Supporting Information

Chemo- and Stereoselective Synthesis of Z-Alkenes via Electrochemical Pd-Catalyzed Alkyne Reduction

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Table Contents:

1.General information

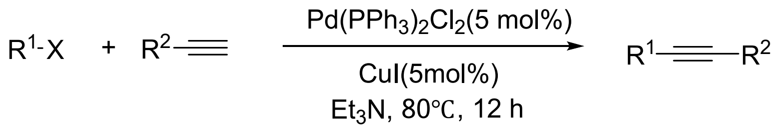
All commercially available reagents were directly used as received without further purification. All organic solvents applied in the reactions were not pre-dried by distillation, and one of the solvents ethanol is Industrial ethanol instead of anhydrous ethanol. The electrochemical reactions were performed on a DJS-292B potentiostat (made in China) in constant current mode. All yields of products refer to the isolated yields after chromatography.

^{1}H NMR (400 MHz), ^{13}C NMR (101 MHz) and ^{19}F NMR (376 MHz) spectra were recorded on a Bruker AV-400 spectrometer or a Quantum-I Plus 400 in Chloroform-d or DMSO-d_6. For ^{1}H NMR, Chloroform-*d* (δ = 7.26 ppm), DMSO-d_6 (δ = 2.50 ppm) or tetramethylsilane (TMS, δ = 0 ppm) serves as the internal standard; for ^{13}C NMR, Chloroform-*d* (δ = 77.16 ppm) or DMSO-d_6 (δ = 39.52 ppm) serves as the internal standard. Data are reported as follows: chemical shift (in ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, hept = heptet, m = multiplet, br = broad), coupling constant (in Hz), and integration.

GC analysis was performed on a 7890B/Agilent, while GC-MS analysis was performed on a 7890A-5975C/Agilent. HR-MS spectra were recorded on a Waters Xevo G2QTOF/UPLC mass spectrometer using electrospray ionization.

2. Substrates preparation

The starting materials were prepared from the corresponding phenyl iodides and terminal alkynes via the Sonogashira coupling method, as previously reported in the literature.[1]

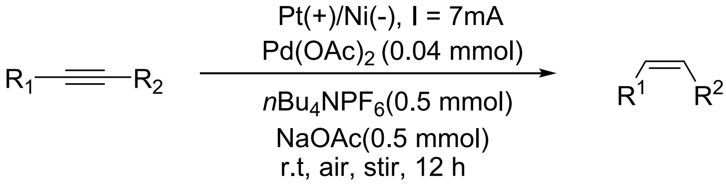


R^1, R^2= aryl, alkyl, heterocyclic

The two components were added to a 100 ml three-neck flask in a 1:1 ratio. To this, 5 mol% bis(triphenylphosphine)palladium(II) chloride and 5 mol% copper(I) iodide were added. The reaction mixture was stirred magnetically in an oil bath at 80°C for 12 hours. After this, the oil bath was removed, and the reaction was allowed to cool to room temperature. The reaction was then quenched with water and extracted with ethyl acetate.

A small amount of silica gel was added to the organic phase, which was then dried under reduced pressure using a rotary evaporator. The product **1** was purified by silica gel column chromatography. The target product was obtained and confirmed by TLC and ^{1}H-NMR analysis.

3. General procedure for the electrochemical synthesis of *Z*-alkenes (1.0 mmol scale)

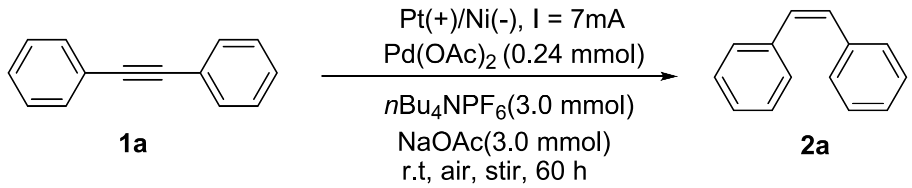


A 25 mL three-necked flask was charged with the substrate (1.0 mmol), $Pd(OAc)_2$ (0.04 mmol), NaOAc (41 mg, 0.5 mmol), and the electrolyte nBu_4NPF_6 (191 mg, 0.5 mmol), followed by the addition of 10 mL of solvent (MeCN:EtOH = 1:1). The solvent did not require anhydrous treatment, and EtOH used was industrial ethanol. The flask was then equipped with platinum plate electrodes (10 × 10 × 0.2 mm) as the anode and nickel plate electrodes (10 × 10 × 0.2 mm) as the cathode, with a distance of approximately 2 cm between them. To minimize the evaporation of the alcohol co-solvent, the system was sealed with a rubber plug (Fig. S1). The reaction was carried out under constant current of 7 mA. Upon completion, the reaction mixture was poured into water and extracted with ethyl acetate (EtOAc) three times. The combined organic layers were dried over anhydrous Na_2SO_4, and the solvent was removed under reduced pressure. The resulting mixture was purified by silica gel column chromatography (eluted with EtOAc/PE) to yield the desired product **2**.

Fig.S1 Reaction plant diagram

4. Procedure for the gram-scale reactions (6.0 mmol scale)

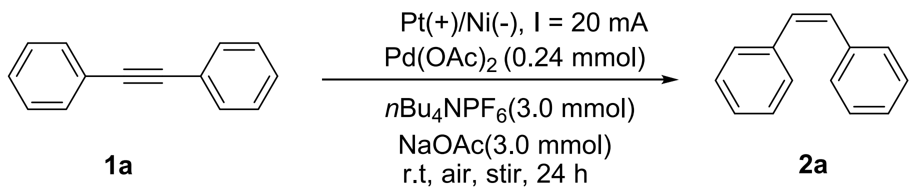
Conditions 1：



A 100 mL beaker was charged with diphenylacetylene (6.0 mmol), $Pd(OAc)_2$ (0.24 mmol), NaOAc (246 mg, 0.6 mmol), and the electrolyte nBu_4NPF_6 (1.15 g, 0.6 mmol), followed by the addition of 60 mL of reaction solvent (MeCN:EtOH = 1:1). The beaker was then equipped with platinum plate electrodes (1 cm × 1 cm × 0.2 mm) as the anode and nickel plate electrodes (1 cm × 1 cm × 0.2 mm) as the cathode, with a distance of approximately 3 cm between them. To minimize the evaporation of the alcohol co-solvent, the system was sealed with cardboard (Fig. S2). The reaction was carried out under constant current of 7 mA.

Upon completion (monitored by GC-MS), the reaction mixture was poured into water and extracted with ethyl acetate (EtOAc) three times. The combined organic layers were dried over anhydrous Na_2SO_4, and the solvent was removed under reduced pressure. The resulting mixture was purified by silica gel column chromatography (eluted with EtOAc/PE) to yield the desired product **2a**.

Conditions 2:

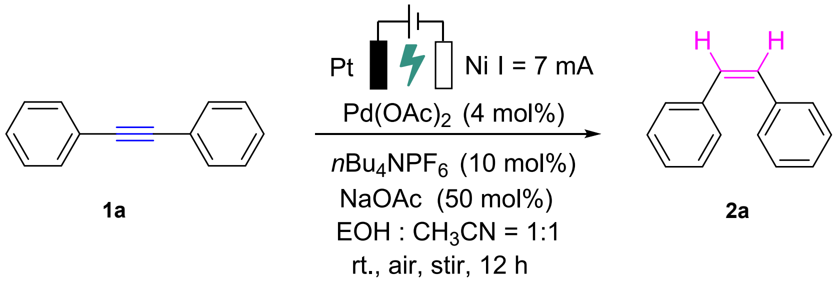


A 100 mL beaker was charged with diphenylacetylene (6.0 mmol), $Pd(OAc)_2$ (0.24 mmol), NaOAc (246 mg, 0.6 mmol), and the electrolyte nBu_4NPF_6 (1.15 g, 0.6 mmol), followed by the addition of 60 mL of reaction solvent (MeCN:EtOH = 1:1). The beaker was then equipped with platinum plate electrodes (3 cm × 3 cm × 0.2 mm) as the anode and nickel plate electrodes (3 cm × 3 cm × 0.2 mm) as the cathode, with a distance of approximately 3 cm between them. To minimize the evaporation of the alcohol co-solvent, the system was sealed with cardboard (Fig. S2). The reaction was carried out under a constant current of 20 mA.

Upon completion (monitored by GC-MS), the reaction mixture was poured into water and extracted with ethyl acetate (EtOAc) three times. The combined organic layers were dried over anhydrous Na_2SO_4, and the solvent was removed under reduced pressure. The resulting mixture was purified by silica gel column chromatography (eluted with EtOAc/PE) to yield the desired product **2a**.

Fig.S2 Gram-scale reactions plant diagram

5. Conditions optimizing



Standard condition: 1,2-diphenylethyne (1.0 mmol), $Pd(OAc)_2$ (0.04 mmol), *n*$BuNPF_6$ (0.5 mmol), NaOAc (0.5 mmol), platinum plate electrodes (10 × 10 × 0.2 mm) as anode, nickel plate electrodes (10 × 10 × 0.2 mm) as cathode. 10 mL ethanol acetonitrile mixed solvent (MeCN : EtOH = 1 : 1) is used as the reaction solvent in undivided cell. At room temperature, the reaction was carried out for 12 hours at 7 mA constant current (3.1 F/mol).

Table S1. Conditions optimizing and control experiments

entry	Deviation from the standard conditions [1]	Yield [2]
1	none	88%
2	Without $Pd(OAc)_2$	0%
3	Without electricity	0%
4	Change Pt (+) to C (+)	80%
5	Change Pt (+) to Cu (+)	36%
6	Change Ni (-) to C (-)	36%
7	Change Ni (-) to Pt (-)	52%
8	Without NaOAc	52%
9	Change NaOAc to K_2HPO_4	44%
10	Change NaOAc to KH_2PO_4	56%
11	Change *n*Bu_4NPF_6 to *n*Bu_4NBr	66%
12	Change *n*Bu_4NPF_6 to *n*Bu_4NBF_4	83%
13	Change $Pd(OAc)_2$ to $Pd(PPh_3)_2Cl_2$	61%
14	Change $Pd(OAc)_2$ to $PdCl_2$	45%
15	Change EtOH to isopropanol	19%
16	Change EtOH to MeOH	67%
17	Change 7 mA to 14 mA	21%
18	Change 7 mA to 3 mA	11%

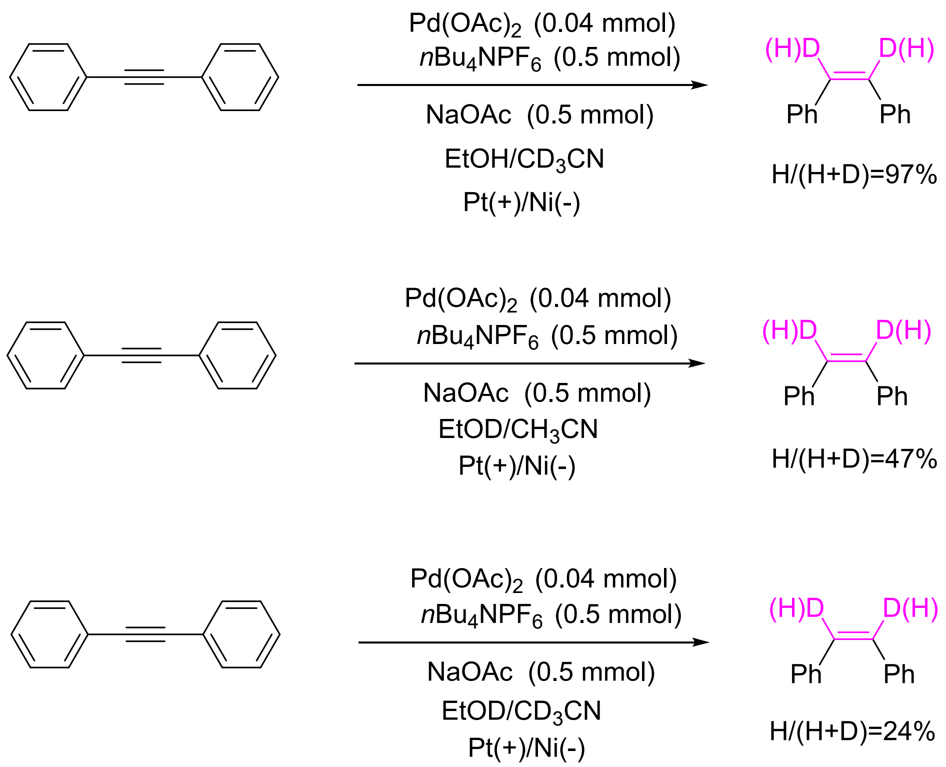
19	Change 12 h to 6 h	41%
20	Change 12 h to 22 h	27%
21	Change Pt (+) to Mg (+)	62%
22	Change Pt (+) to Zn (+)	23%
23	Change Pt (+) to Fe (+)	33%

6. Mechanistic Studies

6.1 Deuterium experiment

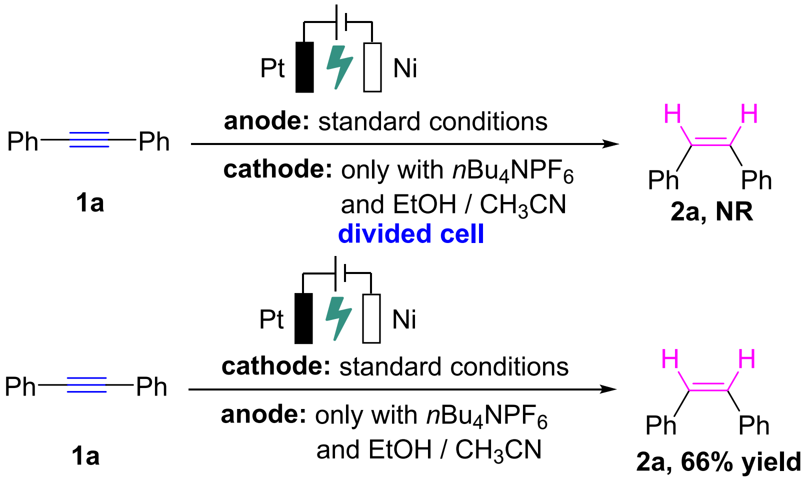
Three 25 mL three-necked flasks were prepared. Each flask was charged with the substrate (1 mmol), $Pd(OAc)_2$ (0.04 mmol), NaOAc (0.5 mmol), and the electrolyte nBu_4NPF_6 (38.2 mg, 0.5 mmol). The solvent did not require anhydrous treatment. Subsequently, each flask was equipped with platinum plate electrodes (10 × 10 × 0.2 mm) as the anode and nickel plate electrodes (10 × 10 × 0.2 mm) as the cathode, with a distance of approximately 2 cm between them. To the first flask, a mixed solvent containing a deuterated reagent was added (10 mL, CD_3CN:EtOH = 1:1). To the second flask, a mixed solvent containing another deuterated reagent was added (10 mL, CH_3CN:EtOD = 1:1). Finally, a mixed solvent of the two deuterated reagents was added to the third flask (10 mL, CD_3CN:EtOD = 1:1). To minimize the evaporation of the alcohol co-solvent, the system was sealed with a rubber plug (Fig. S1). The reaction was conducted under a constant current of 7 mA.

Upon completion, the reaction mixture was poured into water and extracted with ethyl acetate (EtOAc) three times. The combined organic layers were dried over anhydrous Na_2SO_4, and the solvent was removed under reduced pressure. The resulting mixture was purified by silica gel column chromatography (eluted with EtOAc/PE) to yield the desired product **2a**. The deuteration ratio was determined by ^{1}H NMR.



6.2 Divided-cell experiment

The reaction vessel is an H-type divided electrolytic cell (10 mL+ 10 mL) separated by a hydrogen ion permeable membranel (Dupont N-117).

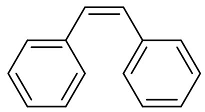


When the part of the cathode was added the substrate (1 mmol), $Pd(OAc)_2$ (0.04 mmol), NaOAc (41 mg, 0.5 mmol), and the electrolyte nBu_4NPF_6 (191 mg, 0.5 mmol), 10 mL of solvent (MeCN:EtOH = 1:1) and a magnetic stirrer bar. The part of the anode was only added the electrolyte nBu_4NPF_6 (191 mg, 0.5 mmol), 10 mL of solvent (MeCN:EtOH = 1:1) and a magnetic stirrer bar. The flask was then equipped with platinum plate electrodes (10 × 10 × 0.2 mm) as the anode and nickel plate electrodes (10 × 10 × 0.2 mm) as the cathode, with a distance of approximately 2 cm between them. To minimize the evaporation of the alcohol co-solvent, the system was sealed with a rubber plug. The reaction was carried out under constant current of 7 mA. Upon completion, the reaction mixture was poured into water and extracted with ethyl acetate (EtOAc) three times.

The combined organic layers were dried over anhydrous Na_2SO_4, and the solvent was removed under reduced pressure. The resulting mixture was purified by silica gel column chromatography (eluted with EtOAc/PE) to yield the desired product **2a** for 66% yield.

However, the same reaction was carried out with the part of the anode was added the substrate (1 mmol), $Pd(OAc)_2$ (0.04 mmol), NaOAc (41 mg, 0.5 mmol), and the electrolyte nBu_4NPF_6 (191 mg, 0.5 mmol), 10 mL of solvent (MeCN:EtOH = 1:1) and a magnetic stirrer bar and the part of the cathode was only added the electrolyte nBu_4NPF_6 (191 mg, 0.5 mmol), 10 mL of solvent (MeCN:EtOH = 1:1) and a magnetic stirrer bar. After sufficient reaction time, no product **2** was detected through TLC and DC-MS analysis.

7. Characterization data



(Z)-1,2-diphenylethene (2a)

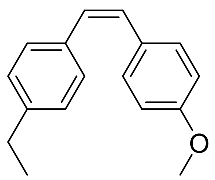
Purification by flash chromatography on silica gel (petroleum ether) afforded 158.4 mg (88% yield) of the title compound **2a**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.17(m,10H), 6.59(s, 2H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.34, 130.33, 128.94, 128.27, 127.15.

Data in accordance with the literature.[1]

HRMS (ESI) calcd for $C_{14}H_{13}^{+}$ m/z $[M+H]^{+}$: 181.1017, found 181.1012.



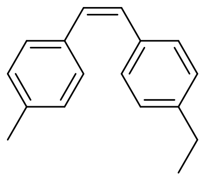
(Z)-1-ethyl-4-(4-methoxystyryl)benzene (2b)

Purification by flash chromatography on silica gel (petroleum ether/EtOAc (10:1)) afforded 218.9 mg (92% yield) of the title compound **2b**.

^{1}H NMR(400MHz,$CDCl_3$) δ 7.21-7.18(m, 4H), 7.07-7.05(d, 2H), 6.77-6.76(d, 2H), 6.47(s, 2H), 3.78(s, 3H), 2.64-2.58(q, 2H), 1.20(t, 3H)

^{13}C NMR(100 MHz, $CDCl_3$) δ 158.65, 143.06, 134.90, 130.13, 130.00, 129.14, 128.83, 128.81, 127.72, 113.63, 55.23, 28.62, 15.42. Data in accordance with the literature[2]

HRMS (ESI) calcd for $C_{17}H_{19}O^+$ m/z $[M+H]^+$: 239.1436, found 239.1431.



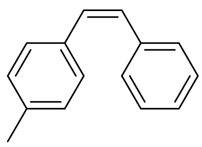
(Z)-1-ethyl-4-(4-methylstyryl)benzene (2c)

Purification by flash chromatography on silica gel (petroleum ether) afforded 175.4 mg (79% yield) of the title compound **2c**.

^{1}H NMR (400 MHz, CDCl3) δ 7.20-7.16(m, 4H), 7.06-7.02(m, 4H), 6.51(s, 2H), 2.61(q, 2H), 2.31(s, 3H), 1.22(t, 3H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.13, 136.74, 134.74, 134.54, 129.55, 129.52, 128.91, 128.82, 128.76, 127.67, 28.61, 21.26, 15.44.

HRMS (ESI) calcd for $C_{17}H_{19}^+$ m/z $[M+H]^+$: 223.1487, found 223.1485.



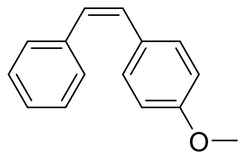
(Z)-1-methyl-4-styrylbenzene (2d)

Purification by flash chromatography on silica gel (petroleum ether) afforded 155.2 mg (80% yield) of the title compound **2d**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.13(m, 8H), 7.02(d, 2H), 6.55(s, 2H), 2.31(s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 137.51, 136.88, 134.27, 130.21, 129.57, 128.92, 128.86, 128.81, 128.21, 126.98, 21.26. Data in accordance with the literature.[1]

HRMS (ESI) calcd for $C_{15}H_{15}^{+}$ m/z $[M+H]^{+}$: 195.1174, found 195.1179.



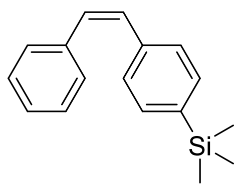
(Z)-1-methoxy-4-styrylbenzene (2e)

Purification by flash chromatography on silica gel (petroleum ether/EtOAc (10:1)) afforded 155.4 mg (74% yield) of the title compound **2e**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.16(m, 7H), 6.75(d, 2H), 6.55-6.48(q, 2H), 3.77(s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.67, 137.62, 130.16, 129.77, 129.66, 128.82, 128.77, 128.24, 126.91, 113.59, 55.19. Data in accordance with the literature.[1]

HRMS (ESI) calcd for $C_{15}H_{15}O^{+}$ m/z $[M+H]^{+}$: 211.1123, found 211.1129.



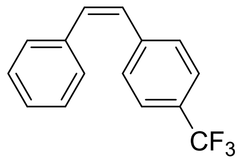
(Z)-trimethyl(4-styrylphenyl)silane (2f)

Purification by flash chromatography on silica gel (petroleum ether) afforded 206.6 mg (82% yield) of the title compound **2f**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37(d, 2H), 7.29-7.17(m, 7H), 6.58(q, J = 12.4Hz, 2H), 0.24(s, 9H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 139.37, 137.56, 137.39, 133.22, 130.41, 130.24, 128.85, 128.26, 128.15, 127.12, -1.09.

HRMS (ESI) calcd for $C_{17}H_{21}Si^+$ m/z $[M+H]^+$: 253.1413, found 253.1416.



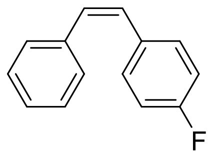
(Z)-1-styryl-4-(trifluoromethyl)benzene (2g)

Purification by flash chromatography on silica gel (petroleum ether) afforded 205.8 mg (83% yield) of the title compound **2g**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46(d, 2H), 7.32(d, 2H), 7.26-7.19(m, 5H), 6.72(d, J = 12.4Hz, 1H), 6.59(d, J = 12.4Hz, 1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 136.7, 132.4, 131.8(2C), 129.2, 128.8(2C), 128.8 (q, $J_{C\text{-}F}$ = 33.9 Hz), 128.5, 128.4(2C), 127.6, 125.2(q, $J_{C\text{-}F}$ = 3.8 Hz, 2C). Data in accordance with the literature.[1]

HRMS (ESI) calcd for $C_{15}H_{12}F_3^+$ m/z $[M+H]^+$: 249.0891, found 249.0899.



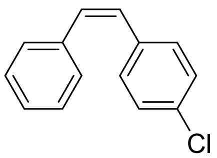
(Z)-1-fluoro-4-styrylbenzene (2h)

Purification by flash chromatography on silica gel (petroleum ether) afforded 136.6 mg (69% yield) of the title compound **2h**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.18(m, 7H), 6.90(t, 2H), 6.59(d, J = 12.4Hz, 1H), 6.54(d, J = 12.4Hz, 1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.05(d, $J_{C\text{-}F}$ = 245.1 Hz), 160.06, 137.04, 133.17 (d, $J_{C\text{-}F}$ = 3.4 Hz), 130.58, 130.5(d, $J_{C\text{-}F}$ = 7.8 Hz), 130.27, 129.09, 128.83, 128.32, 127.21, 115.27 ($J_{C\text{-}F}$ = 21.2 Hz), 115.06. Data in accordance with the literature.[1]

HRMS (ESI) calcd for $C_{14}H_{12}F^+$ m/z $[M+H]^+$: 199.0923, found 199.0917.



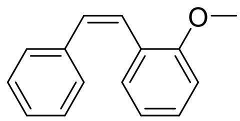
(Z)-1-chloro-4-styrylbenzene (2i)

Purification by flash chromatography on silica gel (petroleum ether) afforded 160.5 mg (75% yield) of the title compound **2i**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23-7.14（m, 9H）, 6.62(d, J = 12.2Hz, 2H), 6.52(d, J = 12.2Hz, 2H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 136.88, 135.66, 132.75, 130.97, 130.23, 128.94, 128.82, 128.42, 128.36, 127.34. Data in accordance with the literature.[1]

HRMS (ESI) calcd for $C_{14}H_{12}Cl^+$ m/z $[M+H]^+$: 215.0628, found 215.0636.



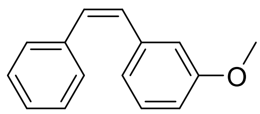
(Z)-1-methoxy-2-styrylbenzene (2j)

Purification by flash chromatography on silica gel (petroleum ether/EtOAc (10:1)) afforded 174.3 mg (83% yield) of the title compound **2j**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.14(m, 7H), 6.90(d, 1H), 6.74(t, 1H)， 6.68（d, *J* = 12.4Hz, 1H）, 6.62(d, *J* = 12.4Hz, 1H), 3.81(s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.19,137.33, 130.24, 130.11, 128.85, 128.60, 128.04, 126.91, 126.22, 125.82, 120.22, 110.67, 55.46. Data in accordance with the literature.[4]

HRMS (ESI) calcd for $C_{15}H_{15}O^{+}$ m/z $[M+H]^{+}$: 211.1123, found 211.1129.



(Z)-1-methoxy-3-styrylbenzene (2k)

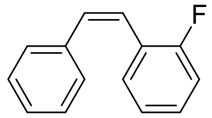
Purification by flash chromatography on silica gel (petroleum ether/EtOAc (10:1)) afforded 176.4mg (84% yield) of the title compound **2k**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.11 (m, 6H), 6.84-6.70 (m, 3H),

6.61 (d, *J* = 12.4 Hz, 1H), 6.56 (d, *J* = 12.4 Hz, 1H), 3.64 (s, 3H).

^{13}C NMR (100 MHz,$CDCl_3$) δ 159.4, 138.6, 137.4 130.6, 130.2, 129.3, 129.0, 128.3, 127.2, 121.6, 113.8, 113.4, 55.1. Data in accordance with the literature.[5]

HRMS (ESI) calcd for $C_{15}H_{15}O^+$ m/z $[M+H]^+$: 211.1123, found 211.1122.



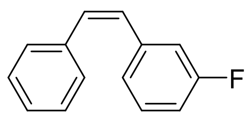
(Z)-1-fluoro-2-styrylbenzene (2l)

Purification by flash chromatography on silica gel (petroleum ether) afforded 180.2mg (91% yield) of the title compound **2l**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.21(m, 7H), 7.10-7.06(m, 1H), 6.99-6.96(m, 1H), 6.77 (d, J = 12.4 Hz 1H), 6.66 (d, J = 12.4 Hz 1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6 ($J_{C\text{-}F}$ = 246.2Hz), 136.9, 132.3, 130.6 (d, $J_{C\text{-}F}$ = 3.5 Hz); 129.1 (d, $J_{C\text{-}F}$ = 8.2Hz), 128.8, 128.3, 127.4, 125.1 (d, $J_{C\text{-}F}$ = 14.4 Hz), 123.6 (d, $J_{C\text{-}F}$ = 3.5 Hz), 122.6 ($J_{C\text{-}F}$ = 3.3 Hz), 115.5 (d, $J_{C\text{-}F}$ = 21.8 Hz). Data in accordance with the literature.[4]

HRMS (ESI) calcd for $C_{14}H_{12}F^+$ m/z $[M+H]^+$: 199.0923, found 199.0926.



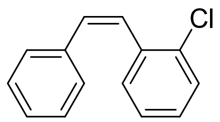
(Z)-1-fluoro-3-styrylbenzene (2m)

Purification by flash chromatography on silica gel (petroleum ether) afforded 152.5mg (77% yield) of the title compound **2m**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.14 (m, 6H), 7.01 (d, J = 7.7 Hz, 1H), 6.96-6.85 (m, 2H), 6.64 (d, J = 12.4 Hz, 1H), 6.54 (d, J = 12.4 Hz, 1H)

^{13}C NMR (100MHz, $CDCl_3$) δ 162.8 (d, $J_{C\text{-}F}$ = 245.1Hz), 139.5 (d, J = 7.9 Hz), 136.7, 131.4, 129.7 (d, $J_{C\text{-}F}$ = 8.4Hz), 129.0 (d, $J_{C\text{-}F}$ = 2.3Hz),128.9, 128.4, 127.5, 124.8 (d, $J_{C\text{-}F}$ = 2.8Hz), 115.7 (d, $J_{C\text{-}F}$ = 21.7Hz),114.1 (d, $J_{C\text{-}F}$ = 21.2Hz) Data in accordance with the literature.[5]

HRMS (ESI) calcd for $C_{14}H_{12}F^+$ m/z $[M+H]^+$: 199.0923, found 199.0916.



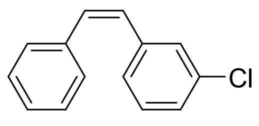
(Z)-1-chloro-2-styrylbenzene (2n)

Purification by flash chromatography on silica gel (petroleum ether) afforded 151.9mg (71% yield) of the title compound **2n**.

^1H NMR(400 MHz, $CDCl_3$) δ 7.41-7.39 (m, 1H), 7.20-7.14 (m, 7H), 7.05 – 7.01 (m, 1H), 6.71 (d, J = 12.4 Hz 1H), 6.67 (d, J = 12.4 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 136.0, 133.7, 131.7, 130.7, 129.5, 129.0, 128.5, 128.2, 127.4, 127.2, 126.4. Data in accordance with the literature.[6]

HRMS (ESI) calcd for $C_{14}H_{12}Cl^+$ m/z $[M+H]^+$: 215.0628, found 215.0632.



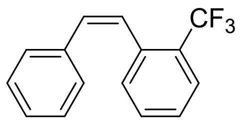
(Z)-1-chloro-3-styrylbenzene (2o)

Purification by flash chromatography on silica gel (petroleum ether) afforded 173.3mg (81% yield) of the title compound **2o**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39(dd,*J* = 8,1.2Hz, 1H), 7.24–7.01 (m, 7H), 7.03(t, 1H), 6.71 (d, *J* = 12.4Hz, 1H), 6.67 (d, *J* = 12.4 Hz, 1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 136.6, 134.0, 131.6, 129.5, 128.8, 128.7, 128.3, 127.5, 127.1, 127.0. Data in accordance with the literature.[1]

HRMS (ESI) calcd for $C_{14}H_{12}Cl^+$ m/z $[M+H]^+$: 215.0628, found 215.0623.



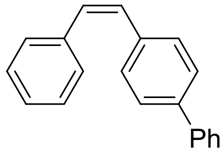
(Z)-1-styryl-2-(trifluoromethyl)benzene (2p)

Purification by flash chromatography on silica gel (petroleum ether) afforded 203.4mg (82% yield) of the title compound **2p**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79(d, 1H), 7.34-7.28(m, 2H), 7.25-7.21(m, 1H), 7.17-7.14(m, 3H), 7.08-7.04(m, 2H), 6.84-6.81(d, *J* = 12Hz, 1H), 76.72(d, *J* = 12.4Hz, 1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 136.2, 132.2, 131.7, 131.3, 129.3(2C), 128.6 (q, $J_{C\text{-}F}$ = 33.9Hz) 128.1(2C), 127.4, 127.2, 126.9, 125.9(q, *J* = 3.8Hz,2C), 124.4(q, $J_{C\text{-}F}$ = 272.3Hz)

HRMS (ESI) calcd for $C_{15}H_{12}F_3^+$ m/z $[M+H]^+$: 249.0891, found 249.0893.



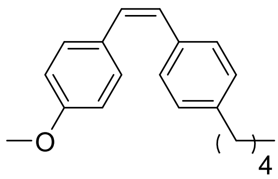
(Z)-4-styryl-1,1'-biphenyl (2q)

Purification by flash chromatography on silica gel (petroleum ether) afforded 235.5mg (92% yield) of the title compound **2q**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57(d, 2H), 7.46-7.38(m, 4H), 7.32-7.29(m, 5H), 7.25-7.19(m, 3H), 6.64-6.58(m, 2H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 139.8, 137.4, 136.2, 130.4, 129.8, 129.4, 128.9, 128.8, 128.3, 127.3, 127.2, 126.9, 126.8. Data in accordance with the literature.[5]

HRMS (ESI) calcd for $C_{20}H_{17}^+$ m/z $[M+H]^+$: 257.1330, found 257.1332.



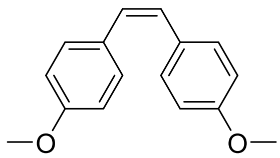
(Z)-1-methoxy-4-(4-pentylstyryl)benzene (2r)

Purification by flash chromatography on silica gel (petroleum ether/EtOAc (10:1)) afforded 212.8mg (76% yield) of the title compound **2r**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19(t, 4H), 7.04(d, 2H), 6.75(d, 2H), 6.47(s, 2H), 3.78(s, 3H), 2.66(t, 2H), 1.61-1.56(m, 2H), 1.36-1.26(m, 4H), 0.89(t, 3H)

^{13}C NMR (100MHz, $CDCl_3$): δ 158.6, 141.8, 134.8, 130.1, 129.9, 129.1, 128.8, 128.7, 128.3, 113.6, 55.2, 35.7, 31.6, 31.1, 22.6, 14.1.

HRMS (ESI) calcd for $C_{17}H_{19}O^+$ m/z $[M+H]^+$: 239.1436, found 239.1435.



(Z)-1,2-bis(4-methoxyphenyl)ethene (2s)

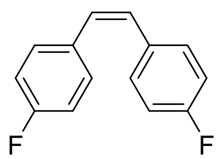
Purification by flash chromatography on silica gel (petroleum ether/EtOAc (10:1)) afforded 194.4mg (81% yield) of the title compound **2s**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (d, J = 8.8Hz, 4H), 6.75 (d, J = 8.8Hz, 4H), 6.42 (s, 2H), 3.76 (s, 6H)

^{13}C NMR (100MHz, $CDCl_3$) δ 158.5, 130.0, 129.9, 128.4, 113.6, 55.2

Data in accordance with the literature.[1]

HRMS (ESI) calcd for $C_{16}H_{17}O_2^+$ m/z $[M+H]^+$: 241.1229, found 241.1221.



(Z)-1,2-bis(4-fluorophenyl)ethene (2t)

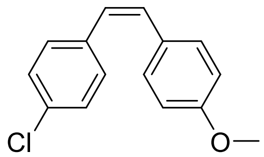
Purification by flash chromatography on silica gel (petroleum ether) afforded 190.1mg (88% yield) of the title compound **2t**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20-7.16(m, 4H), 6.94-6.88(m, 4H), 6.62(s, 2H)

^{13}C NMR (100MHz, $CDCl_3$) δ 161.9(d, J_{C-F} = 245.1Hz), 133.0, 130.5(d, J_{C-F} = 8.0Hz), 129.2, 116.3(d, J_{C-F} =21.2Hz)

Data in accordance with the literature.[6]

HRMS (ESI) calcd for $C_{14}H_{11}F_2^+$ m/z $[M+H]^+$: 217.0829, found 217.0826.



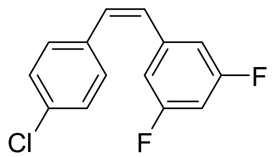
(Z)-1-chloro-4-(4-methoxystyryl)benzene (2u)

Purification by flash chromatography on silica gel (petroleum ether) afforded 158.6mg (65% yield) of the title compound **2u**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19-7.14(m, 6H), 6.76(d, *J* = 8.4Hz,2H), 6.55(s, *J* = 12.4Hz,1H), 6.43(s, *J* = 12.4Hz,1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 136.0, 132.5, 130.5, 130.2, 130.2, 129.3, 128.5, 127.5, 113.8, 55.3.

HRMS (ESI) calcd for $C_{15}H_{14}ClO^+$ m/z $[M+H]^+$: 245.0733, found 245.0731.



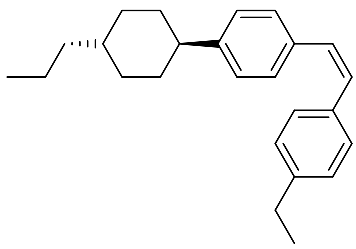
(Z)-1-(4-chlorostyryl)-3,5-difluorobenzene (2v)

Purification by flash chromatography on silica gel (petroleum ether) afforded 195.0mg (78% yield) of the title compound **2v**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22(d, 2H), 7.13(d, 2H), 6.73-6.64(m, 3H), 6.61(d, J = 12.0Hz, 1H), 6.50(d, J = 12.4Hz, 1H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.3, 161.7, 140.2, 140.1, 140.1, 134.6, 133.6, 131.2, 130.2, 128.7, 111.5, 102.8.

HRMS (ESI) calcd for $C_{14}H_{10}ClF_2^+$ m/z $[M+H]^+$: 251.0439, found 251.046.



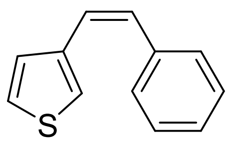
1-ethyl-4-((Z)-4-((1s,4r)-4-propylcyclohexyl)styryl)benzene (2w)

Purification by flash chromatography on silica gel (petroleum ether) afforded 190.0mg (59% yield) of the title compound **2w**.

^{1}H NMR (400 MHz, $CDCl_3$) δ7.22-7.18(m, 4H), 7.06(d, 4H), 6.50(s, 2H), 2.61(q, 2H), 2.45-2.38(m, 1H), 1.90-1.82(m, 4H), 1.47-1.17(m, 11H), 1.08-0.98(m, 2H), 0.90(t, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 146.85, 143.10, 134.88, 134.81, 129.55, 129.46, 128.81, 128.77, 127.68, 126.64, 44.38, 39.76, 37.05, 34.28, 33.59, 28.62, 20.36, 15.45, 14.45. Data in accordance with the literature.[2]

HRMS (ESI) calcd for $C_{25}H_{33}^+$ m/z $[M+H]^+$: 333.2582, found 333.2582.



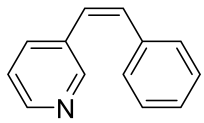
(Z)-3-styrylthiophene (2x)

Purification by flash chromatography on silica gel (petroleum ether) afforded 173.6mg (74% yield) of the title compound **2x**.

^{1}H NMR(400 MHz, $CDCl_3$) δ 7.30-7.21(m, 6H),7.12-7.09(m, 2H), 6.87(dd, *J* = 1.2, 2.8Hz, 1H), 6.58-6.52(q, 2H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 137.8, 129.5, 128.7, 128.3, 128.0, 127.2, 124.9, 124.4, 124.1. Data in accordance with the literature.[2]

HRMS (ESI) calcd for $C_{12}H_{11}S^+$ m/z $[M+H]^+$: 187.0581, found 187.0580.



(Z)-3-styrylpyridine (2y)

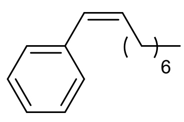
Purification by flash chromatography on silica gel (petroleum ether) afforded 124.9mg (69% yield) of the title compound **2y**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46(m, 2H),7.54(dt, *J* = 8.0, 1.6Hz, 1H)

7.31-7.23(m, 5H), 7.10(dd, *J* = 4.8,8Hz, 2H), 6.78 (d, *J* = 12.4Hz, 1H), 6.57(d, *J* = 12.4Hz, 1H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 150.2, 148.1, 136.6, 135.9, 133.0, 132.7, 128.8, 128.6, 127.7, 126.5, 123.0. Data in accordance with the literature.[6]

HRMS (ESI) calcd for $C_{13}H_{12}N^+$ m/z $[M+H]^+$: 182.0970, found 182.0972.



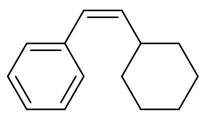
(Z)-non-1-en-1-ylbenzene (2z)

Purification by flash chromatography on silica gel (petroleum ether) afforded 155.5mg (77% yield) of the title compound **2z**.

^{1}H NMR (400MHz, $CDCl_3$) δ 7.34-7.18 (m, 5H), 6.40 (d, *J* = 11.6 Hz, 1H), 5.66 (dt, *J* = 11.6, 7.2 Hz, 1H), 2.35-2.2(m, 2H), 1.48-1.41(m, 2H), 1.33-1.26(m, 8H), 0.87(t, *J* = 6.8Hz, 3H).

^{13}C NMR (100MHz, $CDCl_3$) δ 137.9, 133.4, 128.8, 128.7, 128.2, 126.5, 31.9, 30.1, 29.4, 29.3, 28.7, 22.8, 14.2. Data in accordance with the literature.[9]

HRMS (ESI) calcd for $C_{10}H_{13}^+$ m/z $[M+H]^+$: 133.1017, found 133.1015.



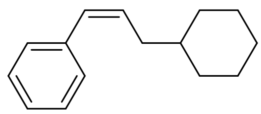
(Z)-(2-cyclohexylvinyl)benzene (2aa)

Purification by flash chromatography on silica gel (petroleum ether) afforded 109.7mg (59% yield) of the title compound **2aa**.

^{1}H NMR (400 MHz, $CDCl_3$) δ7.34-7.20(m, 5H), 6.31(d, *J* = 11.6 Hz, 1H), 5.48(t, *J* = 11.2Hz, 1H), 2.62-2.54(m, 1H), 1.72-1.64(m, 4H), 1.32-1.12(m,6H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 138.1, 128.7, 128.3, 126.9, 126.5, 37.0, 33.4, 26.1, 25.8. Data in accordance with the literature.[7]

HRMS (ESI) calcd for $C_{14}H_{19}^+$ m/z $[M+H]^+$: 187.1487, found 187.1486.



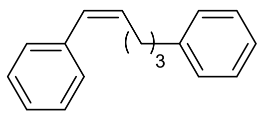
(Z)-(3-cyclohexylprop-1-en-1-yl)benzene (2bb)

Purification by flash chromatography on silica gel (petroleum ether) afforded 118.0mg (59% yield) of the title compound **2bb**.

^{1}H NMR (400MHz, $CDCl_3$) δ 7.34-7.18(m, 5H), 6.40(d, *J* = 11.6Hz, 1H), 5.66(dt, *J* = 11.2,7.6Hz, 1H), 2.35-2.29(m, 2H), 1.48-1.40(m, 2H), 1.36-1.23(m, 6H), 0.87(t, *J* = 7.2Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 133.4, 128.8, 128.8, 128.2, 126.5, 31.9, 30.1, 29.2, 28.8, 22.7, 14.2.

HRMS (ESI) calcd for $C_{15}H_{21}^{+}$ m/z $[M+H]^{+}$: 201.1643, found 201.1646.



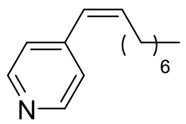
(Z)-pent-1-ene-1,5-diyldibenzene (2cc)

Purification by flash chromatography on silica gel (petroleum ether) afforded 148.7mg (67% yield) of the title compound **2cc**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.12(m, 10H), 6.42(d, *J* = 11.6Hz, 1H), 5.67(q, *J* = 11.2Hz, 1H), 2.63-2.56(m, 2H), 2.39-2.33(m, 2H), 1.80-1.74(m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 142.4, 137.8, 132.7, 129.4, 128.9, 128.6, 128.5, 128.3, 126.7, 125.9, 35.6, 31.89, 28.3. Data in accordance with the literature.[8]

HRMS (ESI) calcd for $C_{15}H_{15}^+$ m/z $[M+H]^+$: 195.1174, found 195.1172.



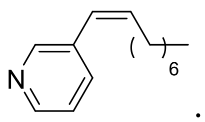
(Z)-4-(non-1-en-1-yl)pyridine (2dd)

Purification by flash chromatography on silica gel (petroleum ether) afforded 144.1mg (71% yield) of the title compound **2dd**.

^1H NMR (400 MHz, $CDCl_3$) δ 8.65(d, 1H), 7.15(d, 1H), 6.32(d, J = 11.6Hz,1H), 5.86(q, J = 11.6Hz, 1H), 2.32(q, 2H), 1.48-1.42(m, 2H), 1.31-1.26(m, 8H), 0.88(t, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 145.3, 137.5, 126.5, 123.5, 31.8, 29.7, 29.3, 29.2, 28.8, 22.7, 14.1

HRMS (ESI) calcd for $C_9H_{12}N^+$ m/z $[M+H]^+$: 134.0970, found 134.0976.



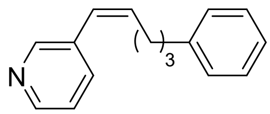
(Z)-3-(non-1-en-1-yl)pyridine (2ee)

Purification by flash chromatography on silica gel (petroleum ether) afforded 111.6mg (55% yield) of the title compound **2ee**.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.53(s, 1H), 8.48(d, *J* = 4.5Hz, 2H), 7.57(d, *J* = 7.7Hz, 1H), 7.28-7.23(m, 1H), 6.35(d, *J* = 11.7Hz, 1H), 5.80(m, 1H), 2.29(m, 2H), 1.47-1.44(m, 2H), 1.33-1.26(m, 8H), 0.87 (t, *J* = 6.4Hz, 3H)

^{13}C NMR (101 MHz, CDCl$_3$) δ 150.0, 147.5, 135.7, 133.4, 125.1, 123.1, 31.8, 29.8, 29.3, 29.2, 28.7, 22.7, 14.1.

HRMS (ESI) calcd for $C_9H_{12}N^+$ m/z [M+H]$^+$: 134.0970, found 134.0972.



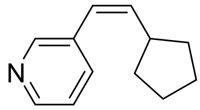
(Z)-3-(5-phenylpent-1-en-1-yl)pyridine (2ff)

Purification by flash chromatography on silica gel (petroleum ether) afforded 160.6 mg (72% yield) of the title compound **2ff**.

^{1}H NMR (400MHz, CDCl$_3$) δ 8.51(d, *J* = 2.0,1H), 8.43(dd, *J* = 3.2,1.6Hz, 1H), 7.50(d, *J* = 8Hz, 1H), 7.28-7.12(m, 6H), 6.37(d, *J* = 11.2Hz, 1H), 5.80(dt, *J* = 12.0,7.2Hz, 1H), 2.62(t, *J* = 8Hz, 2H), 2.36-2.30(m, 2H), 1.83-1.74(m, 2H)

^{13}C NMR (100 MHz, CDCl$_3$) δ 150.0, 147.6, 142.0, 135.7, 135.0, 133.3, 128.5, 128.4, 125.9, 125.7, 123.1, 35.4, 31.6, 28.1.

HRMS (ESI) calcd for $C_{14}H_{14}N^+$ m/z [M+H]$^+$: 196.1126, found 196.1123.



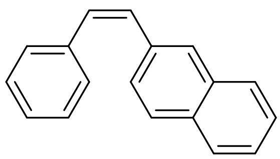
(Z)-3-(2-cyclopentylvinyl)pyridine (2gg)

Purification by flash chromatography on silica gel (petroleum ether) afforded 133.2mg (77% yield) of the title compound **2gg**.

^{1}H NMR (400MHz, $CDCl_3$) δ 8.64(s, 1H), 8.44(d, *J* = 4.8Hz, 1H), 7.56(d, *J* = 8.0 Hz, 1H), 7.24(t, *J* = 4.8Hz, 1H), 6.28(d, *J* = 11.6Hz, 1H), 6.71(t, *J* = 11.2Hz, 1H), 2.87(q, *J* = 8.4Hz, 1H), 1.90-1.82(m, 2H),1.75-1.67(m, 2H), 1.61-1.57(m, 2H), 1.41-1.32(m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 147.5, 140.7, 135.7, 133.5, 123.7, 123.1, 38.9, 34.2, 25.6.

HRMS (ESI) calcd for $C_{12}H_{16}N^+$ m/z $[M+H]^+$: 174.1283, found 174.1286.



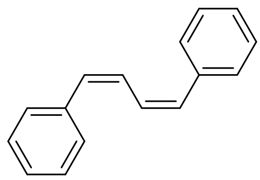
(Z)-2-styrylnaphthalene (2hh)

Purification by flash chromatography on silica gel (petroleum ether) afforded 188.6mg (82% yield) of the title compound **2hh**.

^{1}H NMR(400 MHz, $CDCl_3$) δ 7.77-7.68(m, 3H), 7.62(d, J = 8.6Hz, 1H), 7.43-7.39(m, 2H),7.35-7.32(dd, *J* = 6.8, 1.6Hz, 1H), 7.28-7.25(m, 2H),7.22-7.16(m, 3H), 6.74 (d, *J* = 12.24Hz, 1H), 6.67 (d, *J* = 12.4 Hz, 1H)

^{13}C NMR (100 MHz, CDCl3) δ137.2, 134.9,133.5, 132.6, 130.6, 130.2, 129.0, 128.2, 128.0 (2C), 127.6, 127.5, 127.2, 127.0, 126.0, 125.9. Data in accordance with the literature.[5]

HRMS (ESI) calcd for $C_{18}H_{15}^+$ m/z $[M+H]^+$: 231.1174, found 231.1172.



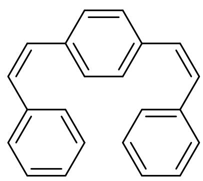
(1Z,3E)-1,4-diphenylbuta-1,3-diene (2ii)

Purification by flash chromatography on silica gel (petroleum ether) afforded 166.9mg (81% yield) of the title compound **2ii**.

^{1}H NMR (400MHz, $CDCl_3$) δ 7.41-7.20(m, 11H), 6.72(d, *J* = 15.6Hz, 1H), 6.53(d, *J* = 11.6Hz, 1H), 6.42(t, *J* = 11.2Hz, 1H)

^{13}C NMR (100MHz, $CDCl_3$) δ 137.7, 137.4, 134.9, 130.5, 130.4, 129.13, 128.7, 128.4, 127.8, 127.1, 126.7, 125.3. Data in accordance with the literature.[10]

HRMS (ESI) calcd for $C_{16}H_{15}^{+}$ m/z $[M+H]^{+}$: 207.1174, found 207.1176.



1,4-di((Z)-styryl)benzene (2jj)

Purification by flash chromatography on silica gel (petroleum ether) afforded 201.6mg (71% yield) of the title compound **2jj**.

^{1}H NMR(400 MHz, $CDCl_3$) δ 7.27-7.17(m, 10H), 7.10(s, 4H), 6.58-6.51(m, 4H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.4, 136.12, 130.4, 130.0, 129.0, 128.8, 128.3, 127.2. Data in accordance with the literature.[2]

HRMS (ESI) calcd for $C_{22}H_{19}^+$ m/z $[M+H]^+$: 283.1487, found 283.1486.

8. References

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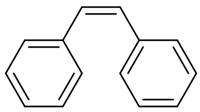
[10] D. E. E. Coyle, B. J. Doonan, A. J. Holohan, K. A. Walsh, D. F. Lavigne, D. E. H. Krenske, D. C. J. O'Brien, Angew. Chem., 2014, **126**, 13121.

9. NMR Spectra



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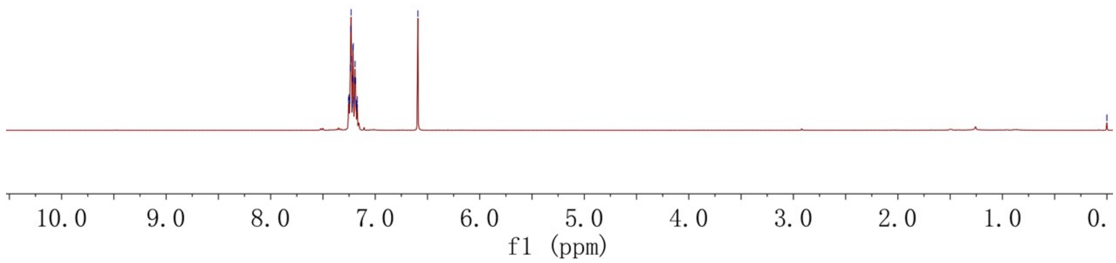

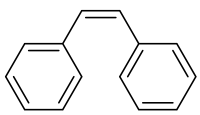

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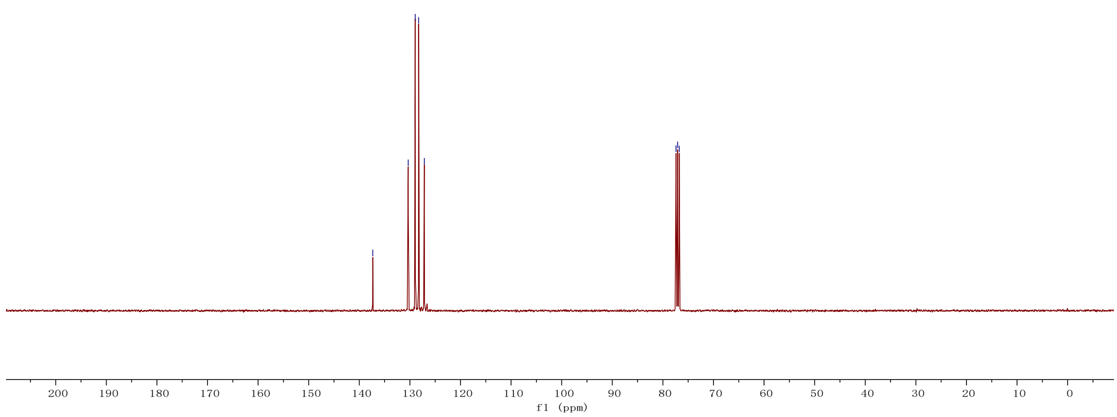

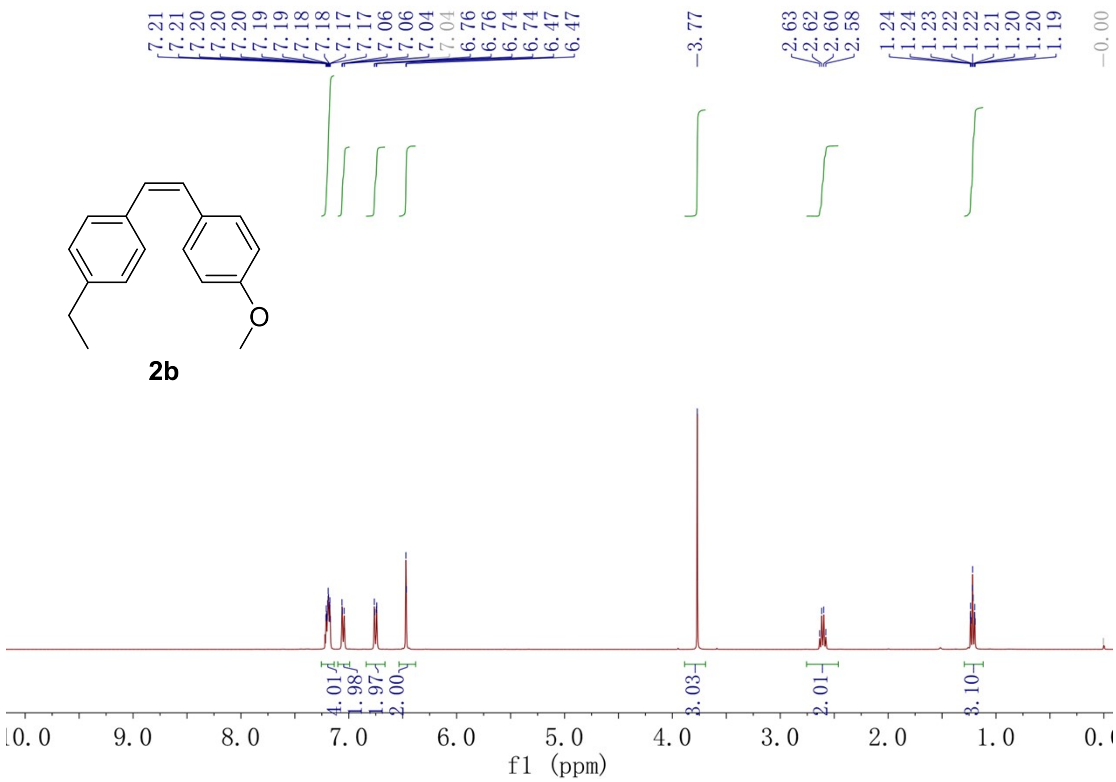

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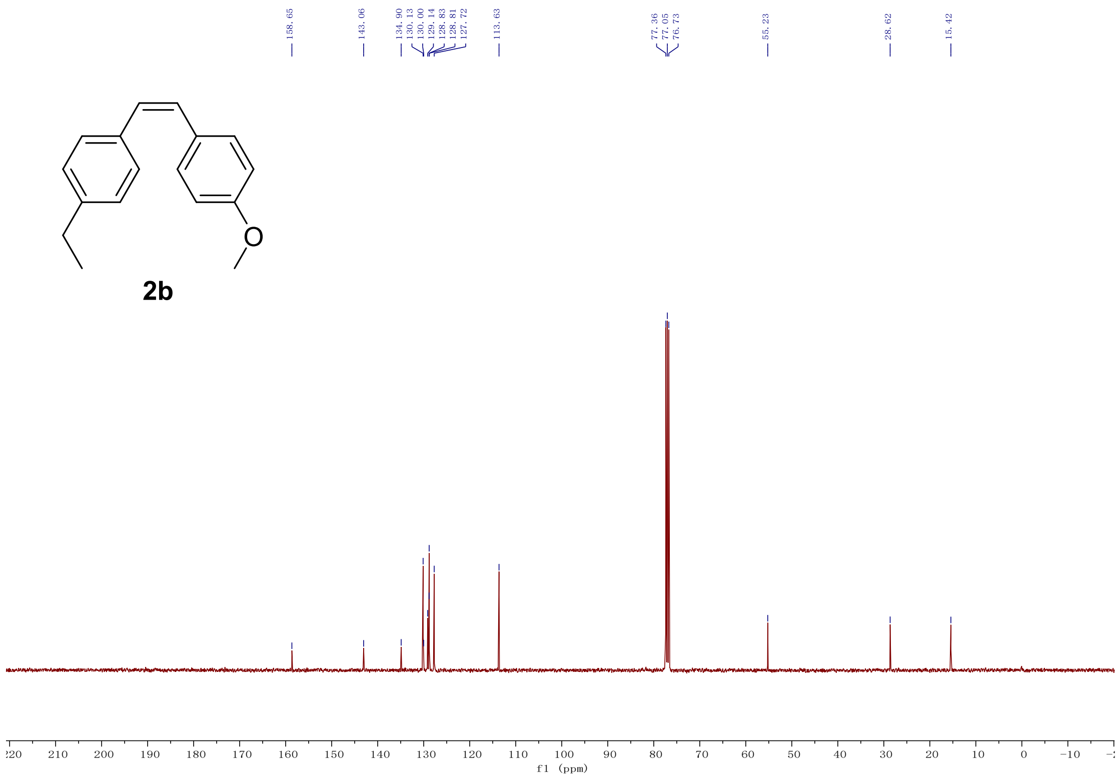

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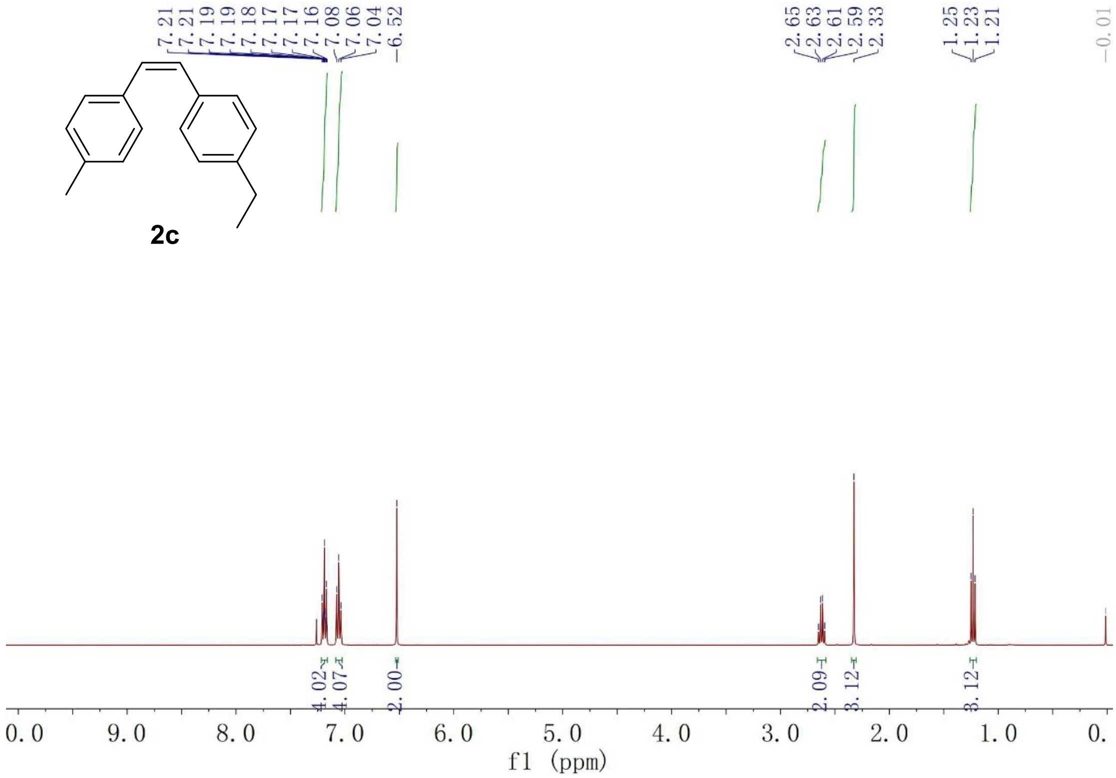
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7.19
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7.17
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7.08
7.06
7.04
6.52
2.65
2.63
2.61
2.59
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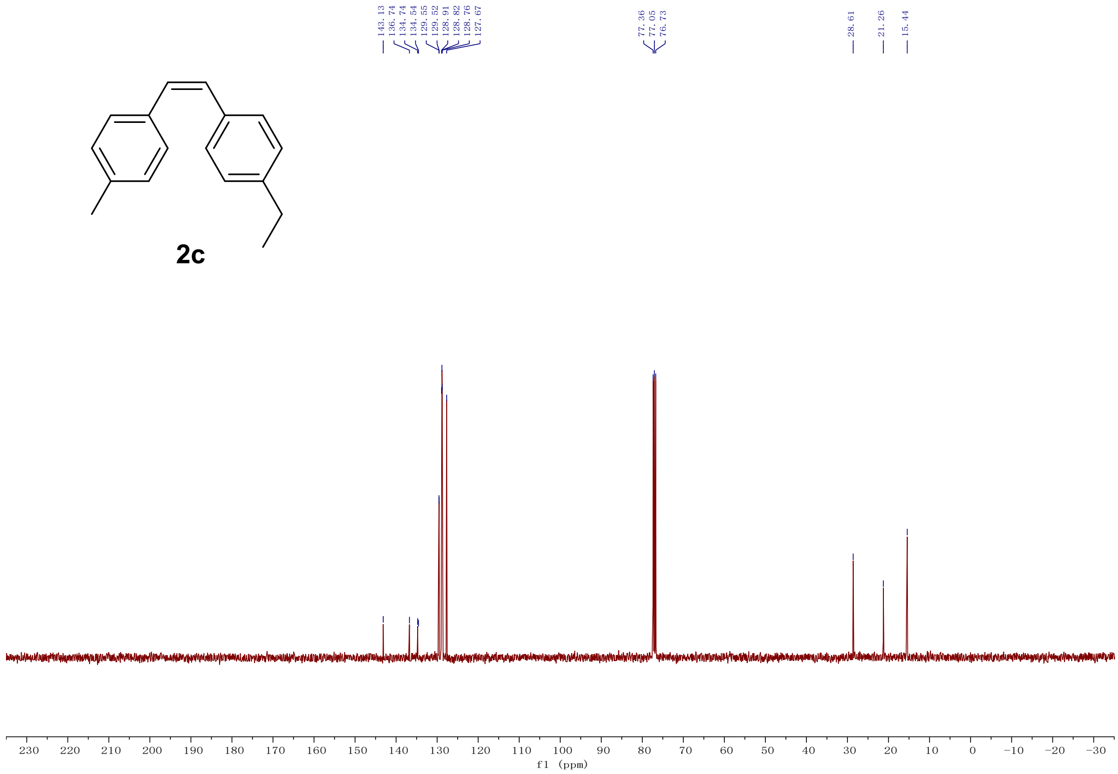
3.12
f1 (ppm)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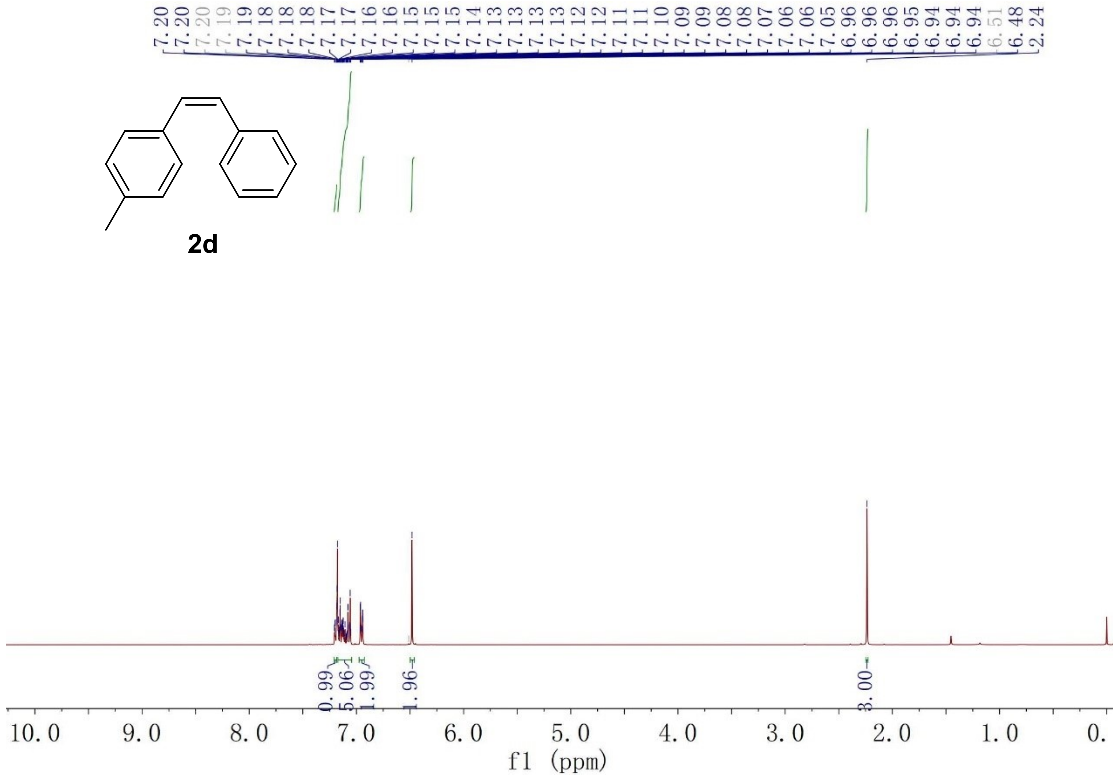
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7.06
7.05
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6.95
6.94
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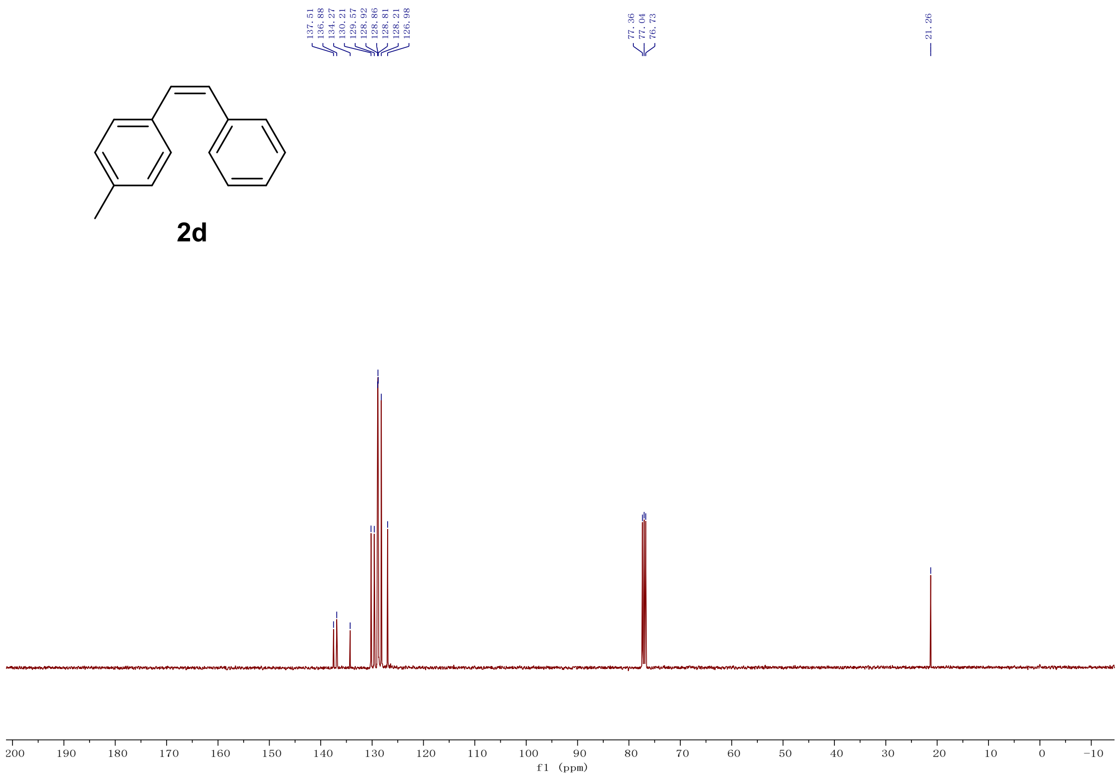
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21.26
2d
200
190
180
170
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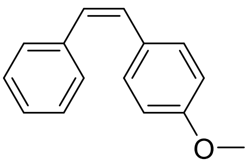
f1 (ppm)



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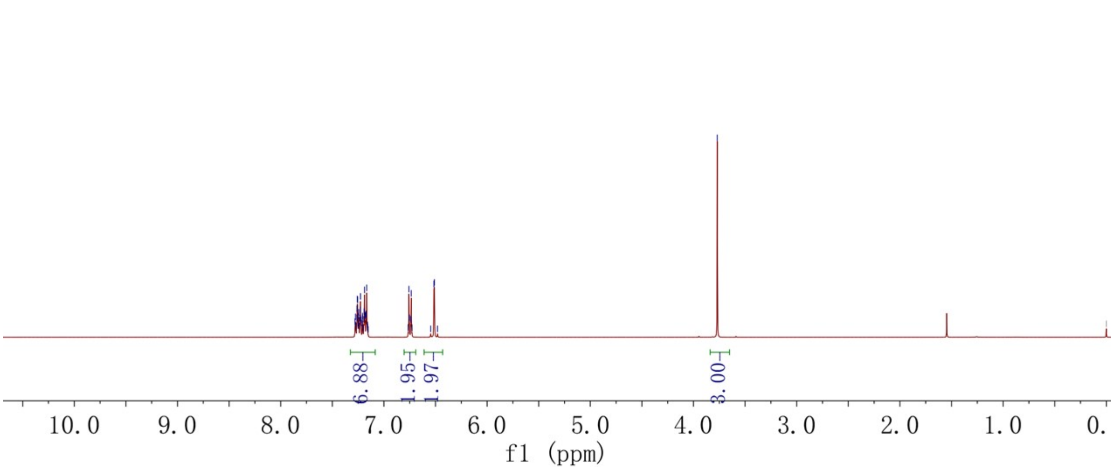

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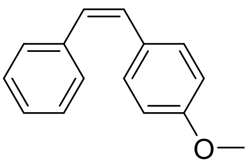

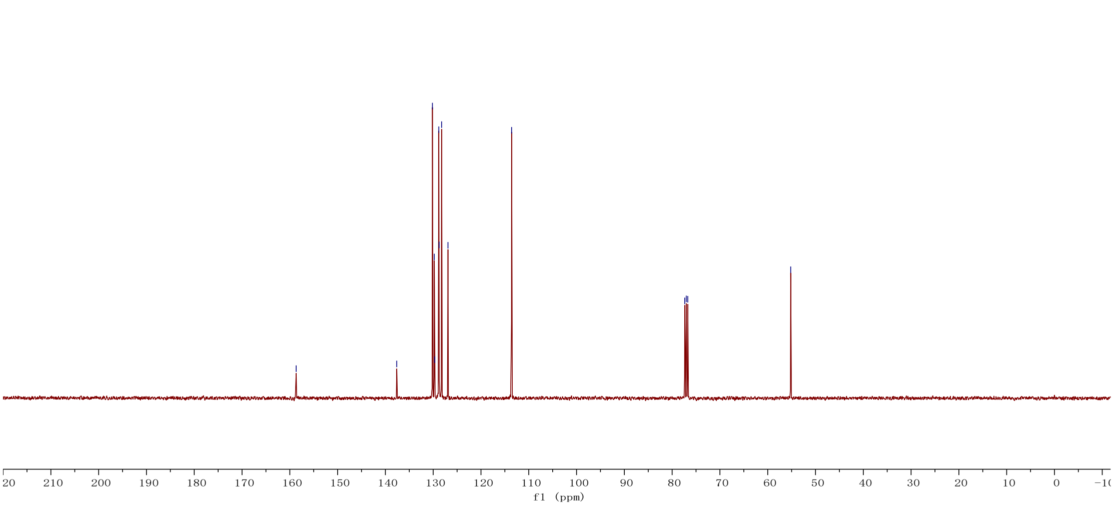

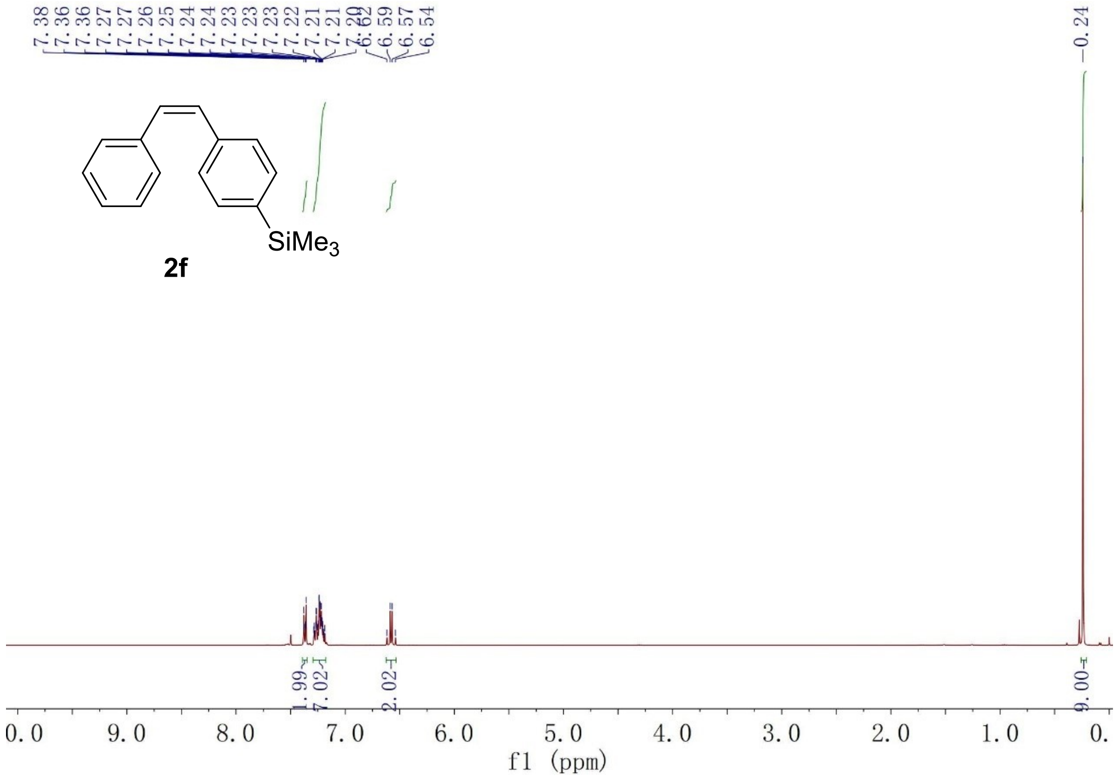
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2.02
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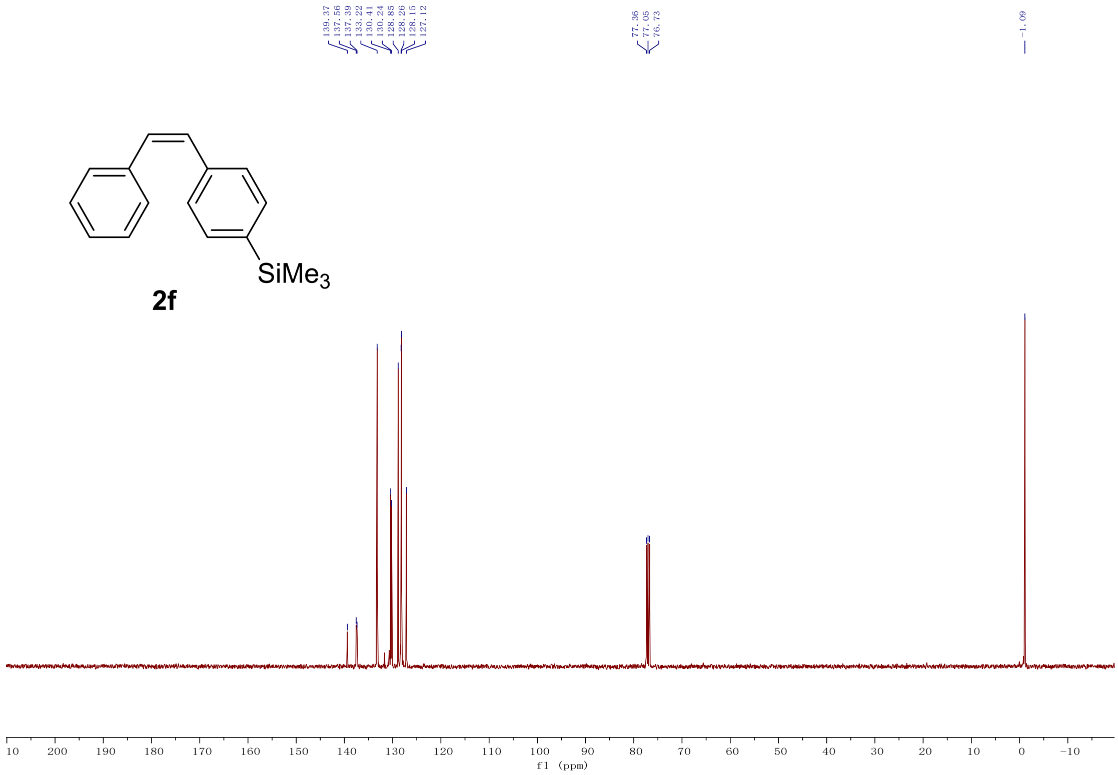
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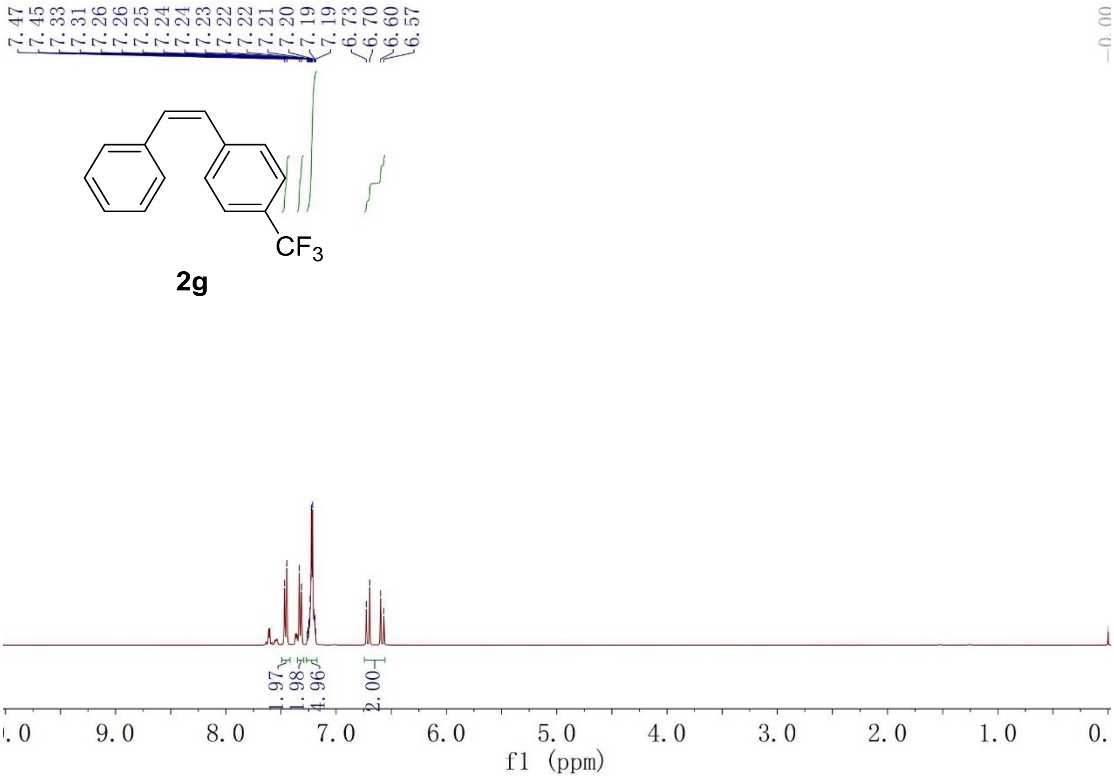
f1 (ppm)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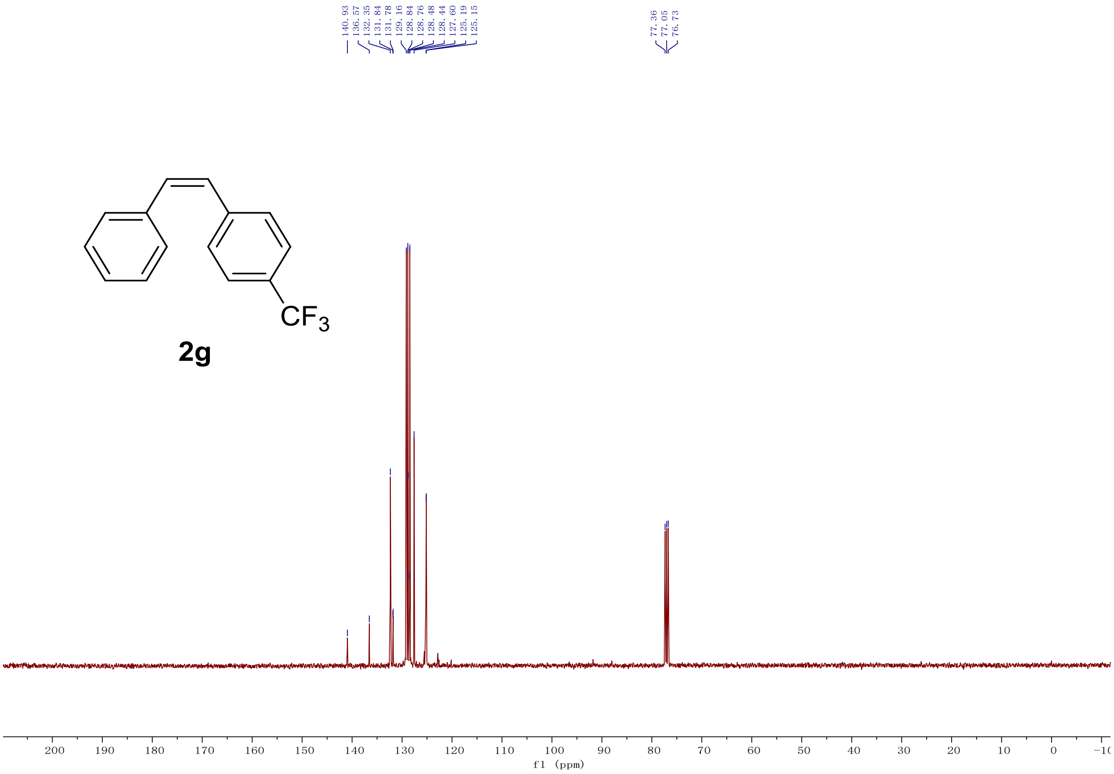
2g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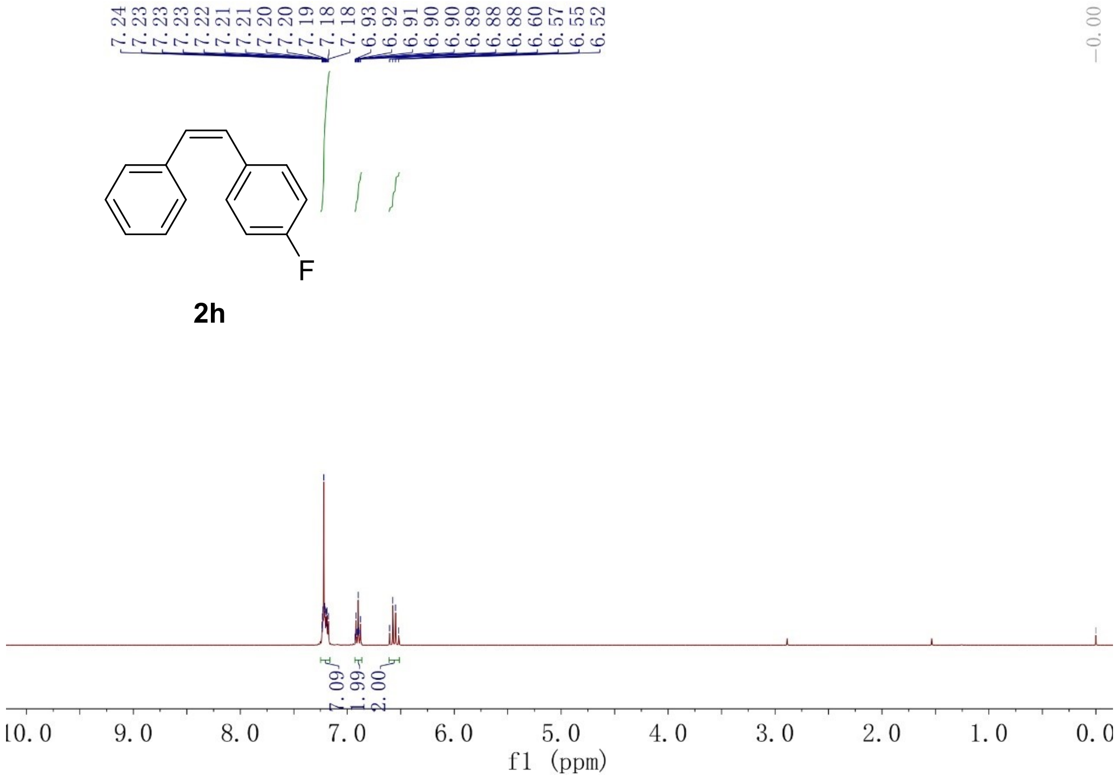

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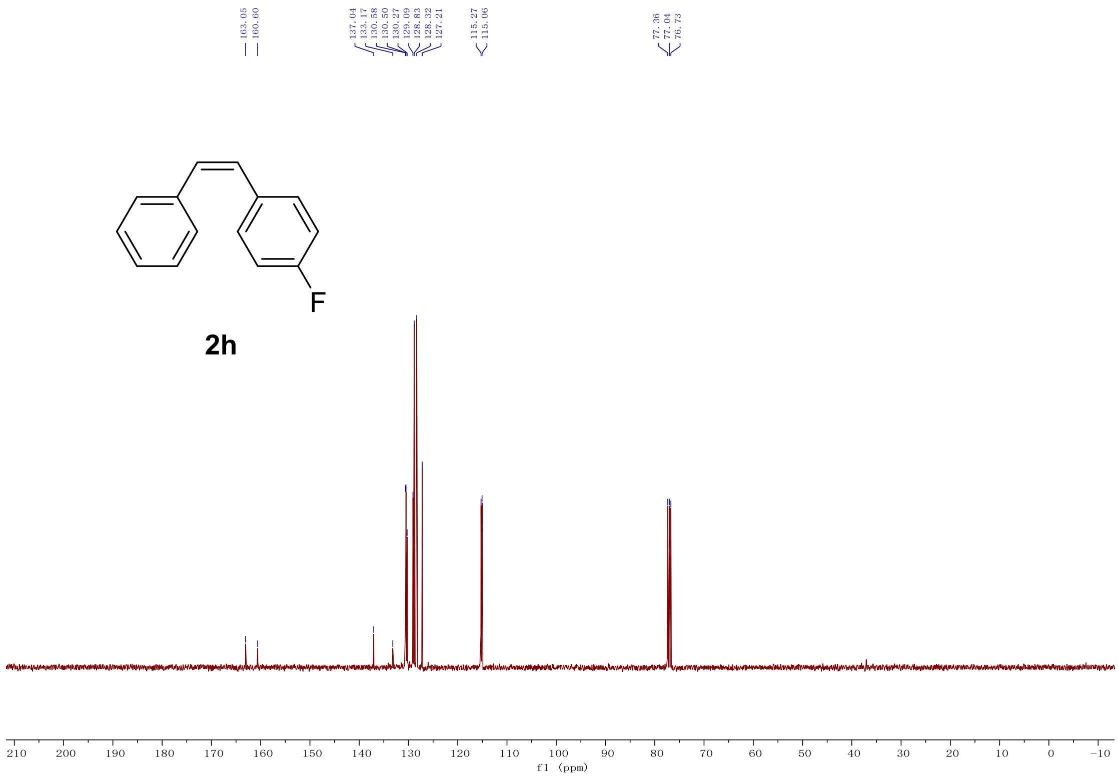

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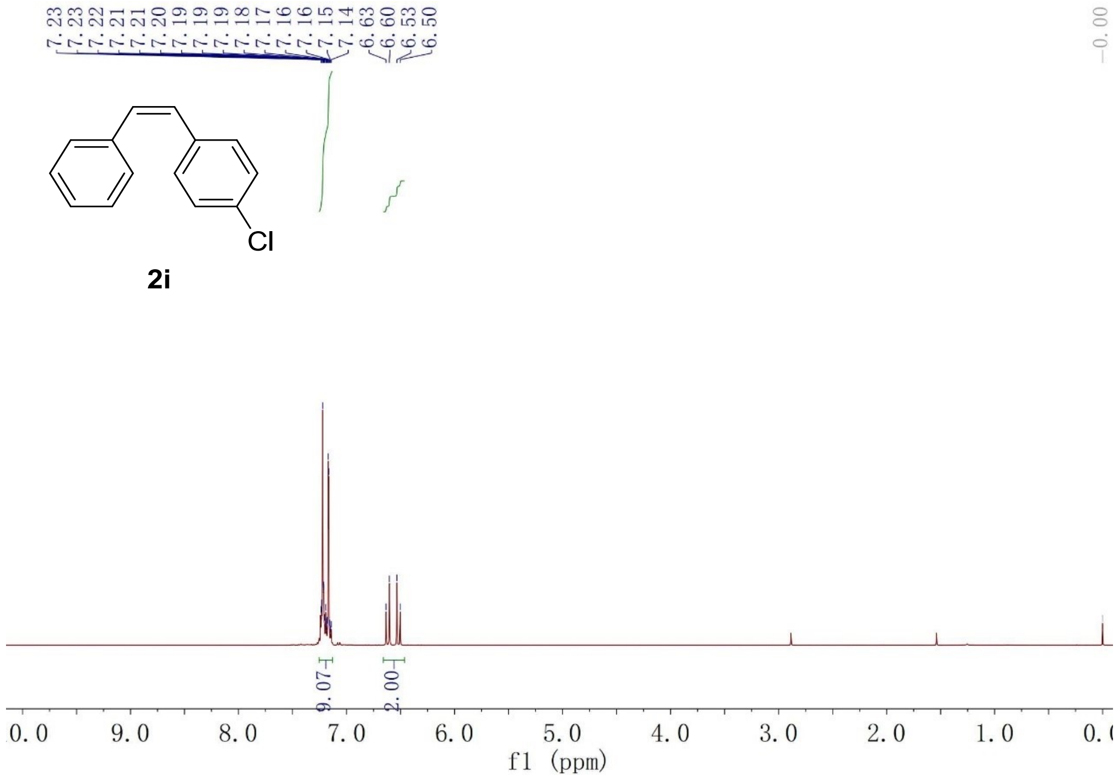
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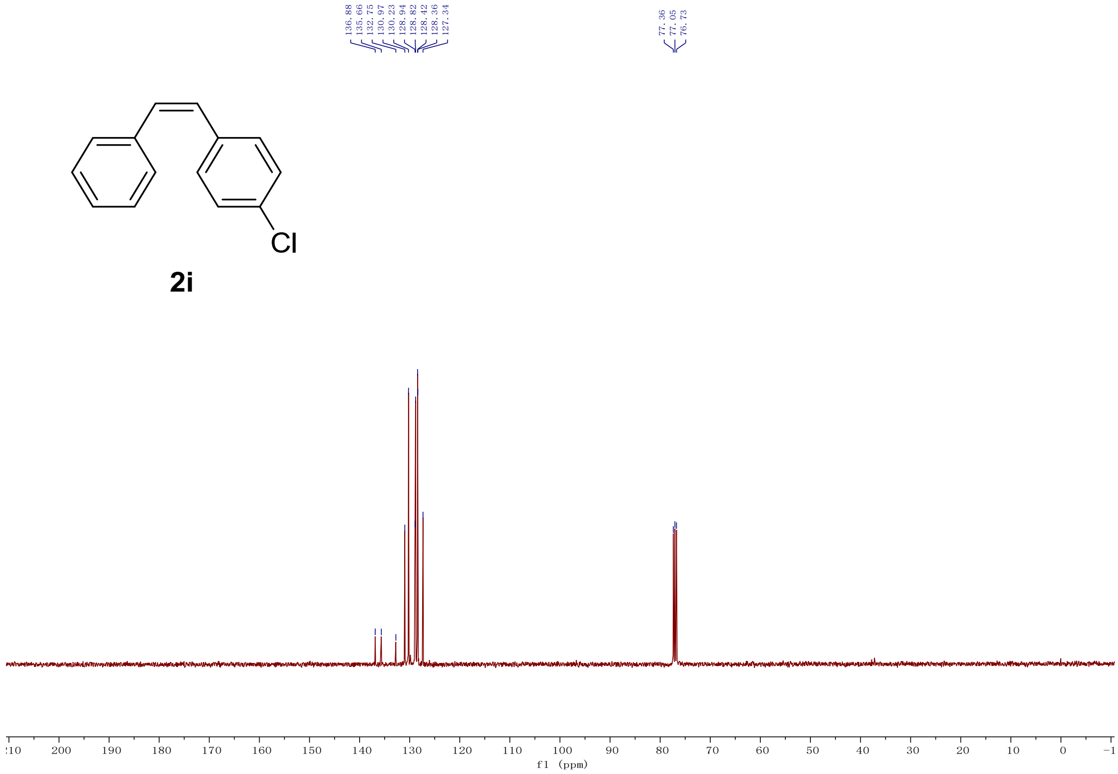
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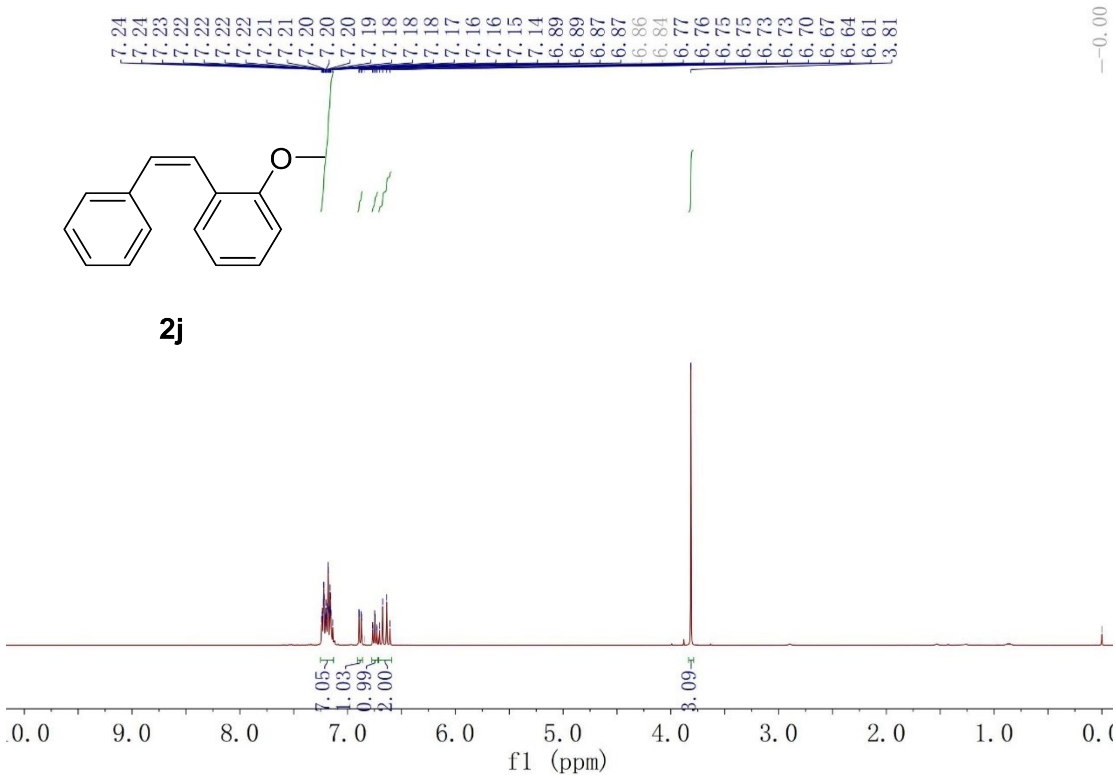
f1 (ppm)



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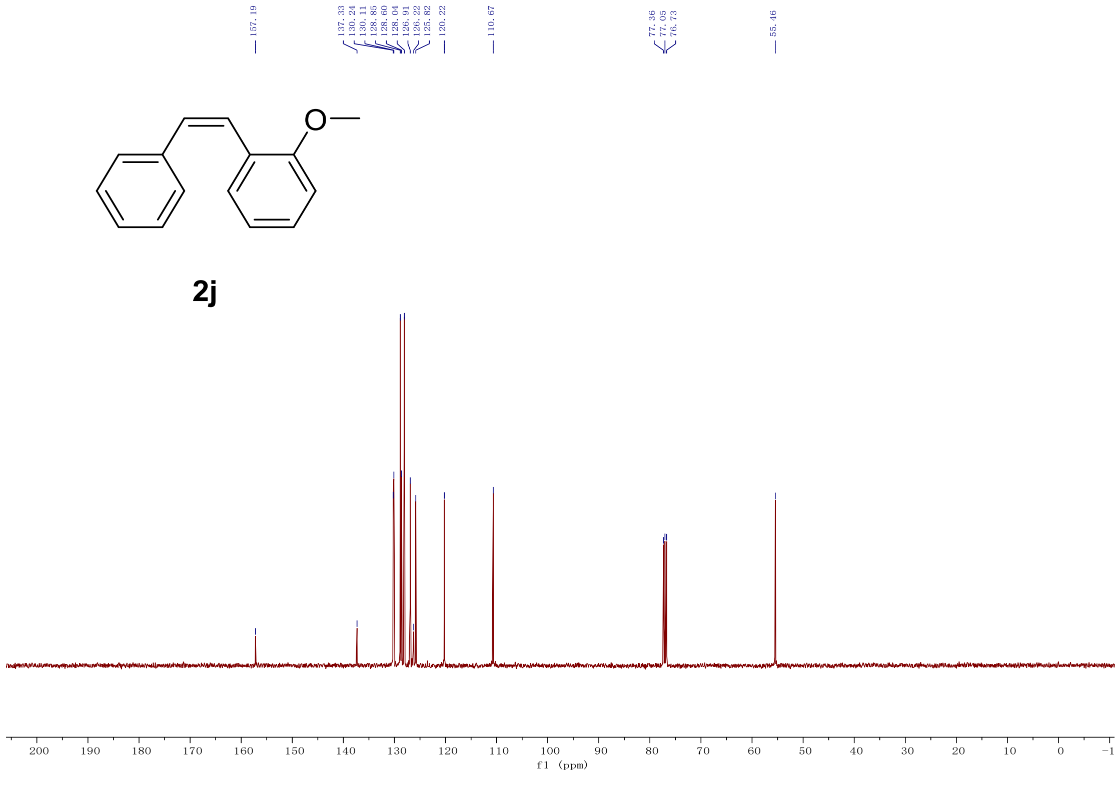
f1 (ppm)

2j



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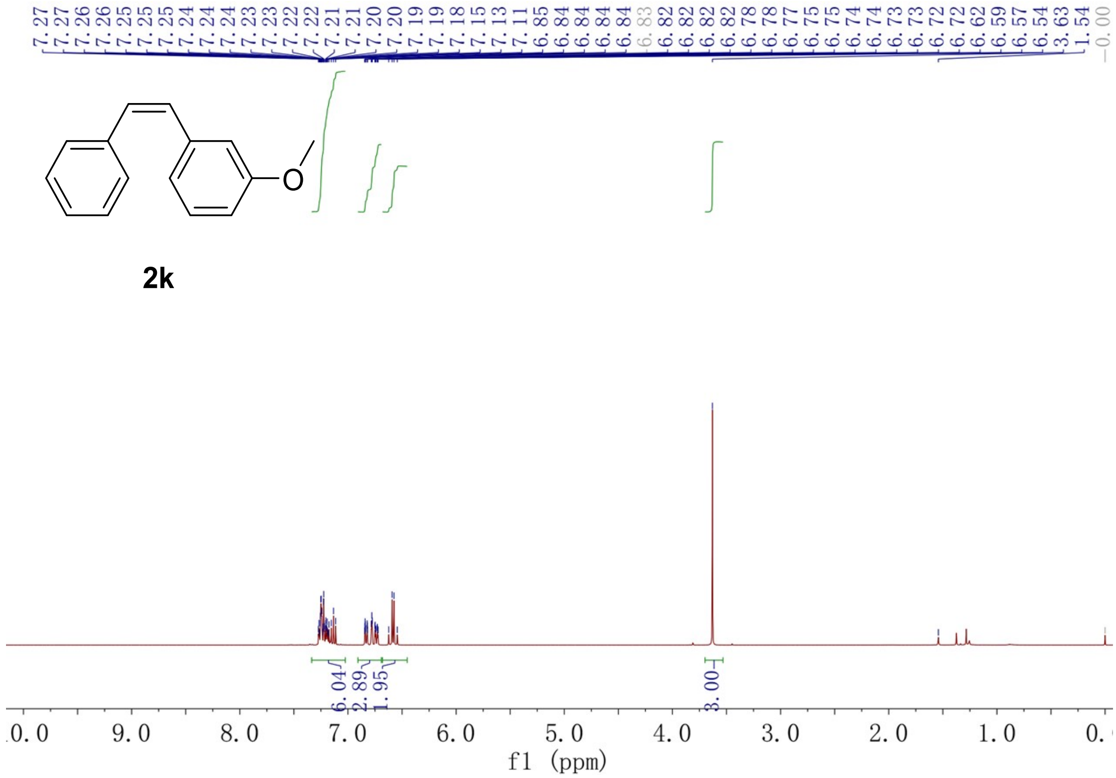
2j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O
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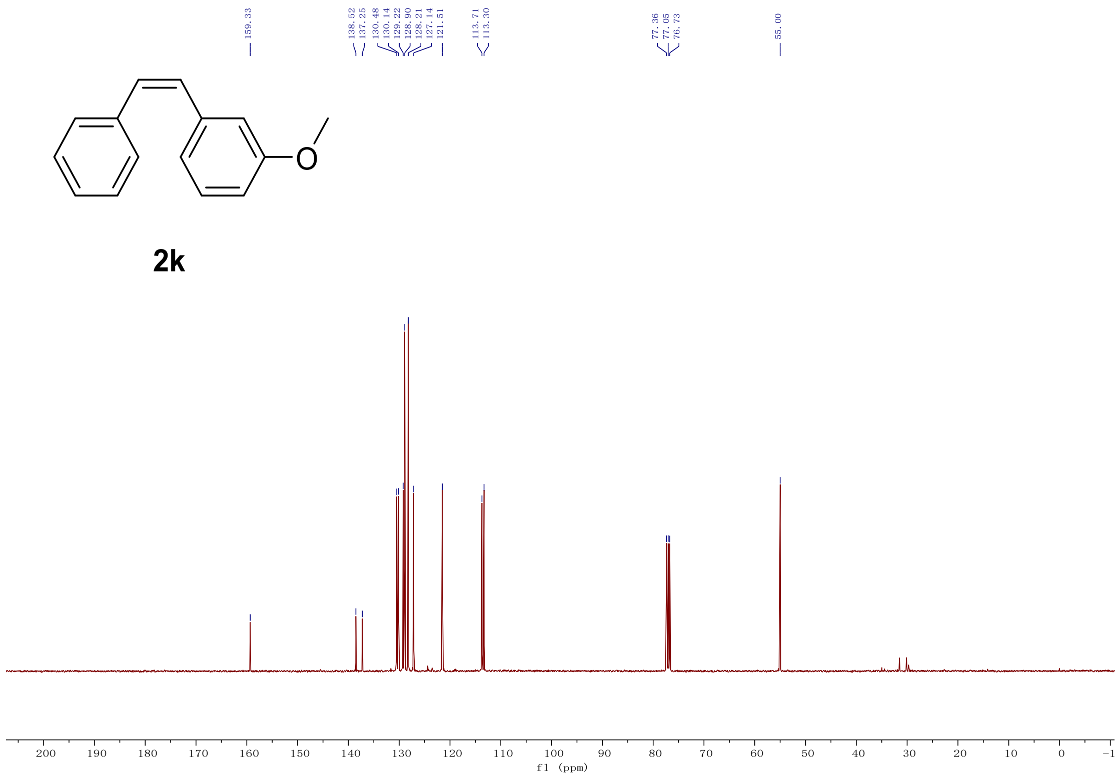
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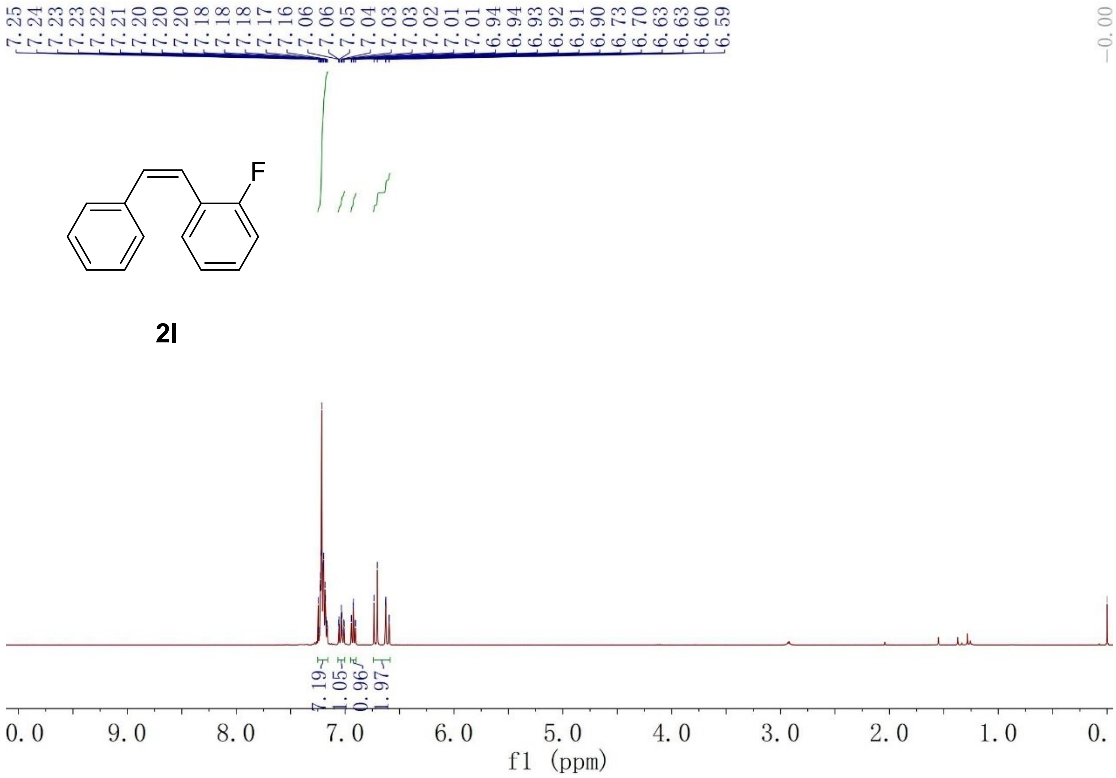

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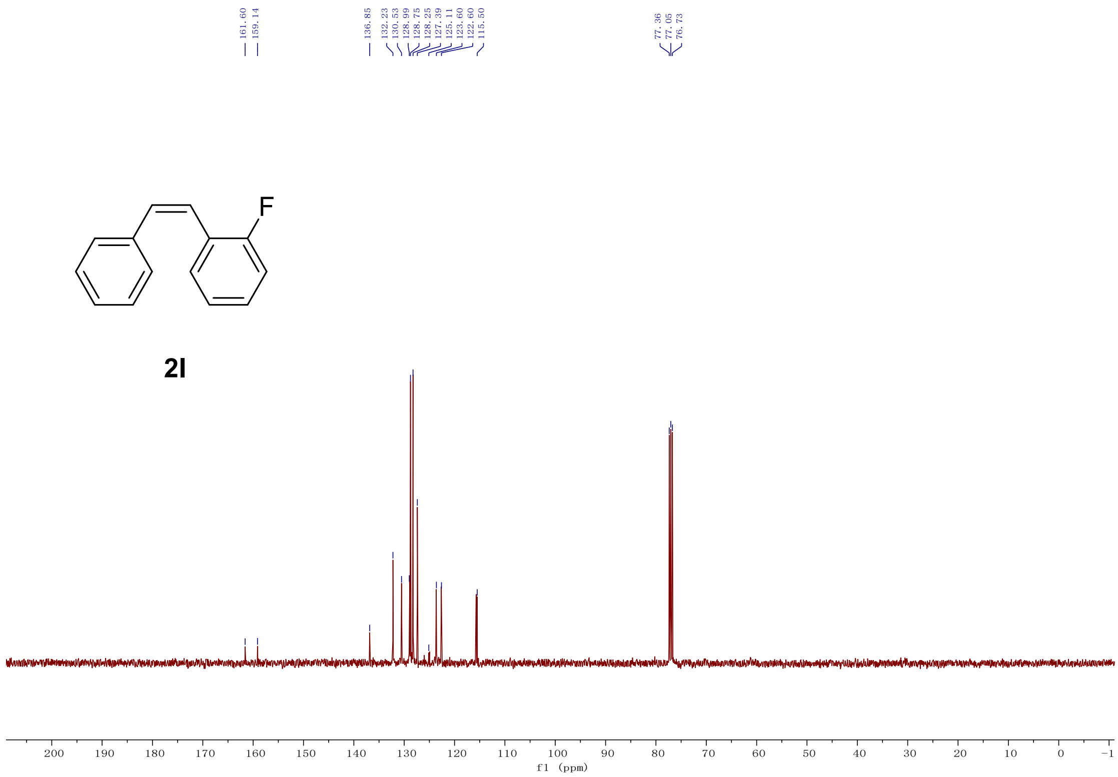

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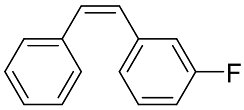
F
2l
f1 (ppm)



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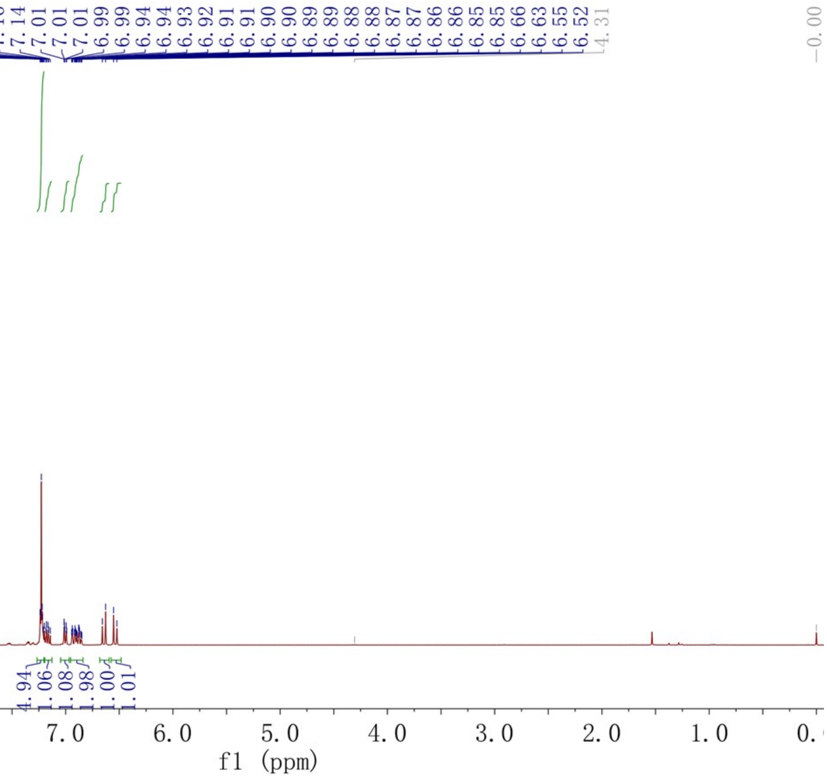

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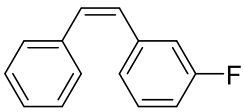

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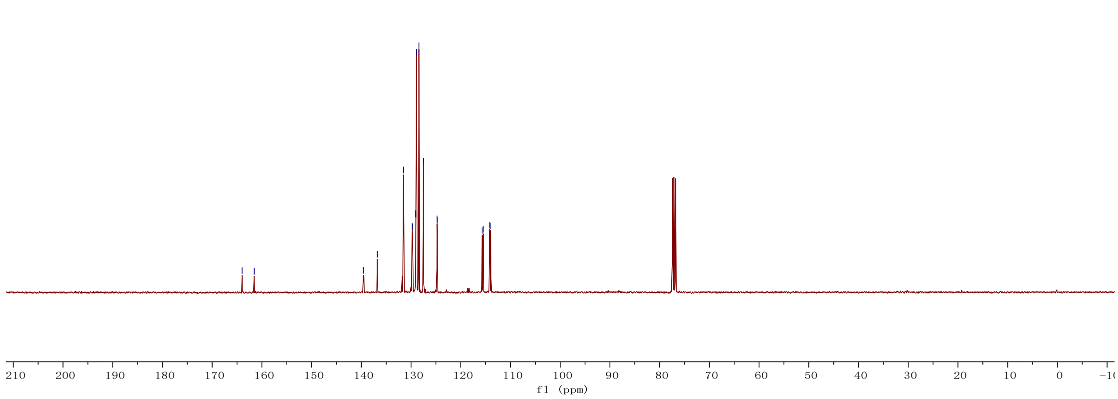

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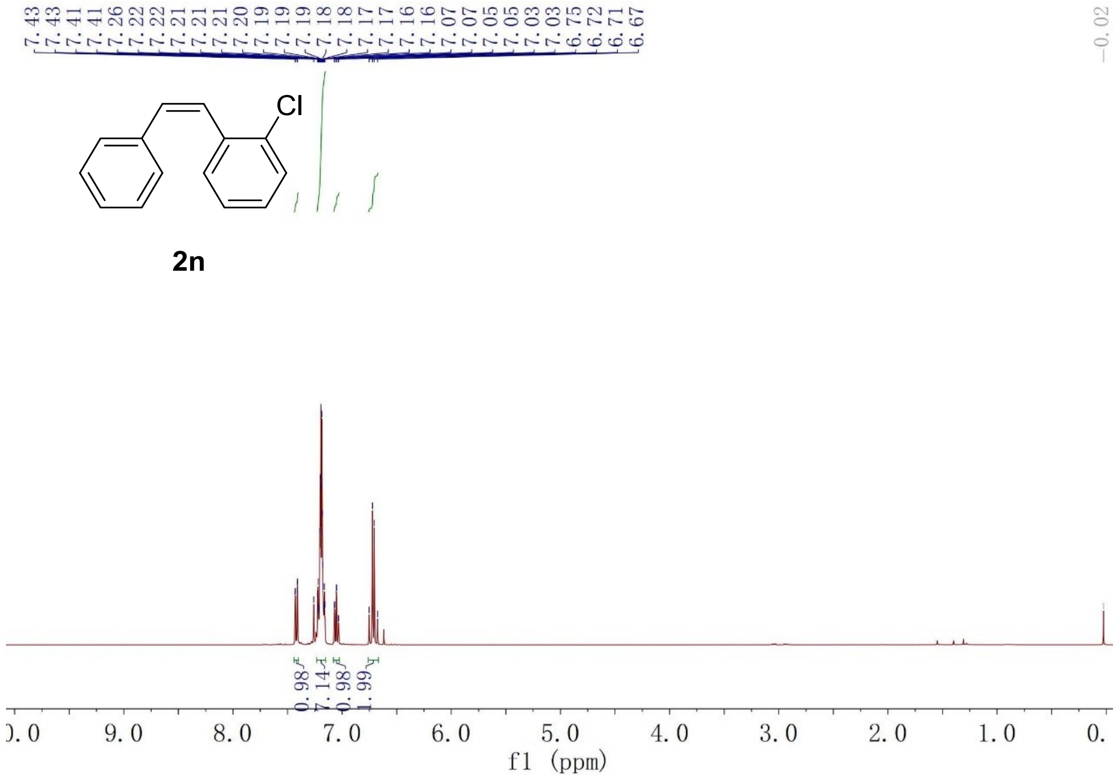
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Cl
2n
0.98
7.14
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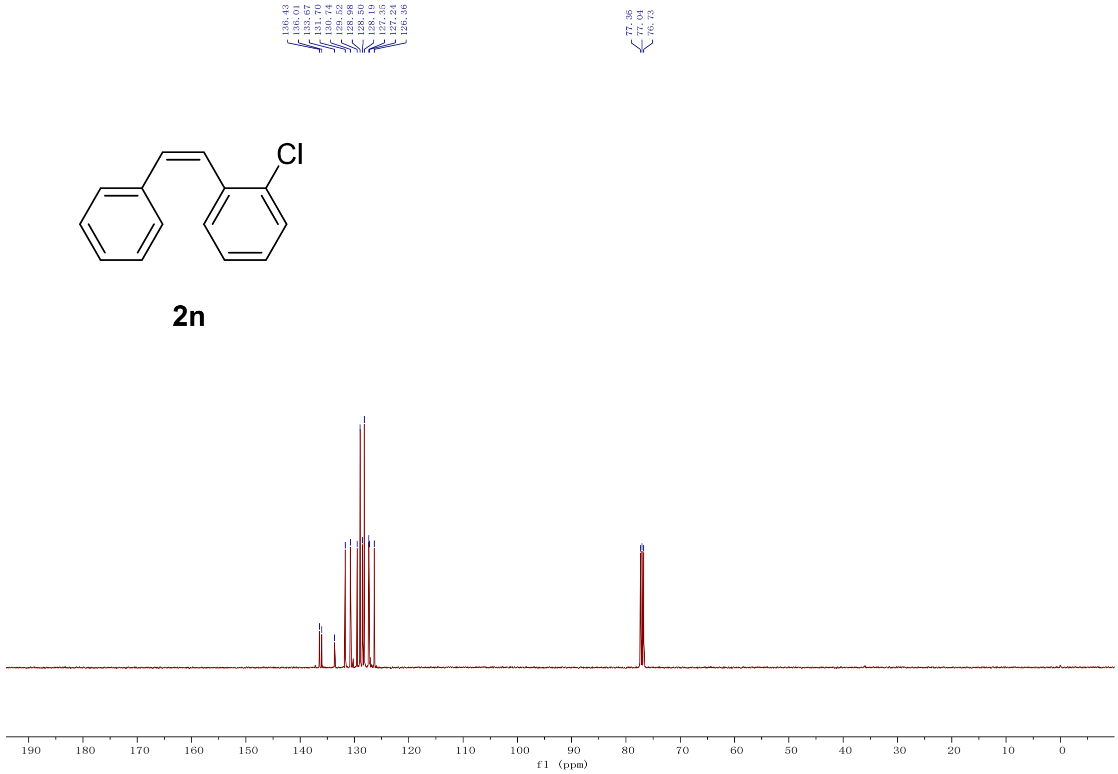
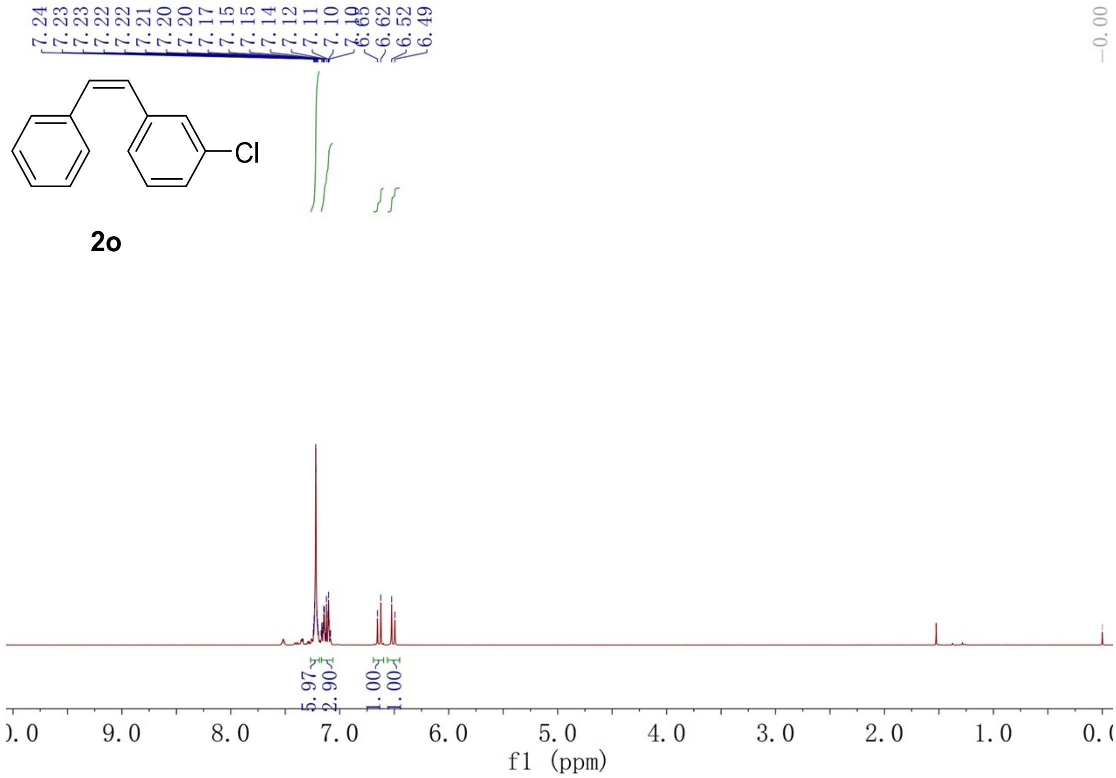
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


136.43 136.01 133.67 131.70 130.74 129.52 128.98 128.50 128.19 127.35 127.24 126.36
77.36 77.04 76.73
Cl
2n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



7.24
7.23
7.23
7.22
7.22
7.21
7.20
7.20
7.17
7.15
7.15
7.14
7.12
7.11
7.10
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6.52
6.49
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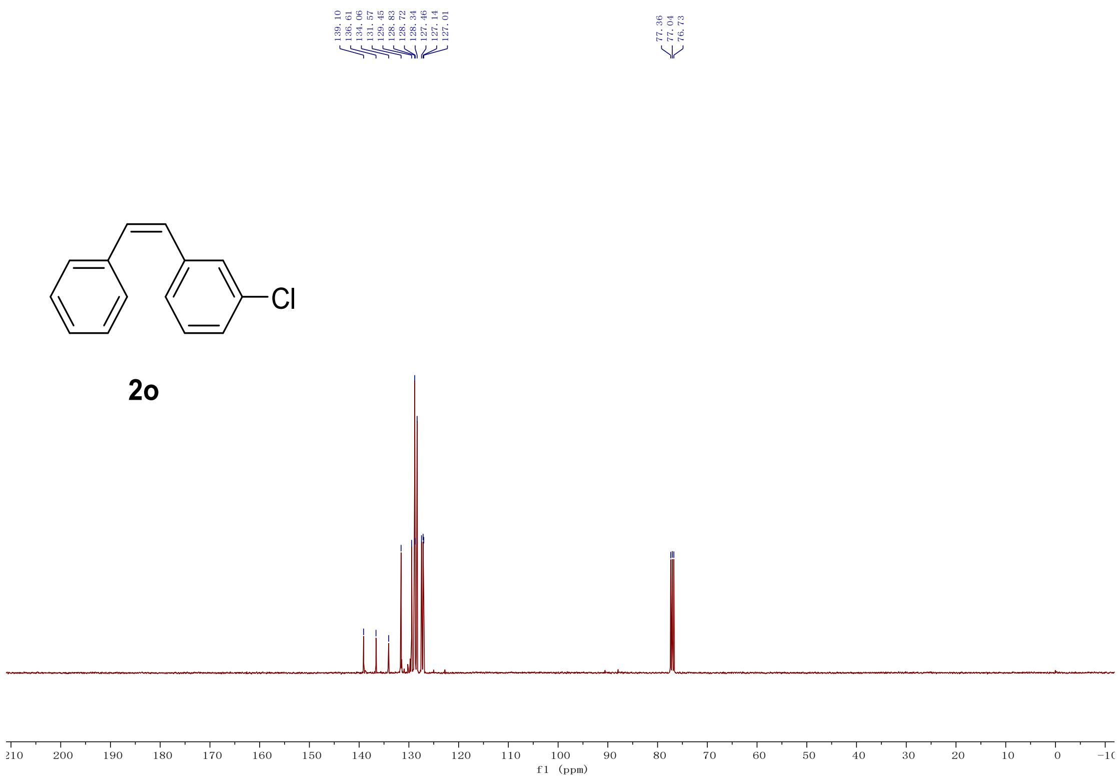
Cl
2o
5.97
2.90
1.00
1.00
f1 (ppm)



139.10
136.61
134.06
131.57
129.45
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128.34
127.46
127.14
127.01
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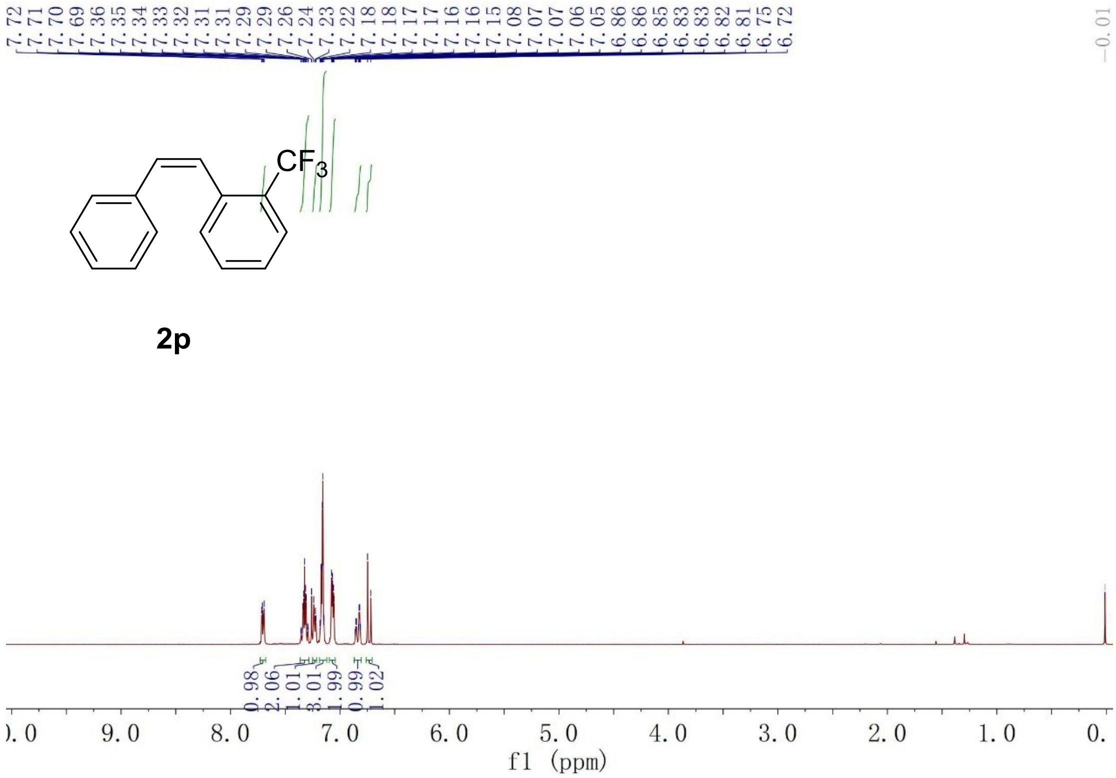
77.04
76.73
Cl
2o
f1 (ppm)



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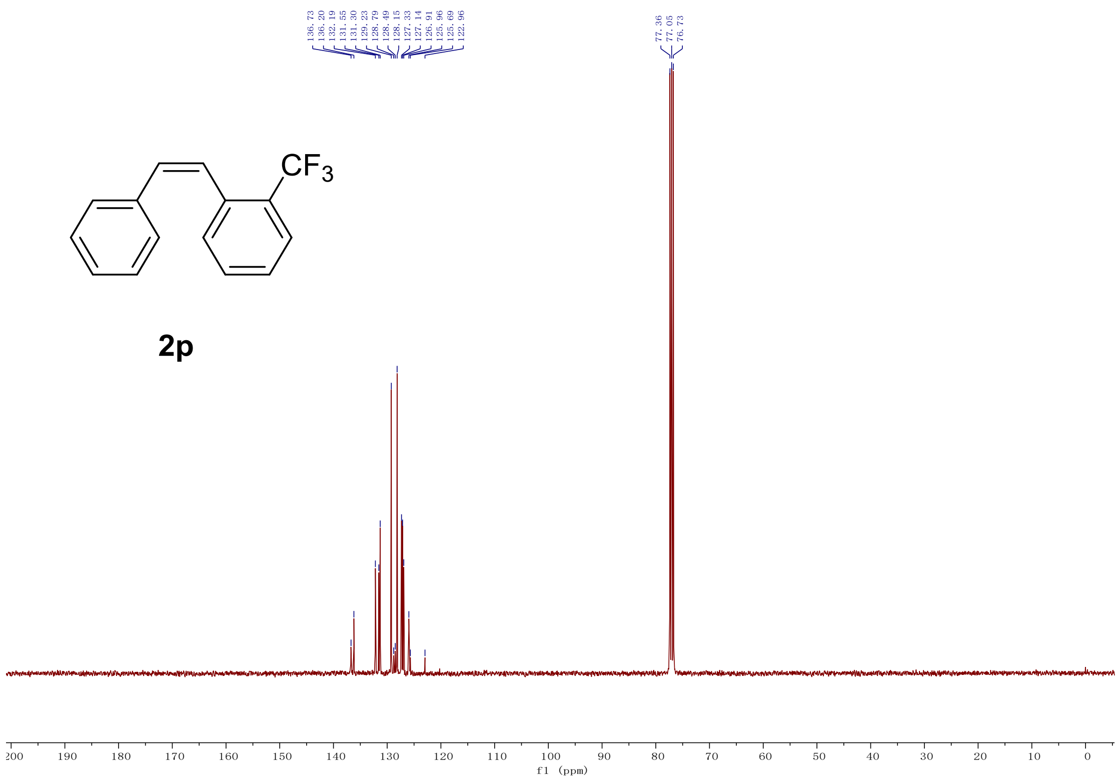

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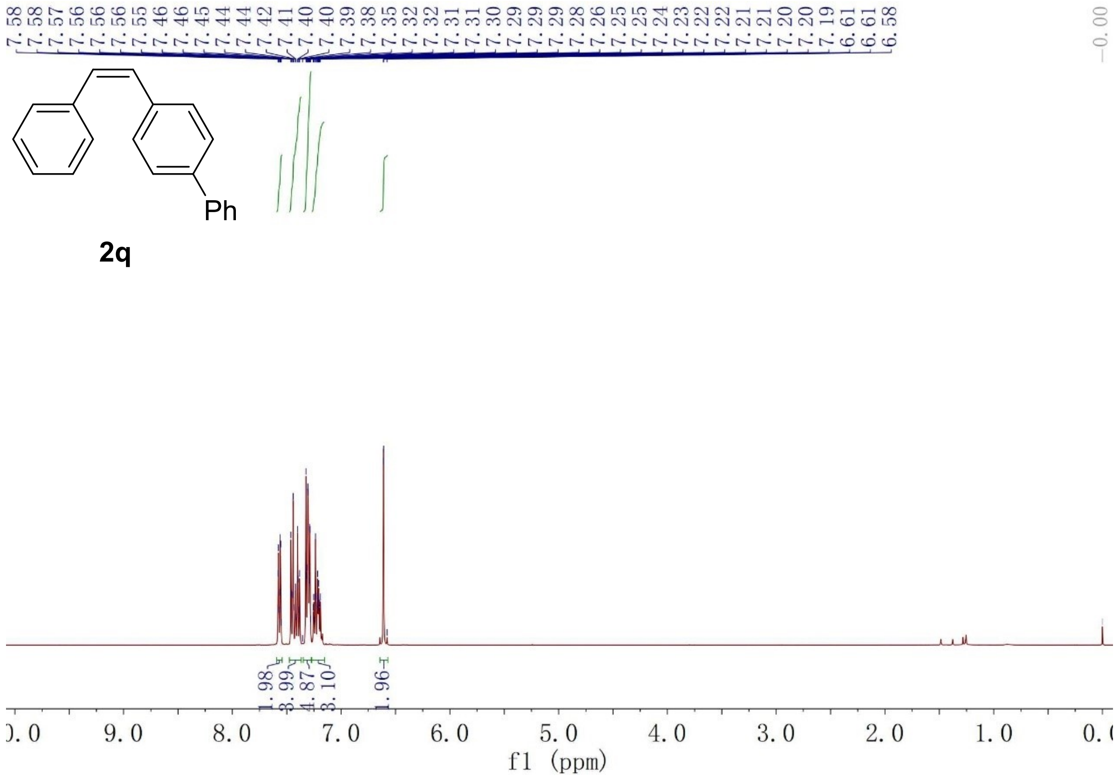
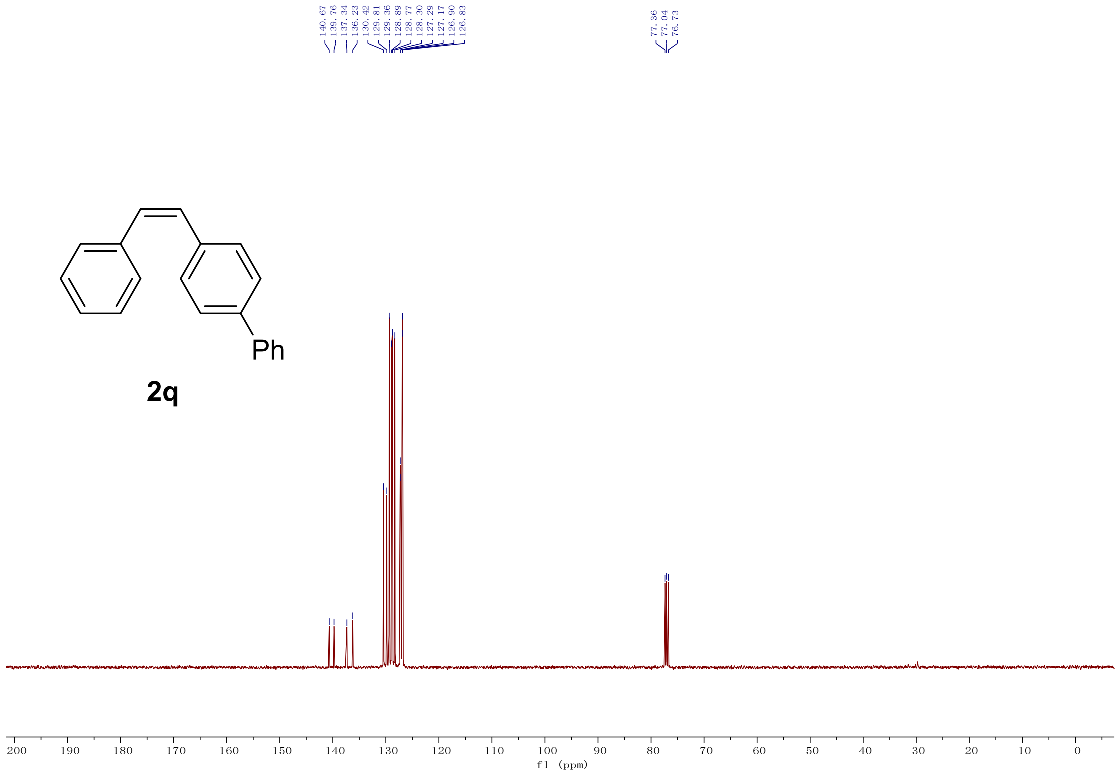
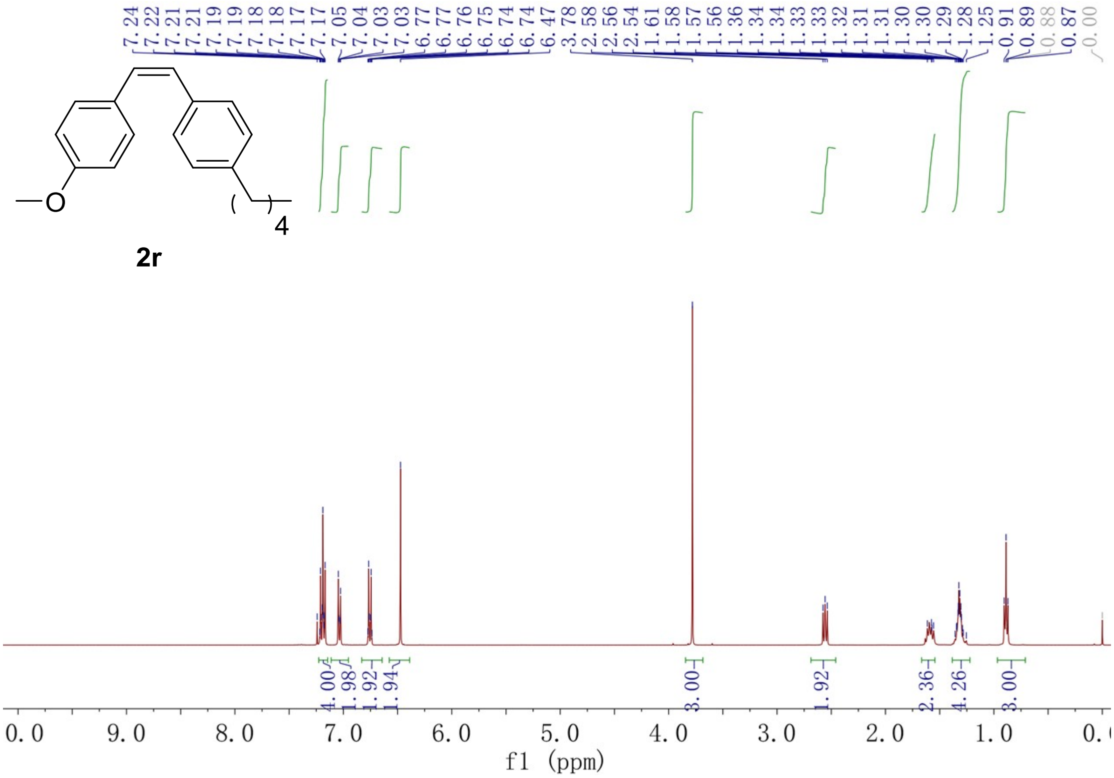
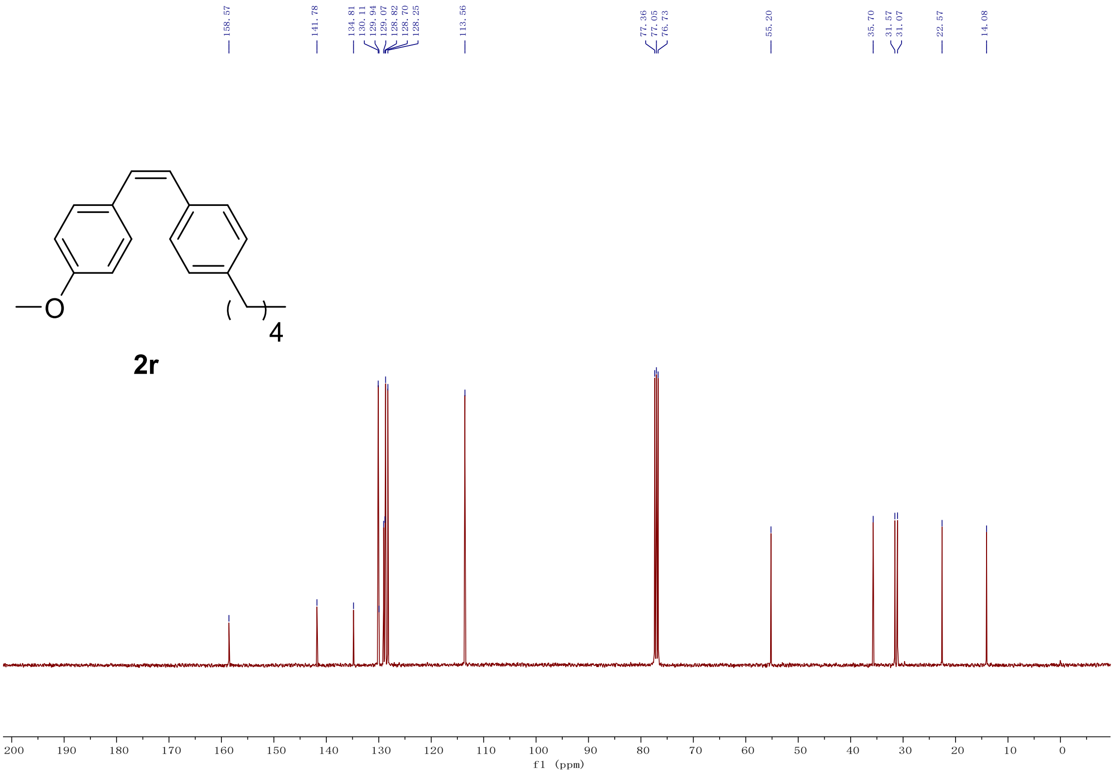

Ph
2q
f1 (ppm)


Ph
2q
f1 (ppm)


2r
f1 (ppm)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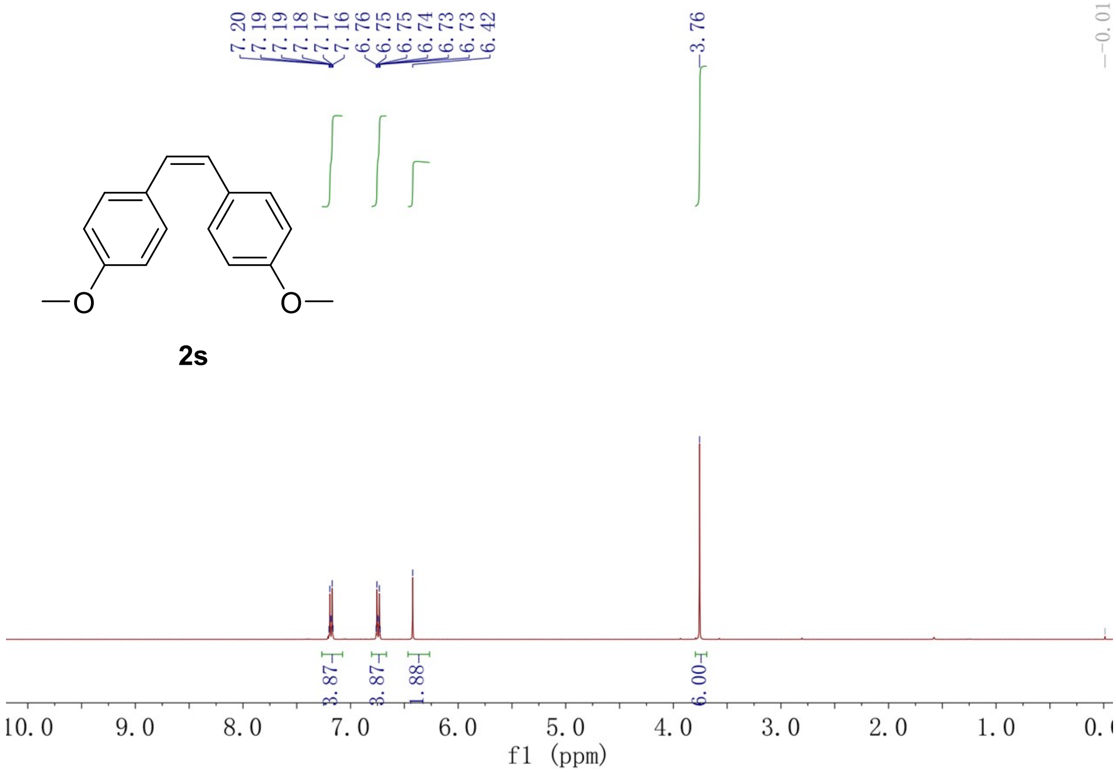
f1 (ppm)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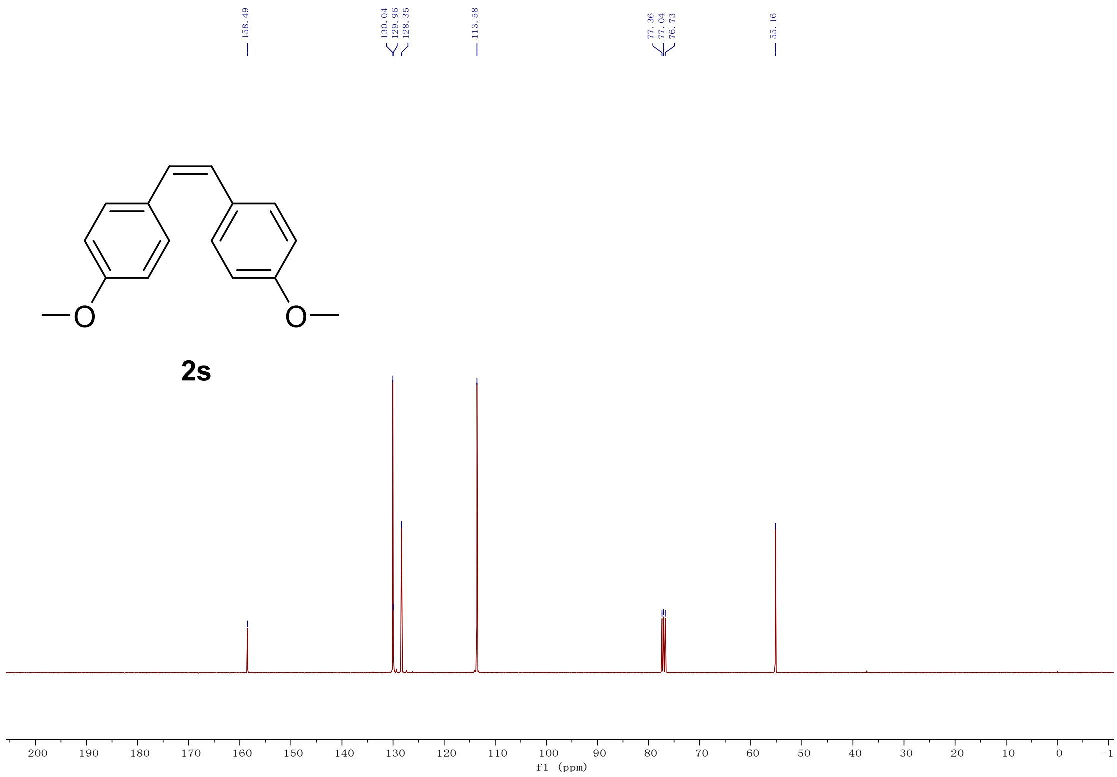
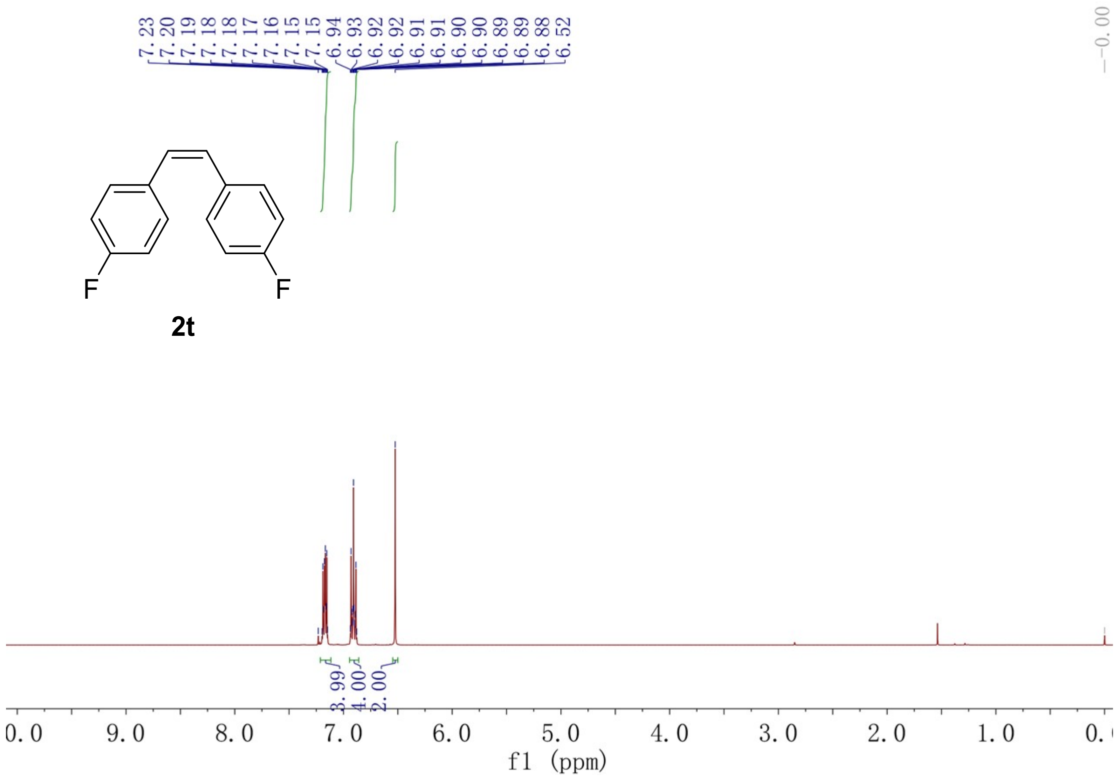
7.19
7.19
7.18
7.17
7.16
6.76
6.75
6.75
6.74
6.73
6.73
6.42
3.76
-0.01
2s
3.87
3.87
1.88
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


158.49
130.04
129.96
128.35
113.58
77.36
77.04
76.73
55.16
2s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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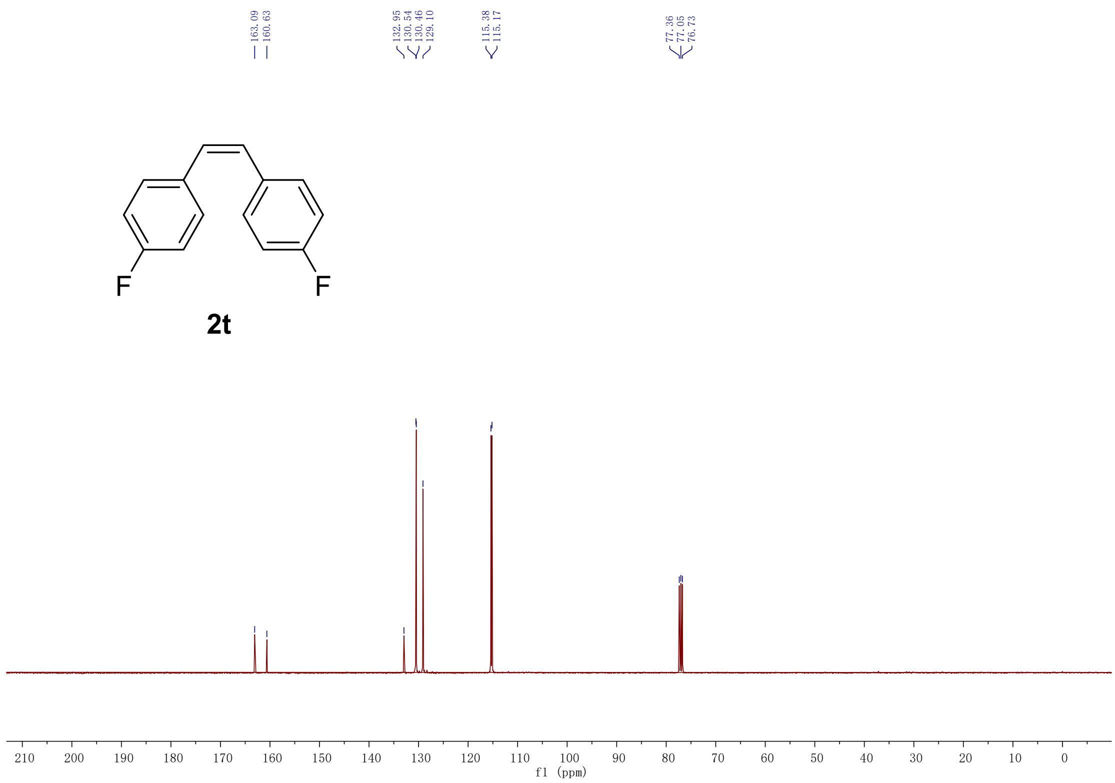
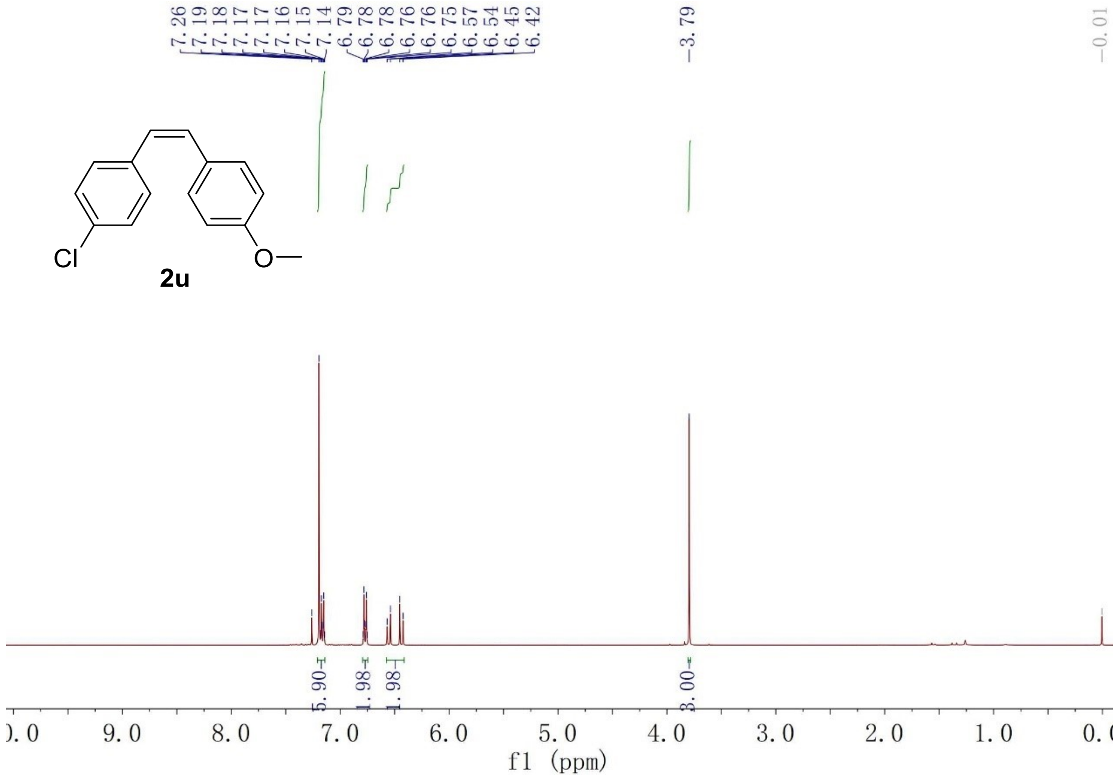
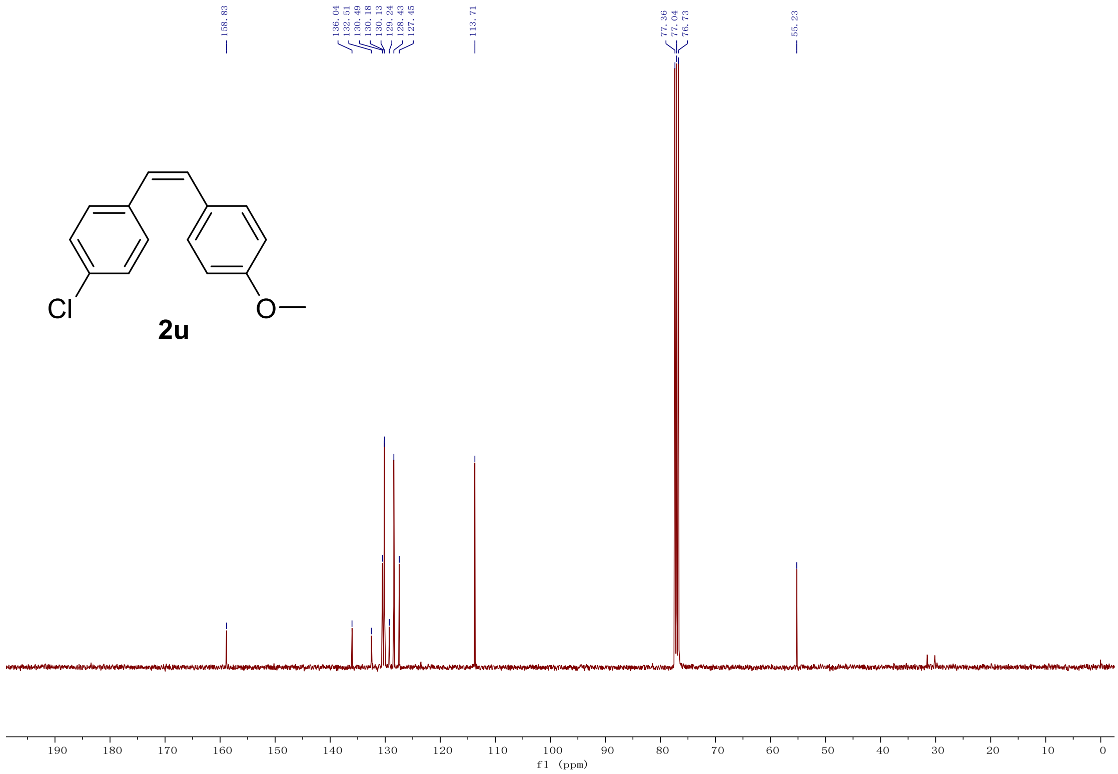
0.00
F
F
2t
3.99
4.00
2.00
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)


163.09 160.63
132.95 130.54 130.46 129.10
115.38 115.17
77.36 77.05 76.73
F
F
2t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.26
7.19
7.18
7.17
7.17
7.16
7.15
7.14
6.79
6.78
6.78
6.76
6.76
6.75
6.57
6.54
6.45
6.42
3.79
-0.01
Cl
O
2u
5.90
1.98
1.98
3.00
f1 (ppm)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130.49
130.18
130.13
129.24
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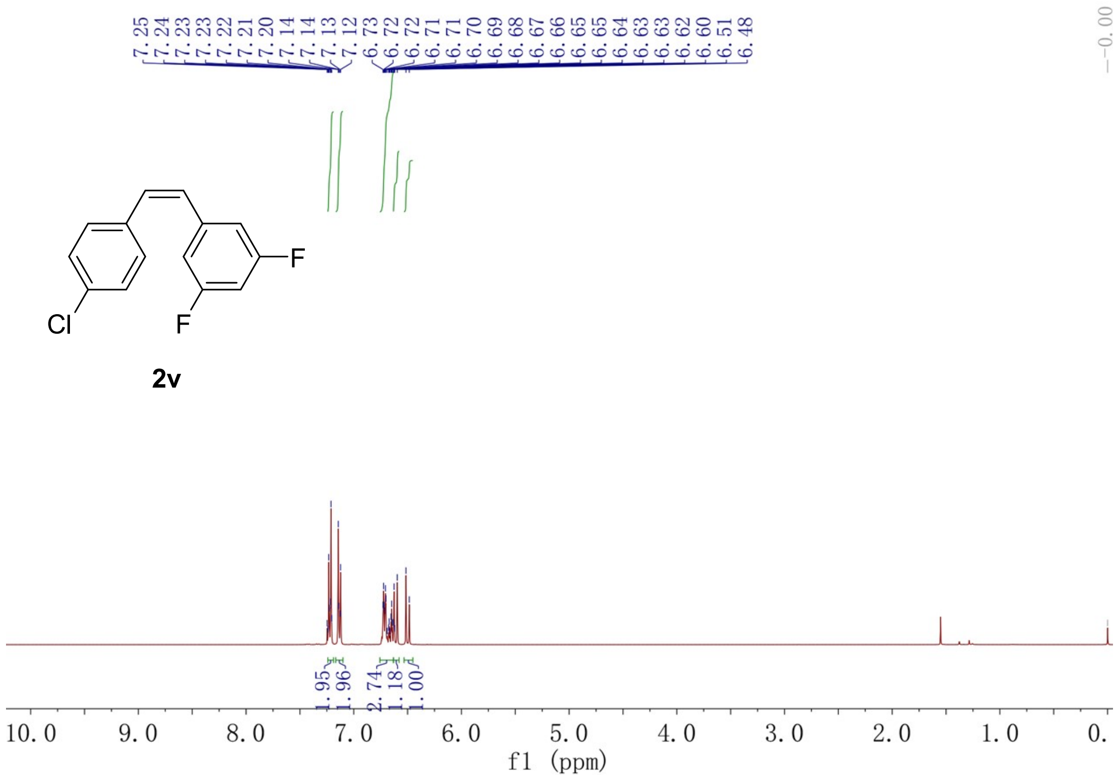
127.45
113.71
77.36
77.04
76.73
55.23
Cl
O
2u
f1 (ppm)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7.14
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7.13
7.12
6.73
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6.72
6.71
6.71
6.70
6.69
6.68
6.67
6.66
6.65
6.65
6.64
6.63
6.63
6.62
6.60
6.51
6.48
0.00
Cl
F
F
2v
1.95
1.96
2.74
1.18
1.00
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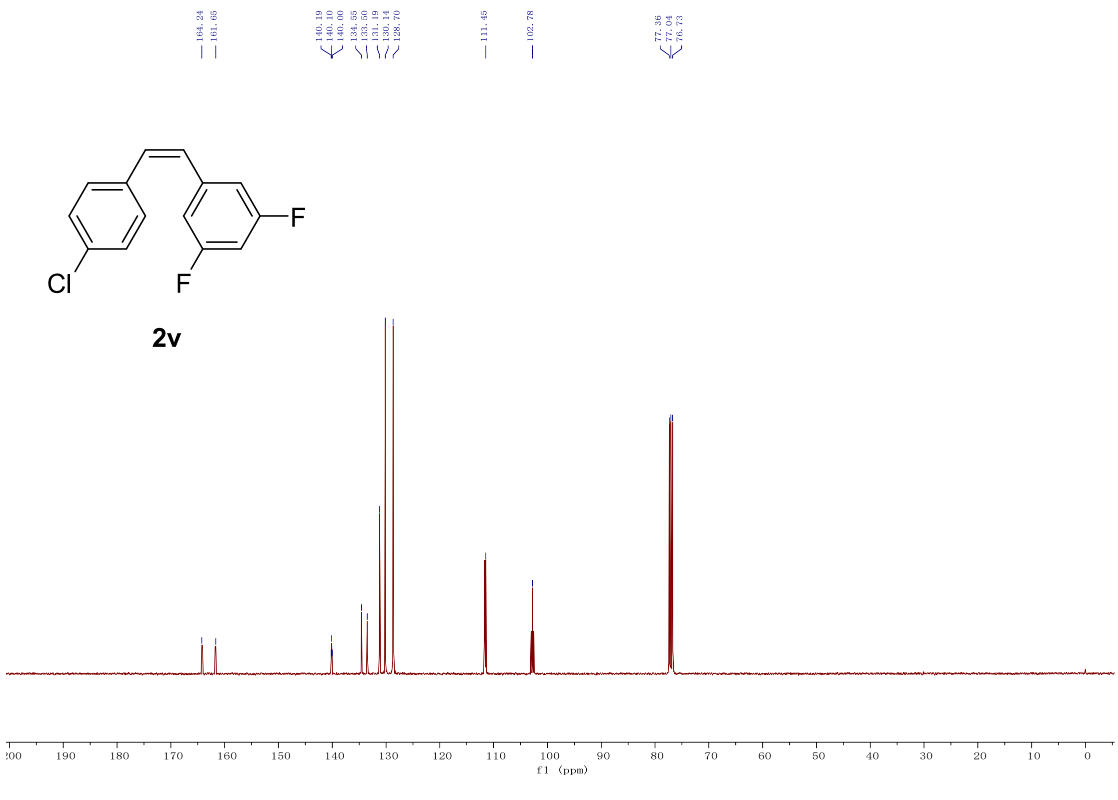
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.
f1 (ppm)


164.24
161.65
140.19
140.10
140.00
134.55
133.50
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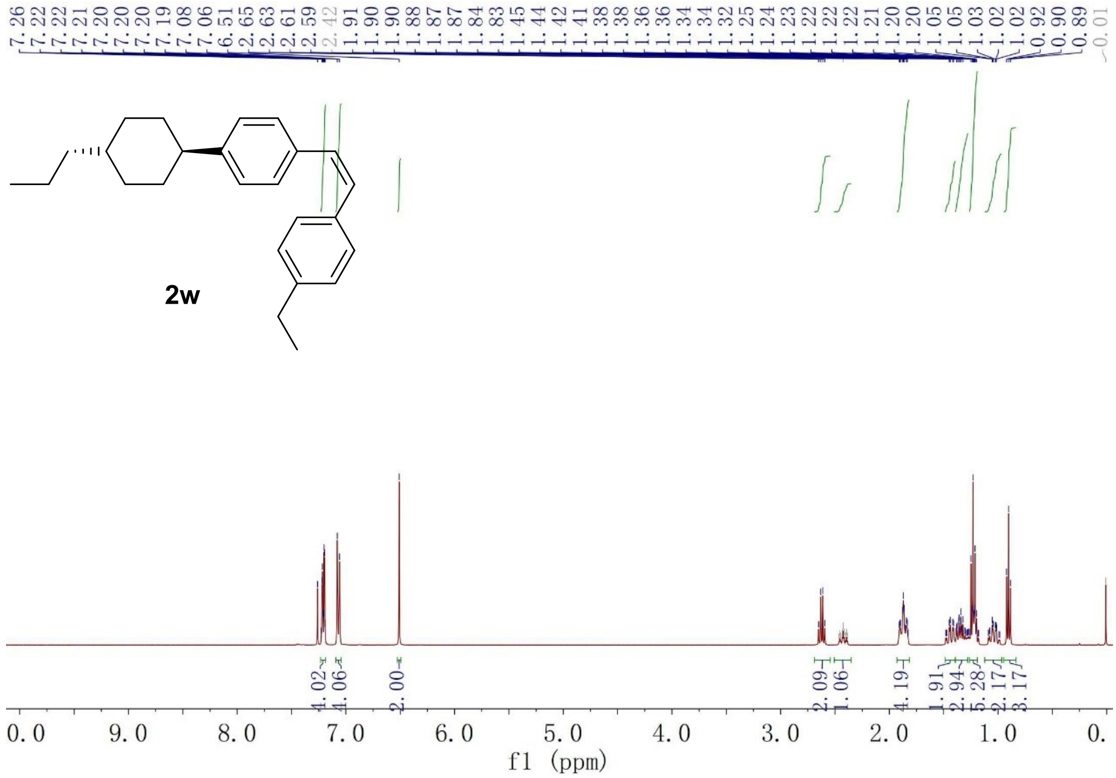
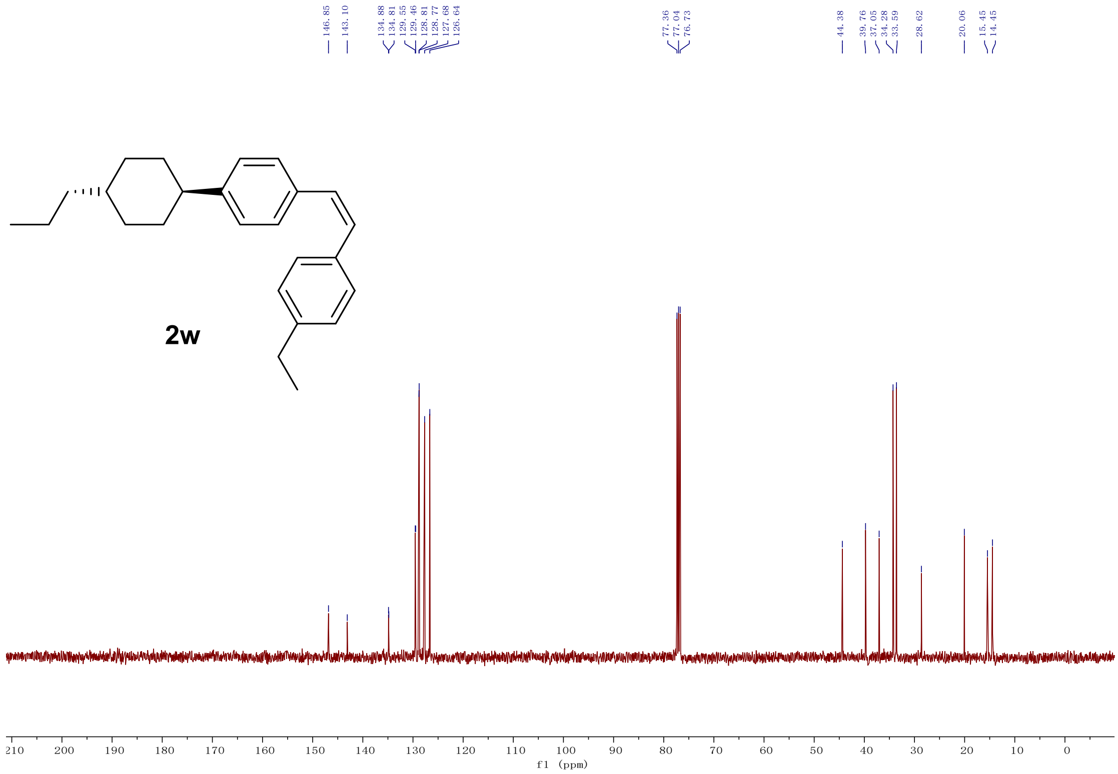
130.14
128.70
111.45
102.78
77.36
77.04
76.73
Cl
F
F
2v
f1 (ppm)


7.26 7.22 7.22 7.21 7.21 7.20 7.20 7.20 7.19 7.08 7.06 6.51 2.65 2.63 2.61 2.59 2.42 1.91 1.90 1.90 1.88 1.87 1.87 1.84 1.83 1.45 1.44 1.42 1.41 1.38 1.38 1.36 1.36 1.34 1.34 1.32 1.25 1.24 1.23 1.22 1.22 1.22 1.21 1.20 1.20 1.05 1.05 1.03 1.02 1.02 0.92 0.90 0.89 0.01
2w
4.02 4.06 2.00 2.09 1.06 4.19 1.91 2.94 5.28 2.17 3.17
0.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.
f1 (ppm)


146.85 143.10 134.88 134.81 129.55 129.46 128.81 128.77 127.68 126.64 77.36 77.04 76.73 44.38 39.76 37.05 34.28 33.59 28.62 20.06 15.45 14.45
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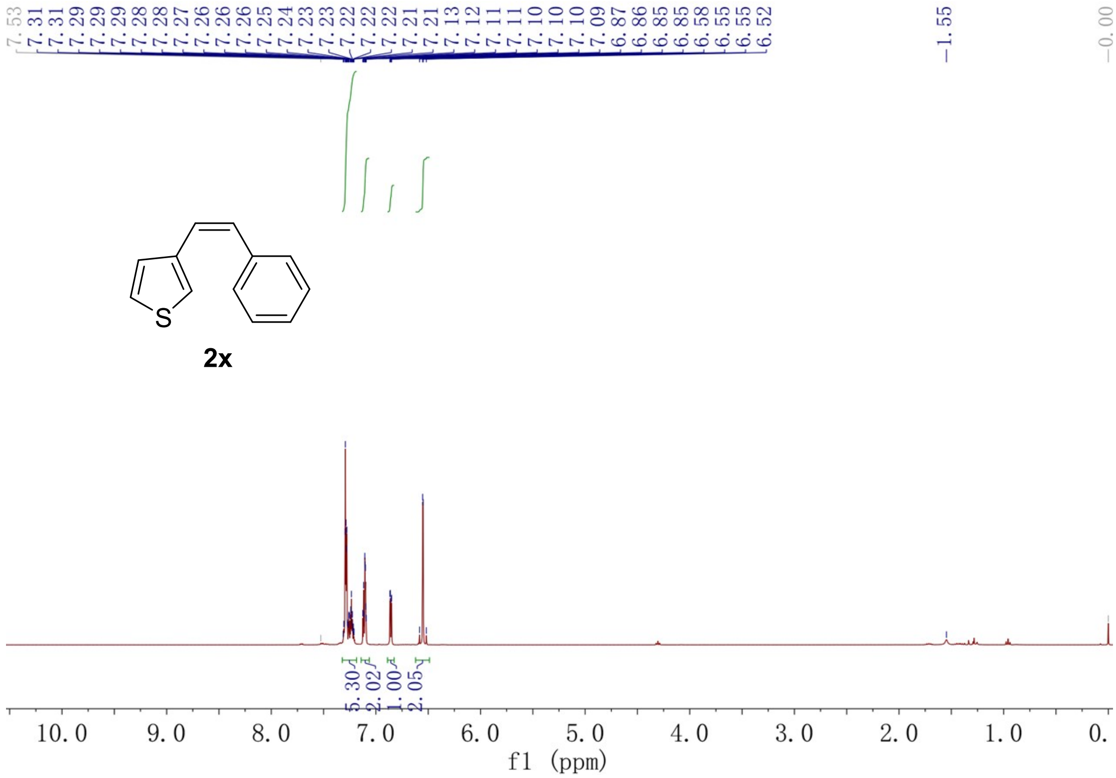
f1 (ppm)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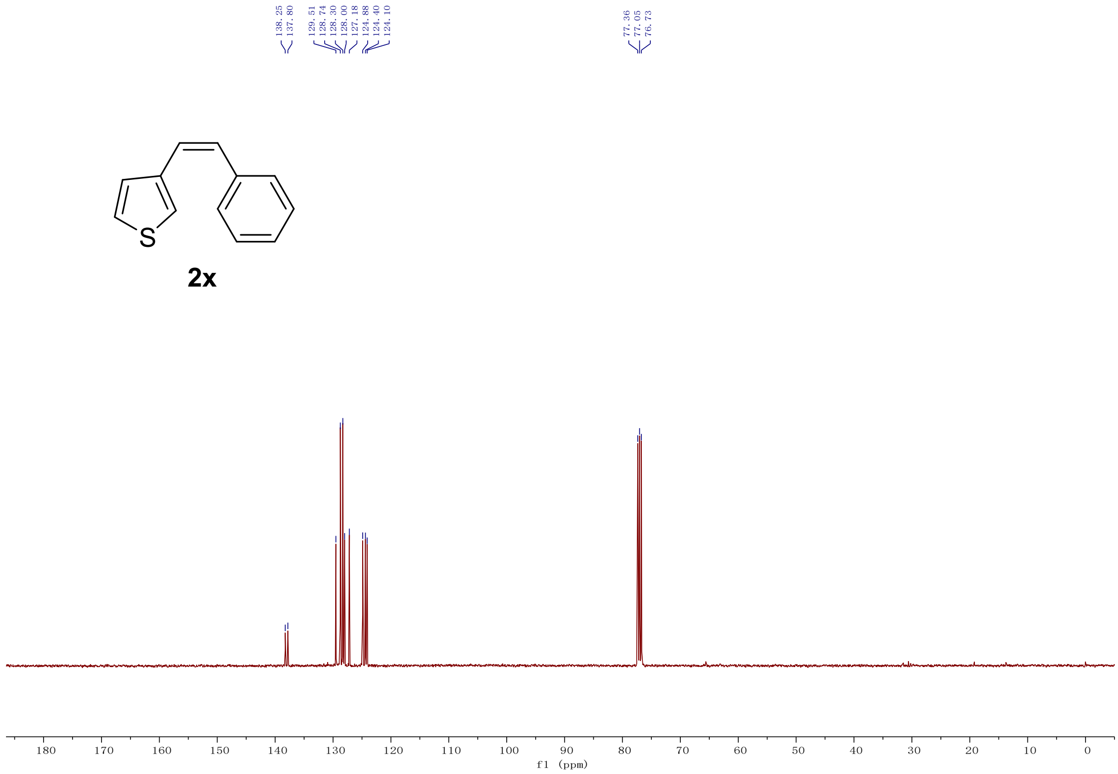
1.55
0.00
5.30
2.02
1.00
2.05
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.
f1 (ppm)

2x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77.36 77.05 76.73
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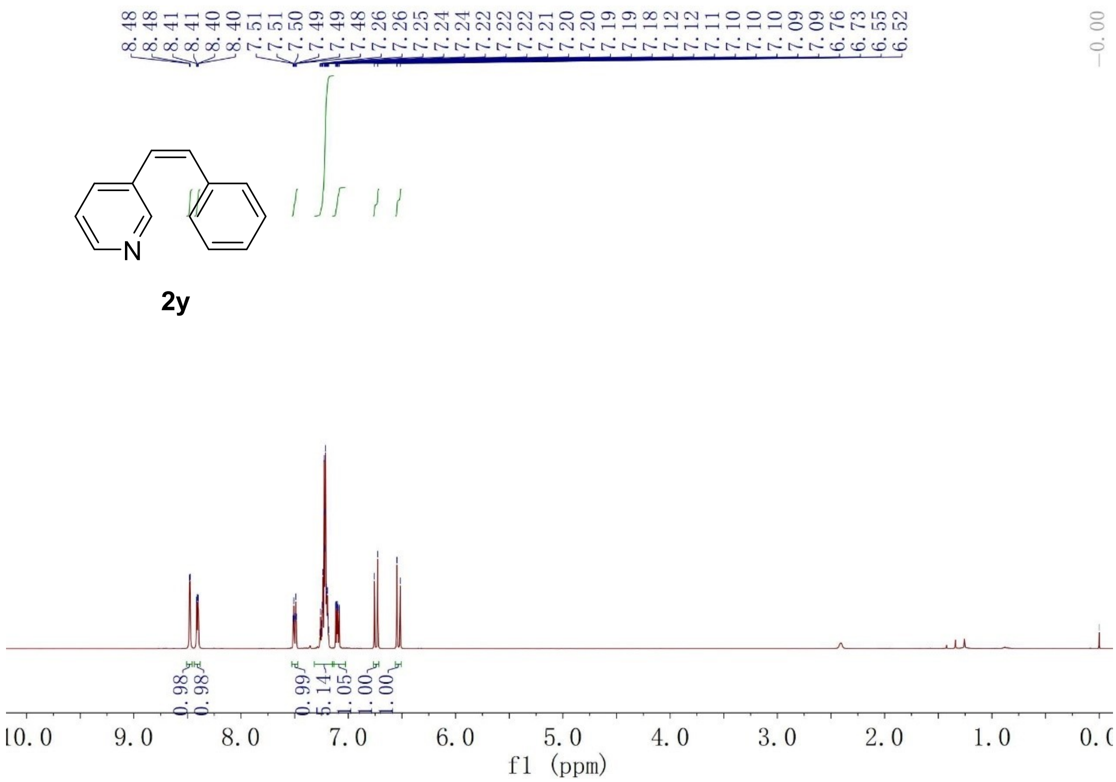
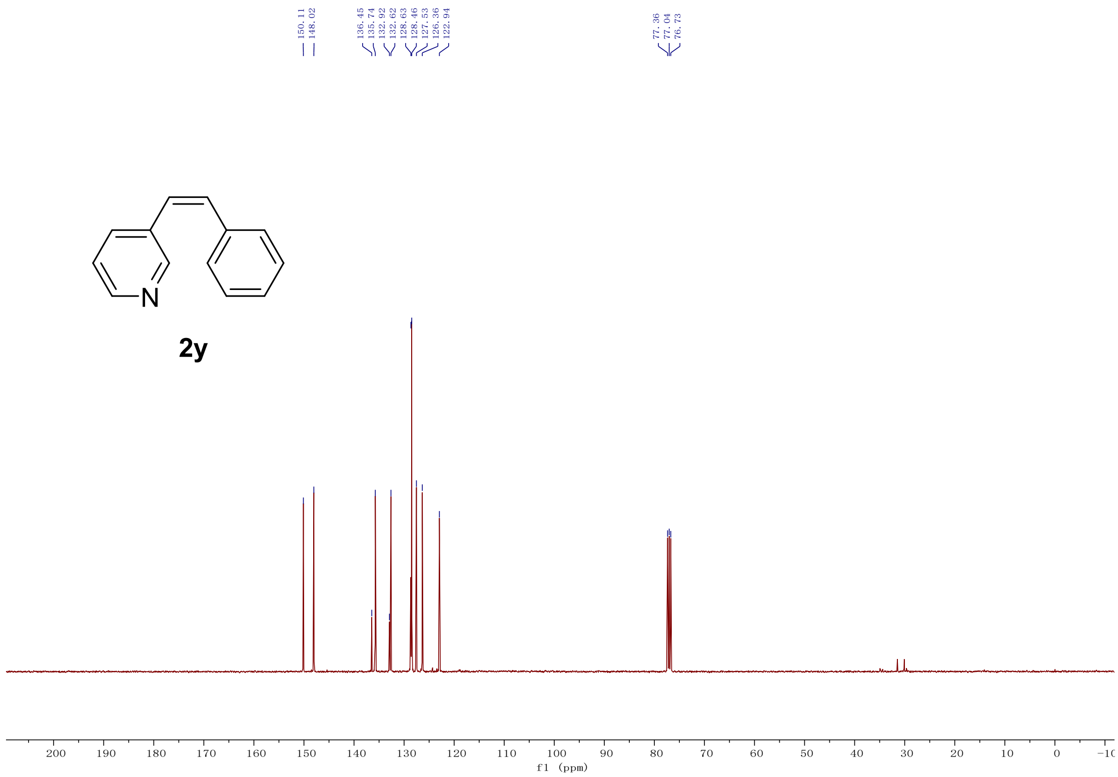
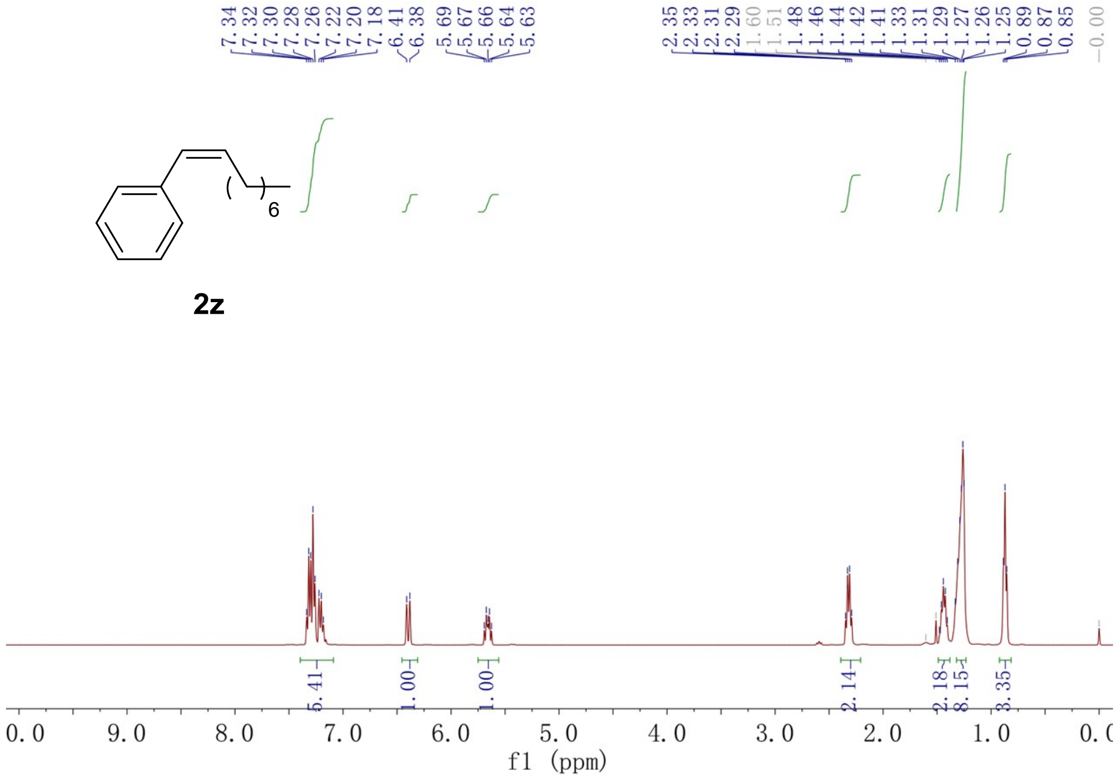
f1 (ppm)

2x



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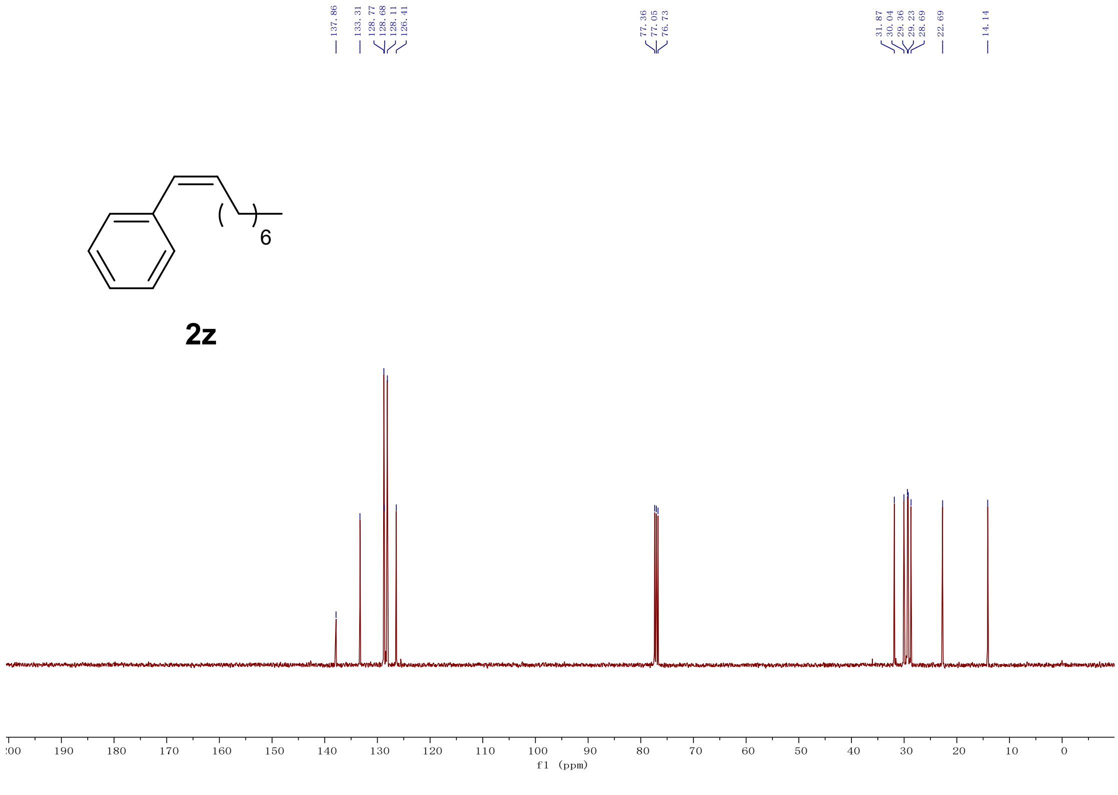
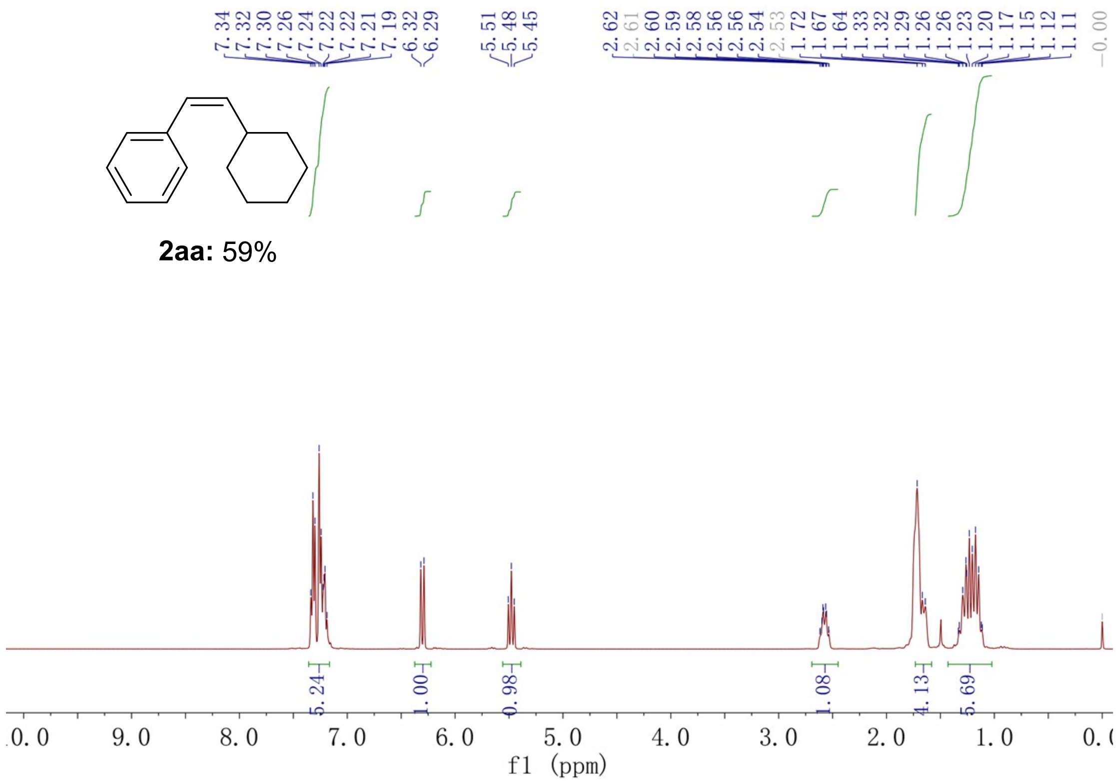
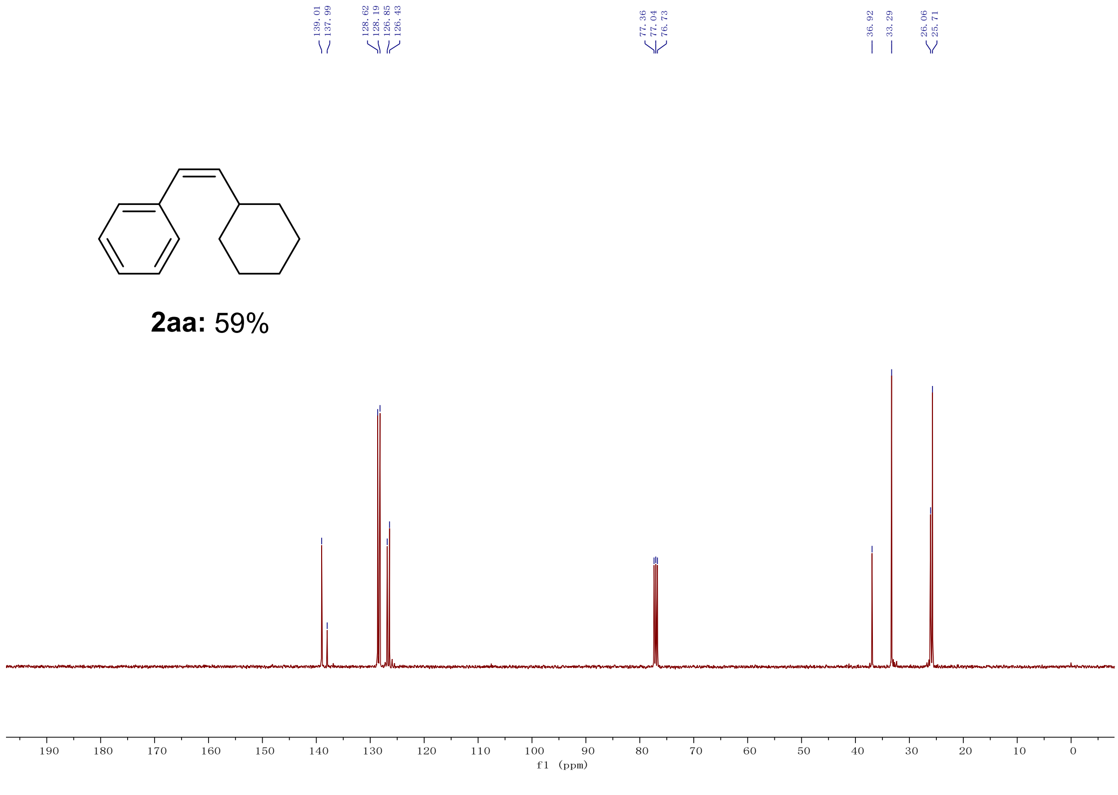
2.35 2.33 2.31 2.29 1.60 1.51 1.48 1.46 1.44 1.42 1.41 1.33 1.31 1.29 1.27 1.26 1.25 0.89 0.87 0.85 0.00
6
2z
5.41 1.00 1.00 2.14 2.18 8.15 3.35
f1 (ppm)


137.86 133.31 128.77 128.68 128.11 126.41
77.36 77.05 76.73
31.87 30.04 29.36 29.23 28.69 22.69 14.14
6
2z
f1 (ppm)


7.34 7.32 7.30 7.26 7.24 7.22 7.22 7.21 7.19 6.32 6.29
5.51 5.48 5.45
2.62 2.61 2.60 2.59 2.58 2.56 2.56 2.54 2.53 1.72 1.67 1.64 1.33 1.32 1.29 1.26 1.26 1.23 1.20 1.17 1.15 1.12 1.11
0.00
5.24 1.00 0.98 1.08 4.13 5.69
f1 (ppm)

2aa: 59%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36.92 33.29 26.06 25.71
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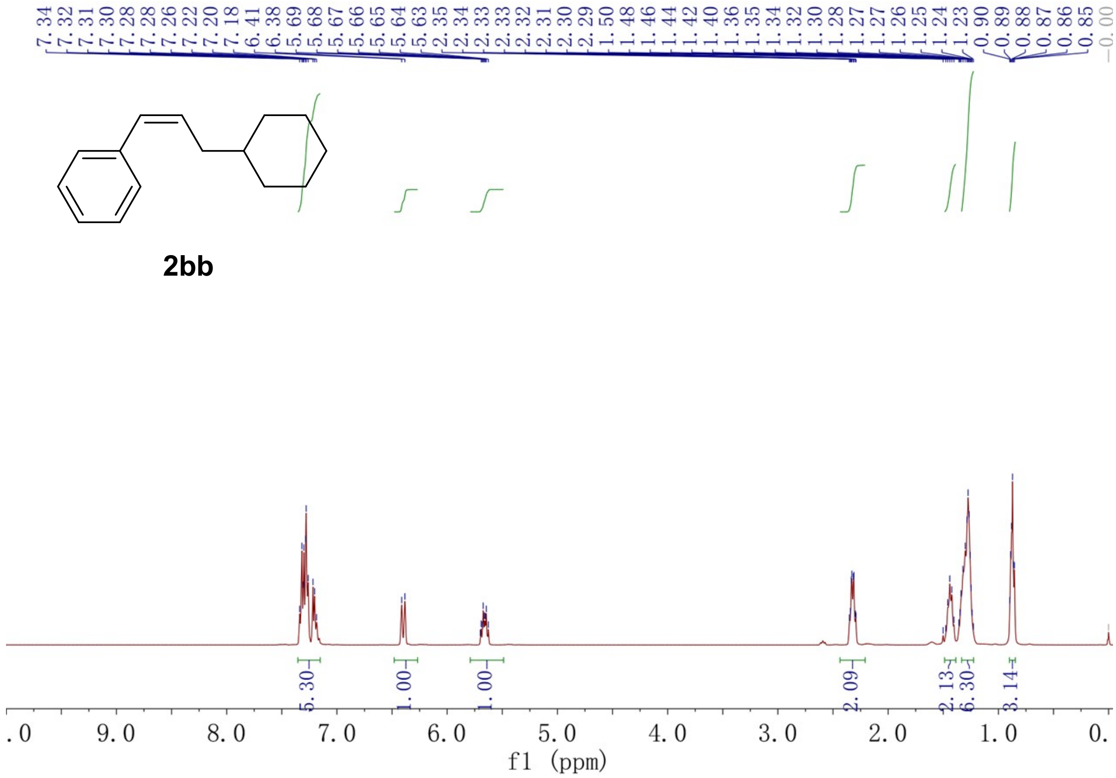
2aa: 59%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1.00
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2.13
6.30
3.14
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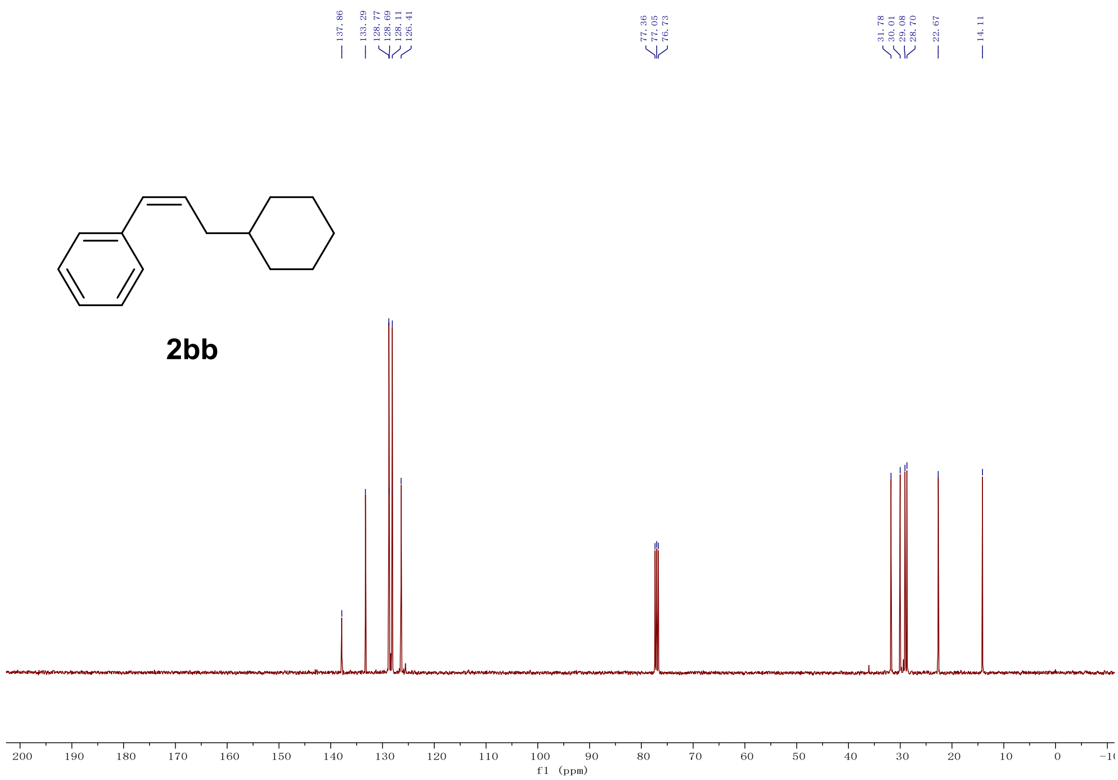
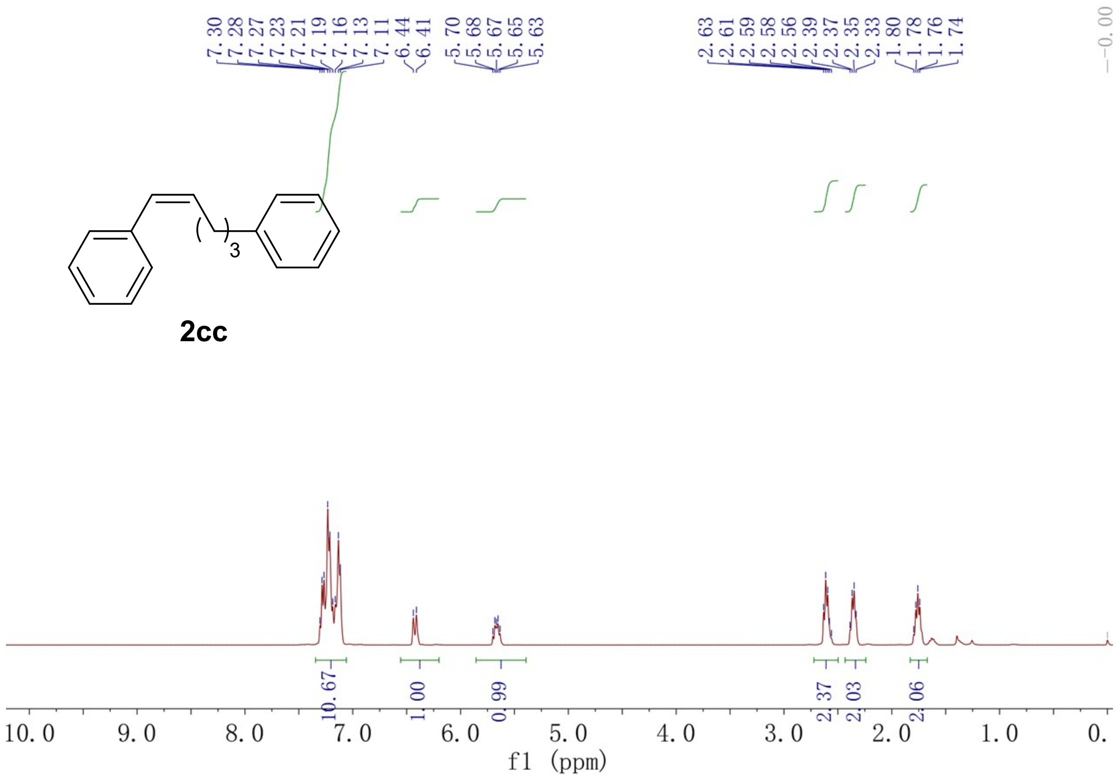

137.86 133.29 128.77 128.69 128.11 126.41
77.36 77.05 76.73
31.78 30.01 29.08 28.70 22.67 14.11
2bb
f1 (ppm)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7.13
7.11
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6.41
5.70
5.68
5.67
5.65
5.63
2.63
2.61
2.59
2.58
2.56
2.39
2.37
2.35
2.33
1.80
1.78
1.76
1.74
0.00
10.67
1.00
0.99
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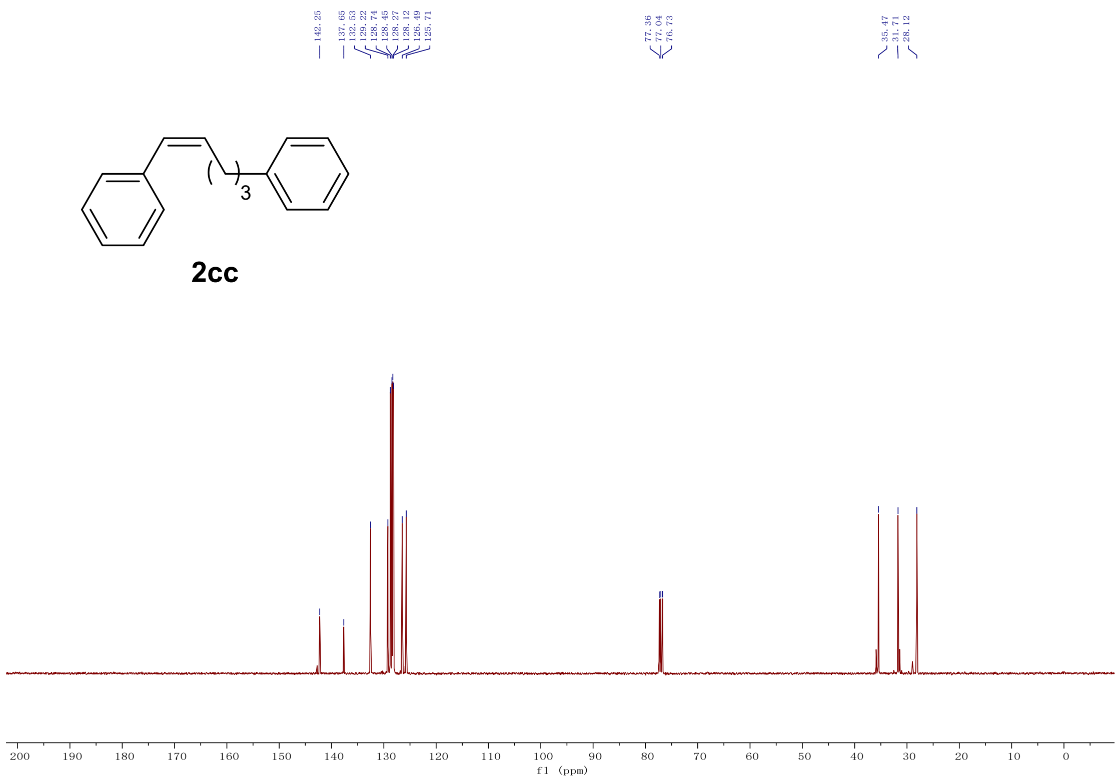
2.03
2.06
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.
f1 (ppm)

2cc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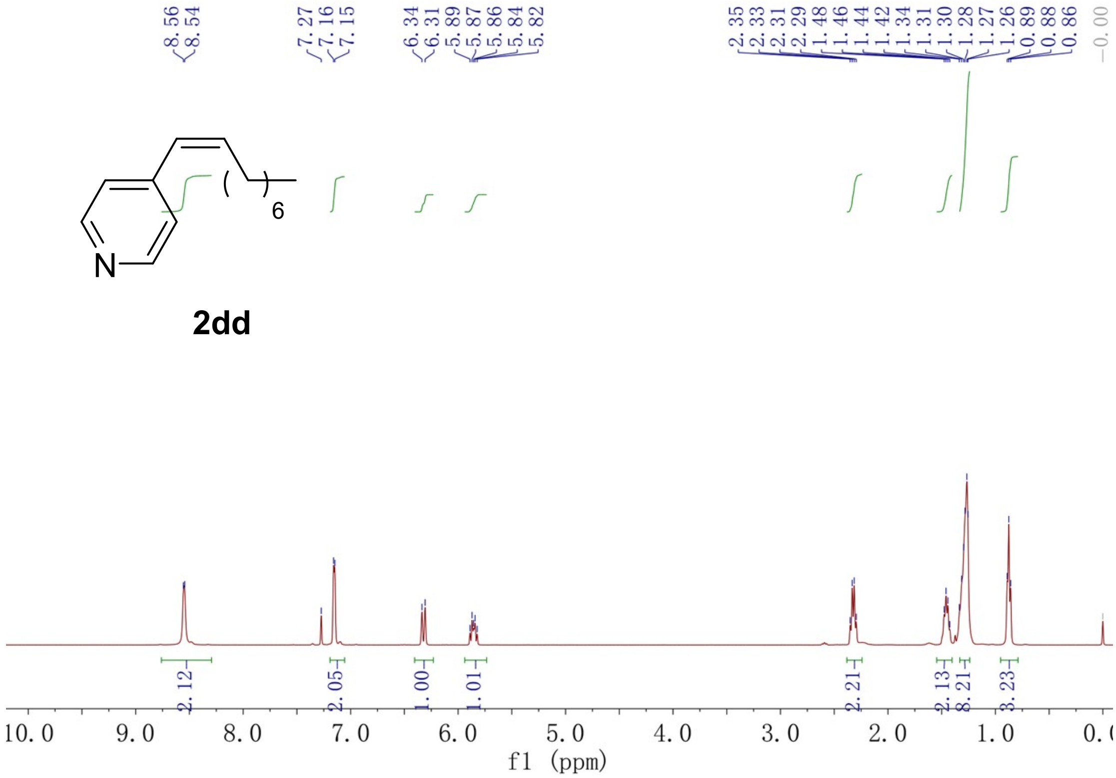
128.27
128.12
126.49
125.71
77.36
77.04
76.73
35.47
31.71
28.12
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2cc



8.56
8.54
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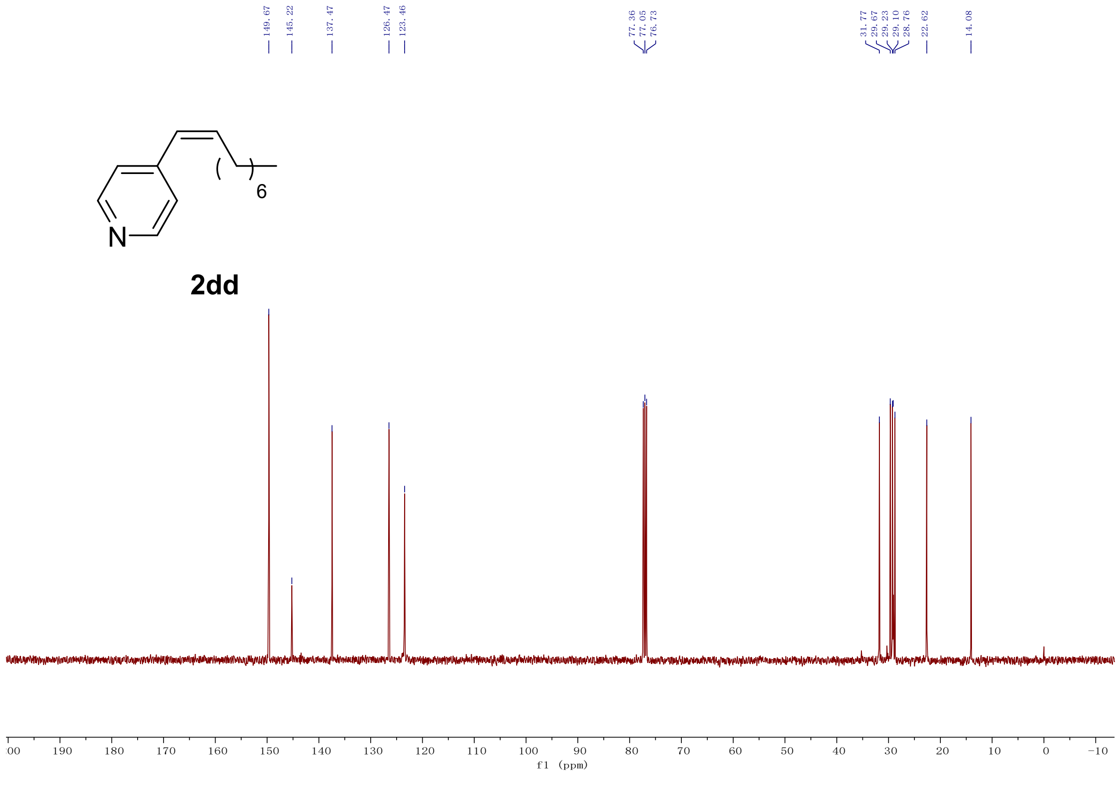
6.34
6.31
5.89
5.87
5.86
5.84
5.82
2.35
2.33
2.31
2.29
1.48
1.46
1.44
1.42
1.34
1.31
1.30
1.28
1.27
1.26
0.89
0.88
0.86
-0.00
N
6
2dd
2.12
2.05
1.00
1.01
2.21
2.13
8.21
3.23
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)



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77.05
76.73
31.77
29.67
29.23
29.10
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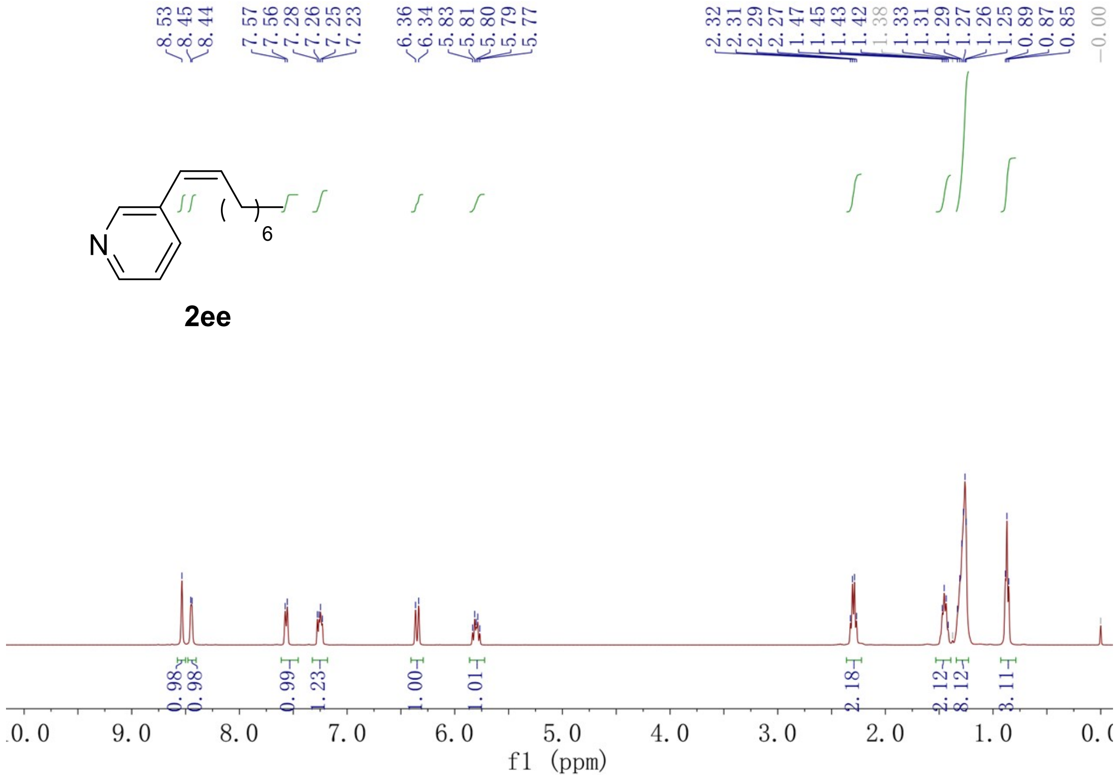
22.62
14.08
N
6
2dd
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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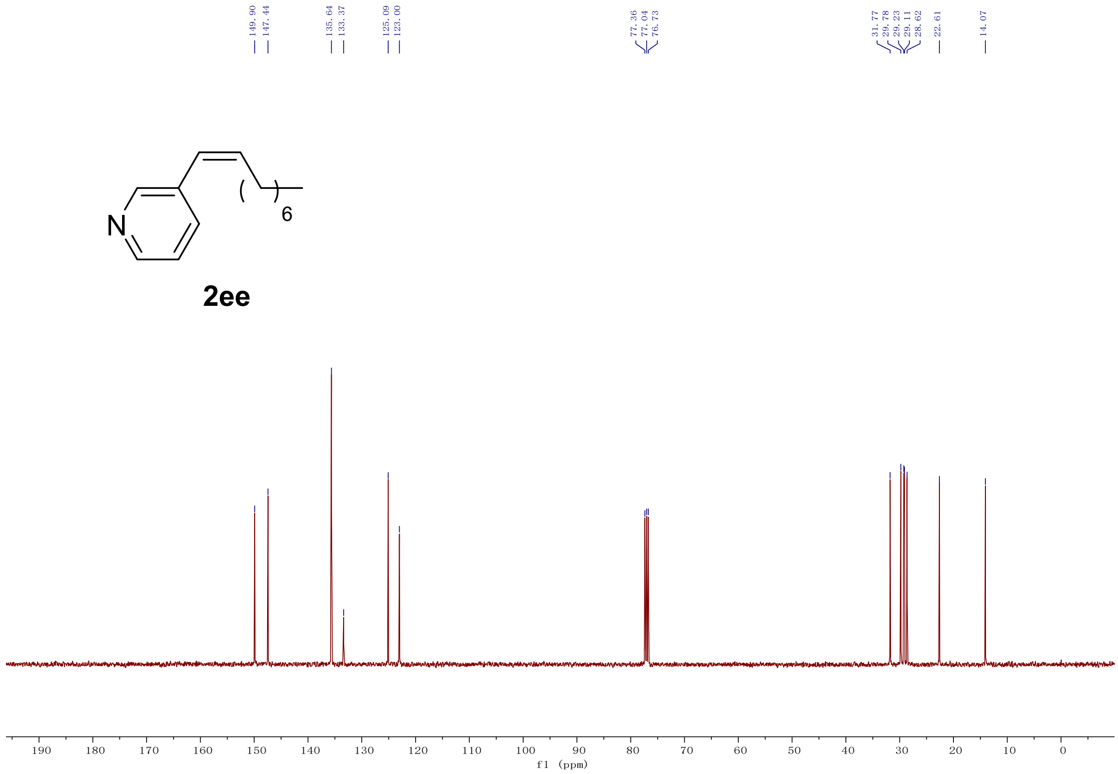
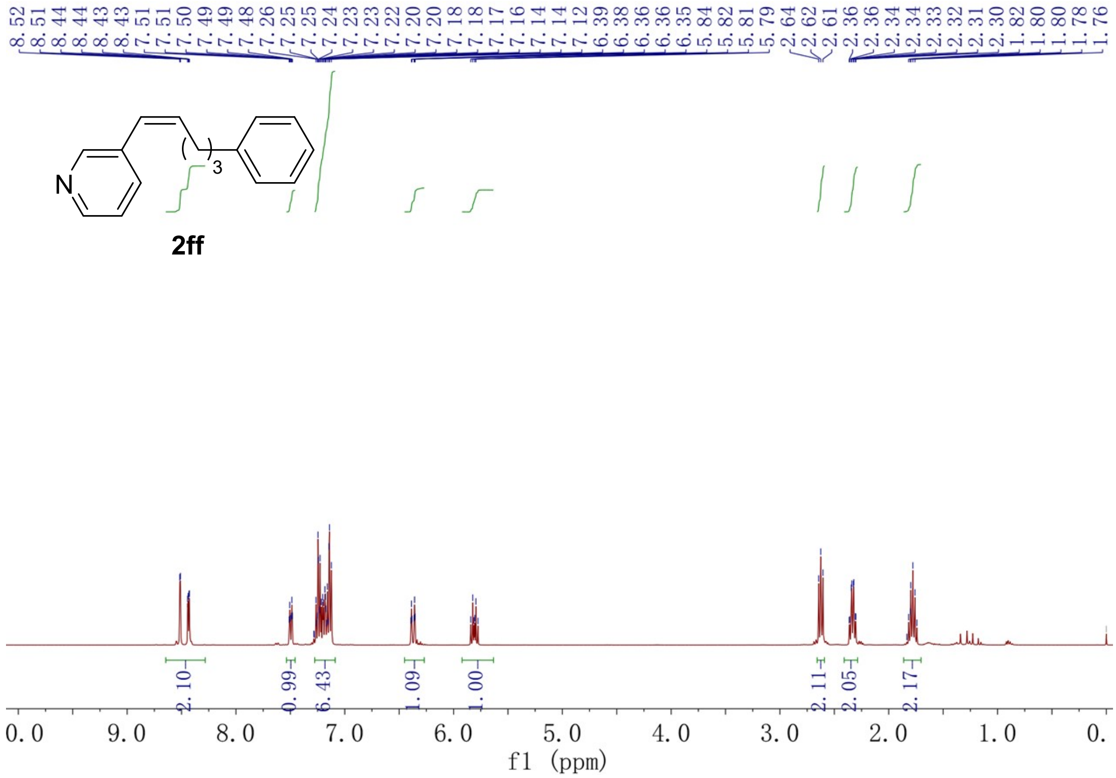
2ee
0.98 0.98 0.99 1.23 1.00 1.01 2.18 2.12 8.12 3.11
f1 (ppm)


149.90 147.44 135.64 133.37 125.09 123.00 77.36 77.04 76.73 31.77 29.78 29.23 29.11 28.62 22.61 14.07
N
6
2ee
f1 (ppm)


8.52 8.51 8.44 8.44 8.43 8.43 7.51 7.51 7.50 7.49 7.49 7.48 7.26 7.25 7.25 7.24 7.23 7.23 7.22 7.20 7.20 7.18 7.18 7.17 7.16 7.14 7.14 7.12 6.39 6.38 6.36 6.36 6.35 5.84 5.82 5.81 5.79 2.64 2.62 2.61 2.36 2.36 2.34 2.34 2.33 2.32 2.31 2.30 1.82 1.80 1.80 1.78 1.76
N
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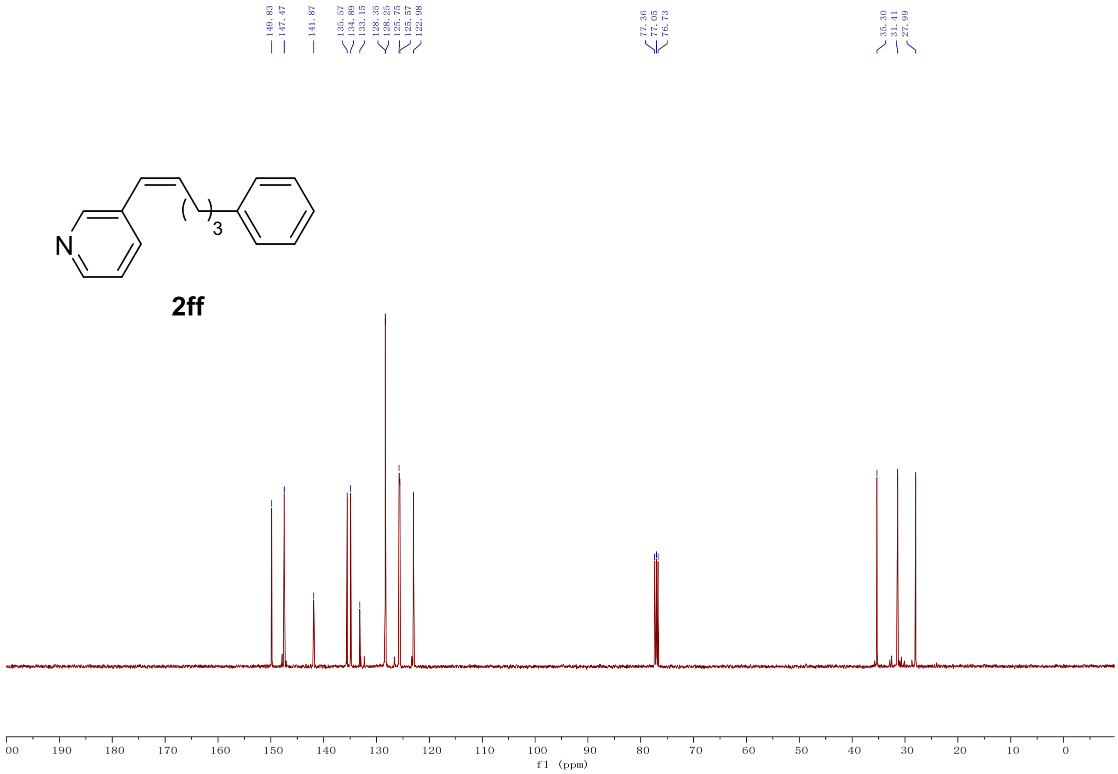
2ff
2.10
0.99
6.43
1.09
1.00
2.11
2.05
2.17
f1 (ppm)


149.83 147.47 141.87 135.57 134.89 133.15 128.35 128.25 125.75 125.57 122.98
77.36 77.05 76.73
35.30 31.41 27.99
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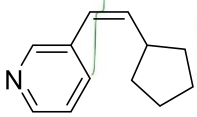
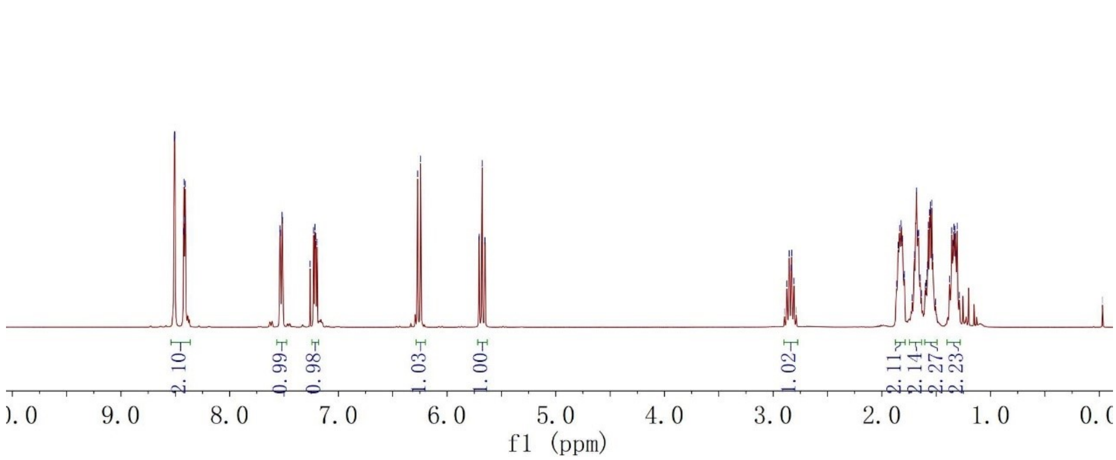
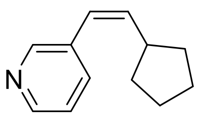
3
2ff
f1 (ppm)



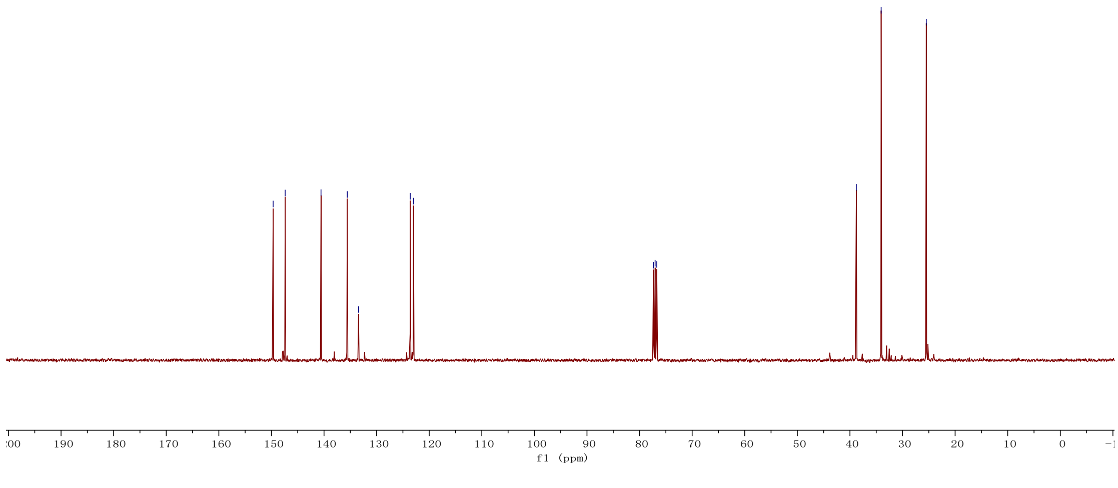
2gg



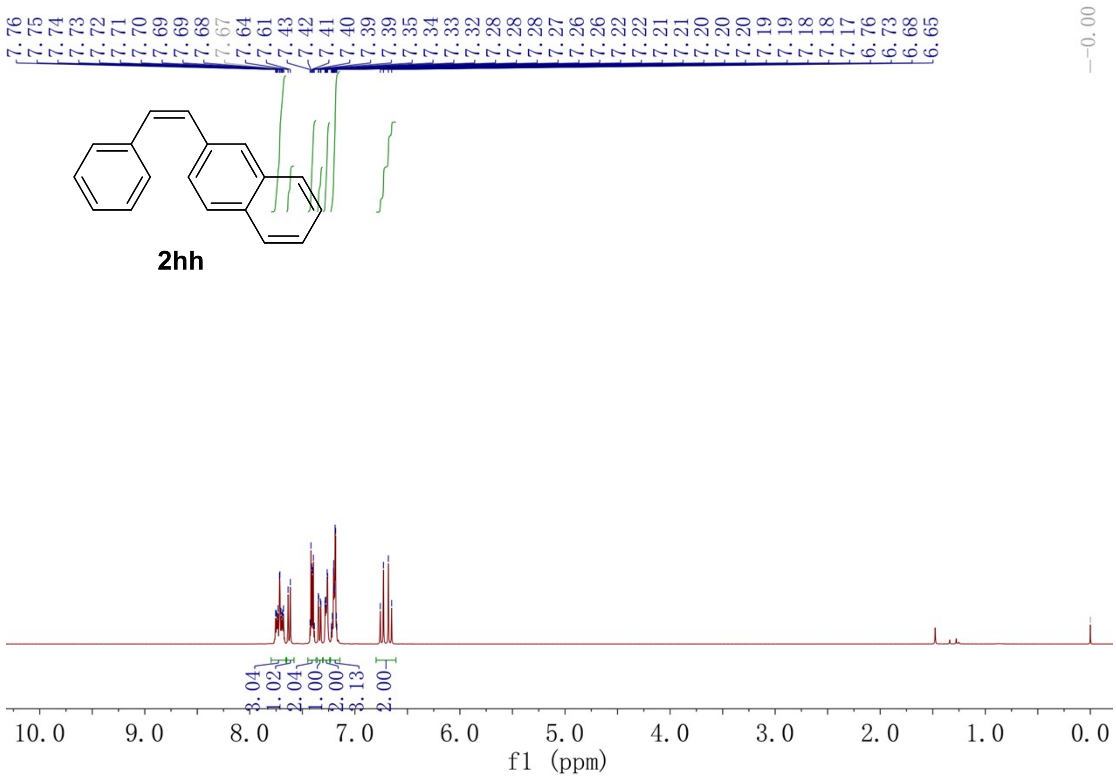
8.51 8.50 8.42 8.42 8.42 8.41 8.41 7.54 7.53 7.52 7.51 7.26 7.23 7.22 7.21 7.20 6.27 6.24 5.70 5.68 5.65 2.85 2.83 2.83 2.81 1.85 1.84 1.82 1.81 1.80 1.79 1.70 1.68 1.67 1.66 1.65 1.59 1.58 1.58 1.57 1.56 1.55 1.55 1.54 1.53 1.38 1.36 1.34 1.33 1.32 1.32 1.31
2.10 0.99 0.98 1.03 1.00 1.02 2.11 2.14 2.27 2.23
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
f1 (ppm)



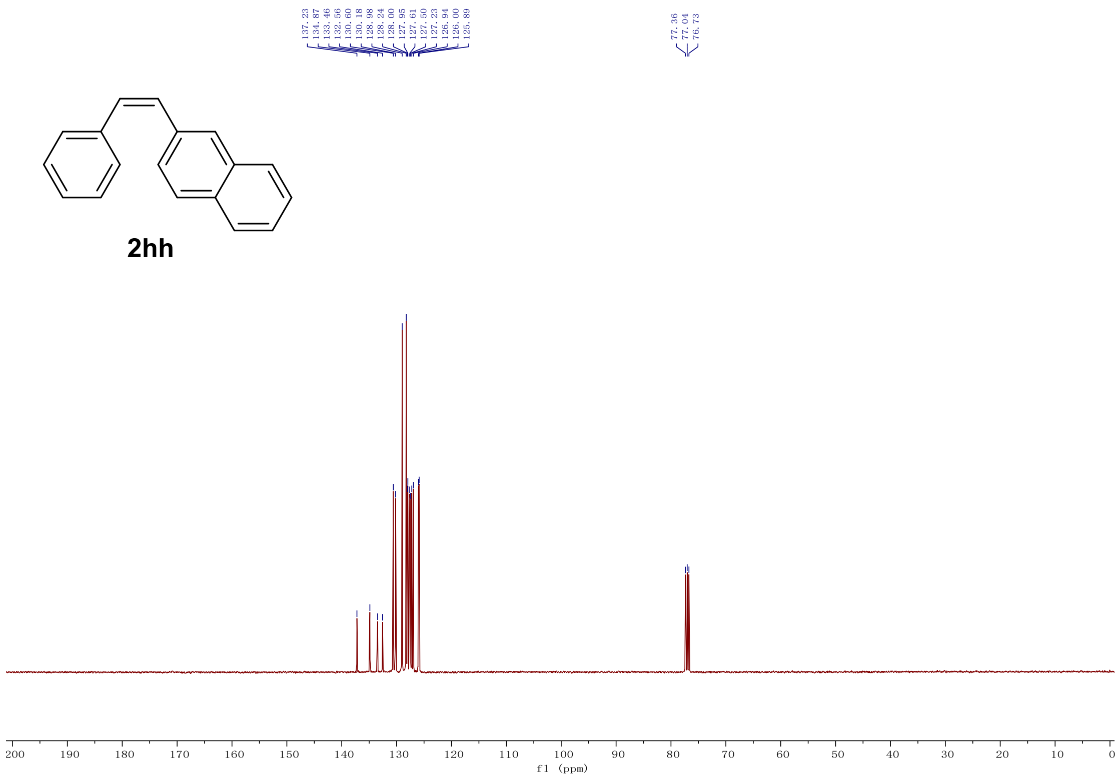
2gg



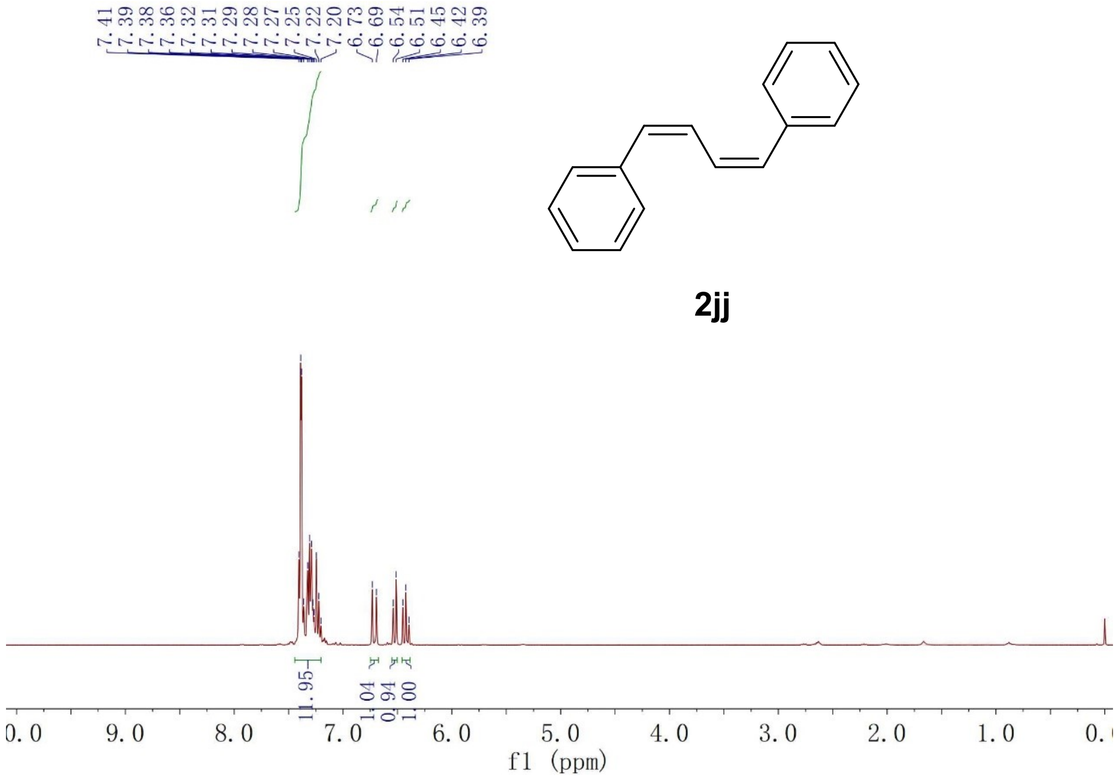
149.68 147.39 140.57 135.58 133.43 123.61 122.99 77.36 77.05 76.73 38.78 34.07 25.49
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

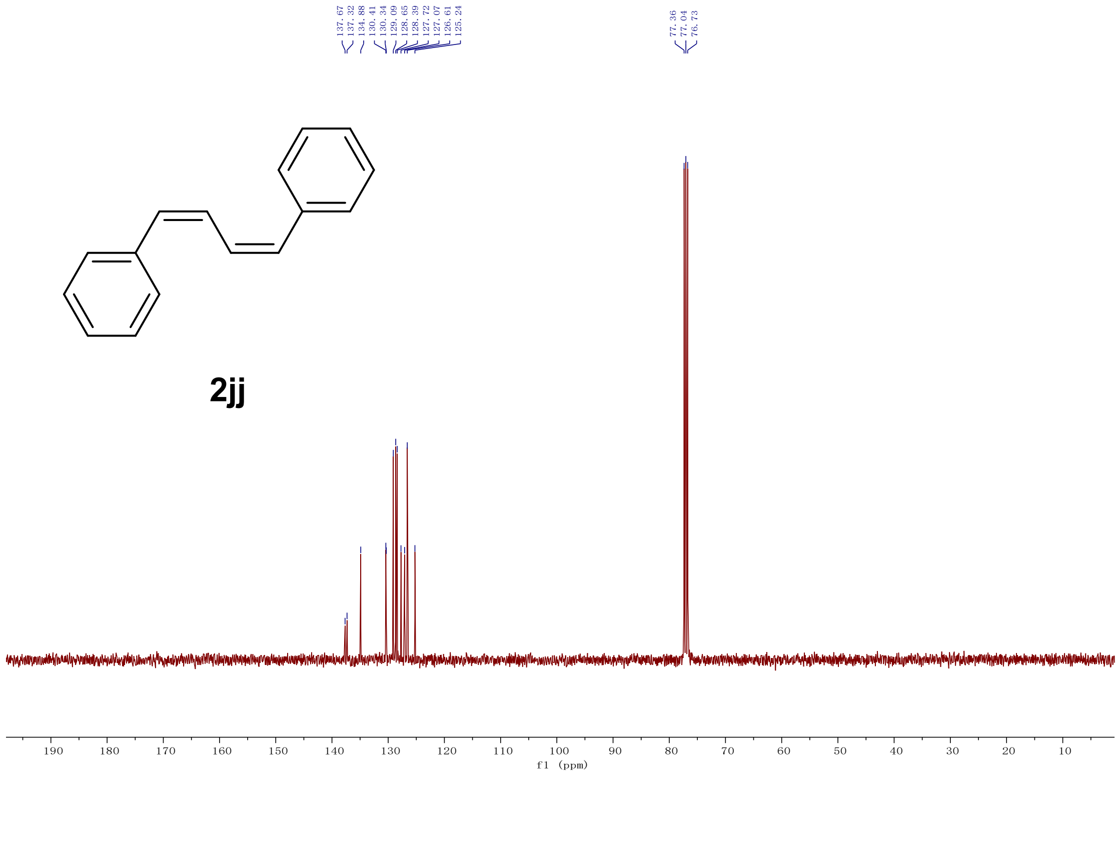


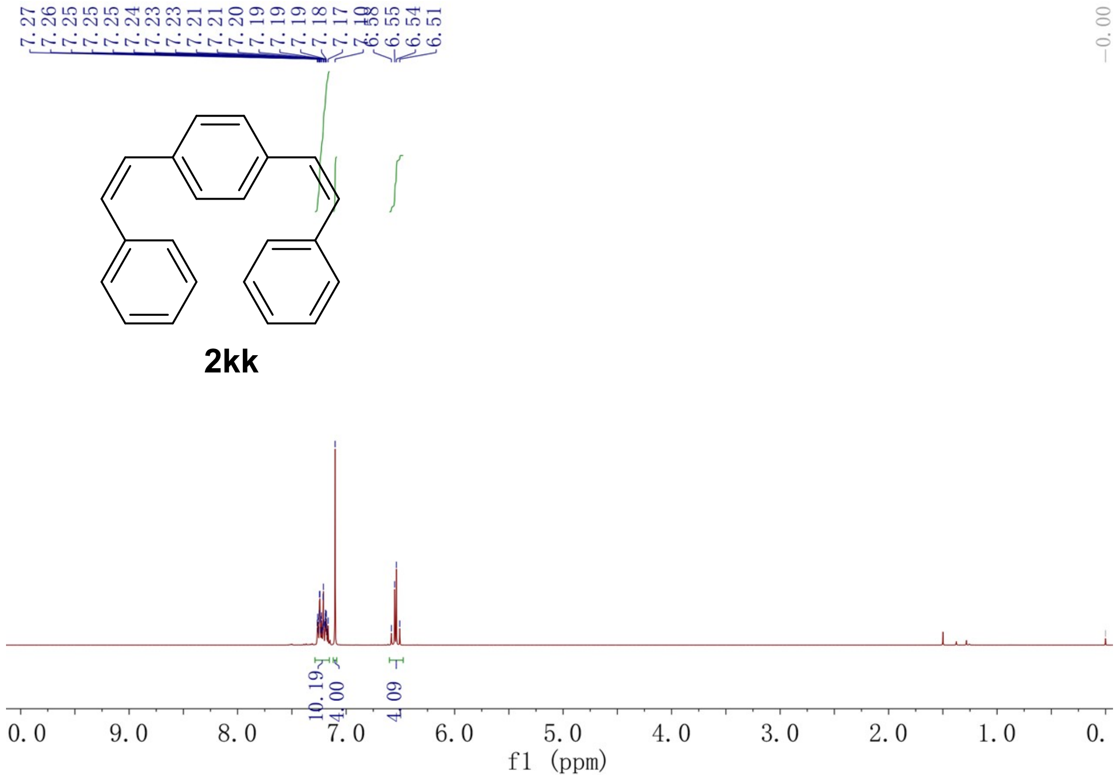
7.76
7.75
7.74
7.73
7.72
7.71
7.70
7.69
7.69
7.68
7.67
7.64
7.61
7.43
7.42
7.41
7.40
7.39
7.39
7.35
7.34
7.33
7.32
7.28
7.28
7.28
7.27
7.26
7.26
7.22
7.22
7.21
7.21
7.20
7.20
7.20
7.19
7.19
7.18
7.18
7.17
6.76
6.73
6.68
6.65
0.00
2hh
3.04
1.02
2.04
1.00
2.00
3.13
2.00
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

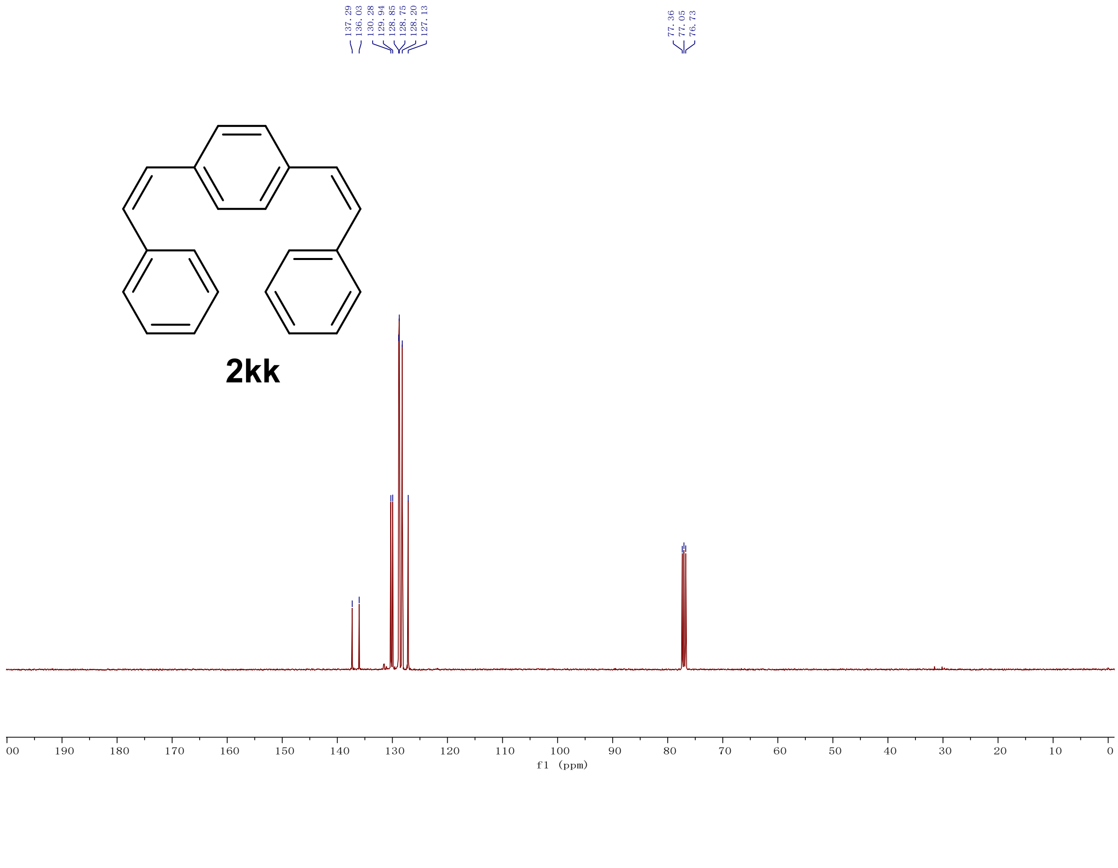


137.23
134.87
133.46
132.56
130.60
130.18
128.98
128.24
128.00
127.95
127.61
127.50
127.23
126.94
126.00
125.89
77.36
77.04
76.73
2hh
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.41 7.39 7.38 7.36 7.32 7.31 7.29 7.28 7.27 7.25 7.22 7.20 6.73 6.69 6.54 6.51 6.45 6.42 6.39
2jj
11.95
1.04
0.94
1.00
f1 (ppm)

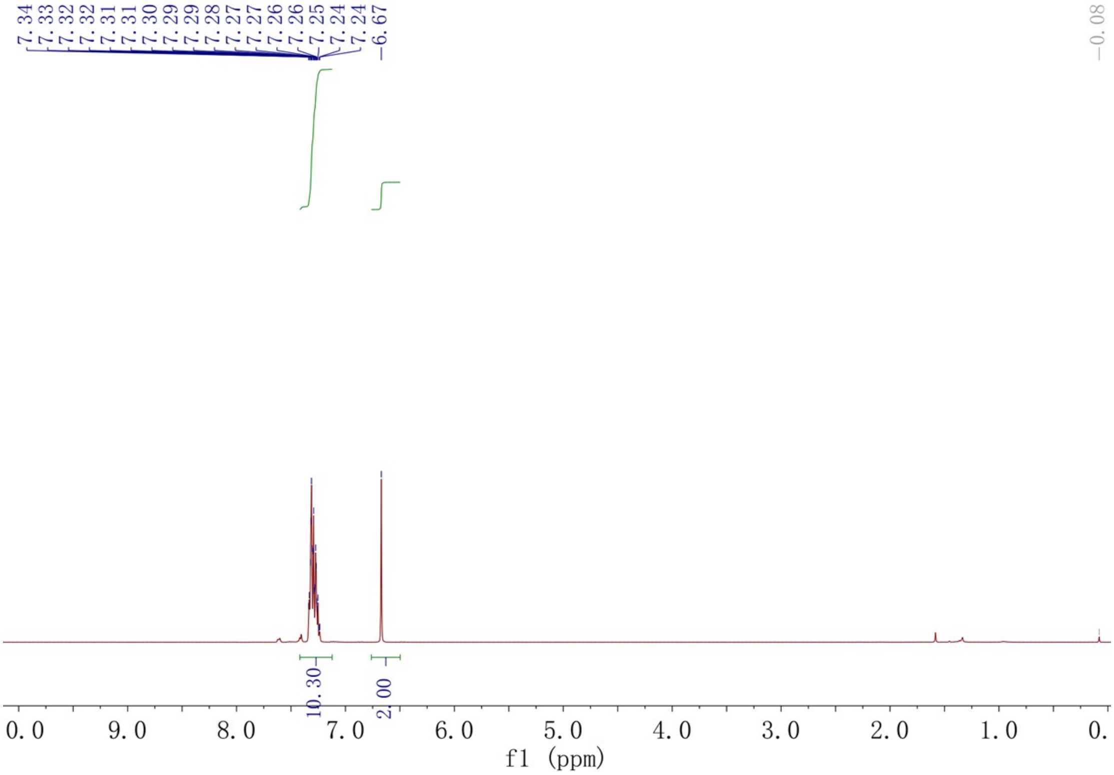

137.67 137.32 134.88 130.41 130.34 129.09 128.65 128.39 127.72 127.07 126.61 125.24
77.36 77.04 76.73
2jj
f1 (ppm)


7.27
7.26
7.25
7.25
7.25
7.24
7.23
7.23
7.21
7.21
7.20
7.19
7.19
7.19
7.18
7.17
7.10
6.58
6.55
6.54
6.51
0.00
2kk
10.19
4.00
4.09
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.
f1 (ppm)

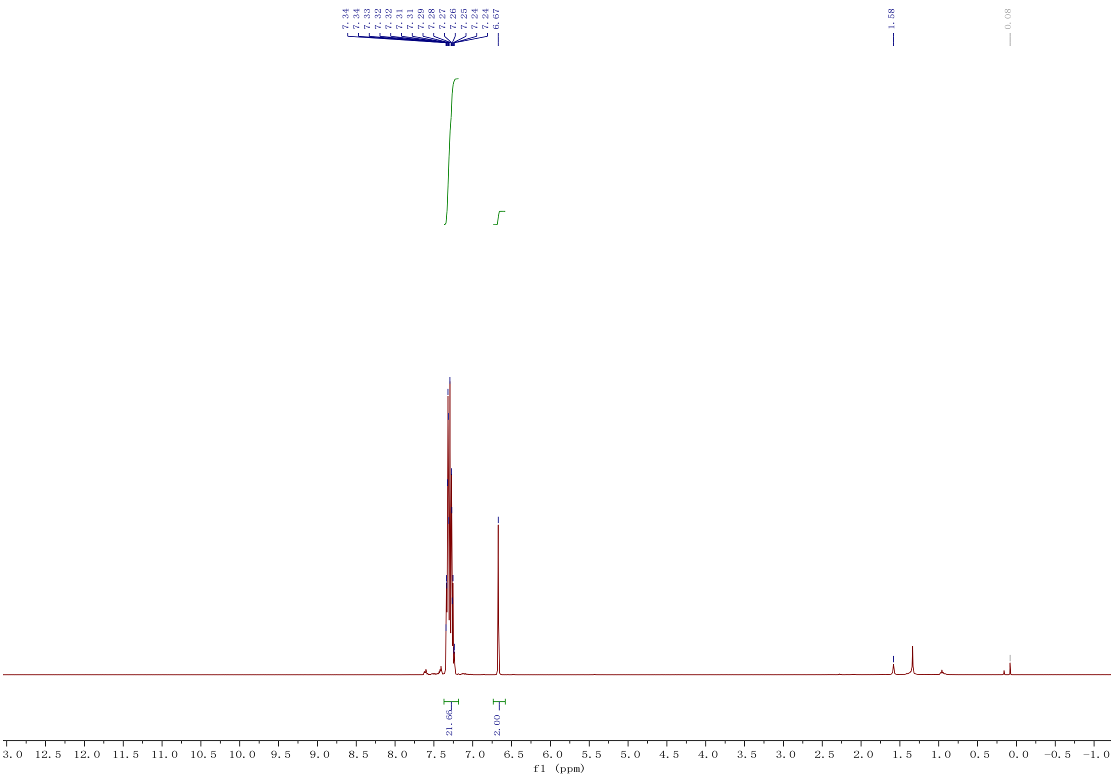

137.29
136.03
130.28
129.94
128.85
128.75
128.20
127.13
77.36
77.05
76.73
2kk
f1 (ppm)

Deuterium experiment：

CD_3CN/EtOH as solvent



CH_3CN/EtOD as solvent



CD_3CN/EtOD as solvent