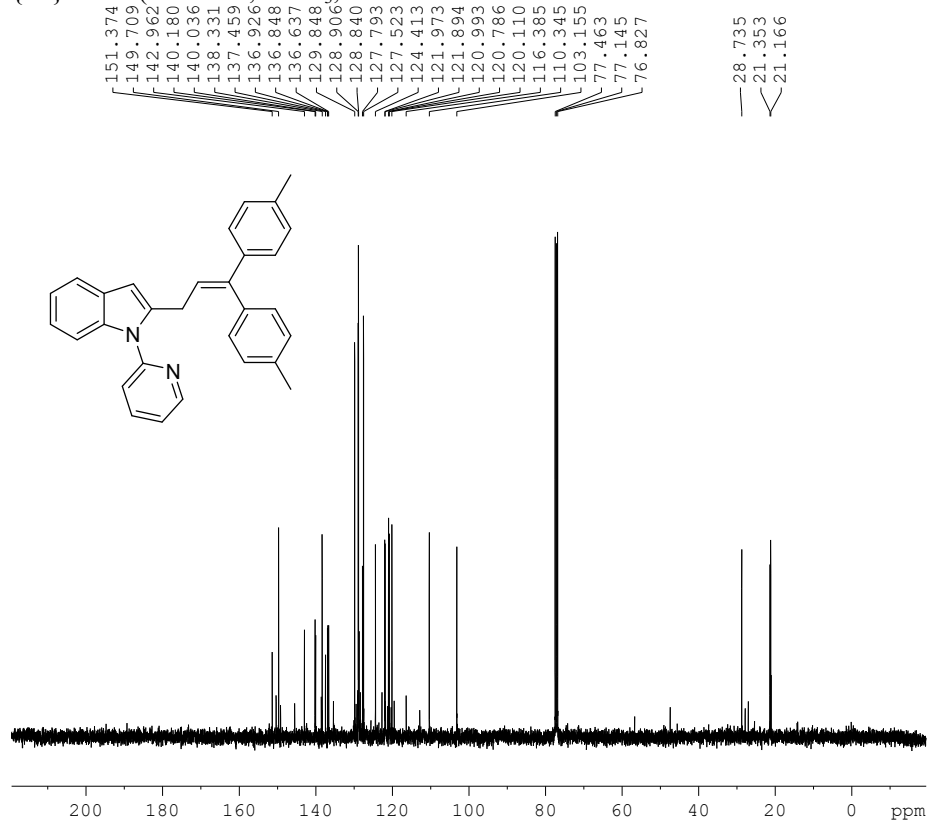
F2 - Acquisition Parameters
Date_ 20171227
Time_ 10.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.51
DW 62.400 usec
DE 6.50 usec
TE 293.5 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300268 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C

{¹H} NMR (100 MHz, CDCl₃, 24 °C):



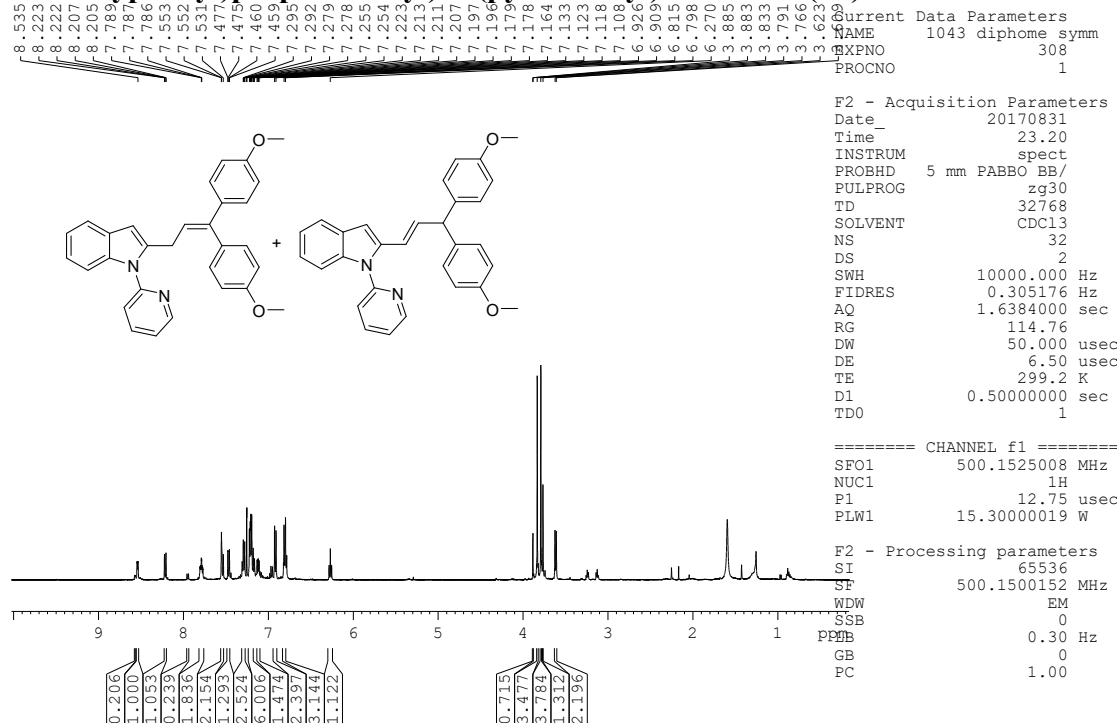
Current Data Parameters
NAME 1171 ph me s
EXPNO 5
PROCNO

F2 - Acquisition Parameters
Date_ 201712
Time_ 10.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 294
D1 1.000000
D11 0.030000
TD0

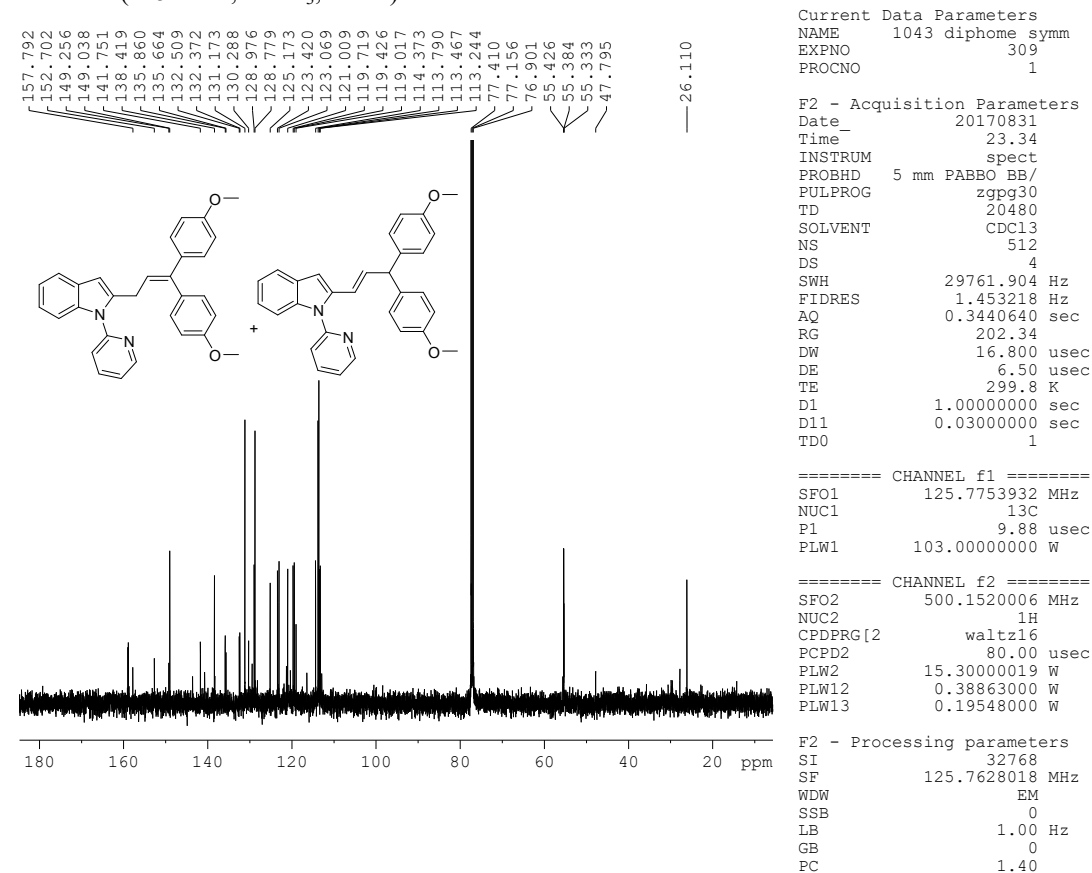
===== CHANNEL f1 =
SFO1 100.62282
NUC1 1
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2 waltz
PCPD2 90.
PRW2 7.750000

2-(3,3-bis(4-methoxyphenyl)allyl)-1-(pyridin-2-yl)-1H-indole and (E)-2-(3,3-bis(4-methoxyphenyl)prop-1-en-1-yl)-1-(pyridin-2-yl)-1H-indole(3u):

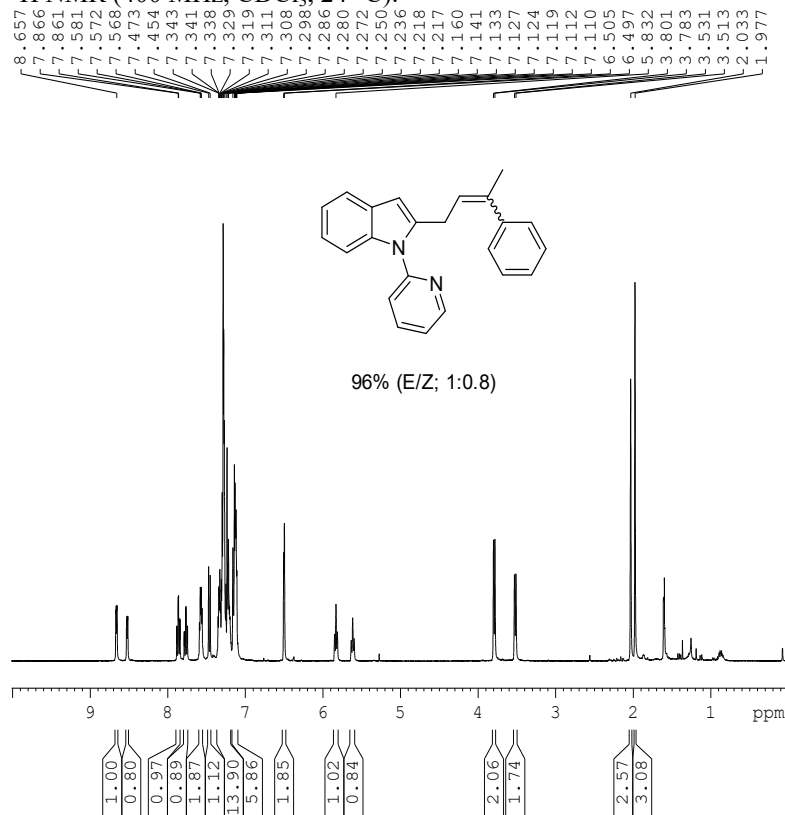


¹³C NMR (125 MHz, CDCl₃, 24 °C):



Mixture of (Z)-2-(3-Phenylbut-2-en-1-yl)-1-(pyridin-2-yl)-1H-indole and (E)-2-(3-Phenylbut-2-en-1-yl)-1-(pyridin-2-yl)-1H-indole (3v):

¹H NMR (400 MHz, CDCl₃, 24 °C):



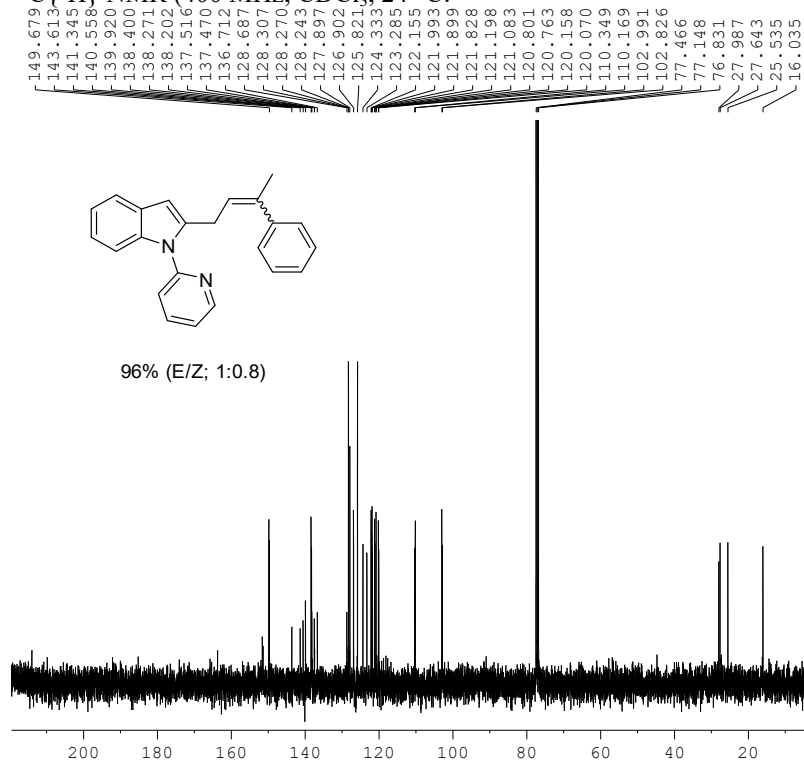
Current Data Parameters
NAME ex.no. 889 and 890
EXPNO 247
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170510
Time_ 1.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300193 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME ex.no. 889 a
EXPNO 2
PROCNO

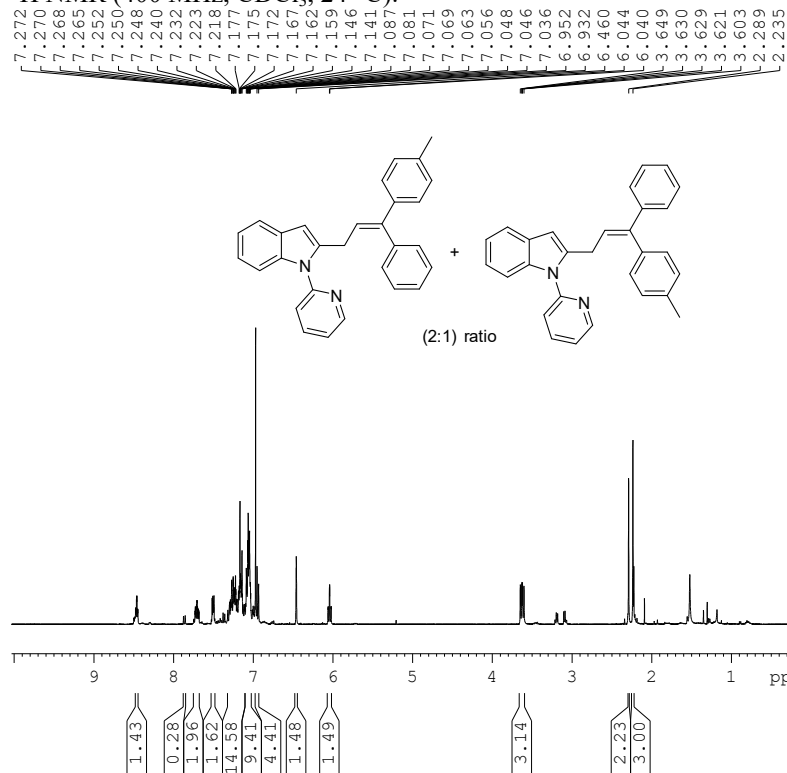
F2 - Acquisition Para
Date_ 201705
Time_ 1.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 1
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 295
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 1
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
P1
PLW1
=====

(E)-2-(3-phenyl-3-(p-tolyl)allyl)-1-(pyridin-2-yl)-1H-indole and (Z)-2-(3-phenyl-3-(p-tolyl)allyl)-1-(pyridin-2-yl)-1H-indole(3w):

¹H NMR (400 MHz, CDCl₃, 24 °C):



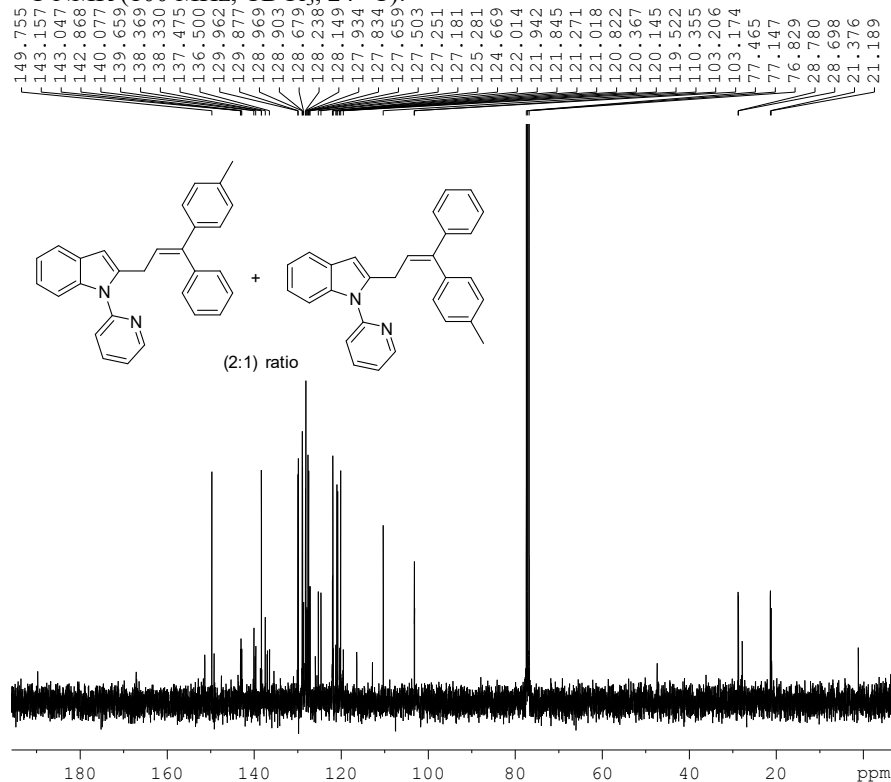
Current Data Parameters
NAME 1158 me ph mix isome
EXPNO 430
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171219
Time 18.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.77
DW 62.400 usec
DE 6.50 usec
TE 293.4 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300469 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1158 me ph m
EXPNO 4
PROCNO

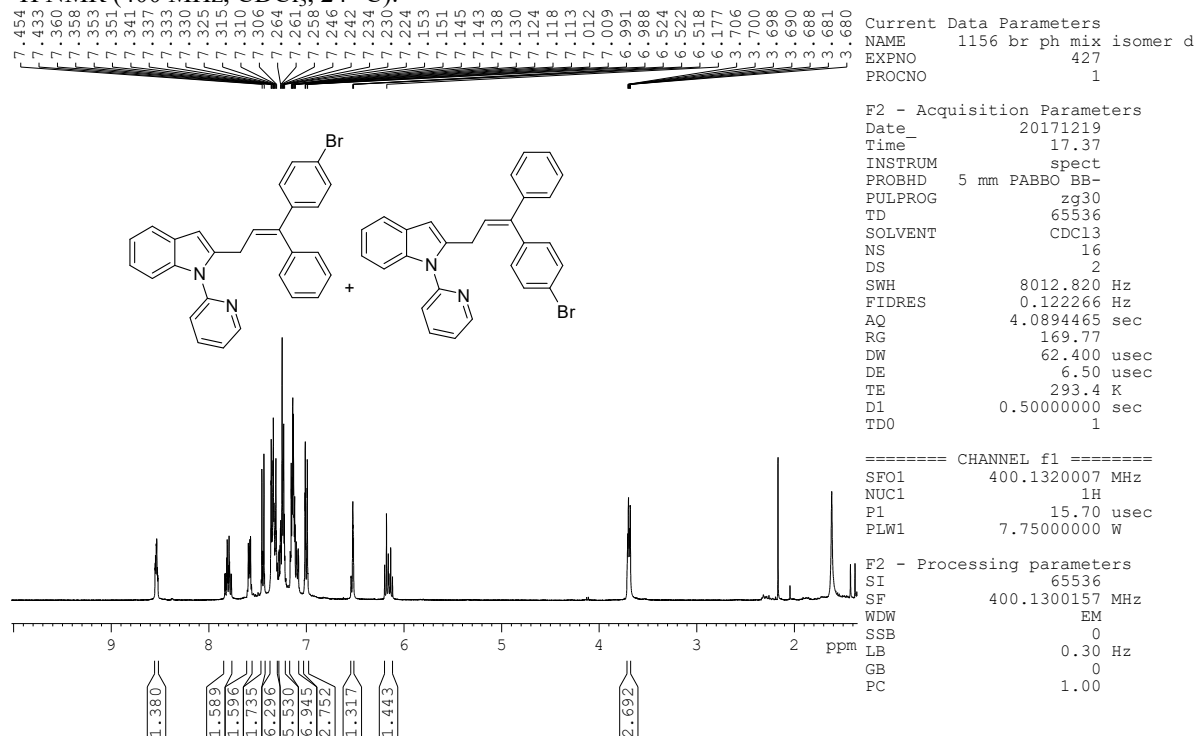
F2 - Acquisition Parameters
Date_ 201712
Time 18.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 293
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SF01 100.62282
NUC1 1
P1 9.
PLW1 47.000000

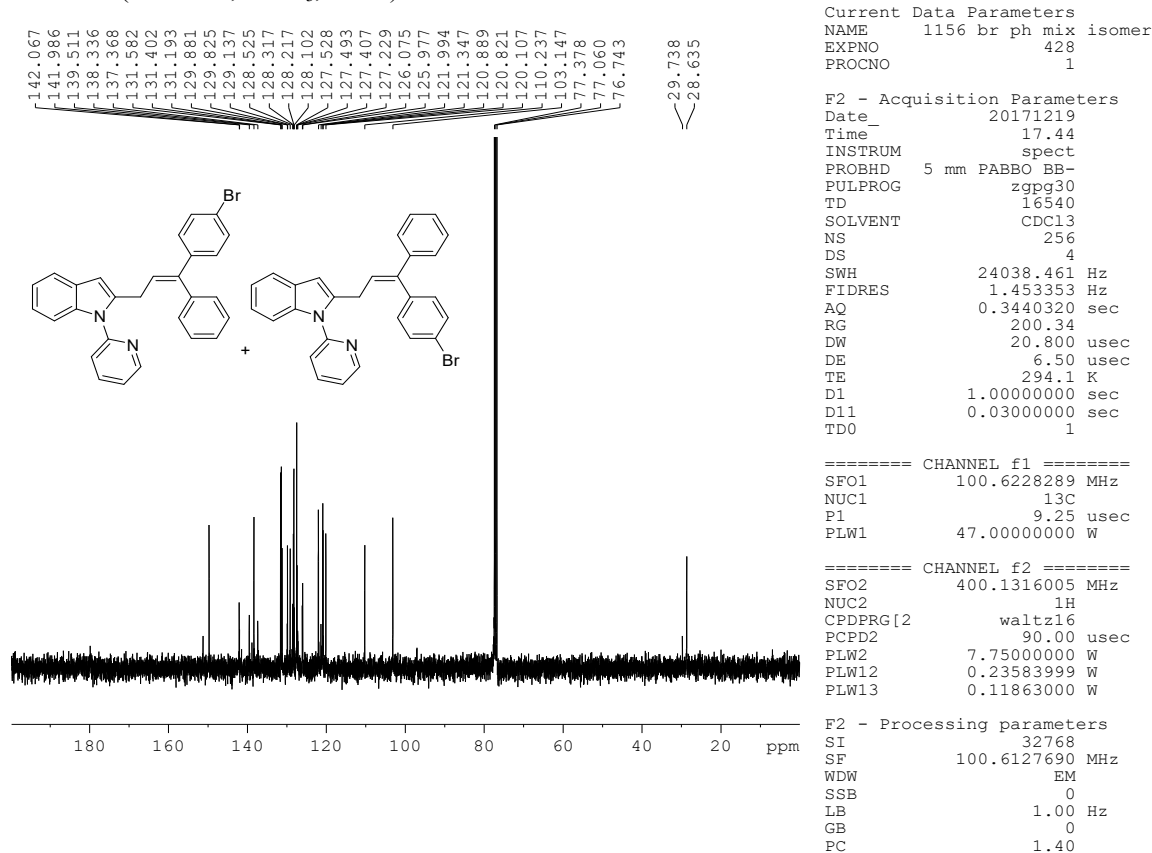
===== CHANNEL f2 =
SF02 400.13160
NUC2
CPDPRG[2 waltz
PCPD2 90.
PLW2 7.750000

(E)-2-(3-(4-bromophenyl)-3-phenylallyl)-1-(pyridin-2-yl)-1H-indole and (Z)-2-(3-(4-bromophenyl)-3-phenylallyl)-1-(pyridin-2-yl)-1H-indole (3x):

¹H NMR (400 MHz, CDCl₃, 24 °C):

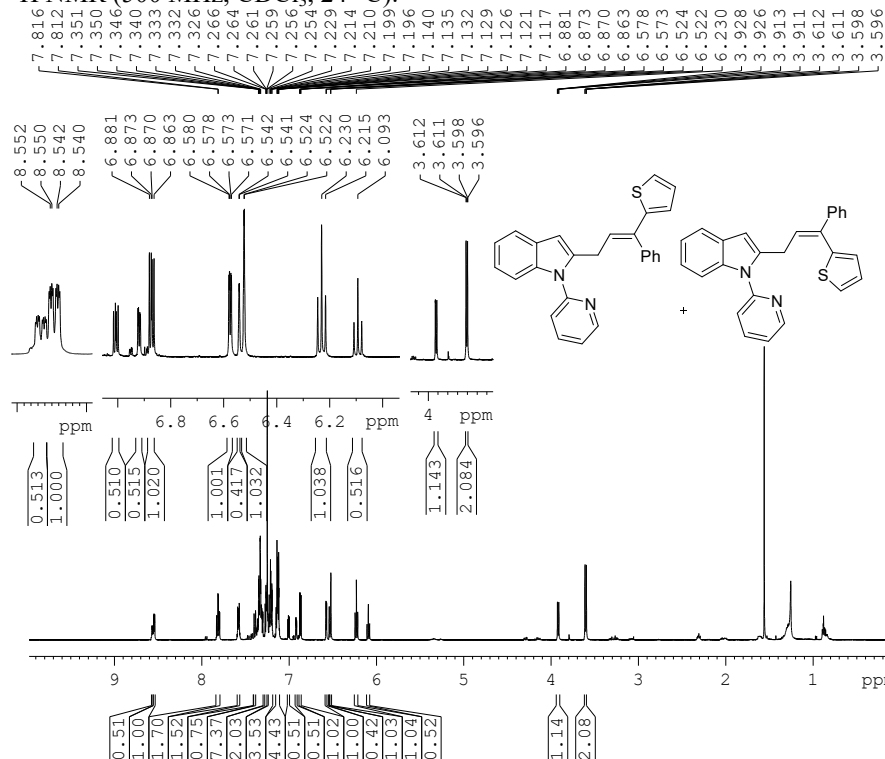


¹³C NMR (100 MHz, CDCl₃, 24 °C):



Mixture of (E)-2-(3-Phenyl-3-(thiophen-2-yl)allyl)-1-(pyridin-2-yl)-1H-indole and (Z)-2-(3-phenyl-3-(thiophen-2-yl)allyl)-1-(pyridin-2-yl)-1H-indole (3y):

¹H NMR (500 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1231thiol allyl arer
EXPNO 15
PROCNO 1

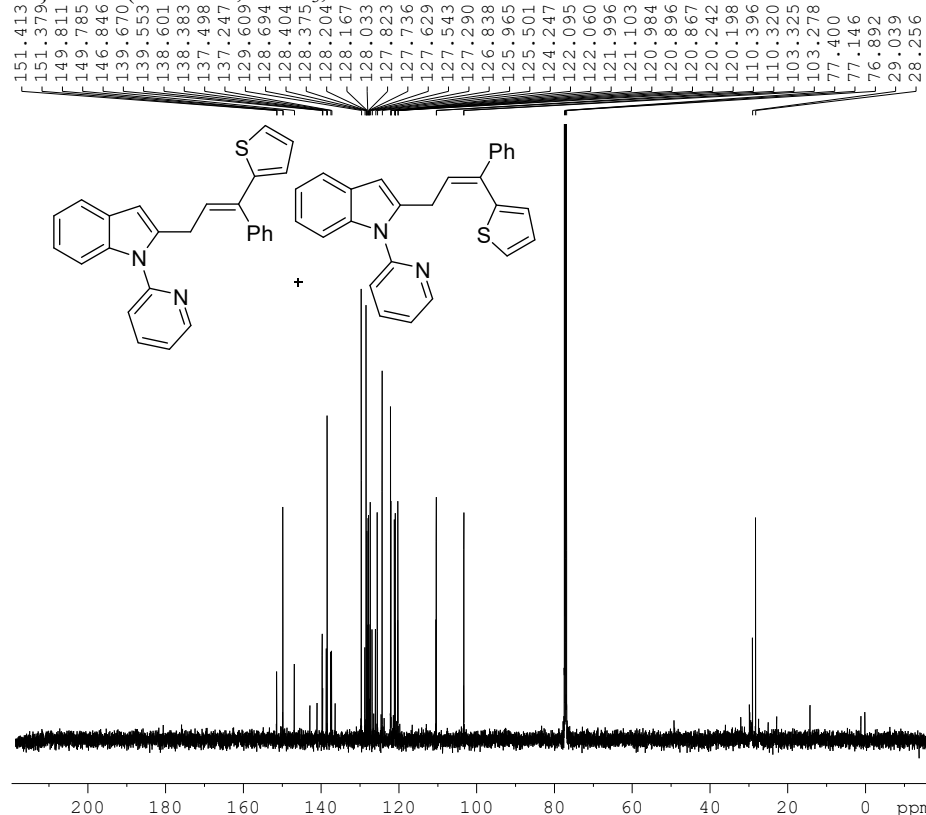
F2 - Acquisition Parameters
Date_ 20180302
Time 7.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 114.76
DW 50.000 usec
DE 6.50 usec
TE 299.4 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 12.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500163 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{

¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME 1231thiol al
EXPNO
PROCNO

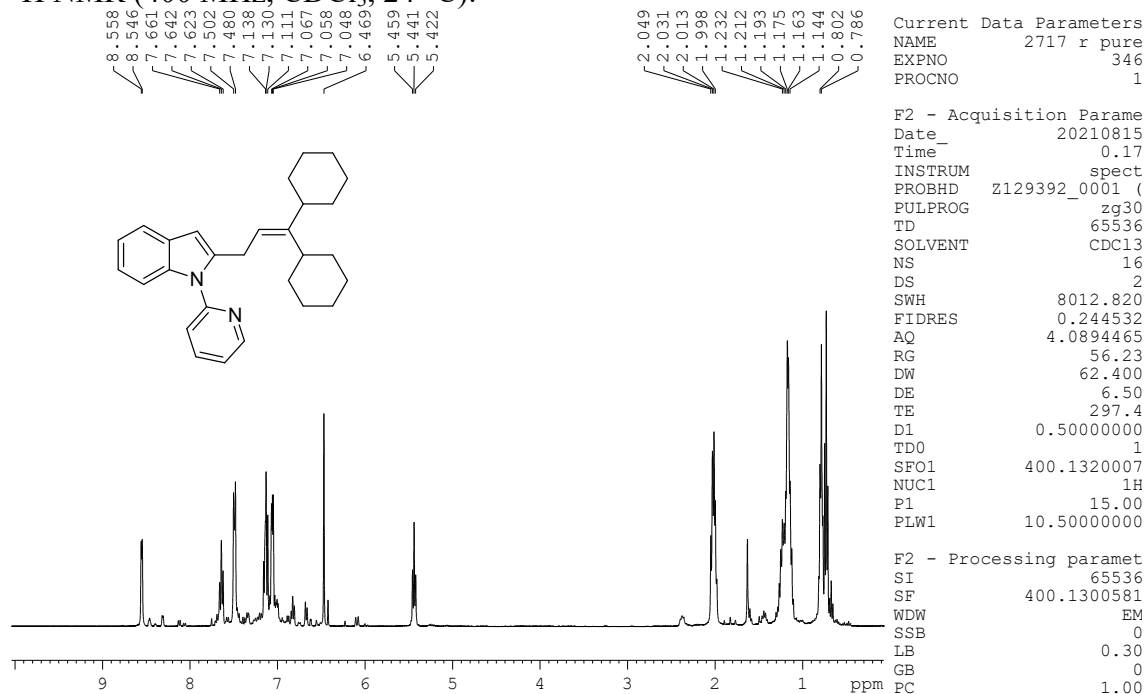
F2 - Acquisition Para
Date_ 201803
Time 8.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 204
SOLVENT CDC
NS 20
DS
SWH 29761.9
FIDRES 1.4532
AQ 0.34406
RG 202.
DW 16.8
DE 6.
TE 300
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 125.77539
NUC1 1
P1 9.
PLW1 103.000000

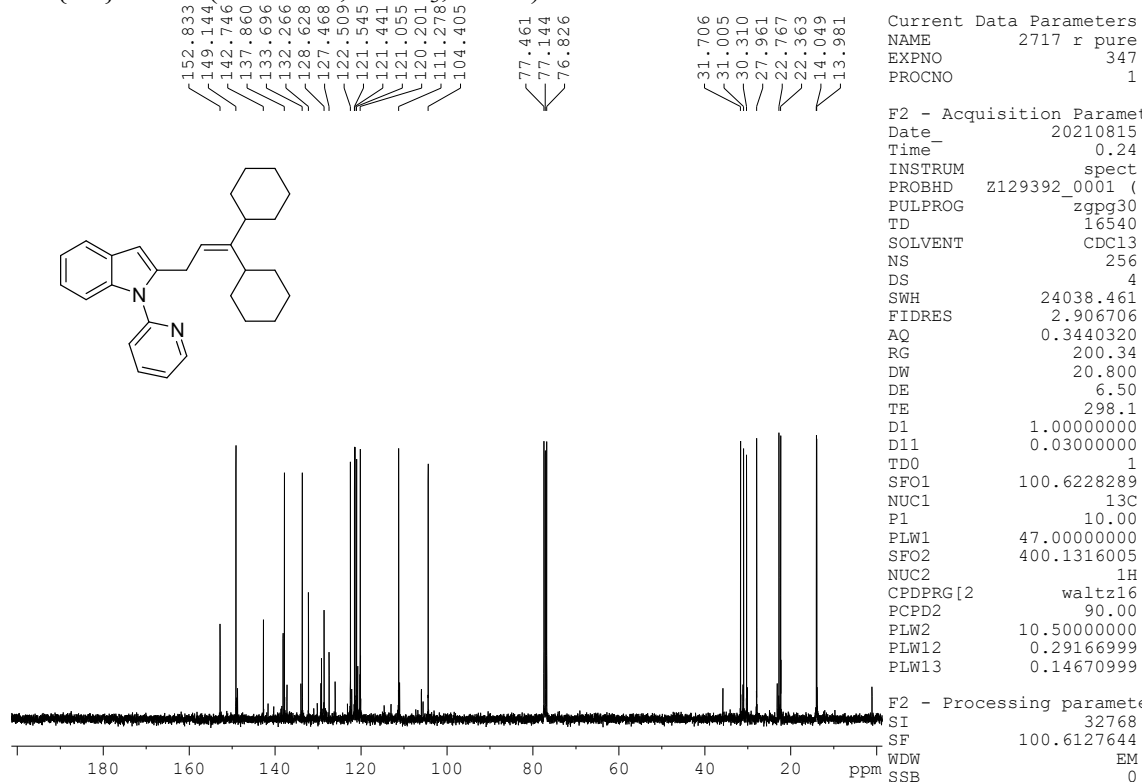
===== CHANNEL f2 =
SFO2 500.15200
NUC2
CPDPRG[2] waltz
PCPD2 80.
PTW2 15.200000

2-(3,3-Dicyclohexylallyl)-1-(pyridin-2-yl)-1H-indole (3z):

¹H NMR (400 MHz, CDCl₃, 24 °C):

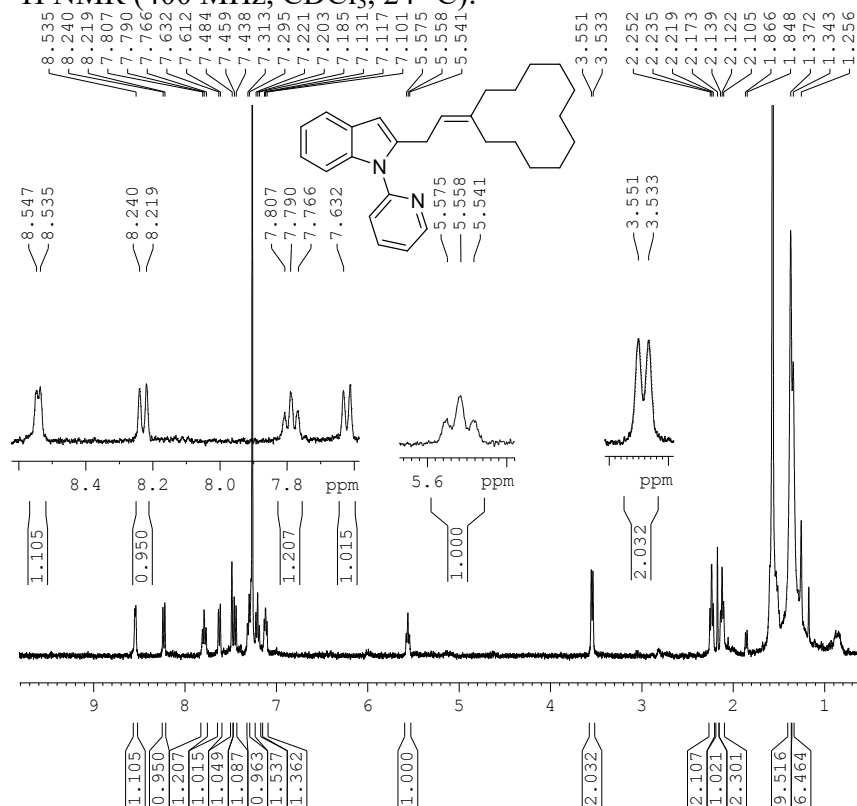


¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



2-(2-Cyclododecylideneethyl)-1-(pyridin-2-yl)-1H-indole (3aa):

¹H NMR (400 MHz, CDCl₃, 24 °C):

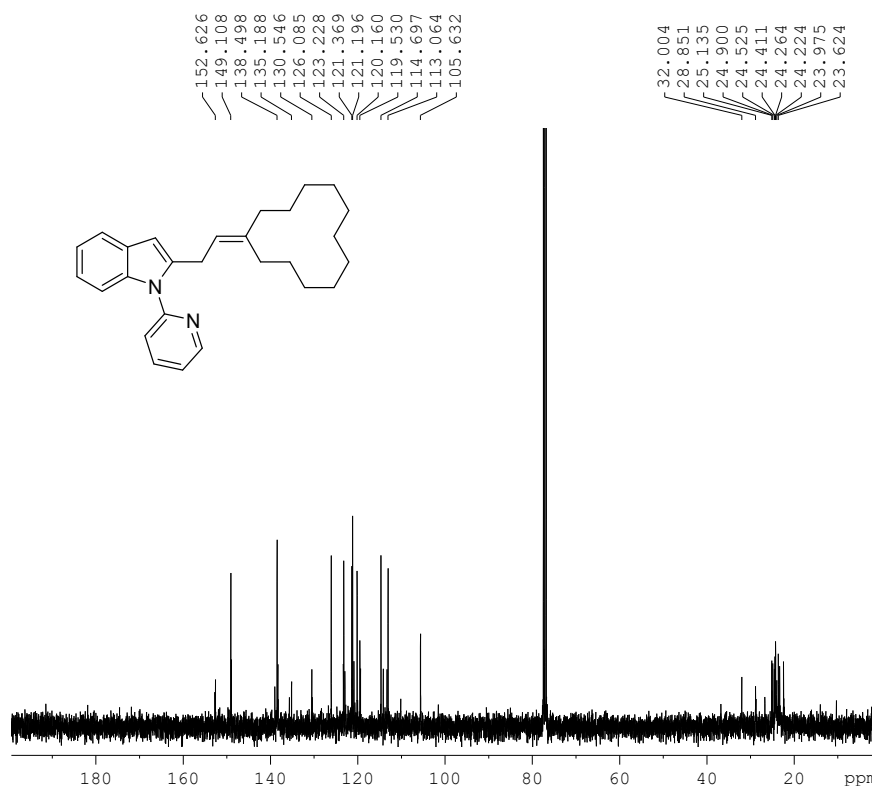


Current Data Parameters
NAME 2711 i final
EXPNO 3
PROCNO 1

F2 - Acquisition Paramet
Date_ 20210802
Time 8.46
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820
FIDRES 0.244532
AQ 4.0894465
RG 200.34
DW 62.400
DE 6.50
TE 297.7
D1 0.50000000
TD0 1
SFO1 400.1320007
NUC1 1H
P1 15.00
PLW1 10.50000000

F2 - Processing paramet
SI 65536
SF 400.1300091
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 2711 i final
EXPNO 10
PROCNO 1

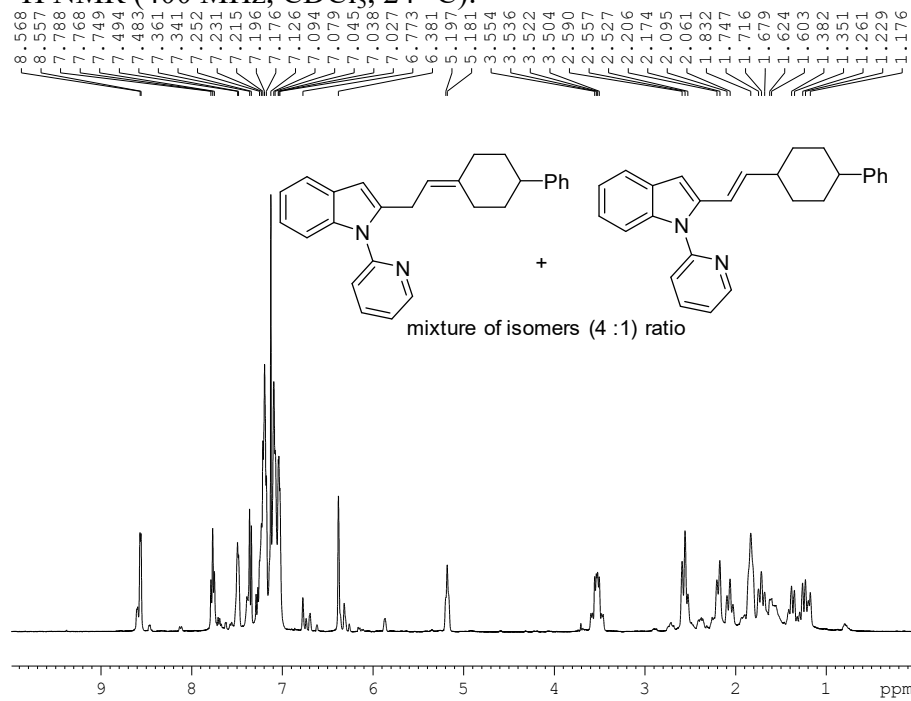
F2 - Acquisition Paramet
Date_ 20210802
Time 12.05
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 188
DS 4
SWH 24038.461
FIDRES 2.906706
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 297.8
D1 1.00000000
D11 0.03000000
TD0 1
SFO1 100.6228289
NUC1 13C
P1 10.00
PLW1 47.00000000
SFO2 400.1316005
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00
PLW2 10.50000000
PLW12 0.29166999
PLW13 0.14670999

F2 - Processing paramet
SI 32768
SF 100.6127599
WDW EM
SSB 0
LB 1.00

2-(2-(4-Phenylcyclohexylidene)ethyl)-1-(pyridin-2-yl)-1H-indole
Phenylcyclohexyl)vinyl)-1-(pyridin-2-yl)-1H-indole (3ab):

and **(E)-2-(2-(4-**

¹H NMR (400 MHz, CDCl₃, 24 °C):

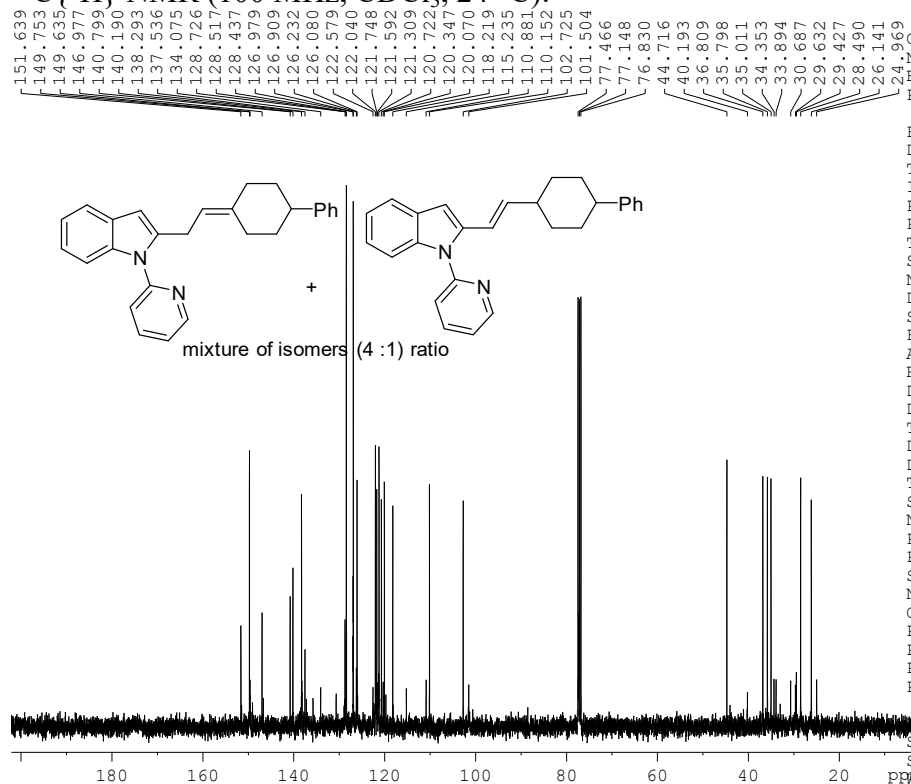


Current Data Parameters
NAME ksr 2710 final
EXPNO 21
PROCNO 1

F2 - Acquisition Paramet
Date_ 20210803
Time_ 11.06
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820
FIDRES 0.244532
AQ 4.0894465
RG 79.8
DW 62.400
DE 6.50
TE 298.2
D1 0.50000000
TD0 1
SFO1 400.1320007
NUC1 1H
P1 15.00
PLW1 10.50000000

F2 - Processing paramet
SI 65536
SF 400.1300629
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



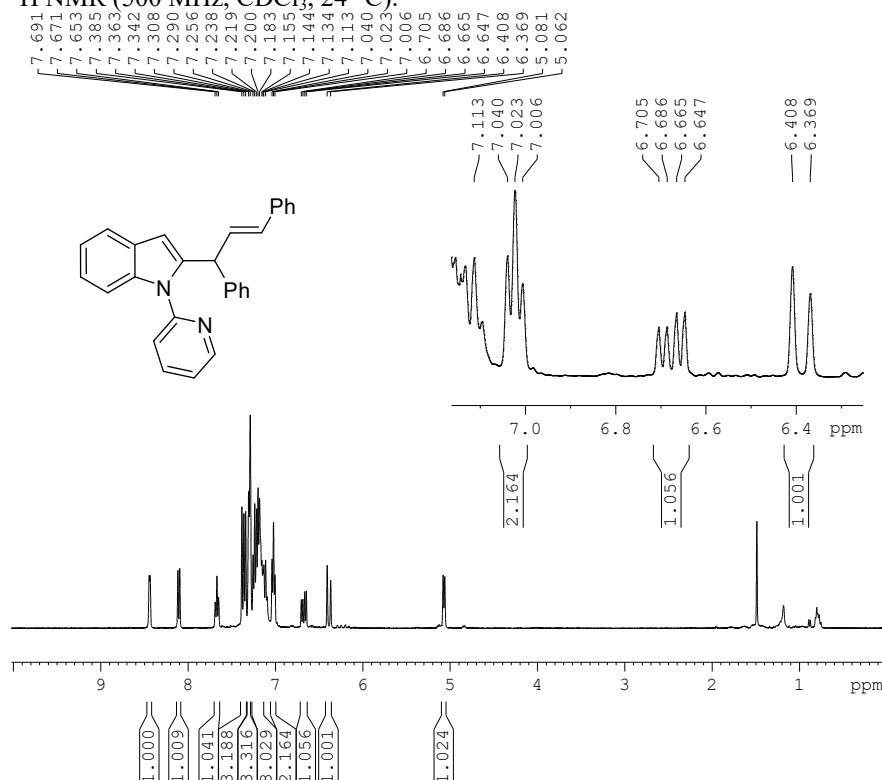
Current Data Parameters
NAME ksr 2710 final
EXPNO 22
PROCNO 1

F2 - Acquisition Paramet
Date_ 20210803
Time_ 11.13
INSTRUM spect
PROBHD Z129392_0001 (
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461
FIDRES 2.906706
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 298.2
D1 1.00000000
D11 0.03000000
TD0 1
SFO1 100.6228289
NUC1 13C
P1 10.00
PLW1 47.00000000
SFO2 400.1316005
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00
PLW2 10.50000000
PLW12 0.29166999
PLW13 0.14670999

F2 - Processing paramet
SI 32768
SF 100.6127647
PPWDW EM

(E)-3-(1,3-diphenylallyl)-1-(pyridin-2-yl)-1H-indole(3ac):

¹H NMR (500 MHz, CDCl₃, 24 °C):



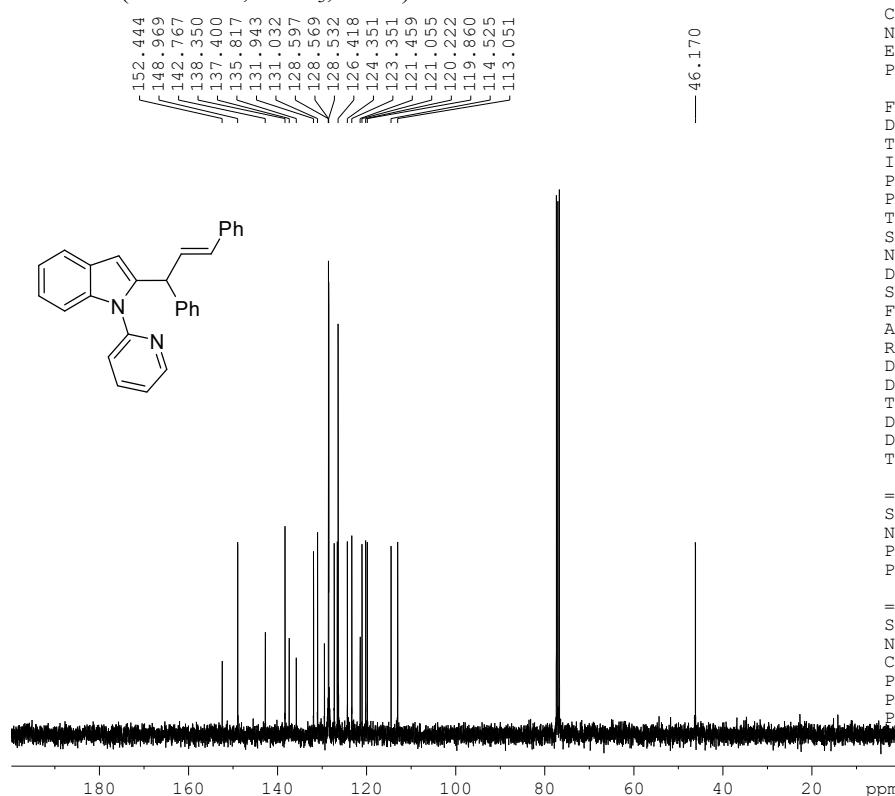
Current Data Parameters
NAME ksr_2082 proto
EXPNO 9
PROCNO 1

F2 - Acquisition Paramet
Date_ 20200503
Time 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 2
SWH 8012.820
FIDRES 0.122266
AQ 4.0894465
RG 169.77
DW 62.400
DE 6.50
TE 297.4
D1 0.50000000
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007
NUC1 1H
P1 15.70
PLW1 7.75000000

F2 - Processing paramet
SI 65536
SF 400.1300558
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME ksr_2082 proton
EXPNO 7
PROCNO 1

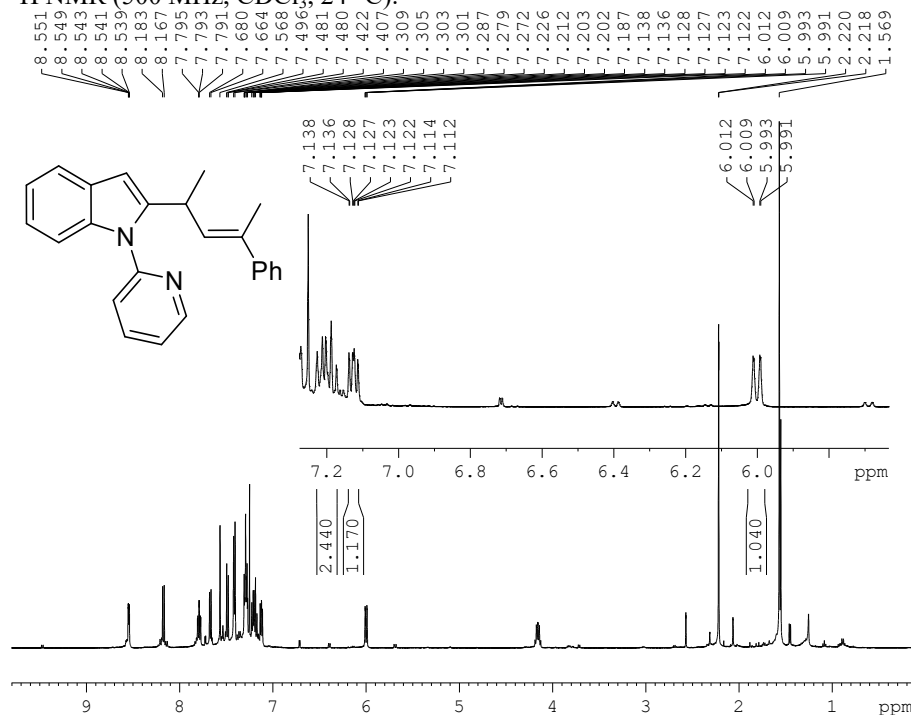
F2 - Acquisition Paramet
Date_ 20200503
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 193
DS 4
SWH 24038.461
FIDRES 1.453353
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 297.5
D1 1.00000000
D11 0.03000000
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228289
NUC1 13C
P1 9.25
PLW1 47.00000000

===== CHANNEL f2 =====
SFO2 400.1316005
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00
PLW2 7.75000000
PLW12 0.23583999
PLW13 0.11863000

(E)-3-(4-phenylpent-3-en-2-yl)-1-(pyridin-2-yl)-1H-indole (3ad):

¹H NMR (500 MHz, CDCl₃, 24 °C):



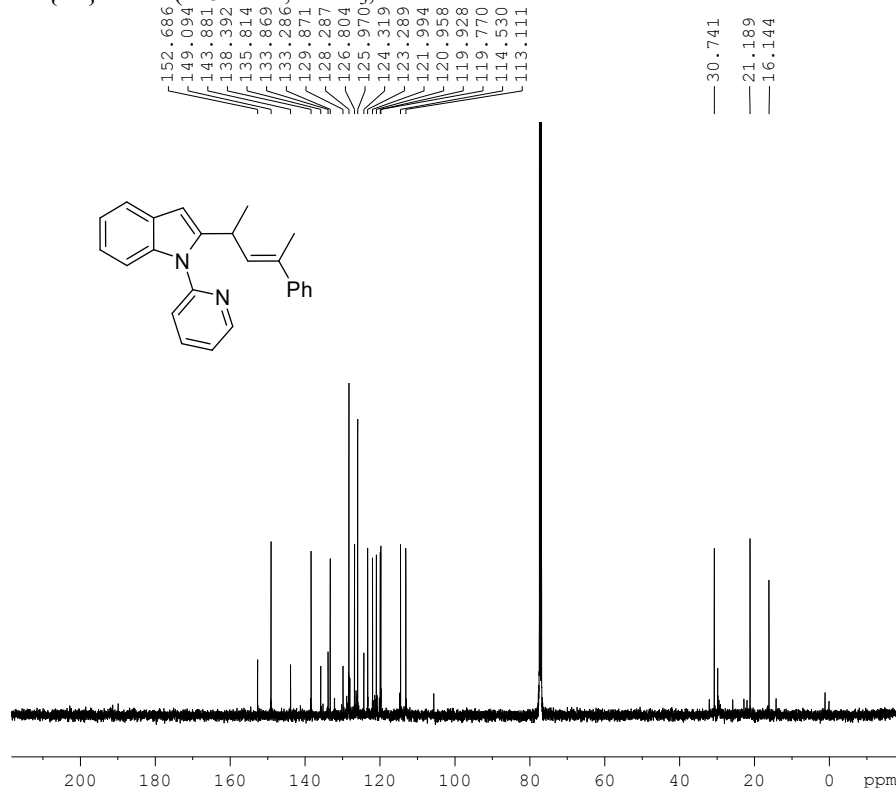
Current Data Parameters
NAME pure
EXPNO 86
PROCNO 1

F2 - Acquisition Paramete
Date_ 20180215
Time 10.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 32
DS 2
SWH 10000.000
FIDRES 0.305176
AQ 1.6384000
RG 124.08
DW 50.000
DE 6.50
TE 300.6
D1 0.50000000
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008
NUC1 1H
P1 12.75
PLW1 15.30000019

F2 - Processing paramet
SI 65536
SF 500.1500164
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME pure
EXPNO 106
PROCNO 1

F2 - Acquisition Paramet
Date_ 20180217
Time 3.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl₃
NS 3000
DS 4
SWH 29761.904
FIDRES 1.453218
AQ 0.3440640
RG 202.34
DW 16.800
DE 6.50
TE 302.0
D1 1.00000000
D11 0.03000000
TD0 1

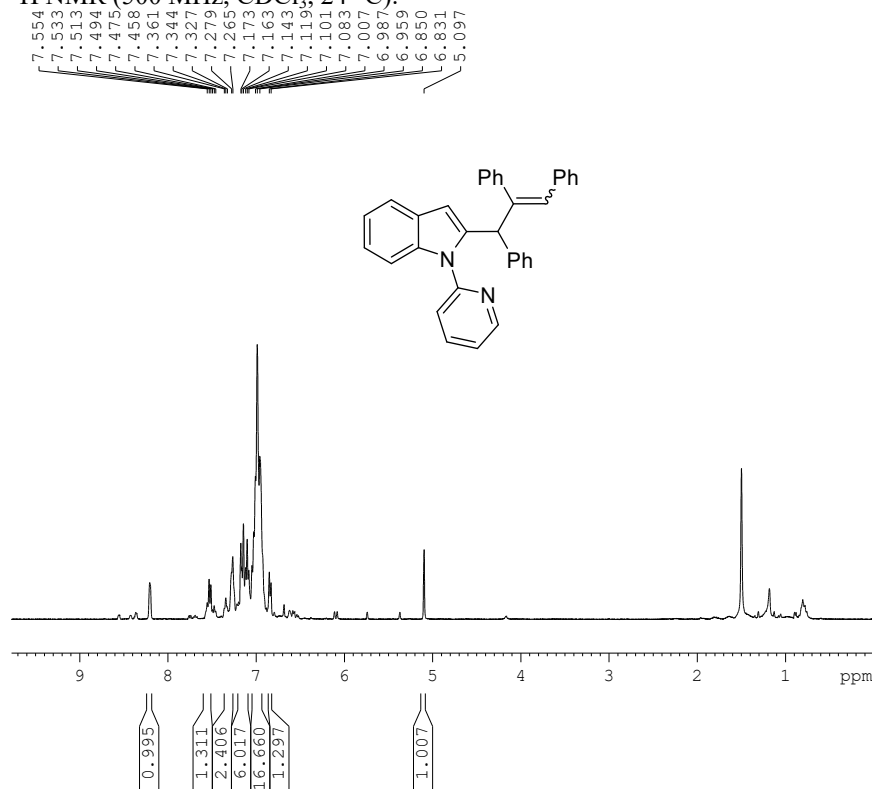
===== CHANNEL f1 =====
SFO1 125.7753932
NUC1 13C
P1 9.88
PLW1 103.00000000

===== CHANNEL f2 =====
SFO2 500.1520006
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00
PLW2 15.30000019
PLW12 0.38863000
PLW13 0.19548000

F2 - Processing paramete

1-(Pyridin-2-yl)-2-(1,2,3-triphenylallyl)-1H-indole (3ae):

¹H NMR (500 MHz, CDCl₃, 24 °C):



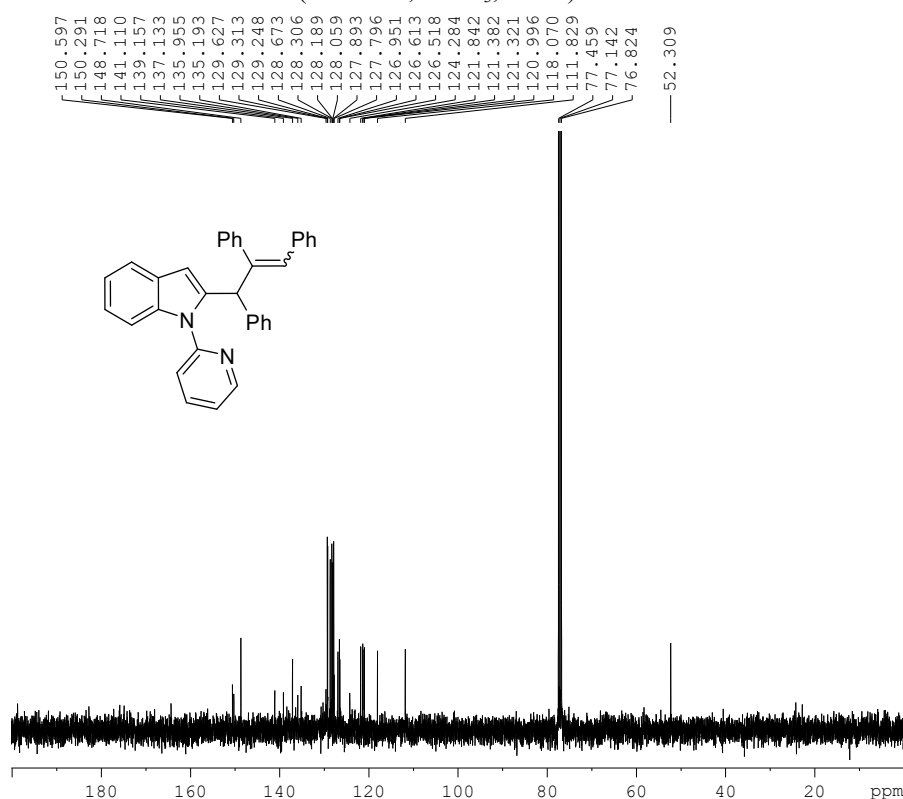
Current Data Parameters
NAME nmr_2085%2f208
EXPNO 38
PROCNO 1

F2 - Acquisition Paramete
Date_ 20200508
Time_ 15.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820
FIDRES 0.122266
AQ 4.0894465
RG 200.34
DW 62.400
DE 6.50
TE 297.1
D1 0.50000000
TD0 1

===== CHANNEL f1 ===
SFO1 400.1320007
NUC1 1H
P1 15.70
PLW1 7.75000000

F2 - Processing paramet
SI 65536
SF 400.1300437
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME nmr_2085%2f2087
EXPNO 39
PROCNO 1

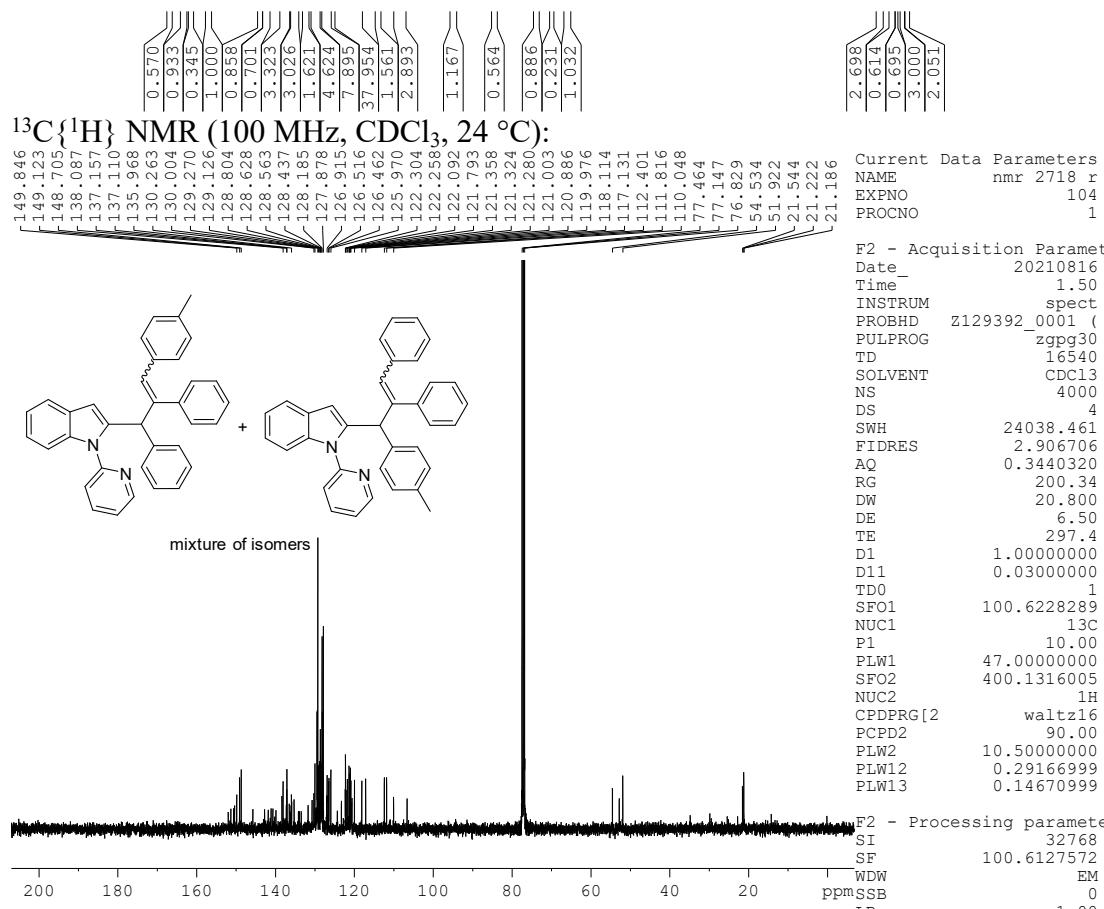
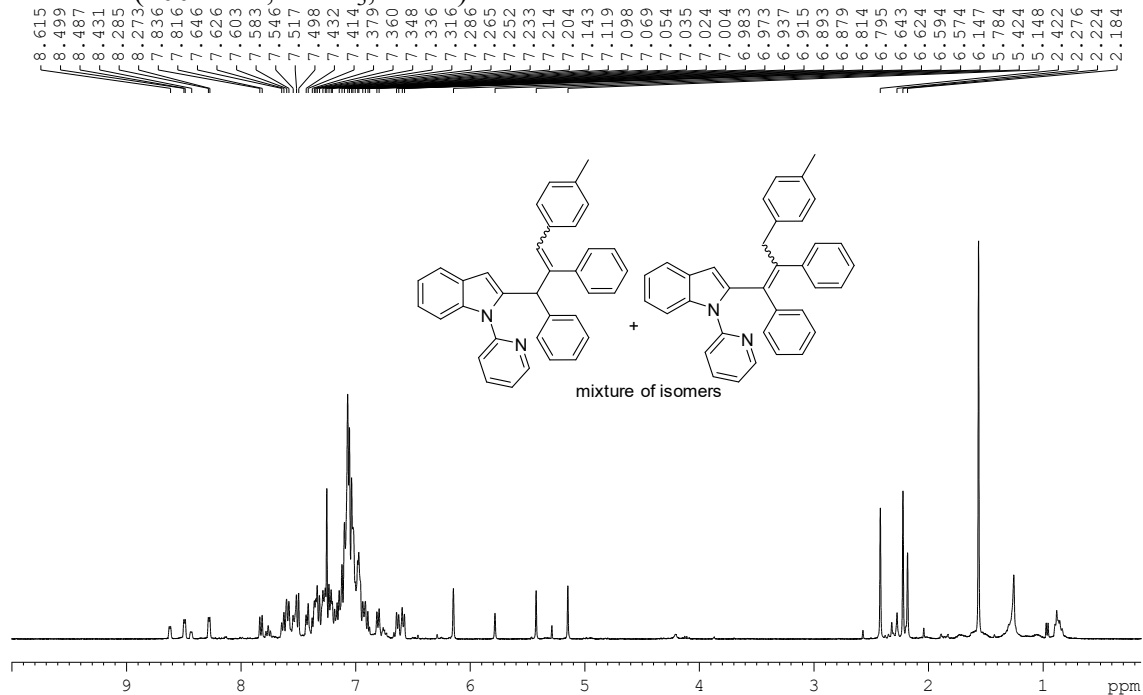
F2 - Acquisition Paramete
Date_ 20200508
Time_ 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 H
FIDRES 1.453353 H
AQ 0.3440320 s
RG 200.34
DW 20.800 u
DE 6.50 u
TE 297.4 K
D1 1.00000000 s
D11 0.03000000 s
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228289 M
NUC1 13C
P1 9.25 u
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 M
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 u
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

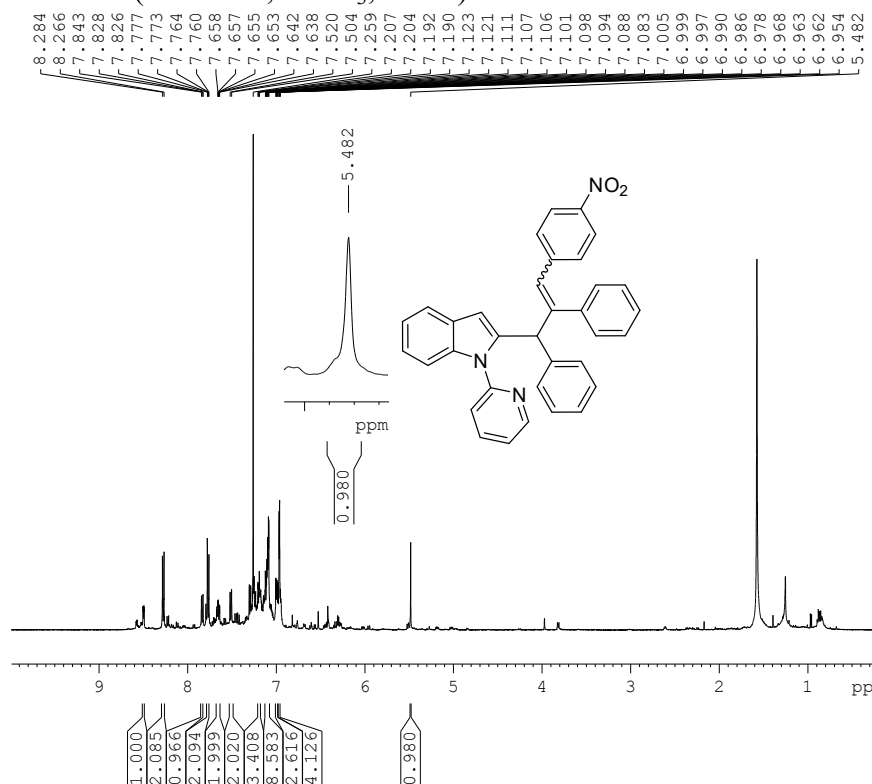
2-(1,2-Diphenyl-3-(p-tolyl)allyl)-1-(pyridin-2-yl)-1*H*-indole and 2-(2,3-Diphenyl-1-(p-tolyl)allyl)-1-(pyridin-2-yl)-1*H*-indole (3af):

¹H NMR (400 MHz, CDCl₃, 24 °C):



2-(3-(4-Nitrophenyl)-1,2-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3ag):

^1H NMR (500 MHz, CDCl_3 , 24 °C):



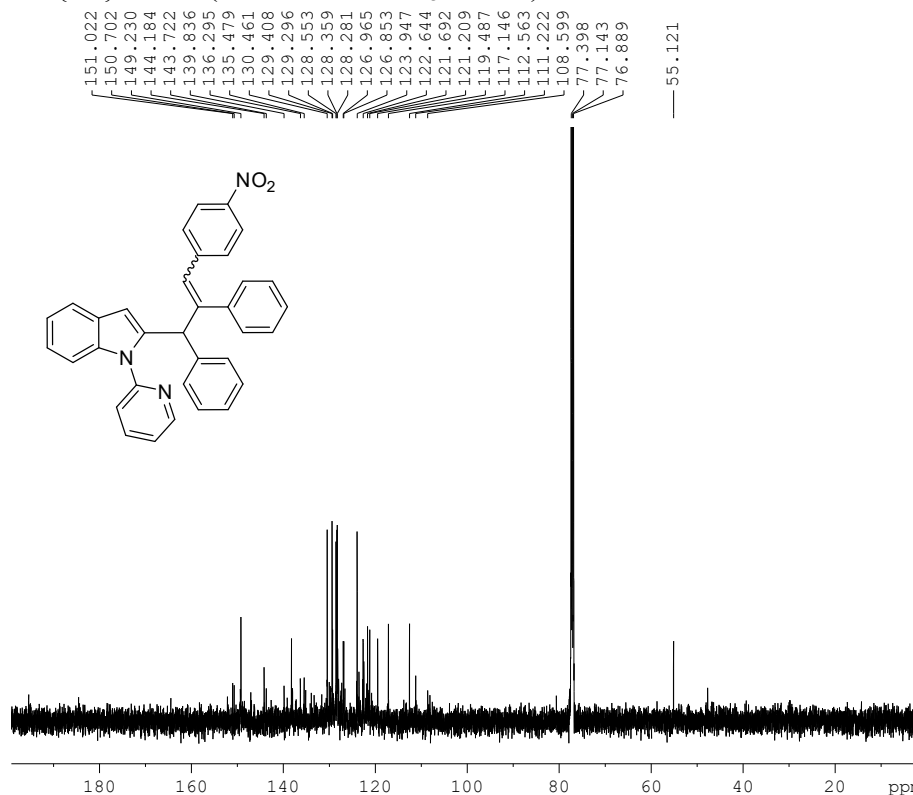
Current Data Parameters
NAME 2730 part 1
EXPNO 64
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210824
Time 23.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl_3
NS 16
DS 2
SWH 10000.000
FIDRES 0.305176
AQ 1.6384000
RG 162.95
DW 50.000
DE 6.50
TE 297.8
D1 0.50000000
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008
NUC1 ^1H
P1 11.75
PLW1 15.30000019

F2 - Processing parameters
SI 65536
SF 500.1500124
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 24 °C):



Current Data Parameters:
NAME 2730 part 1
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210824
Time 1.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 2048
SOLVENT CDCl_3
NS 300
DS 4
SWH 29761.904
FIDRES 1.453214
AQ 0.3440640
RG 202.34
DW 16.800
DE 6.50
TE 298.2
D1 1.00000000
D11 0.03000000
TD0 1

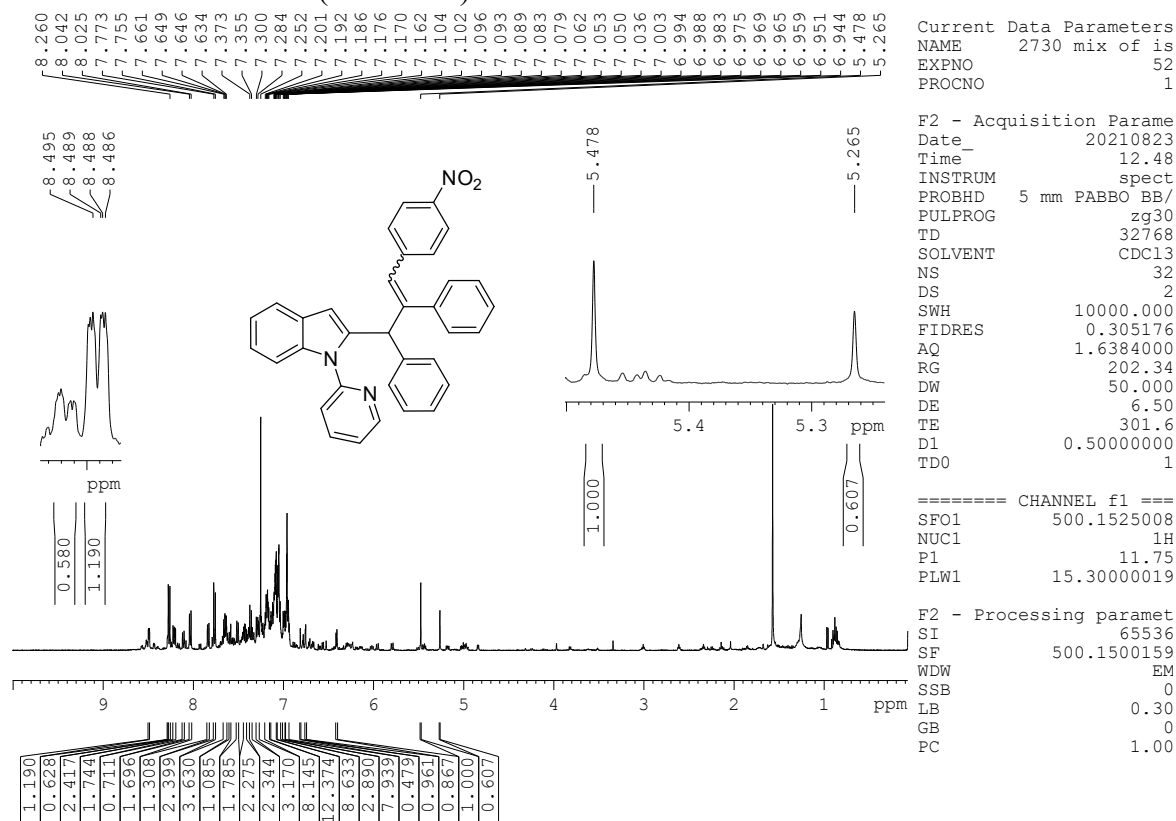
===== CHANNEL f1 =====
SFO1 125.7753932
NUC1 ^{13}C
P1 10.20
PLW1 103.00000000

===== CHANNEL f2 =====
SFO2 500.1520004
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 80.00
PLW2 15.30000019
PLW12 0.39658999
PLW13 0.19948000

F2 - Processing parameters

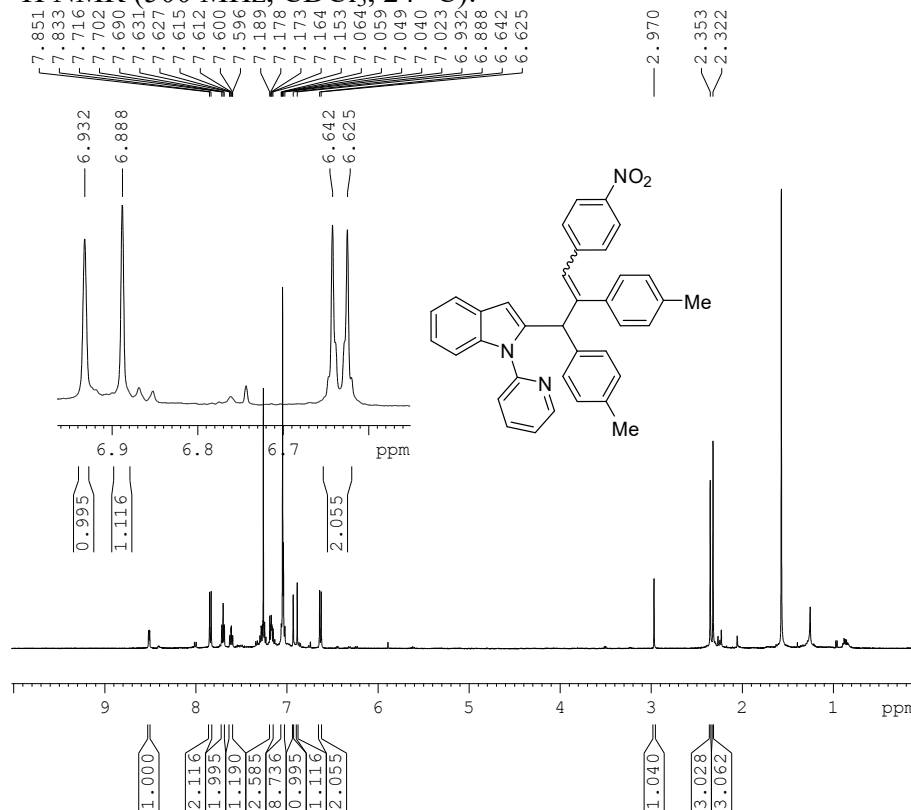
2-(3-(4-Nitrophenyl)-1,2-diphenylallyl)-1-(pyridin-2-yl)-1H-indole (3ag):

Mixture of isomer with (1:0.6 ratio):



3-(3-(4-Nitrophenyl)-1,2-di-*p*-tolylallyl)-1-(pyridin-2-yl)-1*H*-indole (3ah):

¹H NMR (500 MHz, CDCl₃, 24 °C):



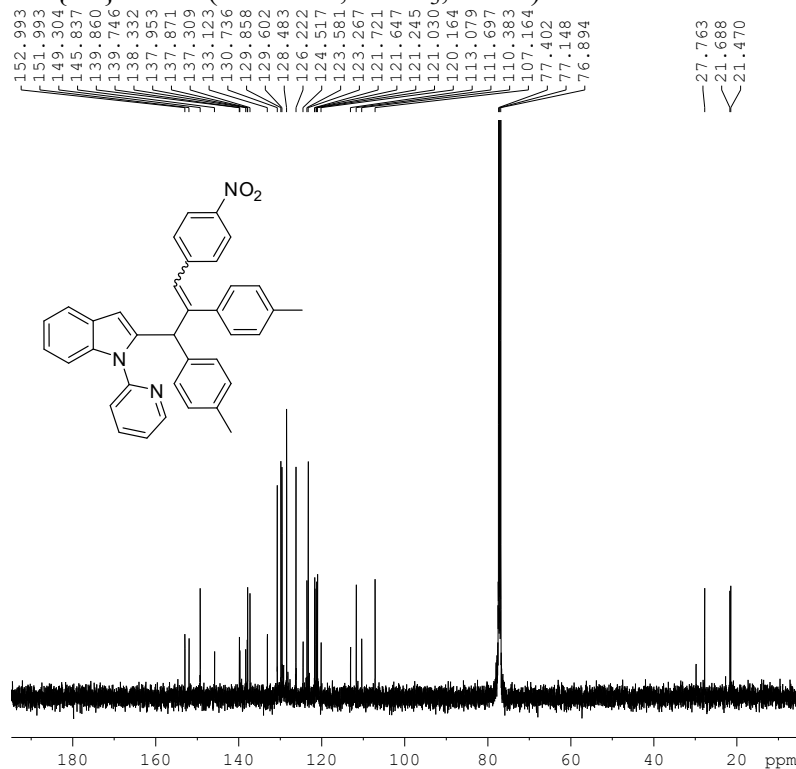
Current Data Parameters
NAME 2735 final
EXPNO 70
PROCNO 1

F2 - Acquisition Paramete
Date_ 20210827
Time_ 1.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000
FIDRES 0.305176
AQ 1.6384000
RG 138.53
DW 50.000
DE 6.50
TE 297.2
D1 0.50000000
TD0 1

===== CHANNEL f1 ===
SFO1 500.1525008
NUC1 1H
P1 11.75
PLW1 15.30000019

F2 - Processing paramet
SI 65536
SF 500.1500124
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 2735 final
EXPNO 71
PROCNO 1

F2 - Acquisition Paramete
Date_ 20210827
Time_ 3.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 3000
DS 4
SWH 29761.904
FIDRES 1.453218
AQ 0.3440640
RG 202.34
DW 16.800
DE 6.50
TE 297.6
D1 1.00000000
D11 0.03000000
TD0 1

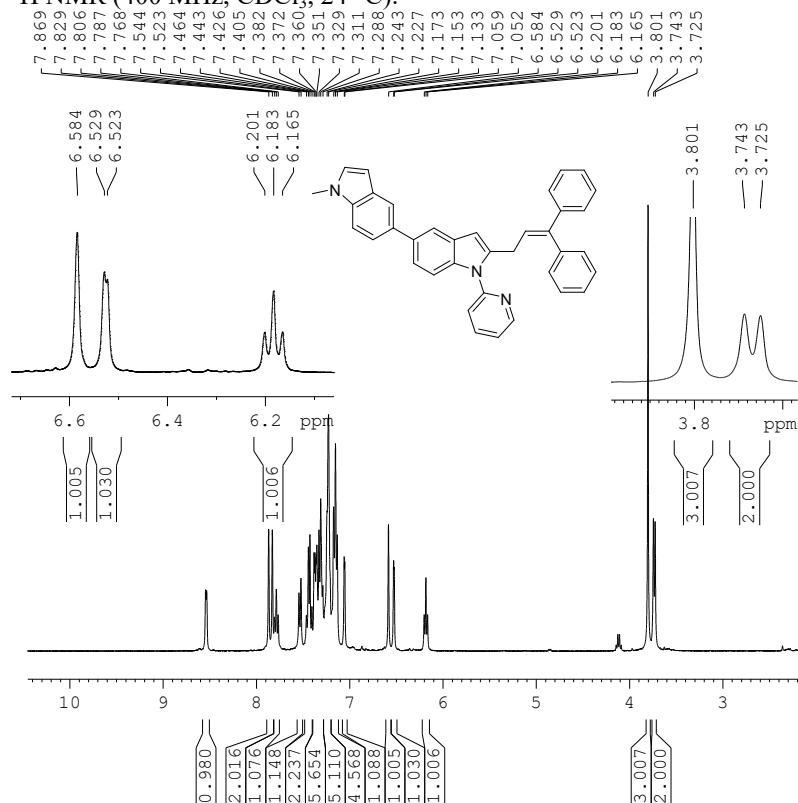
===== CHANNEL f1 ===
SFO1 125.7753932
NUC1 13C
P1 10.20
PLW1 103.00000000

===== CHANNEL f2 ===
SFO2 500.1520006
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00
PLW2 15.30000019
PLW12 0.39658999
PLW13 0.19948000

F2 - Processing paramet
SI 32768

2-(3,3-Diphenylallyl)-1'-methyl-1-(pyridin-2-yl)-1*H*,1'*H*-5,5'-biindole (3ai):

¹H NMR (400 MHz, CDCl₃, 24 °C):



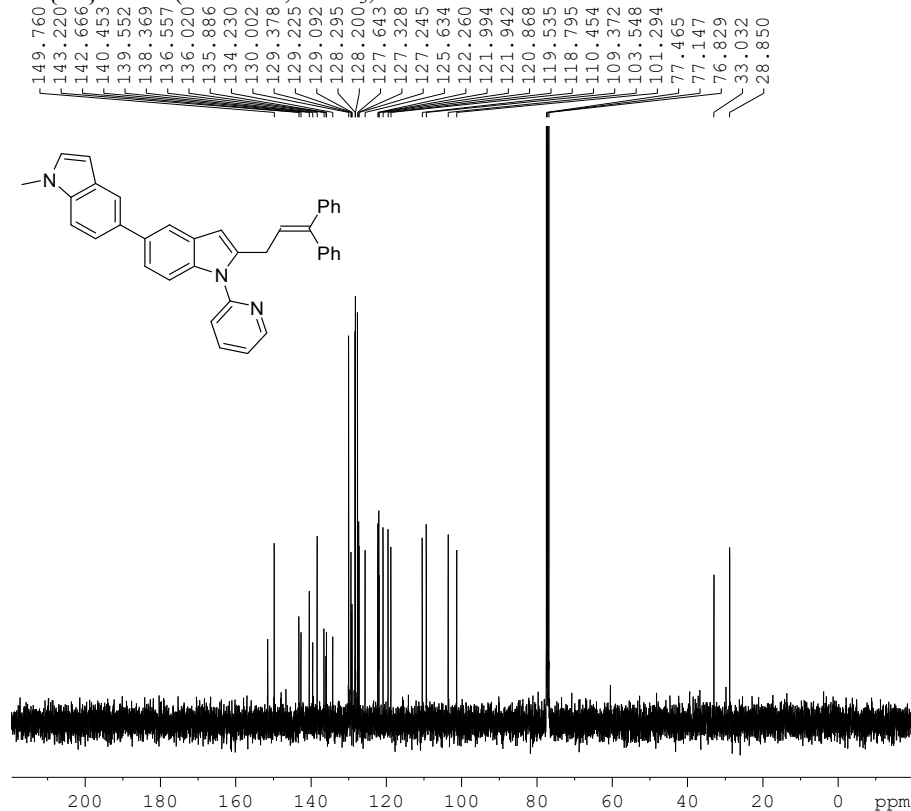
Current Data Parameters
NAME ksr selectivity nmr
EXPNO 383
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190622
Time_ 9.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 153.13
DW 62.400 usec
DE 6.50 usec
TE 297.7 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300209 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME ksr selectiv
EXPNO 3
PROCNO

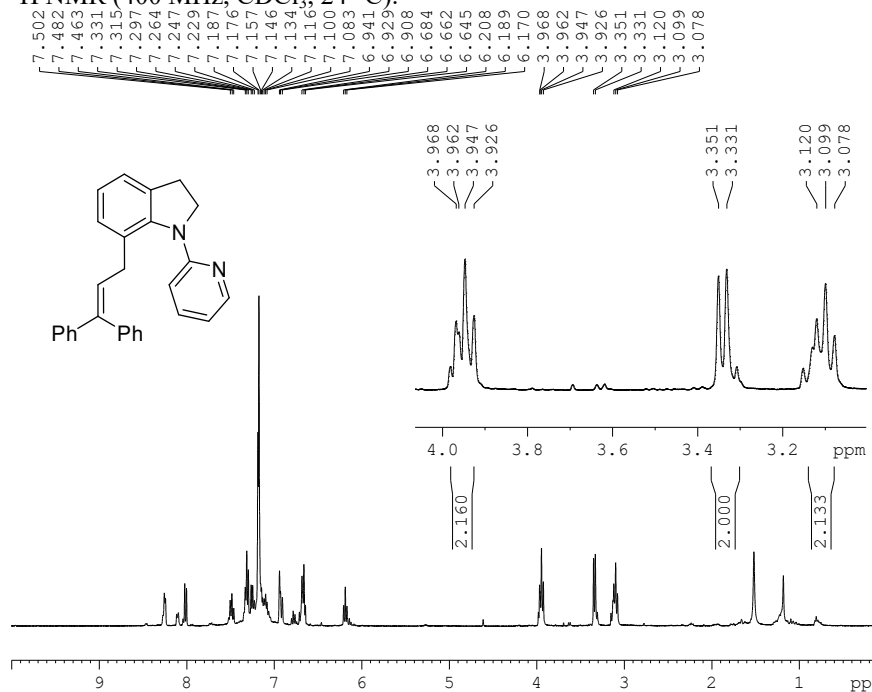
F2 - Acquisition Para
Date_ 201906
Time_ 9.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 298
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 13
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2] waltz
PCPD2 90.
PRG2 7 750000

7-(3,3-Diphenylallyl)-1-(pyridin-2-yl)indoline (3aj):

¹H NMR (400 MHz, CDCl₃, 24 °C):

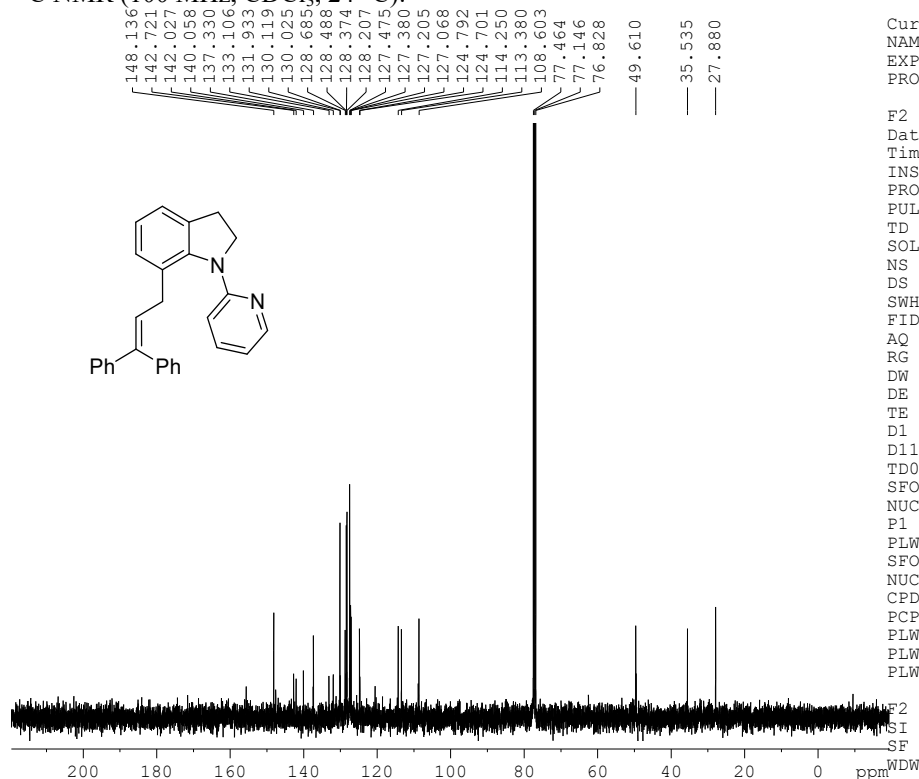


Current Data Parameters
NAME ksr 2700 final
EXPNO 14
PROCNO 1

F2 - Acquisition Param
Date_ 20210804
Time_ 8.38
INSTRUM spect
PROBHD Z129392_0001 (zg30)
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820
FIDRES 0.244532
AQ 4.0894465
RG 200.34
DW 62.400
DE 6.50
TE 298.2
D1 0.50000000
TD0 1
SFO1 400.1320007
NUC1 1H
P1 15.00
PLW1 10.50000000

F2 - Processing paramet
SI 65536
SF 400.1300435
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C NMR (100 MHz, CDCl₃, 24 °C):



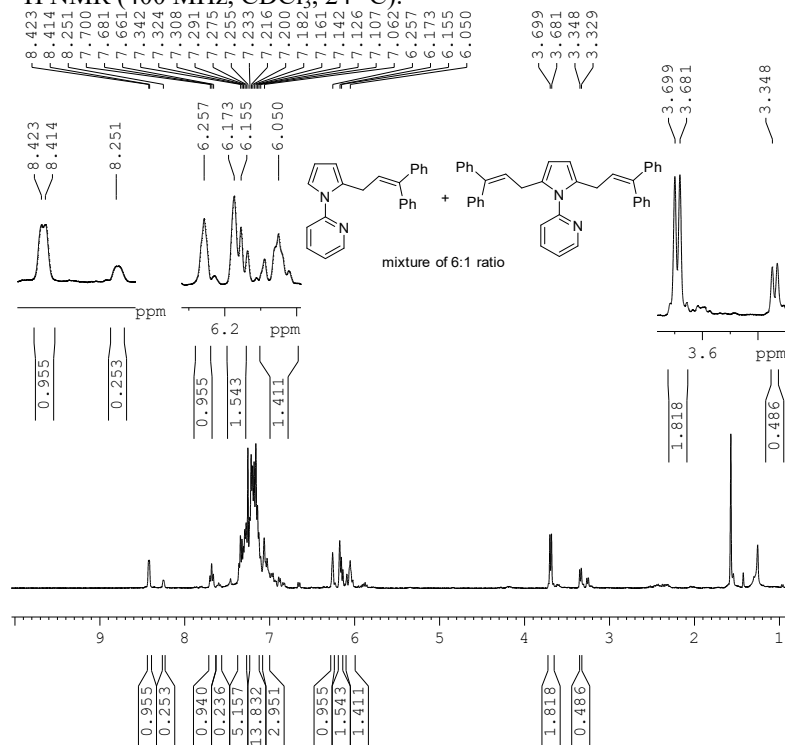
Current Data Parameters
NAME ksr 2700 final
EXPNO 15
PROCNO 1

F2 - Acquisition Paramet
Date_ 20210804
Time_ 8.45
INSTRUM spect
PROBHD Z129392_0001 (zgpg30)
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461
FIDRES 2.906706
AQ 0.3440320
RG 200.34
DW 20.800
DE 6.50
TE 298.5
D1 1.00000000
D11 0.03000000
TD0 1
SFO1 100.6228289
NUC1 13C
P1 10.00
PLW1 47.00000000
SFO2 400.1316005
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00
PLW2 10.50000000
PLW12 0.29166999
PLW13 0.14670999

F2 - Processing paramet
SI 32768
SF 100.6127575
WDW EM

2-(2-(3,3-Diphenylallyl)-1H-pyrrol-1-yl)pyridine (6a):

¹H NMR (400 MHz, CDCl₃, 24 °C):



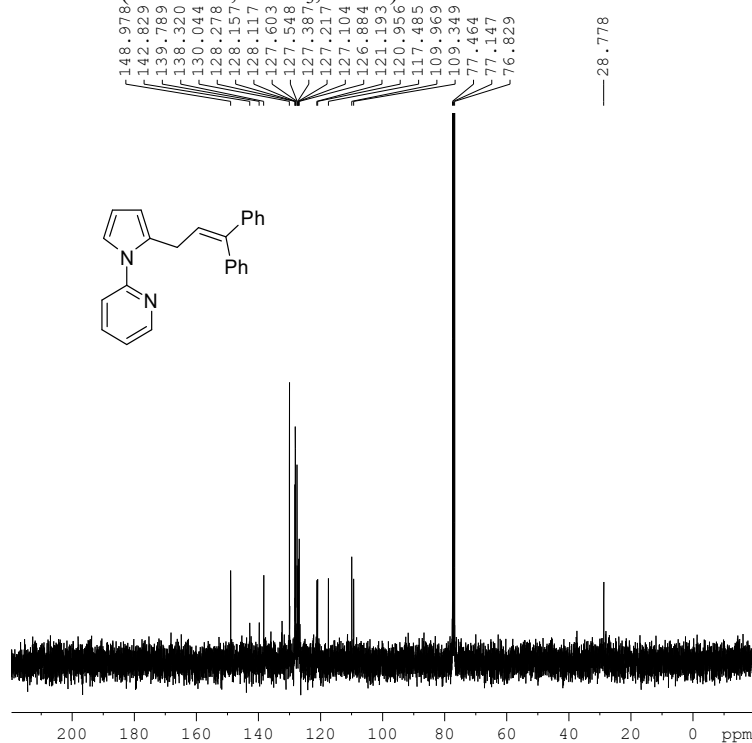
Current Data Parameters
NAME KSR 949
EXPNO 577
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170624
Time_ 1.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 294.4 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300121 MHz
WDW EM
SSB 0
GB 0
PC 1.00

¹³C NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME spa40617
EXPNO 578
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170624
Time_ 2.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

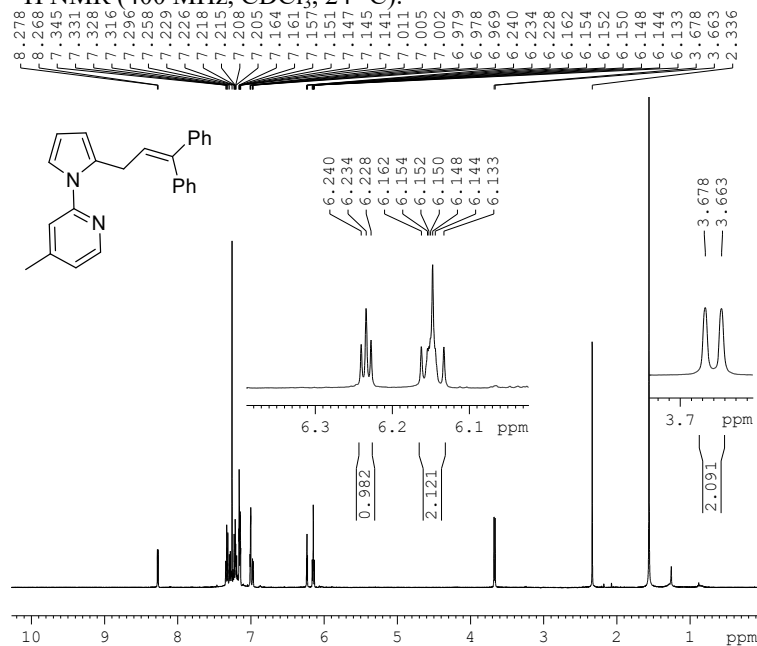
===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.11863000 W

F2 - Processing parameters
SI 32768
SF 100.6127577 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-(2-(3,3-Diphenylallyl)-1H-pyrrol-1-yl)-4-methylpyridine (6b):

¹H NMR (400 MHz, CDCl₃, 24 °C):



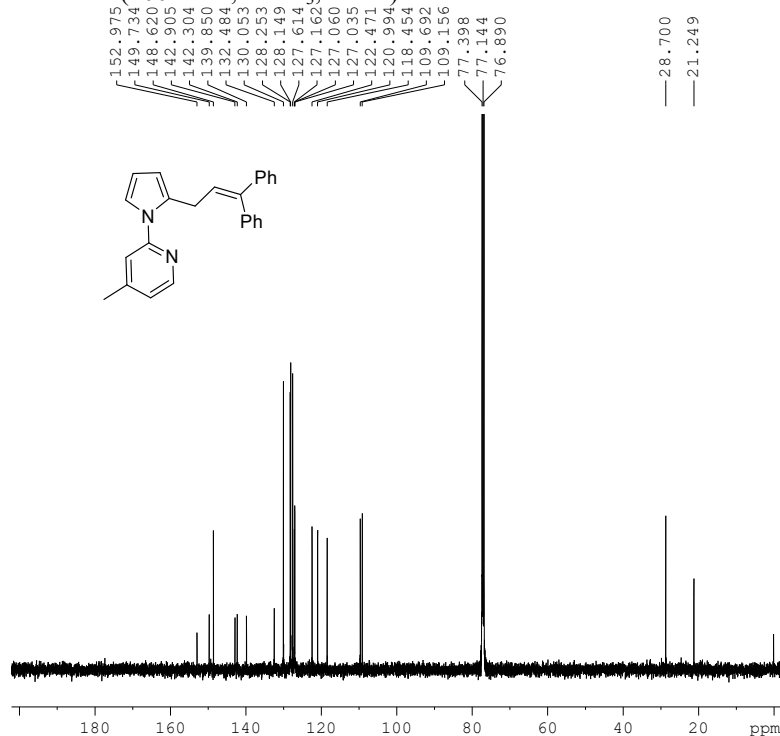
Current Data Parameters
NAME pure
EXPNO 107
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190424
Time 6.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 180.86
DW 50.000 usec
DE 6.50 usec
TE 302.5 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 11.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME pure
EXPNO 108
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190424
Time 8.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl₃
NS 9231
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 303.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

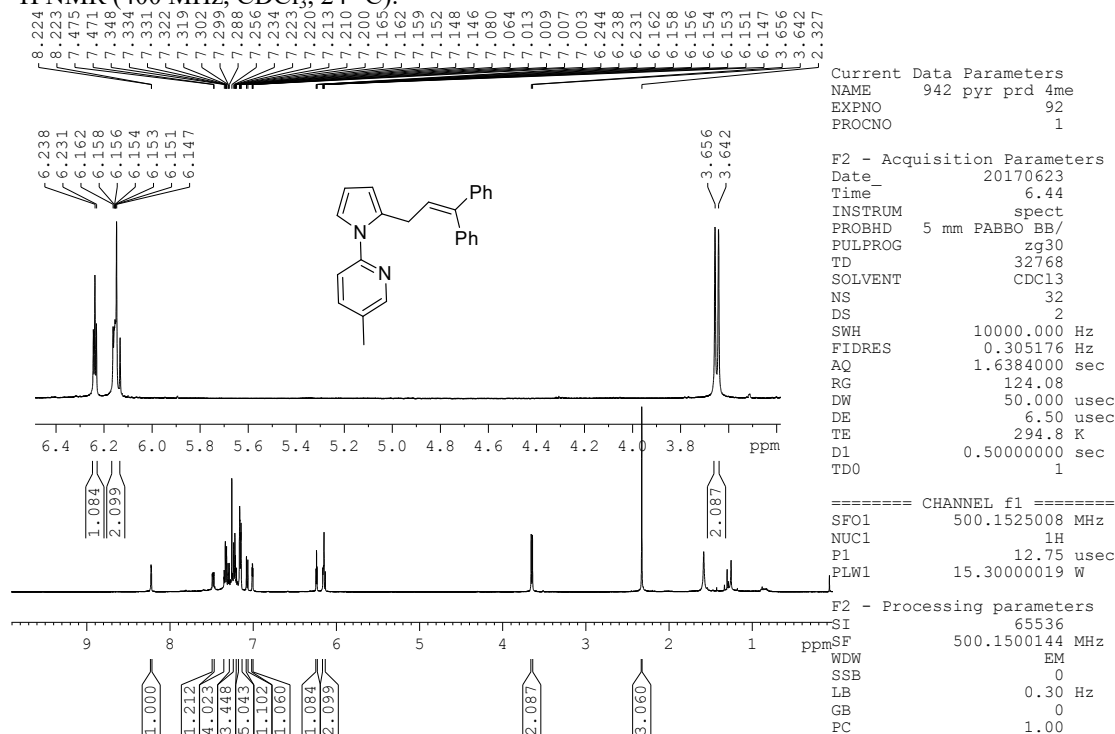
===== CHANNEL f1 =====
SFO1 125.7753932 MHz
NUC1 13C
P1 10.20 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.38863000 W
PLW13 0.19548000 W

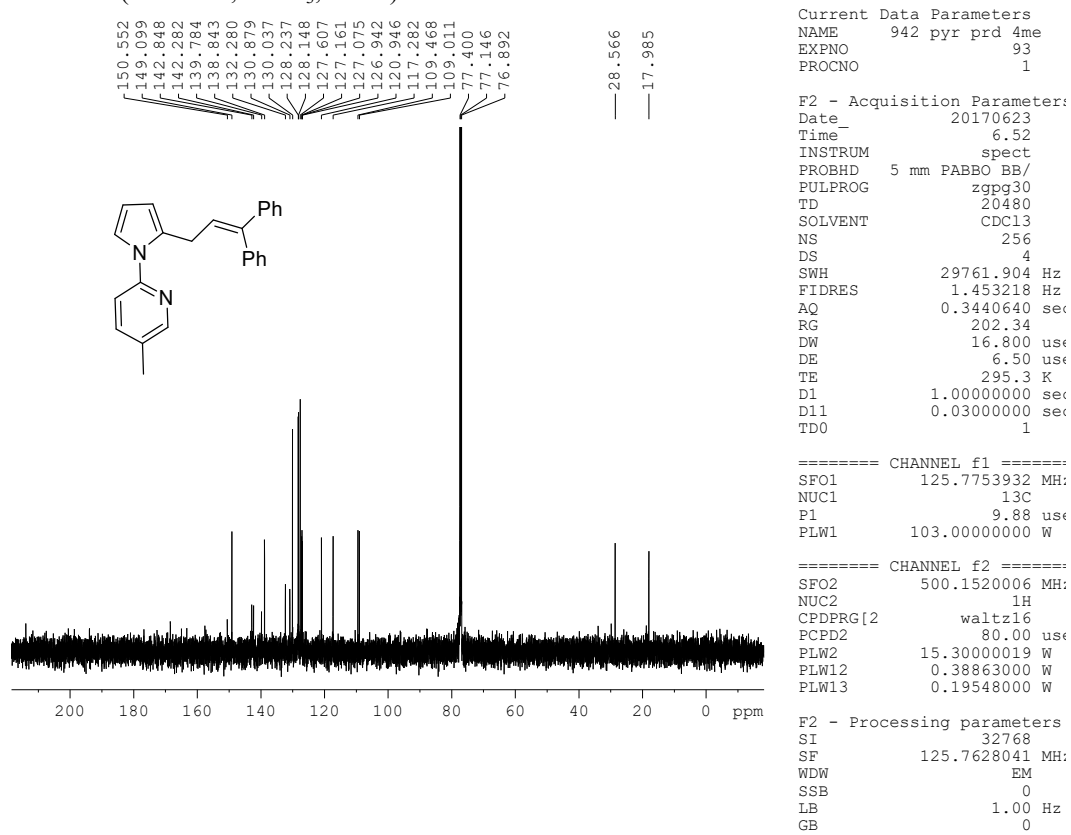
F2 - Processing parameters
SI 32768
SF 125.7628005 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-(2-(3,3-diphenylallyl)-1H-pyrrol-1-yl)-5-methylpyridine(6c):

¹H NMR (400 MHz, CDCl₃, 24 °C):

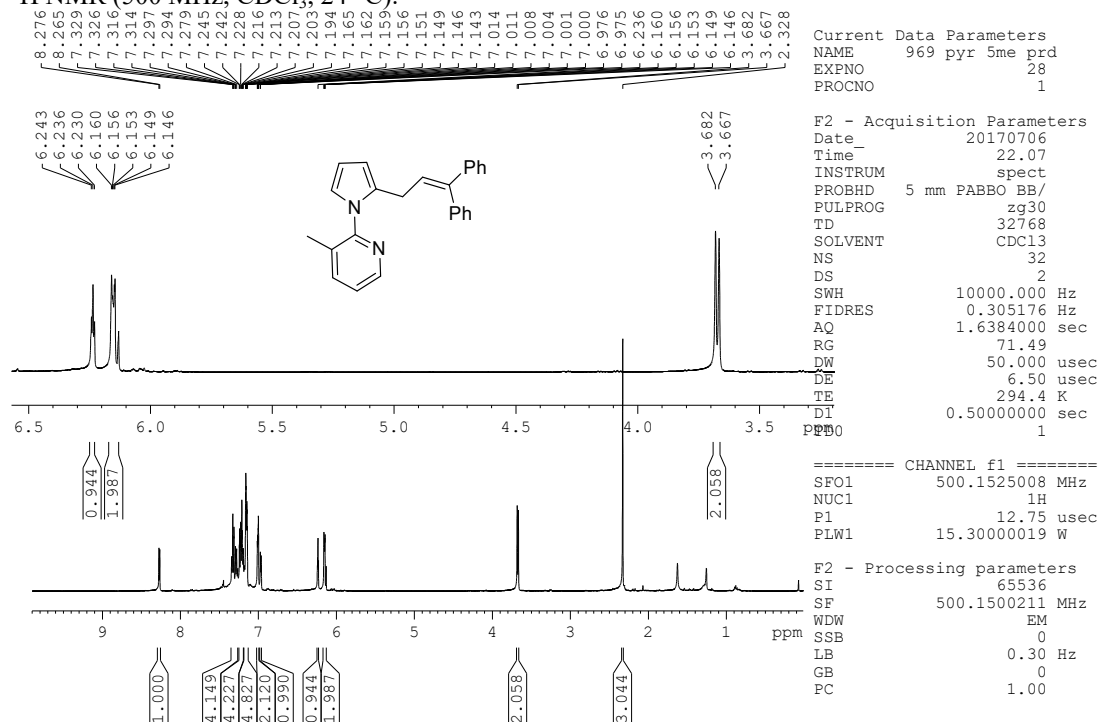


¹³C NMR (125 MHz, CDCl₃, 24 °C):

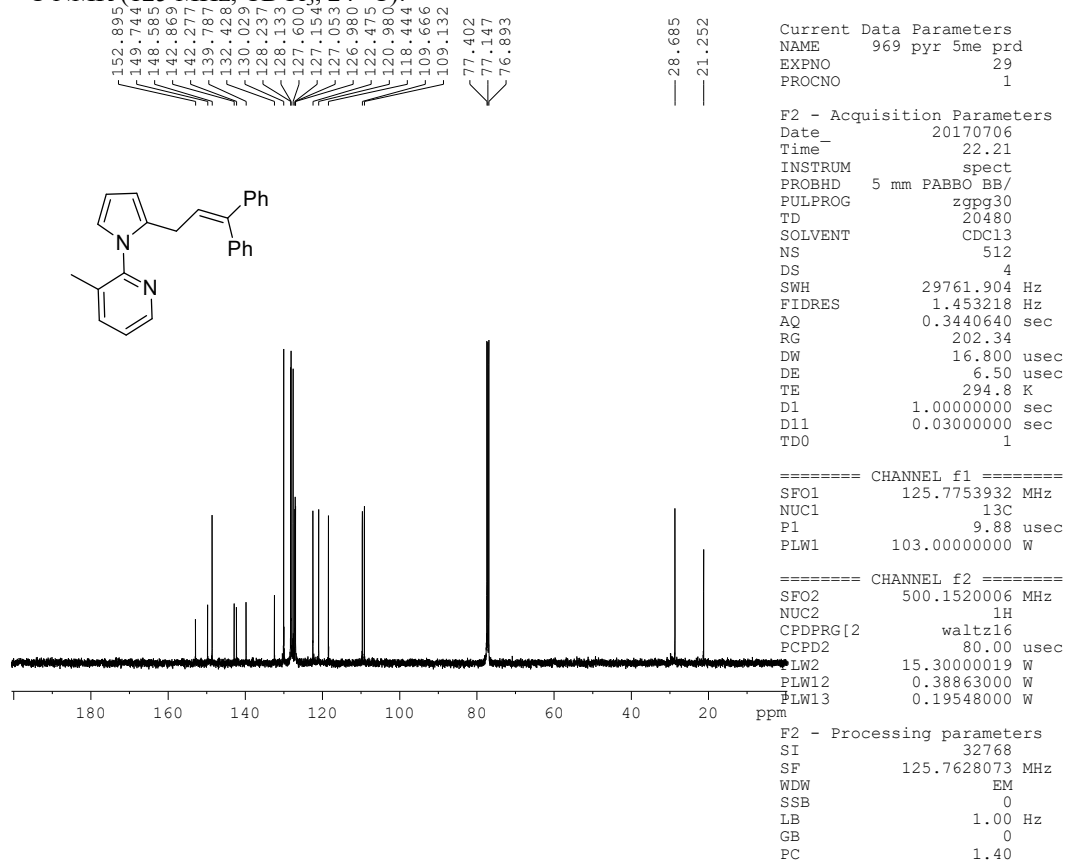


2-(2-(3,3-diphenylallyl)-1H-pyrrol-1-yl)-3-methylpyridine(6d):

¹H NMR (500 MHz, CDCl₃, 24 °C):

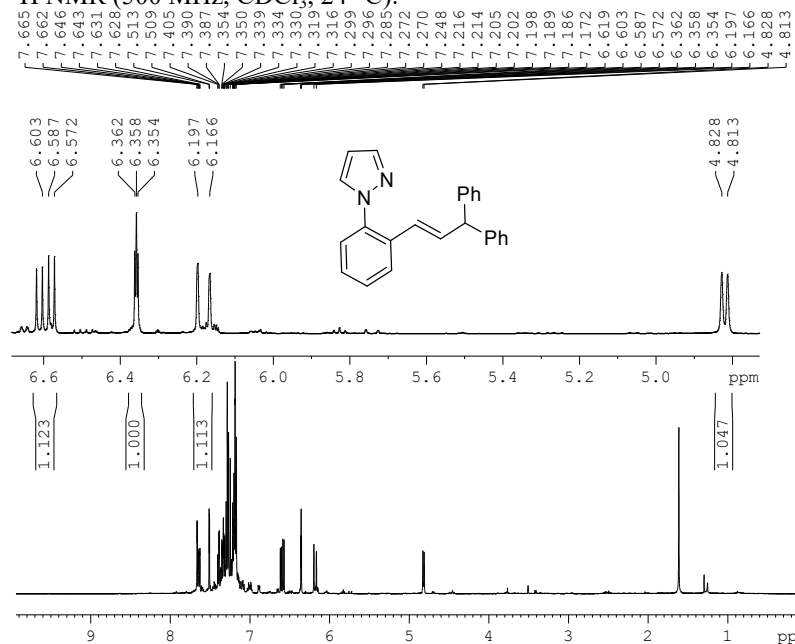


¹³C NMR (125 MHz, CDCl₃, 24 °C):



(E)-1-(2-(3,3-Diphenylprop-1-en-1-yl)phenyl)-1H-pyrazole(7a):

¹H NMR (500 MHz, CDCl₃, 24 °C):



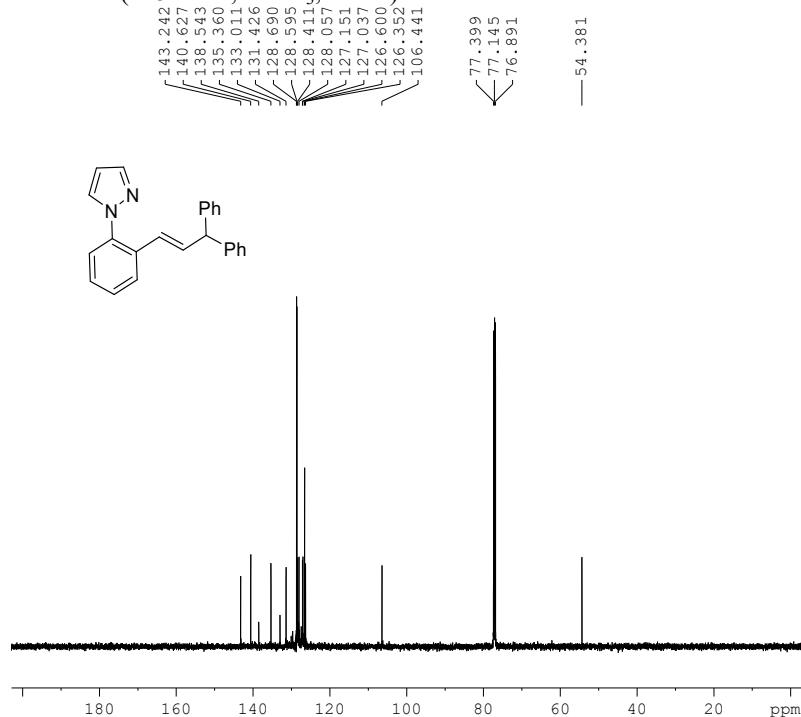
Current Data Parameters
NAME pyrrole parent
EXPNO 121
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190426
Time_ 4.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 101.5
DW 50.000 usec
DE 6.50 usec
TE 296.6 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 11.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500186 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR (125 MHz, CDCl₃, 24 °C):



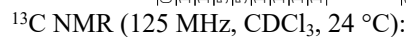
Current Data Parameters
NAME pyrrole parent
EXPNO 122
PROCNO 1

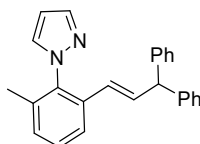
F2 - Acquisition Parameters
Date_ 20190426
Time_ 4.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 sec
RG 202.34
DW 16.800 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7753932 MHz
NUC1 13C
P1 10.20 usec
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.30000019 W
PLW12 0.38863000 W
PLW13 0.19548000 W

F2 - Processing parameters
SI 32768
SF 125.7628053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR (500 MHz, CDCl₃, 24 °C):

¹H NMR (500 MHz, CDCl₃, 24 °C):

```

Current Data Parameters
NAME      pyrrole 2me 1729
EXPNO     38
PROCNO    1

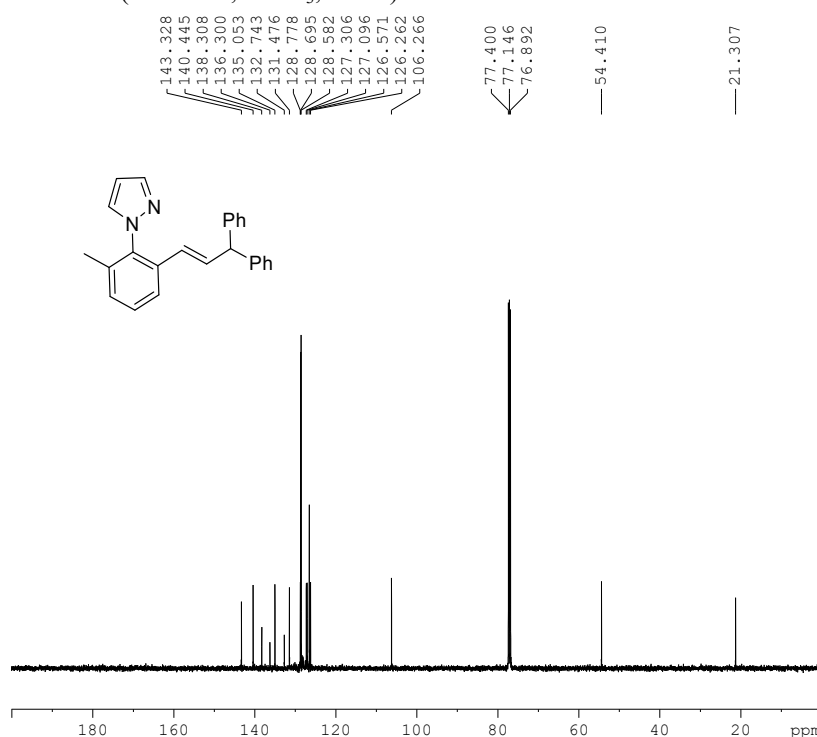
F2 - Acquisition Parameters
Date_     20190508
Time      7.35
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        20480
SOLVENT   CDCl3
NS        1000
DS         4
SWH       29761.904 Hz
FIDRES    1.453218 Hz
AQ        0.3440640 sec
RG         202.34
DW        16.800 usec
DE         6.50 usec
TE        297.0 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     125.7753932 MHz
NUC1      13C
P1        10.20 usec
PLW1     103.0000000 W

===== CHANNEL f2 =====
SFO2     500.1520006 MHz
WALTZ2   1H
CPDPRG2  nutz16
PCPD2    80.00 usec
PLW2     15.30000019 W
PLW12    0.38863000 W
PLW13    0.19548000 W

F2 - Processing parameters
SI        32768
SF        125.7628041 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

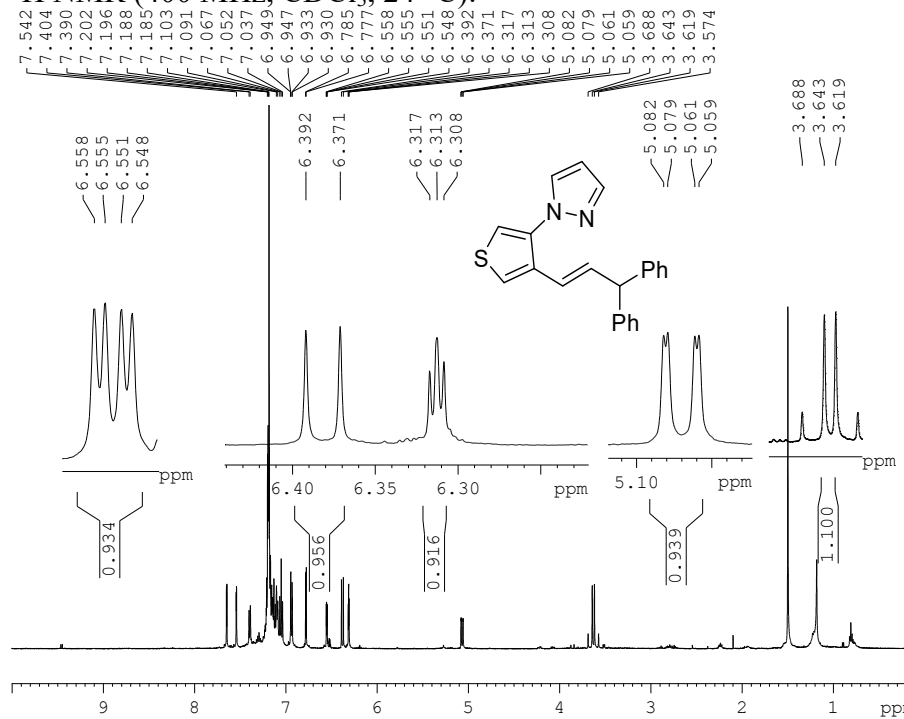
```

¹³C NMR (125 MHz, CDCl₃, 24 °C):

¹H NMR (500 MHz, CDCl₃, 24 °C):

(E)-1-(4-(3,3-Diphenylprop-1-en-1-yl)thiophen-3-yl)-1H-pyrazole (7e):

¹H NMR (400 MHz, CDCl₃, 24 °C):



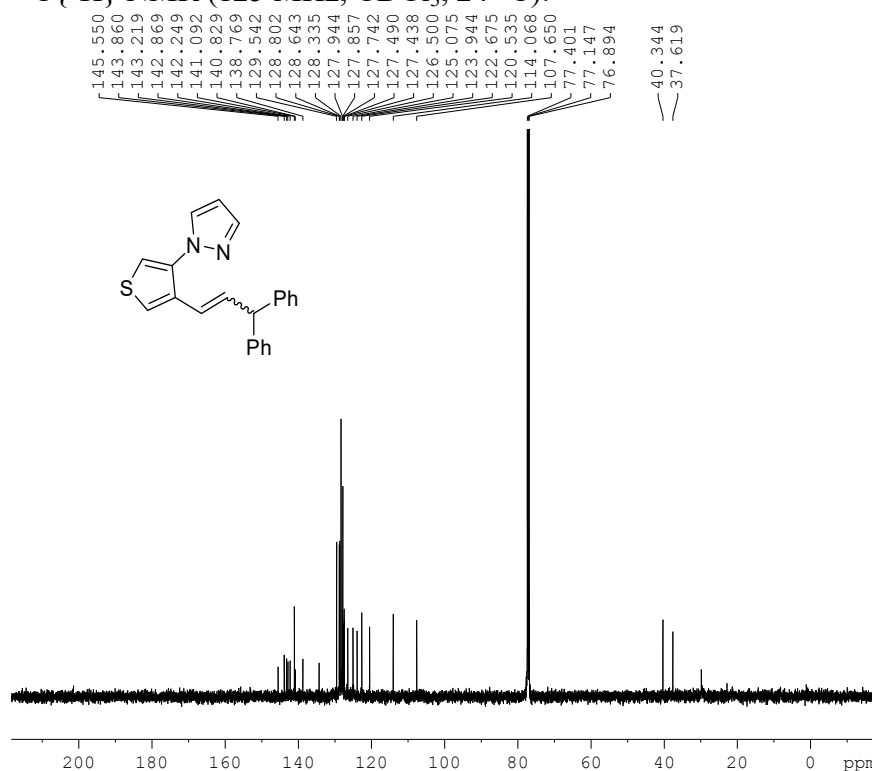
Current Data Parameters
NAME 2715 THIO
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210807
Time_ 11.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 10000.000
FIDRES 0.305176
AQ 1.6384000
RG 138.53
DW 50.000
DE 6.50
TE 296.8
D1 0.50000000
TD0 1

===== CHANNEL f1 =====
SFO1 500.1525008
NUC1 1H
P1 11.75
PLW1 15.30000019

F2 - Processing parameters
SI 65536
SF 500.1500496
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00

¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 2715 THIO
EXPNO 10
PROCNO 1

F2 - Acquisition Parameter
Date_ 20210809
Time_ 13.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 20480
SOLVENT CDCl3
NS 1500
DS 4
SWH 29761.904 Hz
FIDRES 1.453218 Hz
AQ 0.3440640 se
RG 202.34
DW 16.800 us
DE 6.50 us
TE 299.6 K
D1 1.00000000 se
D11 0.03000000 se
TD0 1

===== CHANNEL f1 =====
SFO1 125.7753932 MH
NUC1 13C
P1 10.20 us
PLW1 103.00000000 W

===== CHANNEL f2 =====
SFO2 500.1520006 MH
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 us
PLW2 15.30000019 W
PLW12 0.39658999 W
PLW13 0.19948000 W

F2 - Processing parameters

1,1-Diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10a):

¹H NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1859 application pa
EXPNO 426
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190824
Time_ 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 95.73
DW 62.400 usec
DE 6.50 usec
TE 297.9 K
D1 0.5000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300634 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):

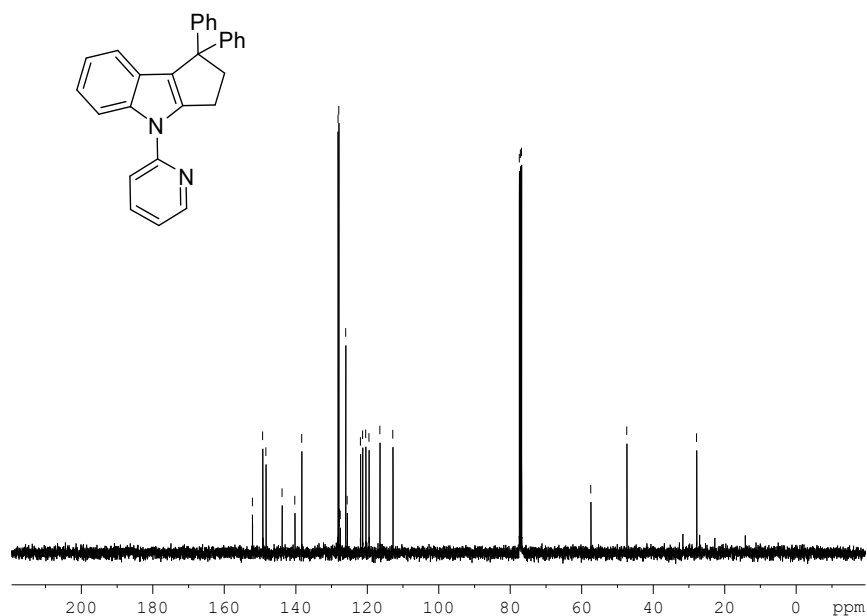


Current Data Paramete
NAME spa411
EXPNO 4
PROCNO

F2 - Acquisition Para
Date_ 201711
Time_ 13.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
LB 20.8
DW 6.
TE 294
D1 1.000000
D11 0.030000
TD0

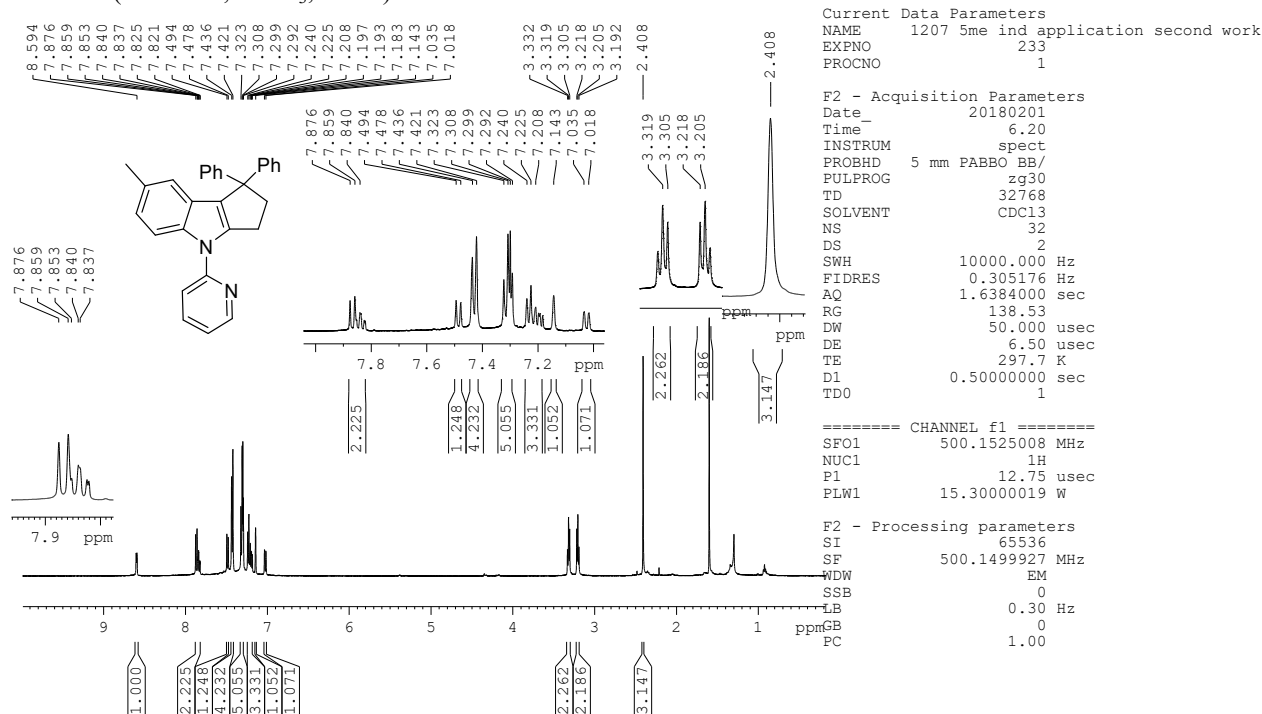
===== CHANNEL f1 =
SFO1 100.62282
NUC1 1
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2] waltz
PCPD2 90.
P1P2 7.750000

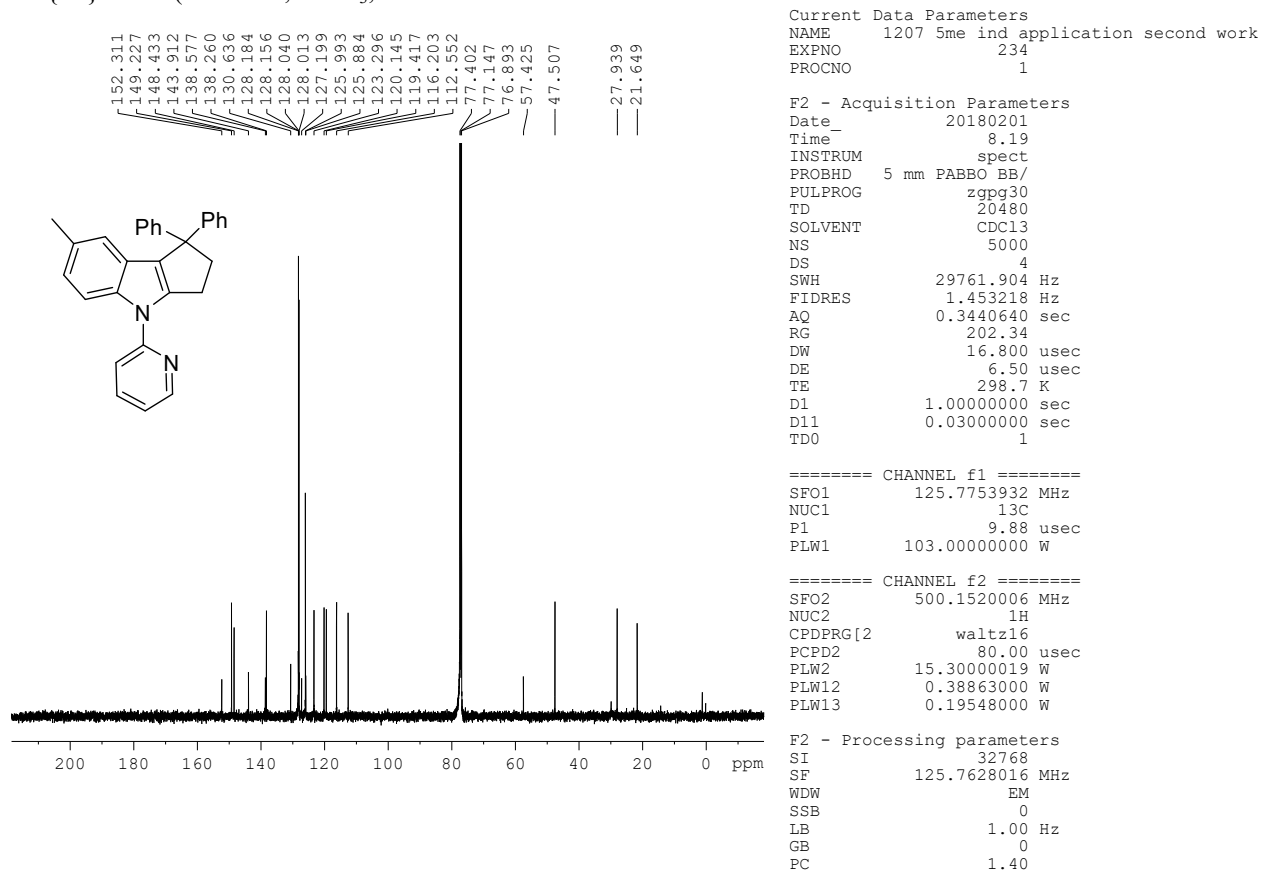


1,1-Diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10b):

¹H NMR (500 MHz, CDCl₃, 24 °C):

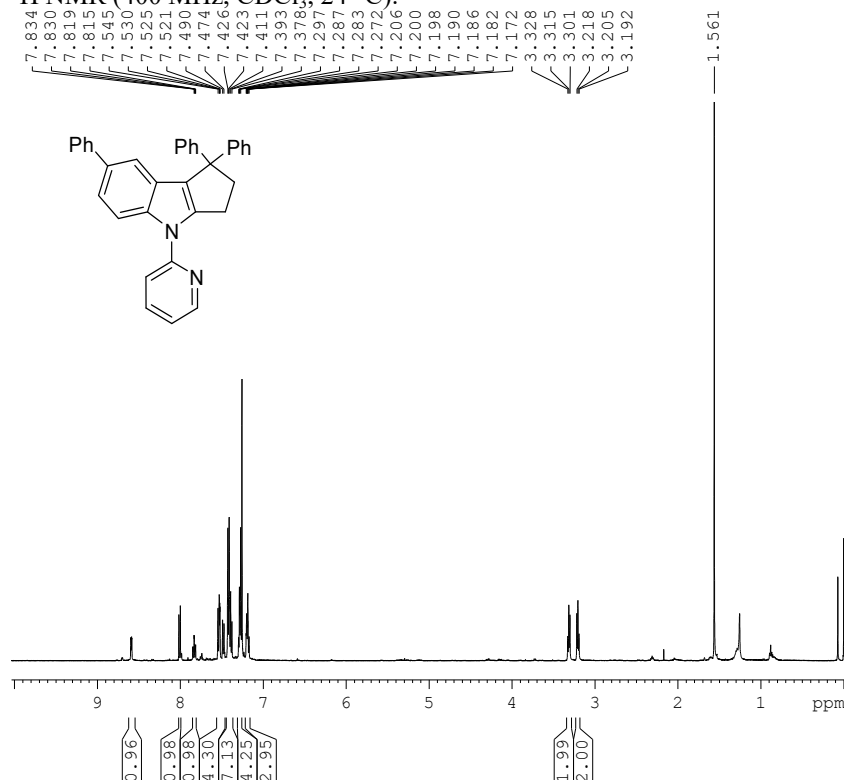


¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



1,1,7-Triphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10c):

¹H NMR (400 MHz, CDCl₃, 24 °C):



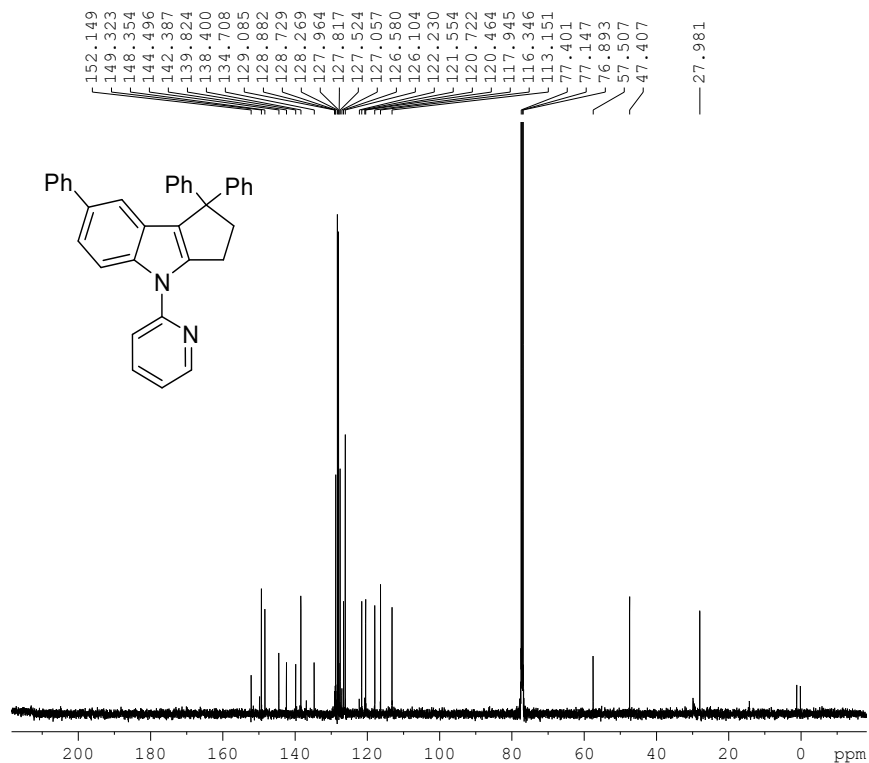
Current Data Parameters
NAME spa502
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_ 201802
Time 20.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zg
TD 327
SOLVENT CDC
NS
DS
SWH 10000.0
FIDRES 0.3051
AQ 1.63840
RG 138.
DW 50.0
DE 6.
TE 297
D1 0.500000
TD0

===== CHANNEL f1 =
SFO1 500.15250
NUC1
P1 12.
PLW1 15.300000

F2 - Processing parameters
SI 655
SF 500.15001
WDW
SSB 0
LB 0.
GB

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME spa502
EXPNO
PROCNO

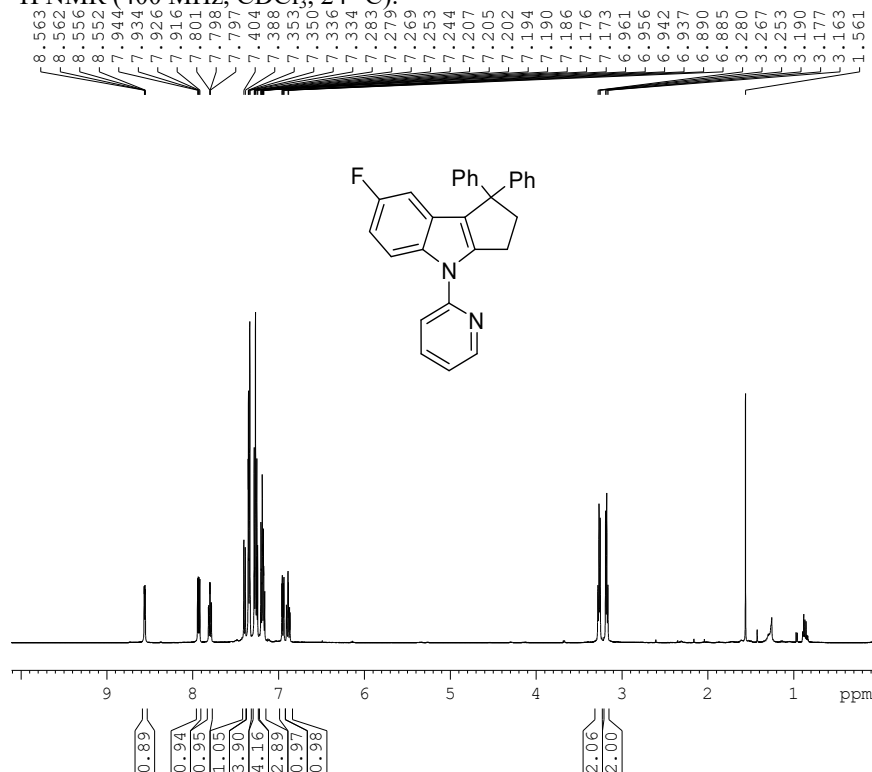
F2 - Acquisition Parameters
Date_ 201802
Time 23.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 204
SOLVENT CDC
NS 80
DS
SWH 29761.9
FIDRES 1.4532
AQ 0.34406
RG 202.
DW 16.8
DE 6.
TE 298
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 125.77539
NUC1 1
P1 9.
PLW1 103.000000

===== CHANNEL f2 =
SFO2 500.15200
NUC2
CPDPRG[2] waltz
PCPD2 80.
P1 15.300000

7-Fluoro-1,1-diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10d):

¹H NMR (400 MHz, CDCl₃, 24 °C):



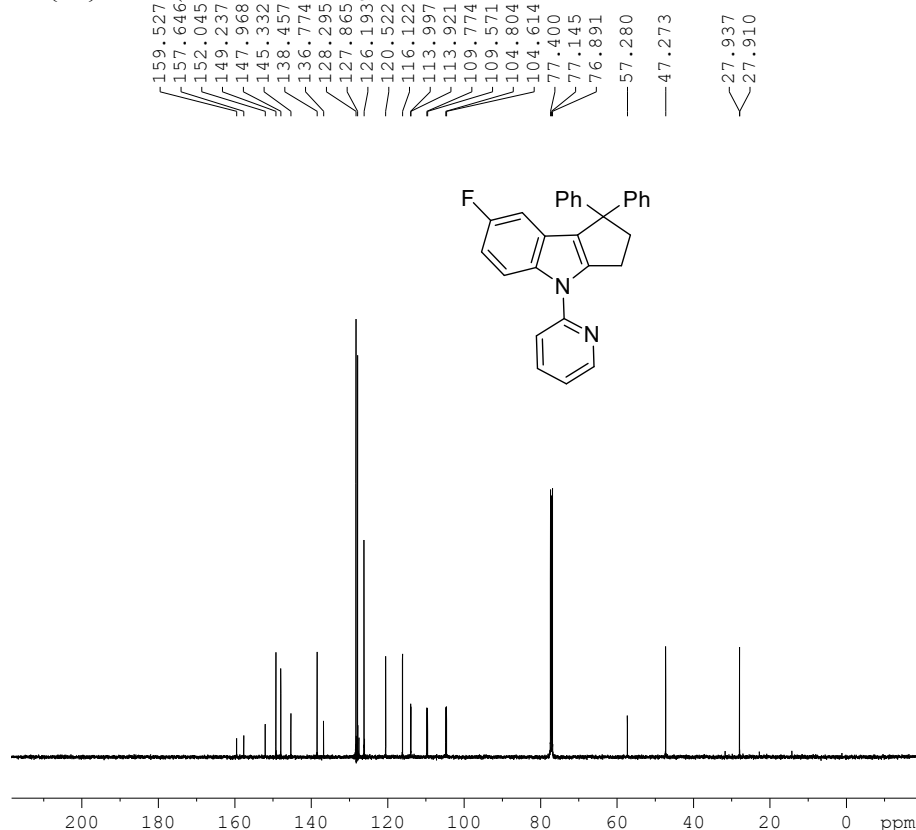
Current Data Parameters
NAME spa502
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_ 201802
Time_ 0.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zg
TD 327
SOLVENT CDC
NS
DS
SWH 10000.0
FIDRES 0.3051
AQ 1.63840
RG 89.
DW 50.0
DE 6.
TE 297
D1 0.500000
TD0

===== CHANNEL f1 =
SFO1 500.15250
NUC1
P1 12.
PLW1 15.300000

F2 - Processing parameters
SI 655
SF 500.15002
WDW
SSB 0
LB 0.
GB

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME pure r
EXPNO
PROCNO

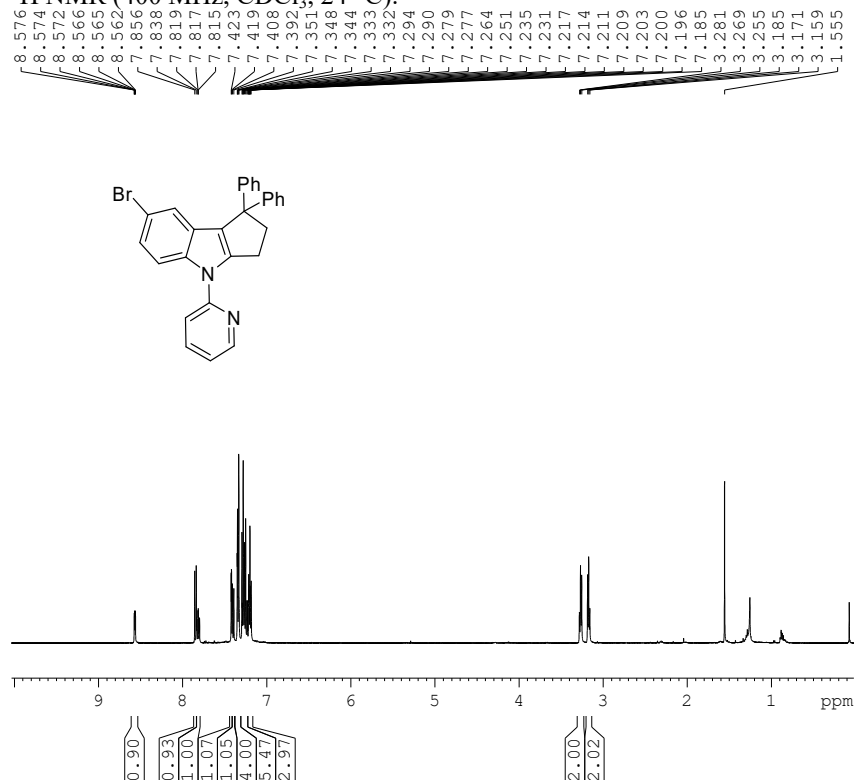
F2 - Acquisition Parameters
Date_ 201802
Time_ 0.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 204
SOLVENT CDC
NS 10
DS
SWH 29761.9
FIDRES 1.4532
AQ 0.34406
RG 202.
DW 16.8
DE 6.
TE 298
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 125.77539
NUC1 1
P1 9.
PLW1 103.000000

===== CHANNEL f2 =
SFO2 500.15200
NUC2
CPDPRG[2] waltz
PCPD2 80.
P1W2 15.300000

7-Bromo-1,1-diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10e):

¹H NMR (400 MHz, CDCl₃, 24 °C):



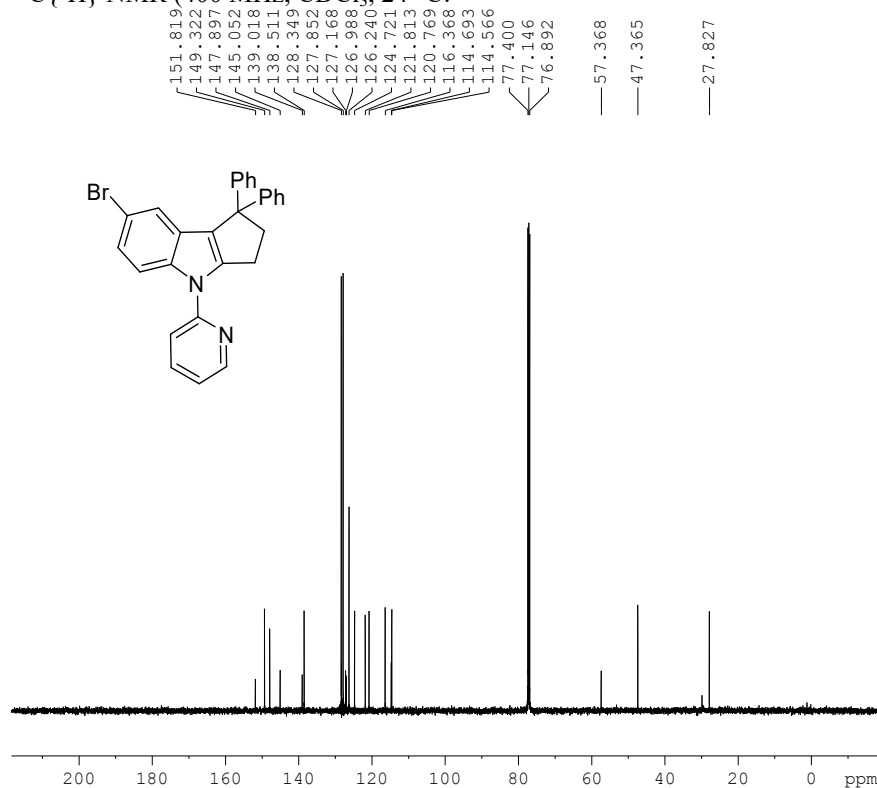
Current Data Parameters
NAME spa502
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_ 201802
Time_ 23.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zg
TD 327
SOLVENT CDC
NS
DS
SWH 10000.0
FIDRES 0.3051
AQ 1.63840
RG 114.
DW 50.0
DE 6.
TE 297
D1 0.500000
TD0

===== CHANNEL f1 =
SFO1 500.15250
NUC1
P1 12.
PLW1 15.300000

F2 - Processing parameters
SI 655
SF 500.15001
WDW
SSB 0
LB 0.
GB

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME spa502
EXPNO
PROCNO

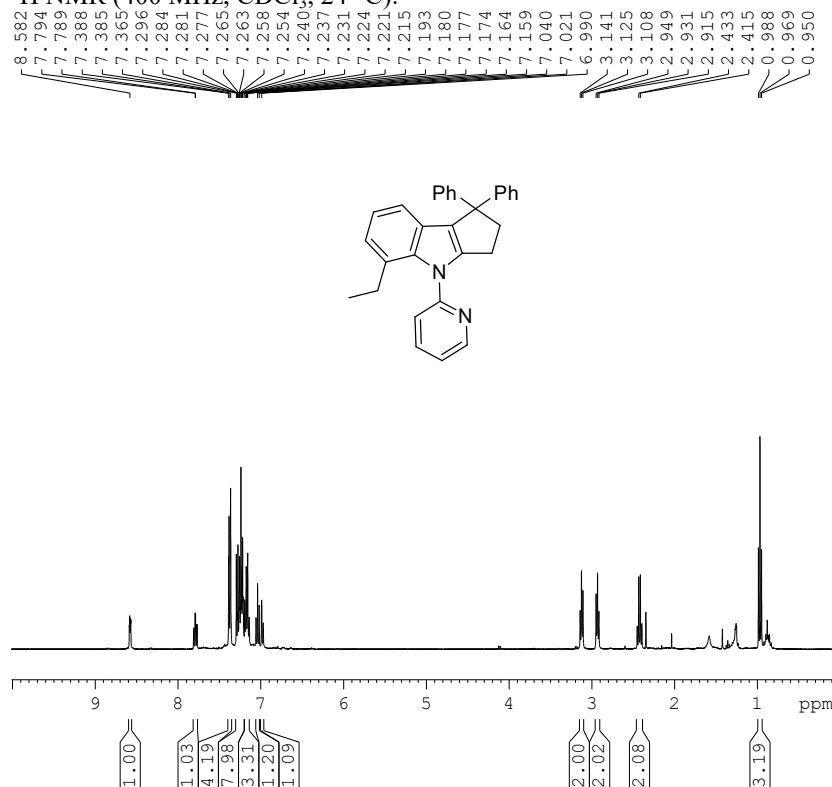
F2 - Acquisition Parameters
Date_ 201802
Time_ 0.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 204
SOLVENT CDC
NS 10
DS
SWH 29761.9
FIDRES 1.4532
AQ 0.34406
RG 202.
DW 16.8
DE 6.
TE 298
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 125.77539
NUC1 1
P1 9.
PLW1 103.000000

===== CHANNEL f2 =
SFO2 500.15200
NUC2
CPDPRG[2] waltz
PCPD2 80.
PLW2 15.300000

5-Ethyl-1,1-diphenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10f):

¹H NMR (400 MHz, CDCl₃, 24 °C):



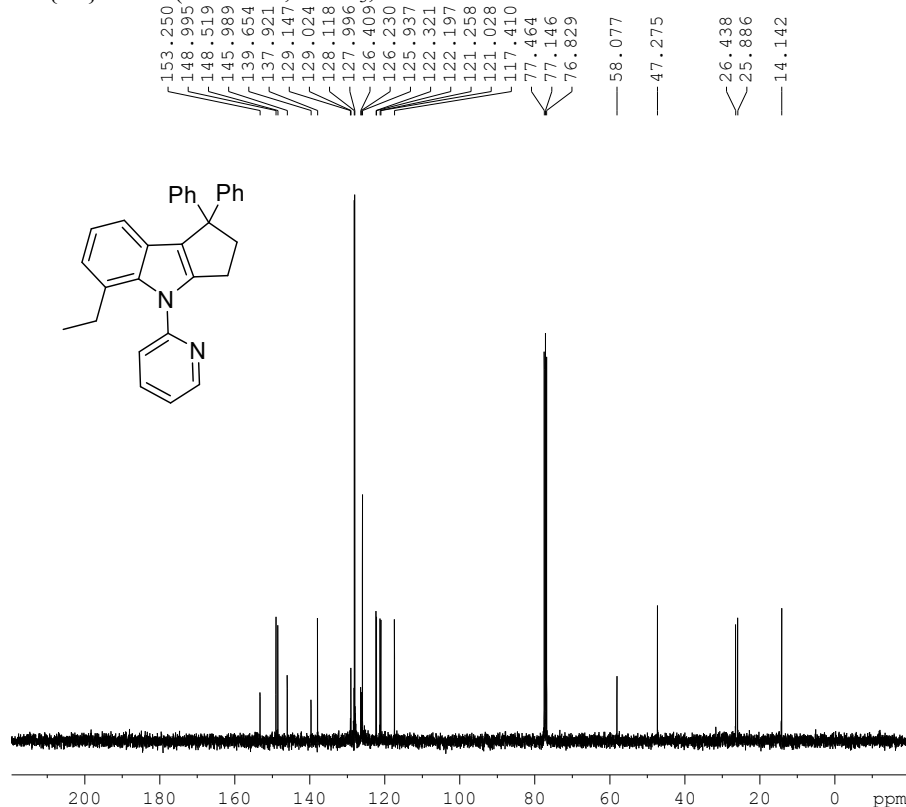
Current Data Parameters
NAME 1205 7 et appli
EXPNO 583
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180131
Time 8.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 124.58
DW 62.400 usec
DE 6.50 usec
TE 296.7 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300217 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME 12
EXPNO 5
PROCNO

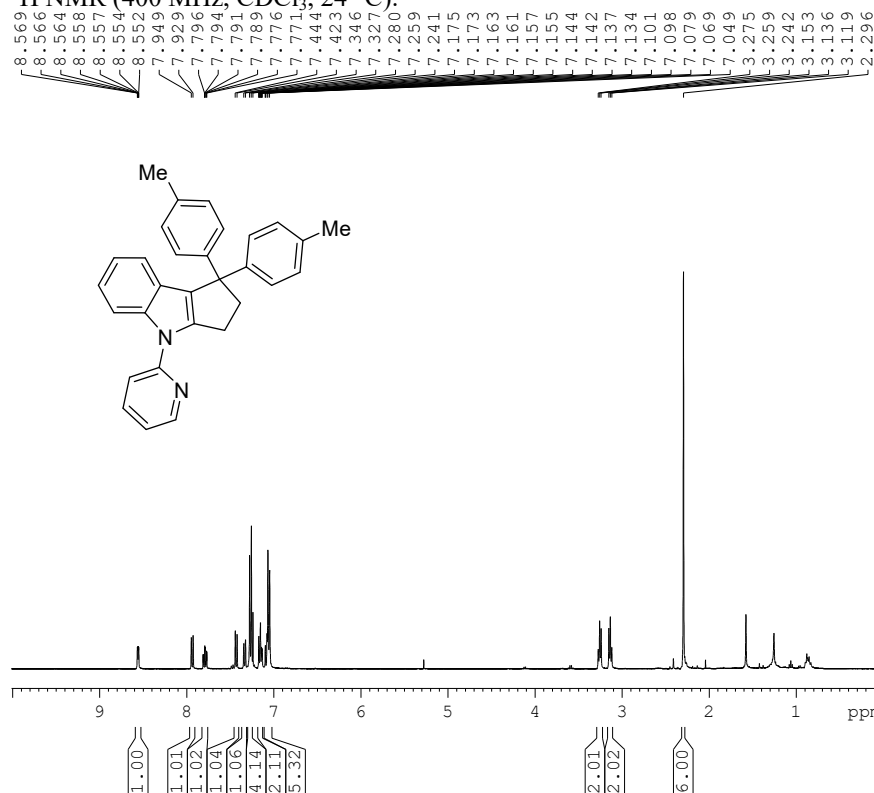
F2 - Acquisition Para
Date_ 201801
Time 8.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 297
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 1
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2 waltz
PCPD2 90.
DTW2 7 7500000

4-(Pyridin-2-yl)-1,1-di-p-tolyl-1,2,3,4-tetrahydrocyclopenta[b]indole (10g):

¹H NMR (400 MHz, CDCl₃, 24 °C):



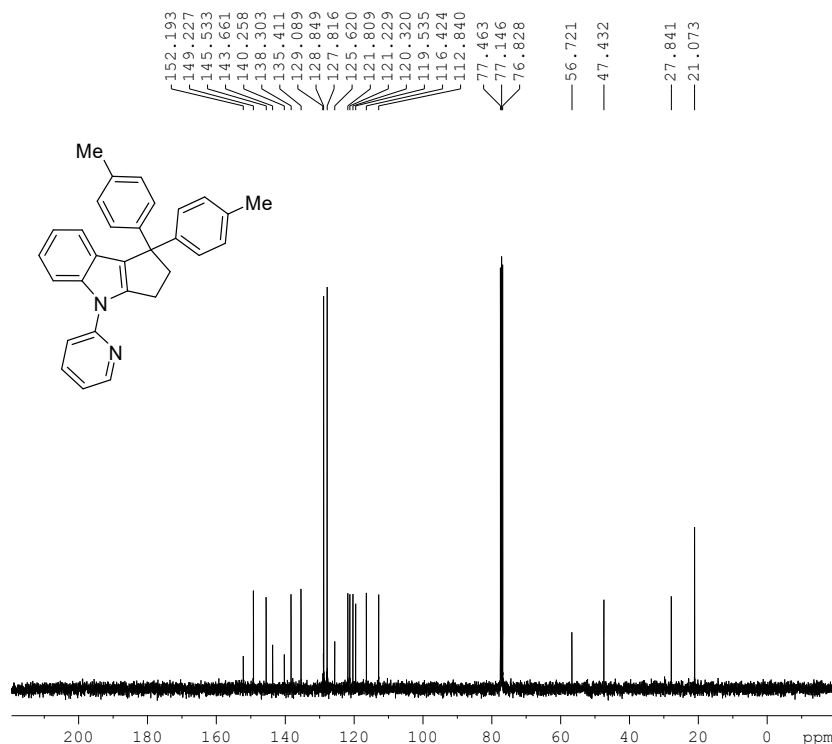
Current Data Parameter
NAME spa412
EXPNO 5
PROCNO

F2 - Acquisition Parameters
Date_ 201712
Time_ 10.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zg
TD 655
SOLVENT CDC
NS
DS
SWH 8012.8
FIDRES 0.1222
AQ 4.08944
RG 138.
DW 62.4
DE 6.
TE 293
D1 0.500000
TD0

===== CHANNEL f1 =
SFO1 400.13200
NUC1
P1 15.
PLW1 7.750000

F2 - Processing parameters
SI 655
SF 400.13001
WDW
SSB 0
LB 0.
GB

¹³C{¹H} NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameter
NAME spa412
EXPNO 5
PROCNO

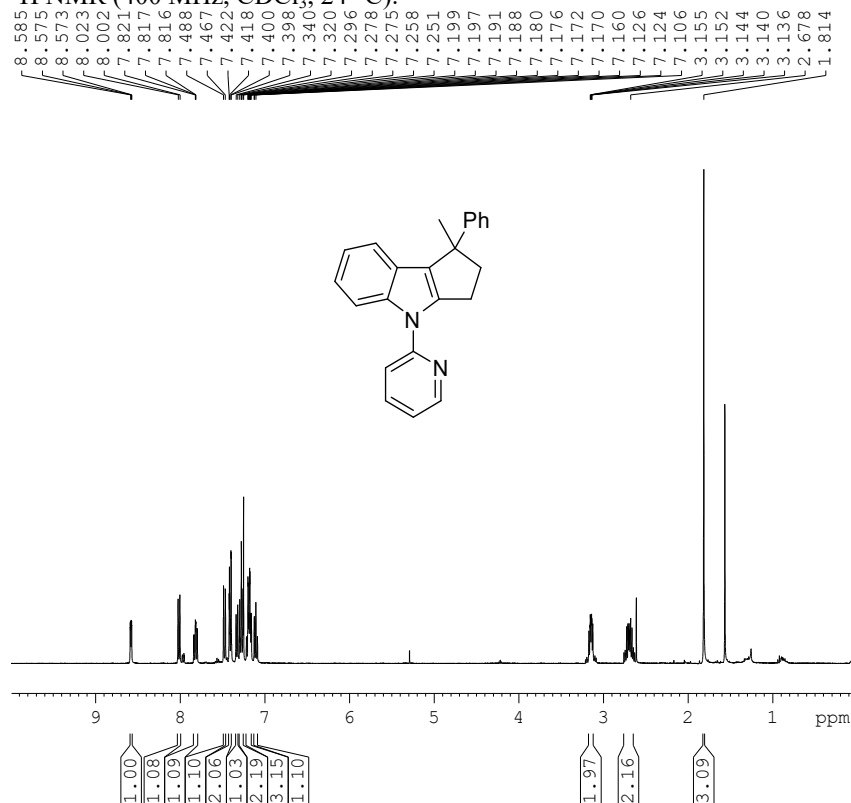
F2 - Acquisition Parameters
Date_ 201712
Time_ 10.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 2
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 293
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 1
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2] waltz
PCPD2 90.
PLW2 7.750000

1-Methyl-1-phenyl-4-(pyridin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10h):

¹H NMR (400 MHz, CDCl₃, 24 °C):



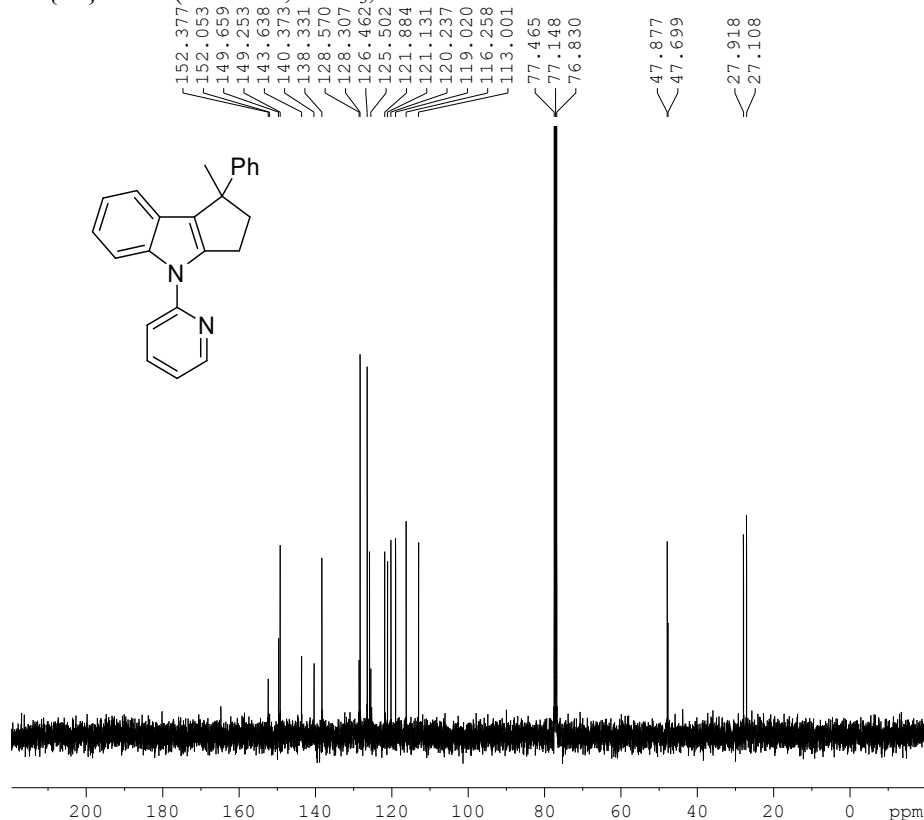
Current Data Parameters
NAME 1212 parent appli me
EXPNO 92
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180203
Time 15.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H} NMR (100 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME 1212 parent
EXPNO
PROCNO

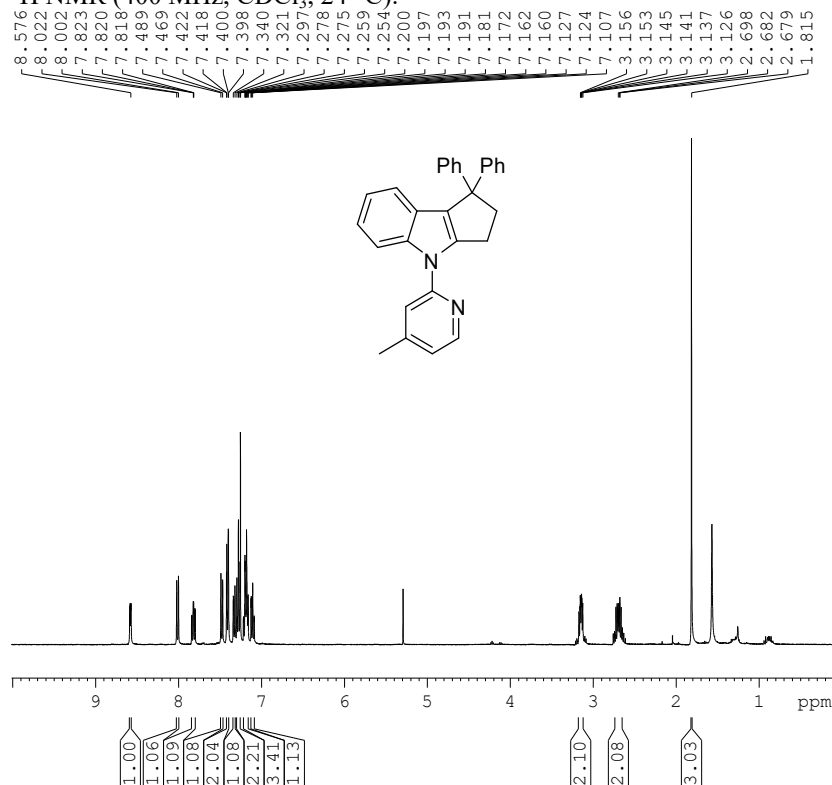
F2 - Acquisition Para
Date_ 201802
Time 15.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 5
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 297
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 1
P1 9.
PLW1 47.000000

===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2] waltz
PCPD2 90.
P1 7.750000

4-(4-Methylpyridin-2-yl)-1,1-diphenyl-1,2,3,4-tetrahydrocyclopenta[b]indole (10i):

¹H NMR (400 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 1213 appli py 4me
EXPNO 155
PROCNO 1

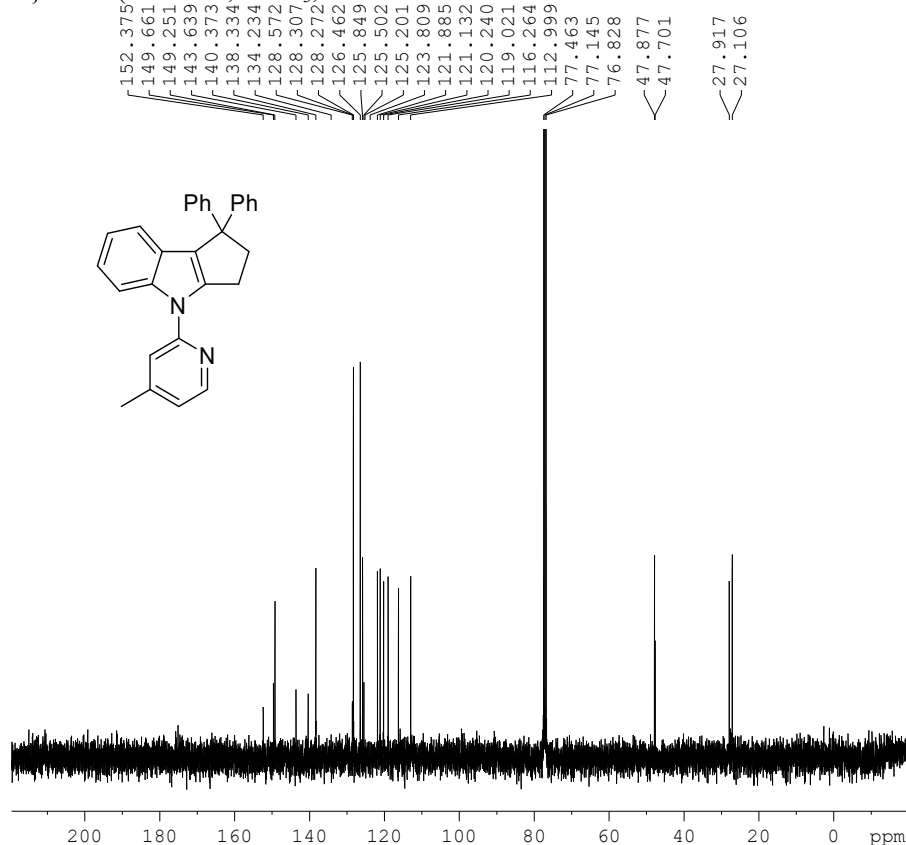
F2 - Acquisition Parameters
Date_ 20180205
Time 8.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 297.1 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W

F2 - Processing parameters
SI 65536
SF 400.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C{¹H}

¹³C NMR (100 MHz, CDCl₃, 24 °C):



Current Data Paramete
NAME 1213 appli
EXPNO 1
PROCNO

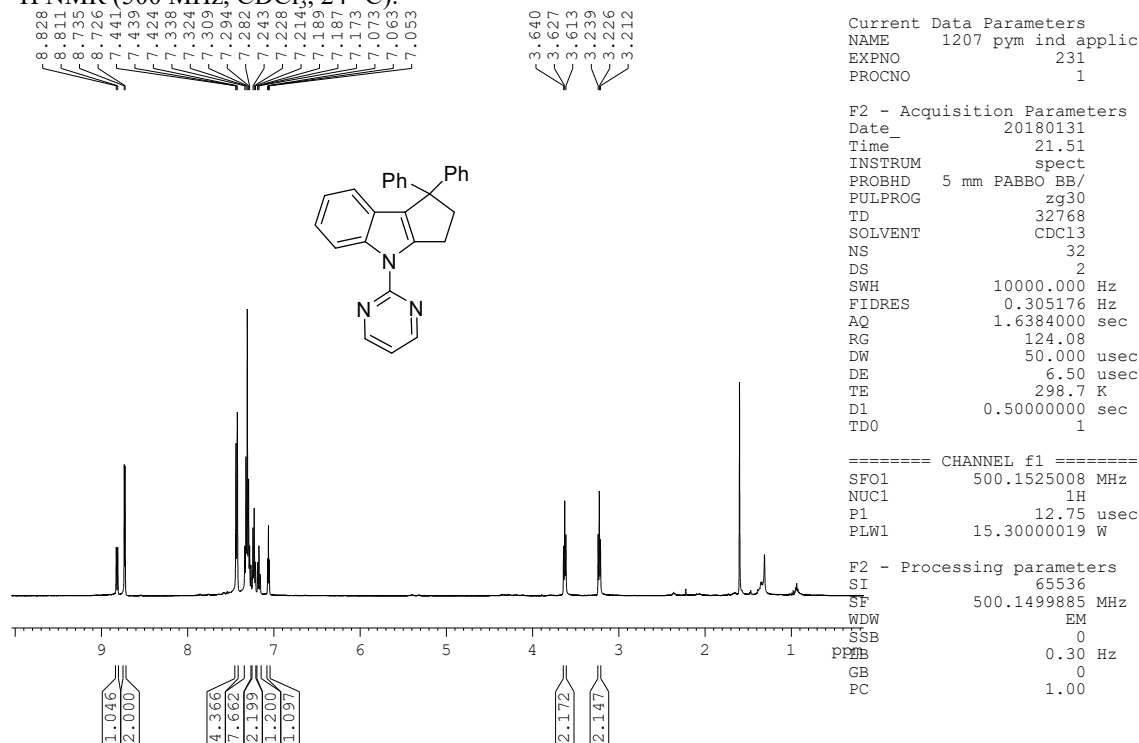
F2 - Acquisition Para
Date_ 201802
Time 8.
INSTRUM spe
PROBHD 5 mm PABBO B
PULPROG zgpg
TD 165
SOLVENT CDC
NS 6
DS
SWH 24038.4
FIDRES 1.4533
AQ 0.34403
RG 200.
DW 20.8
DE 6.
TE 297
D1 1.000000
D11 0.030000
TD0

===== CHANNEL f1 =
SFO1 100.62282
NUC1 1
P1 9.
PLW1 47.000000

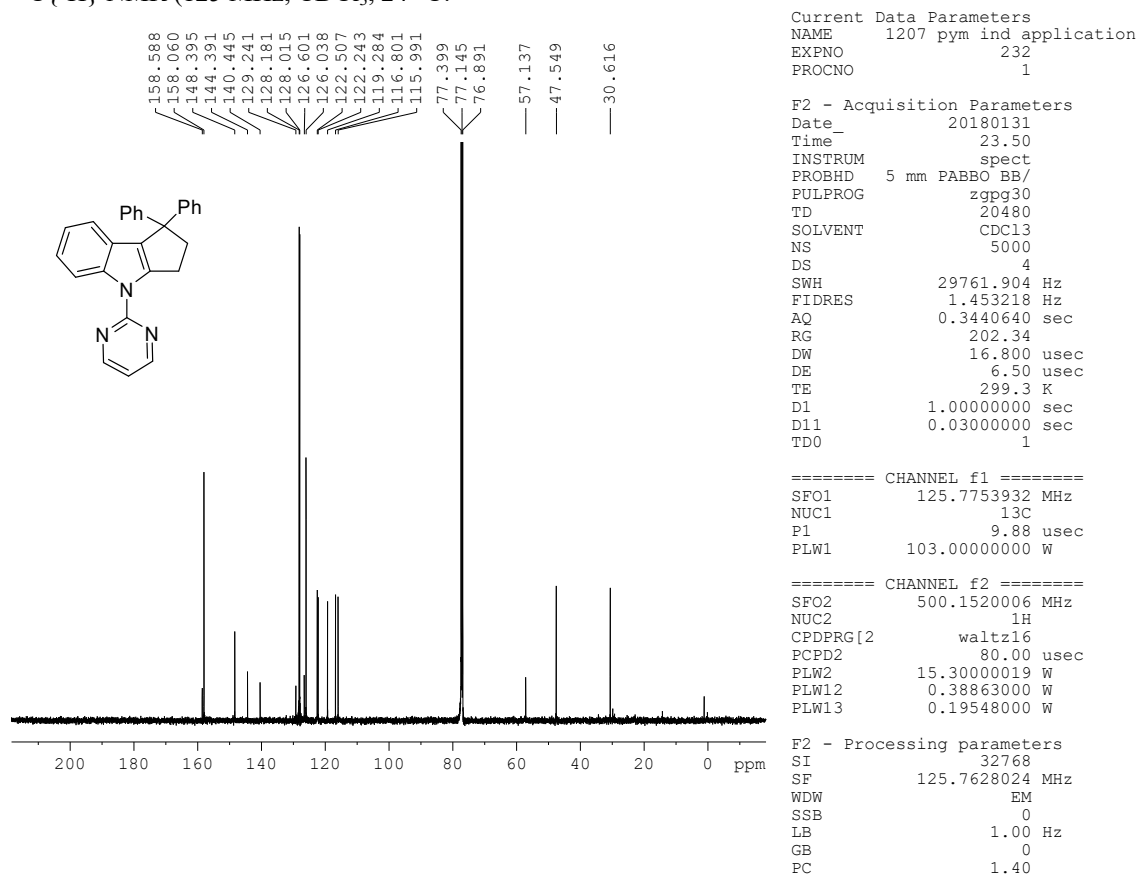
===== CHANNEL f2 =
SFO2 400.13160
NUC2
CPDPRG[2] waltz
PCPD2 90.
PLW2 7.750000

1,1-Diphenyl-4-(pyrimidin-2-yl)-1,2,3,4-tetrahydrocyclopenta[b]indole (10j):

¹H NMR (500 MHz, CDCl₃, 24 °C):

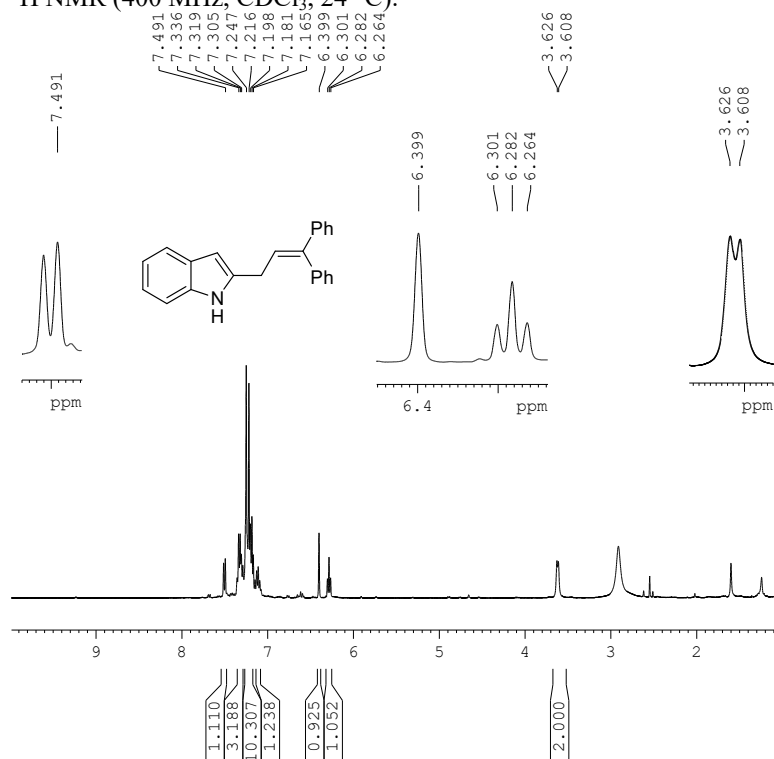


¹³C{¹H} NMR (125 MHz, CDCl₃, 24 °C):



2-(3,3-Diphenylallyl)-1H-indole (9):

¹H NMR (400 MHz, CDCl₃, 24 °C):



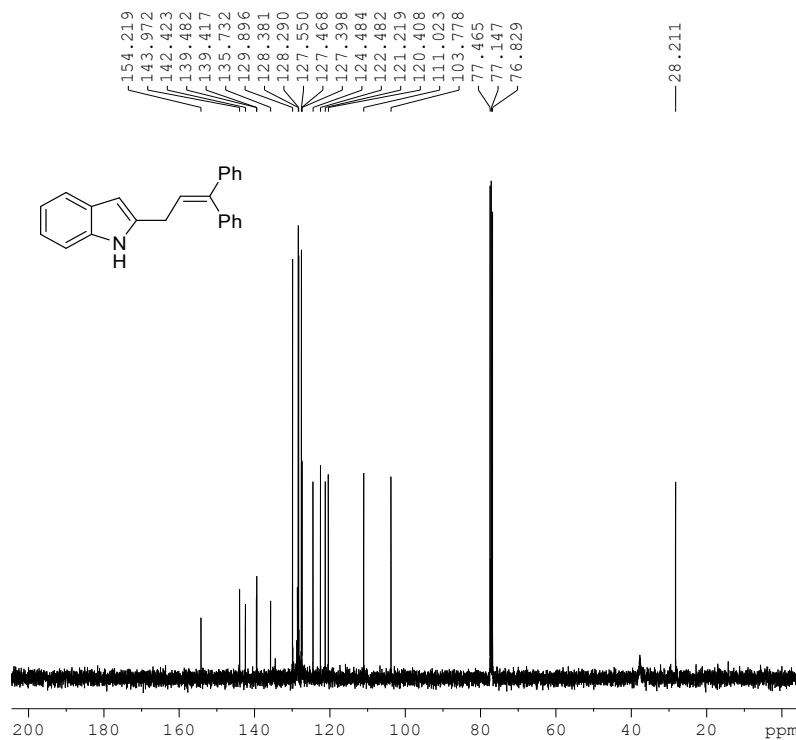
Current Data Parameters
NAME 2666 T2
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210503
Time_ 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 108.26
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1320007 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1300270 MHz
WDW EM
SSB 0
GB 0
PC 1.00

¹³C NMR (100 MHz, CDCl₃, 24 °C):



Current Data Parameters
NAME 2666 T2
EXPNO 33
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210503
Time_ 14.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228289 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 10.50000000 W
PLW12 0.29166999 W
PLW13 0.14670999 W

F2 - Processing parameters
SI 32768
SF 100.6127610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Crystal data of 12: ORTEP diagram

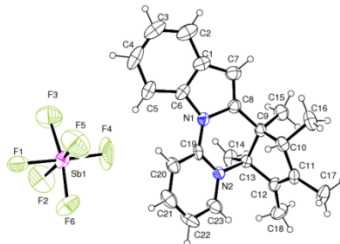


Table 1. Crystal data and structure refinement for col.

Identification code	shelx	
Empirical formula	C ₂₃ H ₂₅ F ₆ N ₂ Sb	
Formula weight	565.20	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /n	
Unit cell dimensions	a = 8.1550(5) Å	$\alpha = 90^\circ$.
	b = 15.9851(10) Å	$\beta = 102.305(2)^\circ$.
	c = 18.1298(11) Å	$\gamma = 90^\circ$.
Volume	2309.1(2) Å ³	
Z	4	
Density (calculated)	1.626 Mg/m ³	
Absorption coefficient	1.256 mm ⁻¹	
F(000)	1128	
Crystal size	0.150 x 0.100 x 0.100 mm ³	
Theta range for data collection	3.308 to 24.997°.	
Index ranges	-9<= <i>h</i> <=9, -19<= <i>k</i> <=19, -21<= <i>l</i> <=21	
Reflections collected	43544	
Independent reflections	4052 [R(int) = 0.0918]	
Completeness to theta = 24.997°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7453 and 0.5799	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4052 / 66 / 350	
Goodness-of-fit on F ²	1.131	
Final R indices [I>2sigma(I)]	R1 = 0.0724, wR2 = 0.1457	
R indices (all data)	R1 = 0.1044, wR2 = 0.1587	
Extinction coefficient	0.0050(5)	

Largest diff. peak and hole

0.607 and -0.480 e.Å⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å² $\times 10^3$) for co1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sb(1)	1383(1)	8076(1)	5512(1)	67(1)
F(1)	1170(40)	8900(20)	6170(20)	151(13)
F(2)	1110(40)	8969(12)	4862(12)	151(8)
F(3)	3629(19)	8300(18)	5748(19)	174(9)
F(4)	1640(50)	7202(17)	4932(19)	199(12)
F(5)	1480(40)	7348(16)	6267(13)	167(8)
F(6)	-945(15)	8025(12)	5346(15)	146(8)
F(1')	640(40)	8660(20)	6219(18)	160(12)
F(2')	2230(40)	8980(16)	5133(19)	208(11)
F(3')	3400(20)	7903(15)	6206(13)	147(8)
F(4')	2230(50)	7608(19)	4773(16)	206(13)
F(5')	920(40)	7067(12)	5870(15)	176(9)
F(6')	-450(30)	8084(15)	4779(13)	172(9)
C(1)	6150(10)	4949(6)	4049(4)	62(2)
C(2)	7629(12)	5083(8)	4596(5)	86(3)
C(3)	7767(14)	5763(9)	5029(6)	96(4)
C(4)	6521(16)	6342(7)	4956(5)	90(4)
C(5)	5007(12)	6252(6)	4412(5)	74(3)
C(6)	4852(10)	5520(5)	3986(4)	56(2)
C(7)	5674(10)	4324(6)	3496(5)	63(2)
C(8)	4123(9)	4487(5)	3103(4)	51(2)
C(9)	2969(9)	4057(4)	2463(4)	47(2)
C(10)	1726(9)	3429(5)	2726(4)	54(2)
C(11)	299(10)	3409(4)	2029(4)	53(2)
C(12)	364(9)	4072(5)	1589(4)	53(2)
C(13)	1745(8)	4663(4)	1963(4)	43(2)
C(14)	2478(11)	5255(5)	1458(4)	63(2)
C(15)	4066(11)	3611(5)	1984(5)	68(2)
C(16)	2481(13)	2588(5)	2978(5)	80(3)
C(17)	-971(12)	2735(6)	1919(6)	81(3)

C(18)	-709(11)	4246(6)	814(4)	81(3)
C(19)	1932(9)	5499(4)	3192(4)	45(2)
C(20)	1184(10)	6005(5)	3646(4)	58(2)
C(21)	-428(12)	6248(5)	3421(5)	71(2)
C(22)	-1347(11)	5993(6)	2732(5)	77(3)
C(23)	-594(11)	5482(5)	2295(5)	65(2)
N(1)	3562(7)	5235(4)	3384(3)	47(1)
N(2)	1028(7)	5233(3)	2514(3)	44(1)

Table 3. Bond lengths [Å] and angles [°] for col.

Sb(1)-F(6')	1.778(11)
Sb(1)-F(5)	1.786(14)
Sb(1)-F(4)	1.788(12)
Sb(1)-F(1')	1.792(14)
Sb(1)-F(4')	1.797(16)
Sb(1)-F(2')	1.799(16)
Sb(1)-F(5')	1.809(14)
Sb(1)-F(1)	1.811(13)
Sb(1)-F(3)	1.825(14)
Sb(1)-F(2)	1.834(13)
Sb(1)-F(6)	1.860(12)
Sb(1)-F(3')	1.867(11)
C(1)-C(6)	1.384(11)
C(1)-C(2)	1.404(12)
C(1)-C(7)	1.410(11)
C(2)-C(3)	1.331(15)
C(2)-H(2)	0.9300
C(3)-C(4)	1.360(15)
C(3)-H(3)	0.9300
C(4)-C(5)	1.415(14)
C(4)-H(4)	0.9300
C(5)-C(6)	1.393(11)
C(5)-H(5)	0.9300
C(6)-N(1)	1.419(9)

C(7)-C(8)	1.339(10)
C(7)-H(7)	0.9300
C(8)-N(1)	1.414(9)
C(8)-C(9)	1.496(10)
C(9)-C(13)	1.540(9)
C(9)-C(15)	1.548(10)
C(9)-C(10)	1.571(10)
C(10)-C(16)	1.508(10)
C(10)-C(11)	1.525(11)
C(10)-H(10)	0.9800
C(11)-C(12)	1.334(10)
C(11)-C(17)	1.479(10)
C(12)-C(18)	1.513(10)
C(12)-C(13)	1.516(9)
C(13)-C(14)	1.525(9)
C(13)-N(2)	1.554(8)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-N(2)	1.361(8)
C(19)-N(1)	1.367(9)
C(19)-C(20)	1.385(10)
C(20)-C(21)	1.348(11)
C(20)-H(20)	0.9300

C(21)-C(22)	1.374(12)
C(21)-H(21)	0.9300
C(22)-C(23)	1.370(11)
C(22)-H(22)	0.9300
C(23)-N(2)	1.357(9)
C(23)-H(23)	0.9300
F(5)-Sb(1)-F(4)	87.2(14)
F(6')-Sb(1)-F(1')	99.9(15)
F(6')-Sb(1)-F(4')	81.0(16)
F(1')-Sb(1)-F(4')	173.0(17)
F(6')-Sb(1)-F(2')	92.2(12)
F(1')-Sb(1)-F(2')	93.9(18)
F(4')-Sb(1)-F(2')	79.1(17)
F(6')-Sb(1)-F(5')	93.8(11)
F(1')-Sb(1)-F(5')	94.6(17)
F(4')-Sb(1)-F(5')	92.3(14)
F(2')-Sb(1)-F(5')	168.6(16)
F(5)-Sb(1)-F(1)	88.0(18)
F(4)-Sb(1)-F(1)	175(2)
F(5)-Sb(1)-F(3)	93.9(13)
F(4)-Sb(1)-F(3)	93.1(14)
F(1)-Sb(1)-F(3)	86.4(12)
F(5)-Sb(1)-F(2)	168.3(11)
F(4)-Sb(1)-F(2)	104.1(15)
F(1)-Sb(1)-F(2)	80.8(17)
F(3)-Sb(1)-F(2)	88.8(11)
F(5)-Sb(1)-F(6)	88.5(11)
F(4)-Sb(1)-F(6)	96.6(13)
F(1)-Sb(1)-F(6)	84.1(11)
F(3)-Sb(1)-F(6)	170.1(11)
F(2)-Sb(1)-F(6)	87.0(10)
F(6')-Sb(1)-F(3')	170.4(10)
F(1')-Sb(1)-F(3')	88.8(14)
F(4')-Sb(1)-F(3')	90.9(15)
F(2')-Sb(1)-F(3')	91.3(11)

F(5')-Sb(1)-F(3')	81.3(10)
C(6)-C(1)-C(2)	119.0(9)
C(6)-C(1)-C(7)	108.6(7)
C(2)-C(1)-C(7)	132.4(10)
C(3)-C(2)-C(1)	119.5(11)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
C(2)-C(3)-C(4)	122.1(10)
C(2)-C(3)-H(3)	119.0
C(4)-C(3)-H(3)	119.0
C(3)-C(4)-C(5)	121.4(10)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
C(6)-C(5)-C(4)	115.8(10)
C(6)-C(5)-H(5)	122.1
C(4)-C(5)-H(5)	122.1
C(1)-C(6)-C(5)	122.1(8)
C(1)-C(6)-N(1)	106.3(7)
C(5)-C(6)-N(1)	131.3(8)
C(8)-C(7)-C(1)	109.0(8)
C(8)-C(7)-H(7)	125.5
C(1)-C(7)-H(7)	125.5
C(7)-C(8)-N(1)	108.3(7)
C(7)-C(8)-C(9)	133.6(7)
N(1)-C(8)-C(9)	118.0(6)
C(8)-C(9)-C(13)	112.9(6)
C(8)-C(9)-C(15)	107.7(6)
C(13)-C(9)-C(15)	109.8(6)
C(8)-C(9)-C(10)	113.4(6)
C(13)-C(9)-C(10)	101.6(5)
C(15)-C(9)-C(10)	111.4(6)
C(16)-C(10)-C(11)	115.0(7)
C(16)-C(10)-C(9)	114.4(7)
C(11)-C(10)-C(9)	100.9(6)
C(16)-C(10)-H(10)	108.7
C(11)-C(10)-H(10)	108.7

C(9)-C(10)-H(10)	108.7
C(12)-C(11)-C(17)	127.9(8)
C(12)-C(11)-C(10)	111.0(6)
C(17)-C(11)-C(10)	121.0(7)
C(11)-C(12)-C(18)	127.8(7)
C(11)-C(12)-C(13)	110.4(6)
C(18)-C(12)-C(13)	121.9(7)
C(12)-C(13)-C(14)	117.8(6)
C(12)-C(13)-C(9)	101.4(6)
C(14)-C(13)-C(9)	117.1(6)
C(12)-C(13)-N(2)	107.9(5)
C(14)-C(13)-N(2)	105.8(5)
C(9)-C(13)-N(2)	106.0(5)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(9)-C(15)-H(15A)	109.5
C(9)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(9)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(10)-C(16)-H(16A)	109.5
C(10)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(10)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(11)-C(17)-H(17A)	109.5
C(11)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(11)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5

H(17B)-C(17)-H(17C)	109.5
C(12)-C(18)-H(18A)	109.5
C(12)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(12)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(2)-C(19)-N(1)	116.4(6)
N(2)-C(19)-C(20)	119.8(7)
N(1)-C(19)-C(20)	123.8(7)
C(21)-C(20)-C(19)	120.9(8)
C(21)-C(20)-H(20)	119.6
C(19)-C(20)-H(20)	119.6
C(20)-C(21)-C(22)	119.8(8)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.1
C(23)-C(22)-C(21)	118.5(8)
C(23)-C(22)-H(22)	120.7
C(21)-C(22)-H(22)	120.7
N(2)-C(23)-C(22)	122.3(8)
N(2)-C(23)-H(23)	118.8
C(22)-C(23)-H(23)	118.8
C(19)-N(1)-C(8)	122.7(6)
C(19)-N(1)-C(6)	128.2(6)
C(8)-N(1)-C(6)	107.8(6)
C(23)-N(2)-C(19)	118.6(6)
C(23)-N(2)-C(13)	117.5(6)
C(19)-N(2)-C(13)	123.9(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for col. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
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Sb(1)	74(1)	68(1)	57(1)	-12(1)	13(1)	-12(1)
F(1)	73(15)	200(20)	160(20)	-101(18)	-25(12)	42(14)
F(2)	190(20)	143(13)	136(14)	50(11)	80(14)	7(14)
F(3)	78(10)	190(20)	270(20)	-35(17)	68(13)	-7(11)
F(4)	290(20)	133(18)	177(19)	-121(17)	56(15)	8(17)
F(5)	200(20)	163(17)	139(15)	53(14)	43(15)	50(15)
F(6)	92(10)	152(13)	177(19)	-26(15)	-9(11)	-39(9)
F(1')	110(20)	270(30)	113(14)	-5(15)	48(15)	78(19)
F(2')	190(20)	168(16)	260(20)	33(16)	39(19)	-71(17)
F(3')	81(10)	159(17)	170(16)	-63(13)	-43(10)	42(10)
F(4')	320(30)	160(20)	141(15)	-20(17)	70(17)	70(20)
F(5')	205(18)	109(12)	182(19)	22(13)	-34(16)	-50(12)
F(6')	135(14)	206(16)	127(14)	-9(14)	-77(11)	10(13)
C(1)	53(5)	78(6)	54(5)	16(4)	7(4)	-13(5)
C(2)	70(6)	124(9)	60(6)	18(6)	3(5)	-29(6)
C(3)	77(7)	141(11)	63(6)	-3(7)	1(5)	-48(8)
C(4)	128(9)	96(8)	48(5)	-22(5)	26(6)	-66(8)
C(5)	87(6)	69(6)	66(5)	-20(5)	15(5)	-28(5)
C(6)	62(5)	62(5)	42(4)	-2(4)	7(4)	-23(4)
C(7)	52(5)	68(5)	69(5)	4(5)	11(4)	0(4)
C(8)	48(4)	50(4)	55(4)	-2(4)	14(4)	-6(3)
C(9)	53(4)	43(4)	46(4)	-8(3)	11(3)	6(3)
C(10)	62(5)	45(4)	58(5)	5(4)	18(4)	4(4)
C(11)	65(5)	35(4)	63(5)	-11(4)	20(4)	-5(4)
C(12)	56(5)	50(5)	50(4)	-14(4)	7(3)	-6(4)
C(13)	45(4)	41(4)	44(4)	-3(3)	11(3)	-3(3)
C(14)	86(6)	56(5)	53(5)	3(4)	27(4)	-9(4)
C(15)	72(6)	72(6)	66(5)	-17(5)	23(4)	8(5)
C(16)	116(8)	41(5)	84(6)	3(5)	26(6)	10(5)
C(17)	92(7)	63(6)	94(7)	-15(5)	31(6)	-39(5)
C(18)	81(6)	95(7)	53(5)	-5(5)	-13(4)	-13(5)
C(19)	67(5)	25(3)	43(4)	0(3)	14(3)	-1(3)
C(20)	76(6)	52(5)	49(4)	-1(4)	20(4)	12(4)
C(21)	100(7)	65(6)	56(5)	7(4)	35(5)	28(5)
C(22)	69(6)	85(7)	78(6)	14(5)	17(5)	44(5)
C(23)	70(5)	66(5)	57(5)	4(4)	8(4)	18(4)

N(1)	50(4)	43(3)	46(3)	-7(3)	10(3)	-1(3)
N(2)	49(3)	40(3)	43(3)	-1(3)	9(3)	3(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for col.

	x	y	z	U(eq)
H(2)	8505	4700	4655	104
H(3)	8746	5845	5392	115
H(4)	6668	6808	5272	108
H(5)	4167	6656	4343	89
H(7)	6332	3871	3417	76
H(10)	1311	3683	3144	65
H(14A)	2831	4939	1068	95
H(14B)	3425	5544	1754	95
H(14C)	1641	5654	1232	95
H(15A)	4732	4018	1790	103
H(15B)	3356	3324	1571	103
H(15C)	4790	3215	2292	103
H(16A)	1759	2294	3244	119
H(16B)	3562	2666	3305	119
H(16C)	2604	2269	2544	119
H(17A)	-1583	2757	2316	122
H(17B)	-422	2202	1929	122
H(17C)	-1733	2807	1441	122
H(18A)	-1806	4012	781	121
H(18B)	-200	3997	436	121
H(18C)	-801	4839	734	121
H(20)	1802	6180	4112	70
H(21)	-917	6587	3731	85
H(22)	-2454	6164	2565	92
H(23)	-1217	5300	1833	78

Table 6. Torsion angles [$^{\circ}$] for co1.

C(6)-C(1)-C(2)-C(3)	-1.5(13)
C(7)-C(1)-C(2)-C(3)	176.6(9)
C(1)-C(2)-C(3)-C(4)	-0.6(15)
C(2)-C(3)-C(4)-C(5)	-0.2(16)
C(3)-C(4)-C(5)-C(6)	2.9(13)
C(2)-C(1)-C(6)-C(5)	4.4(12)
C(7)-C(1)-C(6)-C(5)	-174.1(7)
C(2)-C(1)-C(6)-N(1)	178.6(7)
C(7)-C(1)-C(6)-N(1)	0.2(9)
C(4)-C(5)-C(6)-C(1)	-4.9(12)
C(4)-C(5)-C(6)-N(1)	-177.6(8)
C(6)-C(1)-C(7)-C(8)	-0.8(9)
C(2)-C(1)-C(7)-C(8)	-179.0(9)
C(1)-C(7)-C(8)-N(1)	1.1(9)
C(1)-C(7)-C(8)-C(9)	-179.6(8)
C(7)-C(8)-C(9)-C(13)	-151.9(8)
N(1)-C(8)-C(9)-C(13)	27.4(9)
C(7)-C(8)-C(9)-C(15)	-30.5(12)
N(1)-C(8)-C(9)-C(15)	148.8(6)
C(7)-C(8)-C(9)-C(10)	93.2(10)
N(1)-C(8)-C(9)-C(10)	-87.5(8)
C(8)-C(9)-C(10)-C(16)	-80.5(8)
C(13)-C(9)-C(10)-C(16)	158.1(7)
C(15)-C(9)-C(10)-C(16)	41.2(9)
C(8)-C(9)-C(10)-C(11)	155.5(6)
C(13)-C(9)-C(10)-C(11)	34.0(6)
C(15)-C(9)-C(10)-C(11)	-82.8(7)
C(16)-C(10)-C(11)-C(12)	-142.5(7)
C(9)-C(10)-C(11)-C(12)	-18.9(8)
C(16)-C(10)-C(11)-C(17)	39.7(11)
C(9)-C(10)-C(11)-C(17)	163.3(7)
C(17)-C(11)-C(12)-C(18)	-8.7(14)
C(10)-C(11)-C(12)-C(18)	173.7(8)
C(17)-C(11)-C(12)-C(13)	172.6(7)

C(10)-C(11)-C(12)-C(13)	-5.0(9)
C(11)-C(12)-C(13)-C(14)	156.5(7)
C(18)-C(12)-C(13)-C(14)	-22.3(10)
C(11)-C(12)-C(13)-C(9)	27.3(8)
C(18)-C(12)-C(13)-C(9)	-151.5(7)
C(11)-C(12)-C(13)-N(2)	-83.9(7)
C(18)-C(12)-C(13)-N(2)	97.3(8)
C(8)-C(9)-C(13)-C(12)	-158.7(6)
C(15)-C(9)-C(13)-C(12)	81.1(7)
C(10)-C(9)-C(13)-C(12)	-36.9(6)
C(8)-C(9)-C(13)-C(14)	71.6(8)
C(15)-C(9)-C(13)-C(14)	-48.5(8)
C(10)-C(9)-C(13)-C(14)	-166.5(6)
C(8)-C(9)-C(13)-N(2)	-46.1(7)
C(15)-C(9)-C(13)-N(2)	-166.3(6)
C(10)-C(9)-C(13)-N(2)	75.7(6)
N(2)-C(19)-C(20)-C(21)	-0.8(11)
N(1)-C(19)-C(20)-C(21)	179.5(7)
C(19)-C(20)-C(21)-C(22)	-0.2(13)
C(20)-C(21)-C(22)-C(23)	1.1(14)
C(21)-C(22)-C(23)-N(2)	-1.2(14)
N(2)-C(19)-N(1)-C(8)	-26.3(9)
C(20)-C(19)-N(1)-C(8)	153.4(7)
N(2)-C(19)-N(1)-C(6)	168.7(6)
C(20)-C(19)-N(1)-C(6)	-11.6(11)
C(7)-C(8)-N(1)-C(19)	-168.6(7)
C(9)-C(8)-N(1)-C(19)	11.9(10)
C(7)-C(8)-N(1)-C(6)	-1.0(8)
C(9)-C(8)-N(1)-C(6)	179.6(6)
C(1)-C(6)-N(1)-C(19)	167.3(7)
C(5)-C(6)-N(1)-C(19)	-19.2(13)
C(1)-C(6)-N(1)-C(8)	0.5(8)
C(5)-C(6)-N(1)-C(8)	174.0(8)
C(22)-C(23)-N(2)-C(19)	0.3(12)
C(22)-C(23)-N(2)-C(13)	-179.1(7)
N(1)-C(19)-N(2)-C(23)	-179.6(6)

C(20)-C(19)-N(2)-C(23)	0.7(10)
N(1)-C(19)-N(2)-C(13)	-0.2(9)
C(20)-C(19)-N(2)-C(13)	-179.9(6)
C(12)-C(13)-N(2)-C(23)	-37.0(8)
C(14)-C(13)-N(2)-C(23)	90.0(7)
C(9)-C(13)-N(2)-C(23)	-145.0(6)
C(12)-C(13)-N(2)-C(19)	143.6(6)
C(14)-C(13)-N(2)-C(19)	-89.4(7)
C(9)-C(13)-N(2)-C(19)	35.6(8)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for col [$\text{\AA}$ and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5)...F(4'^b)	0.93	2.44	3.30(3)	154.0
C(7)-H(7)...F(5^a)#1	0.93	2.62	3.50(2)	158.9
C(14)-H(14A)...F(2^a)#2	0.96	2.57	3.530(16)	173.6
C(14)-H(14B)...F(1'^b)#3	0.96	2.56	3.21(3)	125.1
C(20)-H(20)...F(4^a)	0.93	2.23	2.977(18)	136.7
C(20)-H(20)...F(4'^b)	0.93	2.57	3.28(3)	133.3
C(22)-H(22)...F(1^a)#4	0.93	2.54	3.12(3)	120.3
C(22)-H(22)...F(1'^b)#4	0.93	2.61	3.31(4)	132.6
C(23)-H(23)...F(1^a)#4	0.93	2.56	3.13(3)	120.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1/2,y-1/2,-z+1/2 #3 x+1/2,-y+3/2,z-1/2

#4 x-1/2,-y+3/2,z-1/2