Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Mesoporous Carbon Derived from Vitamin B_{12}: A High-Performance Bifunctional Catalyst for Imine Formation

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1. General materials

Commercially available chemicals were used without further purification unless otherwise noted. Products were confirmed by GC-MS (Agilent 7890A GC/5973 MS, SE-54 capillary column) and GC calculations of yields were performed on Agilent 7890A (SE-30 capillary column, FID detector) using N_2 as carrier gas. ^{13}C NMR and ^1H NMR spectrum were recorded on a Bruker DRX-400 spectrometer operating at 400 MHz, using $CDCl_3$ as the solvent with tetramethylsilane as an internal reference.

2. Catalyst preparations

Synthesis of mesoporous carbons 1.25 g of LUDOX® AS-40 colloidal silica was mixed with 50 mL of VB_{12} solution (0.50 g of VB_{12} dissolved in water) under vigorous stirring at room temperature for 30 min. Then, the mixture was heated at 100 °C to volatilize the water under stirring. The obtained VB_{12}/SiO_2 was grinded into powder and pyrolyzed at 600 °C (or 400, 500, 700, 800, 900 °C, ramp rate: 5 °C min-1) for 2 h under flowing nitrogen, then cooled naturally to room temperature. The sample was leached in 10 wt% hydrofluoric acid (HF) for 24 h at room temperature to dissolve the silica template. Finally, the leached sample was thoroughly washed to neutrality with water and dried in vacuum at 100 °C overnight.

Synthesis of mesoporous graphitic carbon nitride (mpg-C_3N_4):[1] Cyanamide was dissolved in a 40% dispersion of 12-nm SiO_2 particles (Ludox HS-40) in water with stirring at 60 °C overnight. After evaporation of the solvent at 100 ^oC, the obtained solid was pyrolyzed at 550 °C (ramp rate: 2.3 °C min^{-1}) for 4 h under flowing nitrogen. The obtained powder was treated with 10 wt % hydrofluoric acid for 12 h, and this procedure was repeated once for removing the silicon template completely. Finally, the powder was thoroughly washed to neutrality with water and dried in vacuum at 100 °C overnight.

3. Catalyst characterizations

Nitrogen sorption isotherms were determined at -196 °C using a QuadraSorb SI4 Station. Piror to the measurement, the samples were degassed in vacuum at 300 °C for 3 h, and the Brunauer-Emmett-Teller (BET) surface areas of the samples were calculated using adsorption data.

Scanning electron microscope (SEM) images were conducted on a JSM-7800F microscope operated at 20 kV landing energy. Transmission electron microscope (TEM) images were acquired with JEM-2100 microscope.

The thermogravimetric analysis (TGA) of the samples were conducted on a Perkin-Elmer TGA-2 thermo gravimetric analyzer from room temperature to 800 °C at a rate of 10 °C min^{-1} under N_2 atmosphere.

X-ray photoelectron spectroscopy (XPS) analysis of the samples were performed on Thermo Scientific ESCALAB 250Xi instrument with Al Ka radiation anode (hv = 1486.6 eV). The C 1s line (284.6 eV) was used as the reference to correct the binding energies (BE).

Power X-ray diffraction (XRD) patterns on a Rigaku D/Max 2500PC diffractometer equipped with a Cu Ka radiation source (λ=1.5418 Å) at a scanning rate of 0.05°/s (2θ from 10° to 80°).

4. Catalytic experiments

Procedures for the cross-coupling of alcohols with amines In a typical oxidation, equimolar amounts of benzyl alcohol (0.5 mmol) and aniline (0.5 mmol), m-VB$_{12}$-8 (10 mg), K_2CO_3 (10 mol %) and heptane (1 mL) were added into a Schlenk tube (10 mL) with a magnetic bar. Then, the tube was vacuumed and purged with air three times before it was finally pressurized with an air balloon, and stirred at 100 °C for 12h. After the reaction, the internal standard (biphenyl, 50 mg) and CH_3CN (2 mL) were added. The liquid mixture analysis were performed on GC and confirmed by GC-MS. For isolated yield: After the reaction completing, the catalyst was separated by centrifugation and washed with ethyl acetate several times. The filtrate was collected and concentrated under reduced pressure to give an analytically pure form of product as confirmed by ^{1}H and ^{13}C NMR spectra.

Procedures for the self-coupling of amines In a typical oxidation, benzylamine (5 mmol) and m-VB$_{12}$-6 (20 mg) were added into a Schlenk tube (10 mL) with a magnetic bar, and then the tube was vacuumed and purged with oxygen three times before it was finally pressurized with an oxygen balloon. Subsequently, the tube was stirred at 100 °C for 8 h. After the reaction, the internal standard (biphenyl, 250 mg) and CH_3CN (12 mL) were added. The liquid mixture was analyzed by GC and confirmed by GC-MS.

Large-scale and recycling test Benzylamine (100 mmol) and m-VB$_{12}$-6 (50 mg) were added into a two-neck flask (50 mL) with a magnetic bar, and then the tube was vacuumed and purged with oxygen three times before it was finally pressurized with double oxygen balloons. Subsequently, the flask was stirred at 120 °C for 48 h. After completion of the reaction, the liquid mixture was analyzed by GC. The solid catalyst was recovered by filtration, washing with hot ethanol and drying under vacuum to remove the residual solvent, and reused for the next run after addition of fresh benzylamine.

5. Results

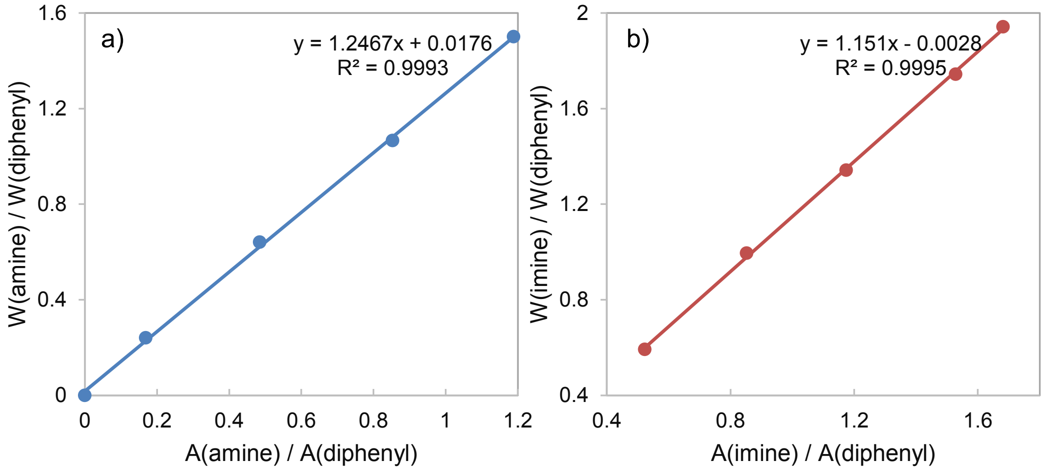


Figure S1. Standard curves for benzylamine oxidation (A: Area, W:weight).

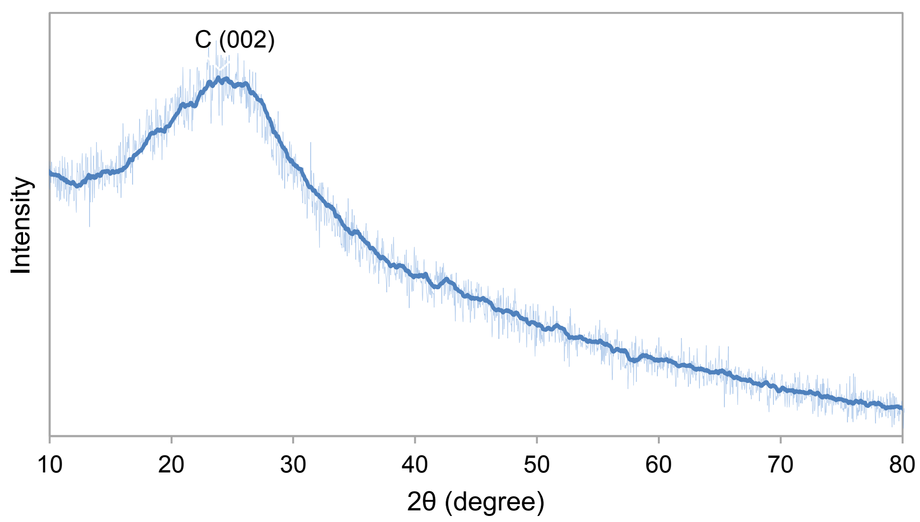


Figure S2. Powder XRD pattern of m-VB_{12}-8.

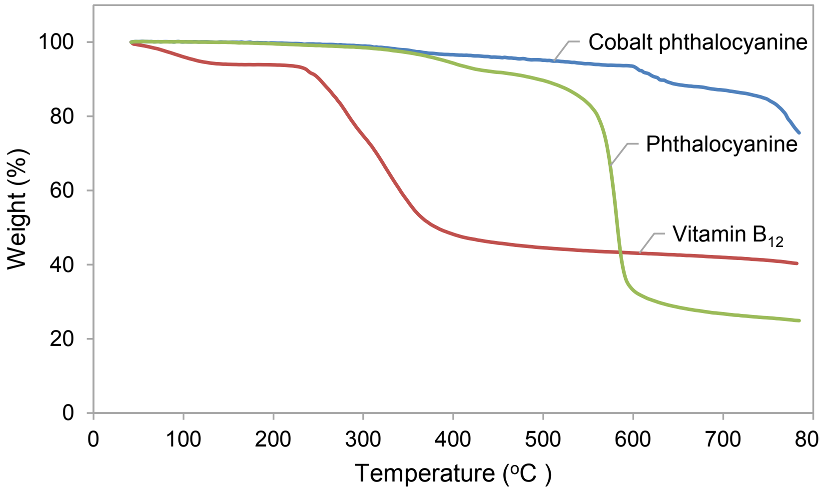


Figure S3. Thermogravimetric curve of different precursor under N_2 atmosphere with a heating rate of 10 °C min^{-1}.

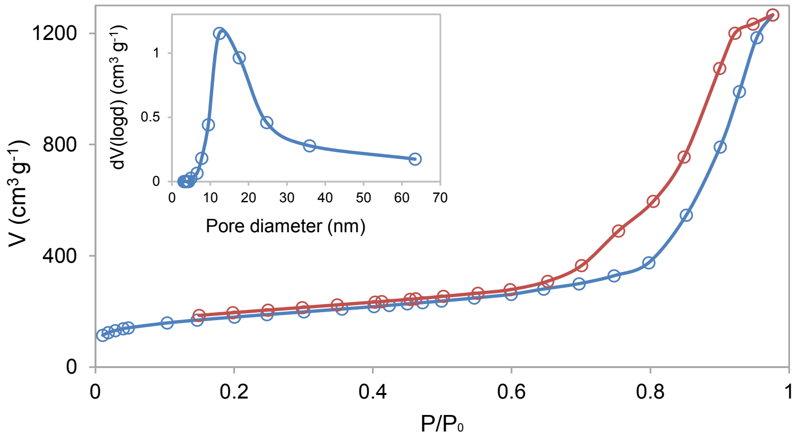


Figure S4. N_2 sorption isotherms and BJH mesopore size distribution (inset) plots of m-VB_{12}-8. (BET surface area and pore size distribution are 637 m^2/g and 12.3 nm, respectively)

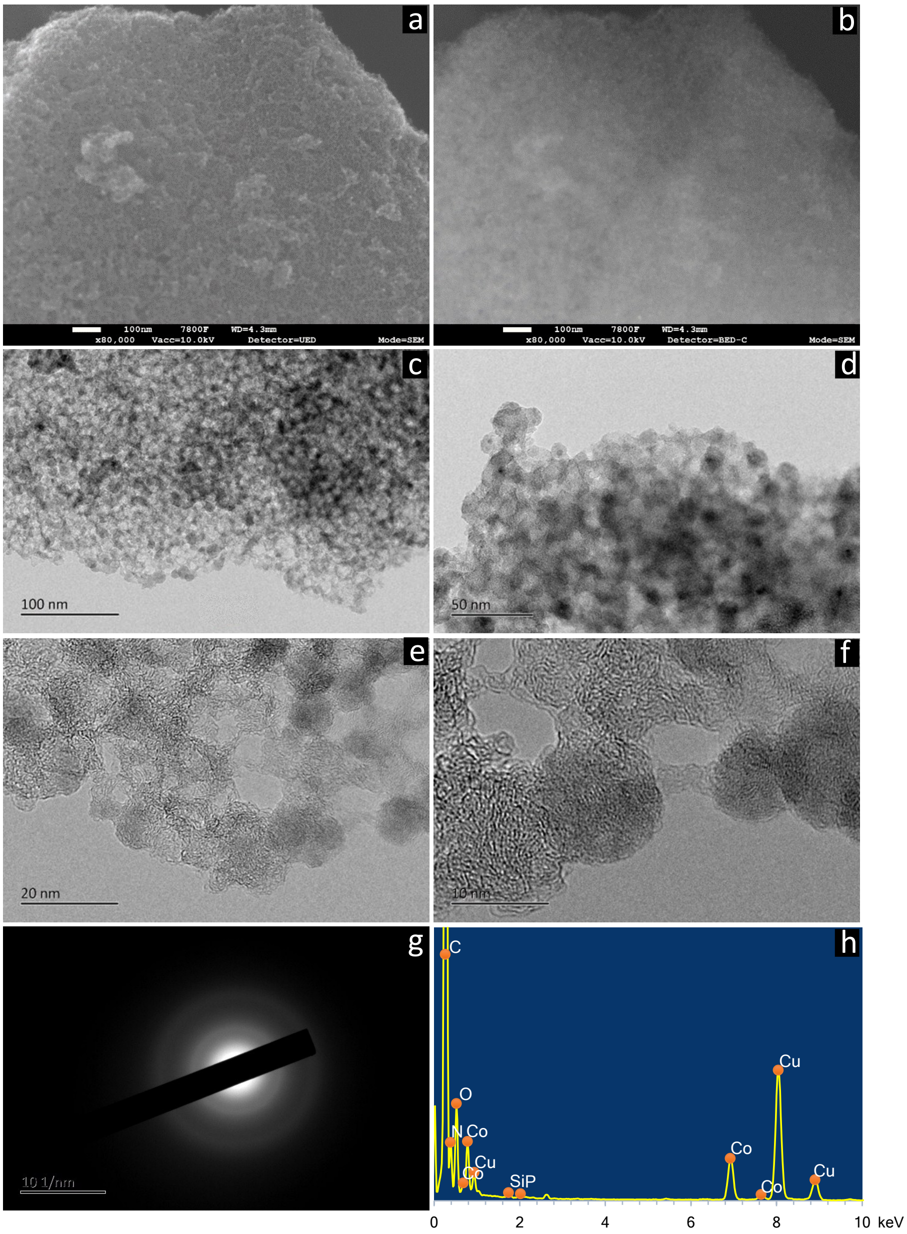


Figure S5. SEM, TEM images (a-b, c-f), SAED image (g) and EDX spectra (h) of m-VB_{12}-8.

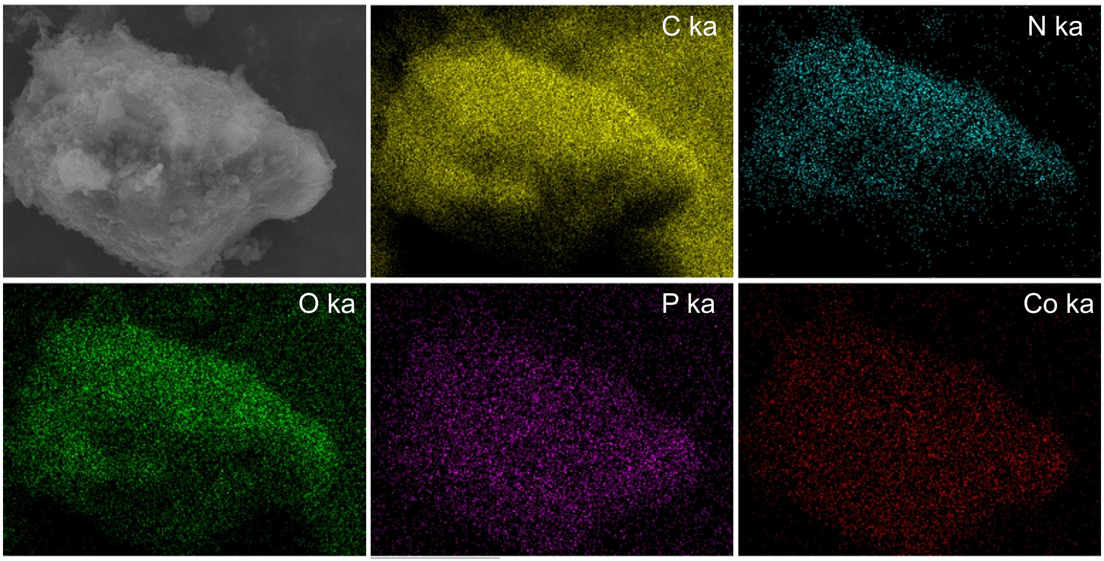


Figure S6. large-area SEM image along with the corresponding C-Ka, N-Ka, O-Ka, P-Ka and Co-Ka elemental maps of m-VB_{12}-8.

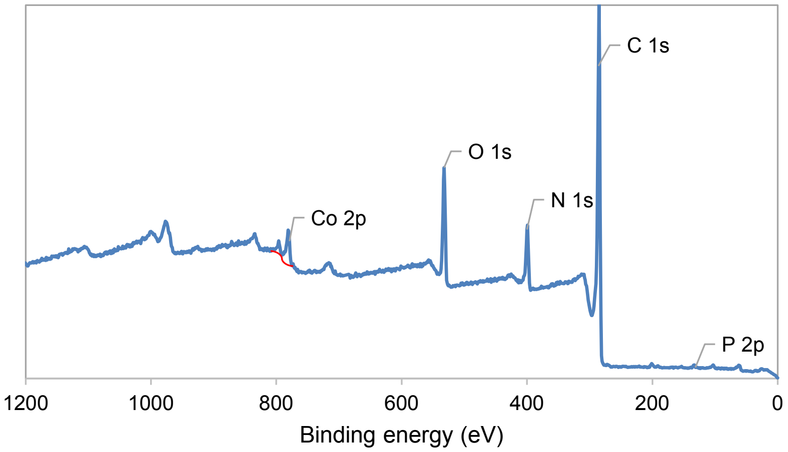


Figure S7. XPS survey spectra of m-VB_{12}-8.

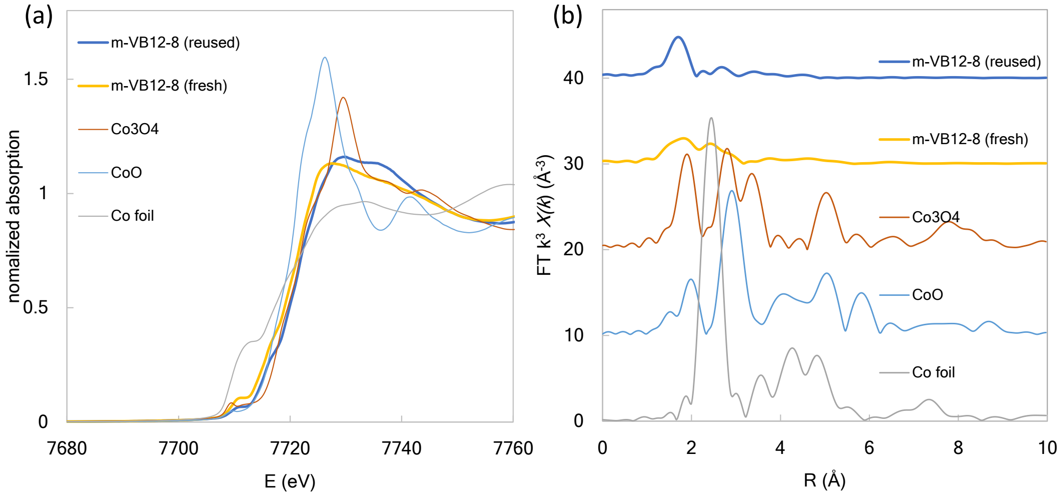


Figure S8. Co-K edge XANES spectra (a) and EXAFS R space (b) of m-VB12-8 (reused and fresh), and the reference compounds

In Figure S8a, the near-edge spectra of the fresh and the reused m-VB12-8 are between that of CoO and Co_3O_4, revealing that the catalysts contain both Co^{3+} and Co^{2+}species. In addition, a small deviation of E_0 was observed between the two catalysts, which may be attributed to the partial oxidation of Co^{2+} species during the reaction under O_2 atmosphere, this is, a little more Co^{3+} species are presented in the reused catalyst. Nevertheless, since no obvious activity loss was observed in the recycle experiments, this change may not greatly affect the active sites of the catalysts. Figure S8b shows the EXAFS spectra of the catalysts and reference samples. The fresh and reused m-VB12-8 cannot be assigned to any structure of Co, CoO or Co_3O_4. By combination of the XRD and XPS results, we propose that the catalysts are probably amorphous structure with Co-N/C shells.

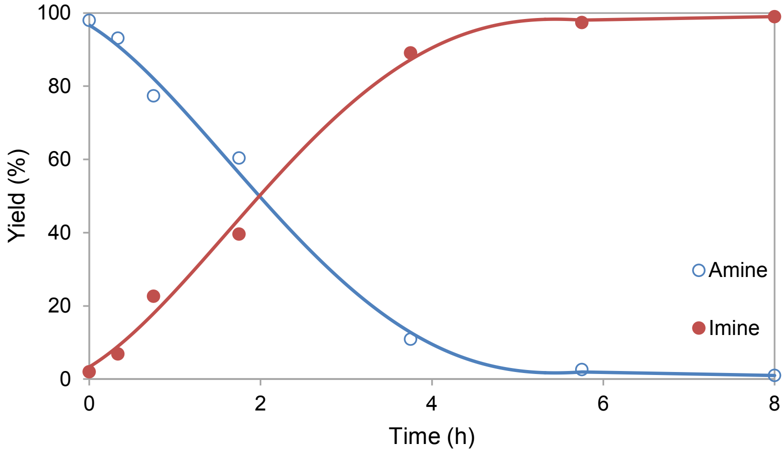


Figure S9. Reaction profile for the formation of imine from benzylamine (5 mmol) over m-VB_{12}-6 (20 mg) at 100 °C under O_2 balloon.

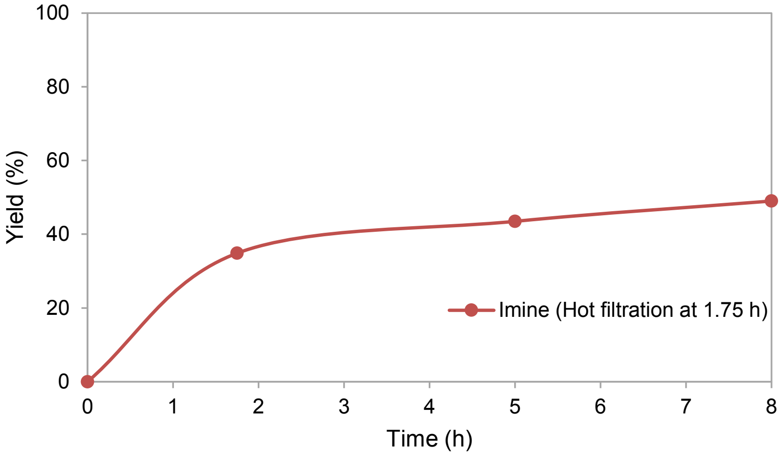
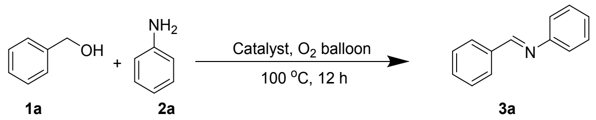


Figure S10. Hot filtration test for the formation of imine from benzylamine (5 mmol) over m-VB_{12}-6 (20 mg) at 100 °C under O_2 balloon.

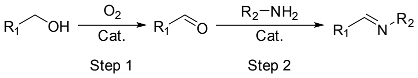
Table S1. Cross-coupling of benzyl alcohol with aniline under different conditions.[a]



Entry	Catalyst	Base (K_2CO_3)	Conversion [%][b]	Selectivity[%][b]
1	m-VB_{12}-6	10%	94	91
2	m-VB_{12}-8	10%	99	97

3	m-VB_{12}-8	5%	86	91
4	m-VB_{12}-8	-	42	98
5[c]	m-VB_{12}-8	10%	74	91
6[d]	**m-VB_{12}-8**	**10%**	**99**	**98**
7	m-Pc-8	10%	16	76
8	m-CoPc-8	10%	75	87
9	m-FePc-8	10%	52	92
10	m-CuPc-8	10%	43	86

[a] Reaction conditions: **1a** (0.5 mmol), **2a** (0.5 mmol), heptane (1 mL), catalyst (10 mg), O_2 balloon, 100 °C, 12 h. [b] Determined by GC using diphenyl as the internal standard and confirmed by GC-MS. [c] The reaction temperature was 80 °C. [d] Air balloon.



$KIE=k_H/k_D=(0.99-0.29)/0.29=2.41$

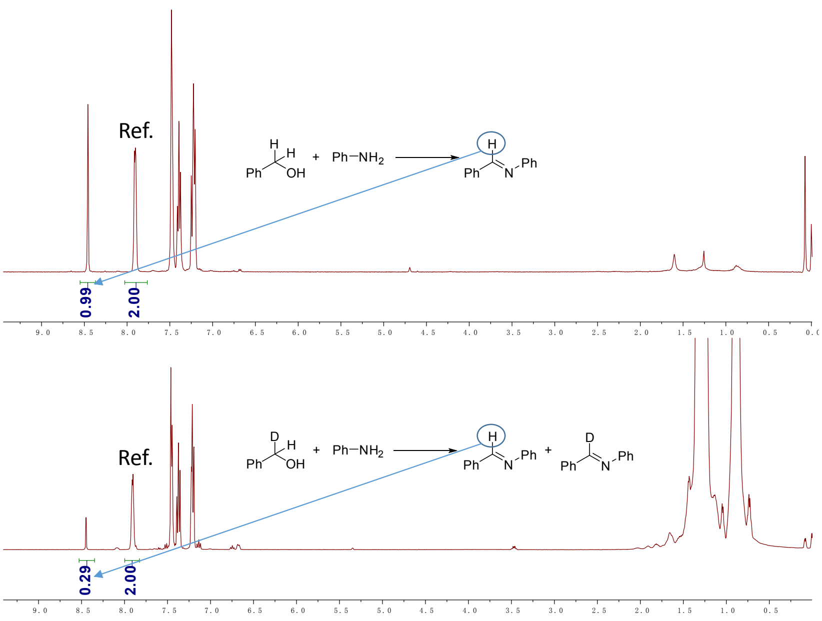
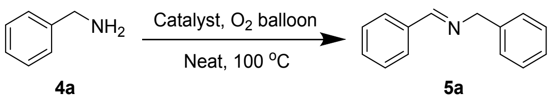


Figure S11. Isotopic labeling experiments for the cross-coupling of benzyl alcohol with aniline.

A primary kinetic isotope effect (KIE=2.41) was observed for the coupling of deuterated benzyl alcohol with aniline, which strongly indicates that the rate-determining step in our system is the oxidation of alcohols into aldehydes (Step 1), and to be more specific, is the cleavage of C-H bond at the benzylic positions.

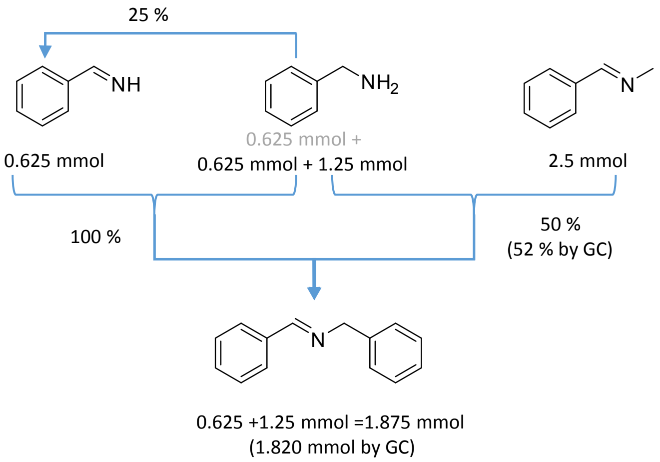
Table S2. Catalytic performance of the catalysts pyrolysed at different temperatures.[a]



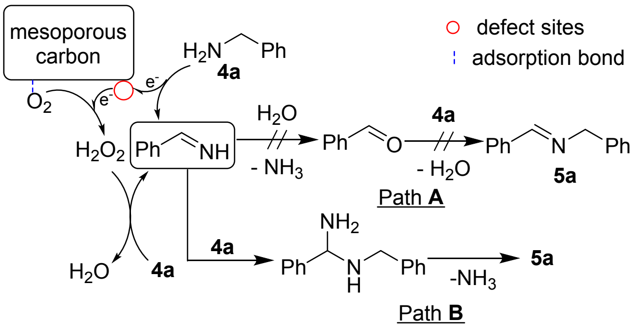
Entry	Catalyst	t [h]	Conversion [%][b]	Selectivity [%][b]

1	m-VB_{12}-4	8	87	87
2	m-VB_{12}-5	3	61	97
3	m-VB_{12}-6	3	66	98
4	**m-VB_{12}-6**	**8**	**97**	**95**
5	m-VB_{12}-7	3	66	98
6	m-VB_{12}-8	3	58	99
7	m-VB_{12}-9	8	91	87
8	-	-	-	-
9[c]	m-VB_{12}-6	8	83	95
10[d]	m-VB_{12}-6	8	56	54
11[e]	m-VB_{12}-6	8	5	5
12[f]	m-VB_{12}-6	8	98	86

[a] Reaction conditions: **4a** (5 mmol), catalyst (20 mg), O_2 balloon, 100 °C. [b] Determined by GC using diphenyl as the internal standard and confirmed by GC-MS. [c] 80 °C. [d] Air balloon. [e] N_2 balloon. [f] The free-radical scavenger 2,6-di-tert-butyl-4-methylphenol (BHT: 5 mol%) was added.



Scheme S1. Cross-coupling of benzylamine with *N*-benzylidenemethyl amine over m-VB_{12}-6. Reaction conditions: benzylamine (2.5 mmol), *N*-benzylidenemethyl amine (2.5 mmol), catalyst (20 mg), O_2 balloon, 8 h, 100 °C.



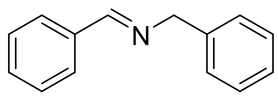
Scheme S2. Proposed mechanism for m-VB_{12}-6-catalyzed the self-coupling of primary amines

We proposed that **4a** was first dehydrogenated into benzaldimine intermediate, and subsequently coupled with a second molecule of **4a** to form **5a** with liberation of ammonia, since no aldehyde was detected via continuous sampling (Figure S8) and also in the 100 mmol scale experiments.

Besides, *N*-methylbenzalimine as the replacement of benzaldimine was reacted with equimolar **4a** under the optimized conditions. After the reation, 52% of *N*-methylbenzalimine was transformed into the desired **5a**, and the residual could be recovered from the reaction mixtures (Schem S1). These results strongly demonstrate that benzaldimine instead of benzylaldehyde (hydrolysis of benzaldimine) was directly attacked by **4a**. Free-radical scavenger (BHT) was failed to disturb the self-coupling of 1a (Table S2, entry 12), indicating the reaction was not involved in a radical process.

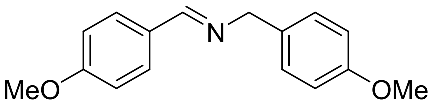
(1) Su, F.; Mathew, S. C.; Möhlmann, L.; Antonietti, M.; Wang, X.; Blechert, S., *Angew. Chem. Int. Ed.* **2011**, *50*, 657-660.

6. Characterizations of typical products



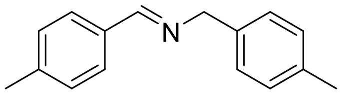
$C_{14}H_{13}N$

***N*-Benzylidenebenzylamine** Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (s, 1H), 7.87 – 7.68 (m, 2H), 7.47 – 7.36 (m, 3H), 7.33 (dd, J = 4.5, 2.0 Hz, 4H), 7.27 – 7.16 (m, 1H), 4.82 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.96 , 139.33 , 136.21 , 130.75 , 128.60 , 128.49 , 128.29 , 127.99 , 126.98 , 65.05 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



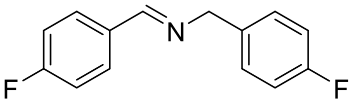
$C_{16}H_{17}NO_2$

***N*-(4-Methoxybenzylidene)-4-methoxyphenylmethyl amine** Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.28 (s, 1H), 7.70 (d, J = 8.8 Hz, 2H), 7.24 (d, J = 8.3 Hz, 2H), 6.91 (d, J = 8.6 Hz, 2H), 6.87 (d, J = 8.6 Hz, 2H), 4.71 (s, 2H), 3.82 (s, 3H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.68 , 160.87 , 158.66 , 131.72 , 129.79 , 129.15 , 113.97 , 113.92 , 64.40 , 55.35 , 55.29 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



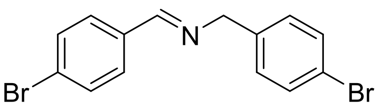
$C_{16}H_{17}N$

***N*-(4-Methylbenzylidene)-4-methylphenylmethylamine** White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 (s, 1H), 7.59 (d, J = 40.1 Hz, 2H), 7.32 – 7.13 (m, 4H), 7.11 (s, 2H), 4.76 (s, 2H), 2.36 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.09 , 139.25 , 138.34 , 138.12 , 136.22 , 131.58 , 128.80 , 128.52 , 128.42 , 127.76 , 125.90 , 125.12 , 65.18 , 21.46 , 21.29 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, 15, 2704-2707.



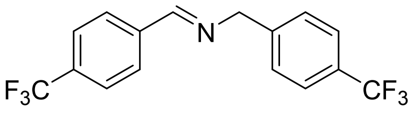
$C_{14}H_{11}F_2N$

***N*-(4-Fluorobenzylidene)-4-fluorophenylmethylamine** Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 7.76 (dd, J = 5.2, 2.1 Hz, 2H), 7.29 (dd, J = 6.4, 2.8 Hz, 2H), 7.08 (t, J = 8.4 Hz, 2H), 7.04 – 6.99 (m, 2H), 4.74 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.02 , 160.79 , 160.47 , 130.85 , 130.21 , 129.50 , 129.43 , 128.63 , 128.28 , 115.83 , 115.61 , 115.41 , 115.20 , 77.33 , 77.02 , 76.70 , 64.14 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



$C_{14}H_{11}Br_2N$

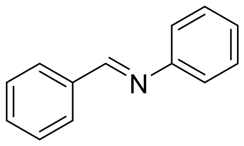
***N*-(4-Bromobenzylidene)-4-bromophenylmethylamine** White solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 7.77 – 7.61 (m, 2H), 7.55 (d, J = 8.5 Hz, 2H), 7.52 – 7.40 (m, 2H), 7.20 (d, J = 8.4 Hz, 2H), 4.74 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.93 , 138.11 , 134.90 , 131.89 , 131.59 , 129.67 , 129.62 , 125.35 , 120.93 , 64.21 . The compound was known: X. Qiu, C. Len, R. Luque, Y. Li, *ChemSusChem* **2014**, *7*, 1684-1688.



$C_{16}H_{11}F_6N$

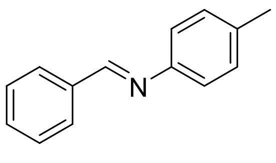
***N*-(4-(Trifluoromethyl)benzylidene)-4-(trifluoromethyl) phenyl)methanimine** Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H), 8.09 – 7.94 (m, 2H), 7.74 –

7.58 (m, 2H), 7.57 – 7.45 (m, 4H), 4.88 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.90 , 139.93 , 136.62 , 131.41 , 131.28 , 129.19 , 128.99 , 127.41 , 125.05 , 124.63 , 123.97 , 64.41 . The compound was known: X. Qiu, C. Len, R. Luque, Y. Li, *ChemSusChem* **2014**, *7*, 1684-1688.



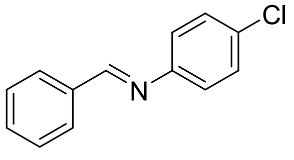
$C_{13}H_{11}N$

***N*-benzylideneaniline** Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (d, *J* = 1.8 Hz, 1H), 7.83 (dt, *J* = 4.9, 2.1 Hz, 2H), 7.44 – 7.36 (m, 3H), 7.31 (d, *J* = 7.1 Hz, 2H), 7.15 (t, *J* = 9.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.96 , 152.67 , 136.81 , 131.94 , 129.71 , 129.38 , 129.34 , 126.49 , 121.43 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



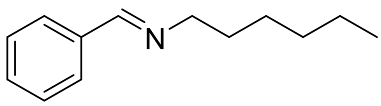
$C_{14}H_{13}N$

***N*-(4-Methylphenyl)-1-phenylmethanimine** Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (s, 1H), 7.90 – 7.78 (m, 2H), 7.46 – 7.29 (m, 3H), 7.11 (d, *J* = 8.1 Hz, 2H), 7.08 – 7.03 (m, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.54 , 149.50 , 136.41 , 135.78 , 131.18 , 129.76 , 128.73 , 128.72 , 120.81 , 21.01 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



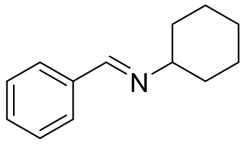
$C_{13}H_{10}ClN$

***N*-(4-Chlorophenyl)-1-phenylmethanimine** Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.34 (s, 1H), 7.77 (d, *J* = 8.5 Hz, 2H), 7.37 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 1.0 Hz, 2H), 7.18 – 7.11 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.75 , 150.69 , 136.35 , 133.72 , 128.92 , 128.17 , 128.05 , 125.16 , 119.82 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



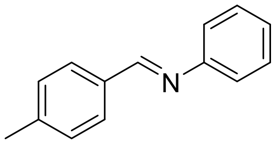
$C_{13}H_{19}N$

***N*-hexyl-1-phenylmethanimine** Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 (s, 1H), 7.83 – 7.67 (m, 2H), 7.43 – 7.37 (m, 3H), 3.60 (td, *J* = 7.1, 1.0 Hz, 2H), 1.69 (p, *J* = 7.0 Hz, 2H), 1.34 (qd, *J* = 8.4, 7.9, 5.1 Hz, 6H), 0.91 – 0.86 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.25 , 130.98 , 129.12 , 128.57 , 62.39 , 32.25 , 31.48 , 27.62 , 23.20 , 14.64 . The compound was known: B. Chen, J. Li, W. Dai, L. Wang, S. Gao, *Green Chem*. **2014**, *16*, 3328-3334.



$C_{13}H_{17}N$

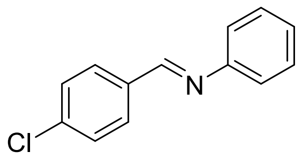
***N*-Benzylidenecyclohexylamine** Yellow oil**.** ^{1}H NMR (400 MHz, Chloroform -*d*) δ 8.28 (s, 1H), 7.74 – 7.65 (m, 2H), 7.42 – 7.31 (m, 3H), 3.17 (tt, *J* = 9.8, 4.1 Hz, 1H), 1.82 (d, *J* = 12.7 Hz, 2H), 1.76 – 1.53 (m, 5H), 1.40 – 1.23 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.14 , 130.90 , 129.10 , 128.67 , 70.58 , 35.00 , 26.29 , 25.43 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



$C_{14}H_{13}N$

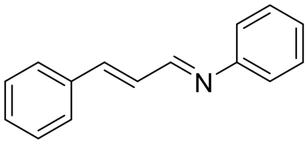
***N*-(4-Methylbenzylidene)aniline** Yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.34 (s, 1H), 7.79 – 7.67 (m, 2H), 7.34 – 7.28 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.11 (m, 3H), 2.34 (s, 3H). ^{13}C NMR

(101 MHz, Chloroform-*d*) δ 160.29 , 152.30 , 141.83 , 133.73 , 129.50 , 129.10 , 128.81 , 125.72 , 120.86 , 21.61 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



$C_{13}H_{10}ClN$

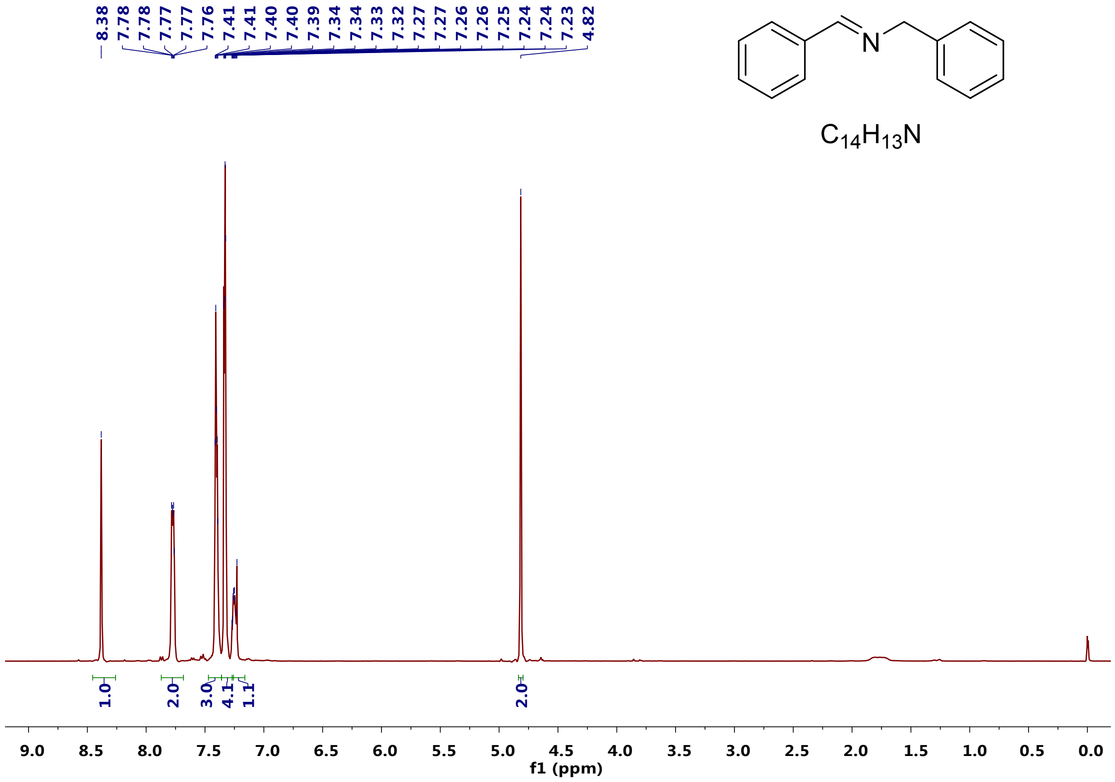
***N*-(4-Chlorobenzylidene)aniline** Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (s, 1H), 7.82 (dd, *J* = 7.4, 2.2 Hz, 2H), 7.44 – 7.36 (m, 3H), 7.30 – 7.25 (m, 2H), 7.11 – 7.04 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.68 , 150.54 , 135.98 , 131.60 , 131.47 , 129.23 , 128.87 , 128.81 , 122.18 . The compound was known: E. L. Zhang, H. W. Tian, S. D. Xu, X. C. Yu, Q. Xu, *Org. Lett.* **2013**, *15*, 2704-2707.



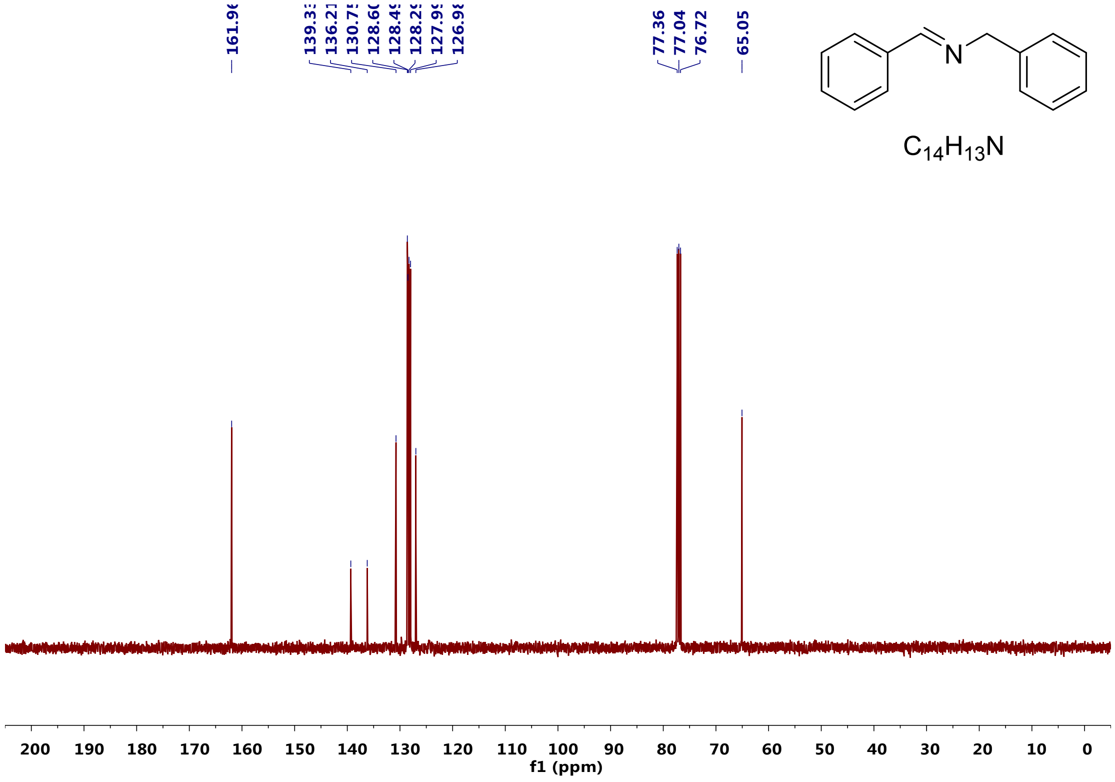
$C_{15}H_{13}N$

***N*-[3-phenyl-2-propenylidene]aniline** Orange solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.47 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.34 – 7.27 (m, 5H), 7.17 – 7.05 (m, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.60 , 151.74 , 143.99 , 135.60 , 129.57 , 129.16 , 128.91 , 128.62 , 127.49 , 126.09 , 120.90 . The compound was known: H. W. Tian, X. C. Yu, Q. Li, J. X. Wang, Q. Xu, *Adv. Synth. Catal.* **2012**, *354*, 2671–2677.

7. ^{1}H NMR and ^{13}C NMR spectra of typical products



$C_{14}H_{13}N$



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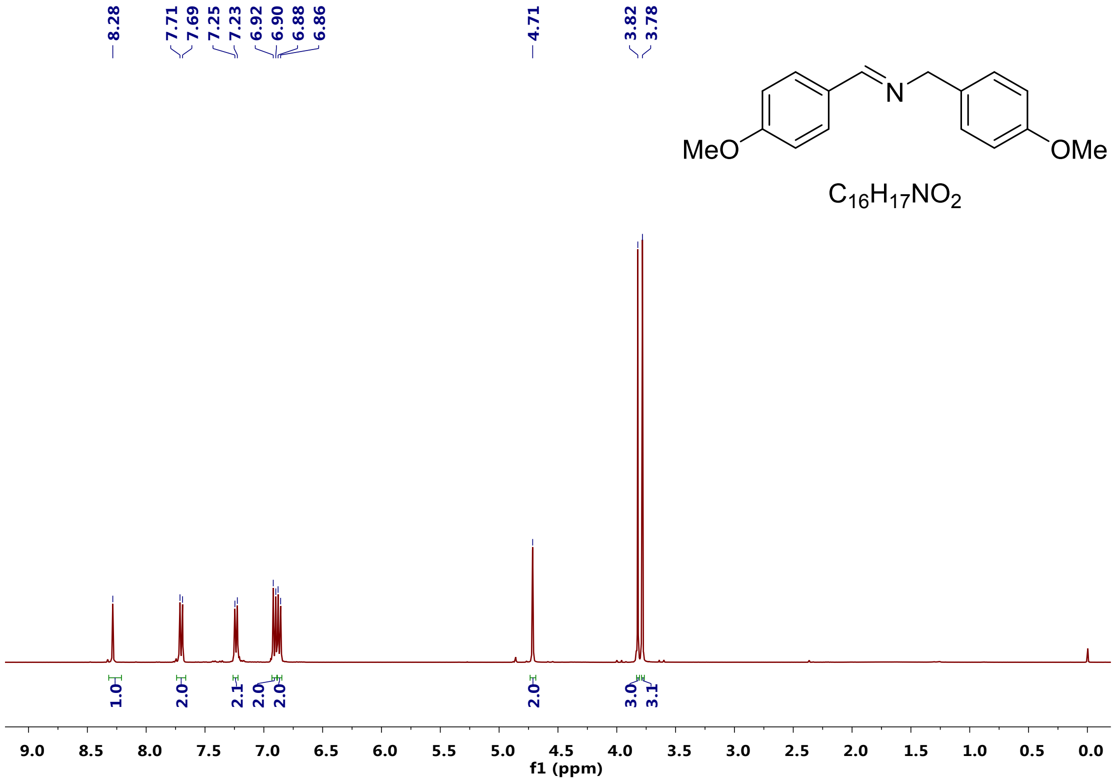
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OMe
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2.0
2.1
2.0
2.0
2.0
3.0
3.1
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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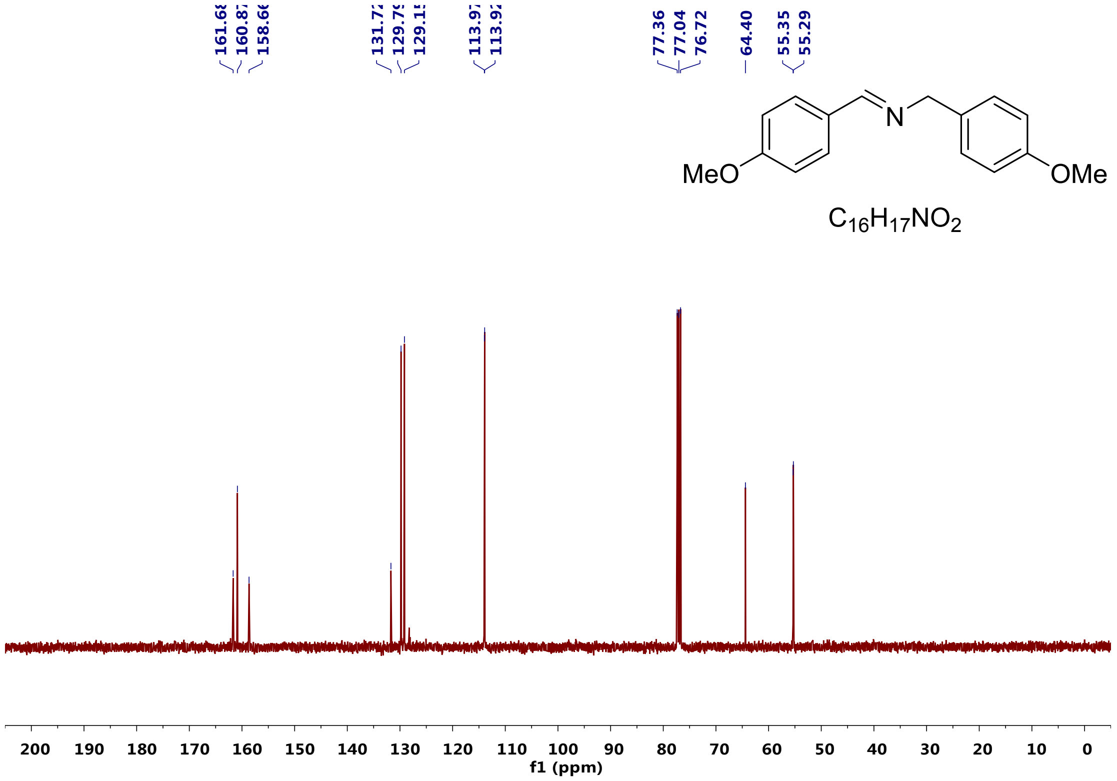
f1 (ppm)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55.29
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N
OMe
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180
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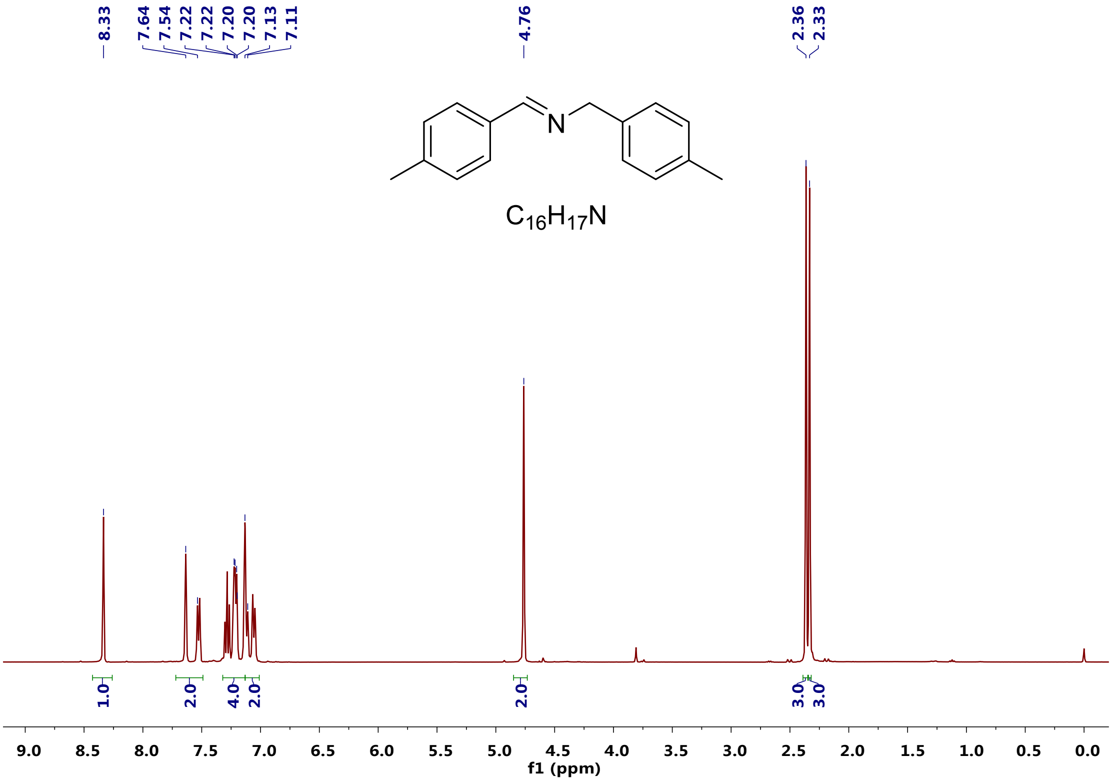
f1 (ppm)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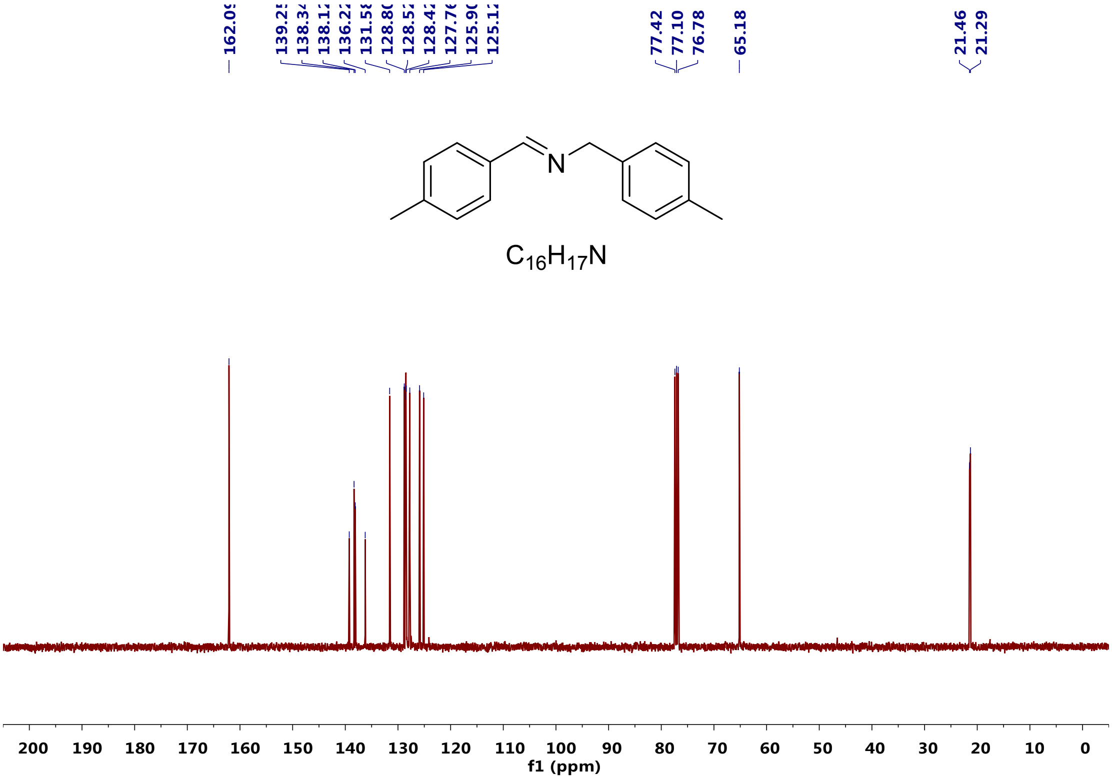
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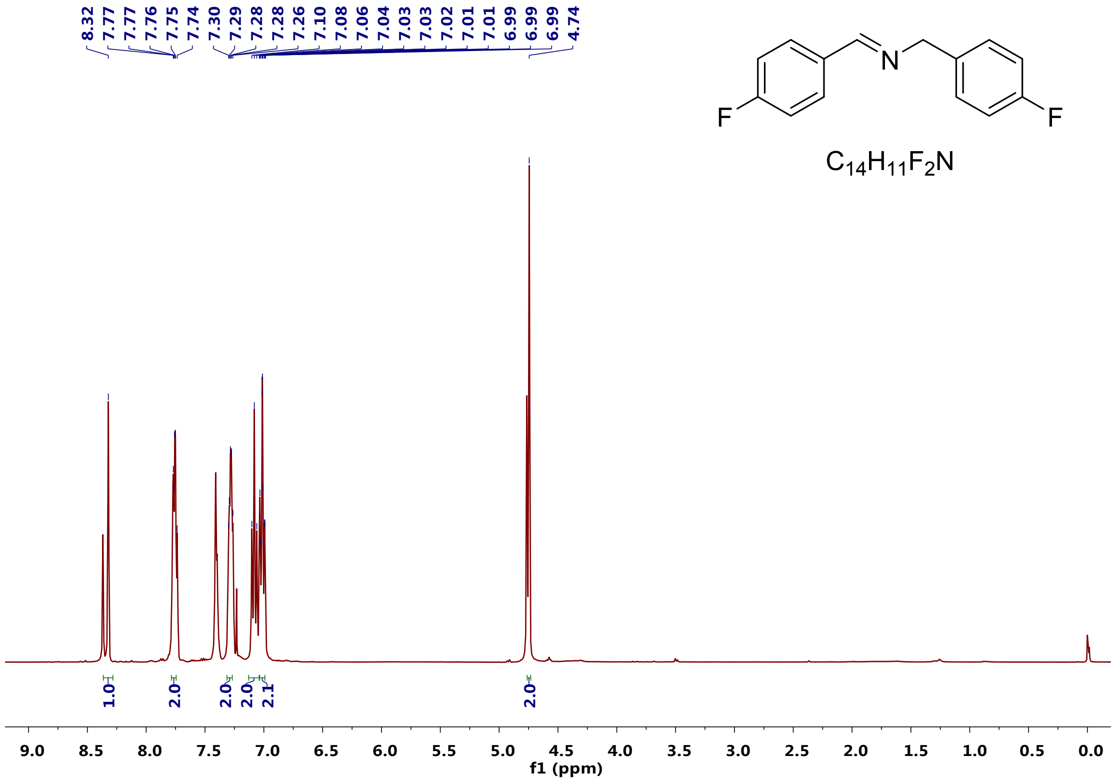
f1 (ppm)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7.01
7.01
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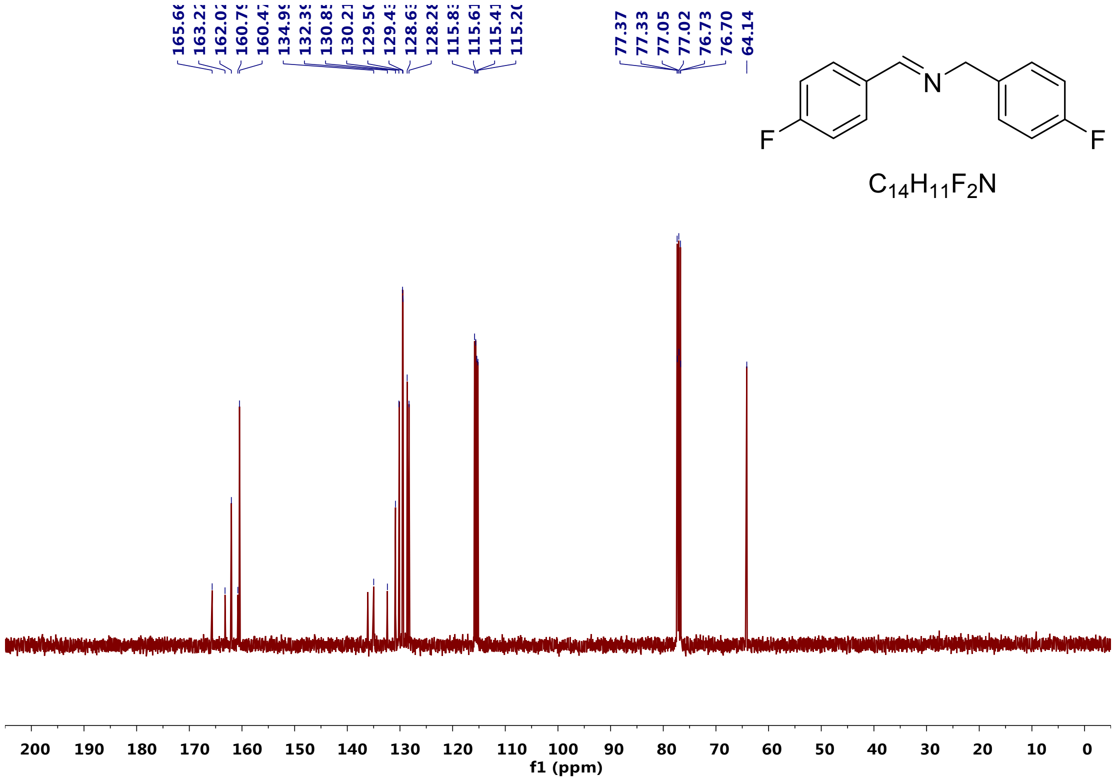
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N
F
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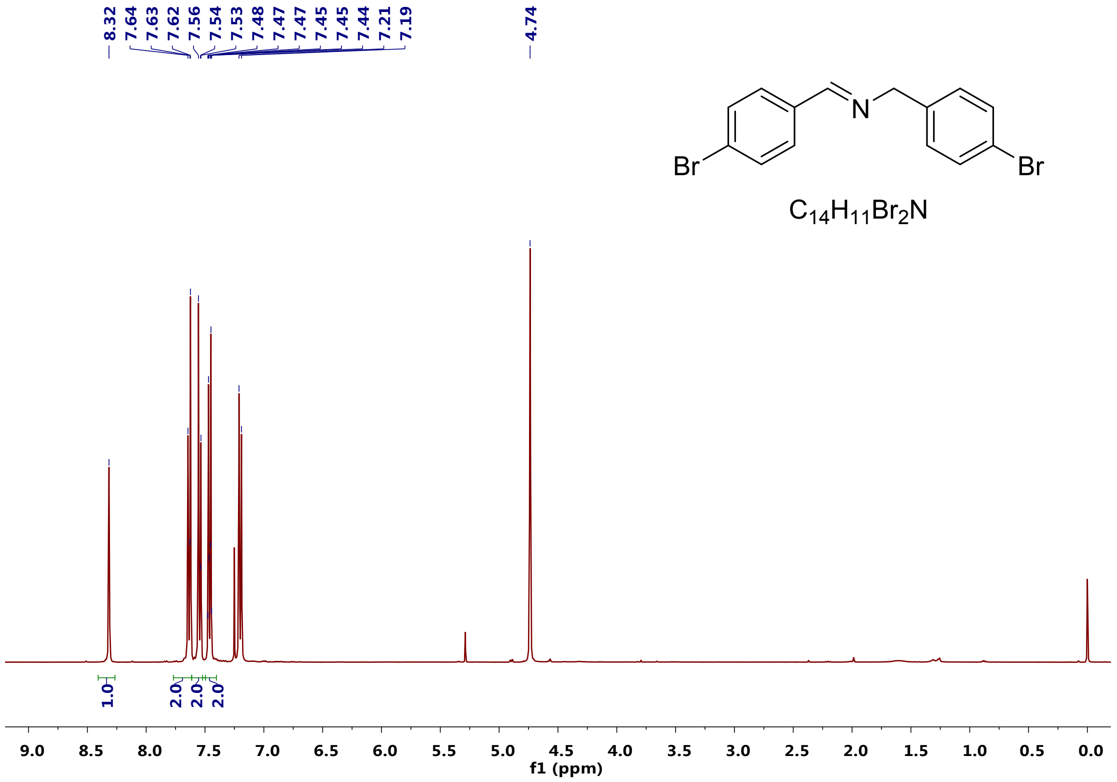
f1 (ppm)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7.19
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9.0
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7.0
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6.0
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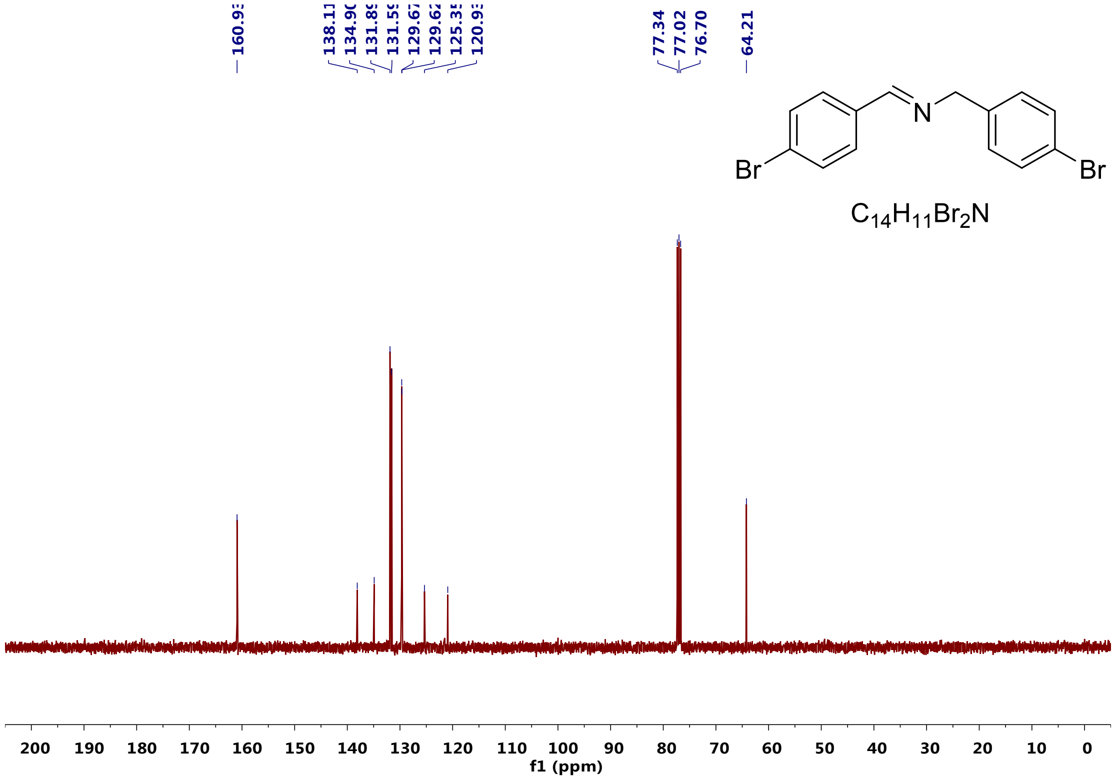
f1 (ppm)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76.70
64.21
Br
N
Br
$C_{14}H_{11}Br_2N$
200
190
180
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90
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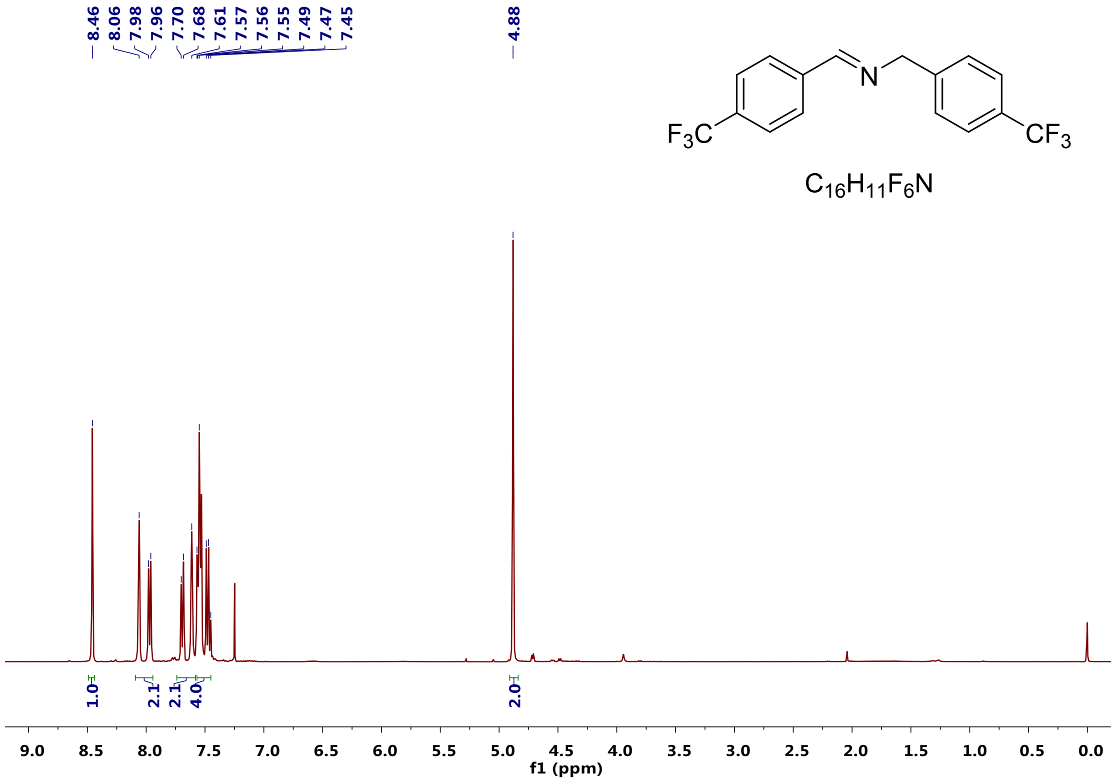
f1 (ppm)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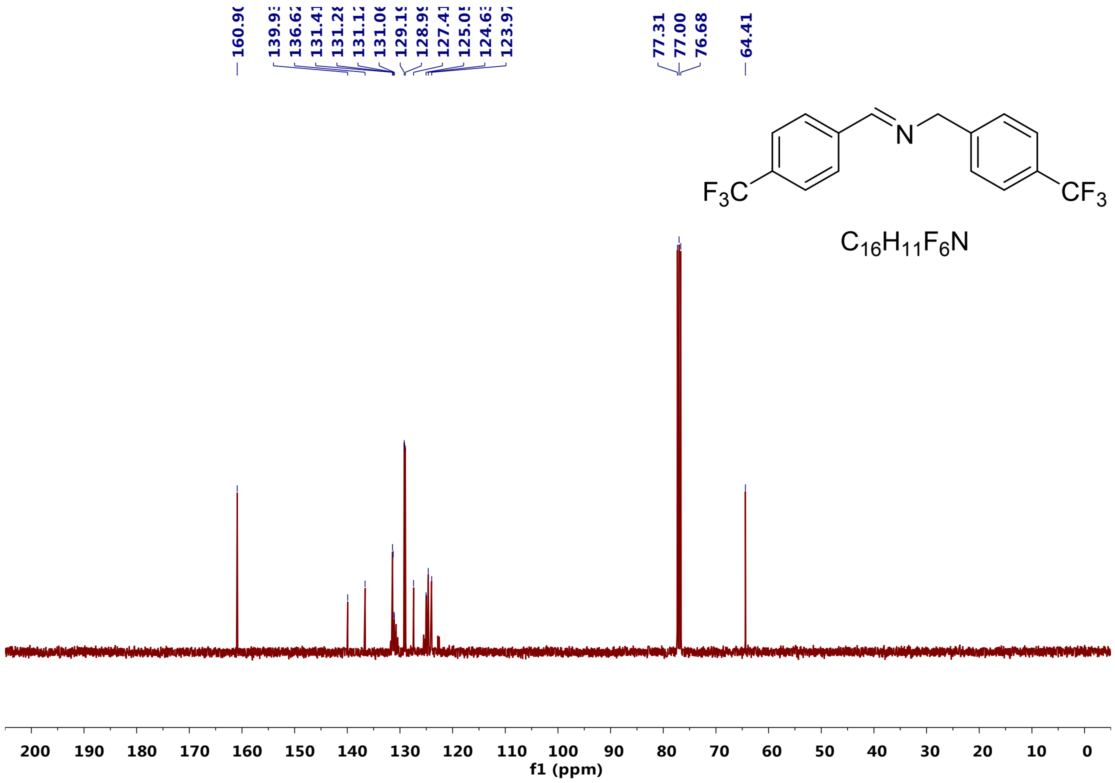
f1 (ppm)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77.00
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64.41
F3C
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CF3
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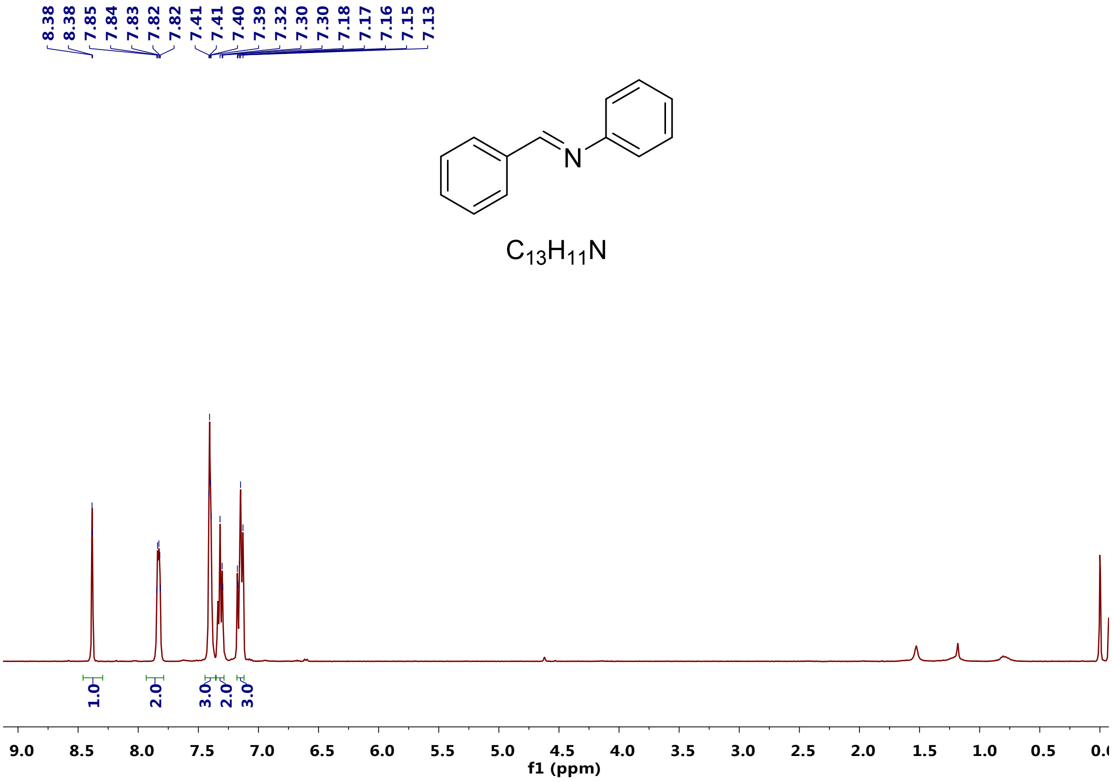
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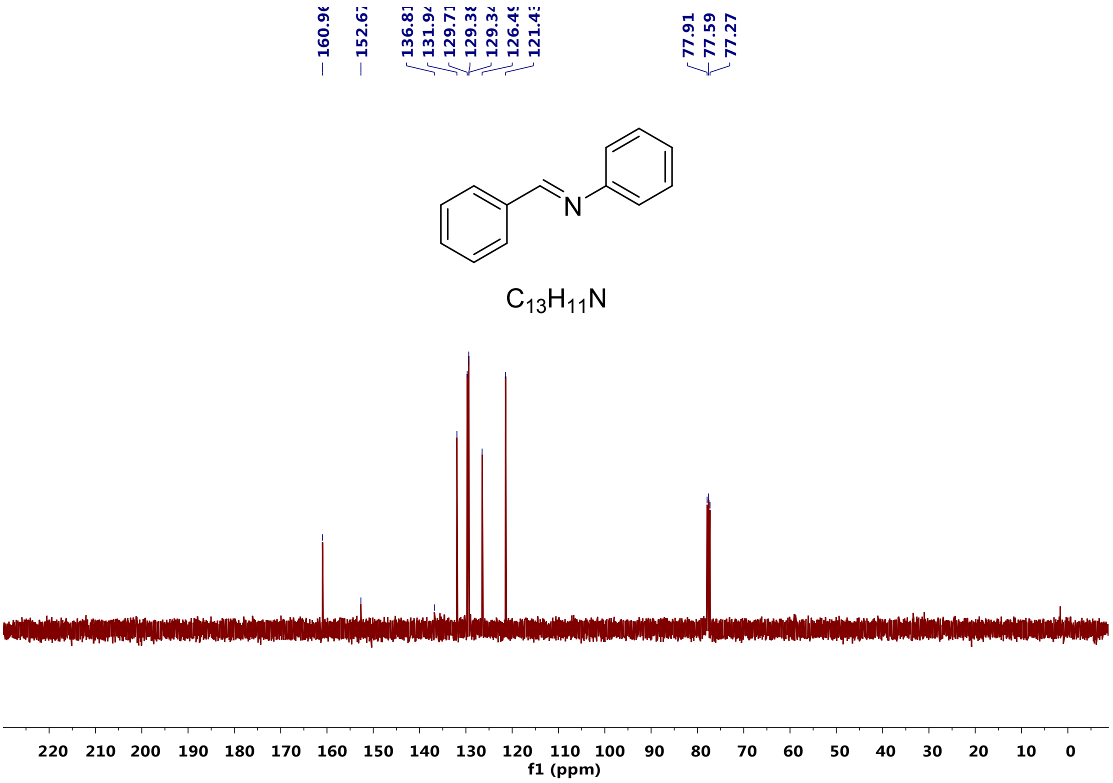
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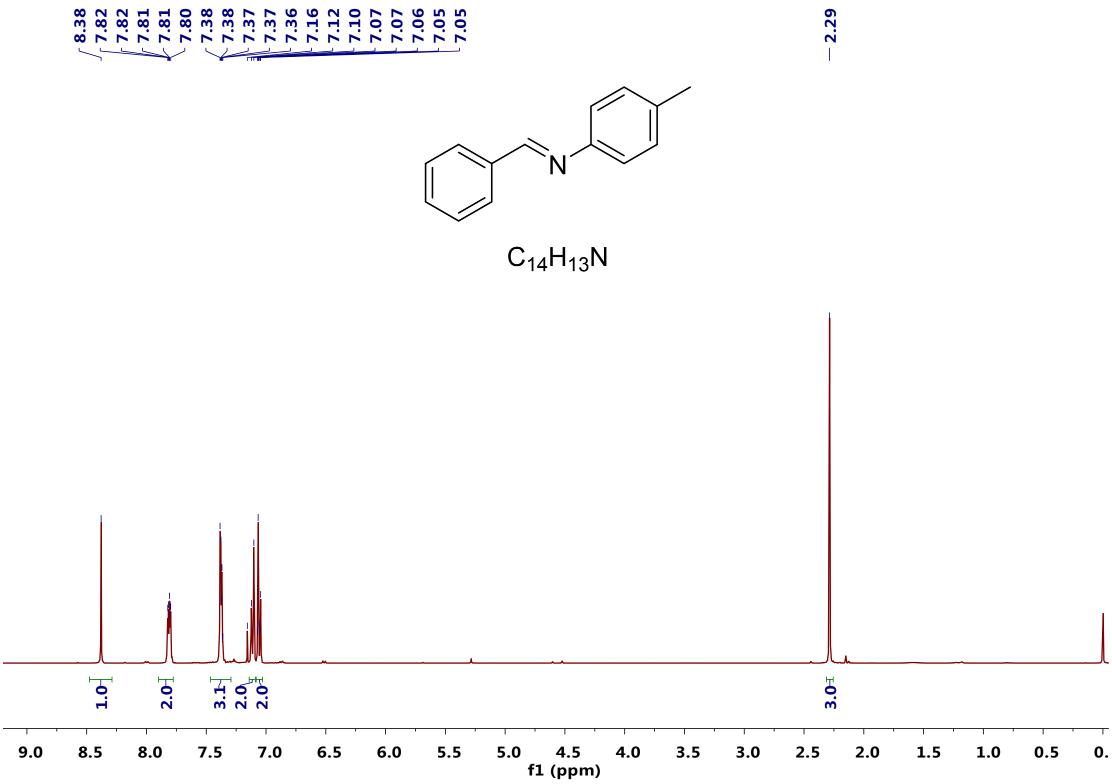
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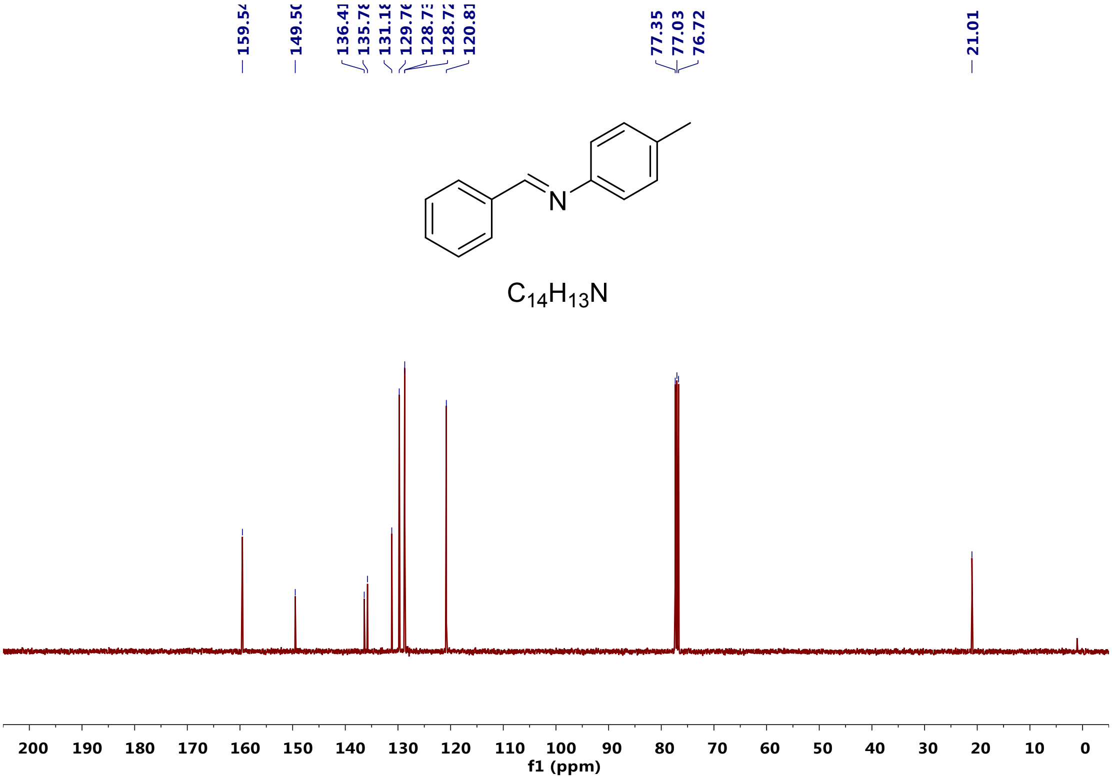
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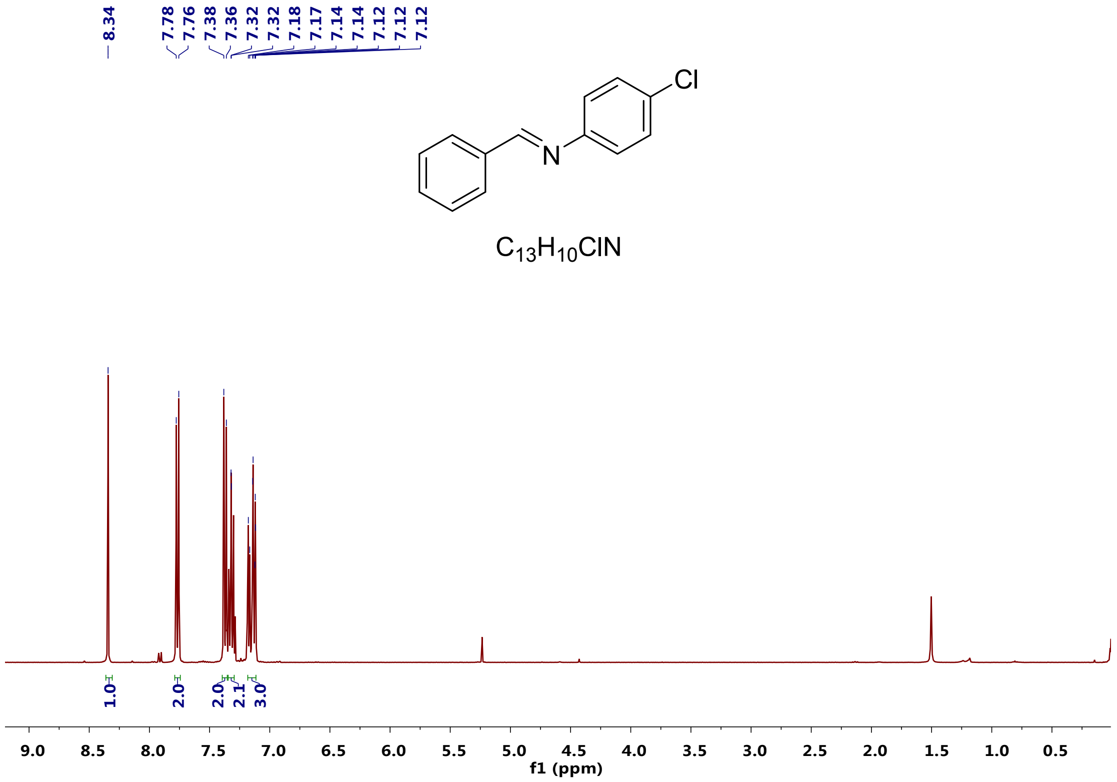
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7.12
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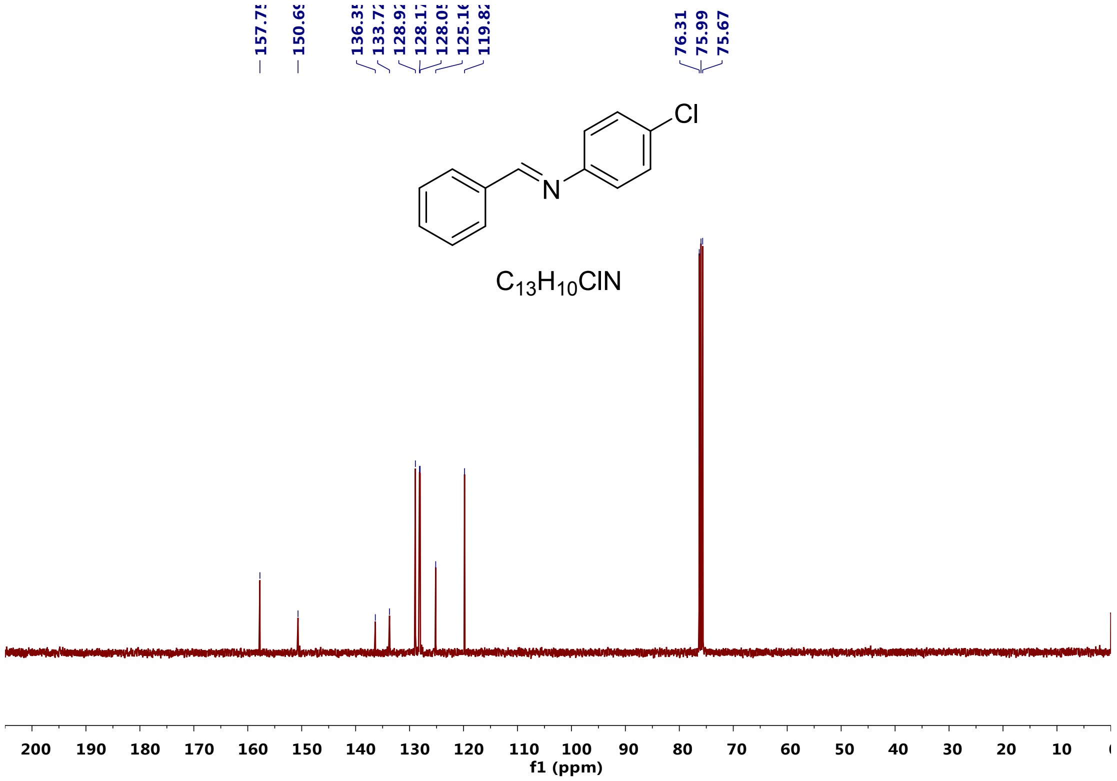
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N
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190
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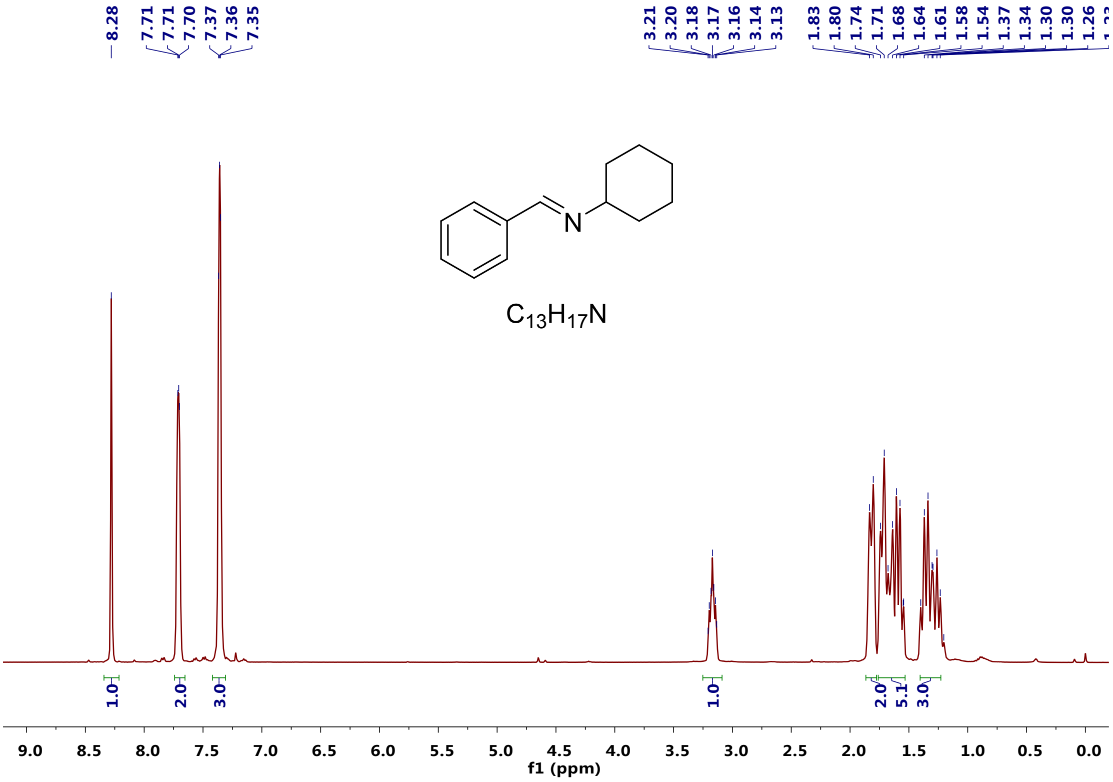
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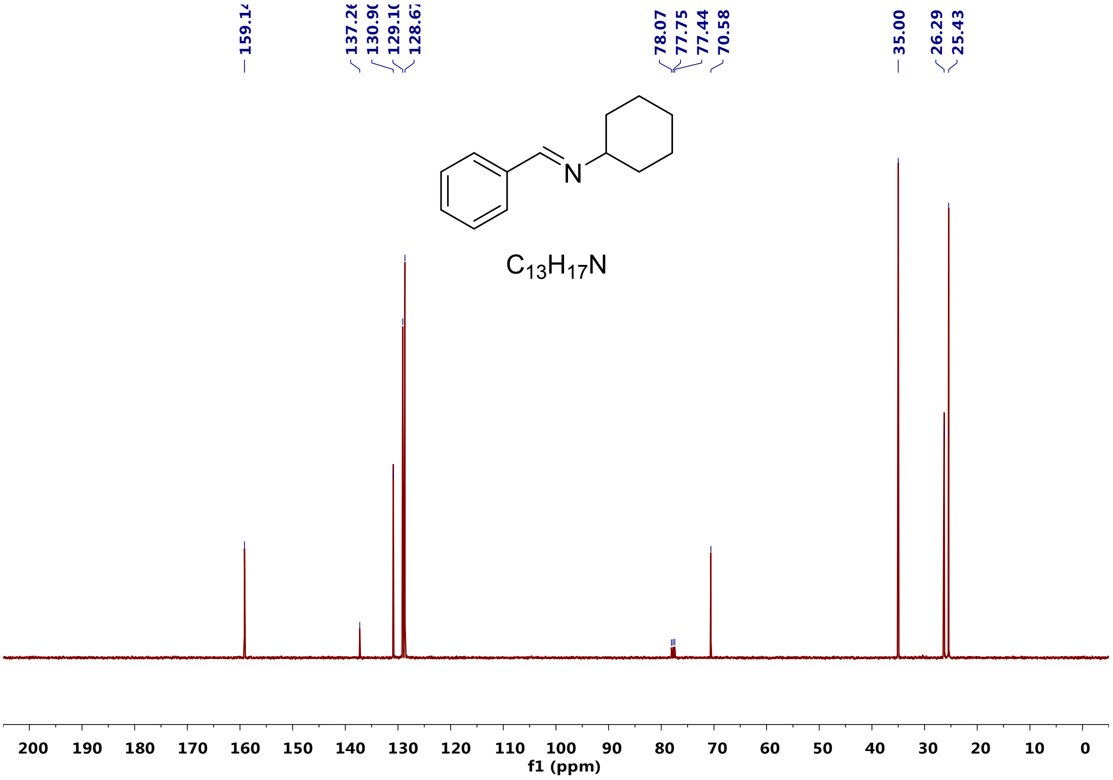
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200
190
180
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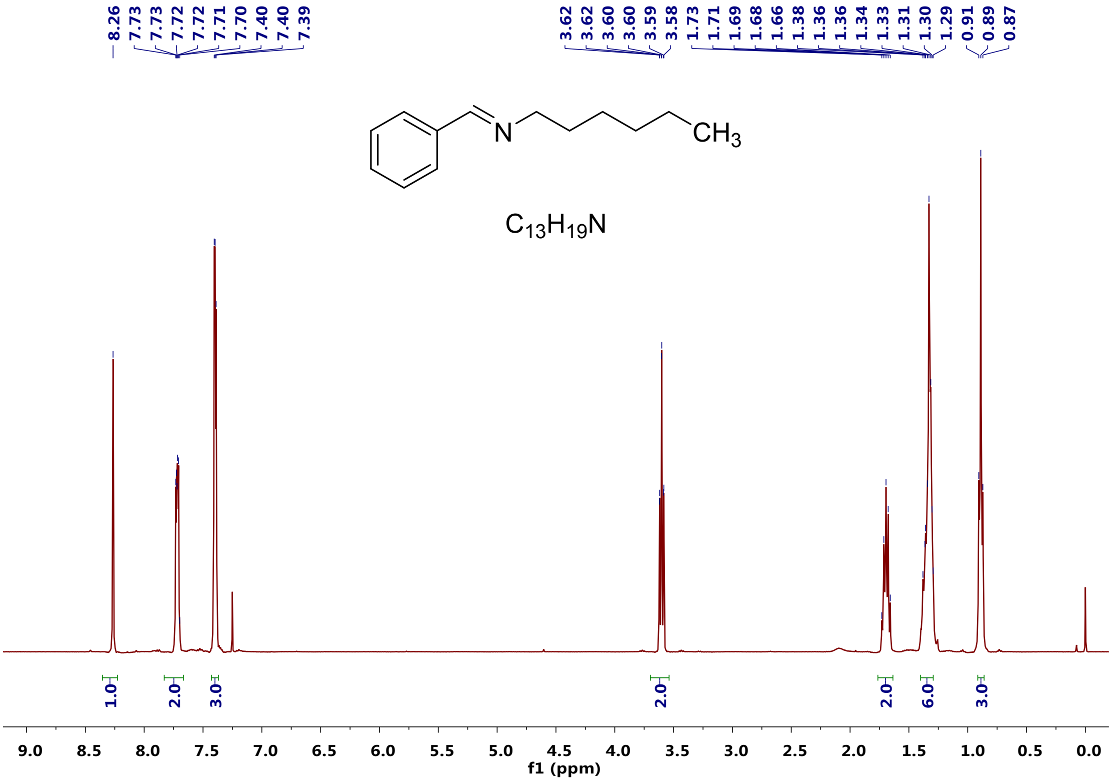
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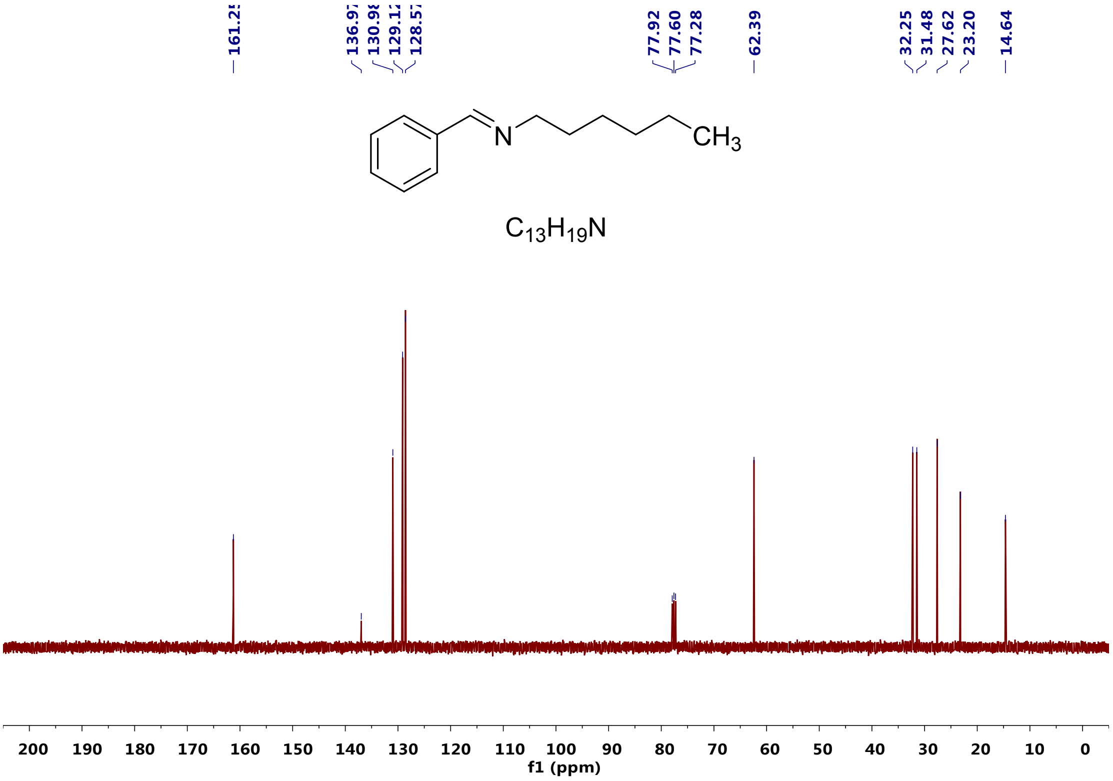
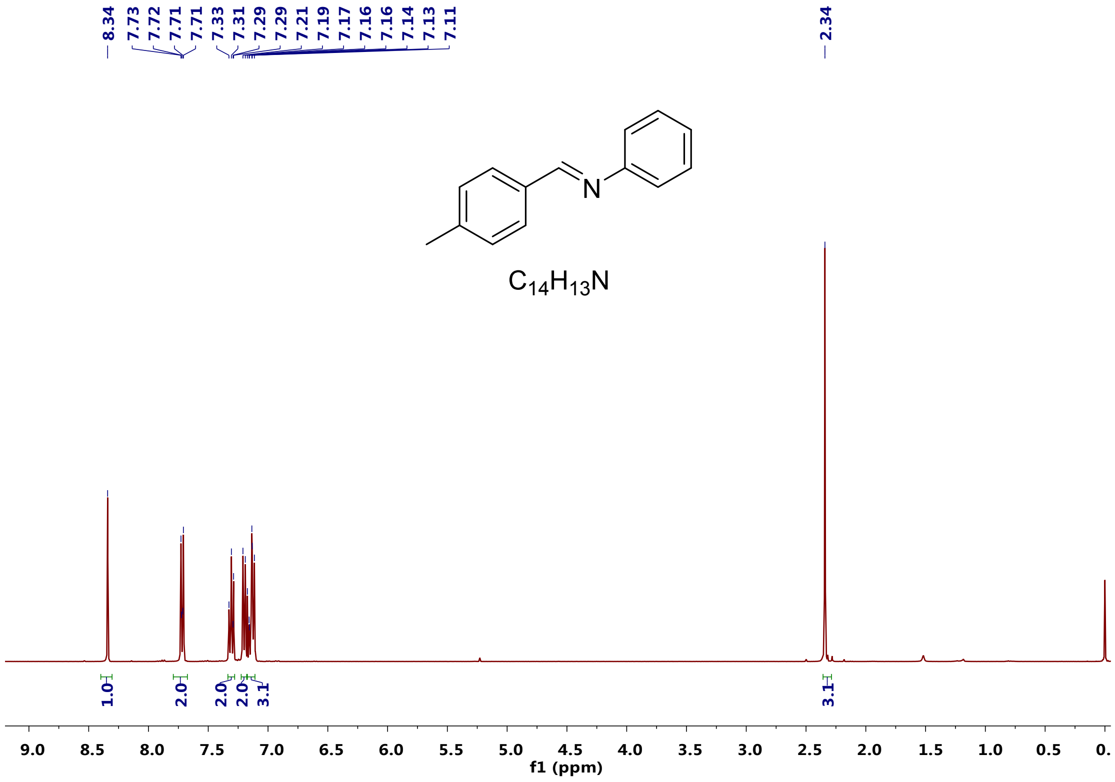
0.5
0.0
f1 (ppm)


161.2
136.9
130.9
129.1
128.5
77.92
77.60
77.28
62.39
32.25
31.48
27.62
23.20
14.64
N
CH3
C13H19N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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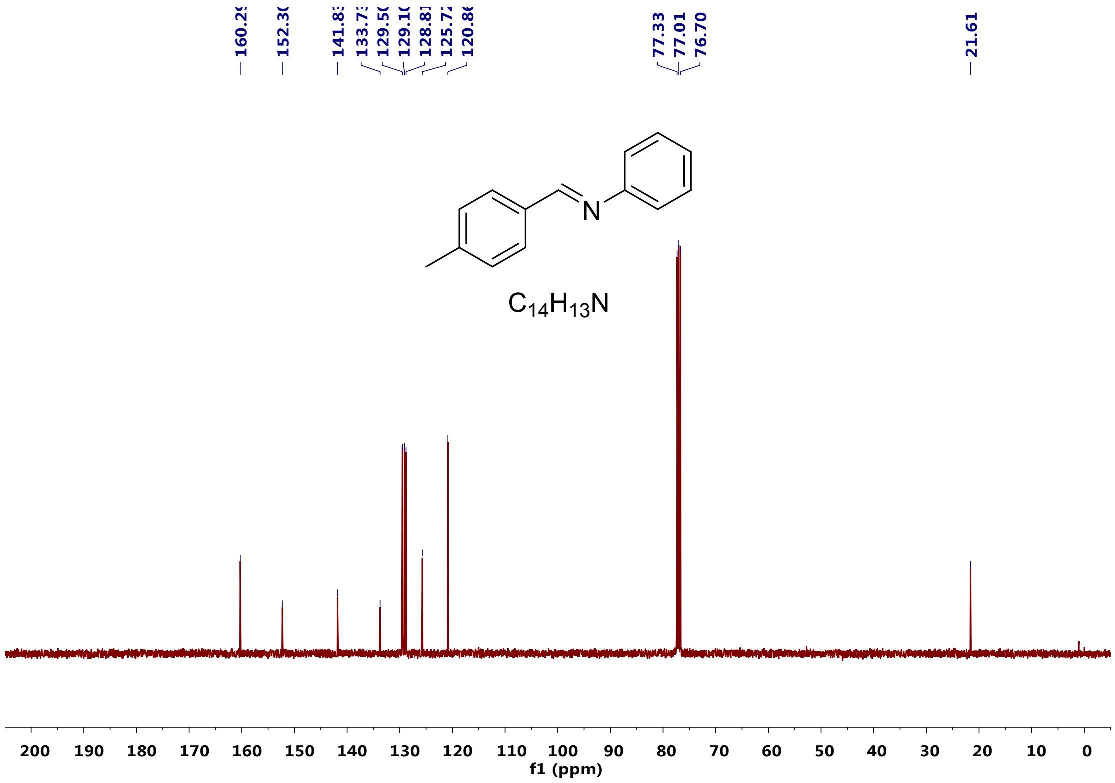
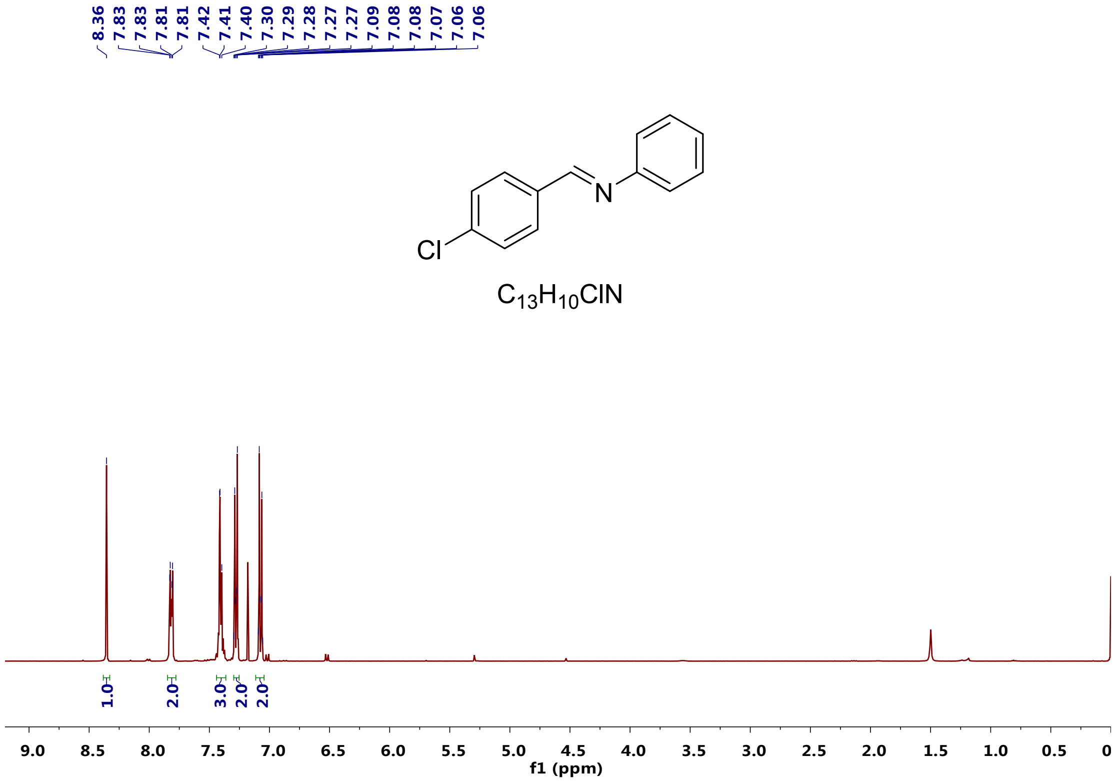
7.71
7.71
7.33
7.31
7.29
7.29
7.21
7.19
7.17
7.16
7.16
7.14
7.13
7.11
2.34
$C_{14}H_{13}N$
1.0
2.0
2.0
2.0
3.1
3.1
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)


160.2
152.3
141.8
133.7
129.5
129.1
128.8
125.7
120.8
77.33
77.01
76.70
21.61
$C_{14}H_{13}N$
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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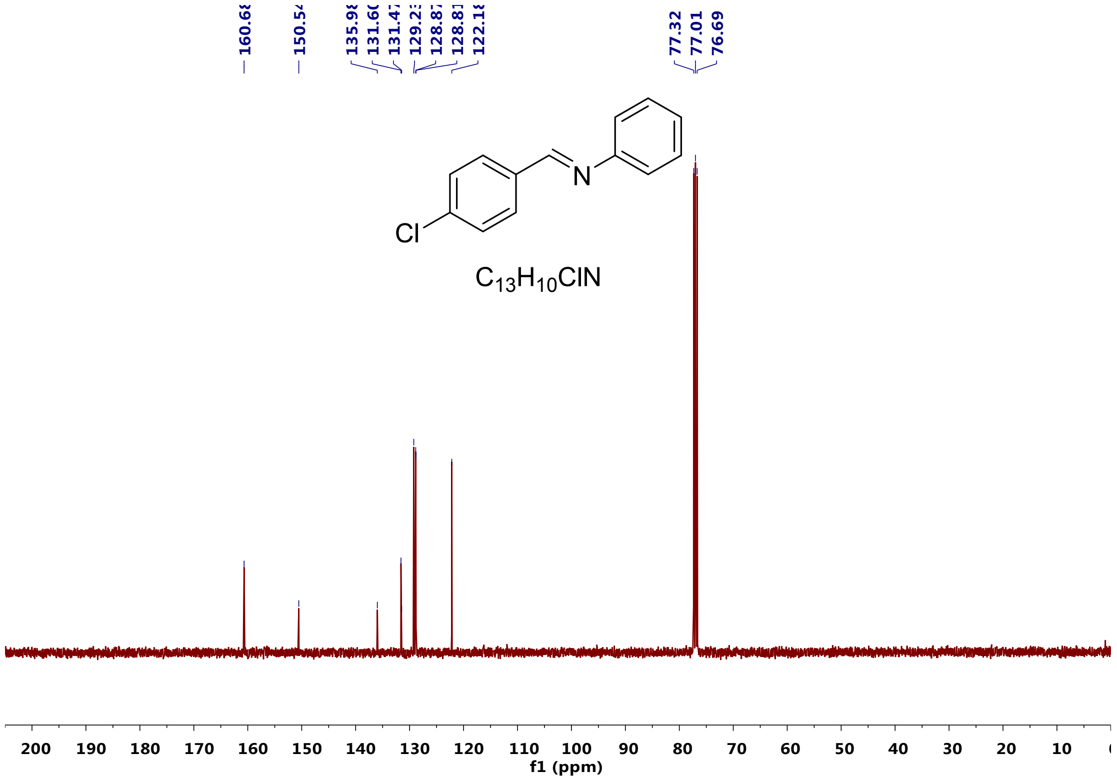
7.83
7.83
7.81
7.81
7.42
7.41
7.40
7.30
7.29
7.28
7.27
7.27
7.09
7.08
7.08
7.07
7.06
7.06
Cl
N
$C_{13}H_{10}ClN$
1.0
2.0
3.0
2.0
2.0
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)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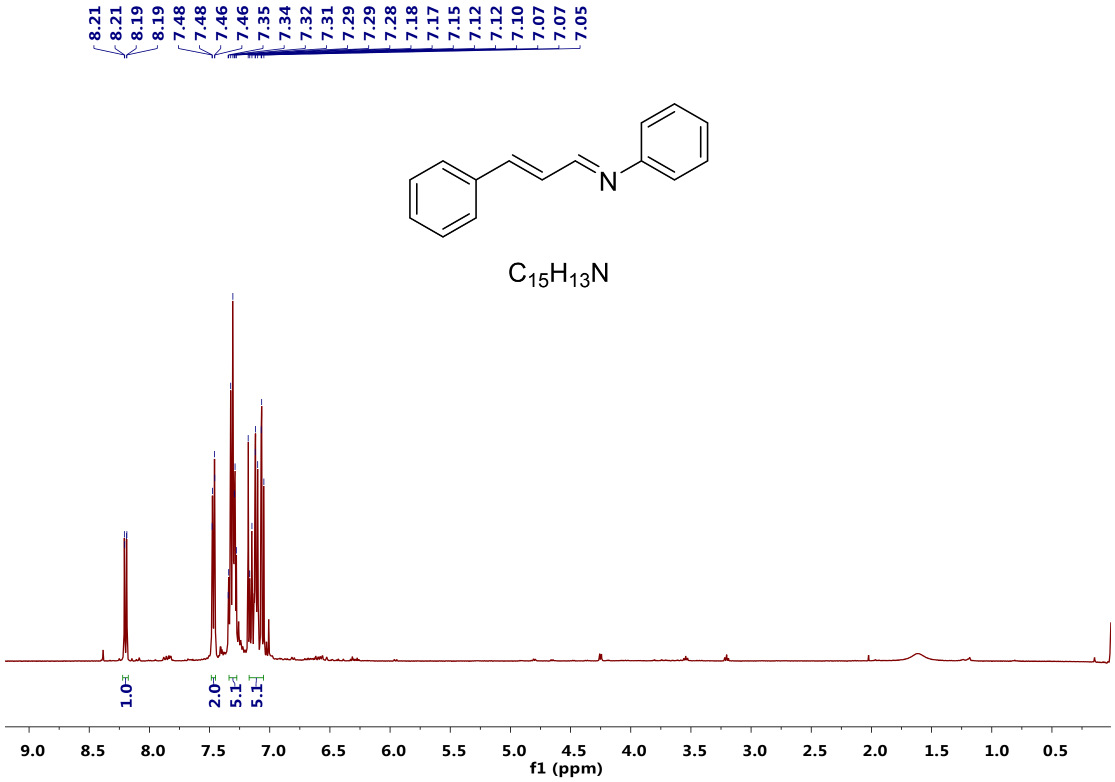
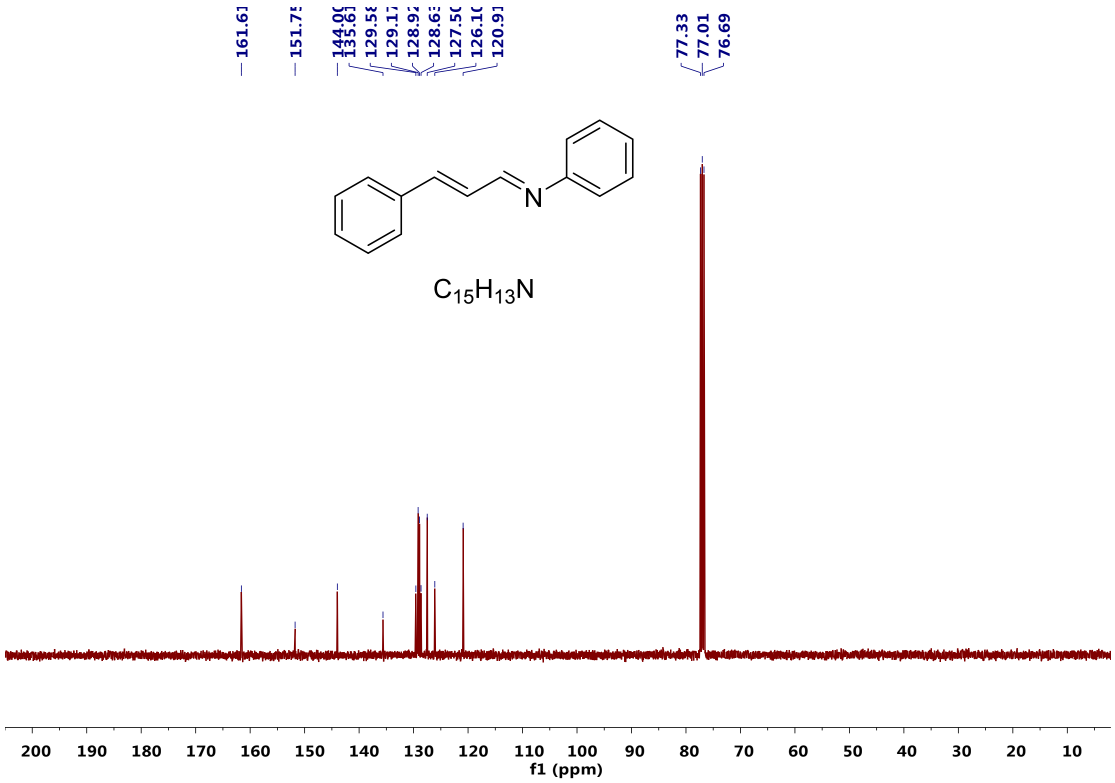
150.5
135.9
131.6
131.4
129.2
128.8
128.8
122.1
77.32
77.01
76.69
Cl
N
$C_{13}H_{10}ClN$
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.21
8.21
8.19
8.19
7.48
7.48
7.46
7.46
7.35
7.34
7.32
7.31
7.29
7.29
7.28
7.18
7.17
7.15
7.12
7.12
7.10
7.07
7.07
7.05
N
$C_{15}H_{13}N$
1.0
2.0
5.1
5.1
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


161.6
151.7
144.0
135.6
129.5
129.1
128.9
128.6
127.5
126.1
120.9
77.33
77.01
76.69
N
$C_{15}H_{13}N$
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)