

SUPPORTING INFORMATION

Immobilize Palladium(II) Acetate on Polymer Anchored Schiff Base as a New Heterogenous Catalyst for the Three Multicomponent One-Pot Mizoroki Heck Coupling via *in situ* Wittig Reaction.

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1. General Information

All the reactions were conducted with N₂ protection. All Chemicals were purchased from Merck(Sigma-Aldrich), TCI, AVRA, and SRL Chemical Company. ¹H NMR and ¹³C NMR spectra were recorded on Bruker Avance neo 400 spectrometers. Chemical shifts are reported in ppm relative to TMS as an internal standard. Chemical shifts were recorded in parts per million (ppm, δ) relative to tetramethylsilane (δ 0.00) or chloroform (d = 7.26, singlet). ¹H-NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublets), m (multiplets). All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet(m) or broad (br). The reactions were monitored by TLC on silica-gel 60 F₂₅₄ plates. IR Spectra were recorded on Bruker spectrometer as KBr pellets. The morphology of the catalyst was examined by scanning electron microscopy field-emission scanning electron microscopy (FESEM, Model-JSM7610F PLUS), and TEM images were recorded using a TEM microscope (JEOL JEM 2100 PLUS). The elemental composition was determined by elemental mapping using TEM (JEOL JEM 2100 PLUS). TG-DTA measurements were carried out on an SII EXTRAR600TG-DTA instrument.

2. Characterization of catalyst

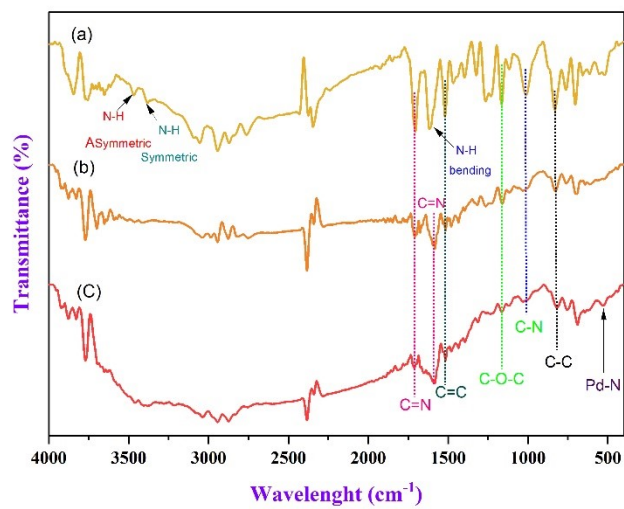


Figure S1. FT-IR spectra of (a) PS-H¹L, (b) PS-H²L, (c) PS@Pd(OAc)₂

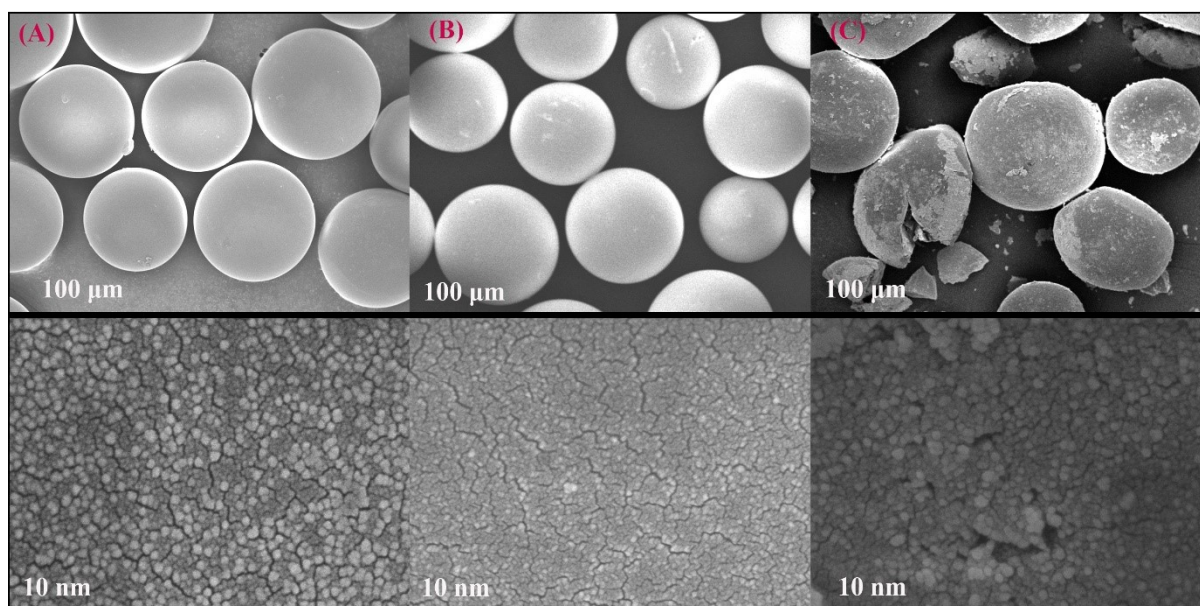


Figure S2. FESEM images of (A) PS-H¹L, (B) PS-H²L, (C) PS@Pd(OAc)₂

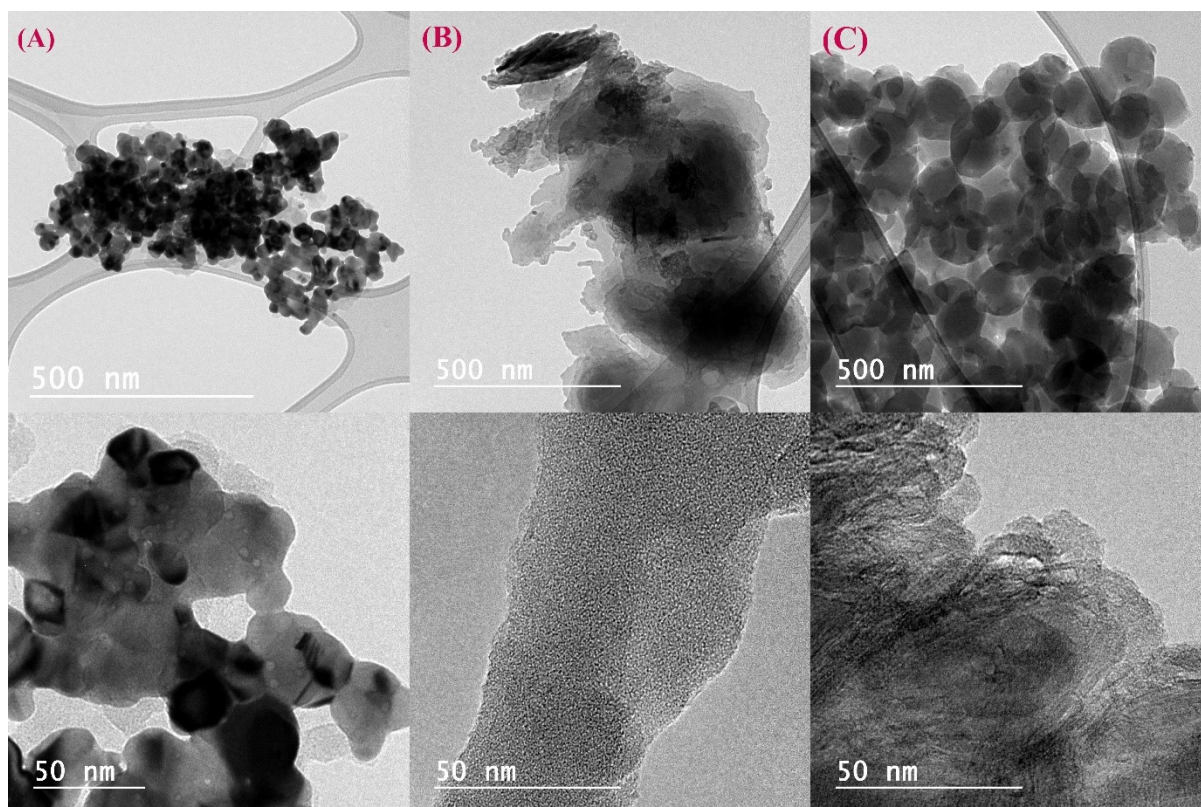


Figure S3. HRTEM images of (a) PS-H¹L, (b) PS-H²L, (c) PS@Pd(OAc)₂

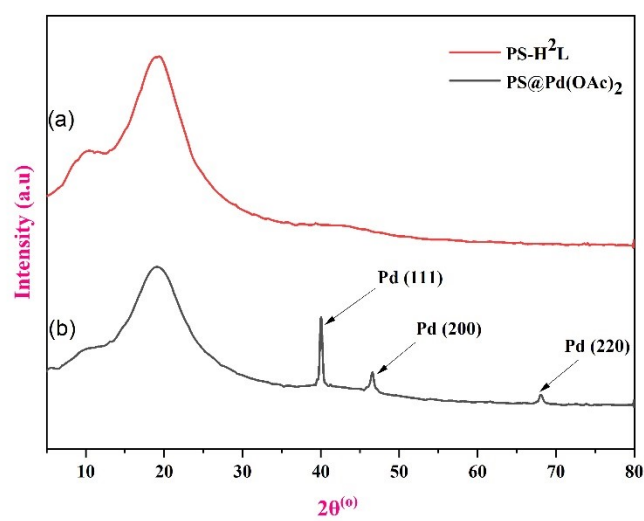


Figure S4. Powder XRD analysis of (a) PS-H²L, (b) PS@Pd(OAc)₂

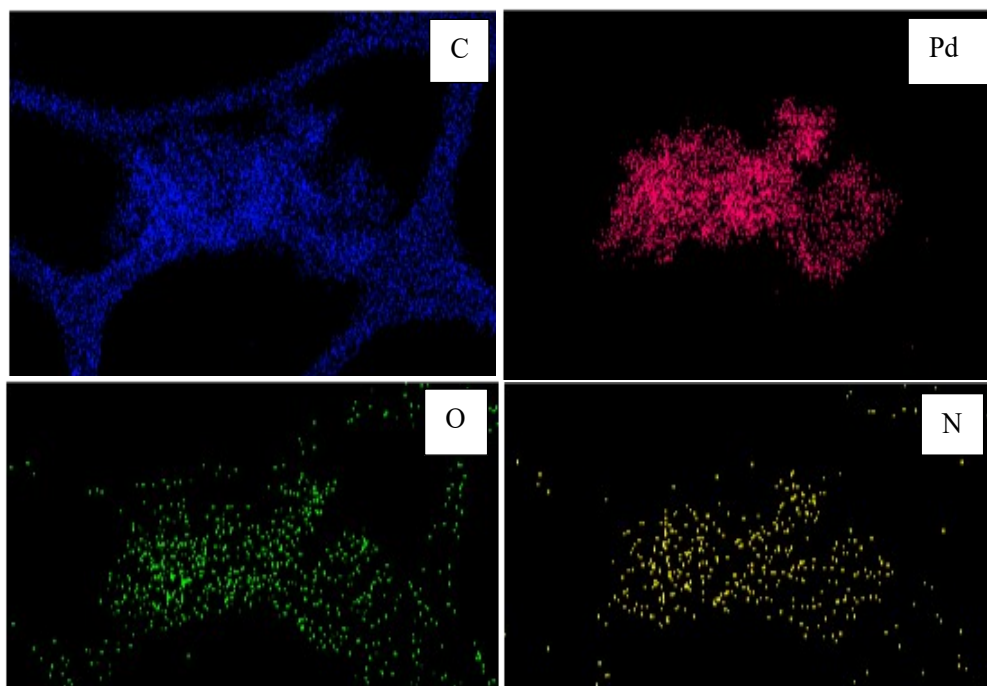


Figure S5. Elemental Mapping analysis images of PS@Pd(OAc)₂ for key elements
(a) C (b) Pd (c) O (d) N

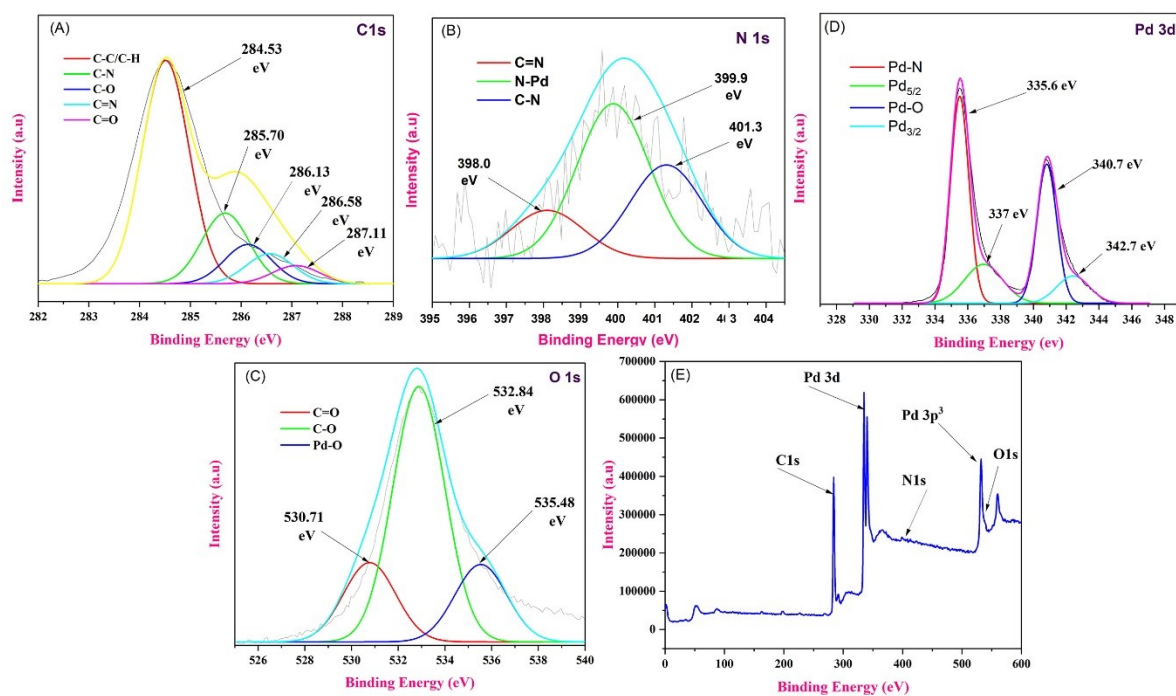


Figure S6. (A) C 1s scan XPS spectrum of PS@Pd(OAc)₂. (B) N 1s scan XPS spectrum of PS@Pd(OAc)₂. (C) O 1s scan XPS spectrum of PS@Pd(OAc)₂. (D) Pd 3d scan XPS spectrum of PS@Pd(OAc)₂ and (E) Full Scan XPS spectrum of PS@Pd(OAc)₂

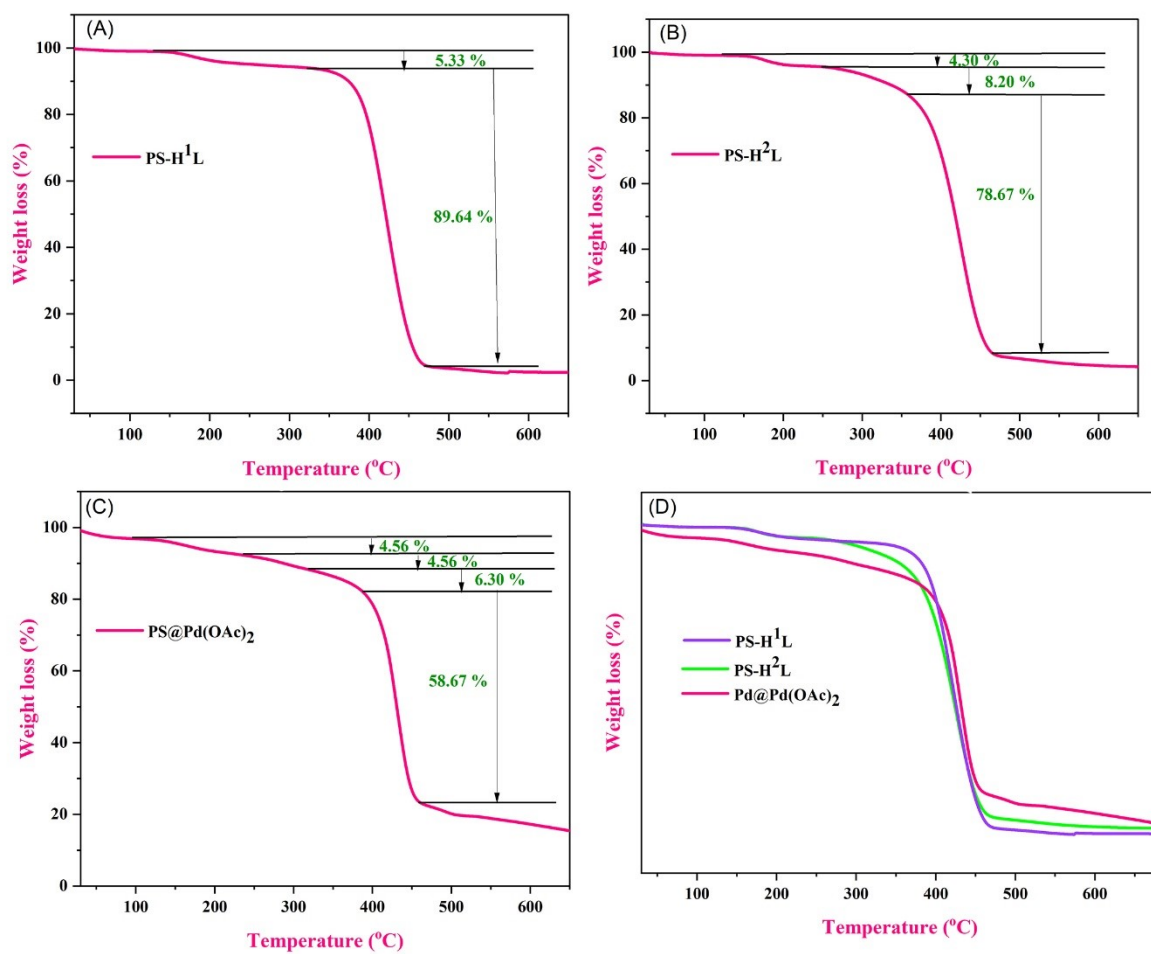


Figure S7. TGA spectra of (a) PS-H¹L, (b) PS-H²L, (c) PS@Pd(OAc)₂ (D) comparison spectra between PS-H¹L, PS-H²L and PS@Pd(OAc)₂

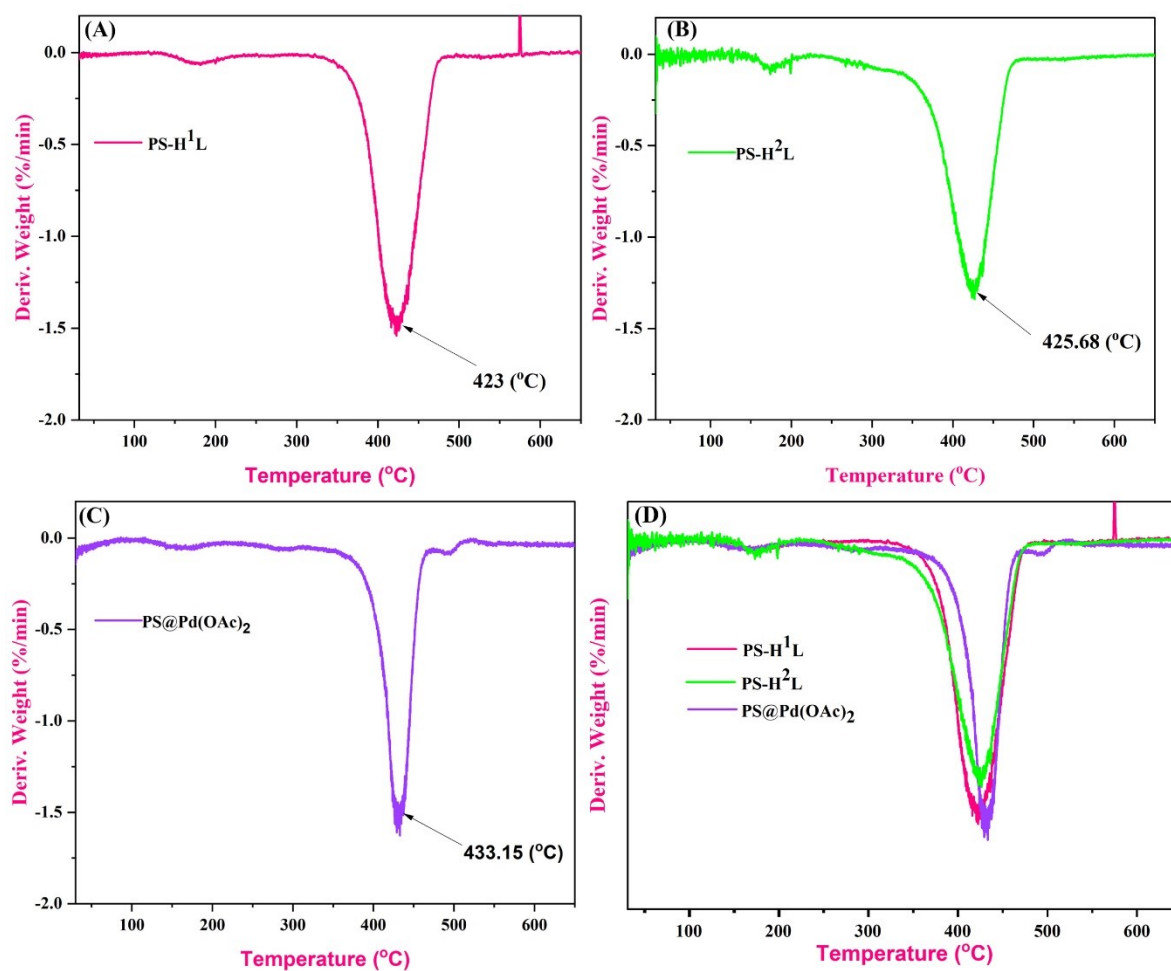
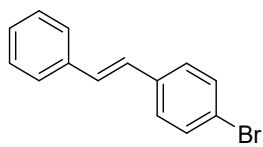


Figure 8. DTGA spectra of (a) PS-H¹L, (b) PS-H²L, (c) PS@Pd(OAc)₂ (D) Comparison spectra between PS-H¹L, PS-H²L and PS@Pd(OAc)₂

3. Characterization data of synthesized compounds

1) (E)-1-bromo-4-styrylbenzene



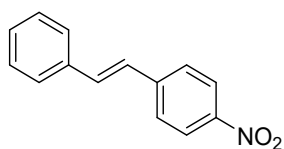
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethyl ether or ethyl acetate in petroleum ether (05:95).

Colour: White solid (90 % yield);

¹H NMR: (400 MHz, CDCl₃): δ 6.64 (d, *J* = 16.0 Hz, 2H), 6.78 (d, *J* = 16.0 Hz, 2H), 7.26 (d, *J* = 6.0 Hz, 2H), 7.35-7.40 (m, 5H), 7.48 (d, *J* = 8.0 Hz, 2H).

¹³C NMR: δ 121.06, 127.45, 128.45, 128.89, 129.03, 130.63, 131.13, 131.46, 136.18, 136.91.

2) (E)-1-nitro-4-styrylbenzene



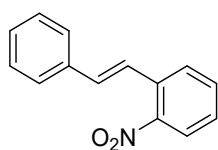
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: Light yellow solid (93 % yield)

¹H NMR: (400 MHz, CDCl₃): δ 6.63 (d, *J* = 16.4 Hz, 1H), 6.86 (d, *J* = 16.4 Hz, 1H), 7.21-7.24 (m, 2H), 7.26-7.28 (m, 3H), 7.39 (d, *J* = 8.8 Hz, 2H), 8.09 (d, *J* = 8.8 Hz, 2H).

¹³C NMR: δ 123.60, 124.20, 126.89, 127.98, 128.58, 129.68, 133.32, 133.96, 136.10, 174.44.

3) (E)-1-nitro-2-styrylbenzene



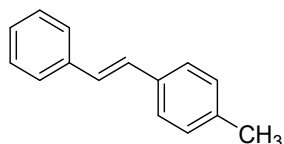
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: Light yellow solid (74 % yield)

¹H NMR: (400 MHz, CDCl₃): δ 6.78 (d, *J* = 16.0 Hz, 1H), 6.91 (d, *J* = 16.0 Hz, 1H), 7.02-7.08 (m, 2H), 7.14-7.24 (m, 4H), 7.40-7.42 (m, 2H), 8.10-8.12 (m 1H).

¹³C NMR: δ 123.89, 124.20, 126.89, 127.98, 128.01, 128.58, 128.88, 128.93, 129.68, 133.96, 136.10, 146.32.

4) (E)-1-methyl-4-styrylbenzene



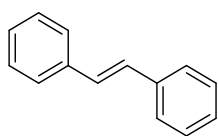
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: White solid (84 % yield)

¹H NMR: (400 MHz, CDCl₃) : δ 2.37 (s, 3H), 6.62 (s, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.23-7.35 (m, 5H).

¹³C NMR: δ 22.71, 126.97, 126.19, 128.79, 120.84, 128.90, 129.55, 130.20, 137.50.

5) (*E*)-1,2-diphenylethene



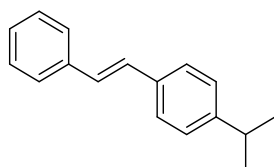
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: White solid (89 % yield)

¹H NMR: (400 MHz, CDCl₃): δ 6.71 (s, 2H), 7.43-7.36 (m, 2H), 7.38-7.40 (m, 3H), 7.42-7.44 (m, 5H).

¹³C NMR: δ 127.09, 128.21, 128.88, 130.25, 137.25.

6) (*E*)-1-isopropyl-4-styrylbenzene



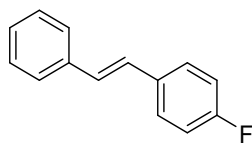
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: White solid (86 % yield)

¹H NMR: (400 MHz, CDCl₃): δ 1.50 (s, 6H), 3.01-3.08 (m, 1H), 6.74-6.78 (m, 2H), 7.25-7.26 (m, 2H), 7.35-7.42 (m, 5H), 7.48-7.50 (m, 2H).

¹³C NMR: δ 24.21, 30.12, 34.12, 126.48, 127.23, 128.47, 129.11, 129.18, 129.80, 130.46, 134.89, 137.82, 148.03.

7) (E)-1-fluoro-4-styrylbenzene



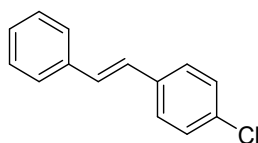
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: White solid (92 % yield)

¹H NMR: (400 MHz, CDCl₃): δ 6.75-6.86 (m, 2H), 7.10-7.14 (m, 2H), 7.44-7.50 (m, 7H).

¹³C NMR: δ 121.06, 127.45, 128.45, 128.89, 129.03, 130.63, 131.13, 131.46, 136.18, 162.91.

8) (E)-1-chloro-4-styrylbenzene



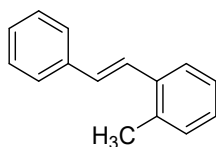
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: White solid (87 % yield)

¹H NMR: (400 MHz, CDCl₃): δ 6.69 (d, *J* = 15.6 Hz, 1H), 6.81 (d, *J* = 15.6 Hz, 1H), 7.29 (m, 2H), 7.35-7.45 (m, 8H)

¹³C NMR: δ 127.40, 128.42, 128.49, 128.88, 128.98, 130.29, 131.01, 132.83, 135.69, 136.92.

09) (E)-1-methyl-2-styrylbenzene



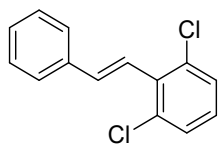
Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: White solid (72 % yield)

¹H NMR: (400 MHz, CDCl₃): δ 2.40 (s, 3H), 6.71-6.80 (m., 2H), 7.15-7.18 (m, 1H), 7.25-7.32 (m, 8H).

¹³C NMR: δ 19.99, 125.83, 127.15, 127.34, 128.19, 128.99, 129.03, 129.64, 130.18, 130.63, 136.18, 137.13, 137.22.

10) (E)-1,3-dichloro-2-styrylbenzene



Following the general procedure, compound was purified by column chromatography over silica gel and mixture of diethylether or ethyl acetate in petroleum ether (05:95).

Colour: White solid (77 % yield)

¹H NMR: (400 MHz, CDCl₃): δ 7.15-7.18 (m, 1H), 7.29-7.34 (m, 2H), 7.45-7.53 (m, 5H), 7.69-7.70 (m, 2H).

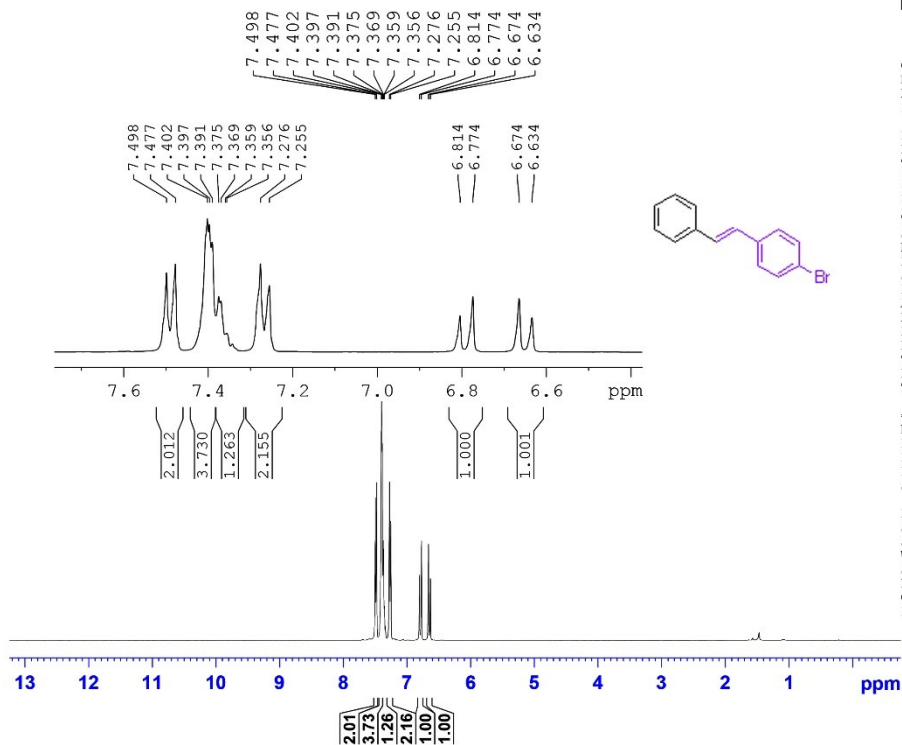
¹³C NMR: δ 122.71, 126.97, 128.17, 128.52, 128.73, 128.90, 134.76, 136.93, 137.20.

4. References.

- (1) Wang, M. L.; Xu, H.; Li, H. Y.; Ma, B.; Wang, Z. Y.; Wang, X.; Dai, H. X. Mizoroki-Heck Reaction of Unstrained Aryl Ketones via Ligand-Promoted C-C Bond Olefination. *Org Lett* 2021, 23 (6), 2147–2152. <https://doi.org/10.1021/acs.orglett.1c00296>.
- (3) Jia, X.; Frye, L. I.; Zhu, W.; Gu, S.; Gunnoe, T. B. Synthesis of Stilbenes by Rhodium-Catalyzed Aerobic Alkenylation of Arenes via C-H Activation. *J Am Chem Soc* 2020, 142 (23), 10534–10543. <https://doi.org/10.1021/jacs.0c03935>.

5. ¹H-NMR and ¹³C-NMR data of synthesized compounds

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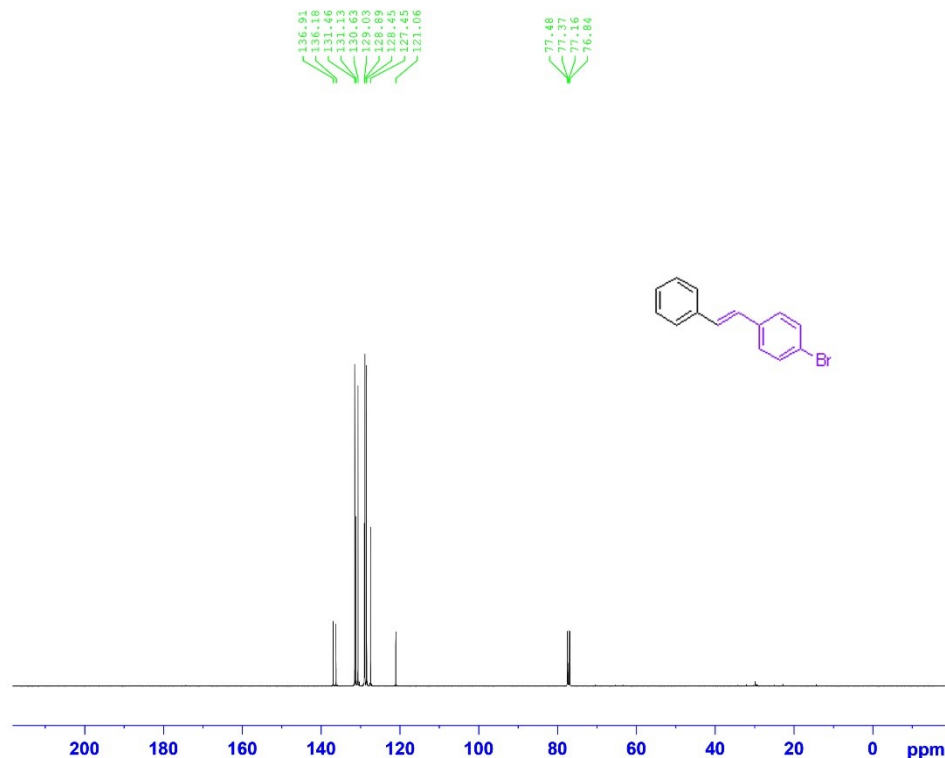
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TDO 1

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JC 1 AKASH CDCL3 13C 22/05/2024

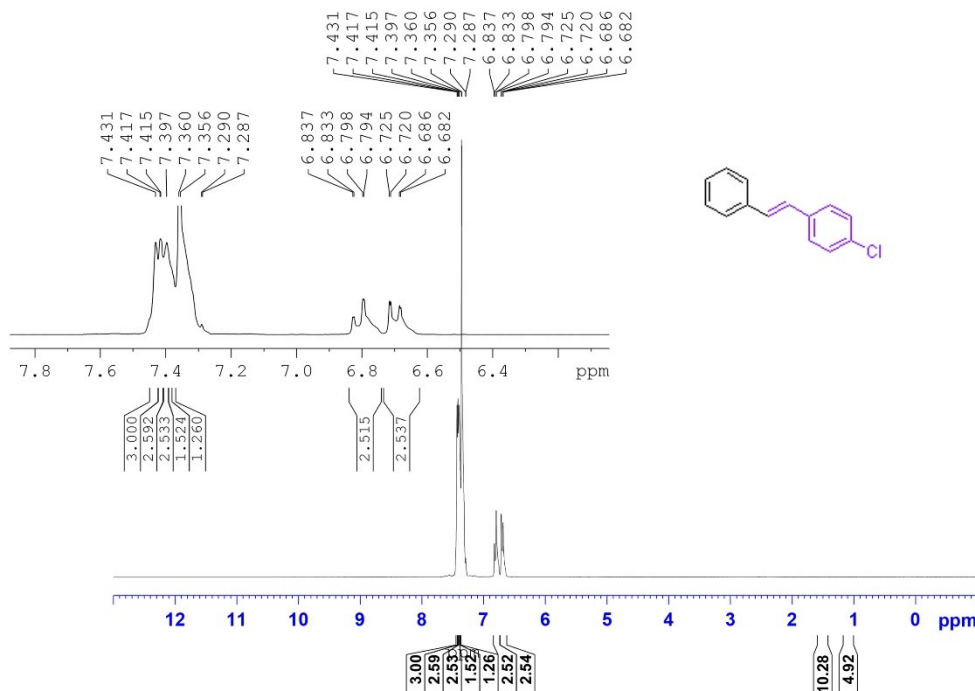


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HC-3 AAKASH 1H 2/1/2024
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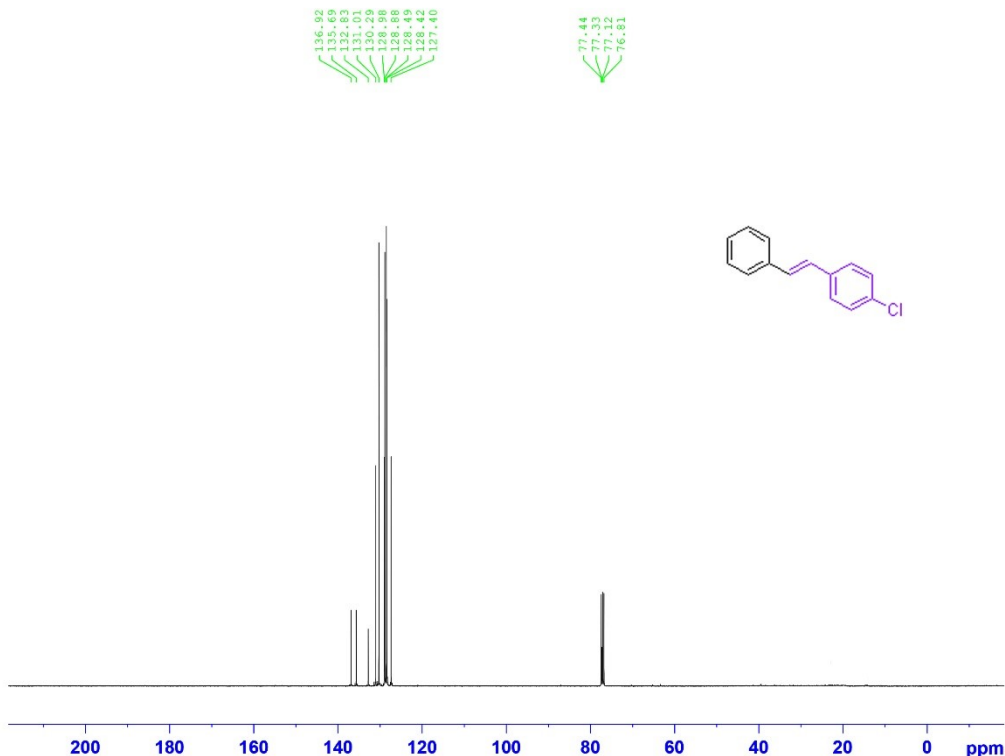
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JC 3 AKASH CDCL3 13C 22/05/2024



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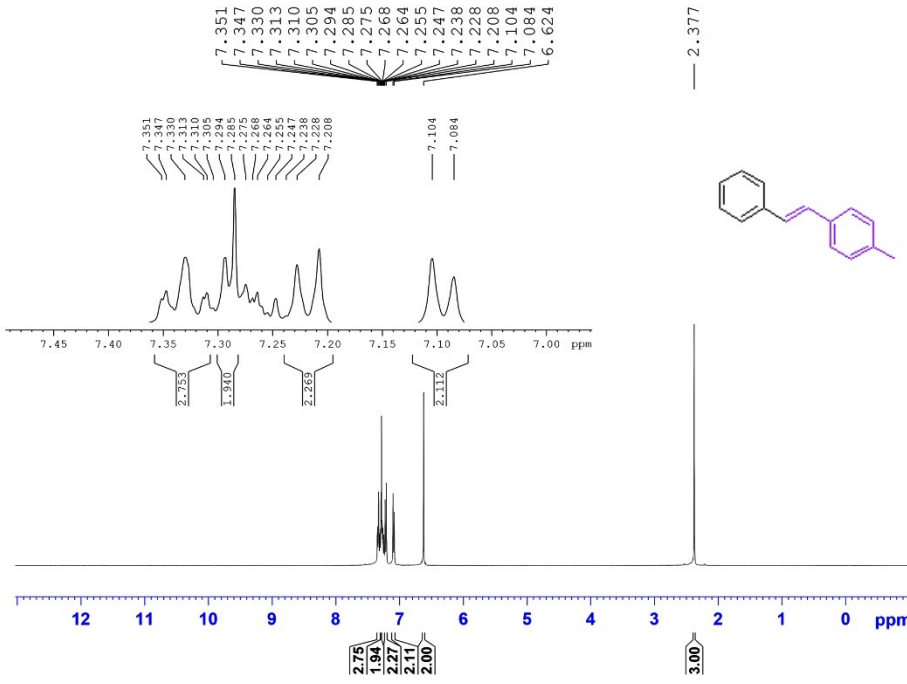
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HC-4 AAKASH 1H 2/1/2024
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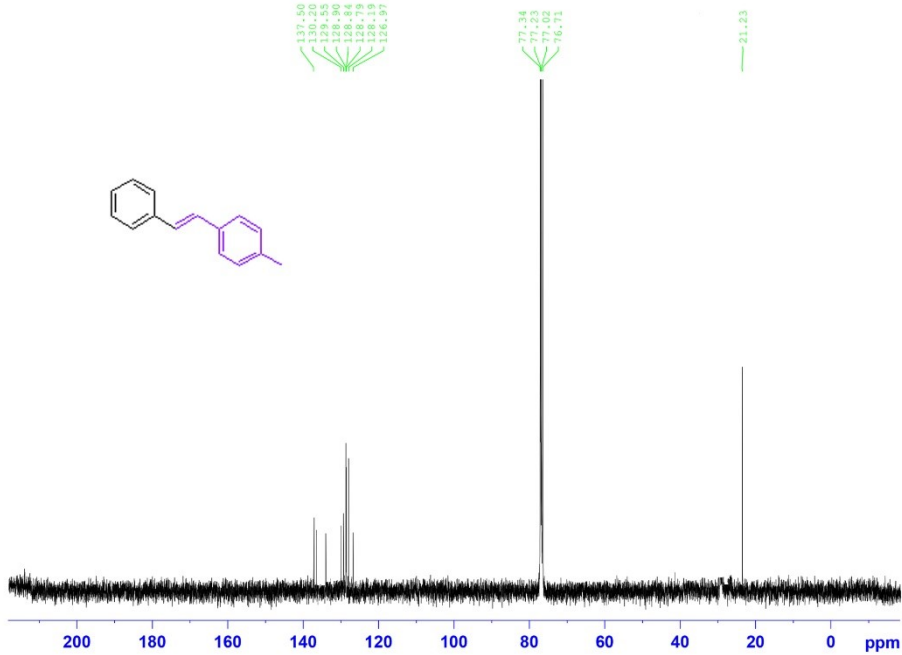
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F2 - Processing parameters
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JC 4 AKASH CDCL3 13C 22/05/2024



Current Data Parameters
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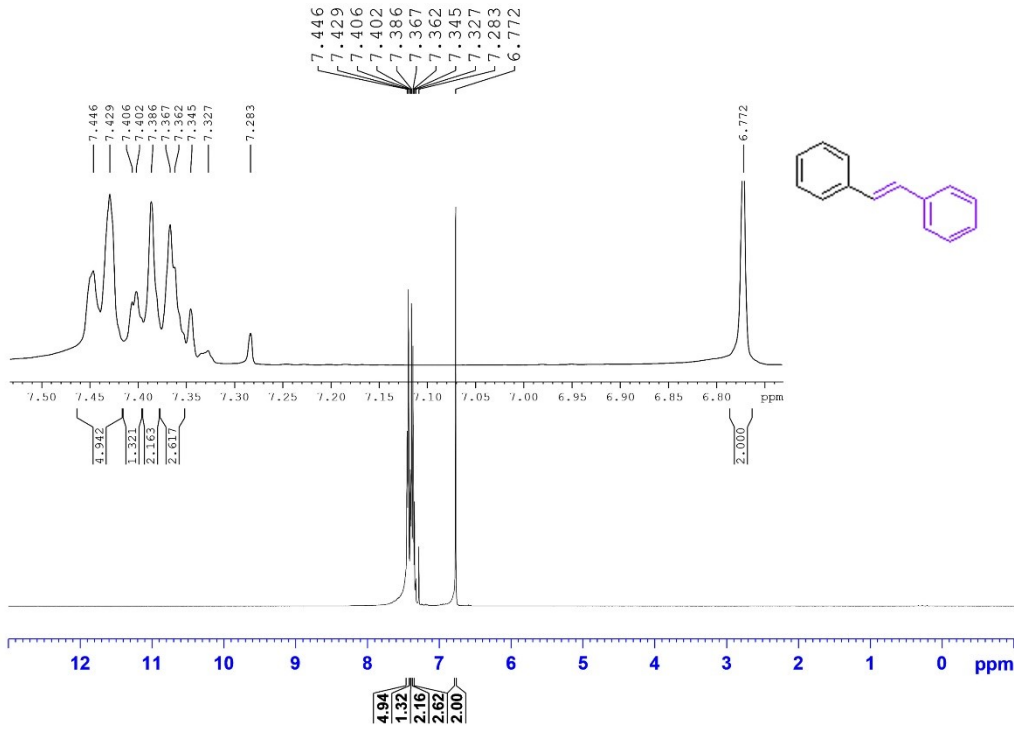
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 PL21 0.17883081 W
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HC-5 AKASH 1H 05/01/2024
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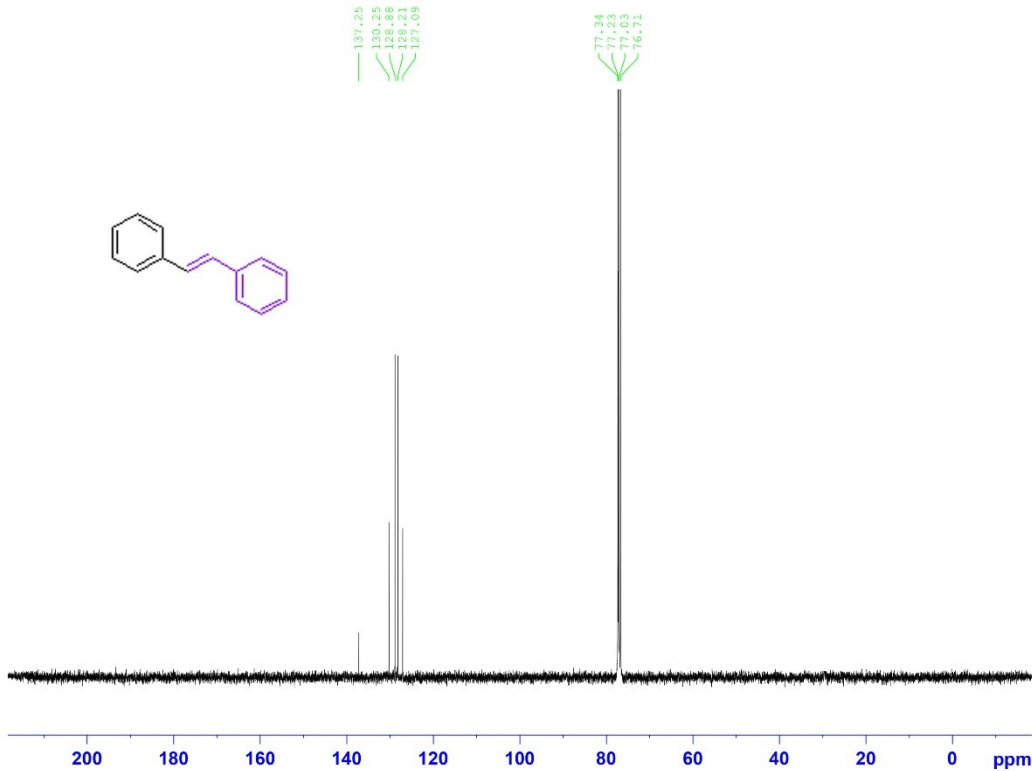
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JC 5 AKASH CDCL3 13C 22/05/2024



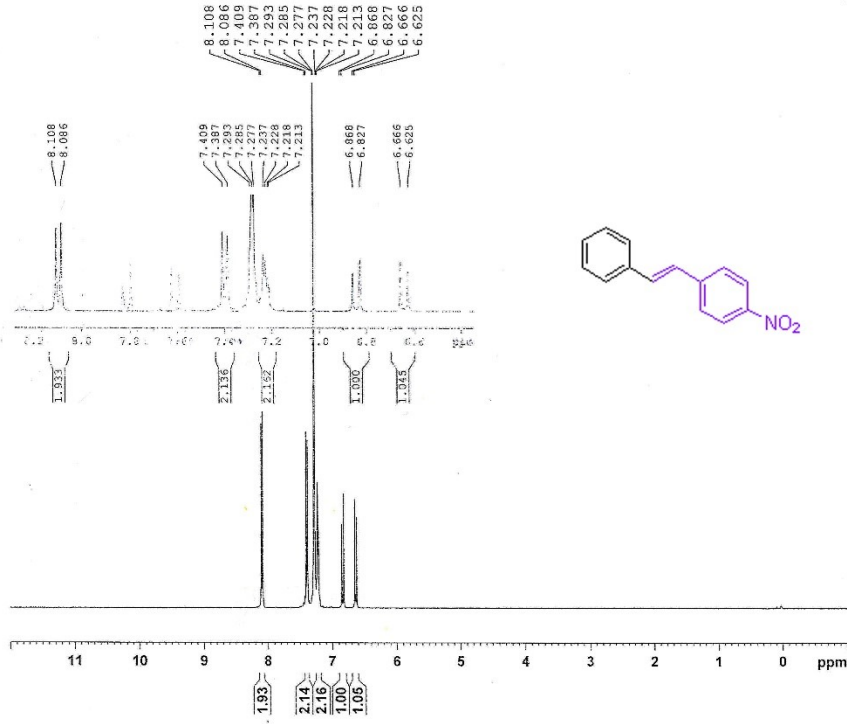
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SWH           23600.514 Hz
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DE            6.50 usec
TE            295.2 K
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PT1           0.00 dB
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NUC2          1H
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NSM12        0.0000100 W

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```


HC-6 AKASH1H 17/01/2024
 (D:\SRC) CDCL3 MSU CHEM-1



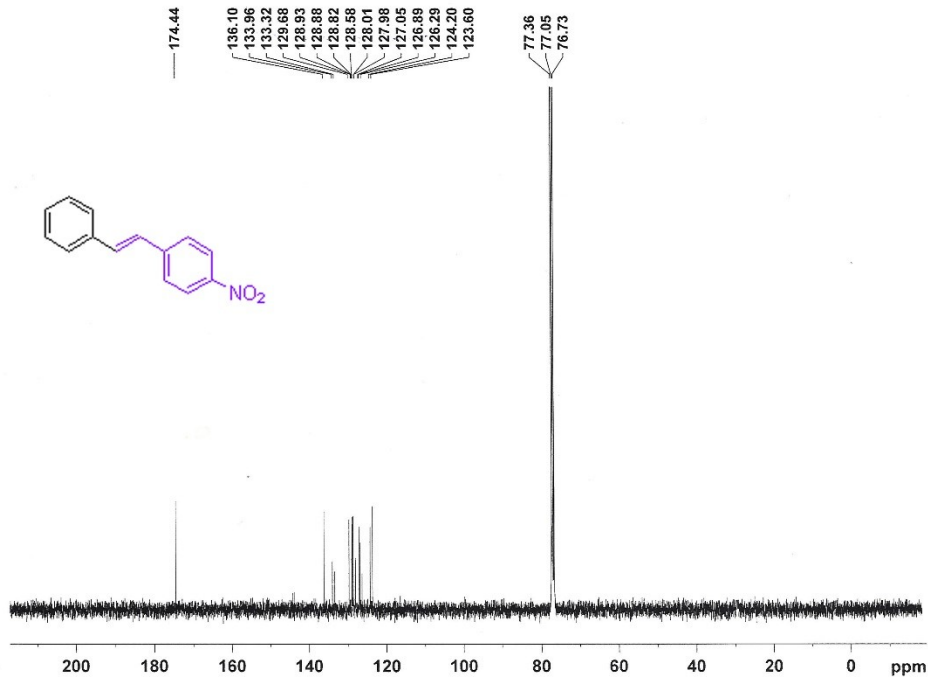
```

NAME      HC -6
EXPNO    5
PROCNO   1
Date_    20240117
Time     17.30
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg
TD        65536
SOLVENT  CDCL3
NS        16
DS        2
SWE       8223.686 Hz
FIDRES   0.129493 Hz
AQ        3.9846397 sec
RG         645
AS         645
DS         60.900 usec
DE         6.30 usec
TE        292.2 K
D1        1.00000000 sec
TDC       1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        16.00 usec
PL1       0.00 dB
PC1       1.00 usec
SFO1      500.136051 MHz
AQ1       3.9846397 sec
RG1       645
AS1       645
DS1       60.900 usec
DE1       6.30 usec
TE1       292.2 K
D11       1.00000000 sec
TDC1      1
  
```

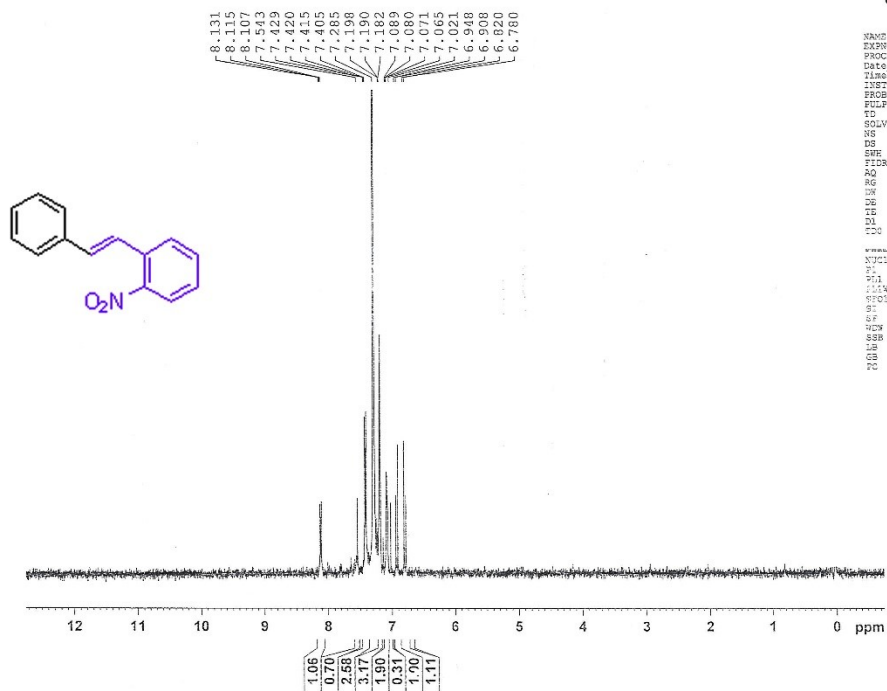
JC-06 13C CDCL3
 D/DP 9/07/24



```

===== CHANNEL f1 =====
NAME      JC-06
EXPNO    1
PROCNO   1
Date_    20240907
Time     10.00
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg
TD        65536
SOLVENT  CDCL3
NS        16
DS        2
SWE       125.761 MHz
FIDRES   0.129493 Hz
AQ        3.9846397 sec
RG         645
AS         645
DS         60.900 usec
DE         6.30 usec
TE        292.2 K
D1        1.00000000 sec
TDC       1
  
```

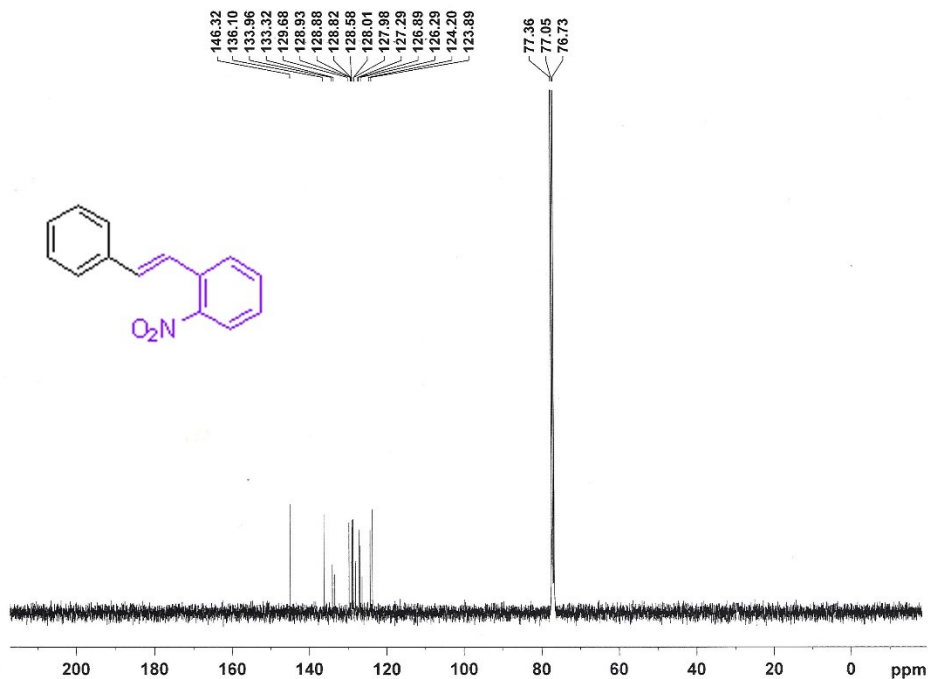
HC-7 AKASH 1H 17/01/2024
 {D:\SRC} CDCL3 MSU CHEM-1



```

NAME      HC-7
EXPNO     1
PROCNO    1
Date_     20240117
Time      17.36
INSTRUM   spect
PROBHD    5 mm PABBO BBI
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.688 Hz
FIDRES     0.129483 Hz
AQ         3.9846387 sec
RG         812
DM         60.600 usec
DE         6.50 usec
TE         292.2 K
D1         1.00000000 sec
T20
===== CHANNEL f1 =====
NUC1       1H
P1         15.00 usec
PL1        0.00 dB
PL12       13.50 dB
SFO1       400.1464010 MHz
SI         32768
SF         400.1500000 MHz
WDW         EM
SSB         0
LB         0.50 Hz
GB         0
PC         1.00
  
```

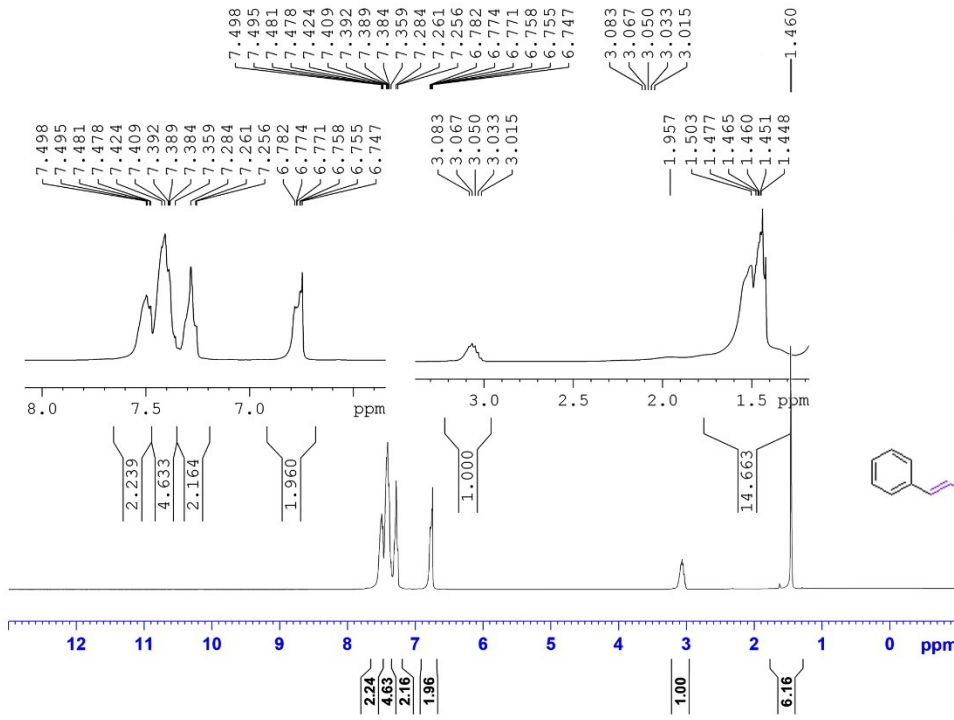
JC-07 13C CDCL3
 D/DP 9/07/24



```

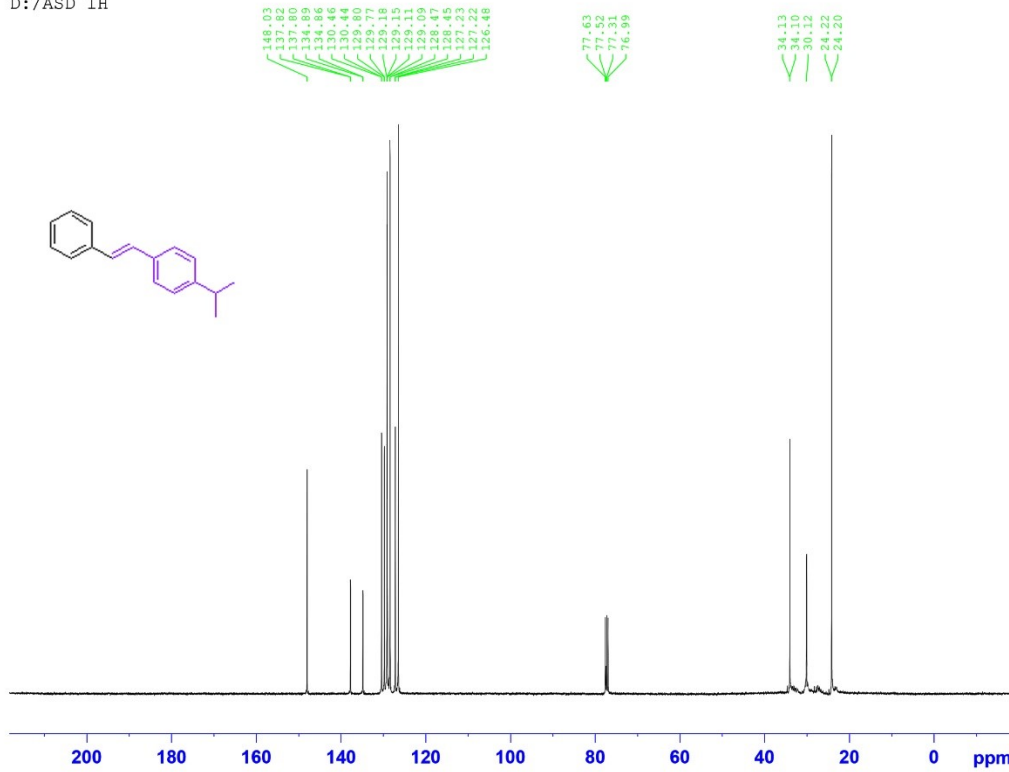
===== CHANNEL f1 =====
NUC1       13C
P1         12.00 usec
PL1        0.00 dB
PL12       19.00 dB
SFO1       101.6255125 MHz
SI         65536
SF         101.6255125 MHz
WDW         EM
SSB         0
LB         0.50 Hz
GB         0
PC         1.00
  
```

HC 11 AKASH CDCL3 1H DT 06/03/2024



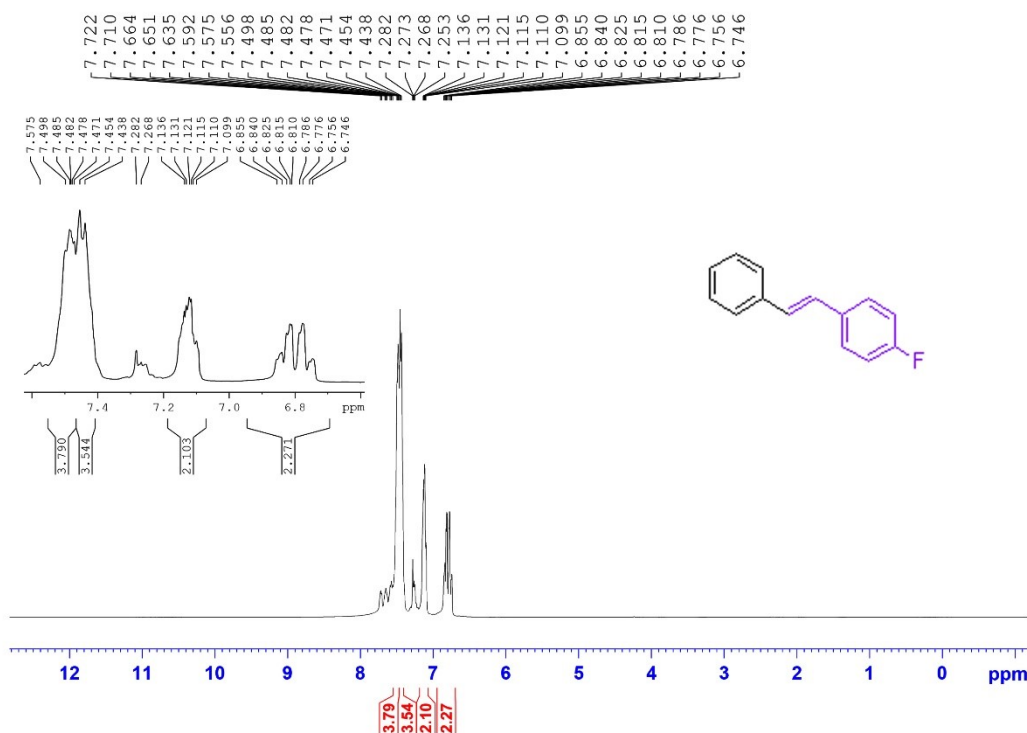
Current Data Parameters
 NAME HC 11
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date 20240306
 Time 17:45 h
 INSTRUM AvanceNeo 400
 PROBRD 1H31P_0922 (1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8196.121 Hz
 FIDRES 0.250144 Hz
 AQ 3.957699 sec
 RG 8
 DM 61.000 usec
 DE 13.89 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.152470 MHz
 NUC1 1H
 PD 2.47 usec
 PL 8.00 usec
 P1M1 22.58300018 W
 F2 - Processing parameters
 SI 62536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

HC 11 AAKASH CDCL3 DT 15/03/2024
 D:/ASD 1H



Current Data Parameters
 NAME HC 11
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date 20240315
 Time 14:56 h
 INSTRUM AvanceNeo 400
 PROBRD 1H31P_0922 (1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 23809.554 Hz
 FIDRES 0.756608 Hz
 AQ 1.3762360 sec
 RG 101
 DM 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 100.4278513 Hz
 SFO1 100.6278513 MHz
 NUC1 13C
 PD 2.47 usec
 PL 8.00 usec
 P1M1 105.2698648 W
 SF2C 400.1516096 MHz
 MCCA
 CPDPRG02 waltz160
 P0C02 50.500 usec
 P1M2 21.58300018 W
 P1M12 0.37830000 W
 P1M13 0.09975100 W
 F2 - Processing parameters
 SI 65536
 SF 100.6177975 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

HC 12 AKASH CDCL3 1H DT 06/03/2024

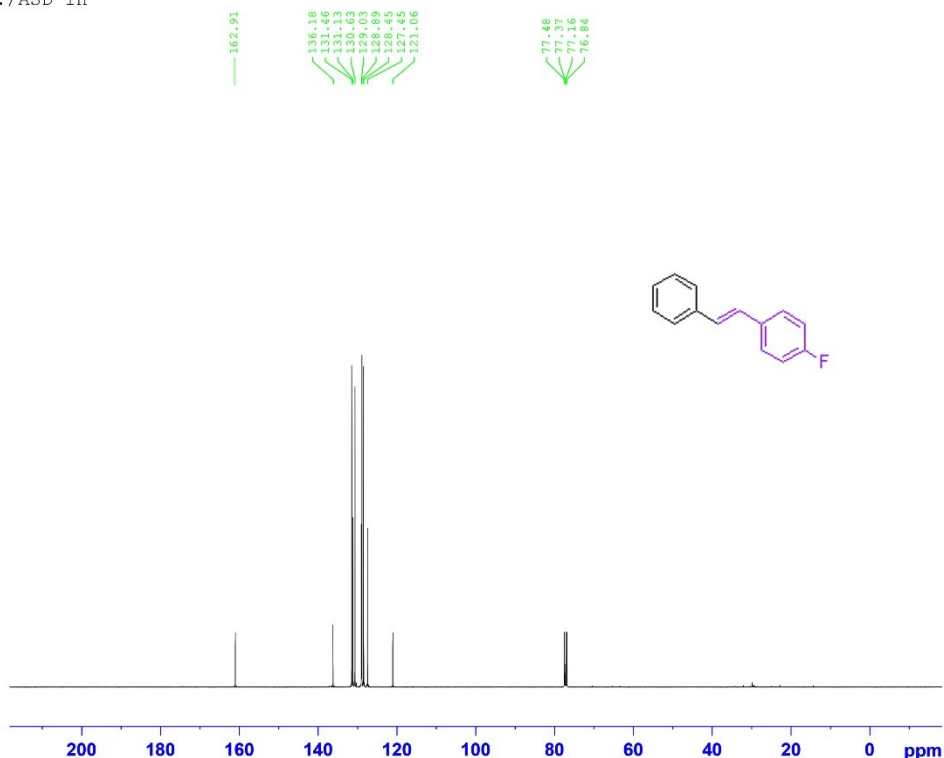


Current Data Parameters
 NAME HC 12
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240306
 Time_ 18.00 h
 INSTRUM AvanceNeo 400
 PROBHD zgpg30 0922 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4
 DS 4
 SWH 816.721 Hz
 FIDRES 0.250144 Hz
 AQ 3.351639 sec
 RG 9
 DW 61.000 usec
 DE 13.89 usec
 TE 298.2 K
 D1 1.0000000 sec
 SFO1 400.1524789 MHz
 NUC1 1H
 P0 2.67 usec
 PL1 22.5830018 W
 PL11 22.5830018 W

F2 - Processing parameters
 SI 65536
 SF 400.150000 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

HC 12 AAKASH CDCL3 DT 15/03/2024
 D:/ASD 1H

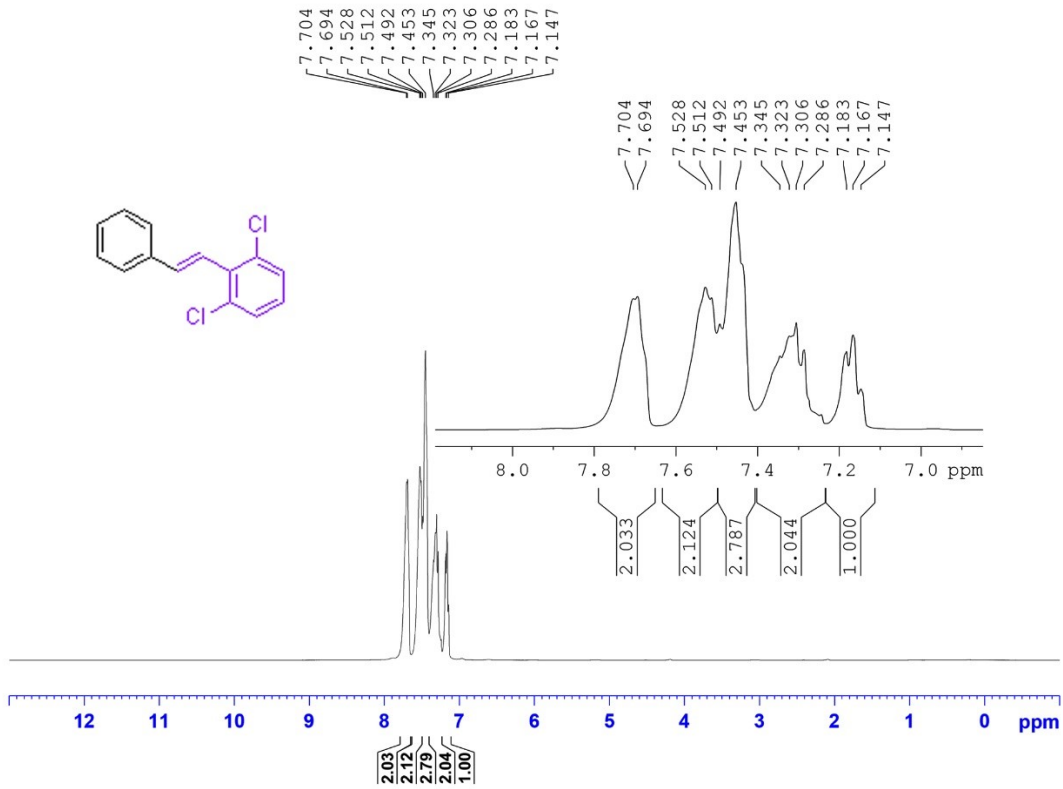


Current Data Parameters
 NAME HC 12
 EXPNO 60
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240316
 Time_ 15.19 h
 INSTRUM AvanceNeo 400
 PROBHD zgpg30 0922 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 23809.524 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6278593 MHz
 NUC1 13C
 P0 2.67 usec
 PL1 8.00 usec
 PLW1 105.2699664 W
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG2 waltz65
 PCPD2 90.00 usec
 PLW2 22.5830018 W
 PLW12 0.17843001 W
 PLW13 0.08975100 W

F2 - Processing parameters
 SI 32768
 SF 100.6177975 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

HC 15 1H CDCL3 20/04/2024



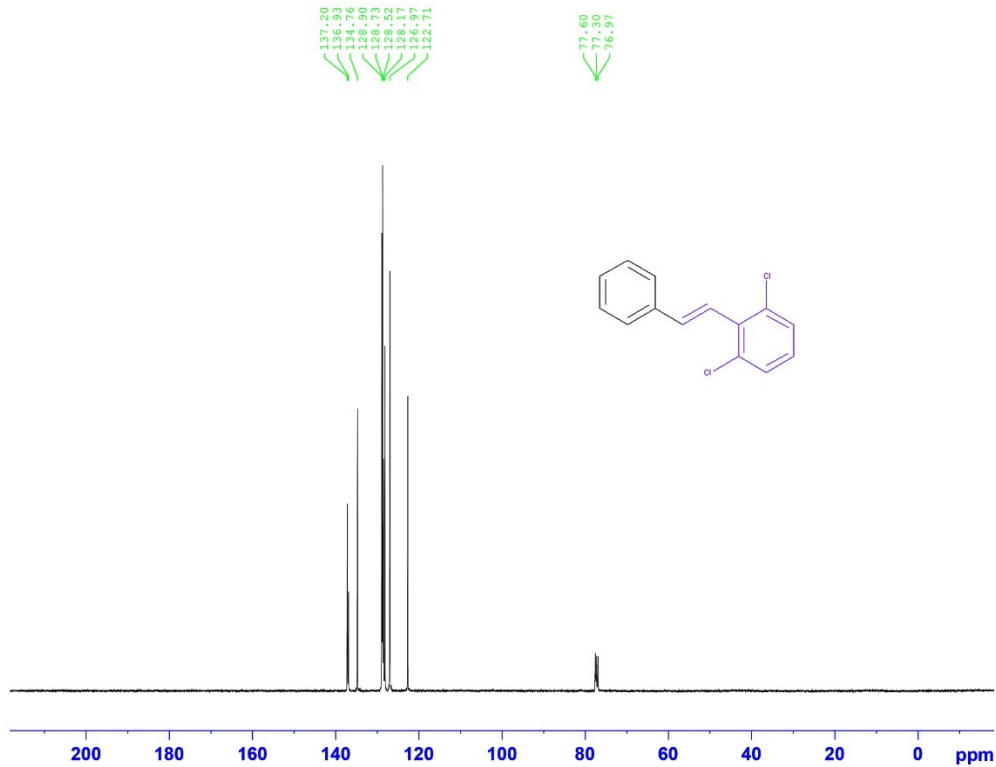
```

Current Data Parameters
NAME          HC 15
EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
Date_         20240420
Time          17:02 h
INSTRUM       AvanceNeo 400
PROBHD        Z163739_0922 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS           16
DS            2
SWE           8196.721 Hz
FIDRES       0.250144 Hz
AQ           3.9976959 sec
RG           9
DW           61.000 usec
DE           13.89 usec
TE           298.0 K
D1           1.00000000 sec
TDO          1
SF01         400.1524709 MHz
NUC1          1H
PQ           2.47 usec
PI           8.00 usec
PLW1         22.58300018 W

F2 - Processing parameters
SI           400.1500000 MHz
SF           EM
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
    
```

HC 15 13C CDCL3 20/04/2024



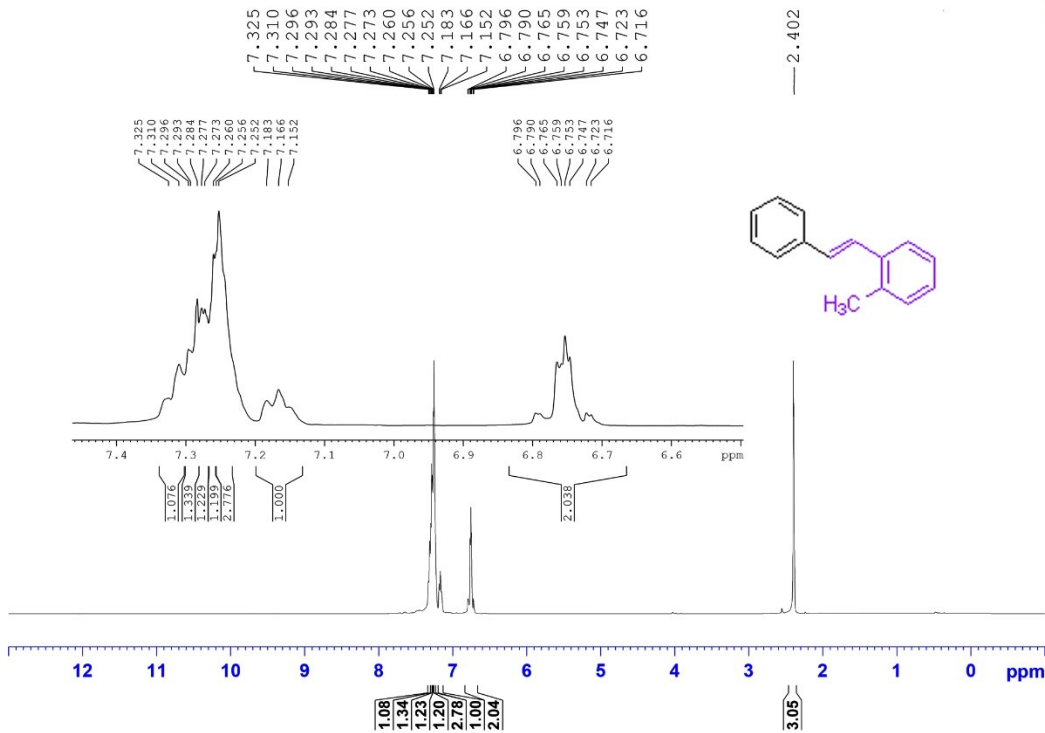
```

Current Data Parameters
NAME          HC 15
EXPNO         8
PROCNO        1

F2 - Acquisition Parameters
Date_         20240420
Time          17:27 h
INSTRUM       AvanceNeo 400
PROBHD        Z163739_0922 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS           256
DS            4
SWE           23809.524 Hz
FIDRES       0.726609 Hz
AQ           1.3762560 sec
RG           101
DW           21.000 usec
DE           6.50 usec
TE           298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TDO          1
SF01         100.6278953 MHz
NUC1          13C
PQ           2.47 usec
PI           8.00 usec
PLW1         105.26999664 W
SFO2         400.1516006 MHz
NUC2          1H
CPDPRG2       waltz16
PCDE2         90.00 usec
PLW2         22.58300018 W
PLW12        0.17849001 W
PLW13        0.08975100 W

F2 - Processing parameters
SI           32768
SF           100.6177715 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

HC 16 1H CDCL3 20/04/2024

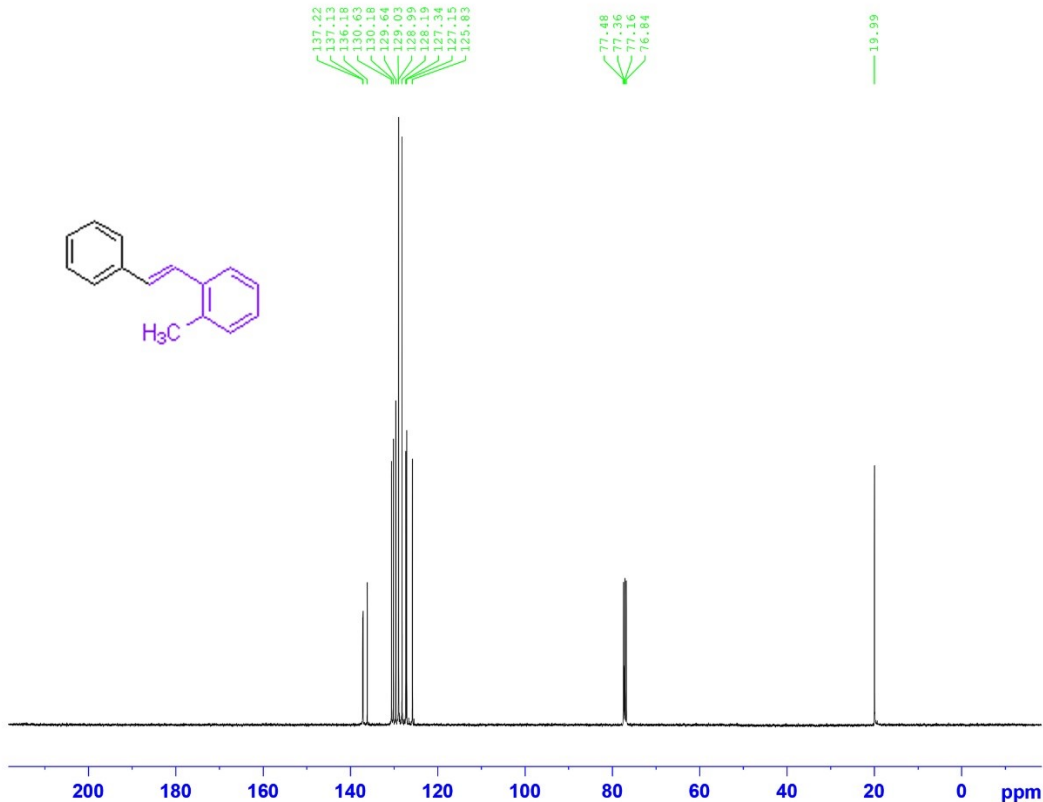


Current Data Parameters
 NAME HC 16
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240420
 Time 17.09 h
 INSTRUM AvanceNeo 400
 PROBHD Z163739_0922 (4
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWE 8156.721 Hz
 FIDRES 0.250144 Hz
 AQ 3.9576959 sec
 RG 16
 DN 61.000 usec
 DE 13.89 usec
 TE 298.0 K
 D1 1.0000000 sec
 TDO 1
 SFO1 400.1524709 MHz
 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 22.58300018 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

HC 16 13C CDCL3 20/04/2024



Current Data Parameters
 NAME HC 16
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240420
 Time 18.00 h
 INSTRUM AvanceNeo 400
 PROBHD Z163739_0922 (4
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 491
 DS 4
 SWE 23809.554 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DN 21.000 usec
 DE 4.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1
 SFO1 100.6278593 MHz
 NUC1 13C
 P0 2.67 usec
 P1 8.00 usec
 PLW1 105.2699664 W
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG2 waltz165
 PCPD2 80.00 usec
 PLW2 22.58300018 W
 PLW12 0.17843001 W
 PLW13 0.08975100 W

F2 - Processing parameters
 SI 65536
 SF 100.6177975 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40