Electronic Supplementary Information (ESI) for

Selective primary aniline synthesis through supported Pd-catalyzed acceptorless dehydrogenative aromatization by utilizing hydrazine

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Experimental

Instruments and Regents

Gas chromatograghy (GC) analyses were performed on Shimadzu GC-2014 equipped with a flame ionization detector (FID) and an InertCap5 capillary column. GC mass spectroscopy (GC-MS) spectra were recorded on Shimadzu GCMS-QP2010 equipped with an InertCap5 capillary column at an ionization voltage of 70 eV. Liquid-state nuclear magnetic resonance (NMR) spectra were recorded on JEOL JNM-ECA-500. ^{1}H and ^{13}C NMR spectra were measured at 500.2 and 125.8 MHz, respectively, using tetramethylsilane (TMS) as an internal standard (δ = 0 ppm). ICP-AES analyses were performed on Shimadzu ICPS-8100. TEM observations were performed on JEOL JEM-2000EX. XRD patterns were measured on Rigaku SmartLab (Cu Kα, λ = 1.5405 Å, 45 kV, 200 mA). XPS spectra were measured on Ulvac-Phi PHI5000 VersaProbe. The binding energies were calibrated by using the C 1s signal at 284.8 eV. Column chromatography on silica gel was performed on Biotage Isolera. IR spectra were measured on Jasco FT/IR-4100 using KBr disks. Hydroxyapatite (HAP, BET surface area: 11 m^2 g^{-1}, 011-14882, FUJIFILM Wako Pure Chemical), Al_2O_3 (BET surface area: 160 m^2 g^{-1} after calcination at 600 °C for 3 h, KHS-24, Sumitomo Chemical), CeO_2 (BET surface area: 92 m^2 g^{-1}, JRC-CEO-5, Daiichi Kigenso Kagaku Kogyo), $Mg_6Al_2(OH)_{16}CO_3 \cdot 4H_2O$ (LDH, BET surface area: 51 m^2 g^{-1}, Tomita Pharmaceutical Co., Ltd.), ZrO_2 (BET surface area: 100.5 m^2 g^{-1}, JRC-ZRO-6, Catalysis Society of Japan), TiO_2 (BET surface area: 316 m^2 g^{-1}, ST-01, Ishihara Sangyo Kaisya), Pd/C (Lot. No. 217-183621, N. E. CHEMCAT), Pt/Al_2O_3 (Lot. No. 137-90020, N. E. CHEMCAT), and Ru/Al_2O_3 (Lot. No. 437-000050, N. E. CHEMCAT) were commercially available. Solvents, substrates, and metal sources were obtained from TCI, Aldrich, Kanto Chemical, FUJIFILM Wako Pure Chemical, Nacalai Tesque, Kojima Chemicals, or Combi-Blocks (reagent grade).

Preparation of Supported Pd Catalysts

The HAP-supported Pd catalyst (Pd/HAP) was prepared as follows. First, HAP (2.0 g) was added to a 60 mL aqueous solution of $PdCl_2$ (8.3 mM) and KCl (2 equivalents with respect to $PdCl_2$, 16.7 mM). After stirring vigorously for 15 min at room temperature, 1 M NaOH aq. was added dropwise to adjust the pH of the solution to 10.0. The resulting slurry was further stirred at room temperature for 24 h. The solid was then filtered off, washed with water (3 L), and dried *in vacuo* overnight to afford the hydroxide precursor (brownish yellow powder). The hydroxide precursor was then dispersed in 50 mL water and reduced by $NaBH_4$ (70 mg). The resulting slurry was further stirred vigorously at room temperature for 2 h. The solid was again filtered off, washed with water (3 L), and dried *in vacuo* overnight to afford the Pd/HAP catalyst (gray powder, Pd: 0.23 mmol g^{-1}). Other supported Pd catalysts such as Pd/Al_2O_3 (Pd: 0.24 mmol g^{-1}), Pd/CeO_2 (Pd: 0.24 mmol g^{-1}), Pd/LDH (Pd: 0.25 mmol g^{-1}), Pd/ZrO_2, (Pd: 0.22 mmol g^{-1}), and Pd/TiO_2 (Pd: 0.21 mmol g^{-1}) were prepared by the similar methods. The supported Pd amounts were determined by ICP-AES analysis.

Catalytic Reaction

The catalytic reactions were typically carried out as follows. 4-Methylcyclohexanone (**1a**, 0.5 mmol), *n*-hexadecane (internal standard, 0.1 mmol), hydrazine monohydrate ($N_2H_4 \cdot H_2O$, 1.0 mmol), *N*,*N*-dimethylacetamide (DMA, 2 mL), and a Teflon-coated magnetic stir bar were successively added into a 20 mL Schlenk flask. The solution was first stirred vigorously at room temperature for 15 minutes under an open air. Then, Pd/HAP (3 mol% with respect to **1a**) was added, and freeze-pump-thaw cycles were carried out. The reactor was connected to a balloon filled with an Ar gas, and the reaction mixture was vigorously stirred at 160 °C for 1 h. After the reaction was completed, the conversion of **1a** and the yields of products were determined by GC analysis. The products were identified by GC-MS analysis.

Isolation of Products

The procedure for isolating the desired primary aniline products were typically carried out as follows. After the reaction was completed, the catalyst was filtered off and EtOAc (20 mL) was added to the filtrate. Next, the solution was washed with brine (20 mL) for three times. The organic phase was dried with Na_2SO_4, and then evaporated to remove solvents. The crude product was subjected to column chromatography on silica gel (using *n*-hexane/EtOAc as an eluent), giving the pure product. The product was identified by GC-MS and NMR (^1H and ^{13}C) analyses.

Leaching Test

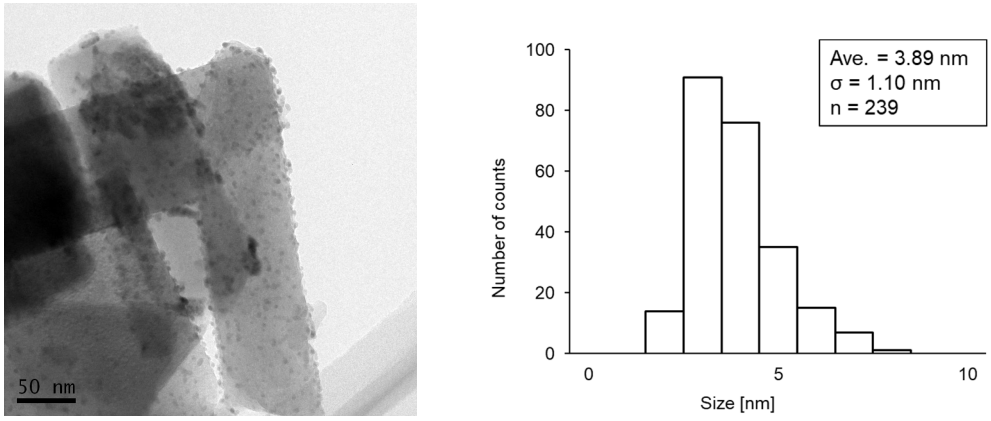
To verify the observed catalysis was truly heterogeneous or not, the Pd/HAP catalyst was removed by hot filtration 15 minutes after the dehydrogenative aromatization was started. The hot filtration test was carried out as follows. 4-Methylcyclohexanone (**1a**, 0.5 mmol), *n*-hexadecane (internal standard, 0.1 mmol), hydrazine monohydrate ($N_2H_4 \cdot H_2O$, 1.0 mmol), *N*,*N*-dimethylacetamide (DMA, 2 mL), and a Teflon-coated magnetic stir bar were successively added into a 20 mL Schlenk flask. The solution was first stirred vigorously at room temperature for 15 minutes under an open air. Then, Pd/HAP (3 mol% with respect to **1a**) was added, and freeze-pump-thaw cycles were carried out. The reactor was connected to a balloon filled with an Ar gas, and the reaction mixture was vigorously stirred at 160 °C. After stirring for 15 minutes, the catalyst was quickly filtered off under an Ar atmosphere *via* cannula filtration to another 20 mL Schlenk flask filled with Ar. Then, the filtrate moved into another 20 mL Schlenk flask was continually stirred at 160 °C. After the removal of the Pd/HAP, the reaction was completely stopped (Fig. S5, ESI†). Besides, the filtrate after the reaction for 1 h was evaporated *in vacuo* and treated with the mixture of concentrated HNO_3 (0.5 mL) and concentrated HCl (1.5 mL). Then, the solution was moved into a 100 mL volumetric flask and the Pd species were analyzed by ICP-AES. It showed that Pd species were not present in the filtrate (below the detection limit, <0.06% of Pd used for the reaction). These results indicated that the observed catalysis was truly heterogeneous.

Reuse Test

After the reaction, the Pd/HAP catalyst could be easily retrieved from the reaction mixture by simple filtration and be reused again. The reuse of catalyst was carried out as follows. The typical catalytic reaction using fresh Pd/HAP was carried out in a 20 mL Schlenk flask. After the reaction, the Pd/HAP catalysts were filtered off, washed with acetone (25 mL), and dried *in vacuo* overnight. The dried catalysts were then directly applied to the reuse reaction using the same reaction conditions. However, from the reaction profiles of three-time reuses, the reaction rates were found to gradually decrease with the reuse times (Fig. S6, ESI†). Although there was no obvious change detected from the XRD and the FT-IR analyses, the TEM images showed that the average particle size of Pd nanoparticles on HAP slightly increased after the reaction, which might be one possible reason for the decreased activity (Fig. S1, S3, and S4, ESI†).

Supplementary Figures

(a) Pd/HAP



(b) Pd/HAP after the 1st use

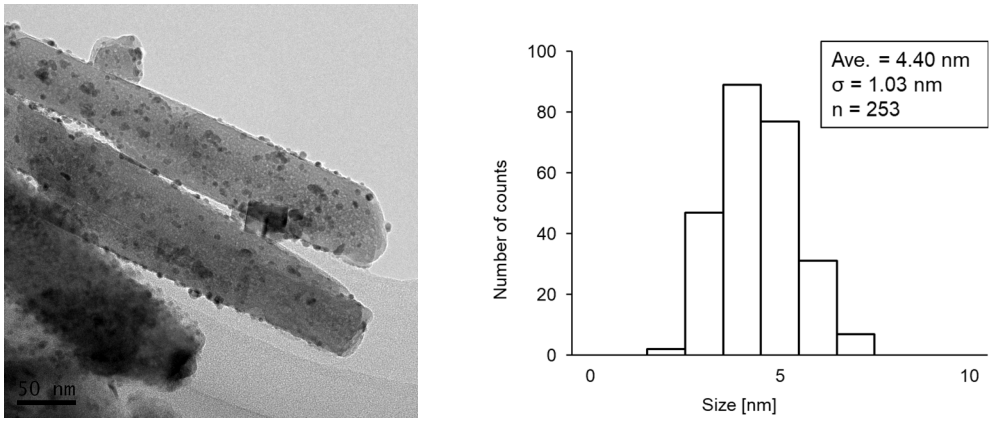


Fig. S1 TEM images and Pd nanoparticle size distributions of (a) Pd/HAP (average particle size (Ave.) = 3.89 nm; standard deviation (σ) = 1.10 nm; total number of counts (n) = 239), (b) Pd/HAP after the 1st use (Ave. = 4.40 nm; σ = 1.03 nm; n = 253).

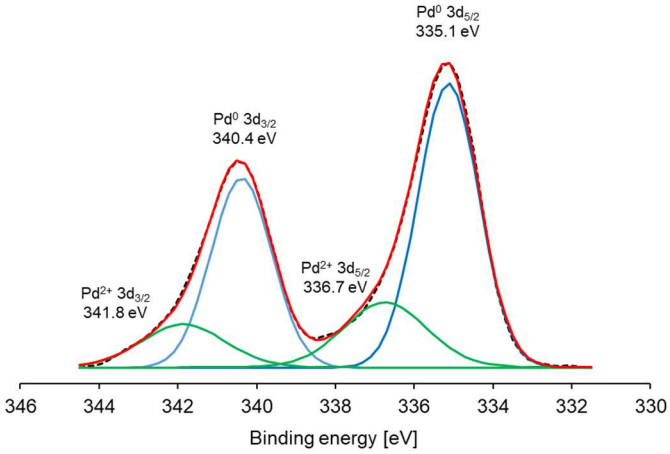


Fig. S2 Pd 3d region XPS spectra of Pd/HAP; the black broken line indicates the data points; the blue and green solid lines indicate the deconvoluted signals; the red solid line indicates the sum of the deconvoluted signals.

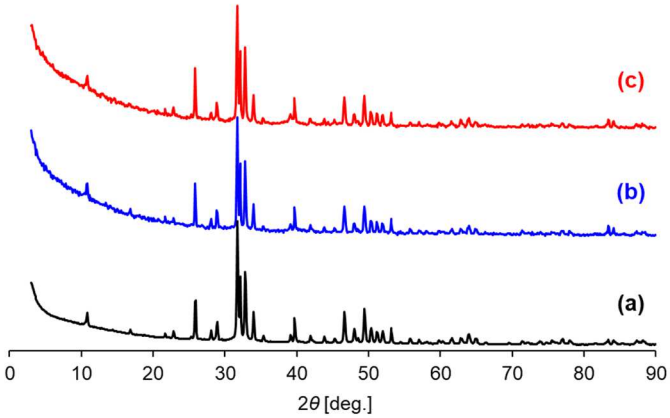
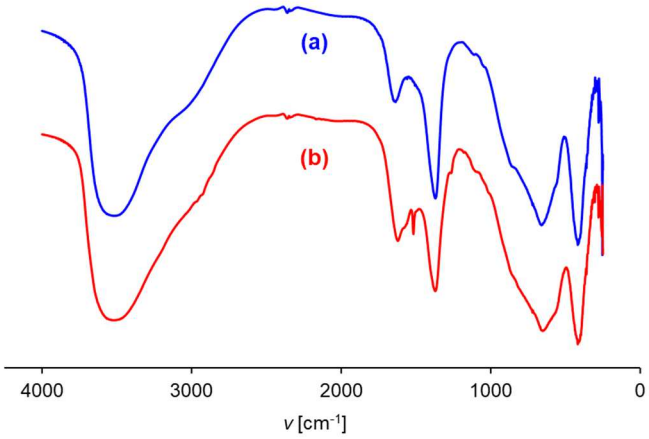


Fig. S3 XRD patterns of (a) HAP support, (b) Pd/HAP, (c) Pd/HAP after the 3rd reuse.

(I) Pd/LDH



(II) Pd/HAP

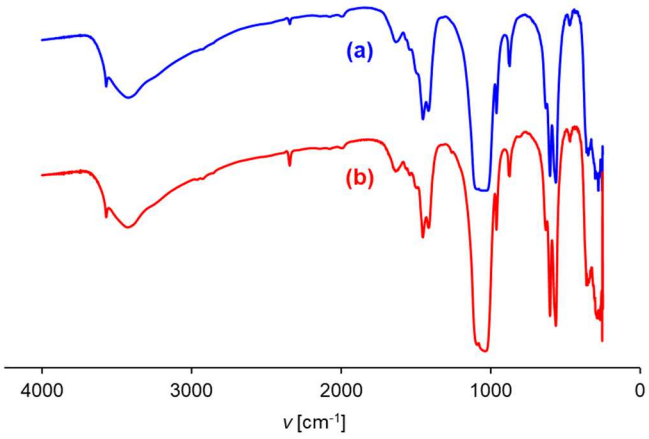


Fig. S4 FT-IR spectra of (I) Pd/LDH (a) fresh, (b) after the 1st use; (II) Pd/HAP (a) fresh, (b) after the 3rd reuse.

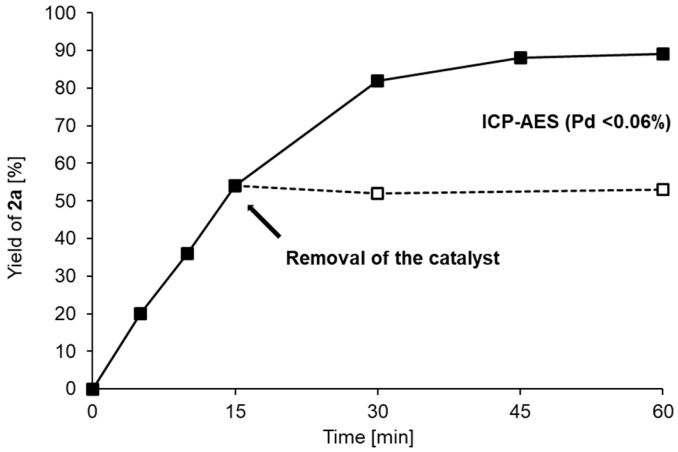


Fig. S5 Effect of removal of the Pd/HAP catalyst on the synthesis of **2a**. The "■" indicates the yields of **2a** without the removal of the catalyst; The "□" indicates the yields of **2a** after the removal of the catalyst. Reaction conditions: (first step) **1a** (0.5 mmol), $N_2H_4 \cdot H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 15 min. (second step) Pd/HAP (Pd: 3 mol% to **1a**), 160 °C, Ar (1 atm). Yields of **2a** was determined by GC analysis using *n*-hexadecane as the internal standard.

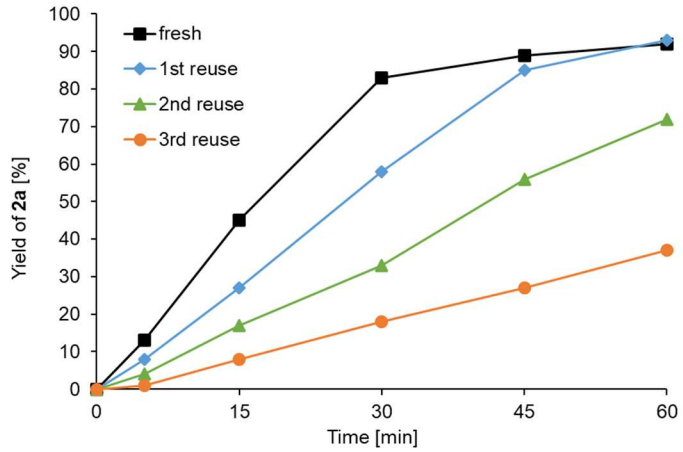


Fig. S6 The reaction profiles for the reuse experiments. Reaction conditions: (first step) **1a** (0.5 mmol), $N_2H_4 \cdot H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 15 min. (second step) Pd/HAP (Pd: 3 mol% to **1a**), 160 °C, Ar (1 atm). Yields of **2a** was determined by GC analysis using *n*-hexadecane as the internal standard.

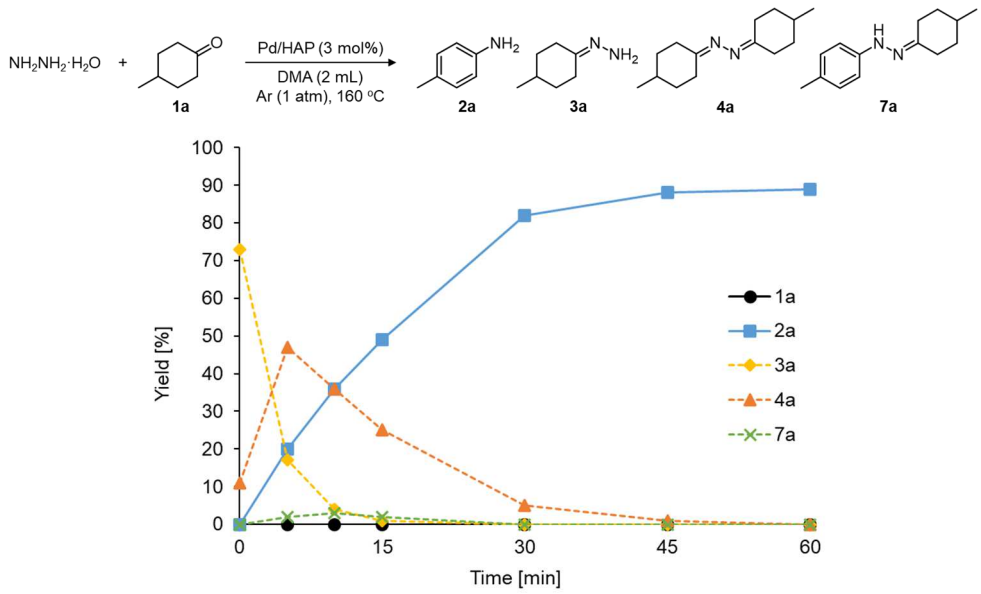


Fig. S7 The dehydrogenative aromatization reaction profile for the synthesis of **2a**. Reaction conditions: (first step) **1a** (0.5 mmol), $N_2H_4 \cdot H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 15 min. (second step) Pd/HAP (Pd: 3 mol% to **1a**), 160 °C, Ar (1 atm), 1 h. Conversions and yields were determined by GC analysis using *n*-hexadecane as the internal standard.

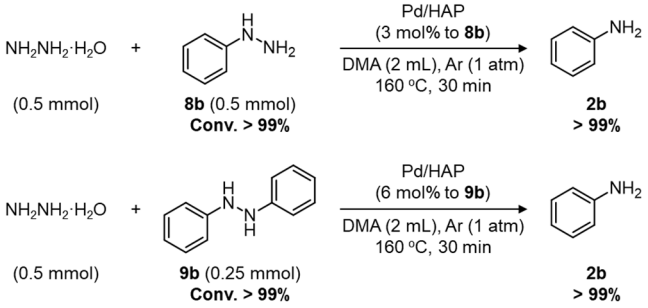


Fig. S8 Reactions starting from **8b** or **9b** under the indicated conditions.

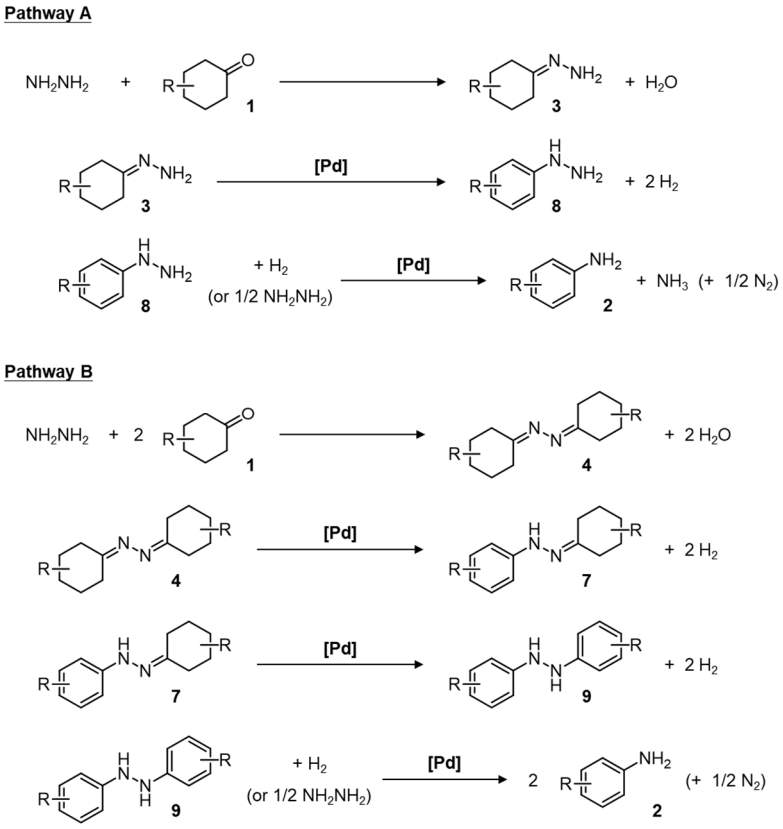
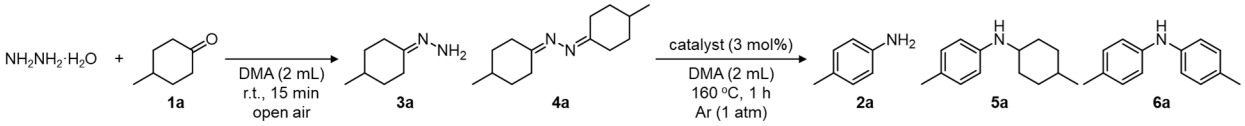


Fig. S9 The proposed reaction pathway for the Pd/HAP-catalyzed acceptorless dehydrogenative aromatization to synthesize primary anilines.

Supplementary Tables

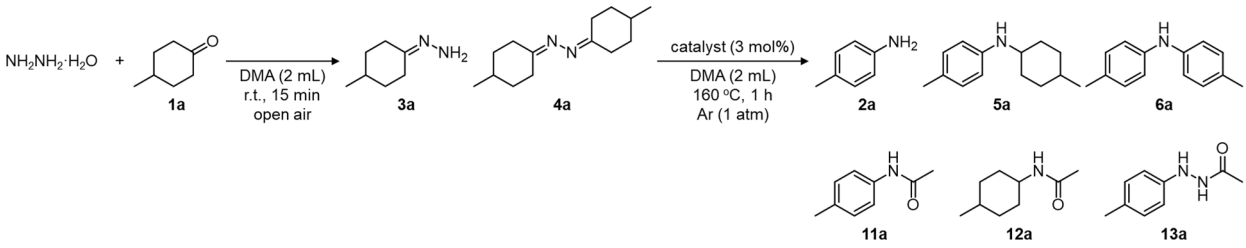
Table S1. Effect of catalysts in the presence of additives[a]



Entry	Catalyst	Conv. [%]	Yield [%]				
		1a	**2a**	**3a**	**4a**	**5a**	**6a**
1	Pd/HAP	>99	87	<1	<1	<1	<1
2[b]	Pd/HAP + LDH	>99	62	<1	<1	<1	<1
3[c]	Pd/HAP + AcOH	>99	42	<1	<1	12	8
4[d,e]	Pd/C + 4A-MS	>99	86	<1	3	<1	<1

[a] Reaction conditions: (first step) **1a** (0.5 mmol), $N_2H_4{\cdot}H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 15 min. (second step) catalyst (Pd: 3 mol% to **1a**), 160 °C, Ar (1 atm), 1 h. [b] LDH (60 mg). [c] AcOH (0.5 mmol). [d] 4A-MS (100 mg). [e] 2 h for the second step. Conversions and yields were determined by GC analysis using *n*-hexadecane as the internal standard.

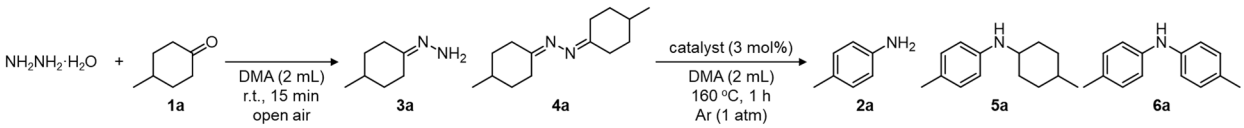
Table S2. Effect of supports on formation of the byproducts derived from DMA[a]



Entry	Catalyst	Conv. [%]	Yield [%]							
		1a	**2a**	**3a**	**4a**	**5a**	**6a**	**11a**	**12a**	**13a**
1	Pd/HAP	>99	87	<1	<1	<1	<1	<1	<1	<1
2	Pd/Al_2O_3	>99	77	<1	<1	1	<1	<1	<1	<1
3	Pd/CeO_2	>99	63	<1	<1	<1	<1	<1	<1	<1
4	Pd/LDH	>99	58	<1	<1	<1	<1	<1	<1	<1
5	Pd/C	>99	58	<1	<1	16	23	<1	<1	<1
6	Pd/ZrO_2	>99	39	<1	<1	2	1	23	9	4
7	Pd/TiO_2	>99	3	<1	29	4	<1	17	4	2

[a] Reaction conditions: (first step) **1a** (0.5 mmol), $N_2H_4{\cdot}H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 15 min. (second step) catalyst (Pd: 3 mol% to **1a**), 160 °C, Ar (1 atm), 1 h. Conversions and yields were determined by GC analysis using *n*-hexadecane as the internal standard.

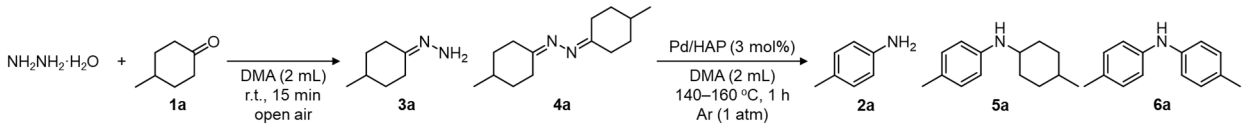
Table S3. Effect of metals[a]



Entry	Catalyst	Conv. [%]	Yield [%]				
		1a	**2a**	**3a**	**4a**	**5a**	**6a**
1	Pd/Al_2O_3	>99	77	<1	<1	1	<1
2	Pt/Al_2O_3	>99	<1	<1	97	<1	<1
3	Ru/Al_2O_3	>99	<1	5	71	<1	<1

[a] Reaction conditions: (first step) **1a** (0.5 mmol), $N_2H_4·H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 15 min. (second step) catalyst (metal: 3 mol% to **1a**), 160 °C, Ar (1 atm), 1 h. Conversions and yields were determined by GC analysis using *n*-hexadecane as the internal standard.

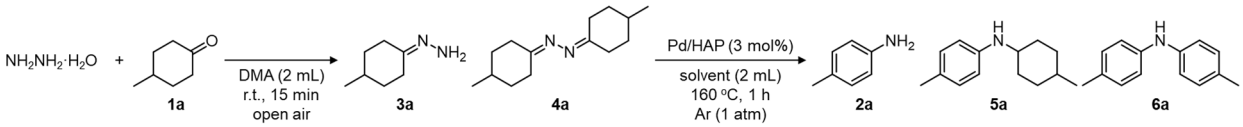
Table S4. Effect of temperatures[a]



Entry	Temperature [°C]	Conv. [%]	Yield [%]				
		1a	**2a**	**3a**	**4a**	**5a**	**6a**
1	160	>99	87	<1	<1	<1	<1
2	150	>99	46	<1	27	<1	<1
3	140	>99	1	<1	88	<1	<1

[a] Reaction conditions: (first step) **1a** (0.5 mmol), $N_2H_4·H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 15 min. (second step) Pd/HAP (Pd: 3 mol% to **1a**), 140–160 °C, Ar (1 atm), 1 h. Conversions and yields were determined by GC analysis using *n*-hexadecane as the internal standard.

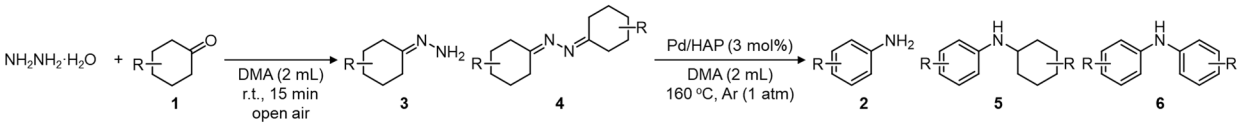
Table S5. Effect of solvents[a]



Entry	Solvent	Conv. [%]	Yield [%]				
		1a	**2a**	**3a**	**4a**	**5a**	**6a**
1	DMA	>99	87	<1	<1	<1	<1
2	NMP	>99	63	<1	2	3	<1
3[b]	diglyme	–	48	<1	<1	<1	<1
4[b]	mesitylene	–	33	<1	19	14	3

[a] Reaction conditions: (first step) **1a** (0.5 mmol), $N_2H_4 \cdot H_2O$ (1.0 mmol), solvent (2 mL), r.t., open air, 15 min. (second step) Pd/HAP (Pd: 3 mol% to **1a**), 160 °C, Ar (1 atm), 1 h. Conversions and yields were determined by GC analysis using *n*-hexadecane as the internal standard. DMA = *N*,*N*-dimethylacetamide, NMP = *N*-methyl-2-pyrrolidone, diglyme = diethylene glycol dimethyl ether. [b] Conversion could not be determined because the peak of **1a** was covered by that of solvent in GC.

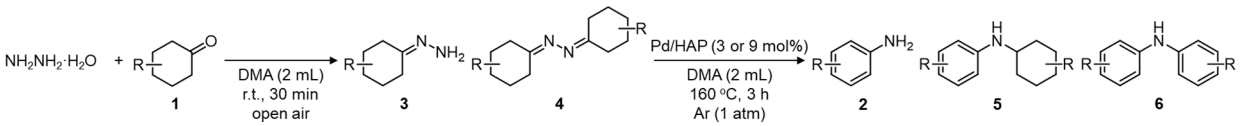
Table S6. Substrate scope[a]



Entry	Desired Product	Time [h]	Conv. [%]	Yield [%]				
				2	**3**	**4**	**5**	**6**
1	**Aniline**	1	>99	95	<1	<1	<1	<1
2	***p*-Toluidine**	1	>99	87	<1	<1	<1	<1
3	***m*-Toluidine**	1	>99	91	<1	<1	<1	<1
4	***o*-Toluidine**	1	>99	84	<1	<1	<1	<1
5[b]	**4-*tert*-Butylaniline**	1	>99	83	<1	6	<1	<1
6[b,c]	**4-Phenylaniline**	1	>99	88	<1	<1	<1	<1
7[b,d]	**2-Phenylaniline**	1	>99	65	<1	<1	<1	<1
8[b,e,f]	**2,6-Dimethylaniline**	3	77	47	1	<1	<1	<1
9[b,g]	**4-(4-Aminophenyl)phenol**	2	>99	77	<1	<1	<1	<1
10[b,e,h]	**4-(Trifluoromethyl)aniline**	2	>99	51	<1	<1	<1	<1
11[b,p]	**2-Methoxyaniline**	2	>99	75	<1	2	1	1
12[b,h,i,p]	**4-(Ethoxycarbonyl)aniline**	4	>99	76	<1	2	<1	<1
13[b,j]	**4-Acetamidoaniline**	2	>99	63	<1	<1	<1	<1
14[b]	**4-(1,4-Dioxaspiro[4,5]decan-8-yl)aniline**	1	>99	85	<1	<1	<1	<1
15[b,k]	**4-(*tert*-Butyldimethylsilyloxy)aniline**	3	>99	50	<1	7	<1	<1
16[b,l,p]	**4-(*tert*-Butoxycarbonylamino)aniline**	2	>99	37	<1	<1	<1	<1
17[m,n,p]	**1,4-Benzenediamine**	1	>99	68	<1	<1	<1	<1
18[m,o]	**1,3-Benzenediamine**	1	>99	50	<1	<1	<1	<1

[a] Reaction conditions: (first step) substrate (0.5 mmol), $N_2H_4 \cdot H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 15 min. (second step) Pd/HAP (Pd: 3 mol% to substrate), 160 °C, Ar (1 atm). Yields were determined by GC analysis. [b] 30 min for the first step. [c] Biphenyl (7% yield) was produced. [d] Biphenyl (9% yield), cyclohexylbenzene (5% yield), and 2-phenylphenol (7% yield) were produced. [e] Pd/HAP (Pd: 9 mol% to substrate). [f] $N_2H_4 \cdot H_2O$ (3.0 mmol). [g] 4-Cyclohexylphenol (2% yield) was produced. [h] 4A-MS (100 mg) was added. [i] Ethyl benzoate (5% yield) and ethyl cyclohexanecarboxylate (3% yield) were produced. [j] *N*-cyclohexylacetamide (8% yield) was produced. [k] Aniline (10% yield) and *tert*-butyldimethylsiloxycyclohexane (5% yield) were produced. [l] *tert*-Butyl *N*-phenylcarbamate (3% yield) and *tert*-butyl *N*-cyclohexylcarbamate (3% yield) was produced. [m] $N_2H_4 \cdot H_2O$ (2.0 mmol). [n] Aniline (13% yield) was produced. [o] Aniline (29% yield) was produced. [p] The values of yields are average of two runs.

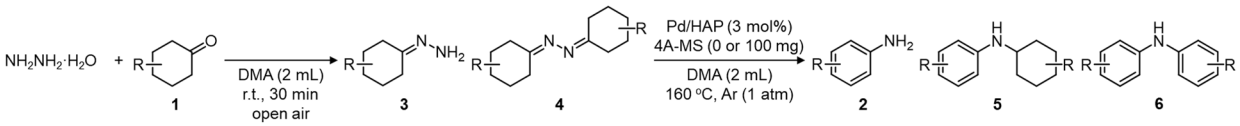
Table S7. Effect of Pd/HAP amount and hydrazine amount on 2,6-dimethylaniline synthesis.



Entry	Substituent	Amount		Conv.	Yield [%]				
		Pd [mol%]	$N_2H_4·H_2O$ [mmol]	[%]	**2**	**3**	**4**	**5**	**6**
1	2,6-Dimethyl	9	3.0	77	47	1	<1	<1	<1
2		3	3.0	87	29	16	19	<1	<1
3		3	1.0	41	16	4	7	<1	<1

[a] Reaction conditions: (first step) substrate (0.5 mmol), $N_2H_4·H_2O$ (1.0 or 3.0 mmol), DMA (2 mL), r.t., open air, 30 min. (second step) Pd/HAP (Pd: 3 or 9 mol% to substrate), 160 °C, Ar (1 atm), 3 h. Conversions and yields were determined by GC analysis using *n*-hexadecane as the internal standard.

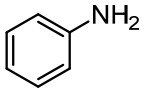
Table S8. Effect of 4A-MS on 4-(trifluoromethyl)aniline and 4-(ethoxycarbonyl)aniline synthesis.



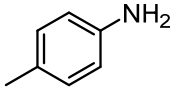
Entry	Substituent	Amount	Time	Conv.	Yield [%]				
		4A-MS (mg)	[h]	[%]	**2**	**3**	**4**	**5**	**6**
1[b]	4-(Trifluoromethyl)	100	2	>99	51	<1	<1	<1	<1
2[b]		100	1	>99	46	<1	6	<1	<1
3[b]		0	1	>99	45	<1	<1	8	<1
4	4-(Ethoxycarbonyl)	100	4	>99	81	<1	1	<1	<1
5		100	2	>99	71	<1	14	<1	<1
6		0	2	>99	71	<1	<1	17	<1

[a] Reaction conditions: (first step) substrate (0.5 mmol), $N_2H_4·H_2O$ (1.0 mmol), DMA (2 mL), r.t., open air, 30 min. (second step) Pd/HAP (Pd: 3 mol% to substrate), 4A-MS (0 or 100 mg), 160 °C, Ar (1 atm). [b] Pd/HAP (Pd: 9 mol% to substrate). Conversions and yields were determined by GC analysis using *n*-hexadecane as the internal standard.

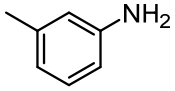
Spectral Data



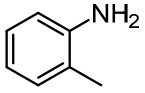
Aniline (2b) (CAS No. 62-53-3): Table 2, entry 1; 95% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 4.3 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.36 (estimated by **2a** and the effective carbon number concept[S1]). MS (70 eV, EI): *m/z* (%): 94 (7), 93 (100) [M^+], 92 (12), 67 (5), 66 (43), 65 (19), 63 (5). This GC-MS spectral data accords with those previously reported.[S2,S3]



***p*-Toluidine (2a) (CAS No. 106-49-0):** Table 2, entry 2; 87% GC yield, 59% isolated yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 6.6 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.43 (determined by calibration curve). Isolated as yellow oil (Silica gel column chromatography; eluent: *n*-hexane/EtOAc = 3/1, R_f = 0.32). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 6.97–6.95 (m, 2H), 6.61–6.59 (m, 2H), 3.50 (brs, 2H), 2.23 (s, 3H). ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$, TMS): δ 143.9, 129.9, 127.9, 115.4, 20.6. MS (70 eV, EI): *m/z* (%): 108 (6), 107 (75) [M^+], 106 (100), 80 (5), 79 (13), 78 (6), 77 (19), 53 (8), 52 (8), 51 (7). These NMR and GC-MS spectral data accord with those previously reported.[S2,S3]

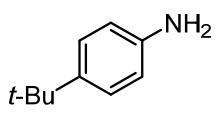


***m*-Toluidine (CAS No. 108-44-1):** Table 2, entry 3; 91% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 6.7 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.43 (estimated to be equal to that of **2a**). MS (70 eV, EI): *m/z* (%): 108 (7), 107 (96) [M^+], 106 (100), 91 (6), 89 (5), 80 (12), 79 (22), 78 (10), 77 (25), 65 (9), 63 (8), 54 (6), 53 (11), 52 (13), 51 (13), 50 (8). This GC-MS spectral data accords with those previously reported.[S2,S3]

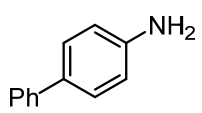


***o*-Toluidine (CAS No. 95-53-4):** Table 2, entry 4; 84% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection

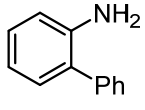
temp., 280 °C; retention time, 6.6 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.43 (estimated to be equal to that of **2a**). MS (70 eV, EI): *m/z* (%): 108 (6), 107 (81) [M^+], 106 (100), 89 (8), 80 (6), 79 (17), 78 (7), 77 (20), 53 (8), 52 (8), 51 (8). This GC-MS spectral data accords with those previously reported.[S2,S3]



4-*tert*-Butylaniline (CAS No. 769-92-6): Table 2, entry 5; 83% GC yield, 56% isolated yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 11.2 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.63 (estimated by **2a** and the effective carbon number concept[S1]). Isolated as yellow oil (Silica gel column chromatography; eluent: *n*-hexane/EtOAc = 3/1, R_f = 0.27). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.19–7.16 (m, 2H), 6.65–6.62 (m, 2H), 3.53 (brs, 2H), 1.27 (s, 9H). ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$, TMS): δ 143.9, 141.5, 126.2, 115.0, 34.0, 31.6. MS (70 eV, EI): *m/z* (%): 149 (22) [M^+], 135 (10), 134 (100), 119 (8), 118 (10), 117 (7), 107 (5), 106 (43), 94 (23), 93 (15), 91 (11), 77 (12), 66 (5), 65 (11), 63 (5), 51 (5). These NMR and GC-MS spectral data accord with those previously reported.[S2,S4]

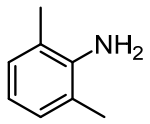


4-Phenylaniline (CAS No. 92-67-1): Table 2, entry 6; 88% GC yield, 66% isolated yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 17.6 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.76 (estimated by **2a** and the effective carbon number concept[S1]). Isolated as white solid (Silica gel column chromatography; eluent: *n*-hexane/EtOAc = 3/1, R_f = 0.25). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.54–7.51 (m, 2H), 7.42–7.36 (m, 4H), 7.27–7.22 (m, 1H), 6.75–6.72 (m, 2H), 3.69 (brs, 2H). ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$, TMS): δ 146.0, 141.3, 131.7, 128.8, 128.1, 126.5, 126.4, 115.5. MS (70 eV, EI): *m/z* (%): 170 (14), 169 (100) [M^+], 168 (21), 167 (13), 141 (9), 139 (5), 115 (14), 89 (5), 84 (12), 77 (5), 63 (7), 52 (5), 51 (7), 50 (5). These NMR and GC-MS spectral data accord with those previously reported.[S3]

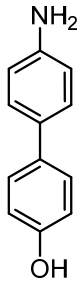


2-Phenylaniline (CAS No. 90-41-5): Table 2, entry 7; 65% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 16.0 min; relative sensitivity for

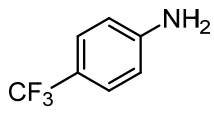
quantification (vs *n*-tetradecane, internal standard), 0.87 (estimated by **2a** and the effective carbon number concept[S1]). MS (70 eV, EI): *m/z* (%):170 (13), 169 (100) [M^+], 168 (93), 167 (43), 166 (8), 154 (5), 141 (5), 140 (5), 139 (9), 115 (16), 102 (5), 89 (9), 84 (20), 83 (5), 77 (9), 76 (6), 75 (5), 74 (6), 65 (7), 63 (14), 62 (6), 52 (9), 51 (13), 50 (8). This GC-MS spectral data accords with those previously reported.[S2]



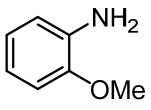
2,6-Dimethylaniline (CAS No. 87-62-7): Table 2, entry 8; 47% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 8.6 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.50 (estimated by **2a** and the effective carbon number concept[S1]). MS (70 eV, EI): *m/z* (%): 122 (9), 121 (100) [M^+], 120 (61), 107 (7), 106 (89), 104 (5), 103 (10), 93 (8), 91 (17), 79 (10), 78 (12), 77 (21), 65 (8), 53 (6), 52 (6), 51 (7). This GC-MS spectral data accords with those previously reported.[S4]



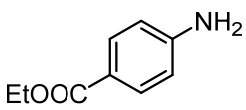
4-(4-Aminophenyl)phenol (CAS No. 1204-79-1): Table 2, entry 9; 77% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 21.3 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.73 (estimated by **2a** and the effective carbon number concept[S1]). MS (70 eV, EI): *m/z* (%): 186 (14), 185 (100) [M^+], 184 (10), 157 (6), 156 (13), 139 (5), 130 (10), 129 (5), 128 (10), 127 (6), 115 (6), 93 (12), 77 (10), 65 (8), 63 (5), 51 (5). This GC-MS spectral data accords with those previously reported.[S2,S3]



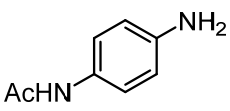
4-(Trifluoromethyl)aniline (CAS No. 455-14-1): Table 2, entry 10; 51% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 6.8 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.43 (estimated by **2a** and the effective carbon number concept[S1]). MS (70 eV, EI): *m/z* (%): 162 (8), 161 (100) [M^+], 160 (8), 143 (5), 142 (56), 140 (7), 115 (5), 114 (19), 113 (8), 111 (54), 95 (6), 88 (5), 84 (6), 83 (6), 75 (6), 71 (5), 69 (9), 65 (16), 64 (6), 63 (12), 62 (5), 52 (7), 51 (6), 50 (5). This GC-MS spectral data accords with those previously reported.[S2,S3]



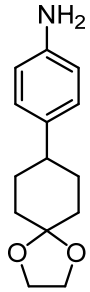
2-Methoxyaniline (CAS No. 90-04-0): Table 2, entry 11; 75% GC yield (average of two runs), 34% isolated yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 8.9 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.36 (estimated by **2a** and the effective carbon number concept[S1]). Isolated as brown oil (Silica gel column chromatography; eluent: *n*-hexane/EtOAc = 3/1, R_f = 0.45). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 6.81–6.77 (m, 2H), 6.75–6.71 (m, 2H), 3.85 (s, 3H), 3.78 (brs, 2H). ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$, TMS): δ 147.4, 136.2, 121.2, 118.6, 115.1, 110.5, 55.5. MS (70 eV, EI): *m/z* (%): 124 (7), 123 (83) [M^+], 109 (7), 108 (100), 92 (5), 81 (6), 80 (96), 65 (14), 63 (5), 54 (5), 53 (26), 52 (16), 51 (8). These NMR and GC-MS spectral data accord with those previously reported.[S2,S3]



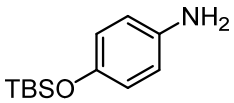
4-(Ethoxycarbonyl)aniline (CAS No. 94-09-7): Table 2, entry 12; 76% GC yield (average of two runs), 45% isolated yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (9 min), 0 °C·min^{-1} (2 min), 10 °C·min^{-1} (11 min), 0 °C·min^{-1} (3 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 15.6 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.43 (estimated by **2a** and the effective carbon number concept[S1]). Isolated as yellow solid (Silica gel column chromatography; eluent: *n*-hexane/EtOAc = 3/1, R_f = 0.31). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.87–7.84 (m, 2H), 6.65–6.62 (m, 2H), 4.32 (q, J = 7.2 Hz, 2H), 4.04 (brs, 2H), 1.36 (t, J = 7.2 Hz, 3H). ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$, TMS): δ 166.8, 150.8, 131.6, 120.2, 113.9, 60.4, 14.5. MS (70 eV, EI): *m/z* (%): 165 (25) [M^+], 137 (16), 121 (11), 120 (100), 93 (6), 92 (29), 65 (27). These NMR and GC-MS spectral data accord with those previously reported.[S2,S3]



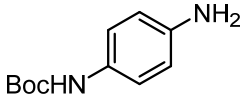
4-Acetamidoaniline (CAS No. 122-80-5): Table 2, entry 13; 63% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 17.2 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.38 (estimated by **2a** and the effective carbon number concept[S1]). MS (70 eV, EI): *m/z* (%): 150 (35) [M^+], 109 (11), 108 (100), 107 (37), 81 (18), 80 (35), 54 (6), 53 (17), 52 (11). This GC-MS spectral data accords with those previously reported.[S2]



4-(1,4-Dioxaspiro[4,5]decan-8-yl)aniline (CAS No. 389602-90-8): Table 2, entry 14; 85% GC yield, 61% isolated yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 21.4 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.76 (estimated by **2a** and the effective carbon number concept[S1]). Isolated as white solid (Silica gel column chromatography; eluent: *n*-hexane/EtOAc = 3/1, R_f = 0.23). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.03–7.01 (m, 2H), 6.63–6.60 (m, 2H), 3.96 (s, 4H), 3.55 (brs, 2H), 2.48–2.42 (m, 1H), 1.85–1.81 (m, 4H), 1.77–1.63 (m, 4H). ^{13}C{^{1}H}NMR (125 MHz, $CDCl_3$, TMS): δ 144.6, 136.9, 127.7, 115.3, 108.7, 64.4, 42.5, 35.3, 31.9. MS (70 eV, EI): *m/z* (%): 234 (6), 233 (37) [M^+], 188 (14), 134 (31), 132 (12), 130 (7), 120 (9), 119 (77), 118 (16), 117 (8), 115 (5), 106 (16), 101 (20), 100 (6), 99 (100), 93 (5), 91 (9), 86 (6), 77 (7), 66 (6), 65 (8), 57 (6), 55 (12). These NMR and GC-MS spectral data accord with those previously reported.[S2,S3]

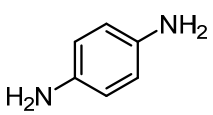


4-(*tert*-Butyldimethylsilyloxy)aniline (CAS No. 111359-74-1): Table 2, entry 15; 50% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (9 min), 0 °C·min^{-1} (2 min), 10 °C·min^{-1} (11 min), 0 °C·min^{-1} (3 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 15.8 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.76 (estimated by **2a** and the effective carbon number concept[S1]). MS (70 eV, EI): *m/z* (%): 224 (8), 223 (42) [M^+], 168 (6), 167 (27), 166 (100), 150 (6), 149 (5), 108 (6), 106 (10), 93 (7), 92 (7), 83 (5), 80 (5), 75 (12), 74 (7), 73 (15), 65 (9), 57 (6). This GC-MS spectral data accords with those previously reported.[S2]

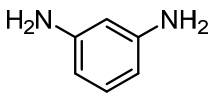


4-(*tert*-Butoxycarbonylamino)aniline (CAS No. 71026-66-9): Table 2, entry 16; 37% GC yield (average of two runs), 17% isolated yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 18.3 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.51 (estimated by **2a** and the effective carbon number concept[S1]). Isolated as brown oil (Silica gel column chromatography; eluent: DCM/EtOAc = 9/1, R_f = 0.35). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.13–7.12 (m, 2H), 6.65–6.62 (m, 2H), 6.27 (brs, 1H), 3.53 (brs,

2H), 1.50 (s, 9H). $^{13}C\{^{1}H\}$NMR (125 MHz, $CDCl_3$, TMS): δ 153.4, 142.5, 129.8, 121.0, 115.7, 80.1, 28.5. MS (70 eV, EI): *m/z* (%): 208 (11) [M^+], 153 (5), 152 (59), 135 (10), 134 (40), 109 (8), 108 (100), 107 (31), 106 (32), 105 (17), 81 (12), 80 (29), 79 (24), 78 (6), 67 (5), 59 (45), 57 (59), 56 (8), 55 (6), 54 (8), 53 (22), 52 (22), 51 (8). These NMR and GC-MS spectral data accord with those previously reported.[S2,S5]



1,4-Benzenediamine (CAS No. 106-50-3): Table 2, entry 17; 68% GC yield (average of two runs), 75% isolated yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 10.5 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.33 (estimated by **2a** and the effective carbon number concept[S1]). Isolated as pink solid (Silica gel column chromatography; eluent: chloroform/methanol = 9/1, R_f = 0.68). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 6.56 (s, 4H), 3.32 (brs, 4H). $^{13}C\{^{1}H\}$NMR (125 MHz, $CDCl_3$, TMS): δ 138.7, 116.8. MS (70 eV, EI): *m/z* (%): 109 (7), 108 (100) [M^+], 107 (28), 81 (28), 80 (55), 63 (5), 54 (18), 53 (23), 52 (22), 51 (6). These NMR and GC-MS spectral data accord with those previously reported.[S4]



1,3-Benzenediamine (CAS No. 108-45-2): Table 2, entry 18; 50% GC yield. GC conditions and analysis: InertCap5 capillary column, 0.25 mm×30 m, GL Science Inc.; carrier gas (N_2) flow rate, 1.6 mL·min^{-1}; initial column temp., 80 °C; final column temp., 280 °C; progress rate, 0 °C·min^{-1} (5 min), 10 °C·min^{-1} (20 min), 0 °C·min^{-1} (5 min); injection temp., 280 °C; detection temp., 280 °C; retention time, 11.1 min; relative sensitivity for quantification (vs *n*-hexadecane, internal standard), 0.33 (estimated by **2a** and the effective carbon number concept[S1]). MS (70 eV, EI): *m/z* (%): 109 (20), 108 (100) [M^+], 107 (12), 91 (7), 82 (5), 81 (43), 80 (69), 67 (6), 66 (5), 65 (9), 64 (8), 63 (7), 54 (18), 53 (23), 52 (17), 51 (8), 50 (6). This GC-MS spectral data accords with those previously reported.[S4]

Supplementary References

S1 (*a*) J. T. Scanlon and D. E. Willis, *J. Chromatographic Sci.*, 1985, **23**, 333–340; (*b*) T. Holm, *J. Chromatography A*, 1999, **842**, 221–227.

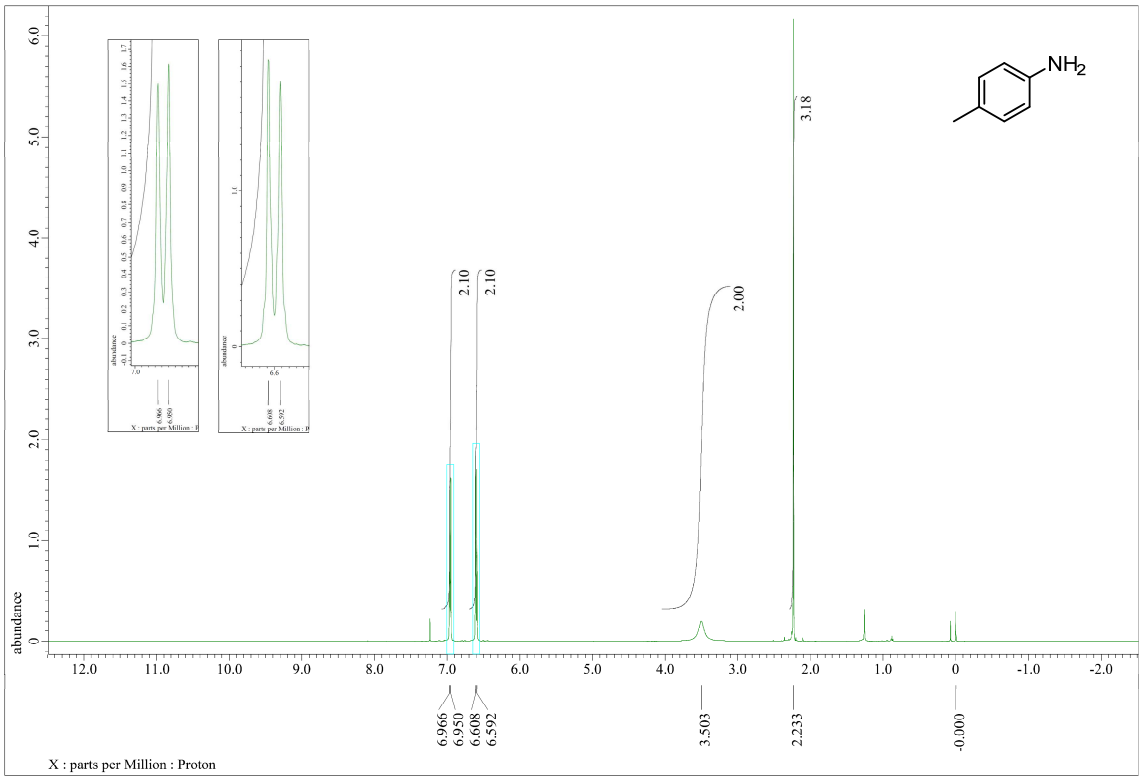
S2 Y. Koizumi, X. Jin, T. Yatabe, R. Miyazaki, J. Hasegawa, K. Nozaki, N. Mizuno and K. Yamaguchi, *Angew. Chem., Int. Ed.*, 2019, **58**, 10893–10897.

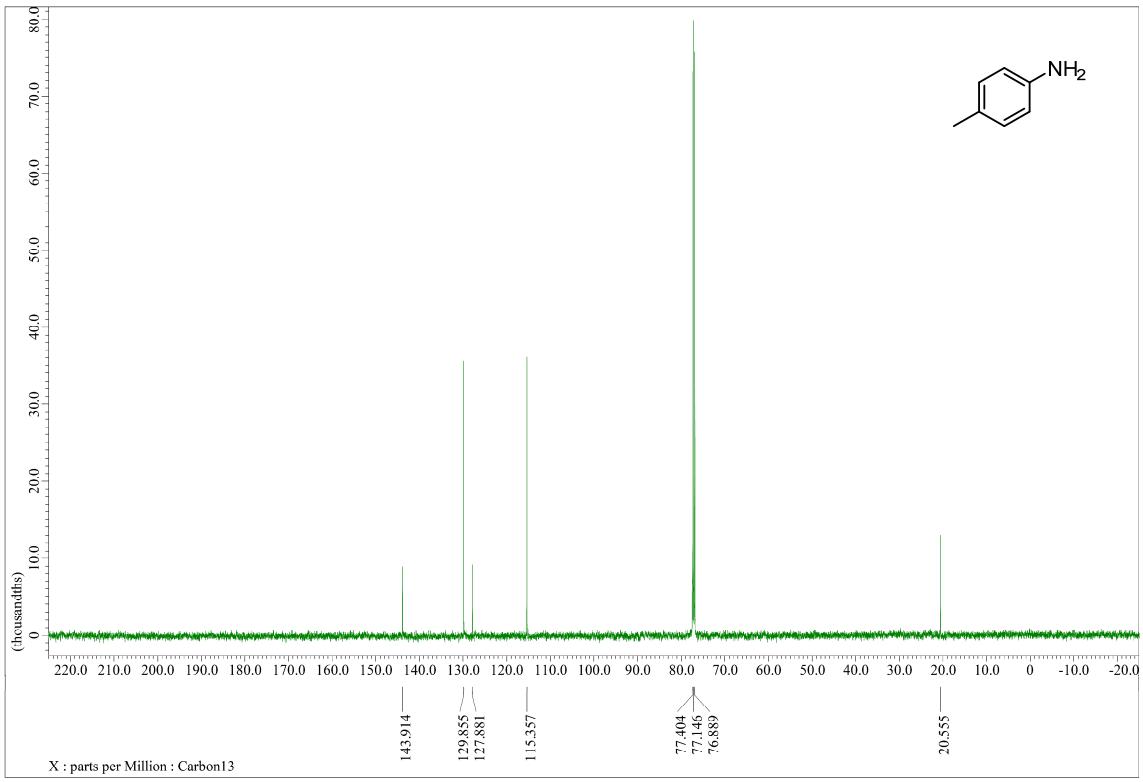
S3 X. Jin, Y. Koizumi, K. Yamaguchi, K. Nozaki and N. Mizuno, *J. Am. Chem. Soc.*, 2017, **139**, 13821–13829.

S4 AIST: National Institute of Advanced Industrial Science and Technology (Japan), URL: https://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi

S5 C. S. Isfort, T. Kreickmann, T. Pape, R. Fröhlich and F. E. Hahn, *Chem. Eur. J.*, 2007, **13**, 2344–2357.

NMR Spectra


NH2
3.18
2.10
2.10
2.00
abundance
6.966
6.950
6.608
6.592
3.503
2.233
-0.000
X : parts per Million : Proton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(thousandths)
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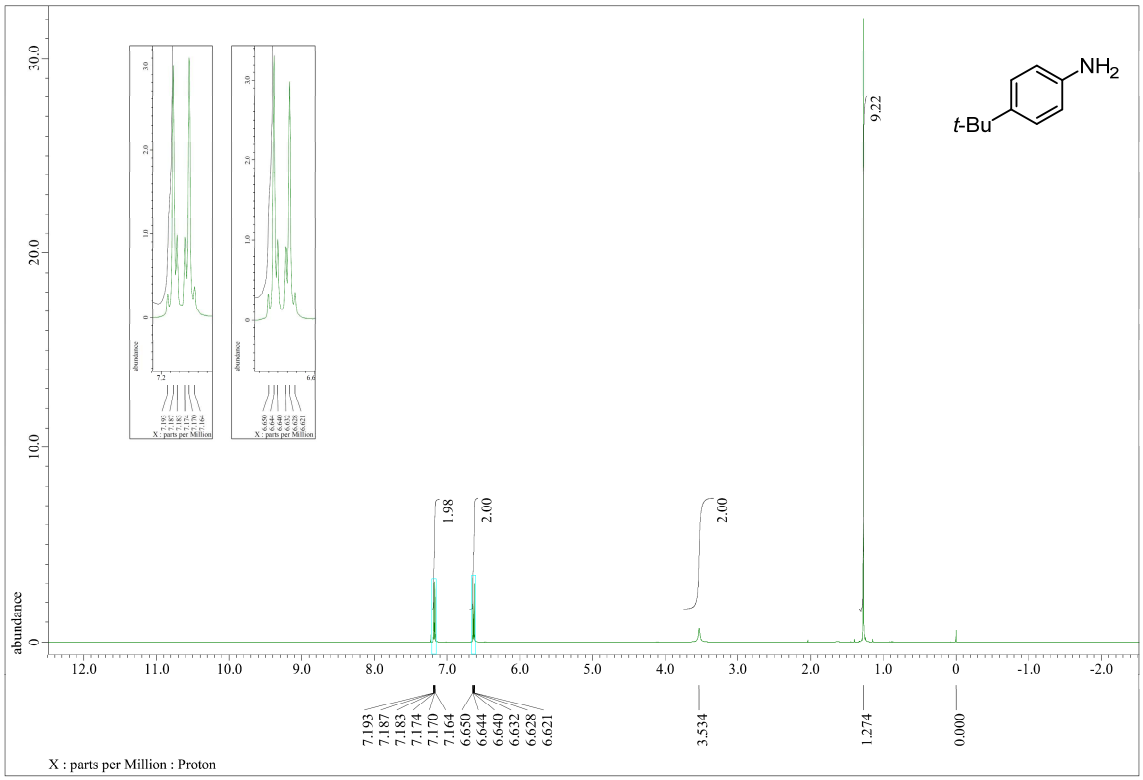
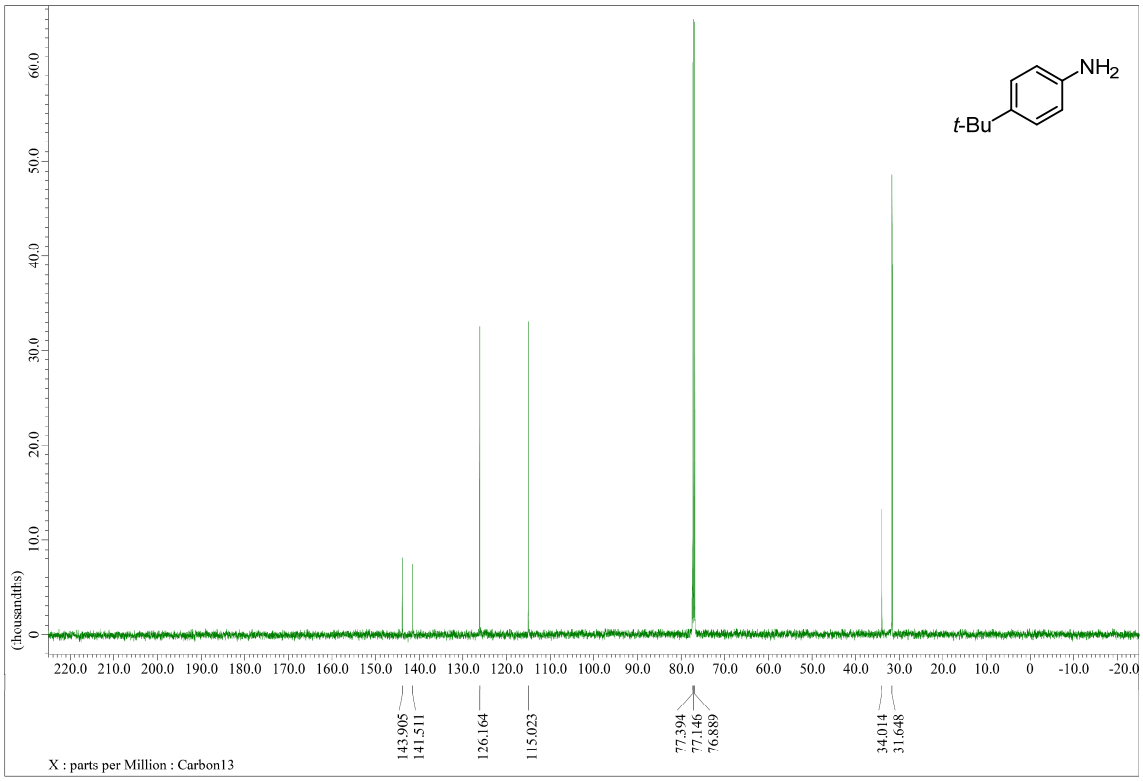
129.855
127.881
115.357
77.404
77.146
76.889
20.555
X : parts per Million : Carbon13


NH2
t-Bu
9.22
1.98
2.00
2.00
abundance
X : parts per Million : Proton
7.193
7.187
7.183
7.174
7.170
7.164
6.650
6.644
6.640
6.632
6.628
6.621
3.534
1.274
0.000


NH2
t-Bu
(thousandth's)
X : parts per Million : Carbon13
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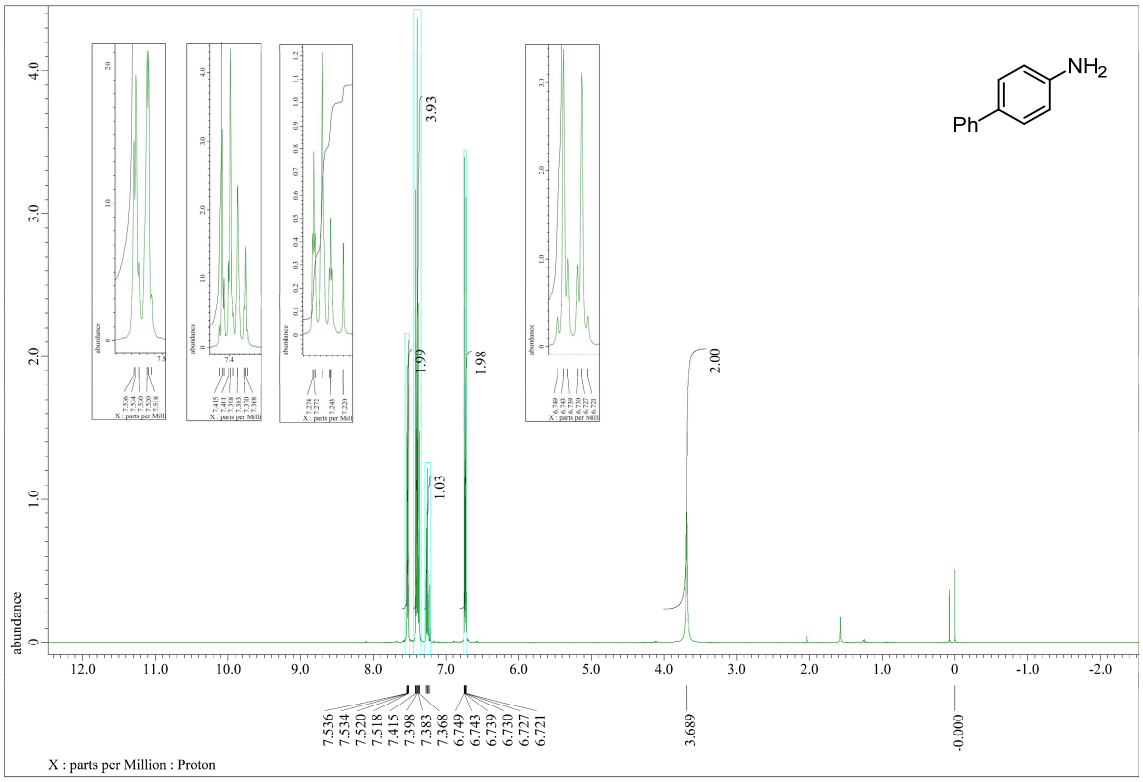
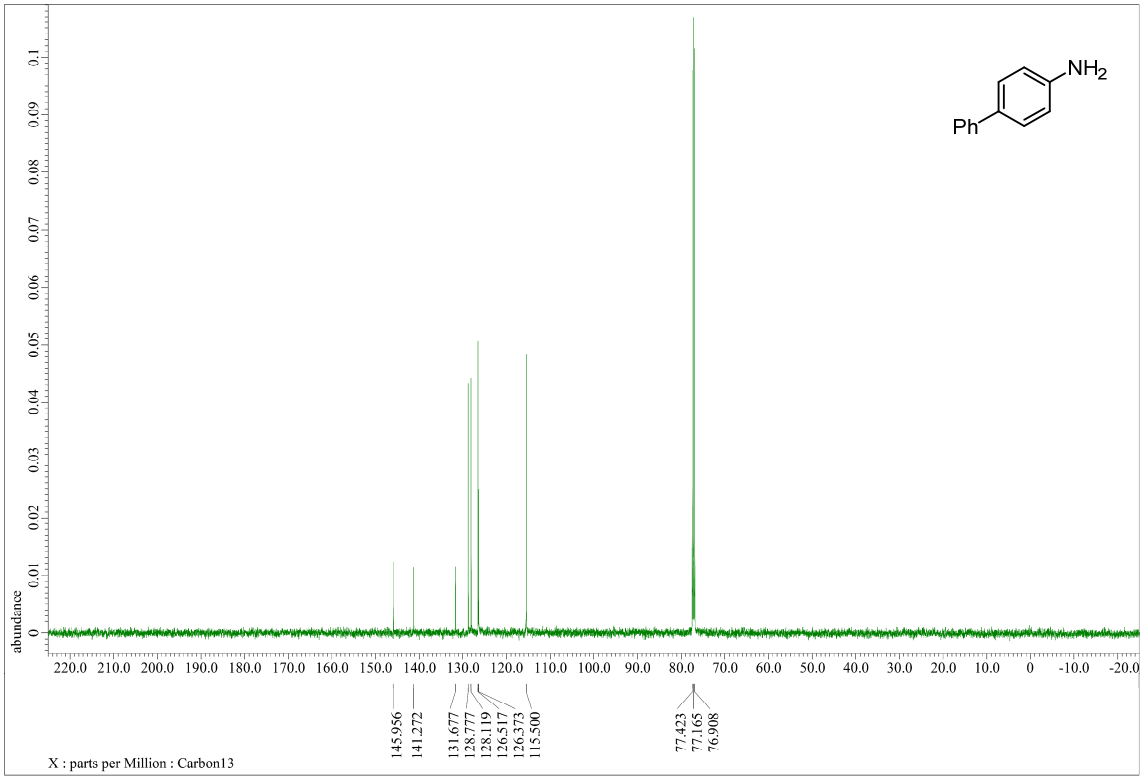
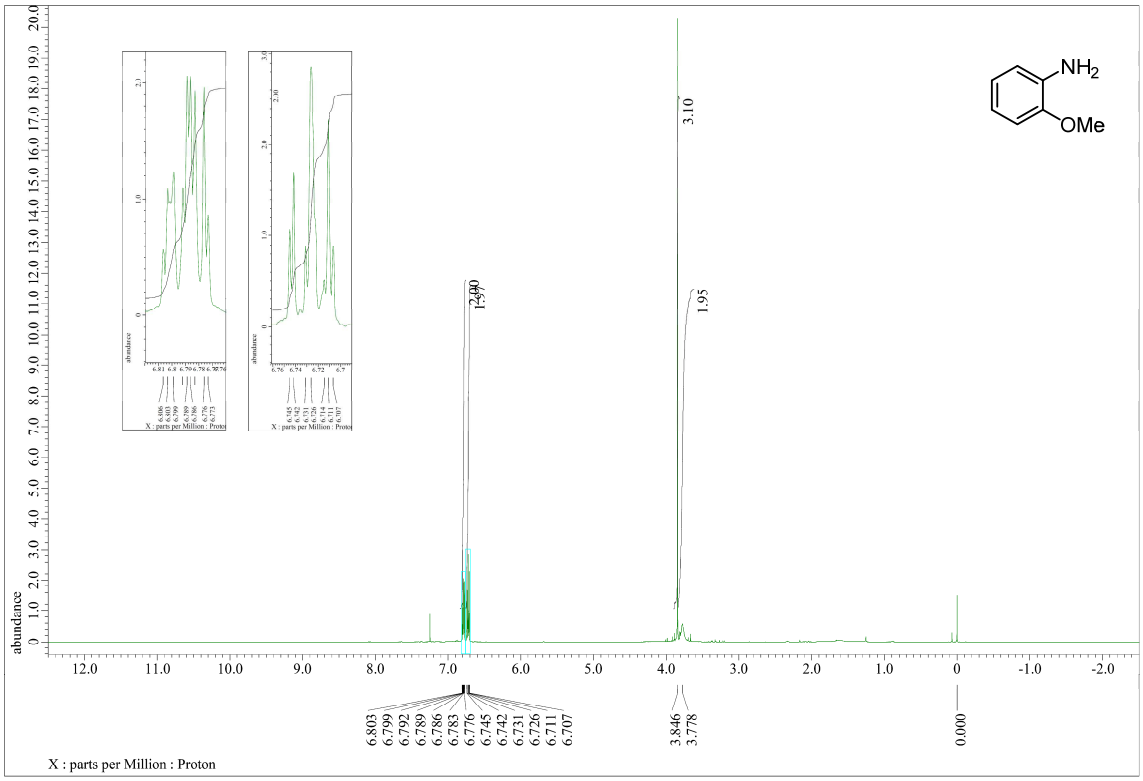
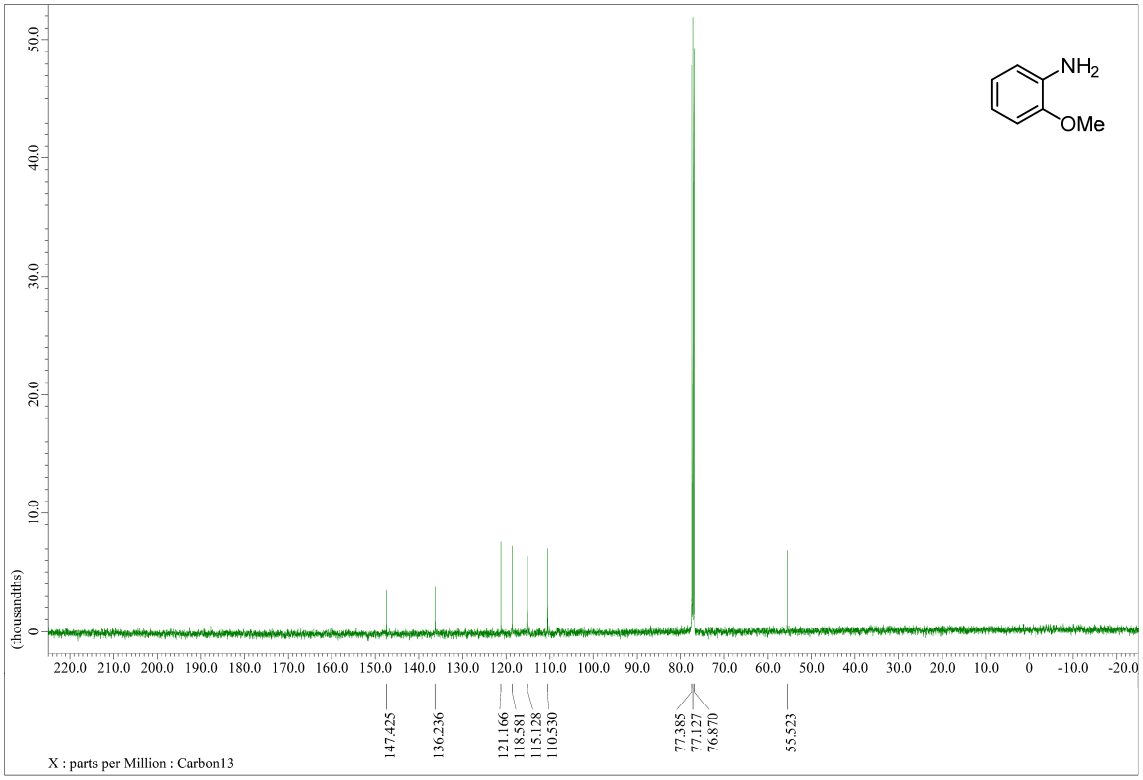
141.511
126.164
115.023
77.394
77.146
76.889
34.014
31.648


NH2
Ph
3.93
1.99
1.98
1.03
2.00
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
7.536 7.534 7.520 7.518 7.415 7.398 7.383 7.368 6.749 6.743 6.739 6.730 6.727 6.721
3.689
-0.000
X : parts per Million : Proton


NH2
Ph
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
145.956 141.272 131.677 128.777 128.119 126.517 126.373 115.500
77.423 77.165 76.908
X : parts per Million : Carbon13


NH2
OMe
3.10
2.00
1.97
1.95
abundance
6.803
6.799
6.792
6.789
6.786
6.783
6.776
6.745
6.742
6.731
6.726
6.711
6.707
3.846
3.778
0.000
X : parts per Million : Proton


NH2
OMe
(thousandths)
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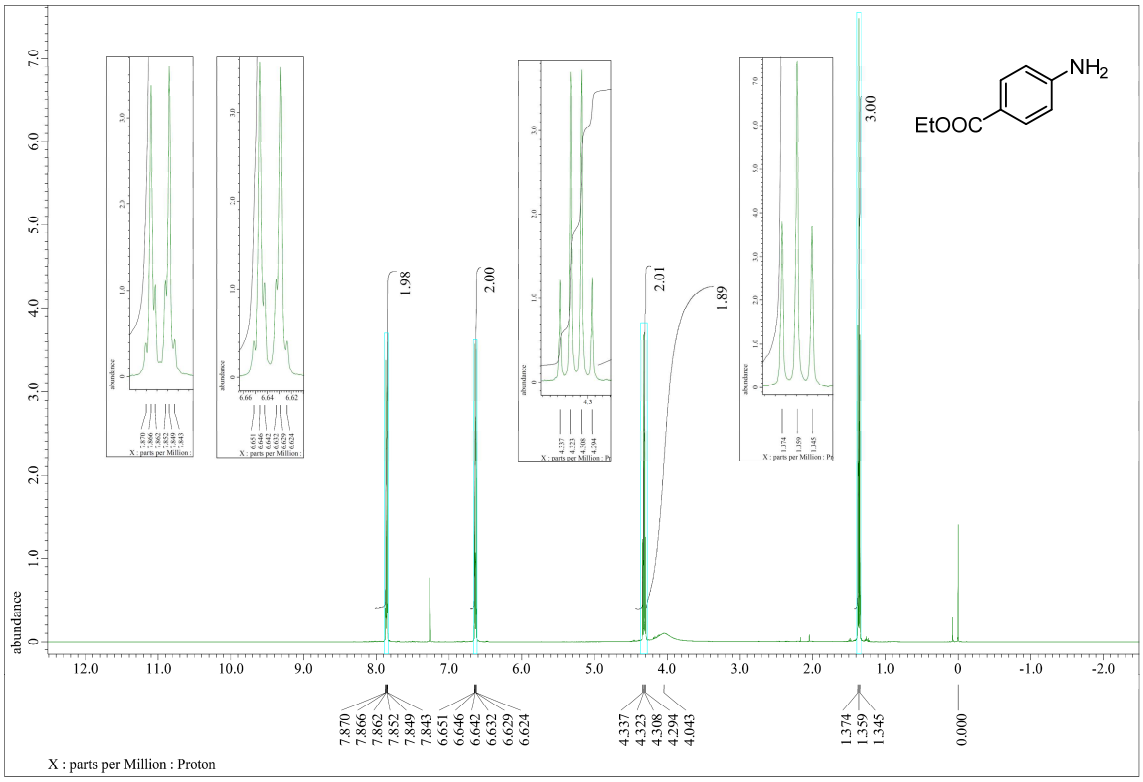
118.581
115.128
110.530
77.385
77.127
76.870
55.523
X : parts per Million : Carbon13


NH2
EtOOC
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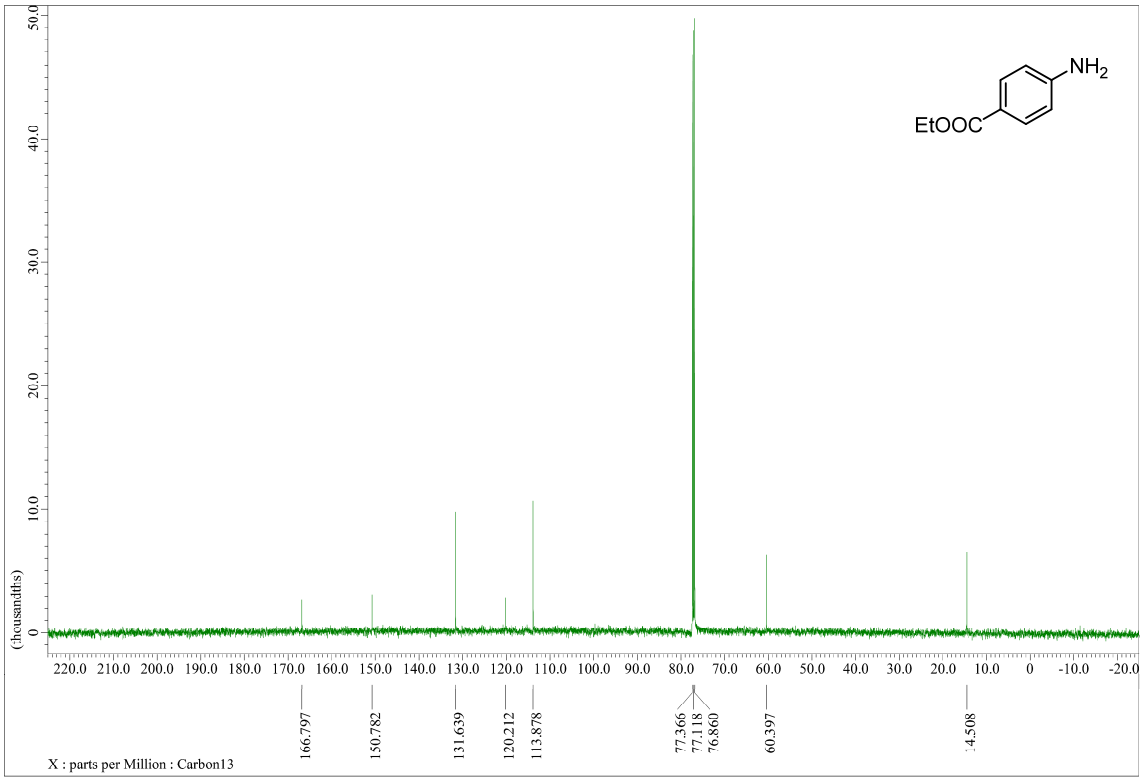
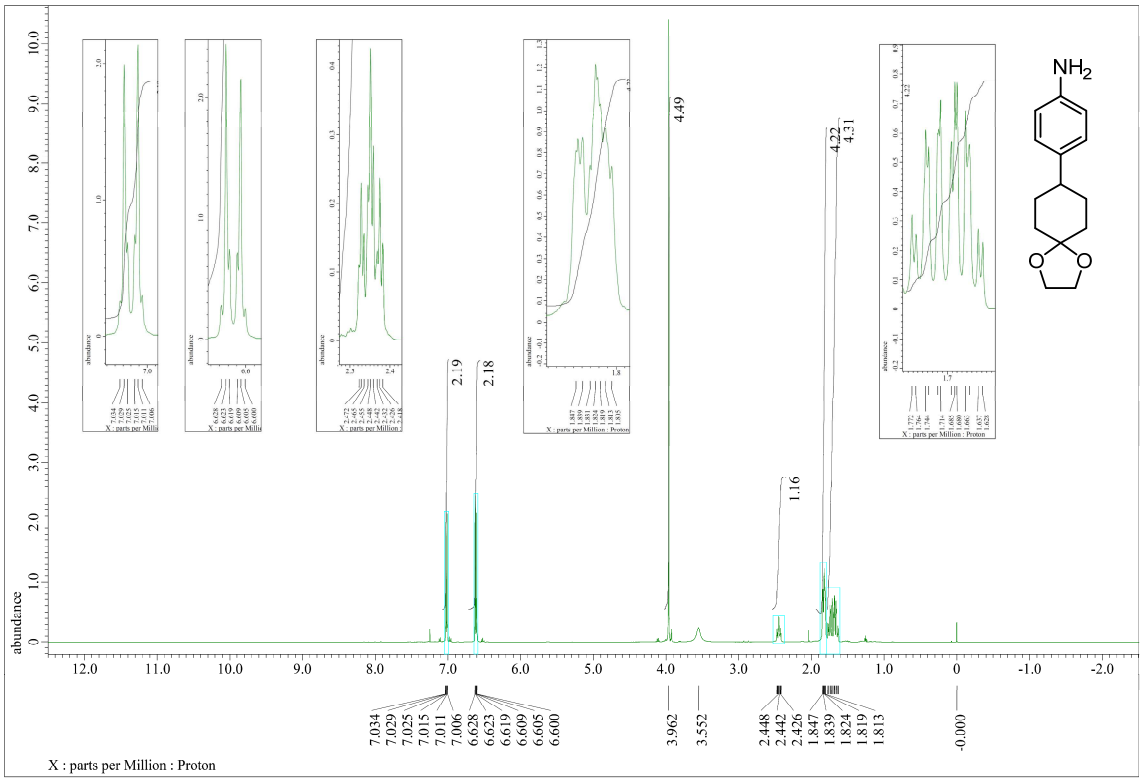
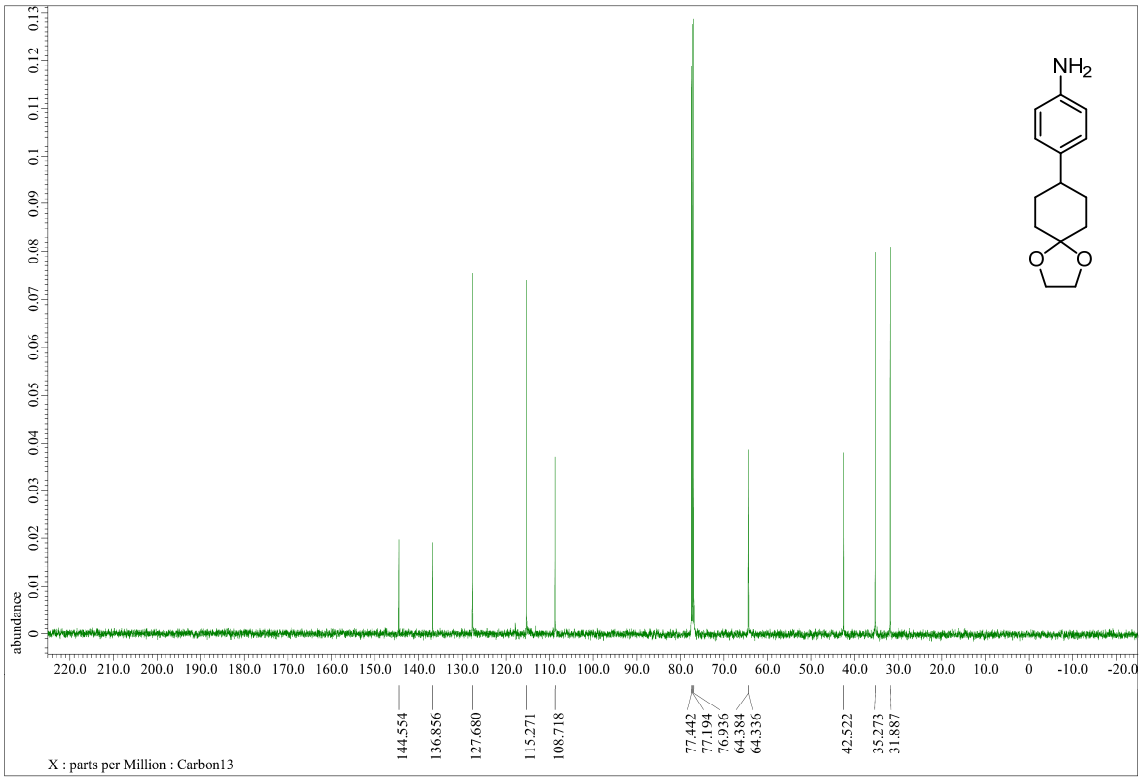
2.00
2.01
1.89
3.00
abundance
X : parts per Million : Proton


NH2
EtOOC
(thousandths)
166.797
150.782
131.639
120.212
113.878
77.366
77.118
76.860
60.397
X : parts per Million : Carbon13


NH2
abundance
X : parts per Million : Proton
7.034
7.029
7.025
7.015
7.011
7.006
6.628
6.623
6.619
6.609
6.605
6.600
3.962
3.552
2.448
2.442
2.426
1.847
1.839
1.824
1.819
1.813
-0.000
2.19
2.18
4.49
4.22
4.31
1.16


NH2
abundance
X : parts per Million : Carbon13
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127.680
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108.718
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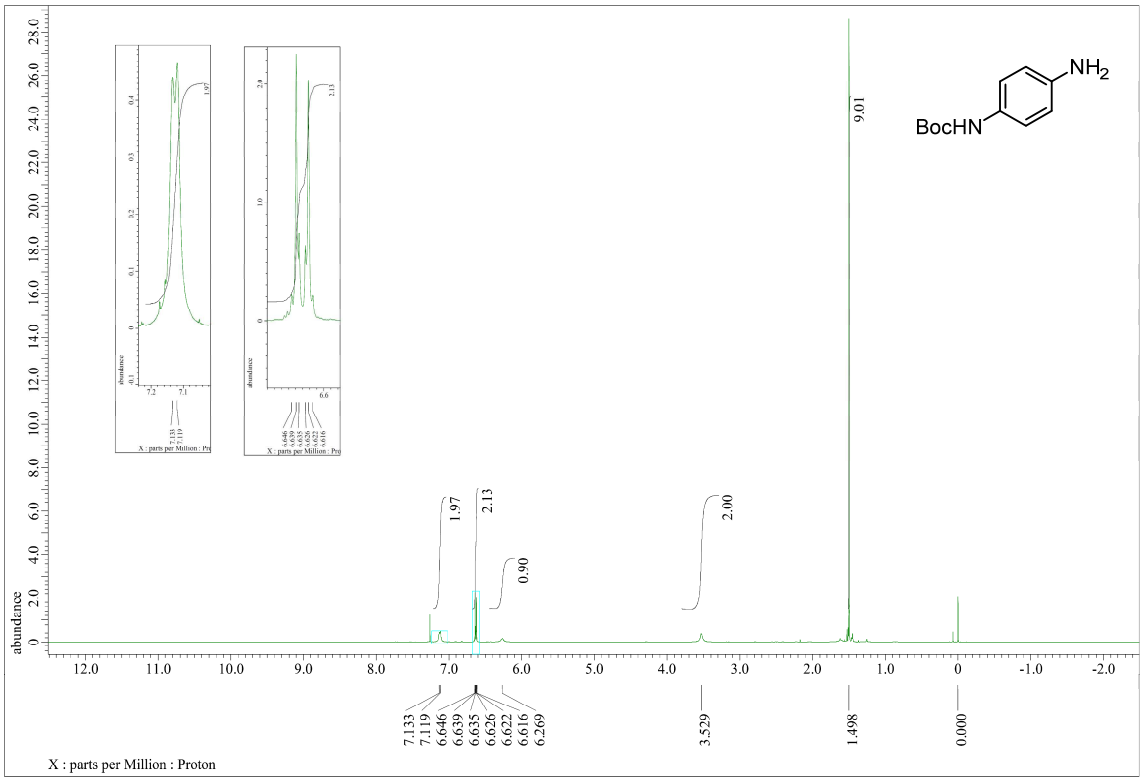
77.194
76.936
64.384
64.336
42.522
35.273
31.887


NH2
BocHN
abundance
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1.97
2.13
0.90
2.00
7.133
7.119
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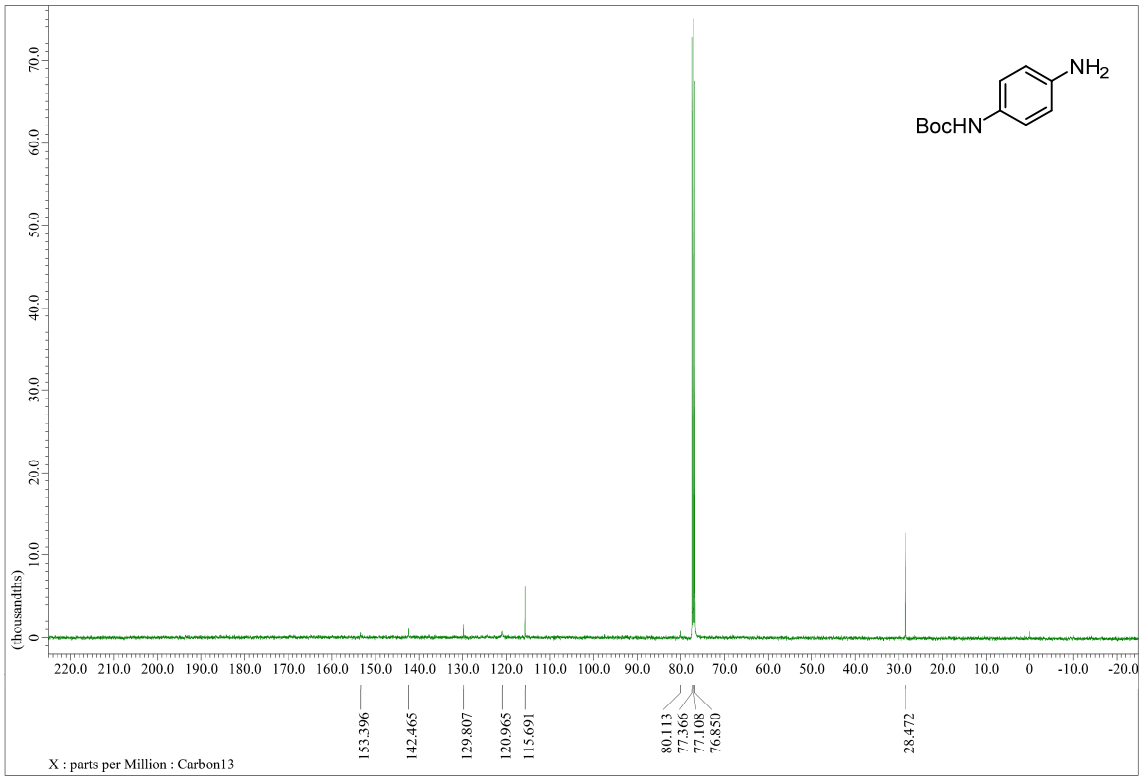
6.639
6.635
6.626
6.622
6.616
6.269
3.529
1.498
0.000
X : parts per Million : Proton


NH2
BocHN
(thousandth's)
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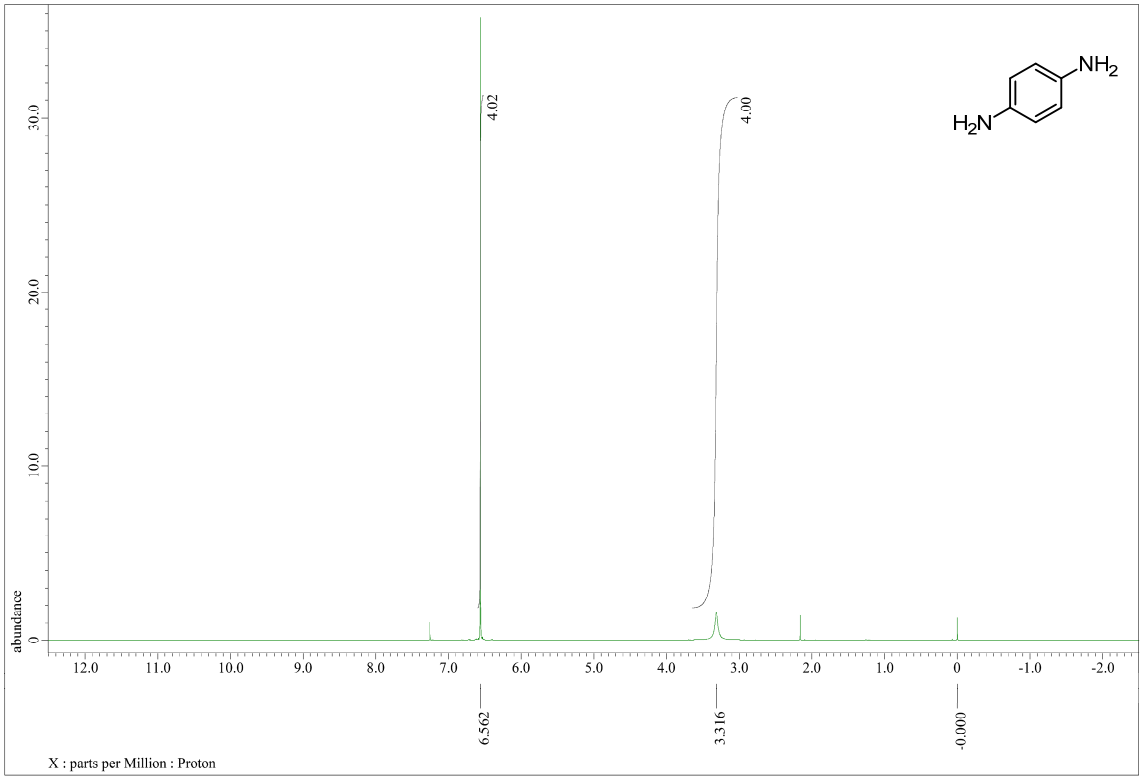
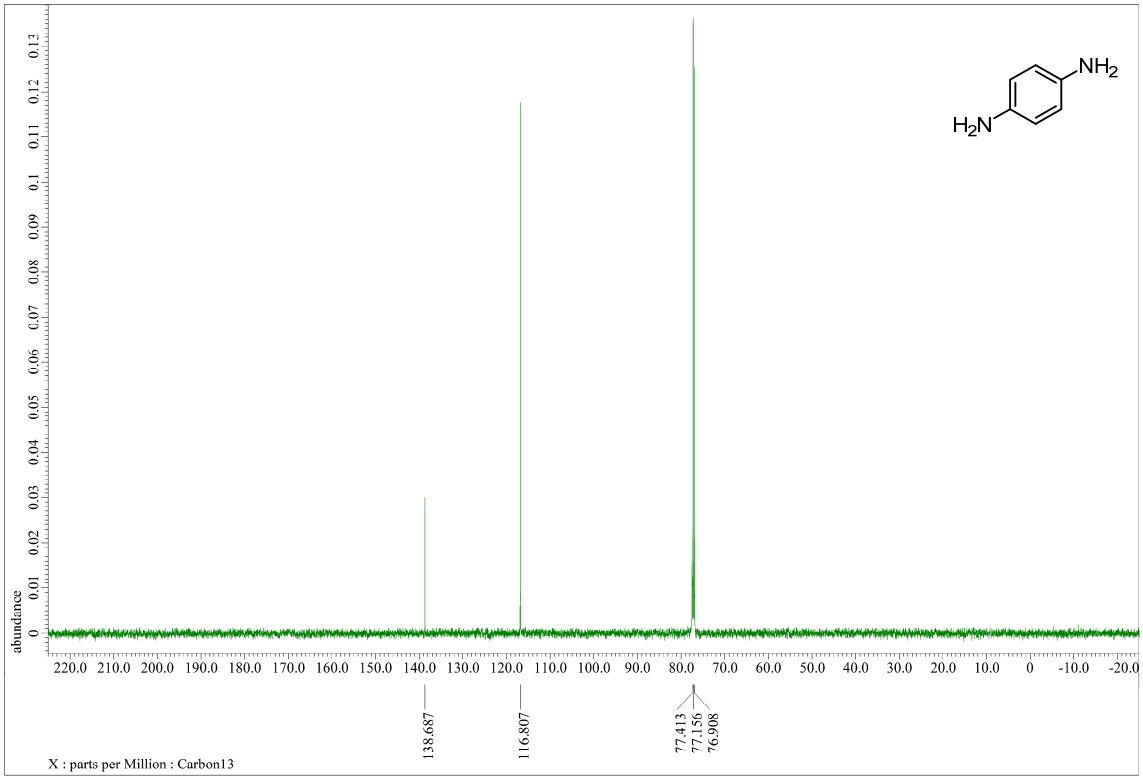
115.691
80.113
77.366
77.108
76.850
28.472
X : parts per Million : Carbon13


4.02
4.00
NH2
H2N
abundance
30.0
20.0
10.0
0
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
6.562
3.316
-0.000
X : parts per Million : Proton


NH2
H2N
abundance
0.13 0.12 0.11 0.1 0.09 0.08 0.07 0.06 0.05 0.04 0.03 0.02 0.01 0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
138.687
116.807
77.413
77.156
76.908
X : parts per Million : Carbon13