Supporting Information

Mesoionic N-heterocyclic Olefin Catalysed Reductive Functionalization of CO_2 for Consecutive N-Methylation of Amines

Subir Maji, Arpan Das and Swadhin K. Mandal*

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India

*Correspondence to: swadhin.mandal@iiserkol.ac.in

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I) General Information

General reagent information

All air- and moisture-sensitive manipulations were carried out using a standard high vacuum line, Schlenk or cannula techniques, or in an MBraun drybox containing an atmosphere of purified argon. All glassware were oven-dried overnight at 130 °C before use. Solvents such as benzene, toluene, diethyl ether, hexane, and tetrahydrofuran were dried by distillation using a Na/benzophenone mixture. Carbon dioxide was purchased from Praxair in a 5.5 purity gas cylinder with 99.995% purity. All solid reagents were purchased (Sigma-Aldrich, Merck, and TCI Chemicals) and used as received. Unless otherwise noted, liquid chemicals were purchased from commercial suppliers (Sigma-Aldrich, Merck, and TCI Chemicals) and dried over molecular sieves (4 Å) prior to use. The molecular sieves (4 Å, Merck) were dried under vacuum at 250 °C for 24 h prior to use. During catalysis, we performed a freeze-pump-thaw cycle to remove dissolved gas from the J. Young pressure tube, and next, we waited

until the temperature reaches to room temperature. The ^{1} H and $^{13}C\{^{1}H\}$ NMR spectroscopic measurements were carried out using a JEOL ECS 400 MHz spectrometer or on a Bruker Avance 500 MHz spectrometer with residual undeuterated solvent as an internal standard. ^{11}B NMR spectroscopy was performed using a Bruker Avance 500 MHz NMR spectrometer. Chemical shifts for $^{11}B\{^{1}H\}$ NMR spectra were referenced using $Et_2O{\cdot}BF_3$ as an external standard. Chemical shifts (δ) are given in ppm, and J values are given in Hz**.**

Mesoionic N-heterocyclic olefin, secondary amines (**2b-2h), 6'** and **6** were synthesized according to the literature procedure.[S1, S2, S3, S4]

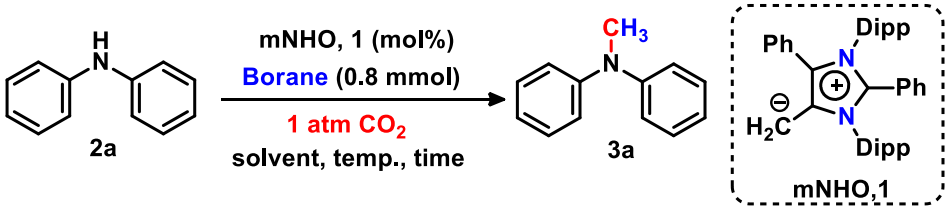
II) Experimental Details

<u>Optimization study for N-methylation of secondary amines catalysed by mesoionic N-heterocyclic olefin</u>

An oven-dried 25 mL Schlenk tube was charged with 0.2 mmol diphenylamine substrate and a magnetic stirring bar. It was kept under high vacuum for 2 h and was transferred into an argon-filled glove box. Inside the glove box, the required amount of mesoionic N-heterocyclic olefin (mNHO) catalyst, 0.8 mmol of different borane source and 0.5 mL anhydrous solvent were added to the reaction tube. Then the tube was sealed tightly with a screw cap equipped with a J. Young valve and removed from the glovebox. Subsequently, the reaction tube was connected through the Schlenk line and the mixture was degassed by two successive freeze-pump-thaw cycles and finally exposed to carbon dioxide (1 atm.). The flask was sealed and the final reaction mixture was allowed to stir for required time at a temperature mentioned in the optimization table below. After completion of the reaction, solvent was removed under reduced pressure and crude product was purified by column chromatography on silica gel (100-200 mesh) using hexane/ethyl acetate mixture (99:1 v/v) to yield the desired products. The product N-methyl diphenylamine (3a) was identified by ^{1}H and $^{13}C\{^{1}H\}$ NMR spectroscopy in $CDCl_3$. From this optimization study, it was established that 9-BBN is the best hydride source delivering the highest isolated yield of 95 % using 5 mol % of mNHO (1) under atmospheric pressure of CO_2 at 40 ^{o}C in THF.

Table S1. Mesoionic N-heterocyclic olefin catalysed N- methylation of amines using CO_2

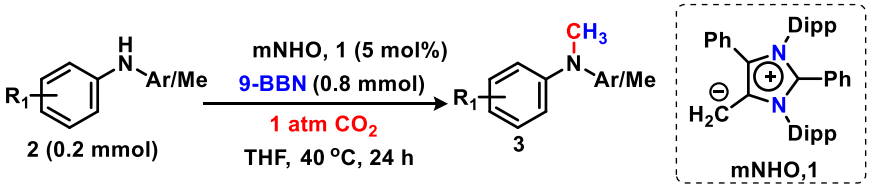
[a]



Entry	mNHO (mol%)	Borane	Solvent	Temp. (°C)	Time (h)	Isolated Yield (%)
1.	-	9-BBN	THF	40	24	-
2.	5	-	THF	40	24	-
3.	5	9-BBN	THF	RT	24	78
4.	**5**	**9-BBN**	THF	**40**	**24**	**95**
5.	5	$Me_2S.BH_3$	THF	40	24	64
6.	5	HBPin	THF	40	24	-
7.	5	9-BBN	Toluene	40	24	82
8.	5	9-BBN	THF	40	12	72
9.	2.5	9-BBN	THF	40	24	65
10.	3	9-BBN	THF	40	24	81
11.	1	9-BBN	THF	40	24	34

[a] Reaction conditions: amine (0.2 mmol), 1 atm CO_2, borane (0.8 mmol), dry solvent (0.5 mL),.

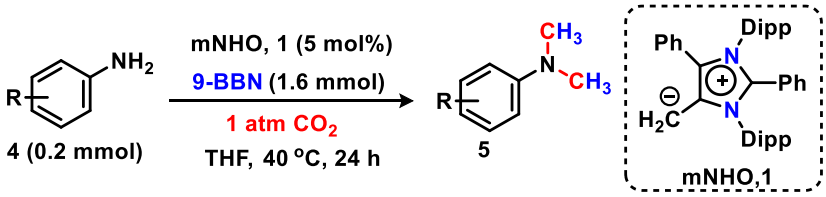
<u>Experimental procedures for mesoionic N-heterocyclic olefin catalysed N-methylation of secondary amines</u>



Scheme S1. General procedure for the N-methylation of secondary amines catalysed by mNHO (1).

Under an argon atmosphere, a 25 mL Schlenk tube equipped with a stir bar and a J. Young valve was charged with secondary amines (0.2 mmol), mNHO (5 mol%), 9-borabicyclo (3,3,1)nonane (9-BBN) (0.8 mmol) and THF (0.5 mL). The mixture was degassed by two successive freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). The tube was sealed and stirred for 24 h at 40 ^{o}C. Next, the reaction mixture was dried using high vacuum pump and purified by column chromatography on silica gel (Merck, 100-200 mesh). The N-methyl diphenylamine was collected in analytically pure form using hexane-ethyl acetate mixture (99:1 v/v) as the eluent. The corresponding N-methyl diphenylamine was identified by ^{1}H and ^{13}C{^{1}H} NMR spectroscopy in $CDCl_3$.

Experimental procedures for mesoionic N-heterocyclic olefin catalysed double N-methylation of primary amines



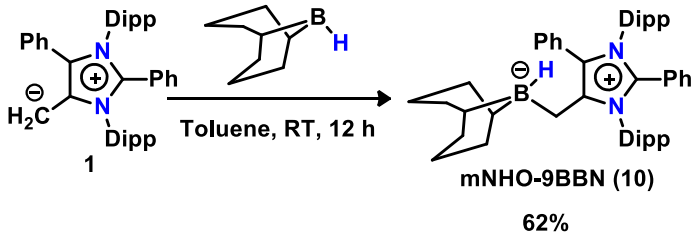
Scheme S2. General procedure for the N, N-dimethylation of primary amines catalysed by mNHO (1).

Under an argon atmosphere, a 25 mL Schlenk tube equipped with a stir bar and a J. Young valve was charged with primary amines (0.2 mmol), mNHO (5 mol%), 9-borabicyclo [3.3.1]nonane (9-BBN) (1.6 mmol) and THF (1 mL). The mixture was degassed by two successive freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). The tube was sealed and stirred for 24 h at 40 ^{o}C. Then the reaction mixture was dried using high vacuum pump and purified by column chromatography on silica gel (Merck, 100-200 mesh). The N, N-dimethylaniline was then collected in analytically pure form using hexane-ethyl acetate mixture (99:1 v/v) as the eluent. The corresponding N, N-dimethylaniline was identified by ^{1}H and ^{13}C{^{1}H} NMR spectroscopy recorded in $CDCl_3$.

Preparation and characterization of reaction intermediate mNHO-9-BBN (10) adduct

An oven-dried 25 mL Schlenk flask equipped with a stirring bar was charged with mesoionic N-heterocyclic olefin, **1** (277 mg, 0.50 mmol, 1 equiv), 9-BBN (0.50 mmol, 1 equiv) and toluene (10 mL) in an argon filled glovebox. Next, the reaction mixture was allowed to stir during 12 h at room temperature. After completion of the reaction, the solvent was dried

under reduced pressure and the final off white solid product was washed with hexane for three times to afford the mNHO-9BBN adduct **10** (62% yield). The colourless crystals were successfully grown from toluene under an argon atmosphere at -25 ^{o}C within one day. The compound **10** was characterized through SCXRD, as well as ^{1}H, ^{13}C{^{1}H}, and ^{11}B{^{1}H} NMR spectroscopies.



Scheme S3. Stoichiometric reaction between mNHO (**1**) and 9-BBN resulting in the formation of the adduct **10.**

^{1}H NMR (500 MHz, C_6D_6:CD_2Cl_2, 25 ^{o}C): δ (ppm) = 7.82 (d, 2H, 8 Hz, Ar-H), 7.25 (t, 1H, 8Hz, Ar-H), 7.13-7.06 (m, 3H, Ar-H), 7.04-6.99 (m, 2H, Ar-H), 6.96-6.89 (m, 3H, Ar-H), 6.81 (d, 2H, 8Hz, Ar-H), 6.54 (t, 1H, 8 Hz, Ar-H), 6.46 (d, 2H, 8 Hz, Ar-H), 2.95-2.87 (m, 2H, $CH(CH_3)_2$), 2.73-2.67 (m, 4H, $CH(CH_3)_2$ and CH(9-BBN)), 2.60-2.50 (m, 5H, CH_2(9-BBN)), 2.32-2.21 (m, 2H, CH_2(9-BBN)), 2.11(s, 2H, CH_2-B), 2.01-1.96 (m, 2H, CH_2(9-BBN)), 1.61 (d, 6H, 5 Hz, $CH(CH_3)_2$), 0.91-.081 (m, 4H, CH_2(9-BBN)), 0.72 (d, 6H, 5Hz, $CH(CH_3)_2$), 0.68-0.64 (dd, 12H, 8 Hz, $CH(CH_3)_2$); **^{13}C{^{1}H} NMR** (125 MHz, C_6D_6:THF-d_8, 25 ^{o}C): δ (ppm) = 151.4 (imidazole-C), 144.5 (Ar-C), 144.4 (Ar-C), 138.2 (imidazole-C), 130.9 (Ar-CH), 130.7 (Ar-CH), 130.3 (Ar-C) , 130.1 (Ar-C), 129.9 (Ar-C), 129.7 (Ar-CH), 129.5 (Ar-CH), 129.1 (Ar-CH), 128.8 (Ar-CH), 128.1 (Ar-CH), 127.4 (Ar-CH), 126.0 (Ar-CH), 124.9 (Ar-CH), 125.6 (Ar-C), 122.5 (imidazole-C), 36.1 CH(9-BBN), 32.6 CH_2(9-BBN), 31.2 ($CH(CH_3)_2$) , 28.5 ($CH(CH_3)_2$), 27.9 ($CH(CH_3)_2$), 26.4 (CH_2(9-BBN)), 25.4 (CH_2(9-BBN)), 23.1 ($CH(CH_3)_2$), 22.8 ($CH(CH_3)_2$), 22.5 ($CH(CH_3)_2$), 22.1 (CH_2-B); **^{11}B{^{1}H} NMR** (160 MHz, C_6D_6: CD_2Cl_2, 25 ^{o}C): δ (ppm) = -11.3.

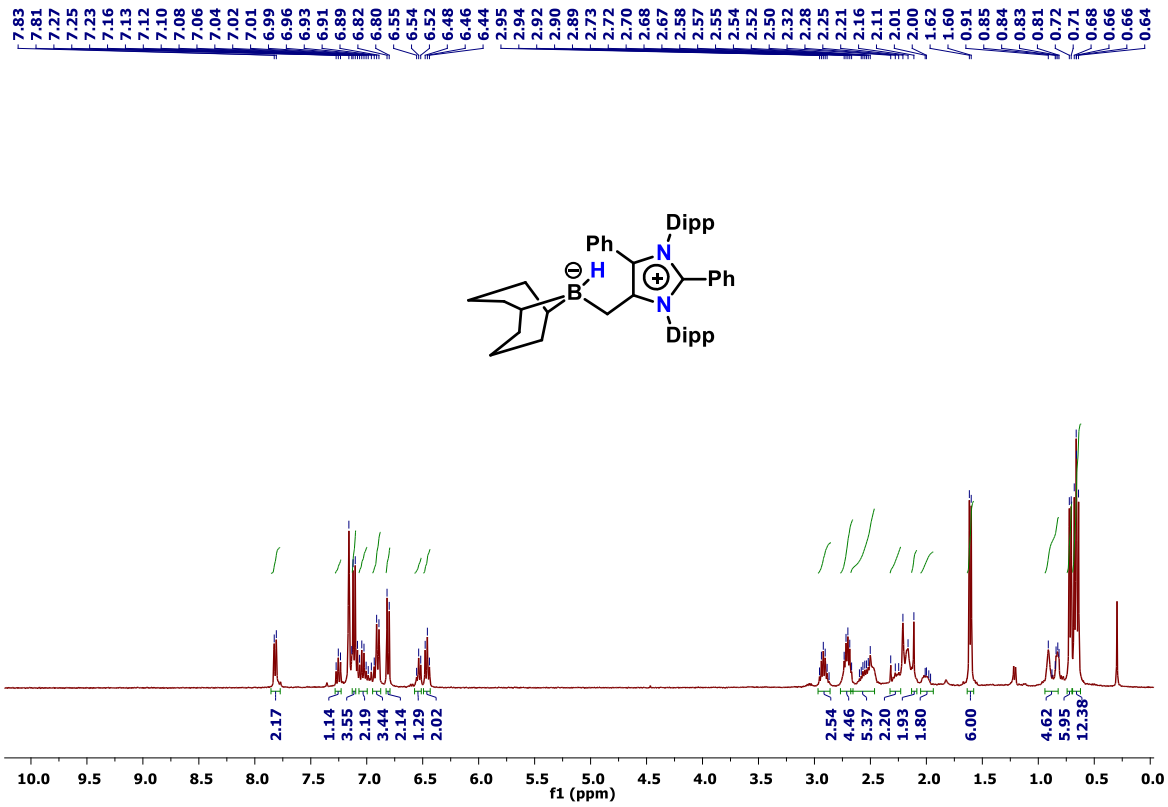


Figure S1. ^{1}H NMR spectrum of compound mNHO-9BBN adduct **10** in C_6D_6:CD_2Cl_2 mixture.

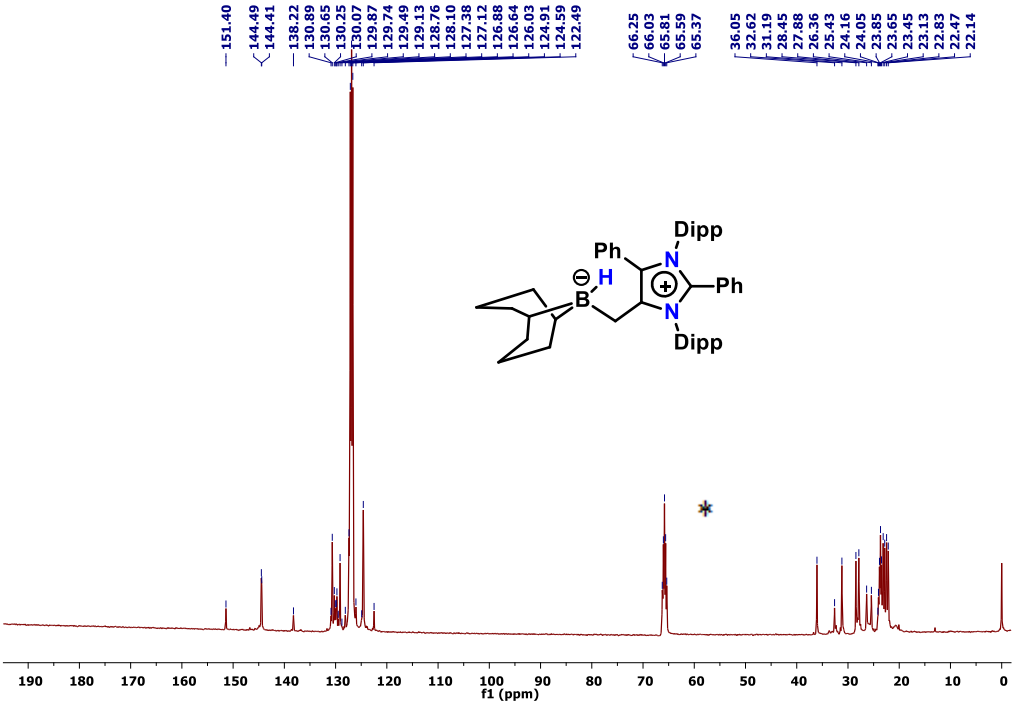


Figure S2. ^{13}C{^{1}H} NMR spectrum of compound mNHO-9BBN adduct **10** in C_6D_6:$THFd_8$ mixture. * The signal at 65.3 to 66.2 ppm indicates the ^{13}C (2, 5) of THF-d_8.

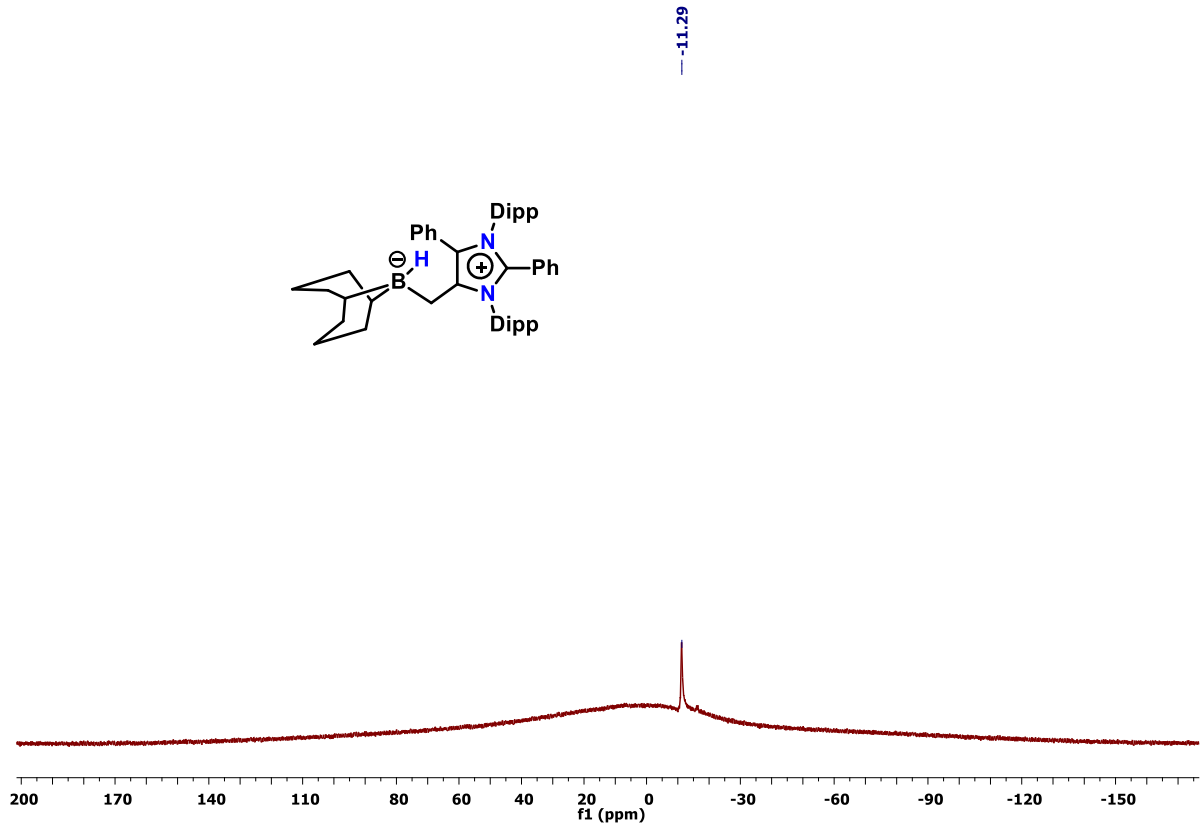
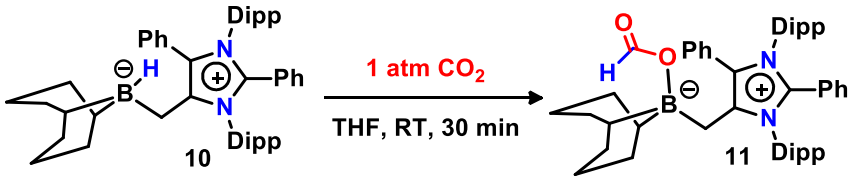


Figure S3. $^{11}B\{^{1}H\}$ NMR spectrum of compound mNHO-9BBN adduct **10** in C_6D_6:CD_2Cl_2 mixture.

Characterization of reaction intermediate boron formate intermediate 11



Scheme S4. Reaction between mNHO and 9-BBN under CO_2 atmosphere.

An oven-dried 25 mL Schlenk flask equipped with a stirring bar was charged with the mesoionic N-heterocyclic olefin, **1** (55.5 mg, 0.10 mmol, 1 equiv), 9-BBN (0.10 mmol, 1 equiv) and THF (2 mL) in an argon filled glovebox. Next, the mixture was degassed by successive two freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). The flask was sealed and allowed to stir during 30 min at room temperature. After completion of the reaction, the solvent was dried under reduced pressure and the white solid product was washed with hexane for three times to afford the boron formate (**11**). The compound **11** was characterized through ^{1}H, $^{13}C\{^{1}H\}$, and $^{11}B\{^{1}H\}$ NMR spectroscopies.

^{1}H NMR (500 MHz, C_6D_6:CD_2Cl_2, 25 ^{o}C): δ (ppm) = 8.67 (s, 1H, OCHO), 7.47 (d, 2H, 5 Hz, Ar-H), 7.22 (t, 1H, 8Hz, Ar-H), 7.09-7.07 (m, 3H, Ar-H), 7.02 (t, 2H, 8Hz, Ar-H), 6.97 (d, 1H, 5 Hz, Ar-H), 6.92 (d, 2H, 8Hz, Ar-H), 6.89 (d, 2H, 5Hz, Ar-H), 6.74-6.69 (m,1H, Ar-H), 6.64 (t, 2H, 8 Hz, Ar-H), 2.98-2.90 (m, 2H, $CH(CH_3)_2$), 2.80-2.72 (m, 2H, $CH(CH_3)_2$), 2.19 (s, 2H, CH_2-B), 2.09-1.96 (m, 3H, CH_2-9BBN), 1.72-1.65 (m, 8H, CH_2-9BBN), 1.45-1.44 (d, 6H, 5 Hz, $CH(CH_3)_2$), 1.28-1.21 (m, 3H, CH_2-9BBN), 0.86 (d, 6H, 8 Hz, $CH(CH_3)_2$), 0.75 (dd, 12H, 5Hz, $CH(CH_3)_2$); **^{13}C{^{1}H} NMR** (125 MHz, C_6D_6:CD_2Cl_2, 25 ^{o}C): δ (ppm) = 166.3 (OCHO), 147.0 (imidazole-C), 146.8 (Ar-C), 146.0 (Ar-C), 142.4 (imidazole-C), 131.7 (Ar-CH), 131.6 (Ar-CH), 131.2 (Ar-C), 130.9 (Ar-C), 130.6 (Ar-C), 129.6 (Ar-CH), 129.2 (Ar-CH), 129.1 (Ar-CH), 128.9 (Ar-CH), 128.4 (Ar-CH), 128.4 (Ar-CH), 128.4 (Ar-CH), 125.9 (Ar-CH), 125.6 (Ar-C), 123.4 (imidazole-C), 33.3 (CH_2-9BBN), 32.0 (CH_2-9BBN), 31.7 ($CH(CH_3)_2$), 29.1 ($CH(CH_3)_2$), 28.8 ($CH(CH_3)_2$, 25.3 ($CH(CH_3)_2$), 24.2 ($CH(CH_3)_2$), 24.1 ($CH(CH_3)_2$), 23.1(CH-9BBN), 14.3 (CH_2-B) ; **^{11}B{^{1}H} NMR** (160 MHz, C_6D_6:CD_2Cl_2, 25 ^{o}C): δ (ppm) = 8.1.

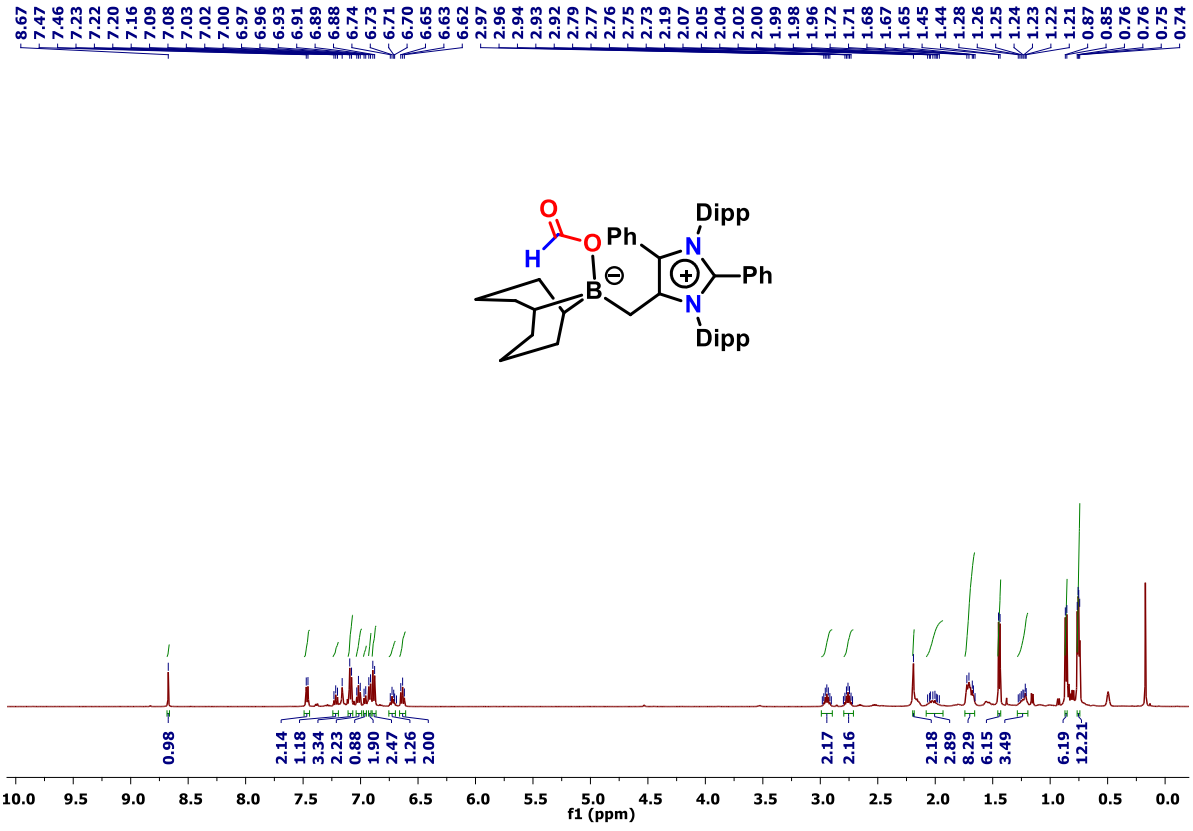


Figure S4. ^{1}H NMR spectrum of compound boron formate **11** in C_6D_6:CD_2Cl_2 mixture.

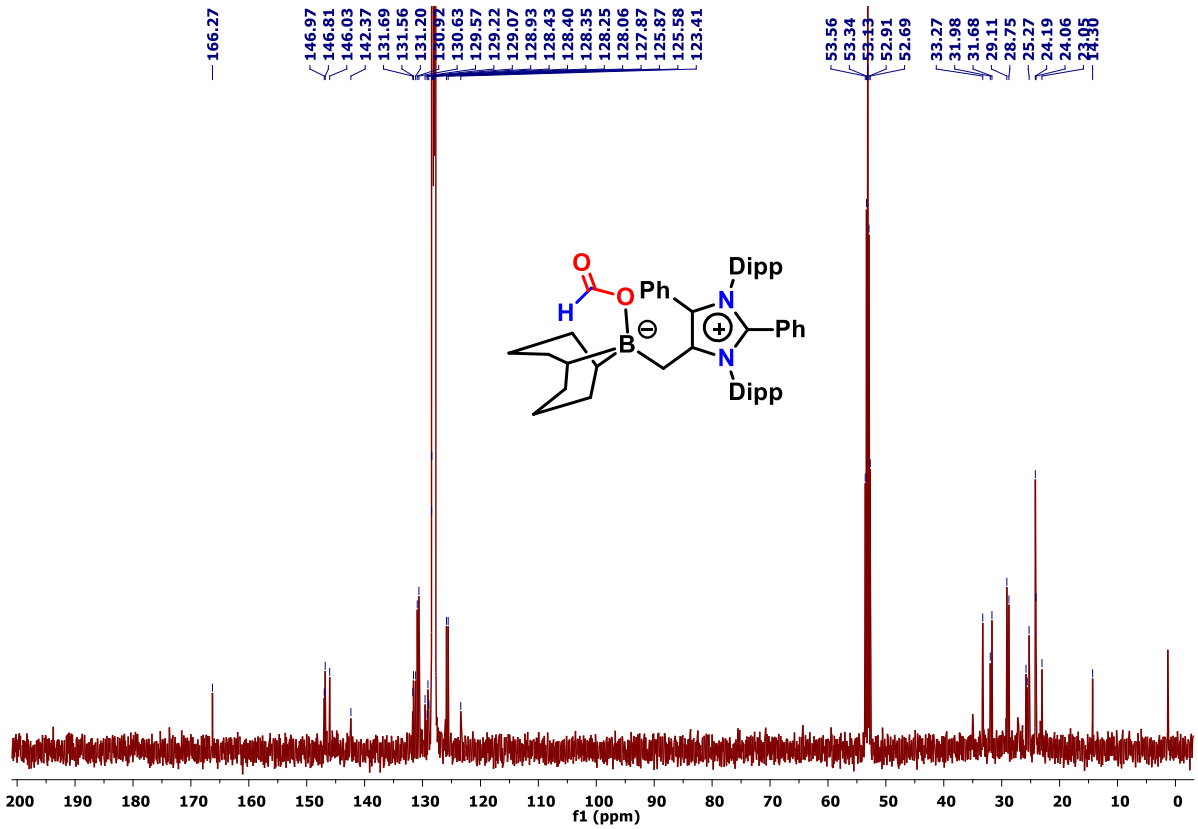


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of compound boron formate **11** in C_6D_6:CD_2Cl_2 mixture.

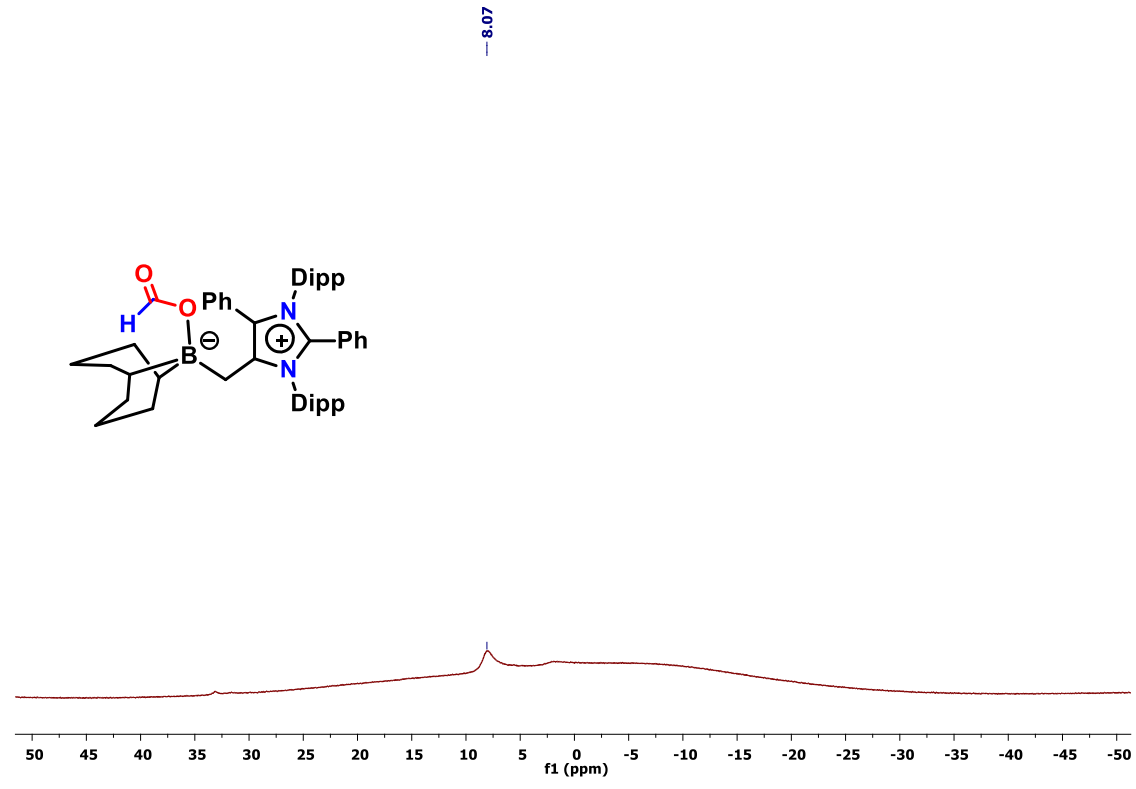
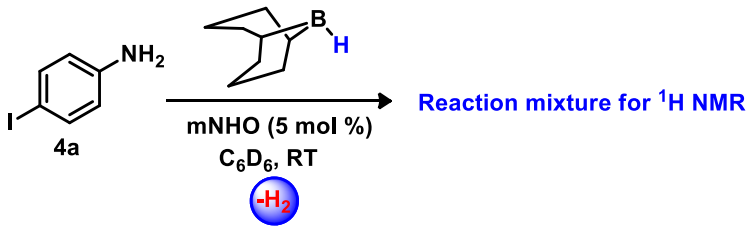


Figure S6. $^{11}B\{^{1}H\}$ NMR spectrum of compound boron formate **11** in C_6D_6:CD_2Cl_2 mixture.

H_2 evolution experiment



Scheme S5. Reaction of amine, 9-BBN and mNHO in benzene-d_6 at room temperature during 10 min.

Under an argon atmosphere, a 2.5 mL screw cap NMR tube was charged with 4-iodo aniline (5.48 mg, 0.025 mmol, 1 equiv.), mNHO (5 mol%), 9-BBN (1 equiv.) and benzene-d_6 (0.6 mL). During the addition of 9-BBN at room temperature, we observed an immediate evolution of a gas which was characterized through ^{1}H NMR (δ = 4.47 ppm) spectroscopy and GC analysis.

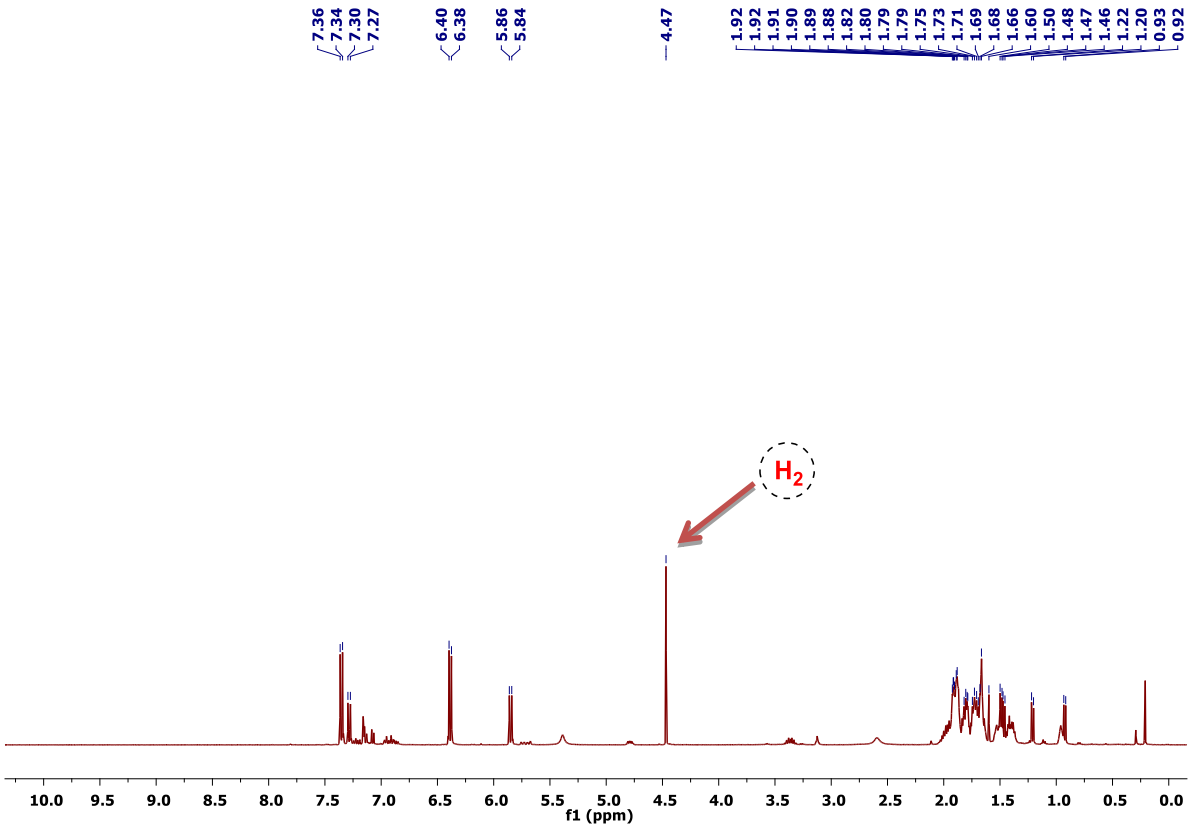


Figure S7. ^{1}H NMR spectrum of the reaction mixture (4-iodo aniline, 9-BBN, and mNHO in benzene-d_6 at room temperature) using a screw cap NMR tube.[S5]

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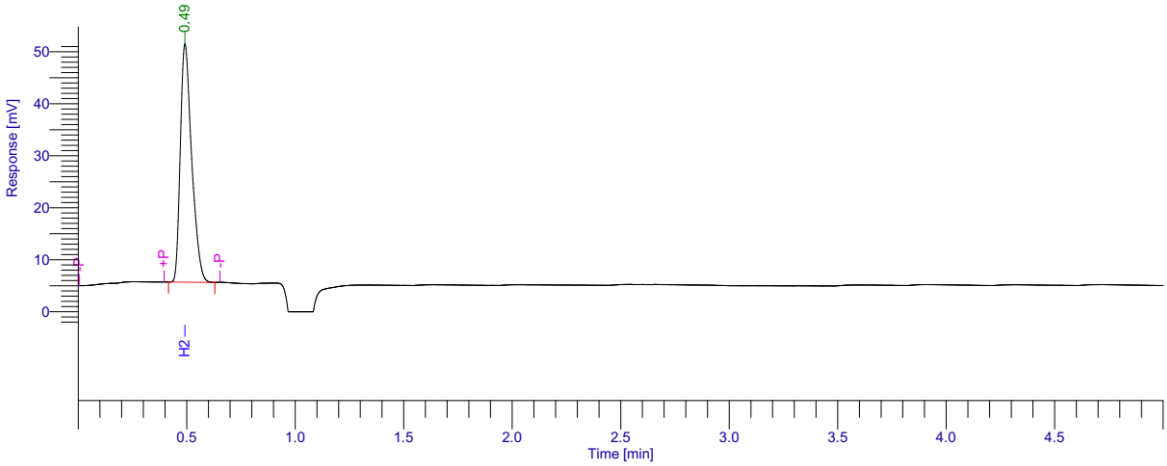
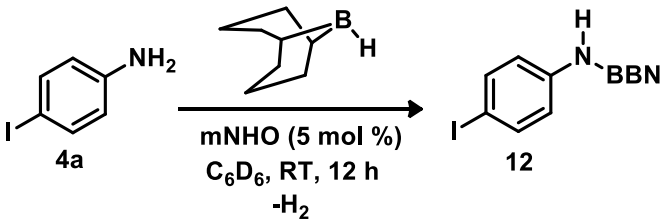


GC REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]
1	H2	0.492	166641.25	45871.26
			166641.25	45871.26

Figure S8. Retention time graph of the reaction mixture (4-iodo aniline, 9-BBN, and mNHO in benzene-d_6 in room temperature) in gas chromatography confirming H_2 evolution.

<u>Characterization of reaction intermediate borylamine using 4-iodo aniline substrate</u>



Scheme S6. Reaction of 4-iodo aniline, 9-BBN and mNHO in benzene-d_6 at room temperature during 12 h.

An oven-dried 25 mL Schlenk tube equipped with a stirring bar and was charged with 4-iodo aniline (21.9 mg, 0.10 mmol, 1 equiv.), mNHO (5 mol %), 9-BBN (1 equiv.) and benzene-d_6 (0.6 mL) in an argon filled glovebox. Next, the reaction mixture was allowed to stir during 12 h at room temperature. After completion of the reaction, the formation of borylamine **12** was characterized by ^{1}H and $^{13}C\{^{1}H\}$ NMR spectroscopies.

^{1}H NMR (400 MHz, C_6D_6, 25 ^{o}C): δ (ppm) = 7.35 (d, 2H, 8Hz, Ar-H), 6.41 (d, 1H, 12Hz, Ar-H), 5.45 (b, 1H, NH) 1.88-1.76 (m, 8H, CH_2-BBN), 1.75-1.68 (m, 3H, CH_2-BBN), 1.44-1.36 (m, 3H, CH_2 and CH-BBN); **^{13}C{^{1}H} NMR** (100 MHz, C_6D_6, 25 ^{o}C): δ (ppm) = 143.4 (Ar-C), 138.1 (Ar-CH), 124.9 (Ar-CH), 86.5 (Ar-C), 34.0 (CH, BBN), 33.2 (CH_2, BBN), 23.8 (CH_2, BBN).

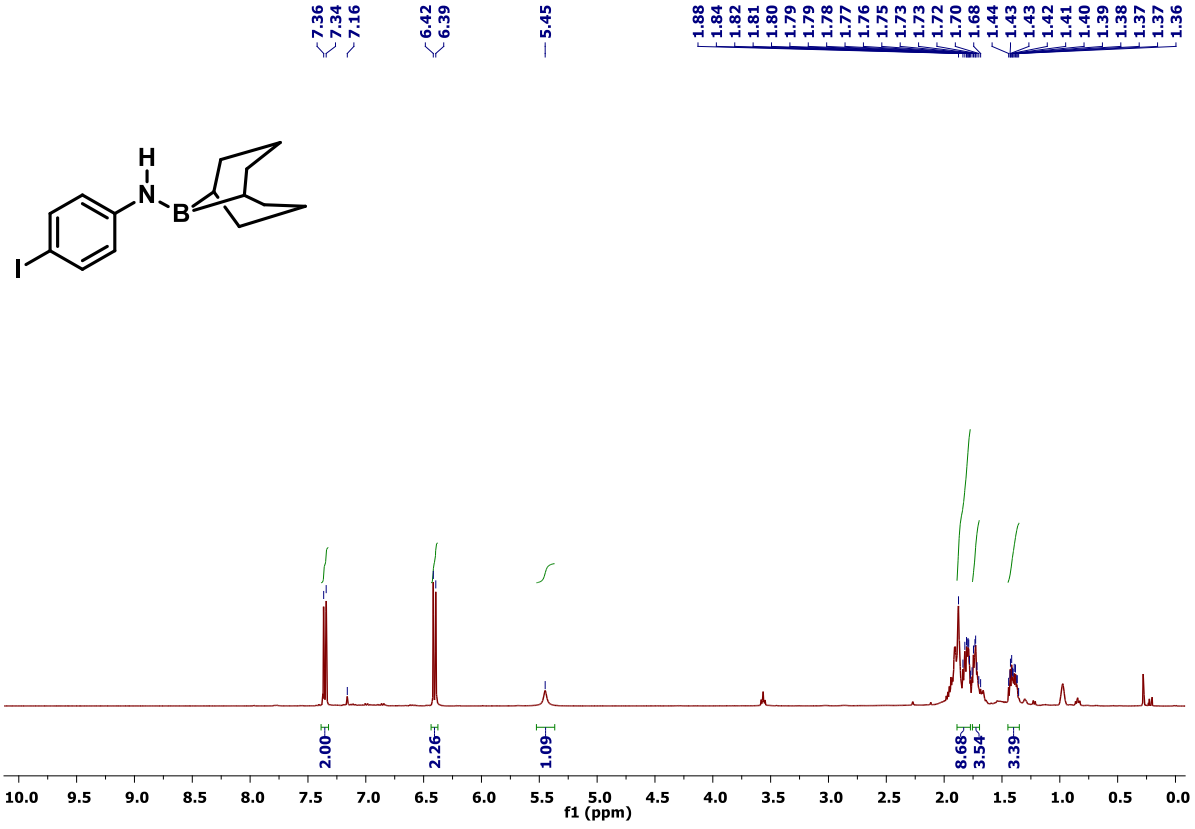


Figure S9. ^{1}H NMR spectrum of the reaction mixture after 12 h (4-iodo aniline, 9-BBN, and mNHO in benzene-d_6 at room temperature).[S6]

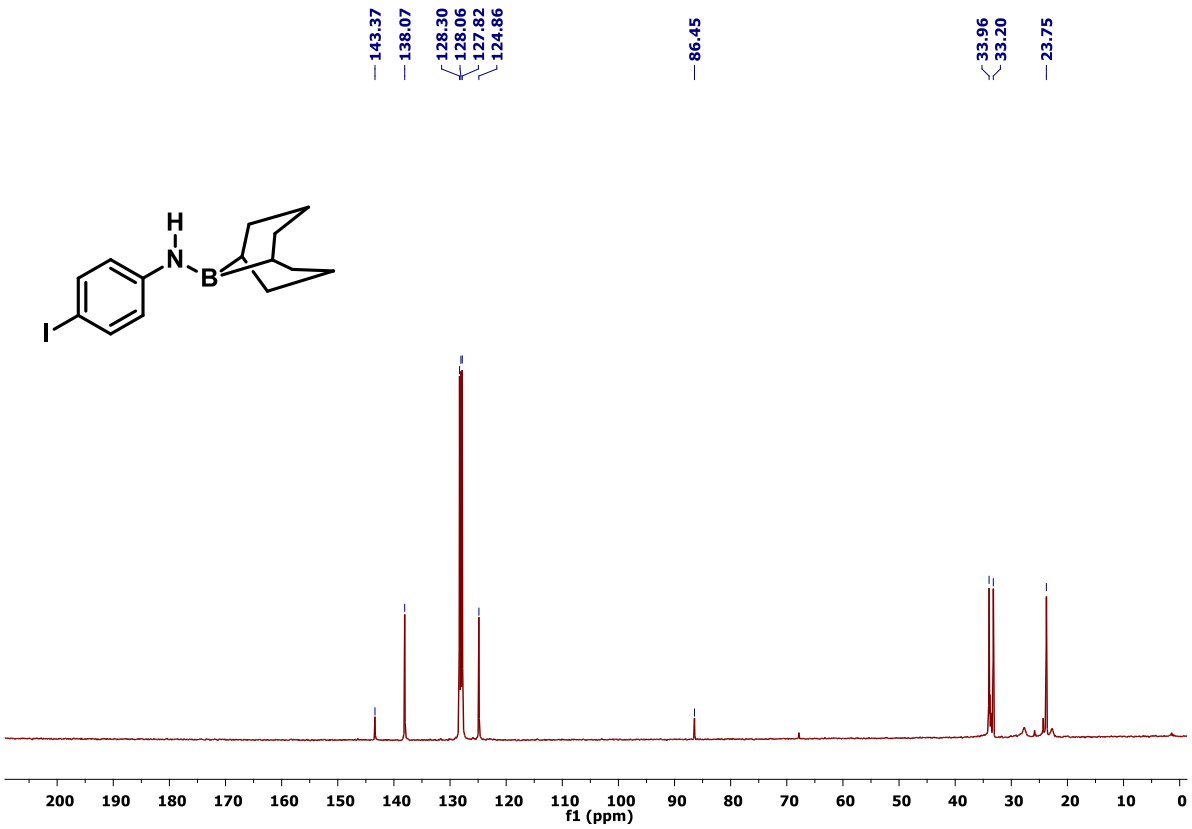
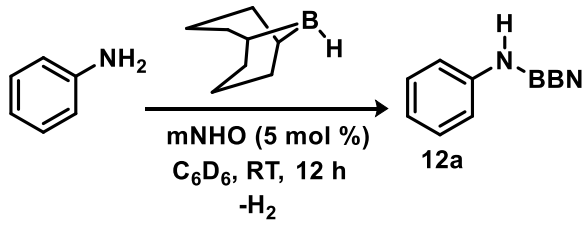


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of the reaction mixture (4-iodo aniline, 9-BBN and mNHO in benzene-d_6 at room temperature) [S6].

Characterization of reaction intermediate N-borylatedamine



Scheme 7. Reaction of aniline, 9-BBN and mNHO in benzene-d_6 at room temperature during 12 h.

An oven-dried 25 mL Schlenk tube equipped with a stirring bar was charged with 0.5 mmol aniline (21.9 mg, 1 equiv.), mNHO (5 mol %), 9-BBN (1 equiv.) and benzene-d_6 (0.8 mL) in an argon filled glovebox. Next, the reaction mixture was allowed to stir during 12 h at room temperature. After completion of the reaction, the formation of borylamine **12a** was characterized by ^{1}H, $^{13}C\{^{1}H\}$ and $^{11}B\{^{1}H\}$ NMR spectroscopies.

^{1}H NMR (400 MHz, C_6D_6, 25 ^{o}C): δ (ppm) = 7.13-7.04 (m, 2H, Ar-H), 6.93-6.87 (m, 2H, Ar-H), 6.35 (d, 1H, 8Hz, Ar-H), 5.67 (b, 1H, NH) 2.00-1.76 (m, 11H, CH_2), 1.48-1.41 (m, 2H, CH), 1.02-1.01 (m, 1H, CH_2); **^{13}C{^{1}H} NMR** (100 MHz, C_6D_6, 25 ^{o}C): δ (ppm) = 143.5 (Ar-C), 129.1 (Ar-CH) 128.8 (Ar-CH), 123.0 (Ar-CH), 122.5 (Ar-CH), 33.7 (CH), 32.9 (CH_2), 23.5 (CH_2).**^{11}B{^{1}H} NMR** (160 MHz, C_6D_6, 25 ^{o}C): δ (ppm) = 50.3.

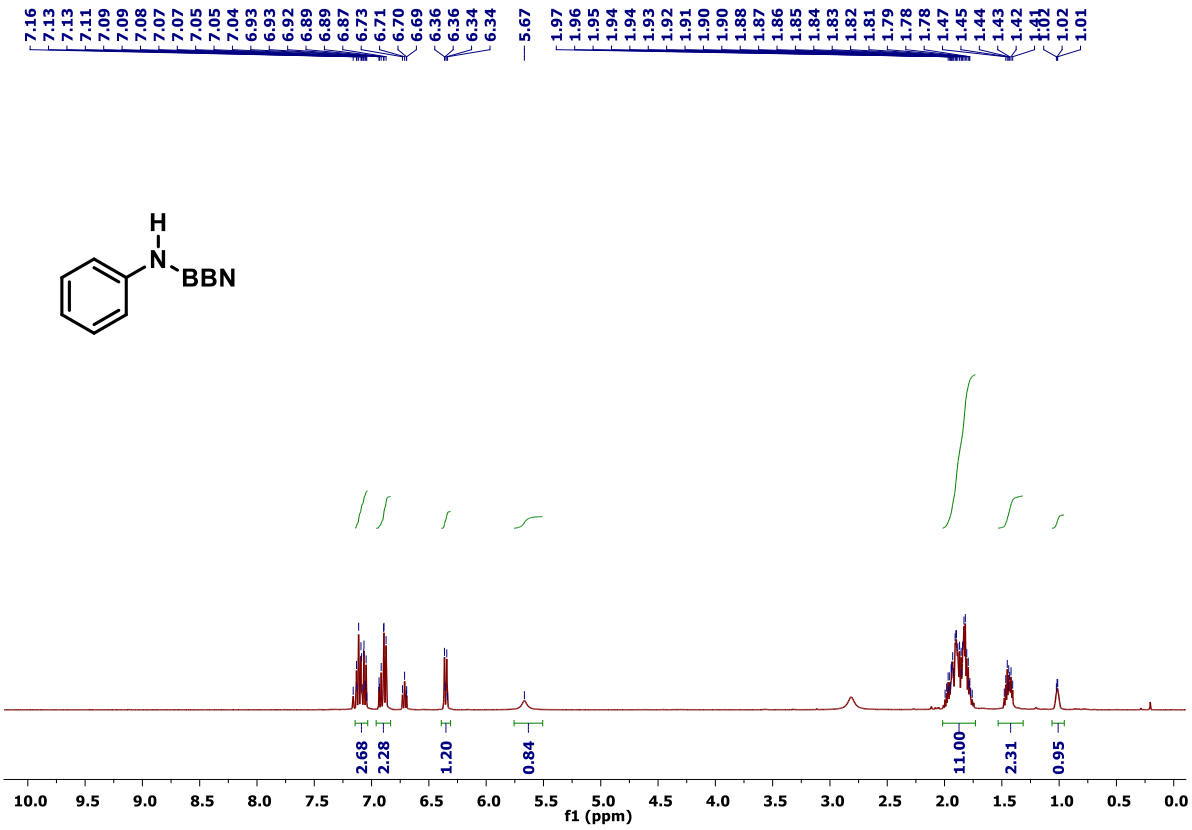


Figure S11. ^{1}H NMR spectrum of the reaction mixture (aniline, 9-BBN, and mNHO in benzene-d_6 at room temperature).[S6]

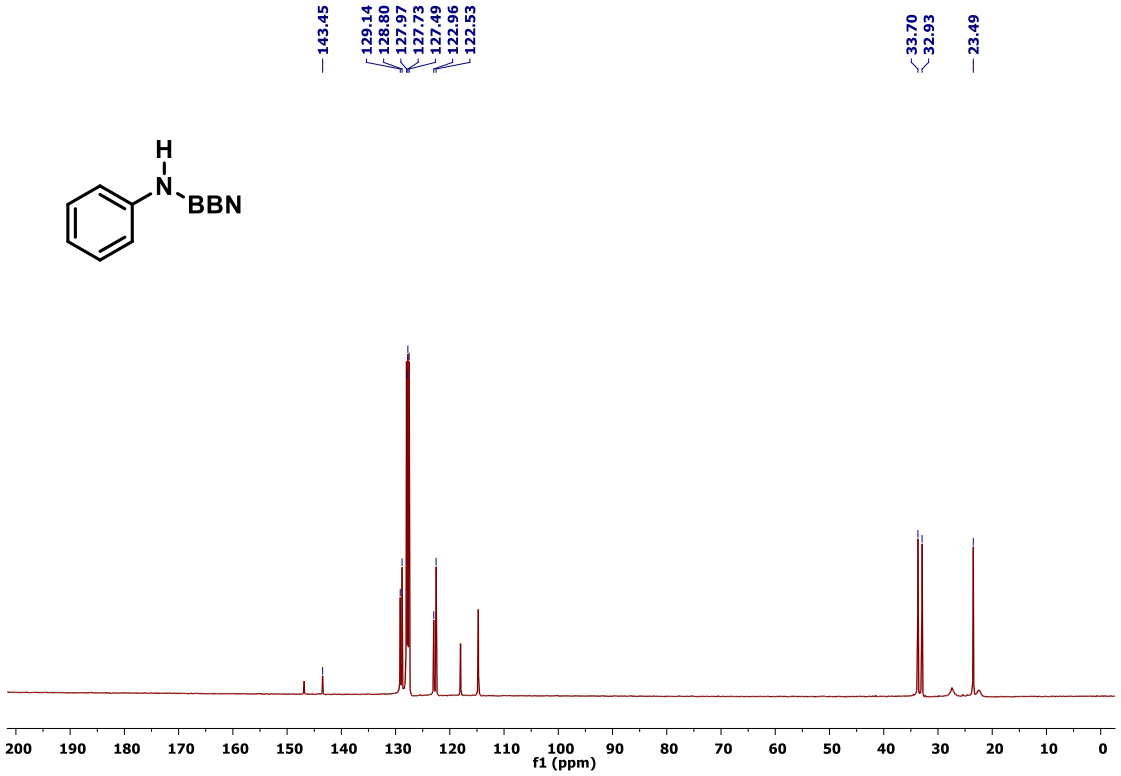


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of the reaction mixture (aniline, 9-BBN and mNHO in benzene-d_6 at room temperature) [S6].

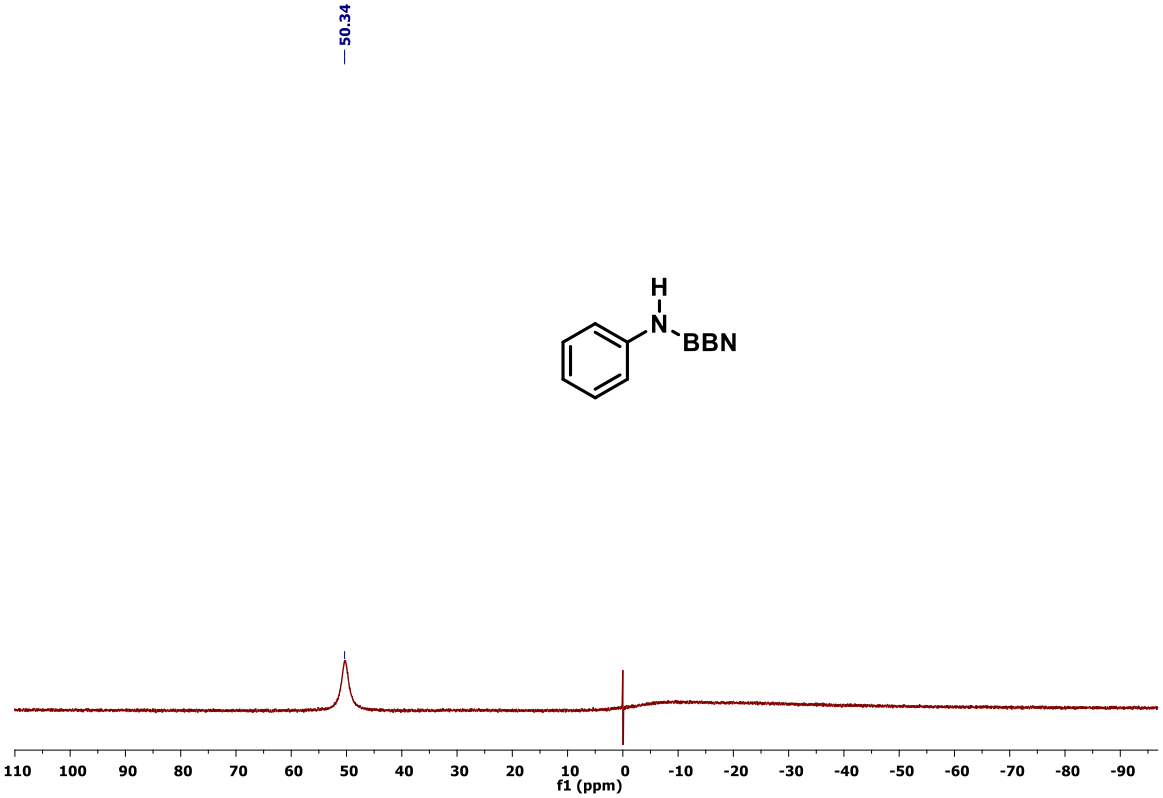
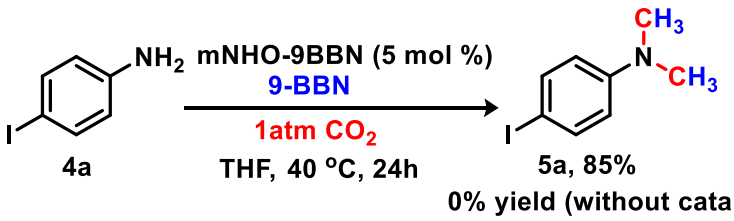


Figure S13. $^{11}B\{^{1}H\}$ NMR spectrum of the reaction mixture (aniline, 9-BBN and mNHO in benzene-d_6 at room temperature) [S6].

Control reactions:

a) mNHO-9BBN adduct (10) catalysed N, N-dimethylation of 4-iodo aniline using CO_2 and 9BBN: As a proof to establish the adduct 10 is catalytically active species

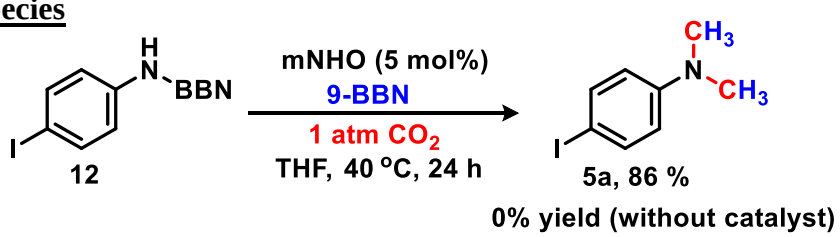


Scheme S8. N, N-dimethylation of 4-iodo aniline catalysed by mNHO-9BBN adduct **10**.

An oven-dried 25 mL Schlenk tube was charged with 0.2 mmol 4-iodo aniline substrate and a magnetic stirring bar. It was kept under high vacuum for 2 h and was transferred into an argon-filled glovebox. Inside the glovebox, mNHO-9BBN adduct (5 mol %), 9-BBN (1.6 mmol) and anhydrous THF (1 mL) were added to the reaction tube. Next, the tube was sealed tightly with a screw cap equipped with a J. Young valve and removed from the glovebox. After that, the reaction tube was connected through the Schlenk line and the mixture was degassed by successive two freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). Subsequently, the flask was sealed and stirred for 24 h at 40 ^{o}C. After completion of the reaction, the solvent was removed by vacuum and the compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99: 1 v/v) as eluent. The corresponding product was identified by ^{1}H and ^{13}C{^{1}H} NMR spectroscopy in $CDCl_3$.

Yellow liquid (85%) [S7]; **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.47 (d, 2H, 8 Hz, Ar-H), 6.49 (d, 2H, 8 Hz, Ar-H), 2.92 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 150.0 (Ar-C), 137.5 (Ar-CH), 114.7 (Ar-CH), 77.4 (Ar-C), 40.4 $N(CH_3)_2$.

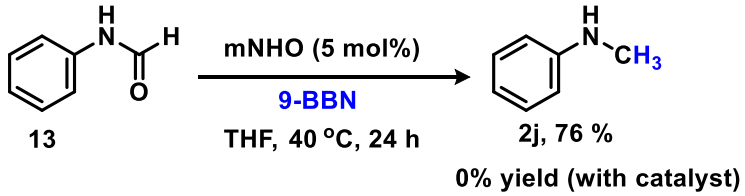
b) mNHO catalysed N, N-dimethylation of 4-iodo borylamine (12) using CO_2 and 9BBN: As a proof to establish the 4-iodo N-borylatedamine 12 is an active intermediate species



Scheme S9. N, N-dimethylation of 4-iodo borylamine catalysed by mNHO.

An oven-dried 25 mL Schlenk tube equipped with a stirring bar was charged with 4-iodo aniline (43.8 mg, 0.2 mmol, 1 equiv.), mNHO (5 mol %), 9-BBN (1 equiv.) and THF (1 mL) in argon filled glove box. Next, the reaction mixture was allowed to stir during 12 h at room temperature. After completion of the reaction, the solvent was removed by vacuum and the semi-liquid borylamine (**12**) was transferred to the glove box. After that, 9-BBN (1.6 mmol) and anhydrous THF (1 mL) were added to the reaction tube. Subsequently the tube was sealed tightly with a screw cap equipped with a J. Young valve and removed from the glove box. Next, the reaction tube was connected through the Schlenk line and the mixture was degassed by successive two freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.) and was stirred for 24 h at 40 ^{o}C. After completion of the reaction, the solvent was removed by vacuum and the compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99: 1 v/v) as eluent. The corresponding product was identified by ^{1}H and ^{13}C{^{1}H} NMR spectroscopy in $CDCl_3$. Yellow liquid (86%) [S7]; **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.47 (d, 2H, 8 Hz, Ar-H), 6.49 (d, 2H, 8 Hz, Ar-H), 2.92 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 150.0 (Ar-C), 137.5 (Ar-CH), 114.7 (Ar-CH), 77.4 (Ar-C), 40.4 ($N(CH_3)_2$) .

c) <u>mNHO catalysed reduction of formanilide (13) to N-methyl amine using 9-BBN: As a proof of N-formyl intermediate during the reaction</u>



Scheme S10. Reduction of formanilide catalysed by mNHO.

An oven-dried 25 mL Schlenk tube equipped with a stirring bar and was charged with formanilide (43.8 mg, 0.2 mmol, 1 equiv.), mNHO (5 mol %), 9-BBN (2.5 equiv.) and THF (0.5 mL) in an argon filled glovebox. Then the reaction mixture was allowed to stir at 40 ^{o}C during 24 h. After completion of the reaction, the solvent was removed by vacuum and the compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99: 1 v/v) as eluent. The desired product was identified by ^{1}H and ^{13}C{^{1}H} NMR spectroscopy in $CDCl_3$.

Yellow liquid (76%); [S8] **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.33 (t, 2H, 8 Hz, Ar-H), 6.85 (t, 1H, 8 Hz, Ar-H), 6.72 (d, 2H, 8 Hz, Ar-H), 3.66 (b, 1H, NH), 2.90 (s, 3H,

NHCH$_3$); **^{13}C{^{1}H} NMR** (100 MHz, CDCl$_3$, 25 ^{o}C): δ (ppm) = 149.2 (Ar-C), 129.0 (Ar-CH), 117.0 (Ar-CH), 112.2 (Ar-CH), 30.5 (NHCH$_3$).

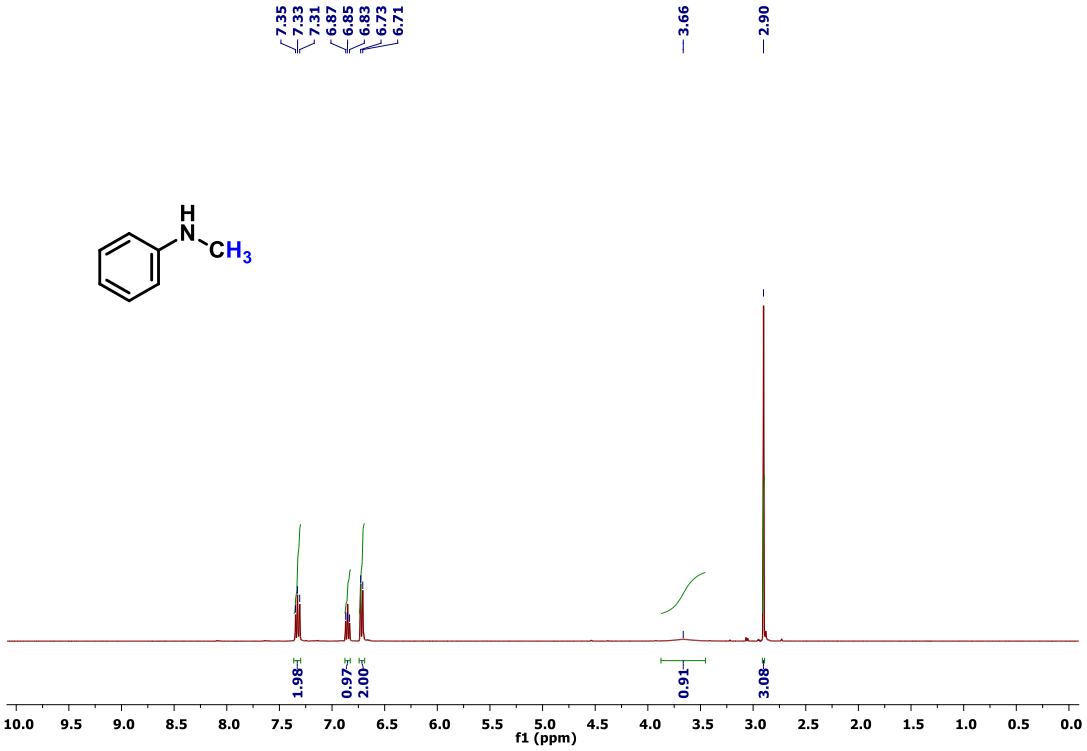


Figure S14. ^{1}H NMR spectrum of N-methyl aniline in CDCl$_3$.[S8]

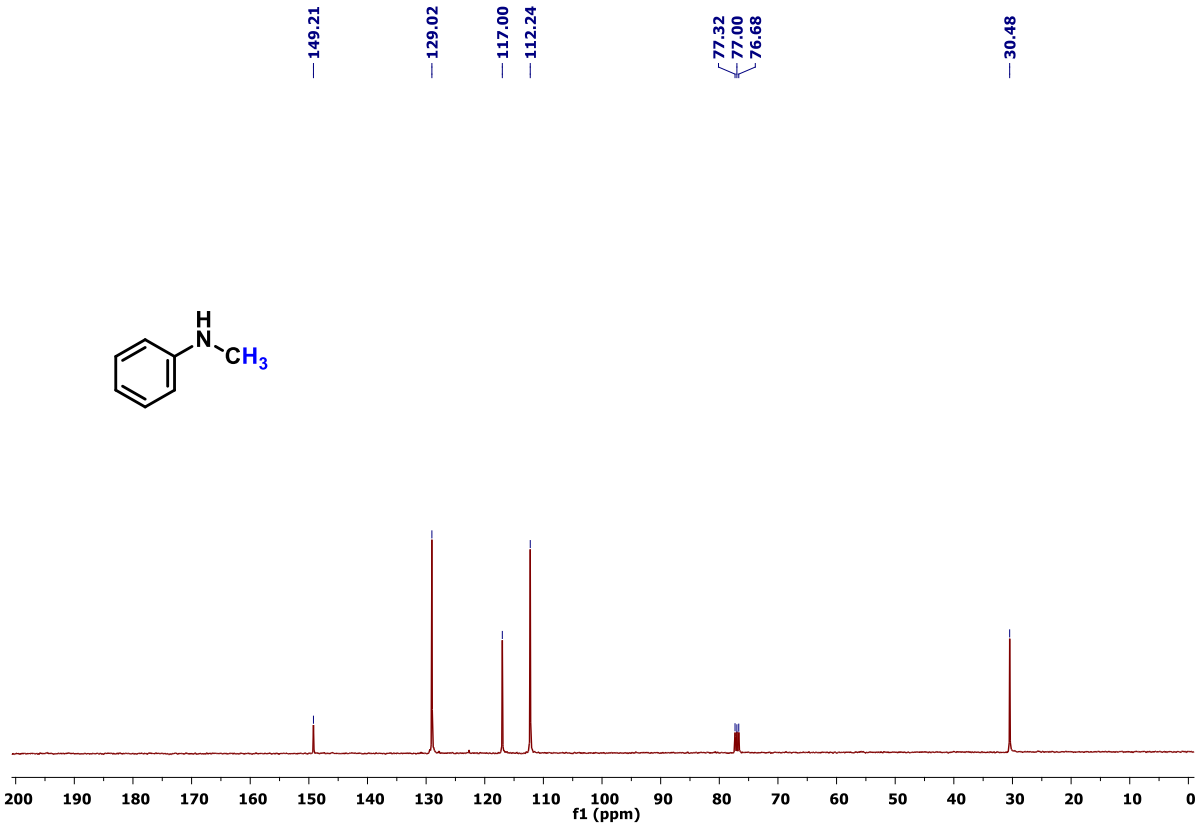
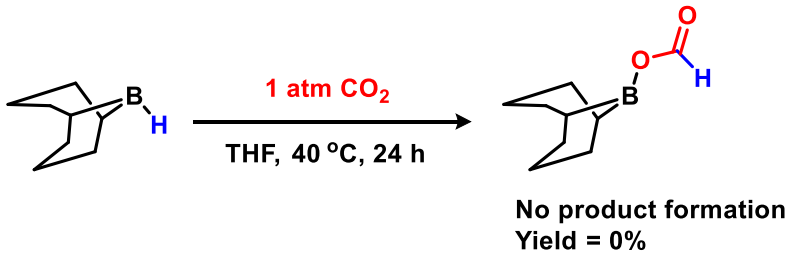


Figure S15. ^{13}C{^{1}H} NMR spectrum of the N-methyl aniline in CDCl$_3$.[S8]

d) <u>Reaction of 9-BBN with CO_2 in absence of catalyst mNHO</u>



Scheme S11. Reaction between 9-BBN and CO_2 in THF at 40 °C.

An oven-dried 25 mL Schlenk tube equipped with a stirring bar was charged with 0.2 mmol 9-BBN (24.5 mg) and THF (0.5 mL) in an argon filled glovebox. The mixture was degassed by two successive freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). Then the reaction mixture was allowed to stir at 40 °C for 24h. After completion of the reaction, the solvent was removed by vacuum. The resulting reaction mixture was dissolved in C_6D_6 and formation of boron-formate was not observed in proton NMR spectrum. This experiment supports the fact that uncatalyzed reaction is not feasible for this step.

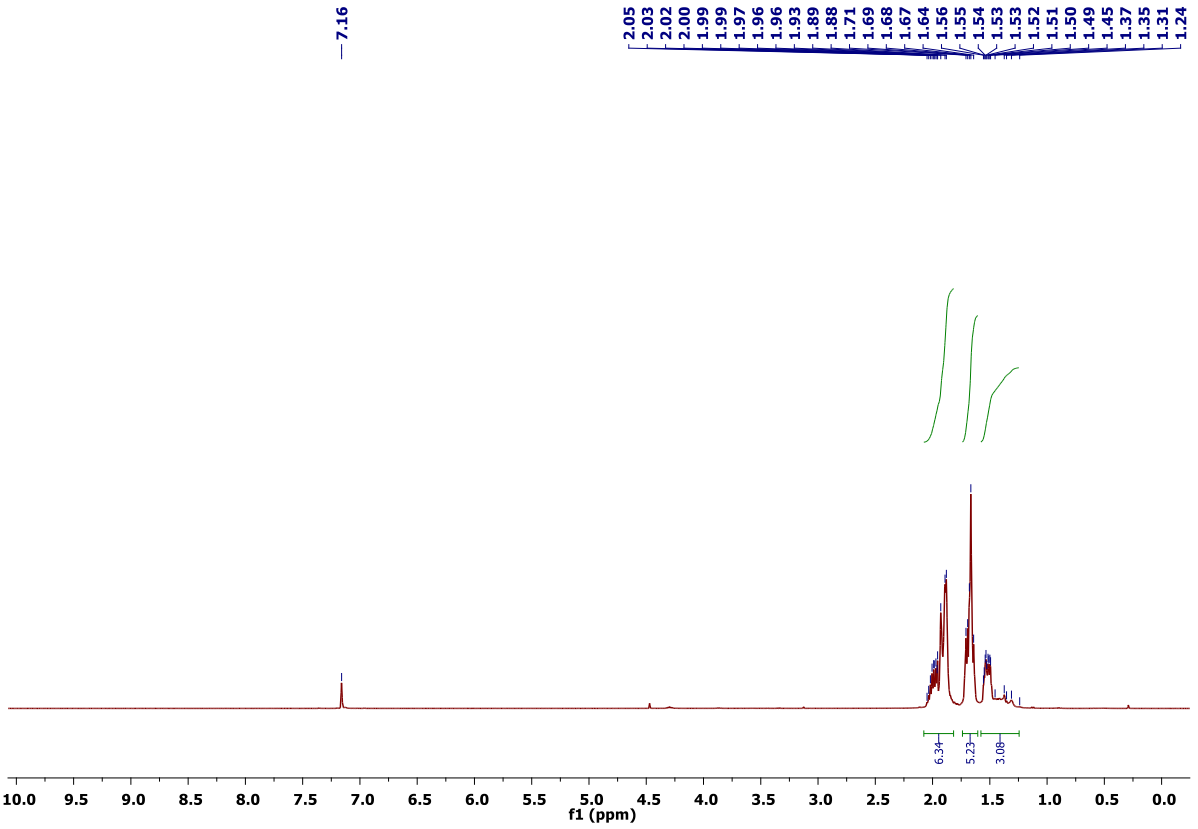
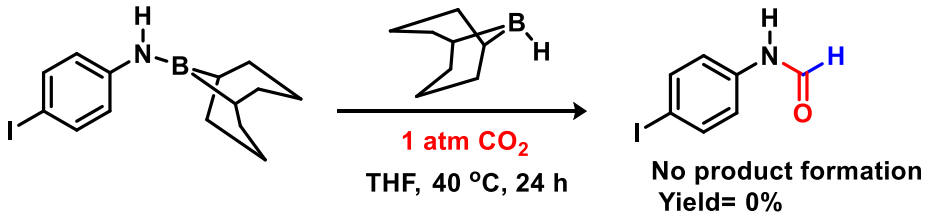


Figure S16. ^{1}H NMR spectrum of the reaction mixture at 40 °C (9-BBN and CO_2 in benzene-d_6).

e) <u>Reaction of 4-iodoaniline-BBN and 9-BBN with CO_2 in absence of catalyst mNHO</u>



Scheme S12. Reaction between 4-Iodoaniline-BBN and 9-BBN with CO_2 in THF at 40 °C.

An oven-dried 25 mL Schlenk tube equipped with a stirring bar was charged with 0.2 mmol 4-iodoaniline-BBN (67.8 mg), 9-BBN (24.5 mg, 1 equiv.) and THF (0.5 mL) in an argon filled glovebox. The mixture was degassed by two successive freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). Next, the reaction mixture was allowed to stir at 40 °C for 24h. After completion of the reaction, the solvent was removed by vacuum. The resulting reaction mixture was dissolved in C_6D_6 and formation of N-formyl 4-iodoaniline was not observed in proton NMR spectrum. This experiment further supports involvement of catalyst during this step.

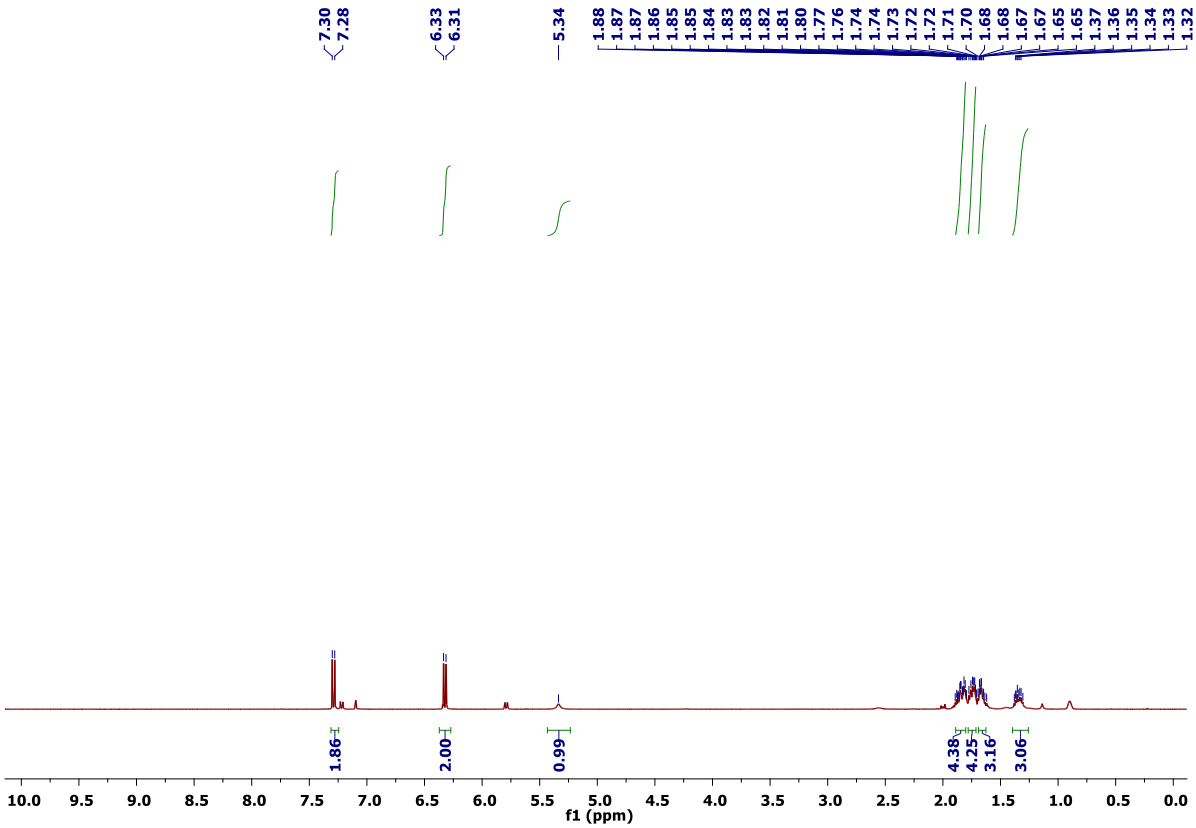
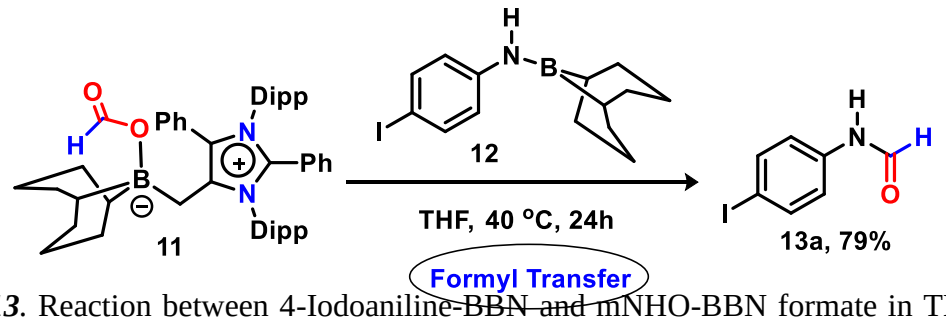


Figure S17. ^{1}H NMR spectrum of the reaction mixture after 24h at 40 °C (4-iodo-BBN, 9-BBN and CO_2 in benzene-d_6).

f) Reaction of 4-iodoaniline-BBN (12) and mNHO-BBN formate (11): Formyl Transfer



Scheme S13. Reaction between 4-Iodoaniline-BBN and mNHO-BBN formate in THF at 40 ^{o}C.

An oven-dried 25 mL Schlenk tube equipped with a stirring bar was charged with 0.05 mmol 4-iodoaniline-BBN **12** (17 mg), mNHO-BBN formate **11** (36 mg, 1 equiv.) and THF (0.5 mL) in an argon filled glovebox. Next, the reaction mixture was allowed to stir at 40 ^{o}C for 24h. After completion of the reaction, the solvent was removed by vacuum. The reaction mixture was dried using high vacuum pump and pass through by column chromatography on silica gel (Merck, 100-200 mesh) using hexane-ethyl acetate mixture (70:30 v/v) as an eluent. The corresponding N-formylated product was identified by ^{1}H and ^{13}C{^{1}H} NMR spectroscopies in $CDCl_3$.

Brown Solid (79%); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 8.65 (d, 8 Hz, 0.51H), 8.35 (d, 0.62H), 7.65-7.60 (m, 2H), 7.31 (d, 2H, 8 Hz, Ar-H), 6.83 (d, 1H, 8 Hz); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 162.3, 159.0, 138.7, 138.0, 136.5, 121.7, 120.4, 88.7, 88.1.

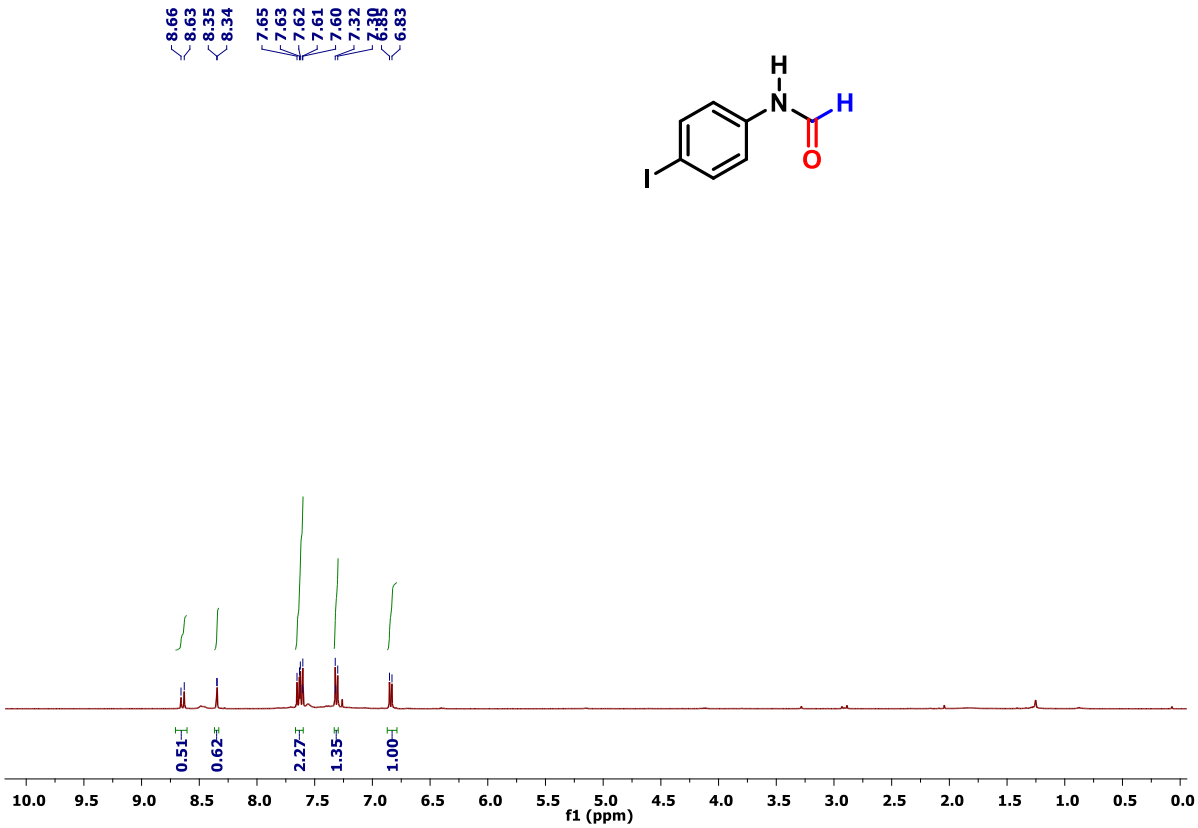


Figure S18. ^{1}H NMR spectrum of the reaction mixture after 24h at 40 ^{o}C (4-iodo-BBN, mNHO-BBN-formate in $CDCl_3$).

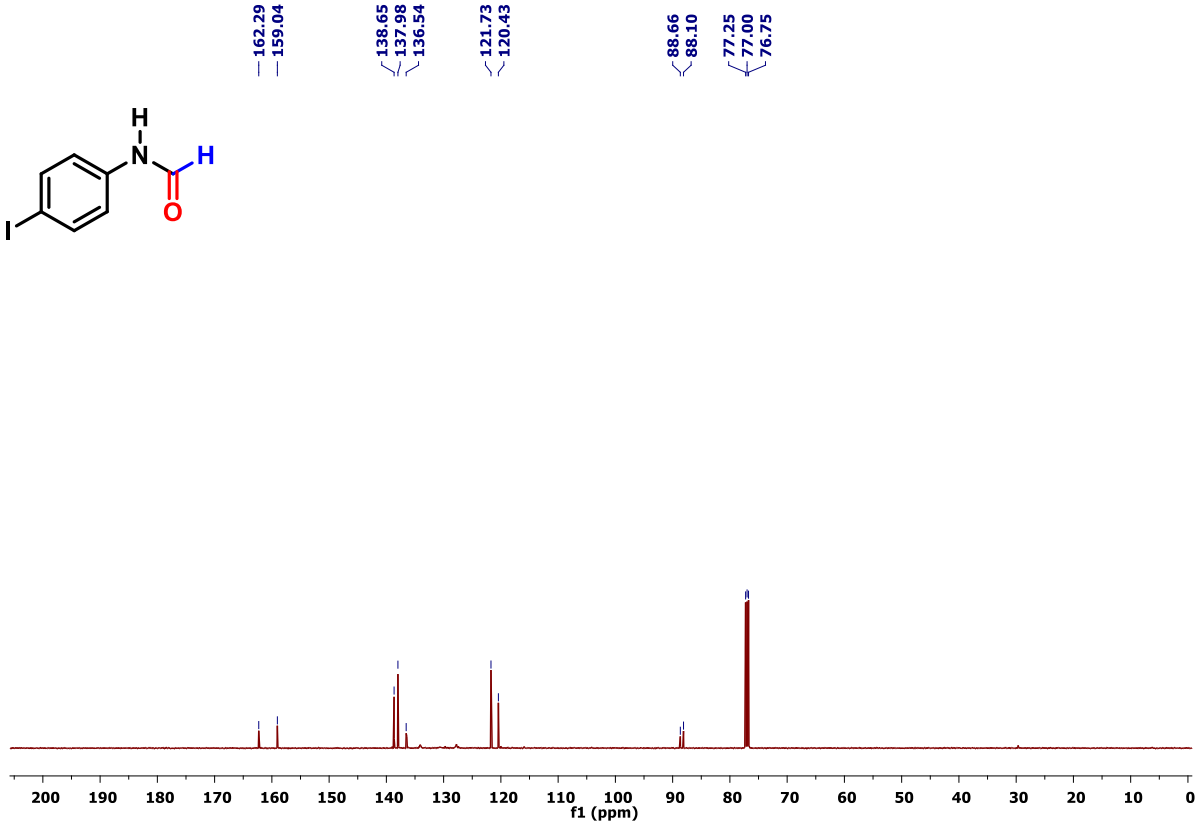
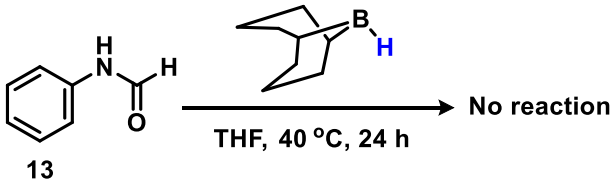


Figure S19. ^{13}C NMR spectrum of the reaction mixture after 24h at 40 ^{o}C (4-iodo-BBN, mNHO-BBN-formate in $CDCl_3$).

g) <u>A control reaction between formanilide 13 and 9-BBN in absence of mNHO</u>



Scheme S14. Reaction of formanilide and 9-BBN.

An oven-dried 25 mL Schlenk tube equipped with a stirring bar was charged with formanilide (43.8 mg, 0.2 mmol, and 1 equiv.), 9-BBN (2.5 equiv.) and THF (0.5 mL) in an argon filled glovebox. Next, the reaction mixture was allowed to stir at 40 ^{o}C during 24h. After completion of the reaction, the solvent was removed by vacuum. Next, the resulting reaction mixture was dissolved in $CDCl_3$ and formation of N-methyl amine product was not observed in proton NMR spectrum.

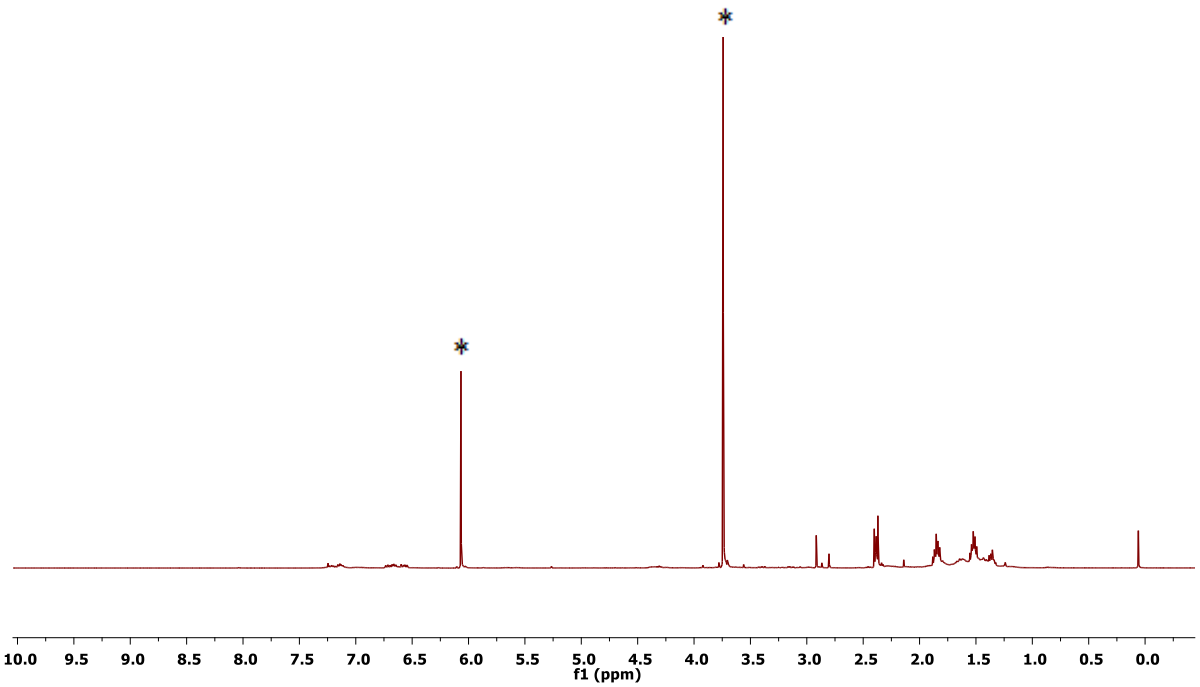
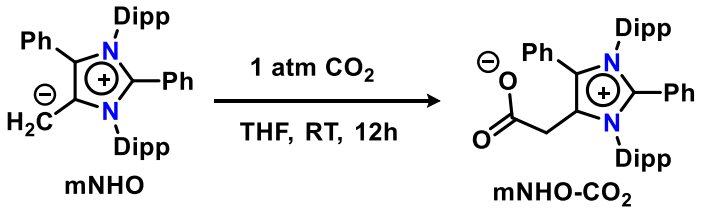


Figure S20. ^{1}H NMR spectrum of the reaction between formanilide and 9-BBN in $CDCl_3$. * indicates peaks arising from 1, 3, 5-trimethoxybenzene.

h) <u>A control reaction between mNHO and CO_2</u>



Scheme S15. Reaction between mNHO and CO_2 in THF at RT.

An oven-dried 25 mL Schlenk flask equipped with a stirring bar was charged with the mesoionic N-heterocyclic olefin, mNHO (111 mg, 0.2 mmol, 1 equiv) and THF (2 mL) in an argon filled glovebox. Next, the solution of mNHO was degassed by successive two freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). The flask was sealed and allowed to stir during 12h at room temperature. After completion of the reaction, the solvent was dried under reduced pressure and the blue solid was washed with hexane for three times and dried. The compound mNHO-CO_2 was characterized through ^{1}H and ^{13}C{^{1}H} NMR spectroscopies.

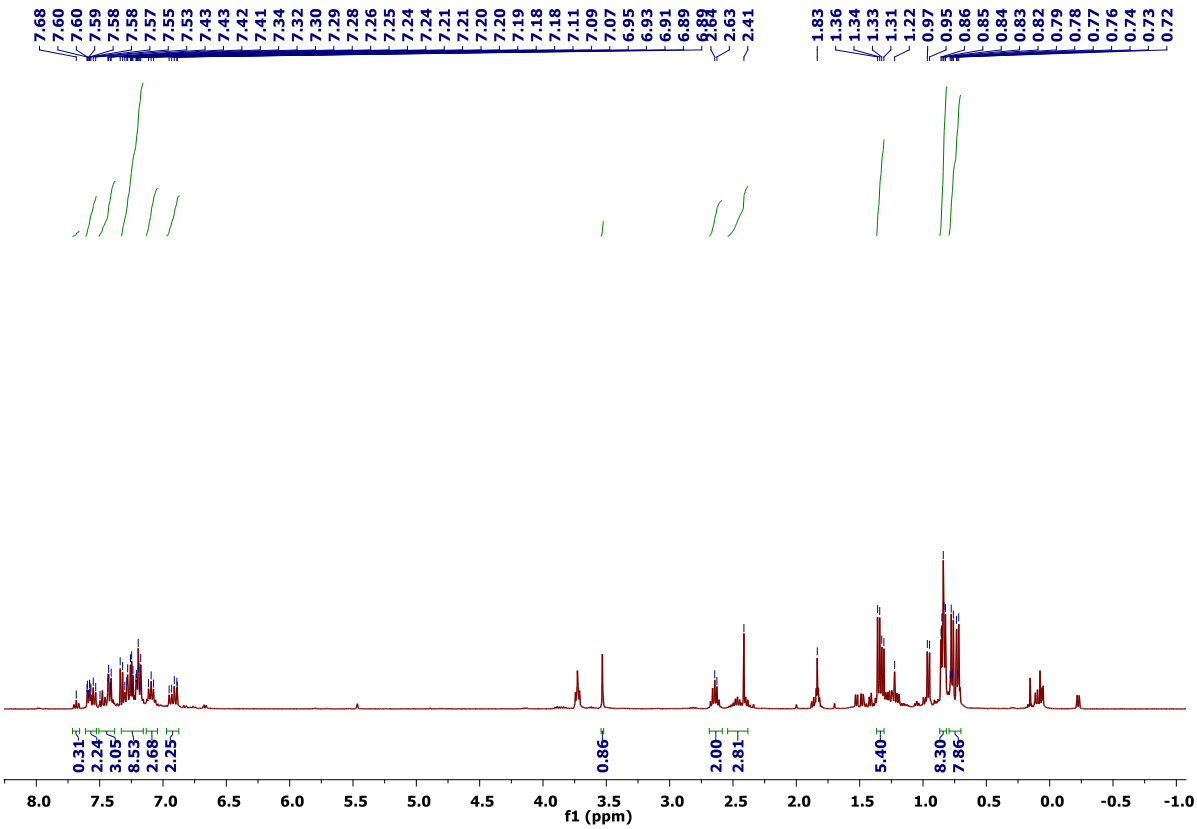


Figure S21. ^{1}H NMR spectrum of the reaction between mNHO and CO_2 in $CDCl_3$.

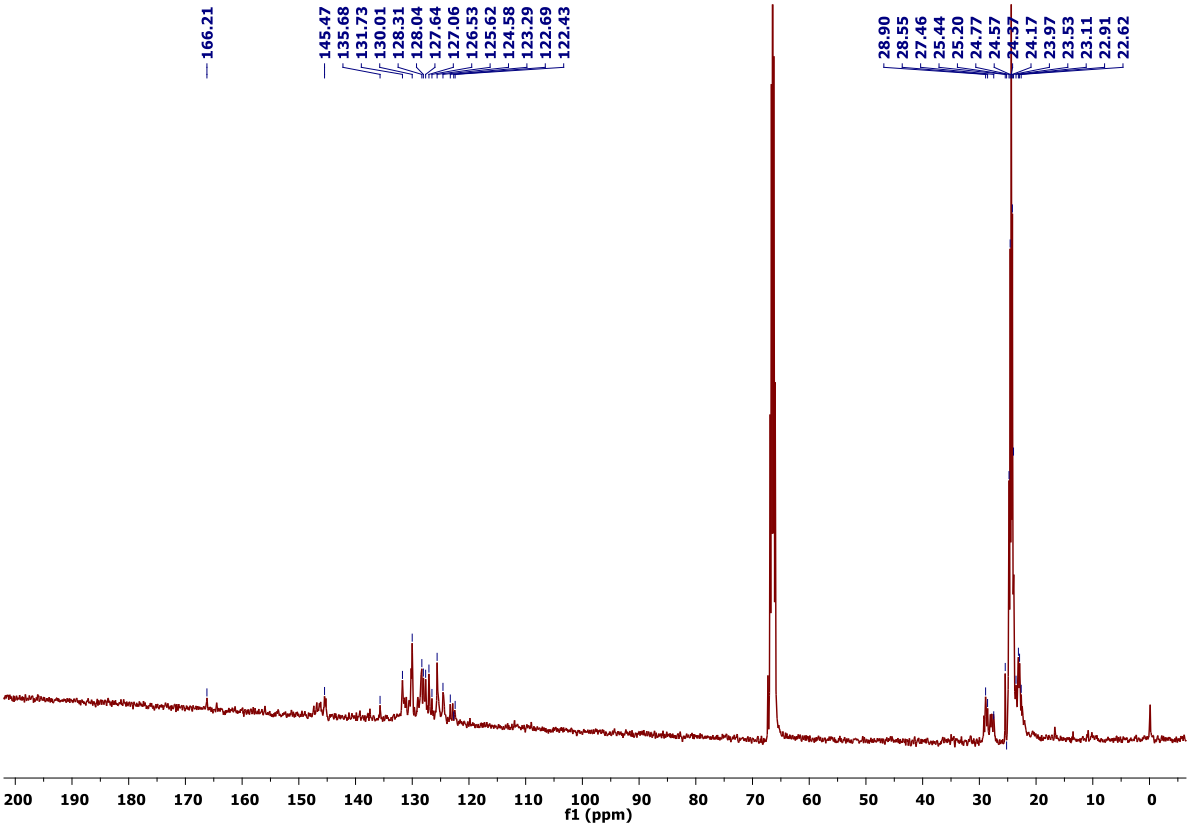
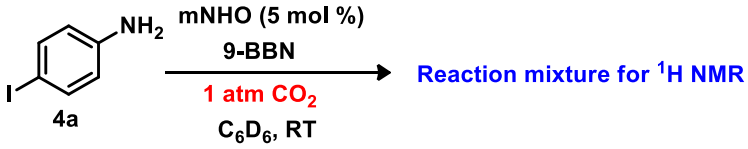


Figure S22. $^{13}C\{^{1}H\}$NMR spectrum of the reaction between mNHO and CO_2 in THF-d_8.

i) <u>Characterization of N-formyl intermediate during the N-methylation reaction catalysed by mNHO</u>



Scheme S16. Reaction of 4-iodo aniline, 9-BBN and mNHO in benzene-d_6 at room temperature under 1 atm CO_2 atmosphere during 10 min.

Under an argon atmosphere, a 2.5 mL screw cap NMR tube equipped with a J. Young valve was charged with 4-iodo aniline (11 mg, 0.05 mmol, 1 equiv.), mNHO (5 mol%), 9-BBN (8 equiv.) and benzene-d_6 (0.6 mL). The mixture was degassed by a freeze-pump-thaw cycle and placed under 1 atm of CO_2 at room temperature. After 10 min, the ^{1}H NMR spectrum of the reaction mixture was recorded confirming the presence of formyl group. This confirms that N-formyl compound acts as an intermediate during the N-methylation process.

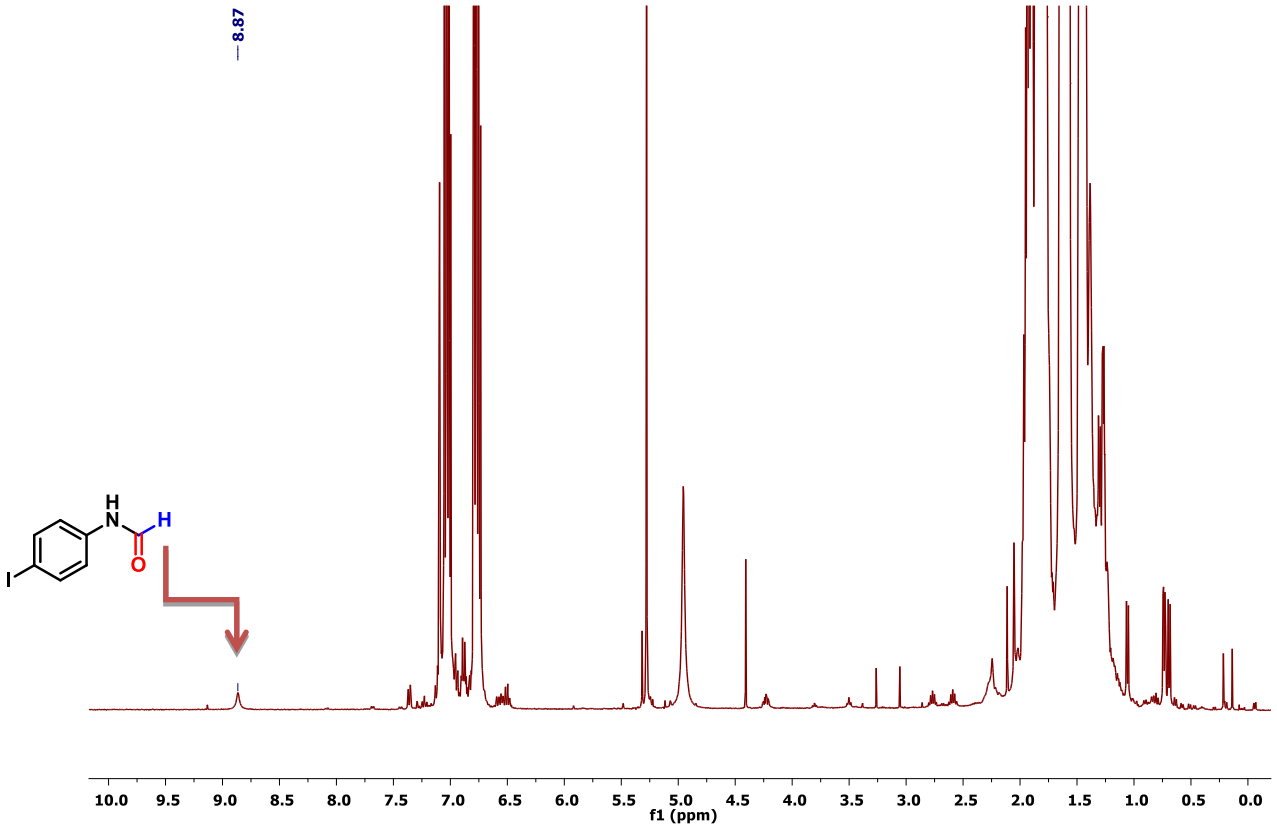
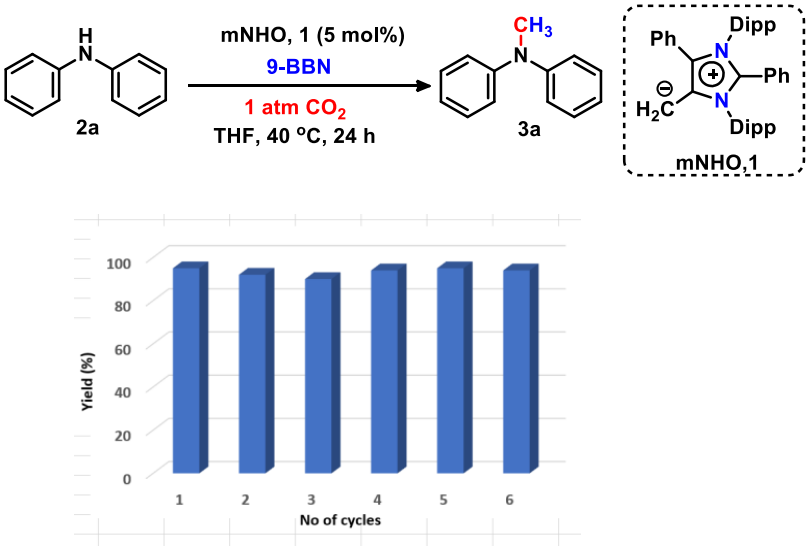


Figure S23. ^{1}H NMR spectrum of the reaction mixture (4-iodo aniline, 9-BBN, and mNHO in benzene-d_6 in room temperature under 1 atm CO_2 atmosphere) using a screw cap NMR tube.

Procedure for testing sustainability of catalyst during six successive catalytic cycles

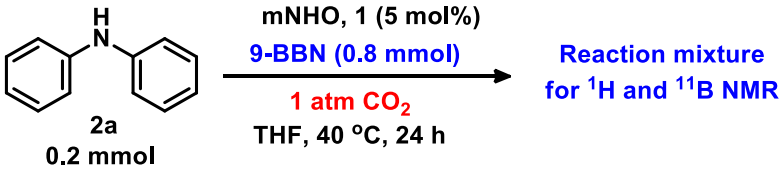
Six oven dried 25 mL Schlenk tubes equipped with magnetic bar were taken and labelled them appropriately; in each of them 0.2 mmol of diphenylamine, mesoionic N-heterocyclic olefin (mNHO) catalyst (5 mol %), 9-BBN (0.8 mmol) and anhydrous THF (0.5 mL) were taken inside a argon filled glovebox. Following this, six tubes were sealed tightly with the screw cap equipped with a J. Young valve and removed from the glove box. Then the six reaction tubes were connected through the Schlenk line and the mixture was degassed by successive two freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). The reaction mixtures were stirred for 24 h at 40 ^{o}C. After the first reaction time span (24h), the first reaction tube was uncapped. The rest 5 tubes were transferred to the glovebox and fresh 0.2 mmol of diphenylamine, 9-BBN (0.8 mmol) were added to all remaining five reaction tubes. Then the five reaction tubes were connected through the Schlenk line and the mixture was degassed by a freeze-pump-thaw cycle and exposed to carbon dioxide (1 atm.). After that, the reaction mixtures were stirred for 24 h at 40 ^{o}C for the second cycle. It may be noted that no further addition of mNHO catalyst was made in any of these reaction tubes. From the 1st reaction tube, the solvent was removed by high vacuum then the product was purified by column chromatography over silica gel (100-200 mesh) using hexane-ethyl acetate mixture (99:1 v/v) and isolated yield (in percentage) was determined. After second reaction time span of 24 h, the 2nd reaction tube was discontinued and worked up as described previously to record the isolated yield. Subtracting the amount of product formed in tube 1 (first cycle), the exclusive amount of product in second cycle was obtained. The remaining 4 tubes were transferred to the glovebox and fresh 0.2 mmol of diphenylamine, 9-BBN (0.8 mmol) were added to the reaction tubes. Then the 4 reaction tubes were connected through the Schlenk line and the mixture was degassed by a freeze-pump-thaw cycle and exposed to carbon dioxide (1 atm.). Following this, the reaction mixtures were stirred for 24 h at 40 ^{o}C for the third cycle. In a similar way, the product was extracted and isolated from tube 3 and amount of product formed had been recorded. Such procedure continued till 6th reaction tube and the yield of product in each cycle was calculated similarly. After calculating yield of product in each cycle, we plot a graph with ‘number of cycles’ in X-axis and ‘yield of product’ in Y-axis using the yield recorded for each cycle. It may be noted that the similar procedure was repeated and the average yield is noted in the graph.



Scheme S17. Checking sustainability of the catalyst mNHO in consecutive six cycles.

Characterization of $(9\text{-BBN})_2O$ dimer as a by-product:

An oven-dried 25 mL Schlenk tube was charged with 0.2 mmol diphenylamine and a magnetic stirring bar. It was kept under high vacuum for 2 h and was transferred into a argon-filled glove box. Inside the glovebox, mesoionic N-heterocyclic olefin (mNHO) catalyst (5 mol %), 9-BBN (0.8 mmol) and anhydrous THF (0.5mL) were added to the reaction tube. Next, the tube was sealed tightly with a screw cap equipped with a J. Young valve and removed from the glovebox. Following this, the reaction tube was connected through the Schlenk line and the mixture was degassed by successive two freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.) and was stirred for 24 h at 40 °C. After completion of the reaction, the solvent was removed by vacuum and the ^{1}H and ^{11}B NMR spectra of the crude mixture were recorded in C_6D_6.



Scheme S18. Reaction of diphenylamine, 9-BBN and mNHO in THF at 40 °C under 1 atm CO_2.

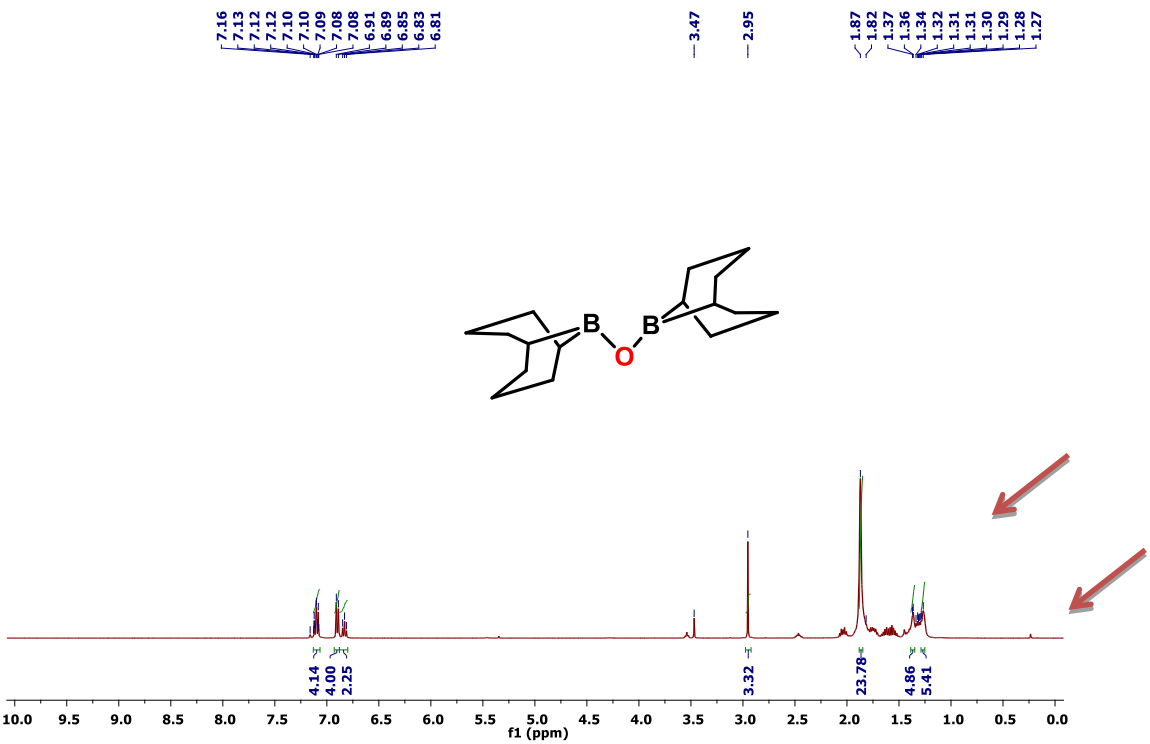


Figure S24. ^{1}H NMR spectrum of the catalytic reaction mixture in C_6D_6 where the peak at (1.87-1.82) ppm and (1.27-1.37) ppm supports the formation of $(9\text{-BBN})_2O$ dimer. [S9]

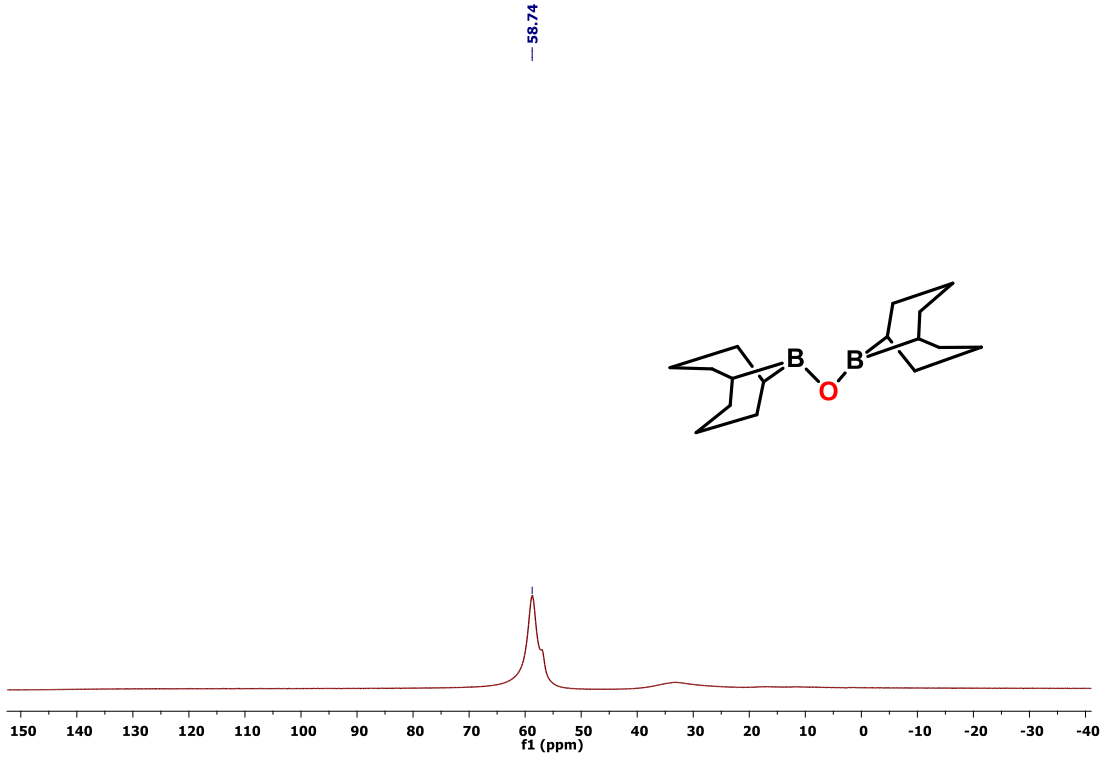
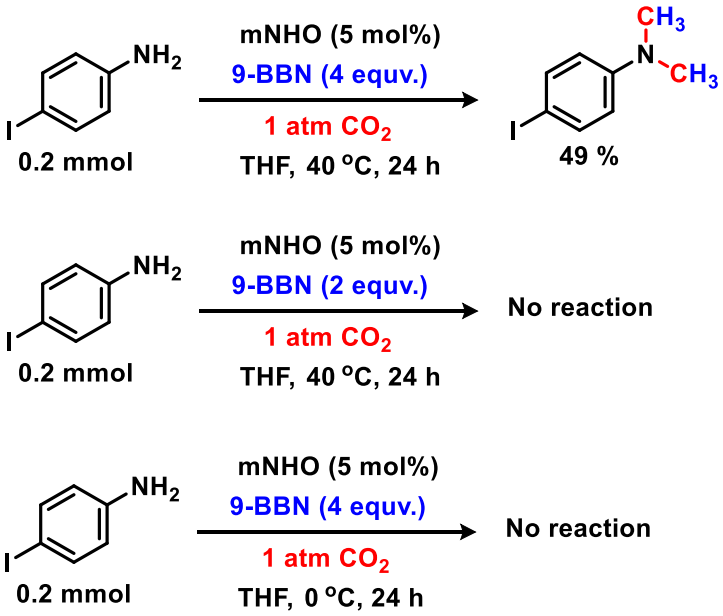


Figure S25. ^{11}B NMR spectrum of the catalytic reaction mixture in C_6D_6 where the peak at 58.7 ppm is attributed to ^{11}B nuclei of boron dimer by comparing the previous reported value.[S9]

Attempts made for selective mono methylation of 4-iodo aniline:

Under an argon atmosphere, a 25 mL Schlenk tube equipped with a stir bar and a J. Young valve was charged with 4-iodo aniline (0.2 mmol), mNHO (5 mol%), required amount of 9-borabicyclo (3,3,1)nonane (9-BBN) and THF (0.5 mL). The mixture was degassed by two successive freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). The tube was sealed and stirred for 24h at varied temperature. Next, the reaction mixture was dried using high vacuum pump and purified by column chromatography on silica gel (Merck, 100-200 mesh). The corresponding product was identified by ^{1}H NMR spectroscopy in $CDCl_3$.

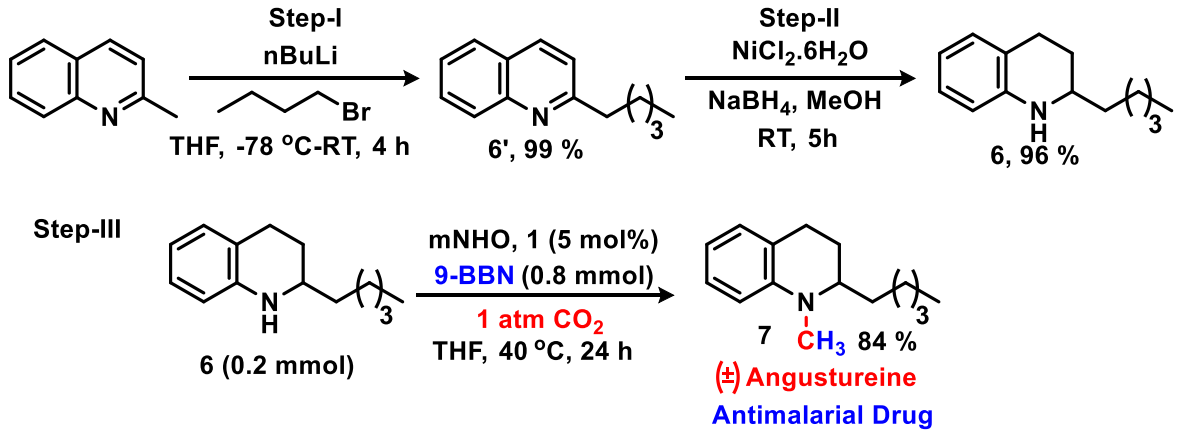
We have tried selective N-monomethylation of primary amines by lowering the amount of 9-BBN and altering the reaction condition, however these attempts were not successful.



Scheme S19. Attempts made for selective mono methylation of 4-iodo aniline.

Synthesis of drug molecules:

a) **Angustureine antimalarial drug synthesis:**



Step-I [S3]: To a solution of 1-methylquinoline (1 mmol) in dry THF (5 ml) at 0°C, n-butyllithium (1equiv.) was added in THF solution (2.5M) dropwise. The mixture was stirred at room temperature for 1.5 h and was cooled to 0 °C. Following this, 1 mmol butyl bromide was added dropwise to the solution. The mixture was stirred overnight. Water was added carefully to quench the reaction and the mixture was extracted by 50 mL ethyl acetate. The extract was dried over sodium sulphate, evaporated and purified by column chromatography to yield the desired product as yellow oil (99% yield). The compound **6'** was identified by ^{1}H and $^{13}C\{^{1}H\}$ NMR spectroscopy in $CDCl_3$.

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ (ppm) = 8.04 (d, 1H, 8Hz, Ar-H), 7.98 (dd, 1H, 8Hz, Ar-H), 7.71-7.69 (m,1H, Ar-H), 7.65-7.61 (m, 1H, Ar-H), 7.43-7.41 (m, 1H, Ar-H), 7.24-7.21 (m, 1H, Ar-H), 2.96-2.92 (m, 2H, CH_2), 1.82-1.75 (m, 2H, CH_2), 1.39-1.32 (m, 4H, CH_2), 0.89-0.86 (m, 3H, CH_3); **$^{13}C\{^{1}H\}$ NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) = 162.9 (Ar-C), 147.3 (Ar-C), 135.9 (Ar-CH), 129.7 (Ar-CH), 128.7 (Ar-CH), 127.3 (Ar-CH), 126.5, (Ar-C), 125.4 (Ar-CH), 121.2 (Ar-CH), 39.2 (CH_2), 31.6 (CH_2), 29.6 (CH_2), 22.4 (CH_2), 13.9 (CH_3). [S4]

Step-II [S4]: The Compound **7** (0.5 mmol) and $NiCl_2.6H_2O$ (5 mol %) were taken in a 100 mL RB flask and dissolved in 10 mL of methanol. Next, $NaBH_4$ (2.0 mmol) was added in portion at 0 °C and stirred for 30 min at RT. After completion of the reaction, methanol was evaporated and black ppt. was dissolved in 10% HCl, the acidic solution was treated with

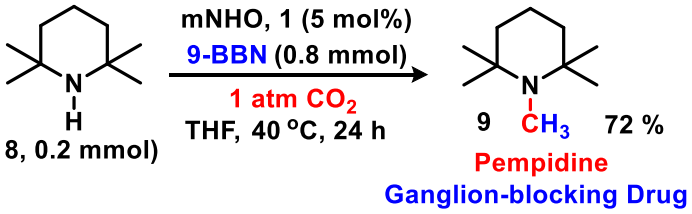
conc. ammonium hydroxide solution and **6** was extracted with ether. The extract was dried over sodium sulphate, evaporated and purified by column chromatography to yield the desired product as yellow oil (96% yield). The compound **6** was identified by ^{1}H and ^{13}C NMR spectroscopy in $CDCl_3$.

^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.05 (t, 2H, 8Hz, Ar-H), 6.69 (t, 1H, 8Hz, Ar-H), 6.54 (d, 1H, 8Hz, Ar-H), 3.8 (b, 1H, NH), 3.33-3.30 (m, 1H, CH), 2.90-2.79 (m, 2H, CH_2), 2.07-2.02 (m, 1H, CH_2), 1.72-1.67 (m, 1H, CH_2), 1.58-1.51 (m, 2H, CH_2), 1.49-1.42 (m, 6H, CH_2), 1.02 (t, 3H, 8 Hz, CH_3); **$^{13}C\{^{1}H\}$ NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 144.7 (Ar-C), 129.1 (Ar-CH), 126.6 (Ar-CH), 121.2 (Ar-C), 116.8 (Ar-CH), 114.0 (Ar-CH), 51.5 (CH), 36.6 (CH_2), 31.9 (CH_2), 28.0 (CH_2), 26.4 (CH_2), 25.3 (CH_2), 22.6 (CH_2), 14.0 (CH_3).[S4]

Step-III: Under an argon atmosphere, a 25 mL Schlenk tube equipped with a stir bar and a J. Young valve was charged with 0.2 mmol **6**, 5 mol% mNHO and 0.8 mmol 9-borabicyclo [3. 3. 1] nonane (9-BBN) in 0.5 mL THF. The mixture was degassed by successive two freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.). The flask was sealed and stirred for 24 h at 40 ^{o}C. Then the reaction mixture was dried using high vacuum pump and purified by column chromatography on silica gel (Merck, 100-200 mesh). The compound **7** (84%) was then collected in analytically pure form using hexane-ethyl acetate mixture (99:1 v/v) as the eluent. The compound **7** was identified by ^{1}H and $^{13}C\{^{1}H\}$ NMR spectroscopy in $CDCl_3$ [S4].

^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) : δ (ppm) = 7.09 (t, 1H, 8Hz, Ar-H), 6.98 (d, 1H, 8Hz, Ar-H), 6.59 (t, 1H, 8Hz, Ar-H), 6.53 (d, 1H, 8Hz, Ar-H), 3.27-3.21(m, 1H, CH), 2.94 (s, 3H, NCH_3), 2.86-2.77 (m, 1H, CH_2), 2.69-2.63 (m, 1H, CH_2), 1.93-1.84 (m, 1H, CH_2), 1.64-1.56 (m, 1H, CH_2), 1.40-1.27 (m,7H, CH_2), 0.91 (t, 3H, 8 Hz, CH_3); **$^{13}C\{^{1}H\}$ NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 145.3 (Ar-C), 128.5 (Ar-CH), 127.8 (Ar-CH), 121.82 (Ar-C) 115.1 (Ar-CH), 110.3 (Ar-CH), 58.9 (CH), 37.9 (NCH_3), 32.0 (CH_2), 31.1 (CH_2), 25.7 (CH_2), 24.3 (CH_2), 23.5 (CH_2), 22.6 (CH_2), 14.0 (CH_3).

b) Pempidine drug synthesis:



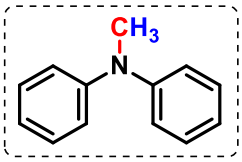
Under an argon atmosphere, a 25 mL Schlenk tube equipped with a stir bar and a J. Young valve was charged with 0.2 mmol 2, 2, 6, 6-tetramethylpiperidine **8**, 5 mol% mNHO and 0.8 mmol 9-borabicyclo (3,3,1)nonane (9-BBN) in 0.5 mL THF . The mixture was degassed by successive two freeze-pump-thaw cycles and exposed to carbon dioxide (1 atm.) and was stirred for 24 h at 40 °C. Next, the reaction mixture was dried using high vacuum pump and purified by column chromatography on silica gel (Merck, 100-200 mesh). The 1, 2, 2, 6, 6-pentamethylpiperidine **9** (72%) was collected in analytically pure form using hexane-ethyl acetate mixture (99:1 v/v) as the eluent. The compound **9** was identified by ^{1}H and $^{13}C\{^{1}H\}$ NMR spectroscopy in $CDCl_3$.[S6]

^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ (ppm) = 2.20 (s, 3H, NCH_3), 1.52-1.46 (m, 2H, CH_2), 1.43-1.40 (m, 4H, CH_2), 1.01(s, 12H, $(CH_3)_4$); **$^{13}C\{^{1}H\}$ NMR** (100 MHz, $CDCl_3$, 25 °C): δ (ppm) = 53.7, $C(CH_3)_4$, 41.2 (NCH_3), 28.5 (CH_2), 16.3 (CH_2), 17.6 $(CH_3)_4$.

III) Characterization of N-methyl and N, N- dimethyl amine compounds

^{1}H and $^{13}C\{^{1}H\}$ NMR Data of Products

N-Methyl-N-phenylaniline (3a)[S10]:

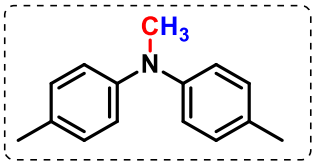


The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99: 1 v/v) as eluent.

Yellow liquid (95% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ (ppm) = 7.36-7.32 (m, 4H, Ar-H), 7.14-7.08 (m, 4H, Ar-H), 7.04-7.00 (m, 1H, Ar-H), 3.38 (s, 3H, NCH_3); **$^{13}C\{^{1}H\}$**

NMR (100 MHz, $CDCl_3$, 25 ^oC): δ (ppm) = 148.9 (Ar-C), 129.1 (Ar-CH), 121.2 (Ar-CH), 120.4 (Ar-CH), 40.1 (NCH_3).

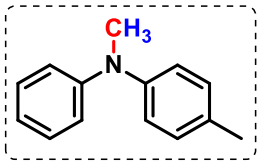
N, 4-dimethyl-N-(p-tolyl)aniline (3b)[S11]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (86% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^oC): δ (ppm) = 7.08 (d, 4H, 8 Hz, Ar-H), 6.91(d, 4H, 6.8 Hz, Ar-H), 3.27(s, 1H, NCH_3), 2.31 (s, 6H, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^oC): δ (ppm) = 147.1(Ar-C), 130.4 (Ar-C), 129.7 (Ar-CH), 120.4 (Ar-CH), 40.4 (NCH_3), 20.6 (CH_3).

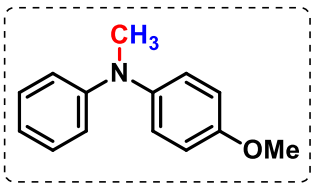
N, 4-dimethyl-N-phenylaniline (3c)[S12]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (79% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^oC): δ (ppm) = 7.23 (t, 2H, 8 Hz, Ar-H), 7.12 (d, 2H, 8 Hz, Ar-H), 7.00 (d, 2H, 8 Hz, Ar-H), 6.92 (d, 2H, 8 Hz, Ar-H), 6.87 (t, 1H, 8 Hz, Ar-H), 3.29 (s, 1H, NCH_3), 2.32 (s, 3H, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^oC): δ (ppm) = 149.4 (Ar-C), 146.6 (Ar-C), 132.0 (Ar-C), 129.9 (Ar-CH), 129.0 (Ar-CH), 122.5 (Ar-CH), 119.8 (Ar-CH), 118.2 (Ar-CH), 40.3 (NCH_3), 20.7 (CH_3).

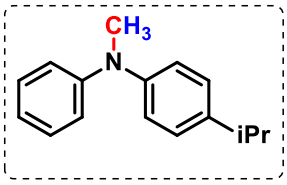
4-methoxy-N-methyl-N-phenylaniline (3d)[S12]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (83% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.21 (t, 2H, 8 Hz, Ar-H), 7.10 (d, 2H, 8 Hz, Ar-H), 6.90 (d, 2H, 8 Hz, Ar-H), 6.79 (t, 1H, 8 Hz, Ar-H), 3.82 (s, 3H, OCH_3), 3.27 (s, 3H, NCH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 156.3 (Ar-C), 149.8 (Ar-C), 142.3 (Ar-C), 128.9 (Ar-CH), 126.2 (Ar-CH), 118.3 (Ar-CH), 115.8 (Ar-CH), 114.8 (Ar-CH), 55.5 (OCH_3), 40.5 (NCH_3).

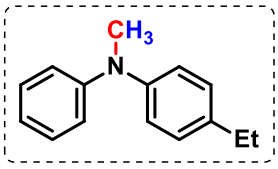
4-isopropyl-N-methyl-N-phenylaniline (3e)[S12]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99: 1 v/v) as eluent.

Yellow liquid (80% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.26 (t, 2H, 8 Hz, Ar-H), 7.18 (d, 2H, 8 Hz, Ar-H), 7.03 (d, 2H, 8 Hz, Ar-H), 6.97 (d, 2H, 8 Hz, Ar-H), 6.90 (t, 1H, 8 Hz, Ar-H), 3.32 (s, 3H, NCH_3), 2.95-2.86 (m, 1H, CH_2), 1.28 (d, 6H, 4 Hz, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 149.3 (Ar-C), 146.8 (Ar-C), 142.8 (Ar-C), 129.0 (Ar-CH), 127.2 (Ar-CH), 122.0 (Ar-CH), 120.0 (Ar-CH), 118.6 (Ar-CH), 40.3 (NCH_3), 33.4 (CH_2), 24.1(CH_3).

4-ethyl-N-methyl-N-phenylaniline (3f):



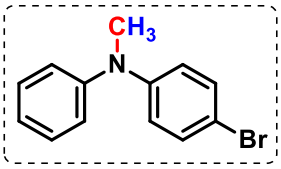
The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99: 1 v/v) as eluent.

Yellow liquid (81% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.27 (t, 2H, 8 Hz, Ar-H), 7.17 (d, 2H, 8 Hz, Ar-H), 7.05 (d, 2H, 8 Hz, Ar-H), 6.97 (d, 2H, 8 Hz, Ar-H), 6.91 (t, 1H, 8 Hz, Ar-H), 3.33 (s, 3H, NCH_3), 2.66 (q, 2H, 8 Hz, CH_2), 1.28 (t, 3H, 8 Hz, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 149.3 (Ar-C), 146.8 (Ar-C), 138.3 (Ar-

C), 129.0 (Ar-CH), 128.6 (Ar-CH), 122.3 (Ar-CH), 119.9 (Ar-CH), 118.3 (Ar-CH), 40.3 (NCH_3), 28.2 (CH_2), 15.6 (CH_3).

HRMS: m/z calc. for $C_{15}H_{17}N$ $[M+H]^+$ 212.1434, found 212.1425.

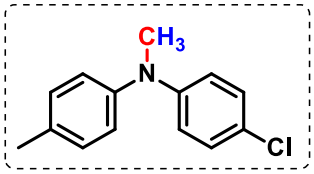
4-bromo-N-methyl-N-phenylaniline (3g)[S13]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (73% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.33 (q, 4H, 8 Hz, Ar-H), 7.07-7.02 (m, 3H, Ar-H), 6.84 (d, 2H, 8 Hz, Ar-H), 3.29 (s, 3H, NCH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 148.5 (Ar-C), 148.1 (Ar-C), 131.9 (Ar-CH), 129.4 (Ar-CH), 122.6 (Ar-CH), 121.9 (Ar-CH), 120.6 (Ar-CH), 112.7 (Ar-C), 40.3 (NCH_3).

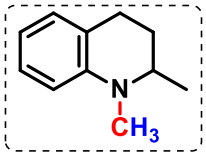
4-chloro-N-methyl-N-(p-tolyl) aniline (3h)[S14]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (76% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.15 (t, 4H, 8 Hz, Ar-H), 7.00 (d, 2H, 8Hz, Ar-H), 6.80 (d, 2H, 8 Hz, Ar-H), 3.26 (s, 3H, NCH_3), 2.33 (s, 3H, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 148.0 (Ar-C), 146.2 (Ar-C), 132.9 (Ar-C), 130.1 (Ar-CH), 128.8 (Ar-CH), 124.2 (Ar-C), 123.3 (Ar-CH), 118.6 (Ar-CH), 40.4 (NCH_3), 20.8 (CH_3).

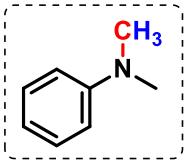
1, 2-dimethyl-1, 2, 3,4-tetrahydroquinoline (3i)[S15]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (73% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.10 (t, 1H, 7.6 Hz, Ar-H), 6.98 (d, 1H, 7.6 Hz, Ar-H), 6.62-6.55 (m, 2H, Ar-H), 3.49-3.42 (m, 1H, NCH), 2.91 (s, 3H, NCH_3), 2.90-2.81 (m, 1H, CH_2), 2.73-2.67 (m, 1H, CH_2), 2.04-1.95 (m, 1H, CH_2), 1.79-1.75 (m, 1H, CH_2), 1.15 (m, 3H, 6.8 Hz, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 145.5 (Ar-C), 128.5 (Ar-CH), 127.1 (Ar-CH), 122.1 (Ar-C), 115.4 (Ar-CH), 110.6 (Ar-CH), 53.8 (NCH), 37.0 (NCH_3), 28.1 (CH_2), 23.8 (CH_2), 17.6 (CH_3).

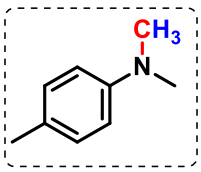
N, N-dimethylaniline (3j)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (80% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.41-7.38 (m, 2H, Ar-H), 6.91-6.89 (m, 3H, Ar-H), 3.07 (s, 6H, $N(CH_3)_2$): **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 150.6 (Ar-C), 128.9 (Ar-CH), 116.5 (Ar-CH), 112.6 (Ar-CH), 40.4 ($N(CH_3)_2$).

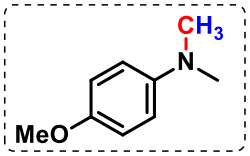
4-methyl-N, N-aniline (3k)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (79% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.08 (d, 2H, 8 Hz, Ar-H), 6.72 (d, 2H, 8Hz, Ar-H), 2.92 (s, 6H, $N(CH_3)_2$), 2.29 (s, 3H, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 148.6 (Ar-C), 129.6 (Ar-CH), 126.1 (Ar-C), 113.2 (Ar-CH), 41.0 ($N(CH_3)_2$), 20.2 (CH_3).

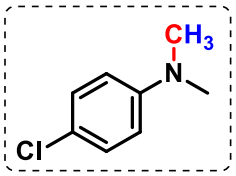
4-methoxy-N, N-dimethylaniline (3l)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (74% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 6.87 (d, 2H, 8 Hz, Ar-H), 6.77 (d, 2H, 7.6 Hz, Ar-H), 3.78 (s, 3H, OCH_3), 2.88 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 152.0 (Ar-C), 145.8 (Ar-C), 114.9 (Ar-CH), 114.6 (Ar-CH), 55.7 (OCH_3), 41.8 ($N(CH_3)_2$).

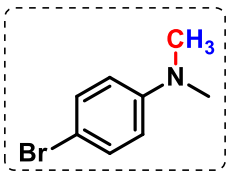
4-chloro-N, N-dimethylaniline (3m)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (72% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.18 (d, 2H, 8 Hz, Ar-H), 6.65 (d, 2H, 12 Hz, Ar-H), 2.93 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 149.2 (Ar-C), 128.8 (Ar-CH), 121.4 (Ar-C), 113.6 (Ar-CH), 40.6 ($N(CH_3)_2$).

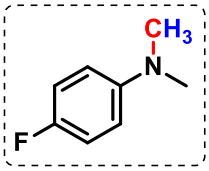
4-bromo-N, N-dimethylaniline (3n)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (79% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.31 (d, 2H, 8 Hz, Ar-H), 6.59 (d, 2H, 8 Hz, Ar-H), 2.93 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 149.5 (Ar-C), 131.6 (Ar-CH), 114.1 (Ar-CH), 108.5 (Ar-C), 40.5 ($N(CH_3)_2$).

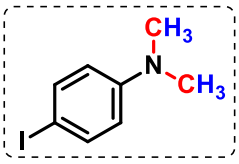
4-fluoro-N, N-dimethylaniline (3o)[S7]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (55% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 6.96 (t, 2H, 8 Hz, Ar-H), 6.71-6.68 (m, 2H, Ar-H), 2.91 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 155.6 (d, $^{1}J_{C-F}$=236 Hz, Ar-C), 147.5 (Ar-C), 115.3 (d, $^{2}J_{C-F}$=22 Hz, Ar-CH), 113.9 (d, $^{3}J_{C-F}$=7 Hz, Ar-CH), 41.3 ($N(CH_3)_2$).

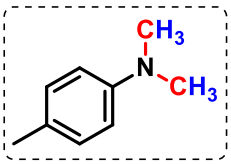
4-iodo-N, N-dimethylaniline (5a)[S7]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (88% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.47 (d, 2H, 8 Hz, Ar-H), 6.49 (d, 2H, 8 Hz, Ar-H), 2.92 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 150.0 (Ar-C), 137.5 (Ar-CH), 114.7 (Ar-CH), 77.4 (Ar-C), 40.4 ($N(CH_3)_2$).

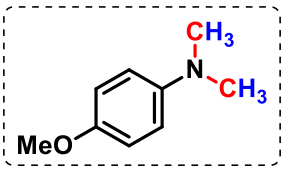
4-methyl-N, N- dimethylaniline (5b)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (84% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.08 (d, 2H, 8 Hz, Ar-H), 6.72 (d, 2H, 8Hz, Ar-H), 2.92 (s, 6H, $N(CH_3)_2$), 2.29 (s, 3H, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 148.6 (Ar-C), 129.6 (Ar-CH), 126.1 (Ar-C), 113.2 (Ar-CH), 41.0 ($N(CH_3)_2$), 20.2 (CH_3).

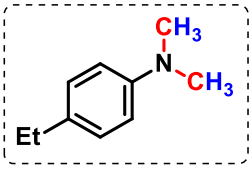
4-methoxy-N, N-dimethylaniline (5c)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (81% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 6.87 (d, 2H, 8 Hz, Ar-H), 6.77 (d, 2H, 7.6 Hz, Ar-H), 3.78 (s, 3H, OCH_3), 2.88 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 152.0 (Ar-C), 145.8 (Ar-C), 114.9 (Ar-CH), 114.6 (Ar-CH), 55.7 (OCH_3), 41.8 ($N(CH_3)_2$).

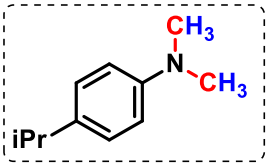
4-ethyl-N, N-dimethylaniline (5d)[7]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (71% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.13 (d, 2H, 8 Hz, Ar-H), 6.76 (d, 2H, 8 Hz, Ar-H), 2.95 (s, 6H, $N(CH_3)_2$), 2.63-2.58 (q, 2H, 8 Hz, $CH_2(CH_3)_2$), 1.27-1.23 (t, 3H, 8Hz, $(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 148.9 (Ar-C), 132.6 (Ar-C), 128.3 (Ar-CH), 113.1 (Ar-CH), 40.9 ($N(CH_3)_2$), 27.8 ($CH_2(CH_3)_2$), 15.9 ($(CH_3)_2$).

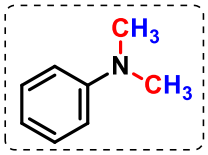
4-isopropyl-N, N-dimethylaniline (5e)[S18]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (66% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.29 (d, 2H, 8 Hz, Ar-H), 6.89 (d, 2H, 8 Hz, Ar-H), 3.07 (s, 6H, $N(CH_3)_2$), 3.04-2.98 (m, 1H, $CH(CH_3)_2$), 1.42-1.40 (d, 6H, 8Hz, $(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 149.0 (Ar-C), 137.1 (Ar-C), 126.9 (Ar-CH), 113.0 (Ar-CH), 40.8 ($N(CH_3)_2$), 33.0 ($CH(CH_3)_2$) , 24.2 (($CH_3)_2$).

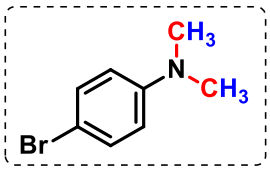
N, N-dimethylaniline (5f)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (82% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.41-7.38 (m, 2H, Ar-H), 6.91-6.89 (m, 3H, Ar-H), 3.07 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 150.6 (Ar-C), 128.9 (Ar-CH), 116.5 (Ar-CH), 112.6 (Ar-CH), 40.4 ($N(CH_3)_2$).

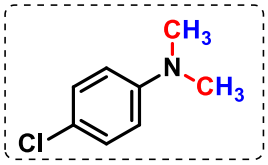
4-bromo-N, N-dimethylaniline (5g)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (78% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.31 (d, 2H, 8 Hz, Ar-H), 6.59 (d, 2H, 8 Hz, Ar-H), 2.93 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 149.5 (Ar-C), 131.6 (Ar-CH), 114.1 (Ar-CH), 108.6 (Ar-C), 40.5 ($N(CH_3)_2$).

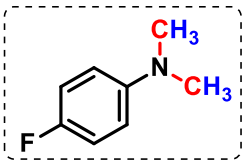
4-chloro-N, N-dimethylaniline (5h)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (74% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.18 (d, 2H, 8 Hz, Ar-H), 6.65 (d, 2H, 12 Hz, Ar-H), 2.93 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 149.2 (Ar-C), 128.8 (Ar-CH), 121.4 (Ar-C), 113.6 (Ar-CH), 40.6 ($N(CH_3)_2$).

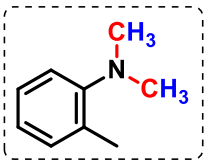
4-fluoro-N, N-dimethylaniline (5i)[S7]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (52% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 6.96 (t, 2H, 8 Hz, Ar-H), 6.71-6.68 (m, 2H, Ar-H), 2.91 (s, 6H, $NCH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 155.6 (d, $^{1}J_{C-F}$=236 Hz, Ar-C), 147.5 (Ar-C), 115.3 (d, $^{2}J_{C-F}$=22 Hz, Ar-CH), 113.9 (d, $^{3}J_{C-F}$=7 Hz, Ar-CH), 41.3 ($N(CH_3)_2$).

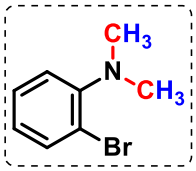
N, N, 2-trimethylaniline (5j)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (77% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.21 (t, 2H, 8 Hz, Ar-H), 7.07 (d, 1H, 8 Hz, Ar-H), 7.00 (t, 1H, 8 Hz, Ar-H), 2.75 (s, 6H, $N(CH_3)_2$), 2.38 (s, 3H, CH_3); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 152.7 (Ar-C), 132.1 (Ar-C), 131.1 (Ar-CH), 126.4 (Ar-CH), 122.5 (Ar-CH), 118.3 (Ar-CH), 44.2 ($N(CH_3)_2$), 18.3 (CH_3).

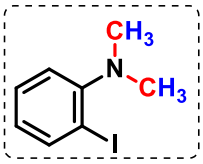
2-bromo-N, N-dimethylaniline (5k)[S17]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (73% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.58 (dd, 1H, 8 Hz, Ar-H), 7.29 (dt, 1H, 8 Hz, Ar-H), 7.11 (dd, 1H, 8 Hz, Ar-H), 6.91 (dt, 1H, 8 Hz, Ar-H), 2.83 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 151.7 (Ar-C), 133.7 (Ar-CH), 128.0 (Ar-CH), 123.8 (Ar-CH), 120.4 (Ar-CH), 119.0 (Ar-C), 44.6 ($N(CH_3)_2$).

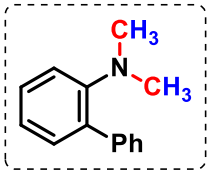
2-iodo-N, N-dimethylaniline (5l)[S19]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (68% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.89 (d, 1H, 8 Hz, Ar-H), 7.35 (t, 1H, 8 Hz, Ar-H), 7.11 (d,1H, 8 Hz, Ar-H), 6.81 (t, 1H, 8 Hz, Ar-H), 2.81 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 154.8 (Ar-C), 139.9 (Ar-CH), 128.8 (Ar-CH), 124.7 (Ar-CH), 120.2 (Ar-CH), 97.0 (Ar-C), 44.7 ($N(CH_3)_2$).

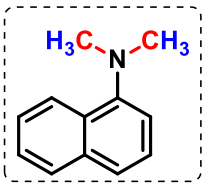
N, N-dimethyl-[1, 1'-biphenyl]-2-amine (5m)[S8]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (59% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.67 (d, 2H, 8 Hz, Ar-H), 7.47 (t, 2H, 8 Hz, Ar-H), 7.38-7.30 (m, 3H, Ar-H), 7.10 (q, 2H, 8 Hz, Ar-H), 2.62 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 151.2 (Ar-C) , 142.0 (Ar-C), 134.1 (Ar-C), 131.7 (Ar-CH), 128.6 (Ar-CH), 128.3 (Ar-CH), 128.0 (Ar-CH), 126.4 (Ar-CH), 121.4 (Ar-CH), 117.5 (Ar-CH), 43.3 ($N(CH_3)_2$).

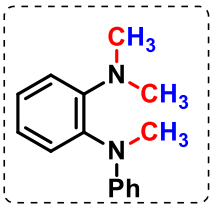
N, N-dimethylnapthalen-1-amine (5n)[S10]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (73% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 8.25 (d, 1H, 8 Hz, Ar-H), 7.83 (d, 1H, 8 Hz, Ar-H), 7.54-7.45 (m, 3H, Ar-H), 7.41 (t, 1H, 8 Hz, Ar-H), 7.09 (d, 1H, 8 Hz, Ar-H) 2.92 (s, 6H, $N(CH_3)_2$); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 150.9 (Ar-C), 134.8 (Ar-C), 128.8 (Ar-C), 128.3 (Ar-CH), 125.7 (Ar-CH), 125.7 (Ar-CH), 125.1 (Ar-CH), 124.1 (Ar-CH), 122.8 (Ar-CH), 113.9 (Ar-CH), 45.2 ($N(CH_3)_2$).

N^1, N^1, N^2-trimrthyl-N^2-phenylbenzene -1, 2-diamine (5q)[S16]:



The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (99:1 v/v) as eluent.

Yellow liquid (61% yield); **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 7.21-7.11 (m, 4H, Ar-H), 6.99 (dd, 1H, 8Hz, Ar-H), 6.90 (d, 1H, 8 Hz, Ar-H), 6.71-6.75 (m, 3H, Ar-H), 3.18 (s, 3H, NCH_3), 2.74 (s, 6H, $N(CH_3)_2$); **^{13}C {^{1}H} NMR** (100 MHz, $CDCl_3$, 25 ^{o}C): δ (ppm) = 149.3 (Ar-C), 148.6 (Ar-C), 139.1 (Ar-C), 129.2 (Ar-CH), 128.8 (Ar-CH), 126.1 (Ar-CH), 121.2 (Ar-CH), 118.2 (Ar-CH), 117.0 (Ar-CH), 113.5 (Ar-CH), 42.2 (NCH_3), 37.2 ($N(CH_3)_2$).

IV) X-ray crystallographic details

Single crystals of compound **10** were mounted on a glass pip. Intensity data were collected on a SuperNova, Dual, Mo at zero, Eos diffractometer. The crystals were kept at 100.6 K during data collection. Atomic coordinates, isotropic and anisotropic displacement parameters of all the non-hydrogen atoms of two compounds were refined using Olex2, [S20] and the structure was solved with the Superflip[S21] structure solution program using Charge Flipping and refined with the ShelXL[S22] refinement package using Least Squares minimization. Structure graphic shown in the figure was created using the Olex2 and X-Seed software package version 2.0.

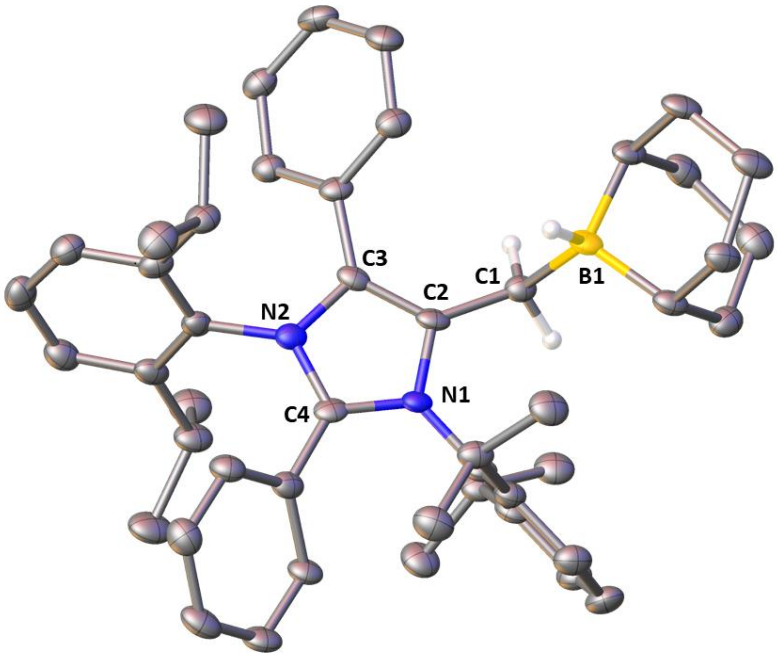


Figure S26. View of the molecular structure of **10.** Ellipsoids are set at the 50% probability level; hydrogen atoms expect $–CH_2$ and the B-H hydrogen's have been omitted for the sake of clarity.

Table S2 Crystal data and structure refinement data for 10.	
CCDC No	2065467
Identification code	mo_TKP180121_0ma_a
Empirical formula	$C_{96}H_{122}B_2N_4$
Formula weight	1353.59
Temperature/K	100.61
Crystal system	triclinic
Space group	P-1
a/Å	13.9680(11)
b/Å	15.6349(13)
c/Å	22.5739(17)
α/°	90.009(3)
β/°	93.393(2)
γ/°	90.024(3)
Volume/Å^3	4921.2(7)
Z	2
ρ_{calc}g/cm^3	0.913
μ/mm^{-1}	0.052
F(000)	1472.0
Crystal size/mm^3	0.2 × 0.15 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.382 to 50.888
Index ranges	$-16 \leq h \leq 16$, $-18 \leq k \leq 18$, $-27 \leq l \leq 25$
Reflections collected	50073
Independent reflections	18007 [R_{int} = 0.1058, R_{sigma} = 0.1239]
Data/restraints/parameters	18007/0/935
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0761, wR_2 = 0.2034
Final R indexes [all data]	R_1 = 0.1184, wR_2 = 0.2410
Largest diff. peak/hole / e Å^{-3}	0.35/-0.35

V) ^{1}H and $^{13}C\{^{1}H\}$ NMR Spectra

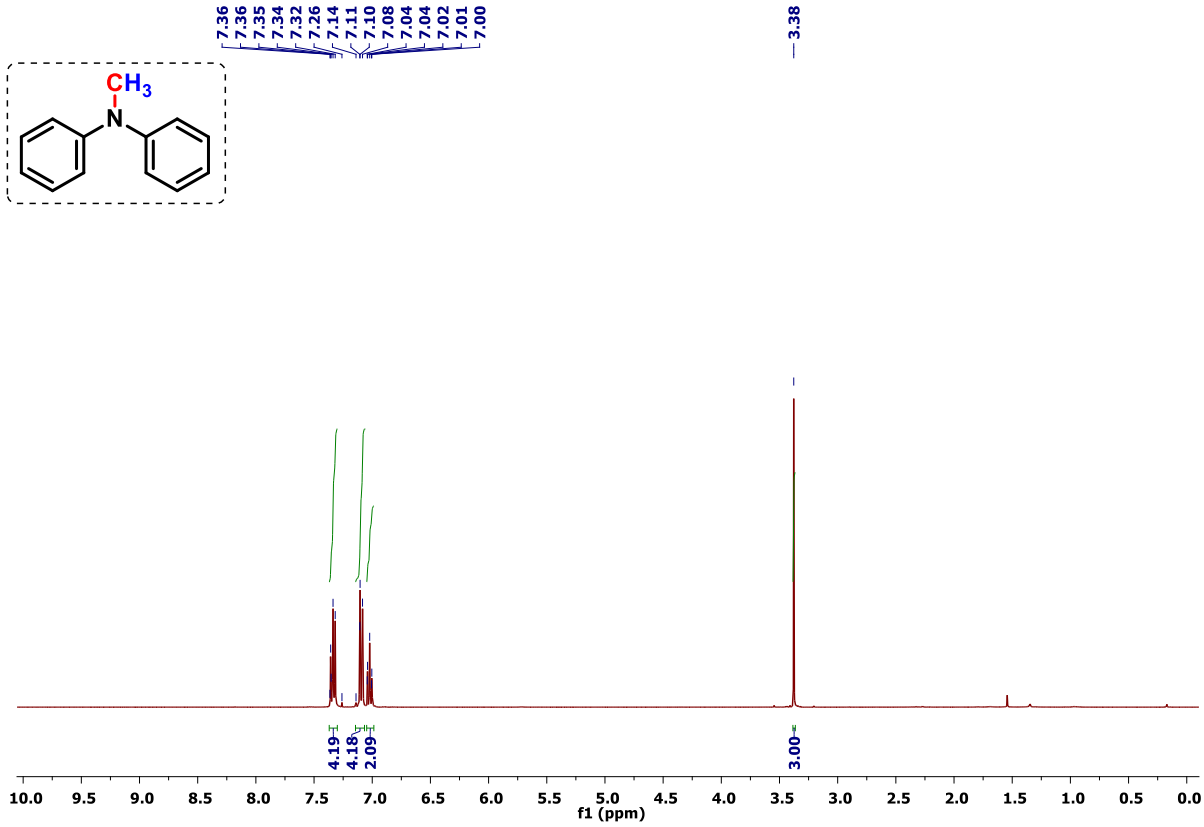


Figure S27. ^{1}H NMR spectrum of **3a** in $CDCl_3$.

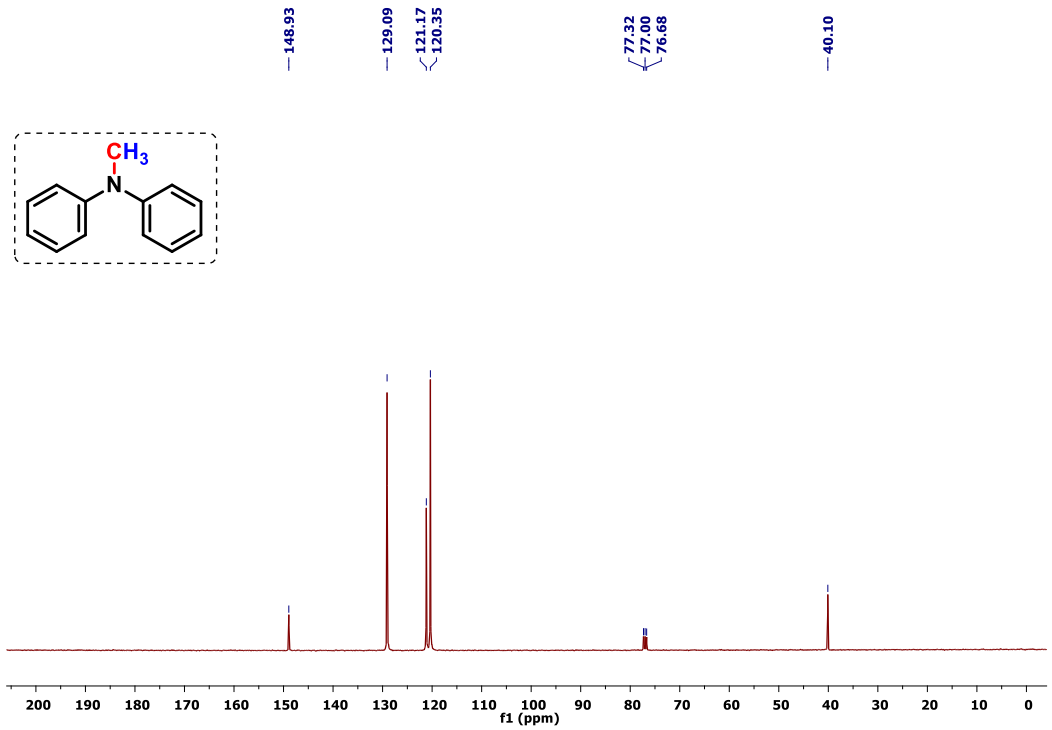


Figure S28. $^{13}C\{^{1}H\}$ NMR spectrum of **3a** in $CDCl_3$.

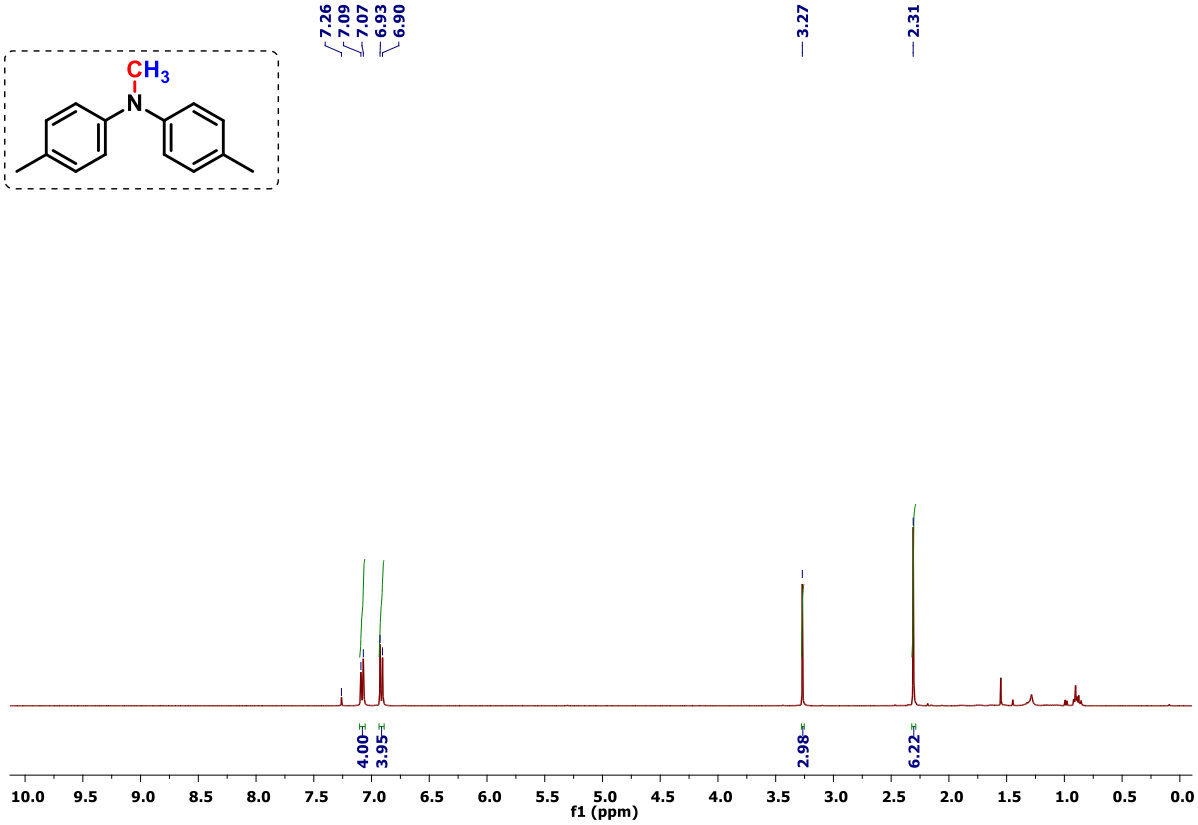


Figure S29. ^{1}H NMR spectrum of **3b** in $CDCl_3$.

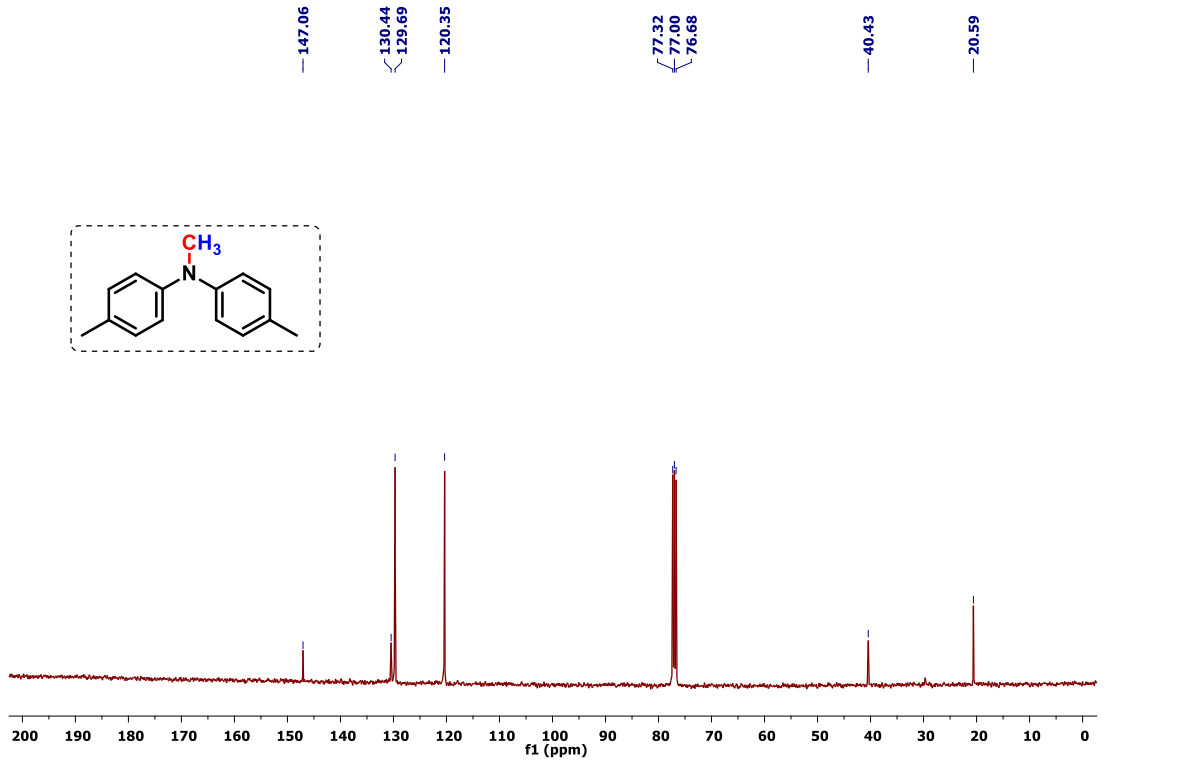


Figure S30. $^{13}C\{^{1}H\}$ NMR spectrum of **3b** in $CDCl_3$.

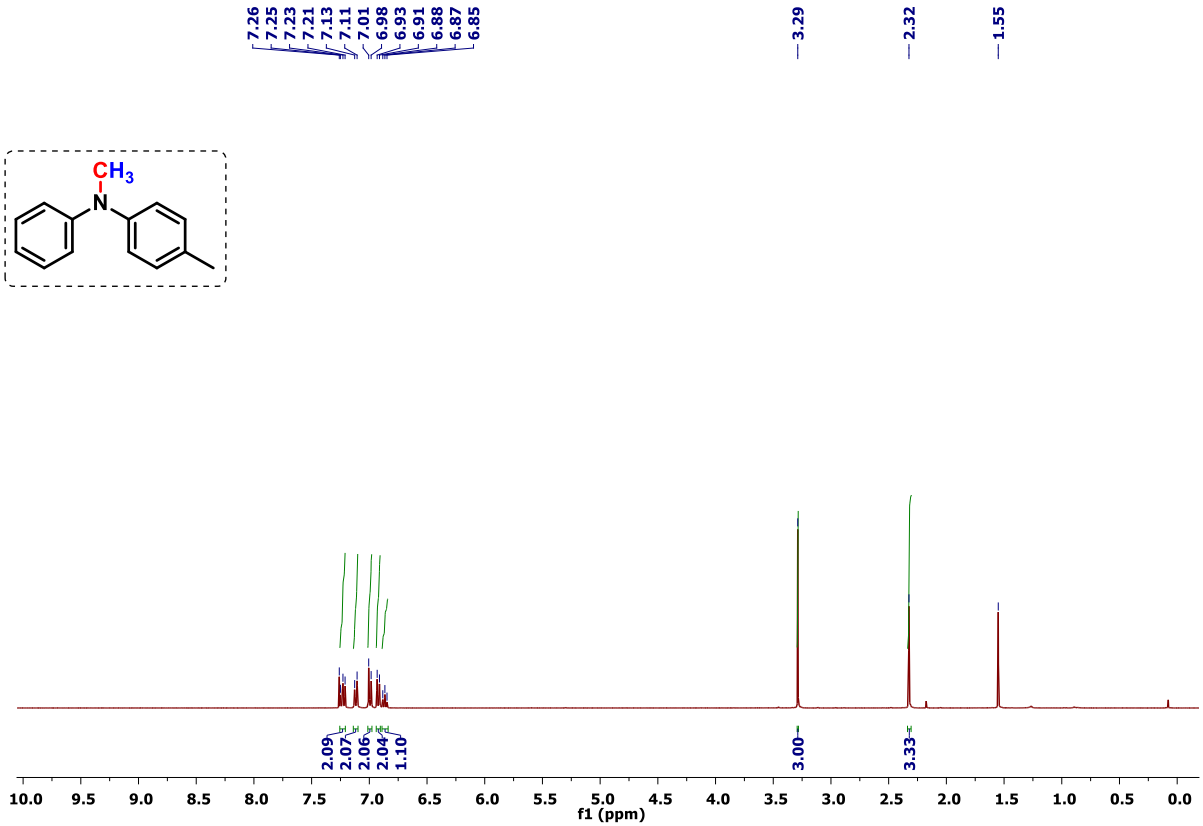


Figure S31. ^{1}H NMR spectrum **3c** in $CDCl_3$.

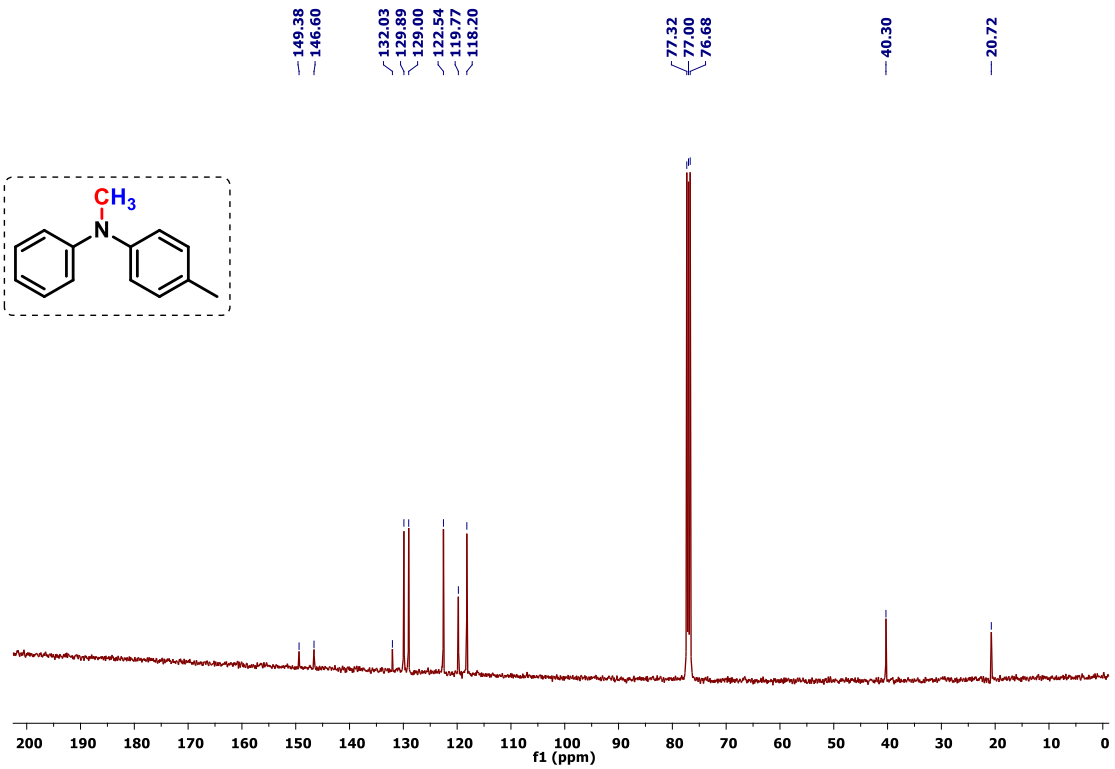


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum of **3c** in $CDCl_3$.

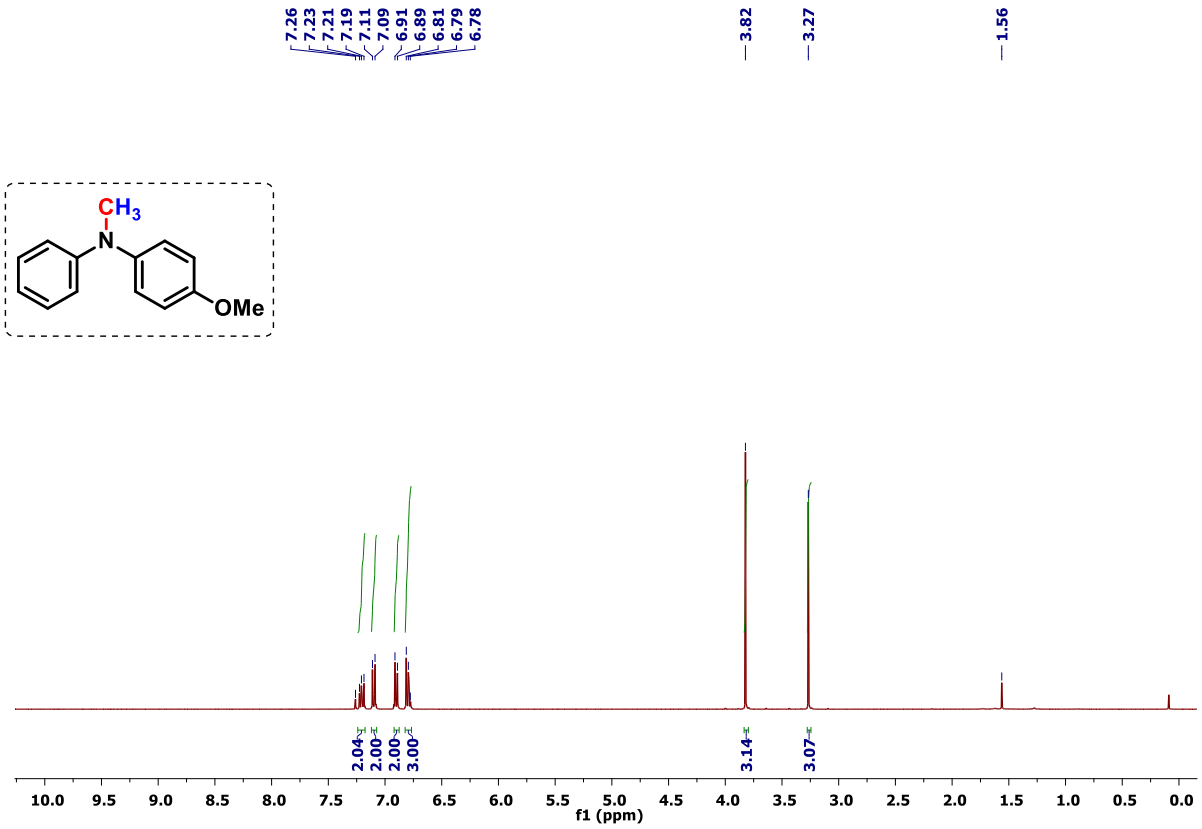


Figure S33. ^{1}H NMR spectrum of **3d** in $CDCl_3$.

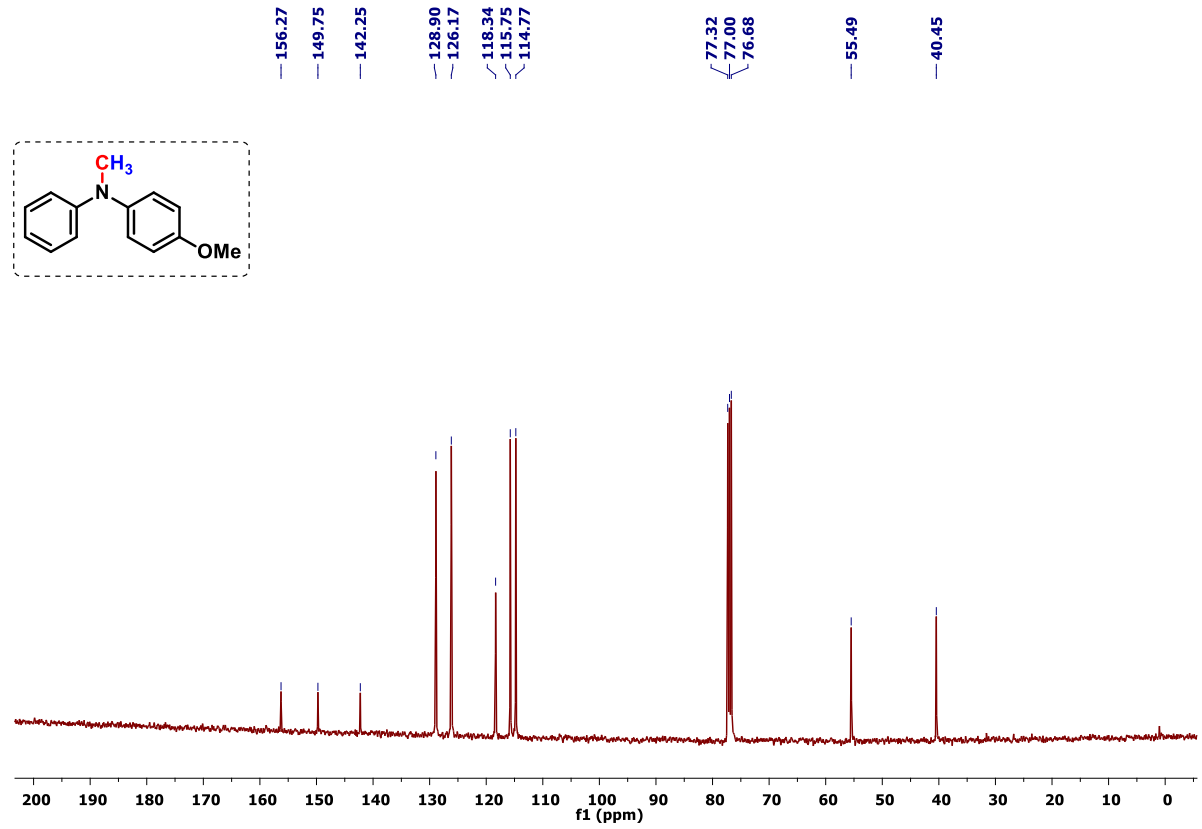


Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum of **3d** in $CDCl_3$.

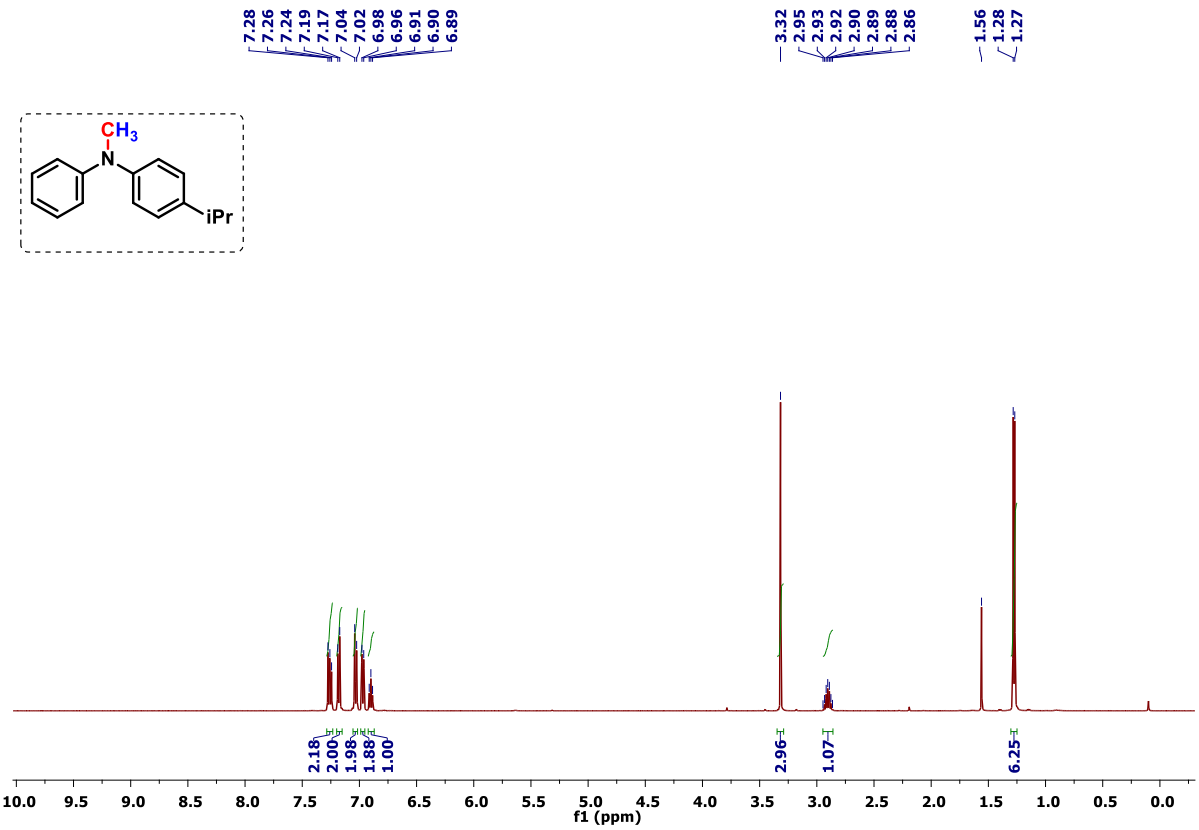


Figure S35. ^{1}H NMR spectrum of **3e** in $CDCl_3$.

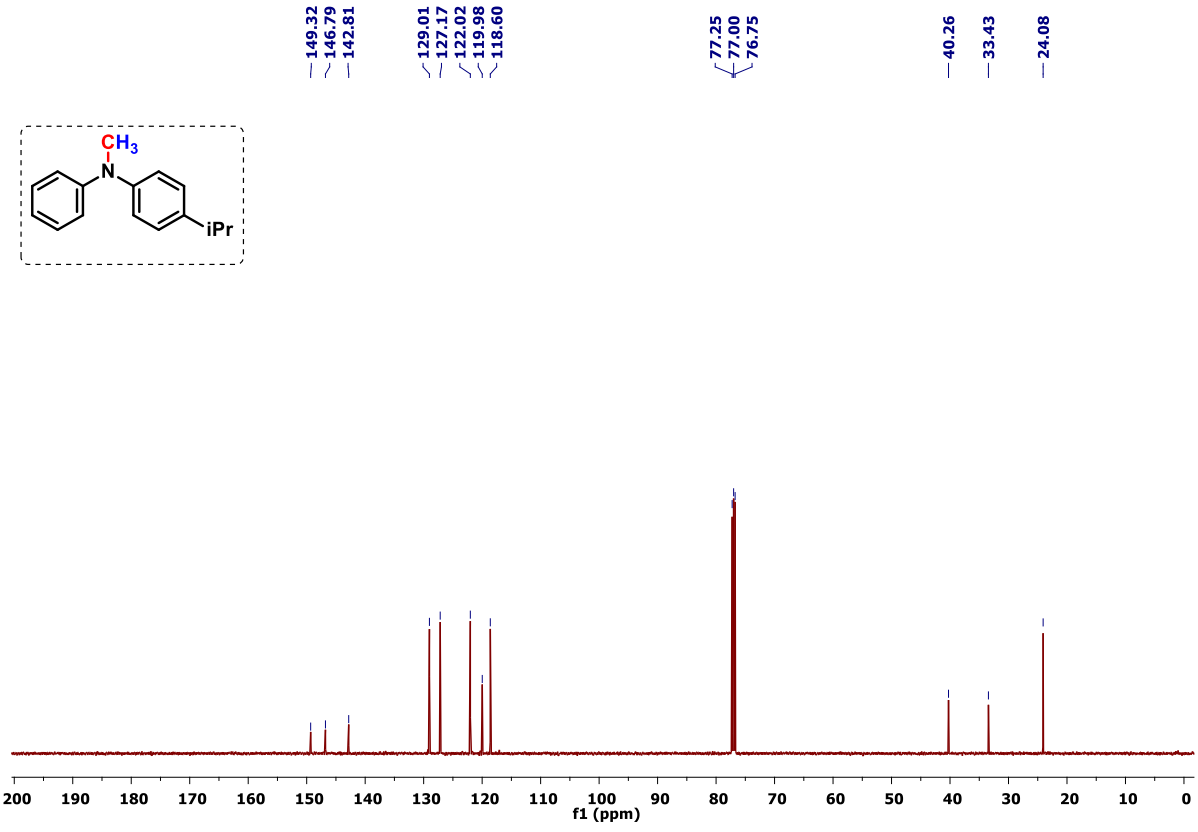


Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum of **3e** in $CDCl_3$.

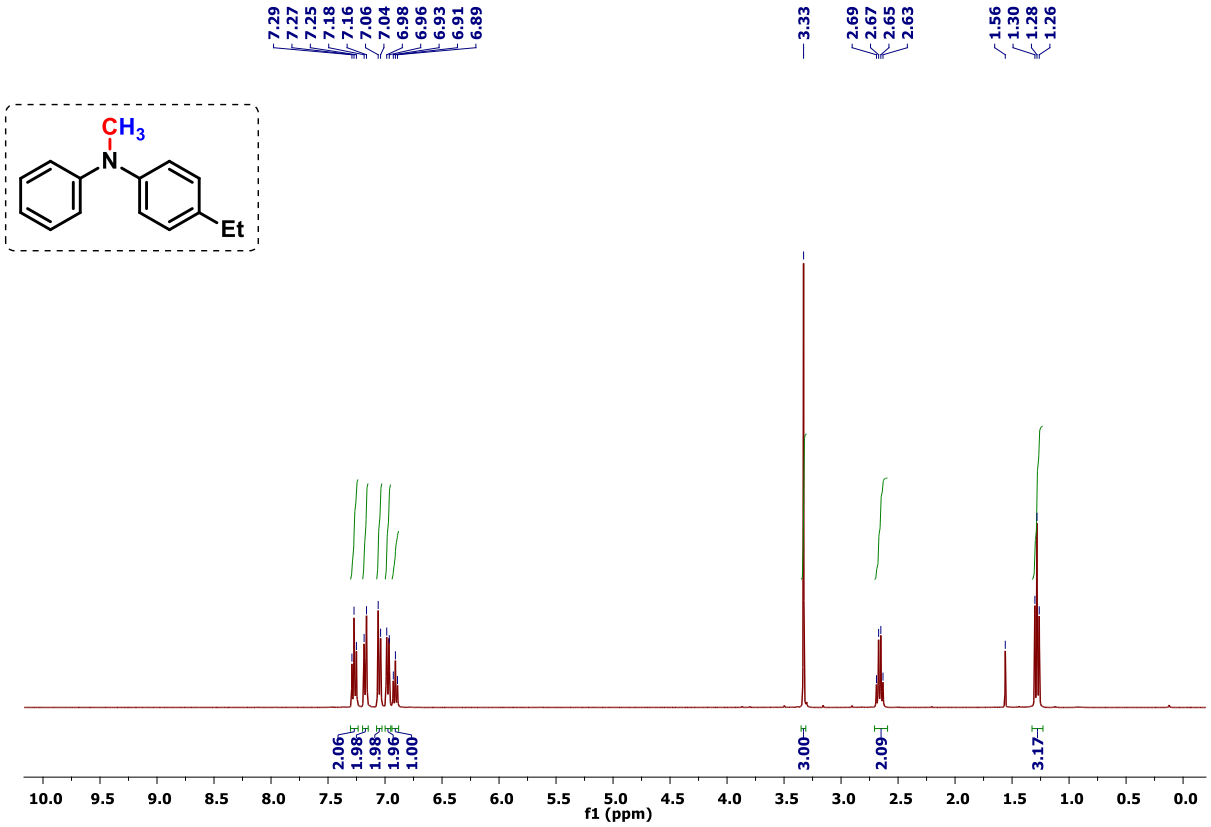


Figure S37. ^{1}H NMR spectrum of **3f** in $CDCl_3$.

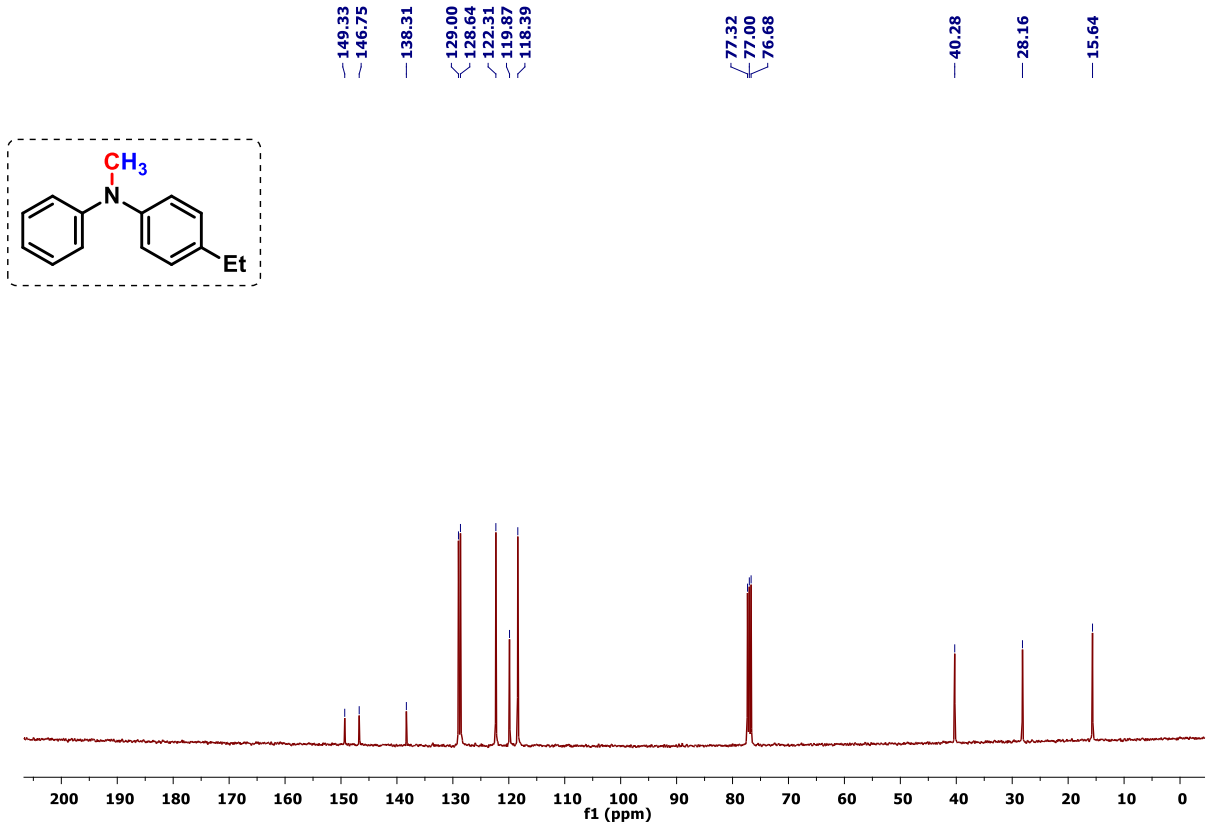


Figure S38. $^{13}C\{^{1}H\}$ NMR spectrum of **3f** in $CDCl_3$.

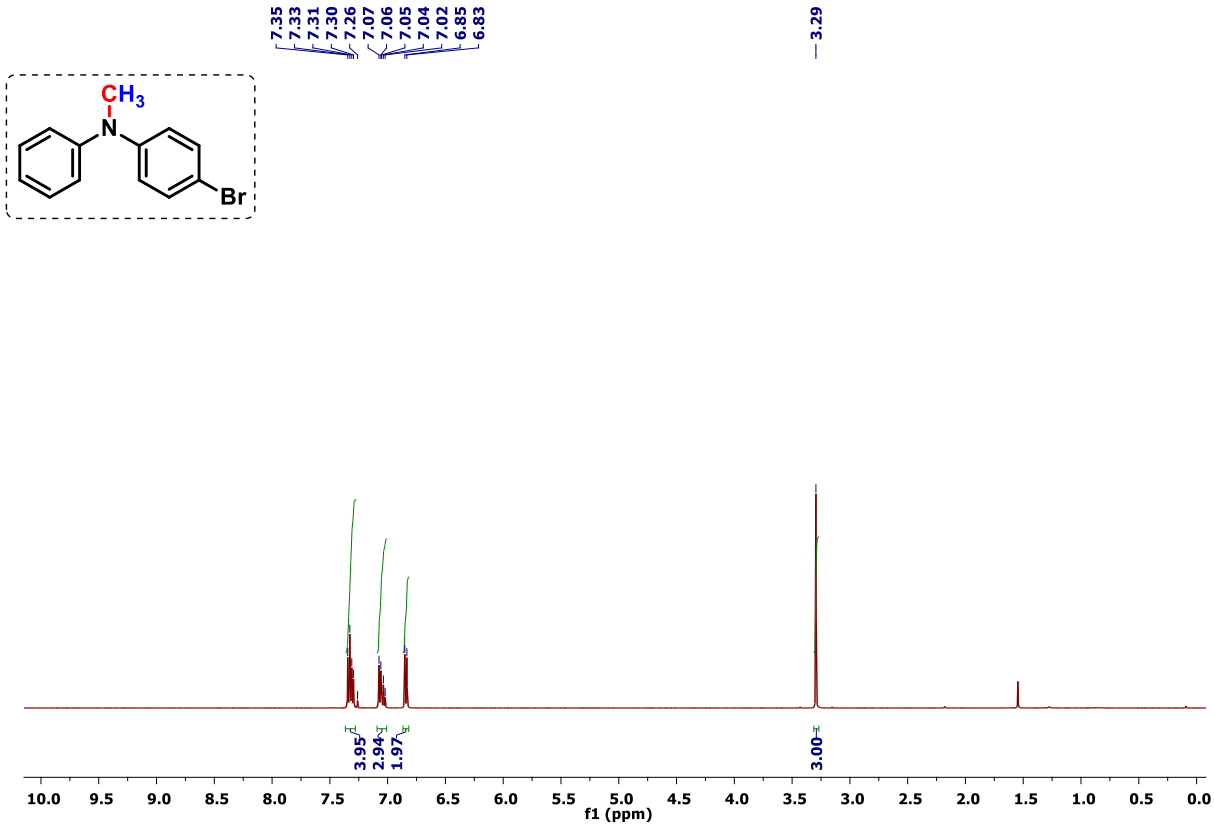


Figure S39. ^{1}H NMR spectrum of **3g** in $CDCl_3$.

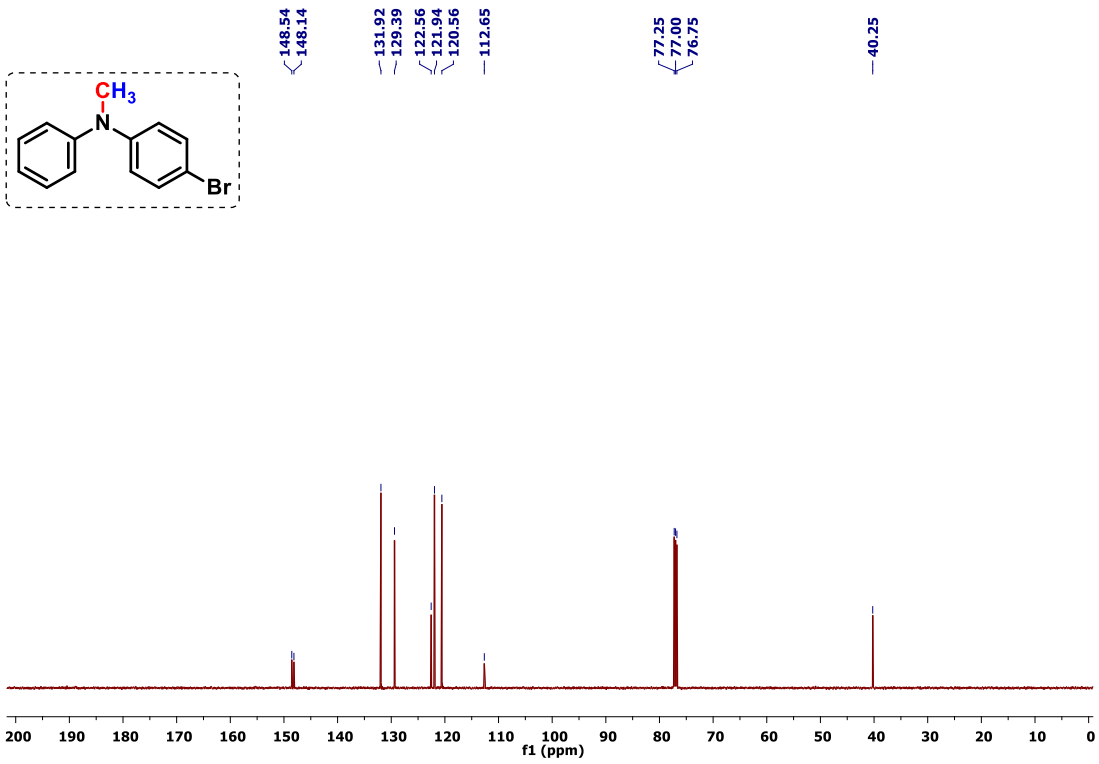


Figure S40. $^{13}C\{^{1}H\}$ NMR spectrum of **3g** in $CDCl_3$.

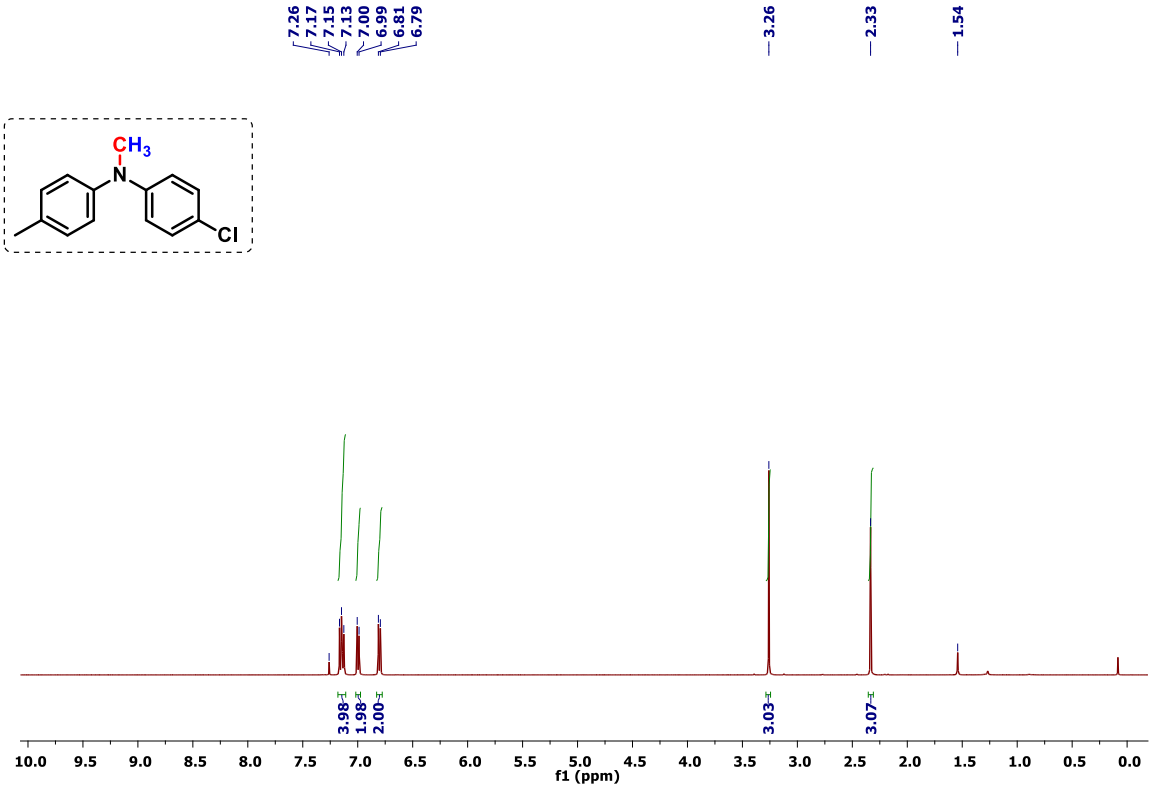


Figure S41. ^{1}H NMR spectrum of **3h** in $CDCl_3$.

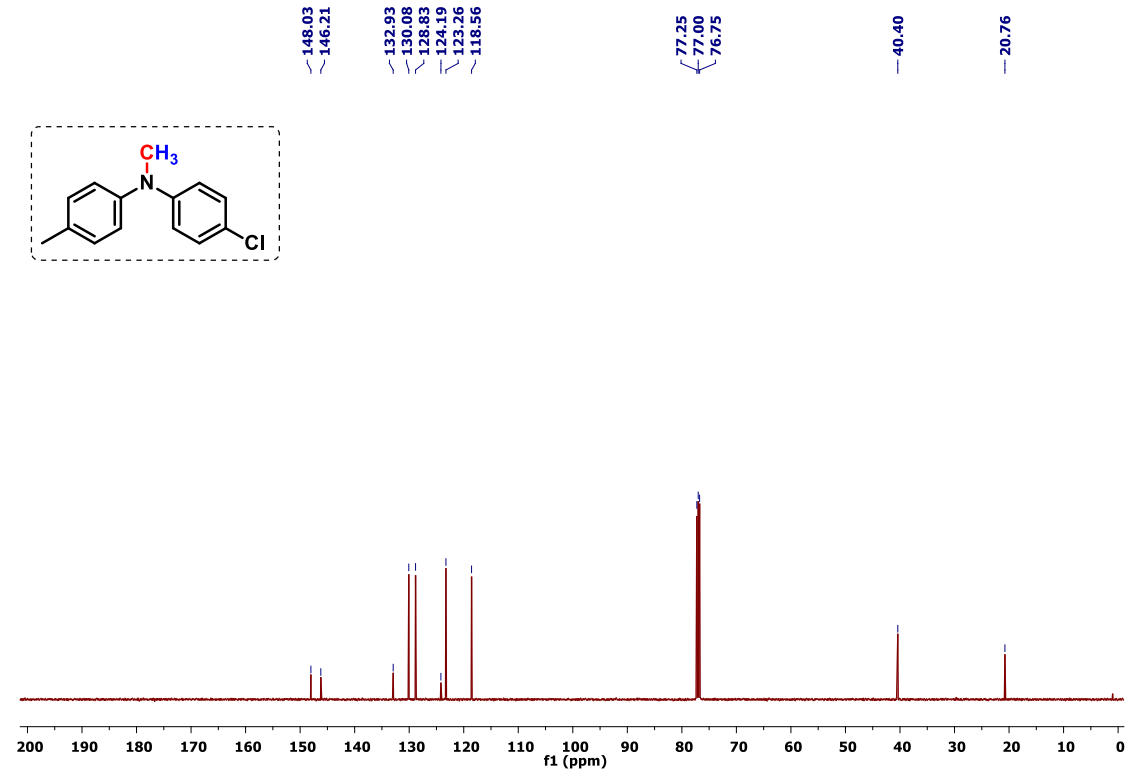


Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of **3h** in $CDCl_3$.

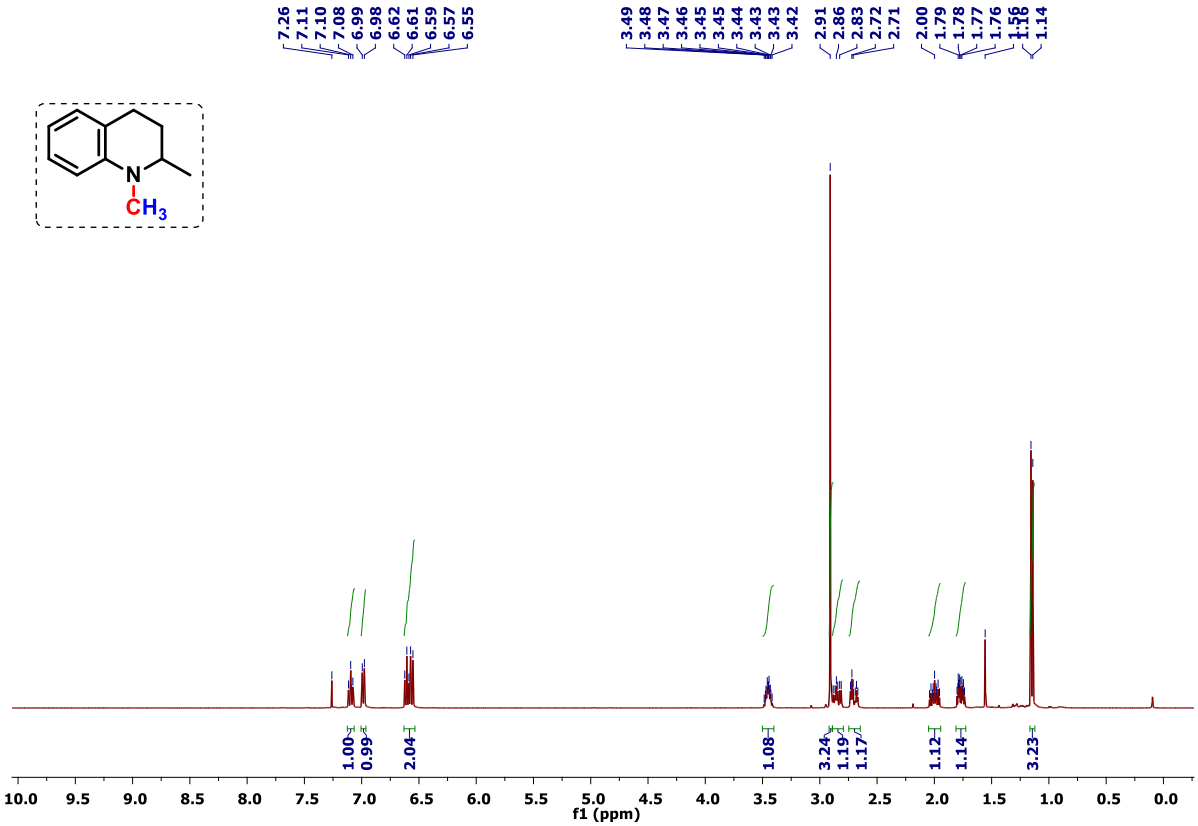


Figure S43. ^{1}H NMR spectrum of **3i** in $CDCl_3$.

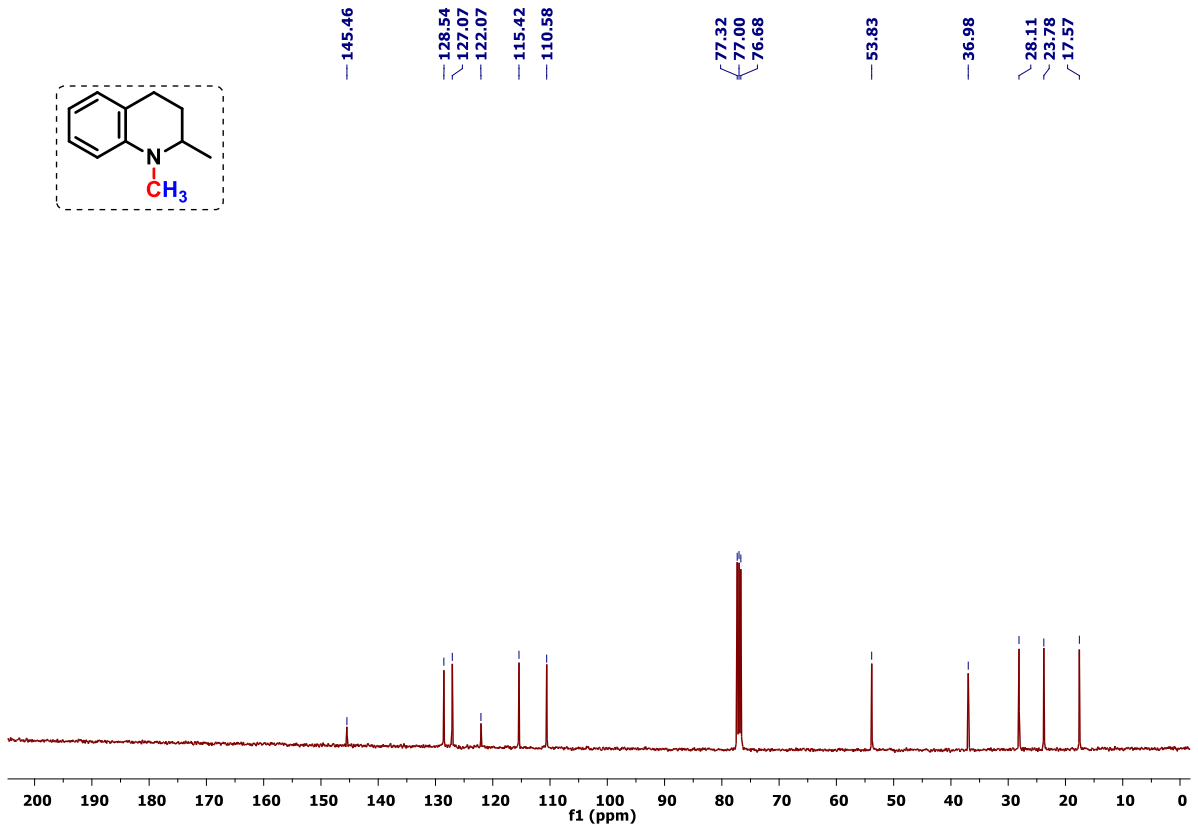


Figure. S44. $^{13}C\{^{1}H\}$ NMR spectrum of **3i** in $CDCl_3$.

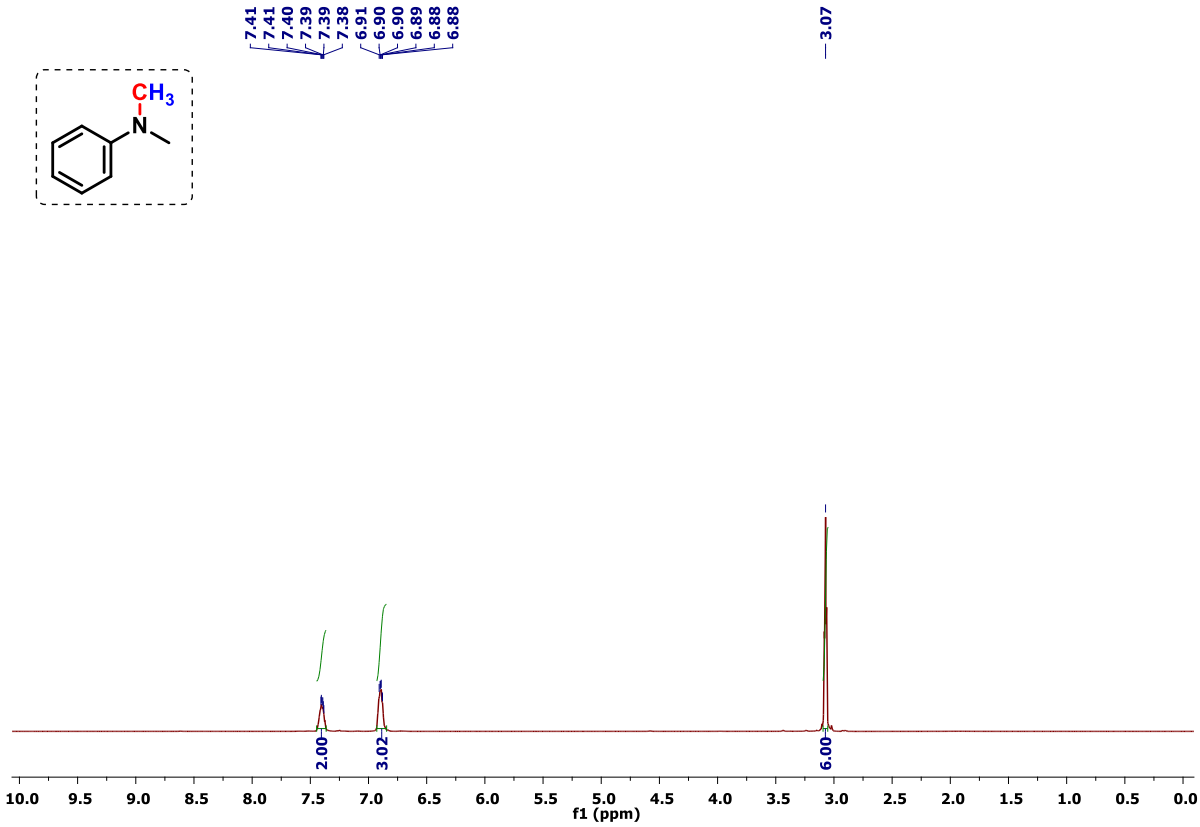


Figure S45. ^{1}H NMR spectrum of **3j** in $CDCl_3$.

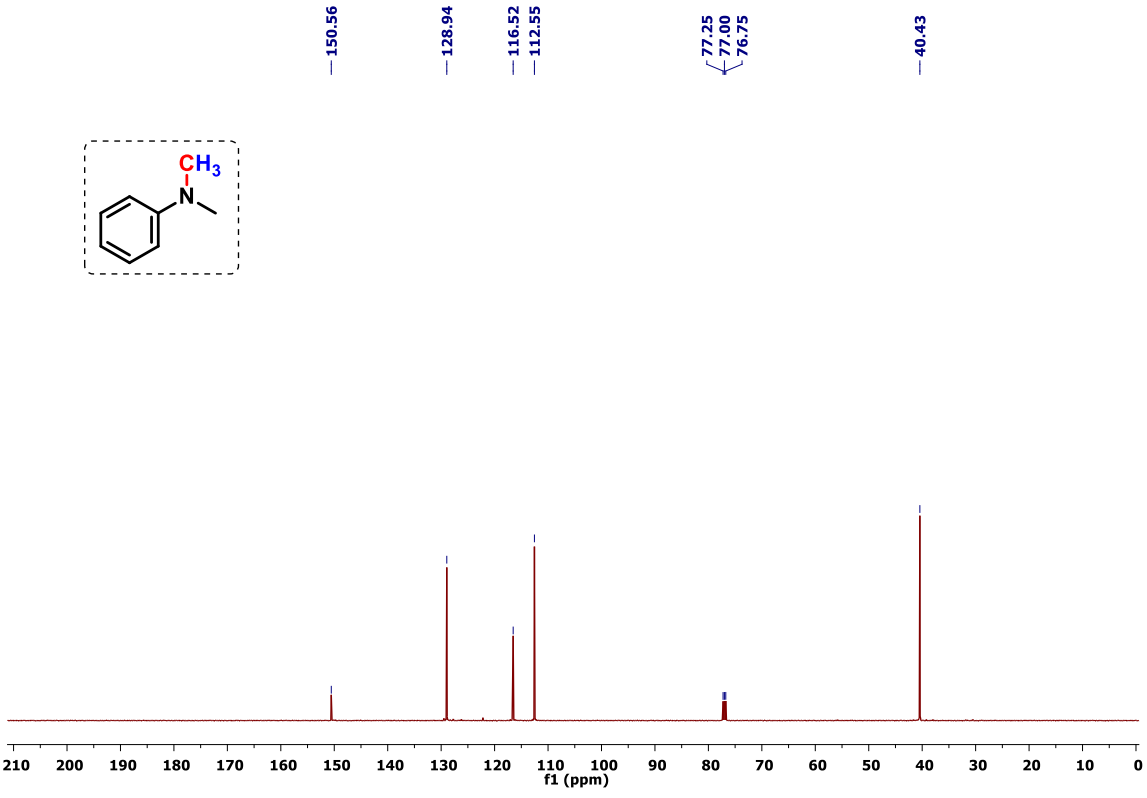


Figure S46. $^{13}C\{^{1}H\}$ NMR spectrum of **3j** in $CDCl_3$.

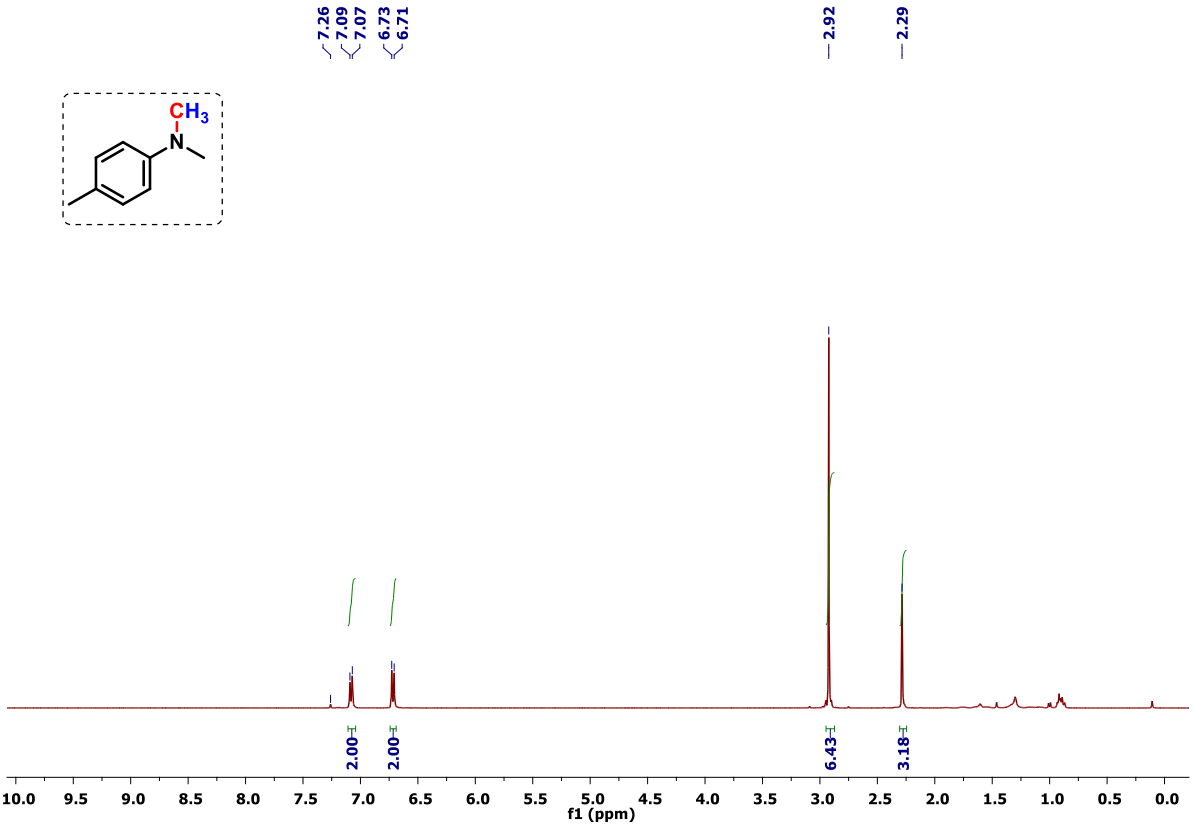


Figure S47. ^{1}H NMR spectrum of **3k** in $CDCl_3$.

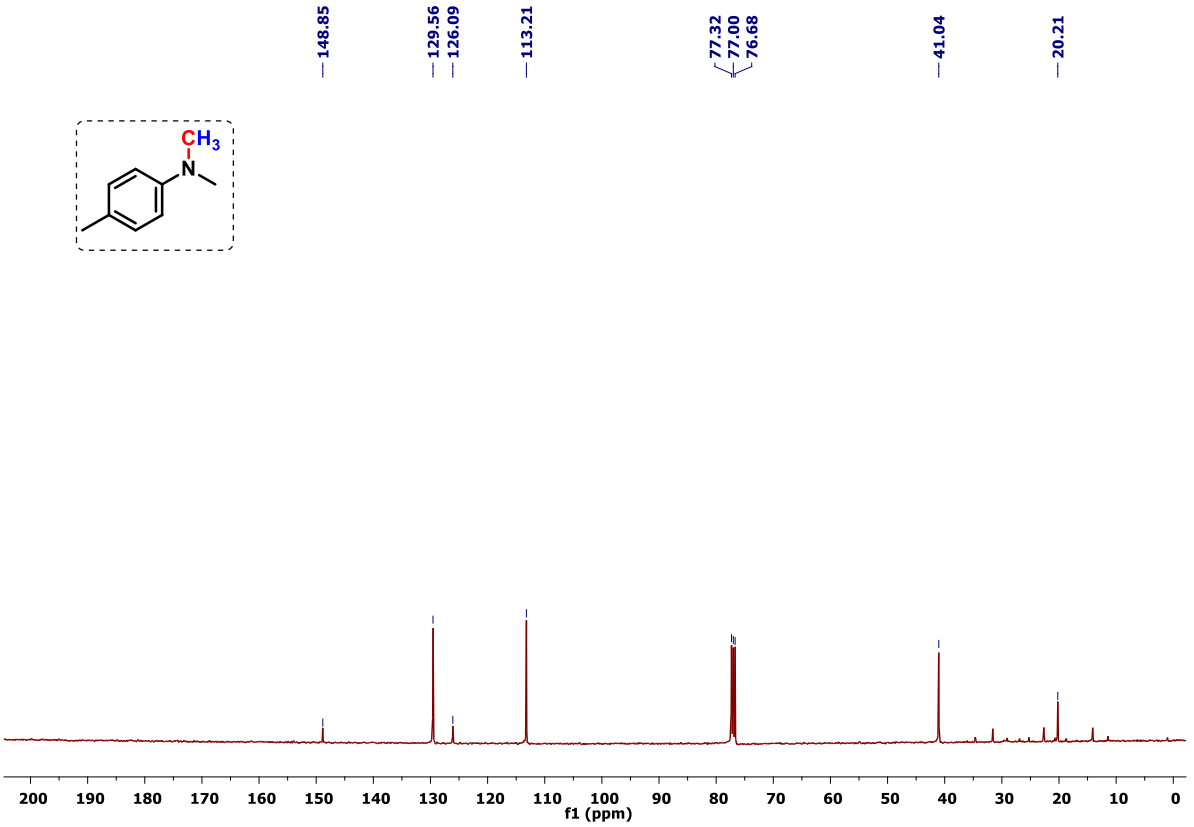


Figure S48. $^{13}C\{^{1}H\}$ NMR spectrum of **3k** in $CDCl_3$.

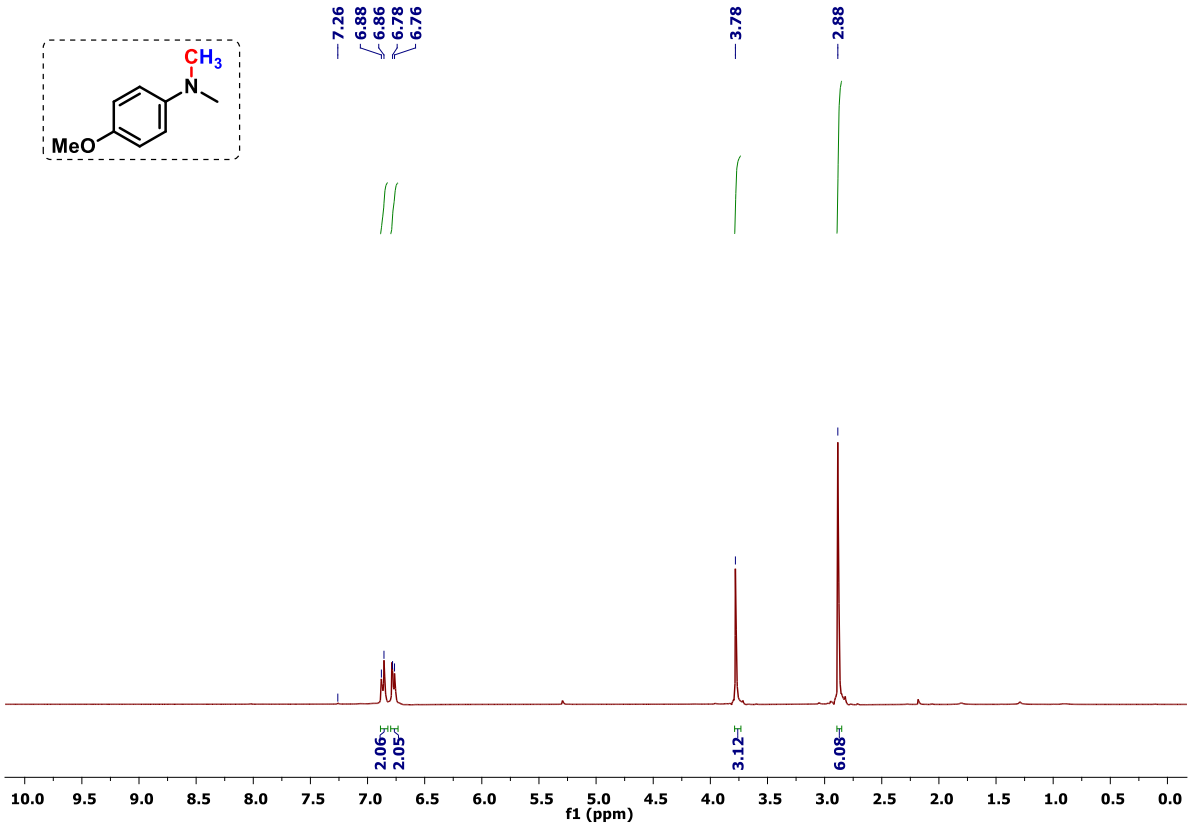


Figure S49. ^{1}H NMR spectrum of **3l** in $CDCl_3$.

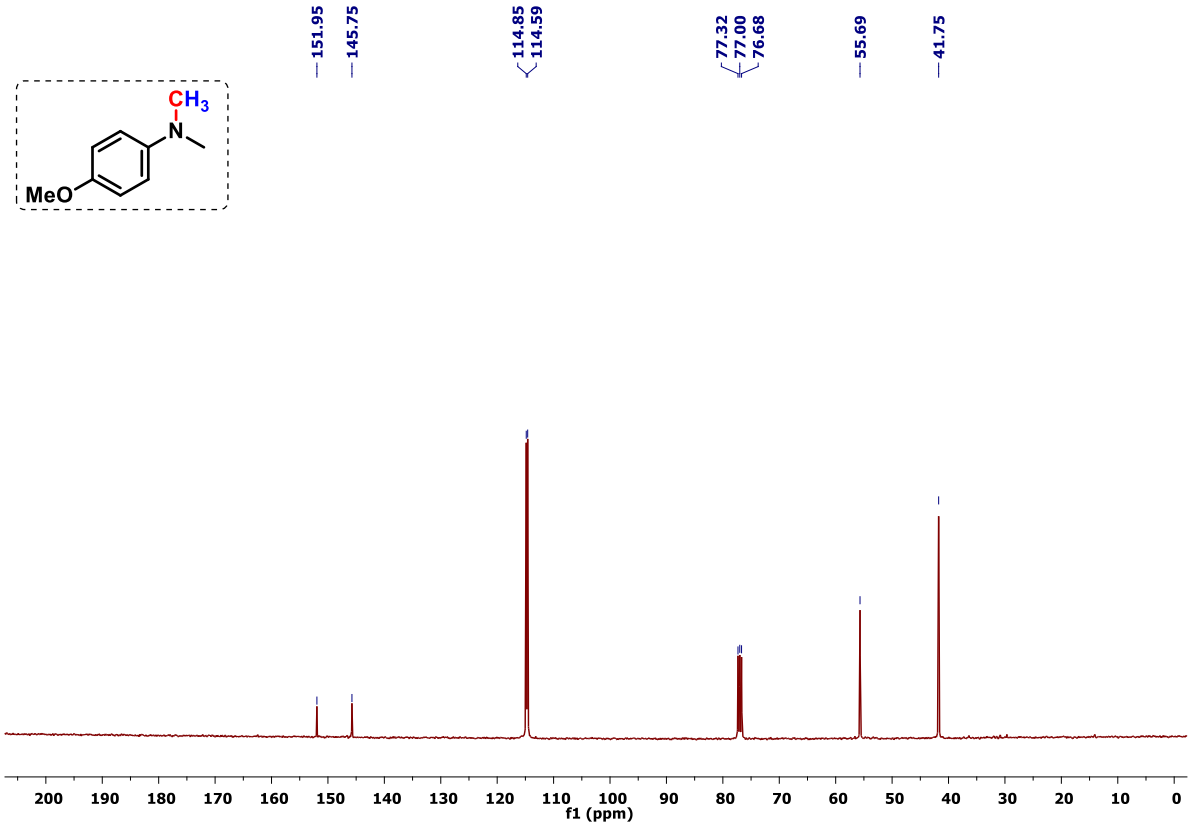


Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum of **3l** in $CDCl_3$.

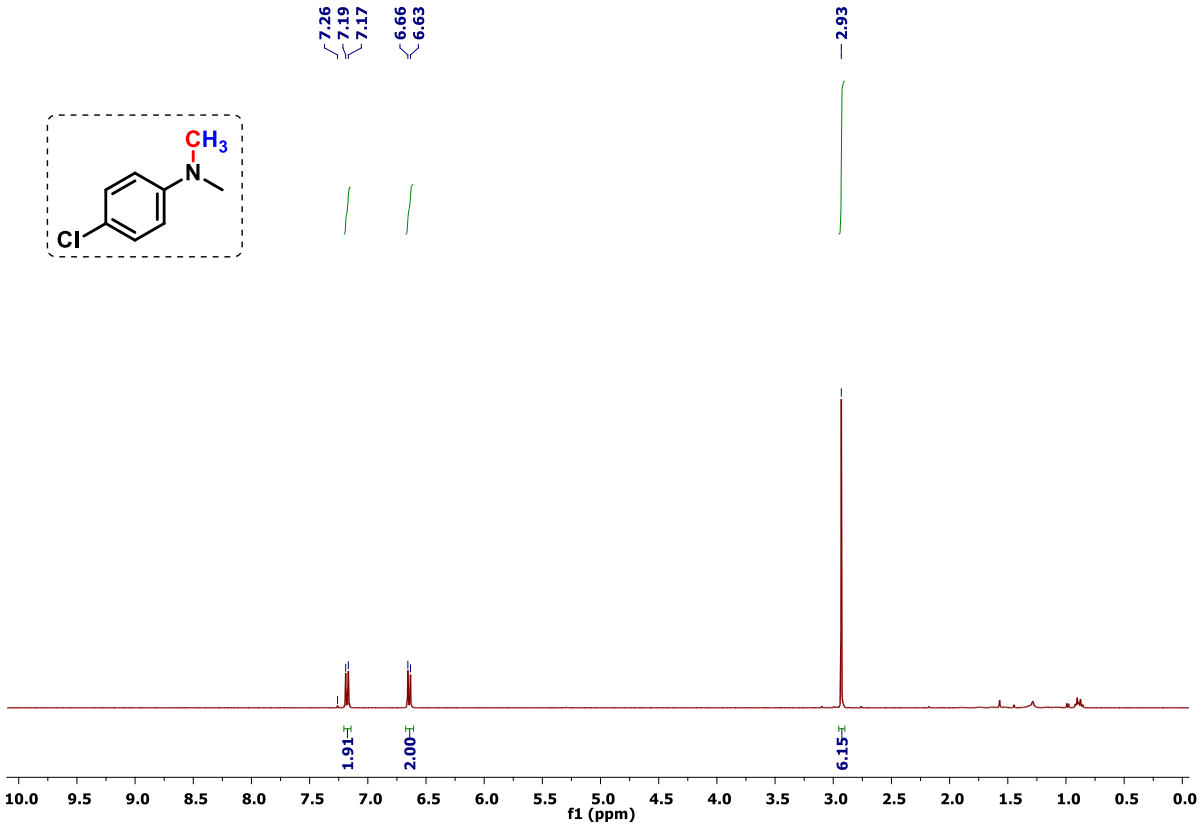


Figure S51. ^{1}H NMR spectrum of **3m** in $CDCl_3$.

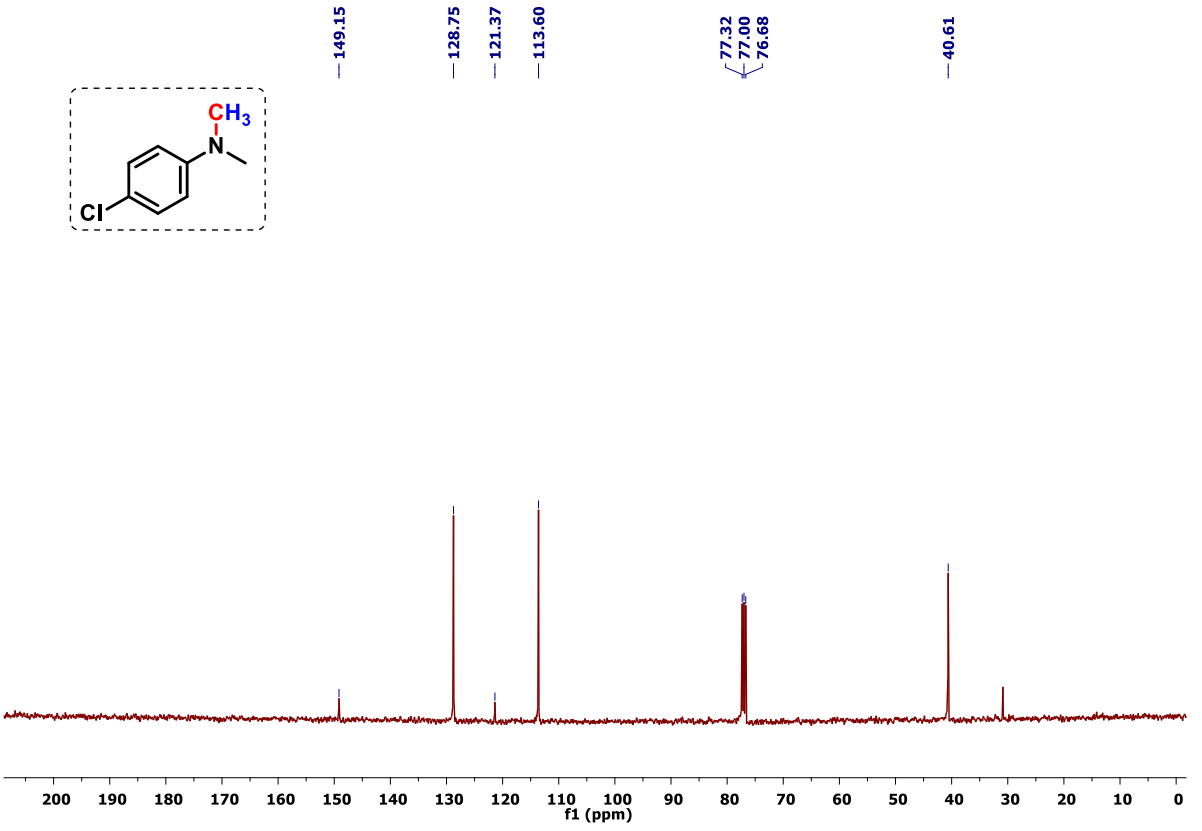


Figure S52. $^{13}C\{^{1}H\}$ NMR spectrum of **3m** in $CDCl_3$.

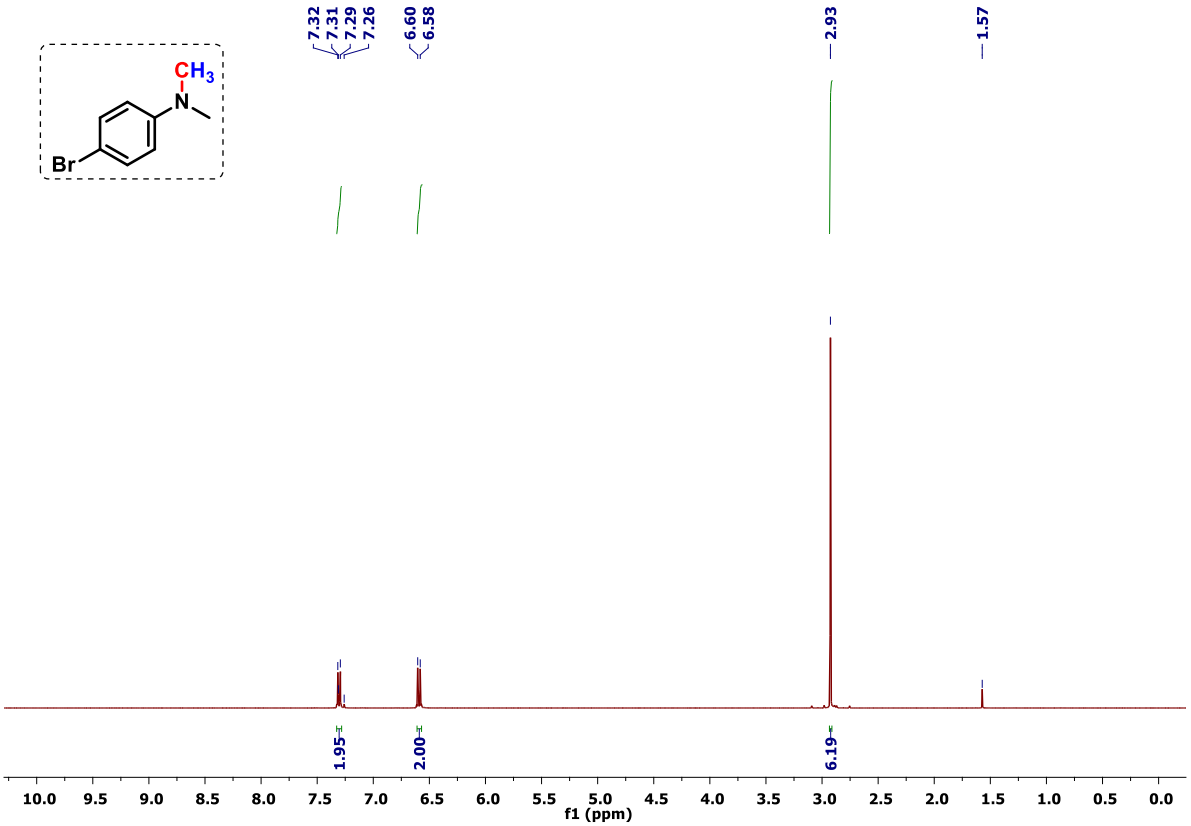


Figure S53. ^{1}H NMR spectrum of **3n** in $CDCl_3$.

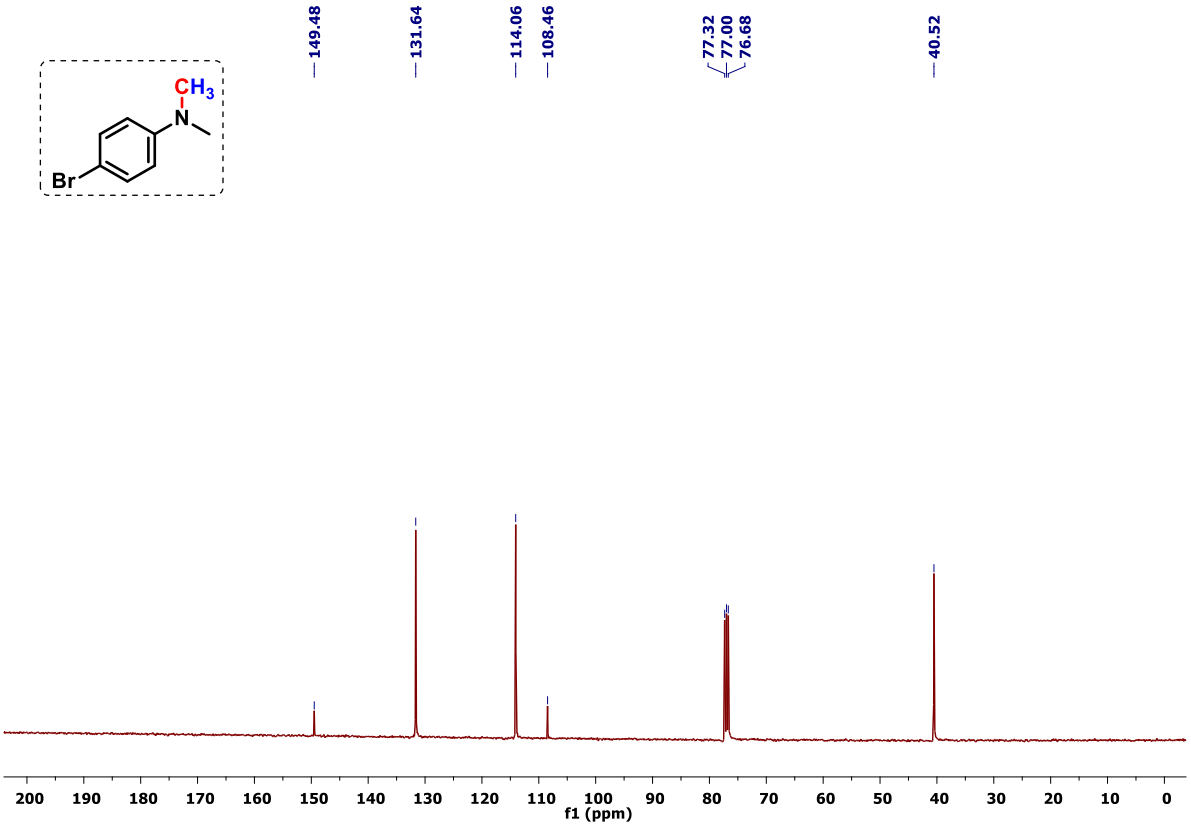


Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of **3n** in $CDCl_3$.

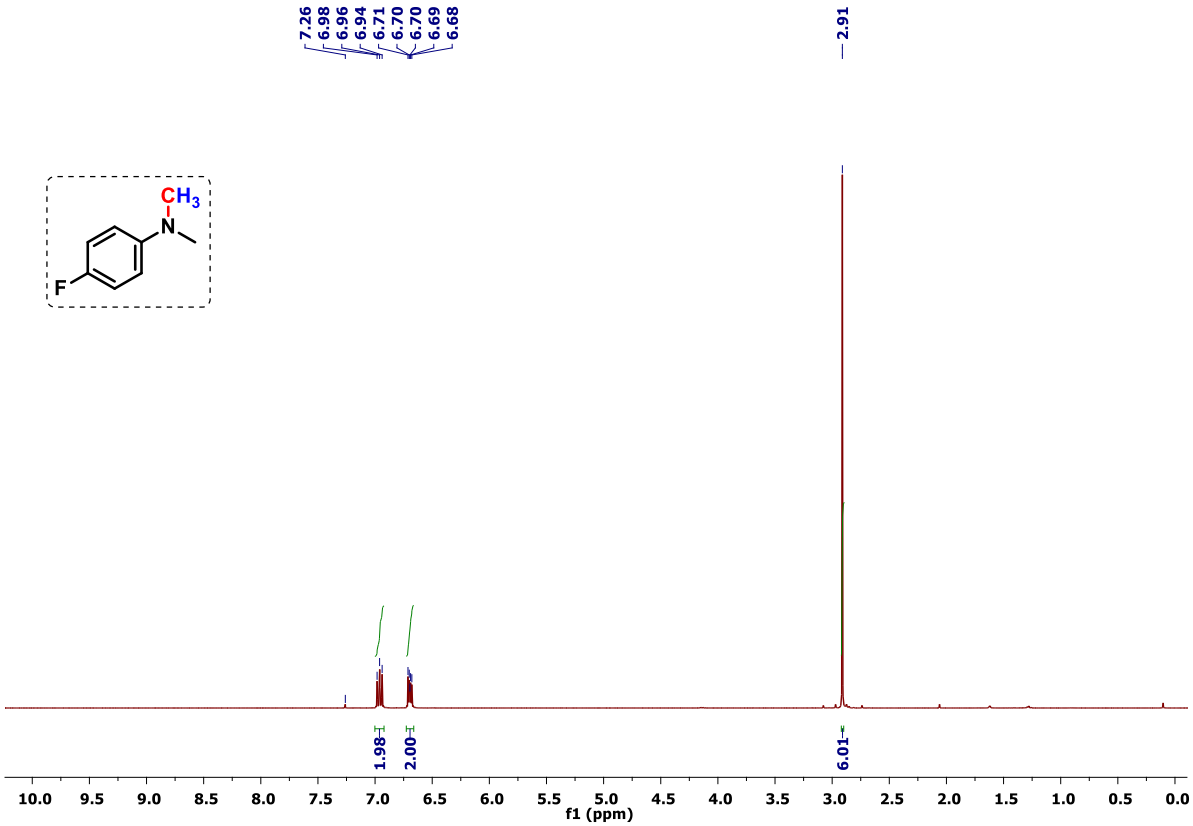


Figure S55. ^{1}H NMR spectrum of **3o** in $CDCl_3$.

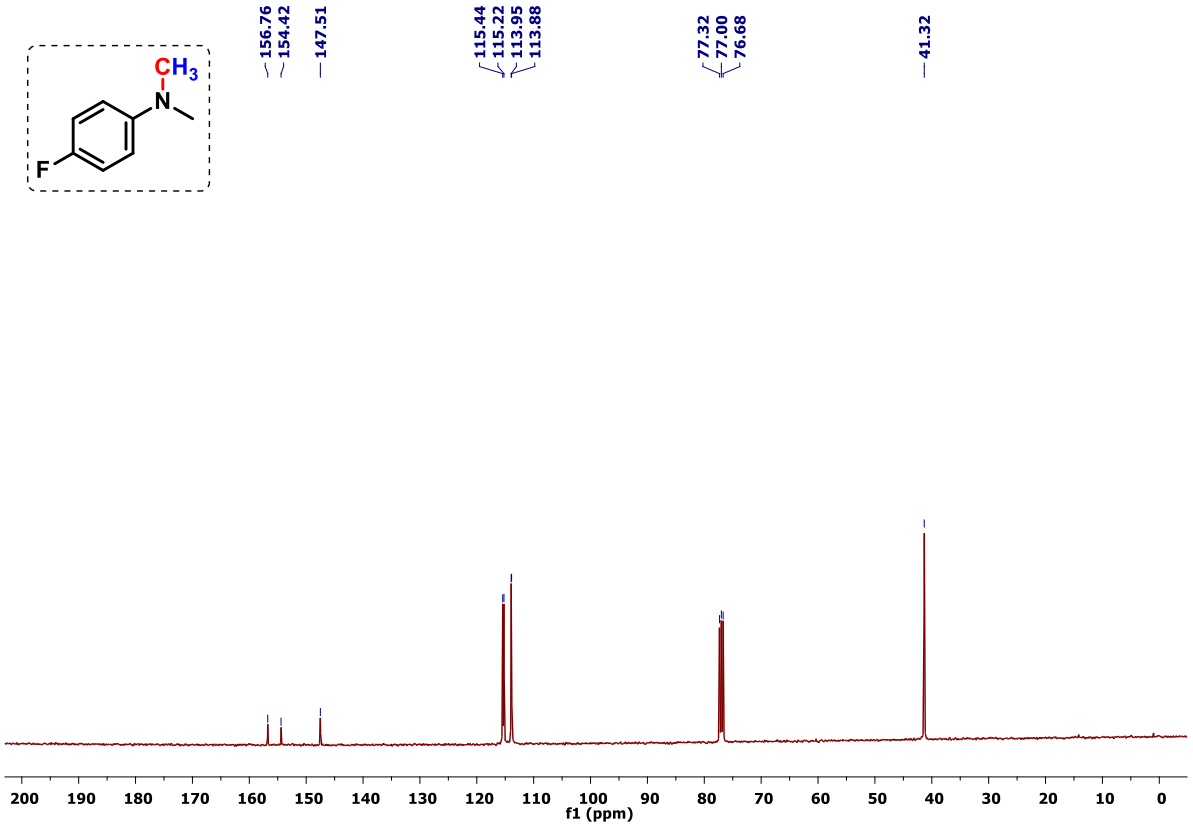


Figure S56. $^{13}C\{^{1}H\}$ NMR spectrum of **3o** in $CDCl_3$.

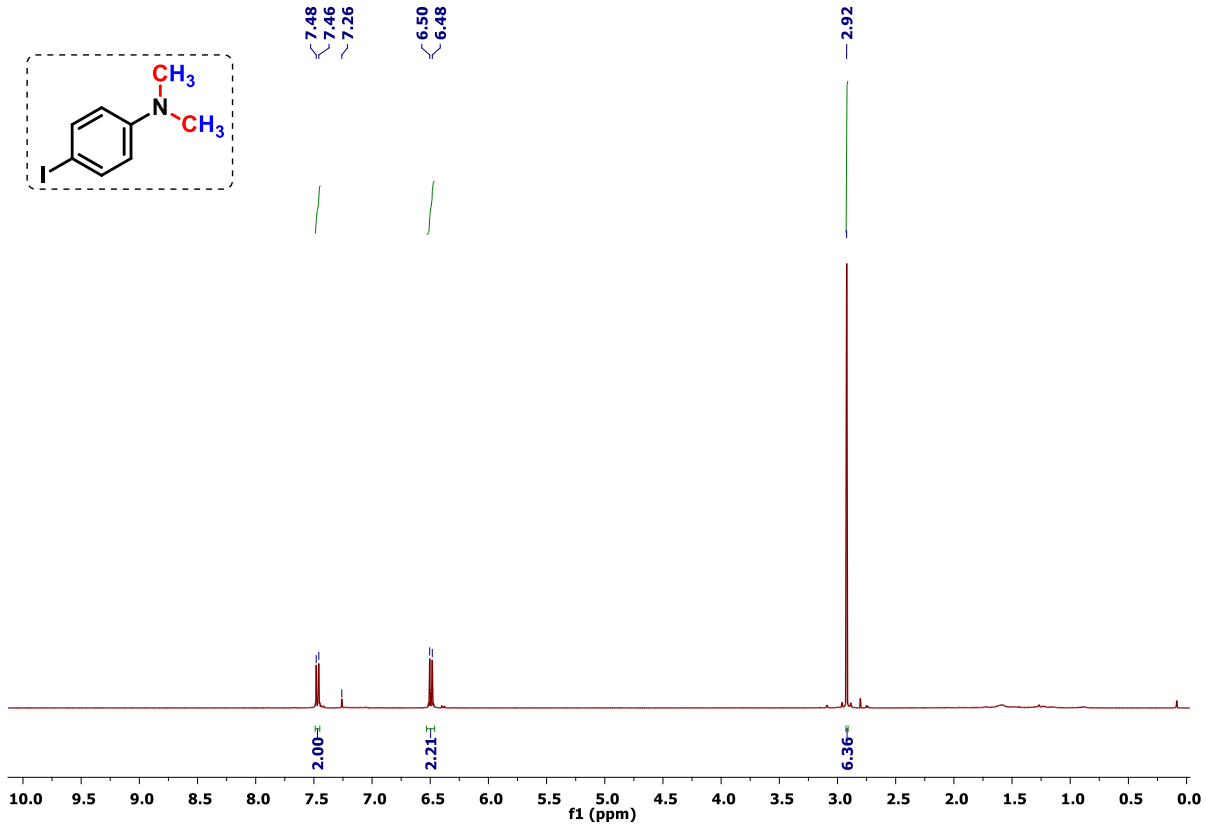


Figure S57. ^{1}H NMR spectrum of **5a** in $CDCl_3$.

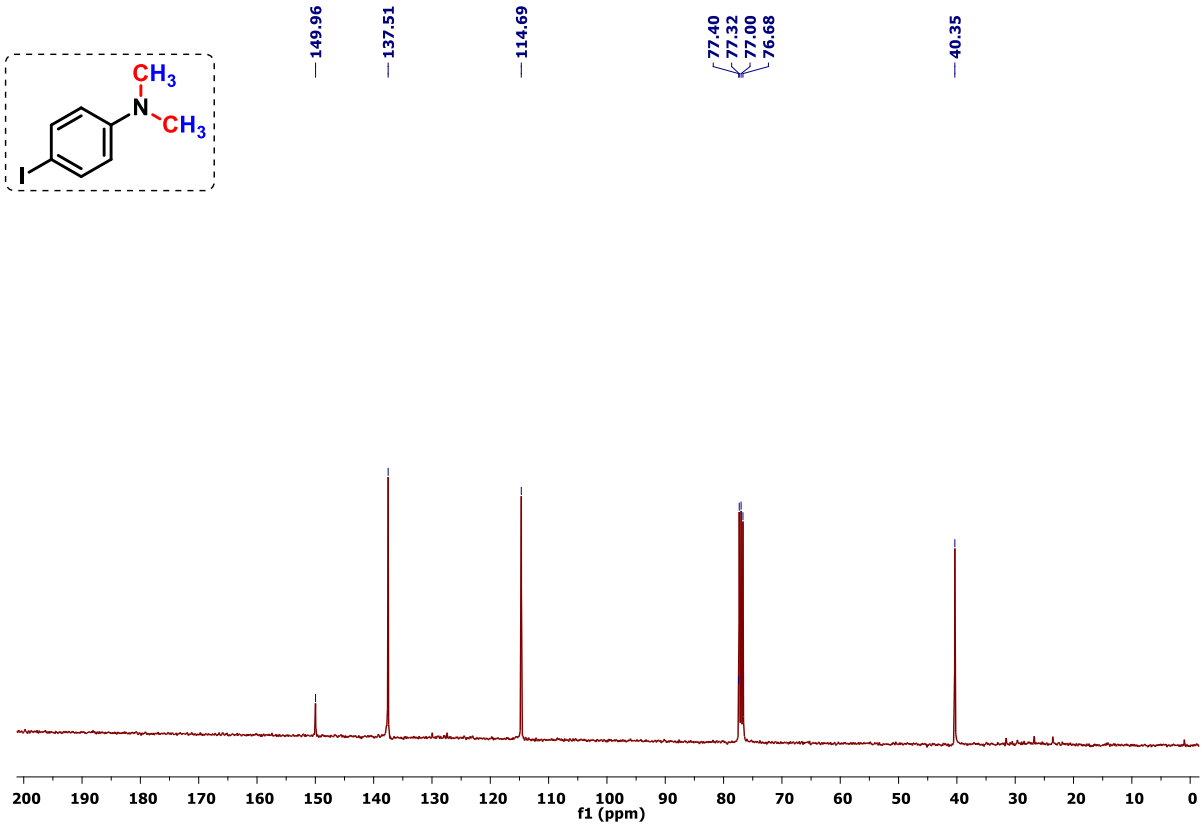


Figure S58. $^{13}C\{^{1}H\}$ NMR spectrum of **5a** in $CDCl_3$.

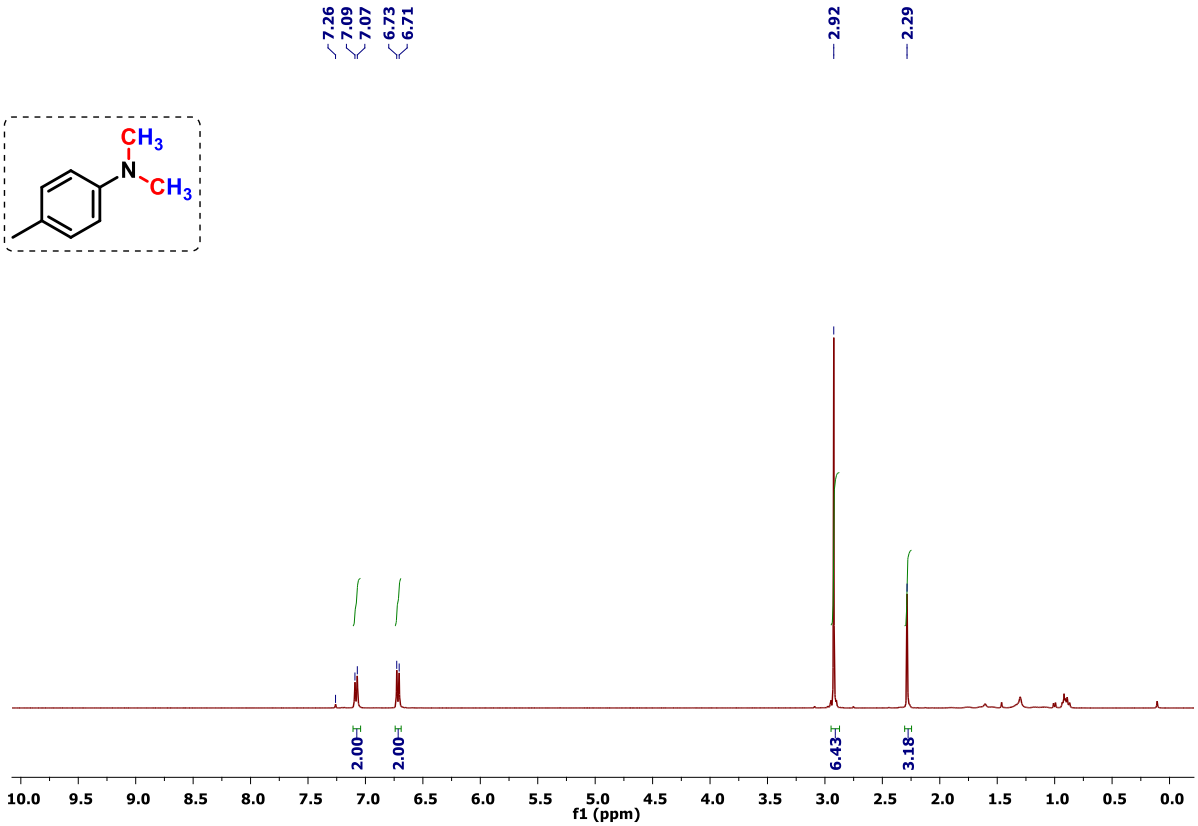


Figure S59. ^{1}H NMR spectrum of **5b** in $CDCl_3$.

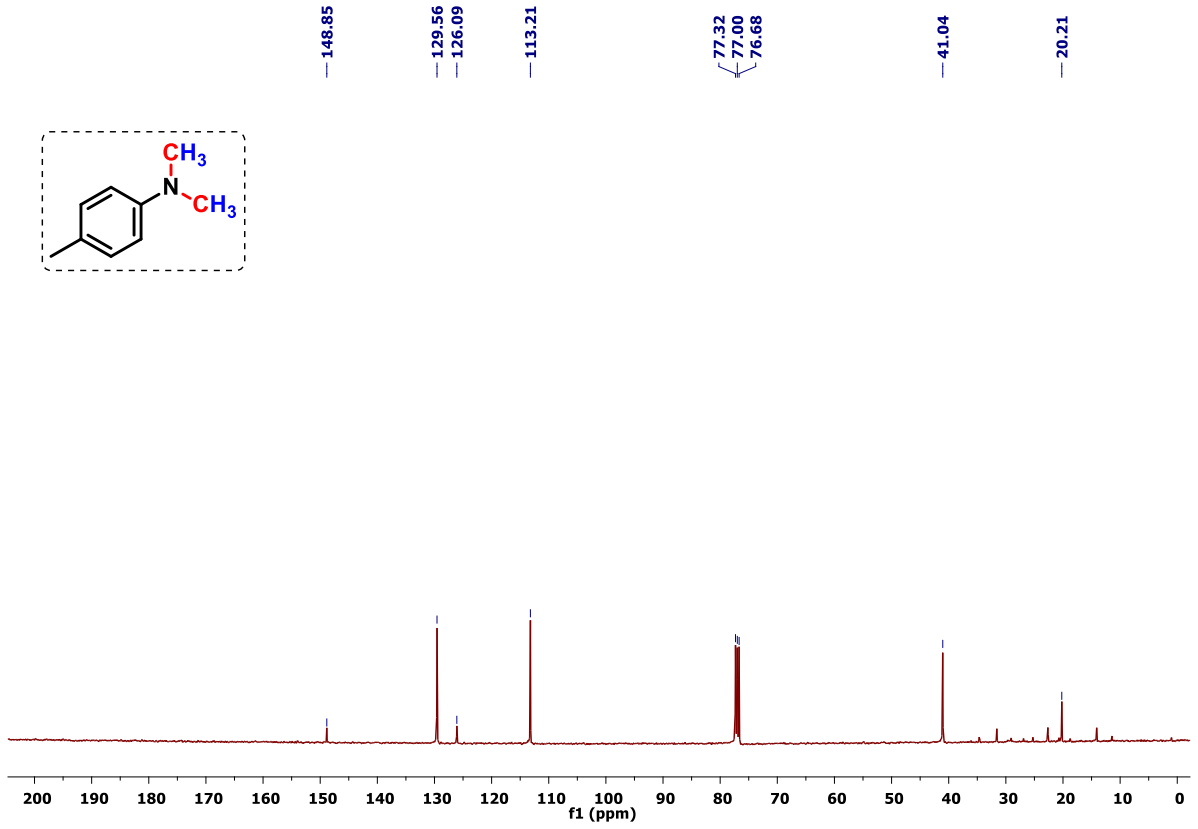


Figure S60. $^{13}C\{^{1}H\}$ NMR spectrum of **5b** in $CDCl_3$.

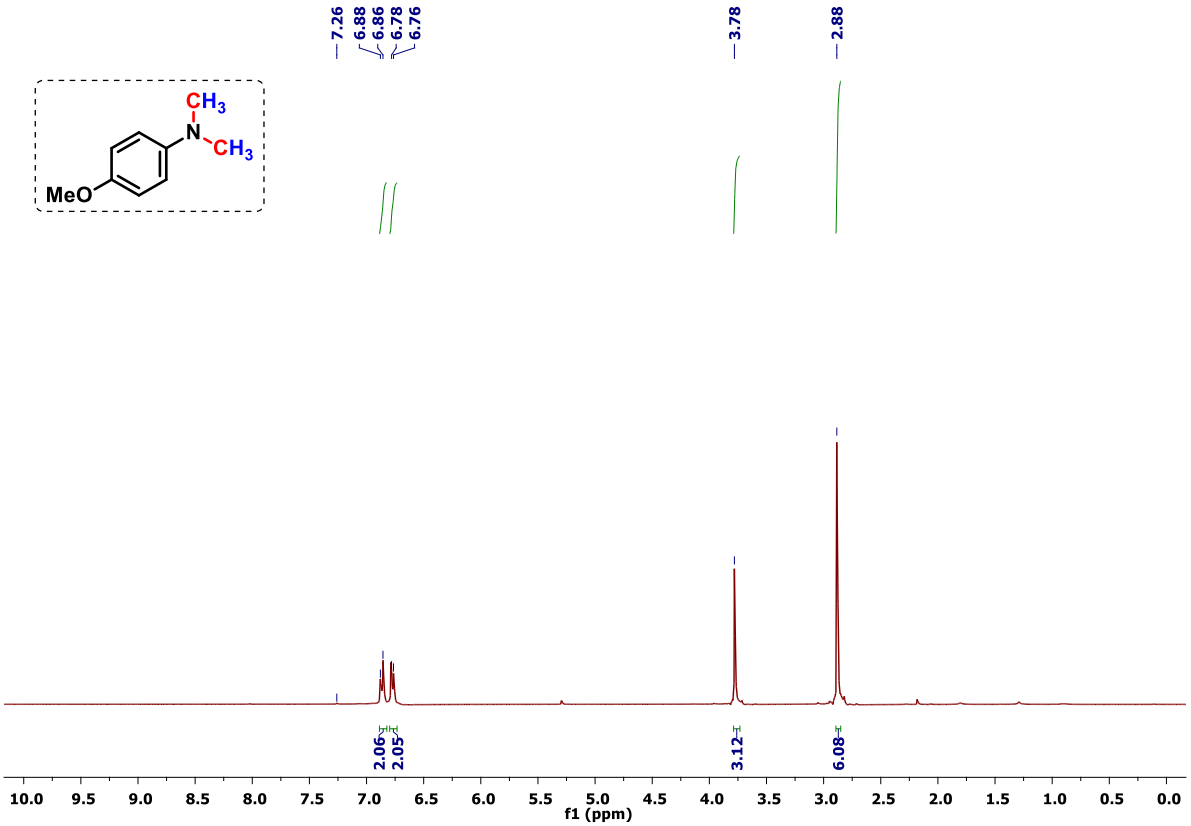


Figure S61. ^{1}H NMR spectrum of **5c** in $CDCl_3$.

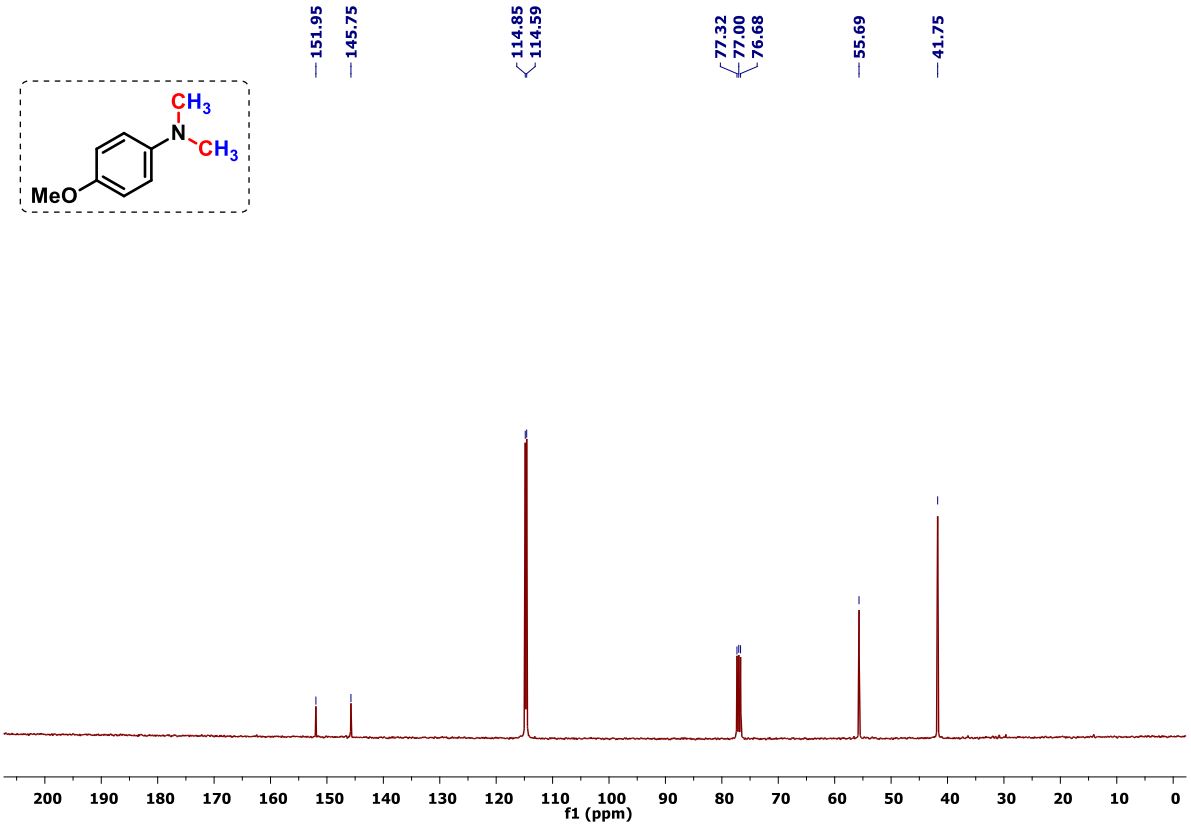


Figure S62. $^{13}C\{^{1}H\}$ NMR spectrum of **5c** in $CDCl_3$.

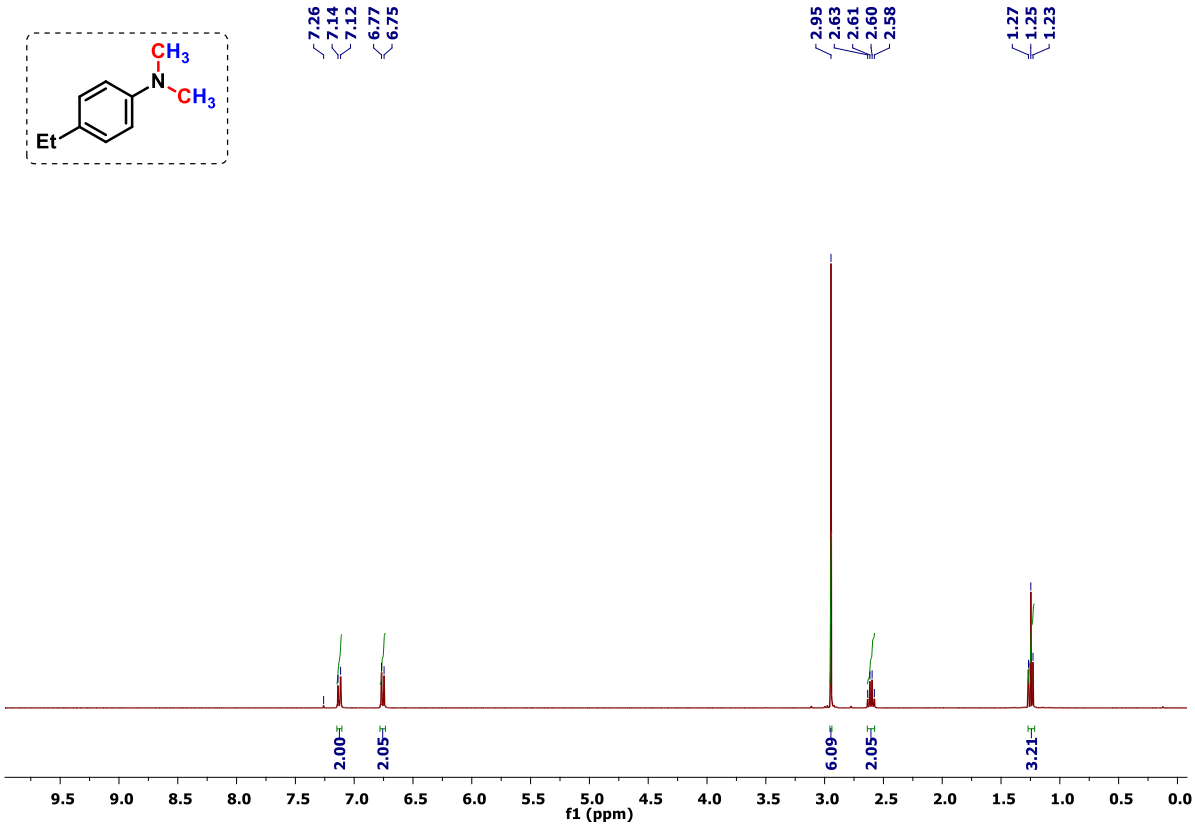


Figure S63. ^{1}H NMR spectrum of **5d** in $CDCl_3$.

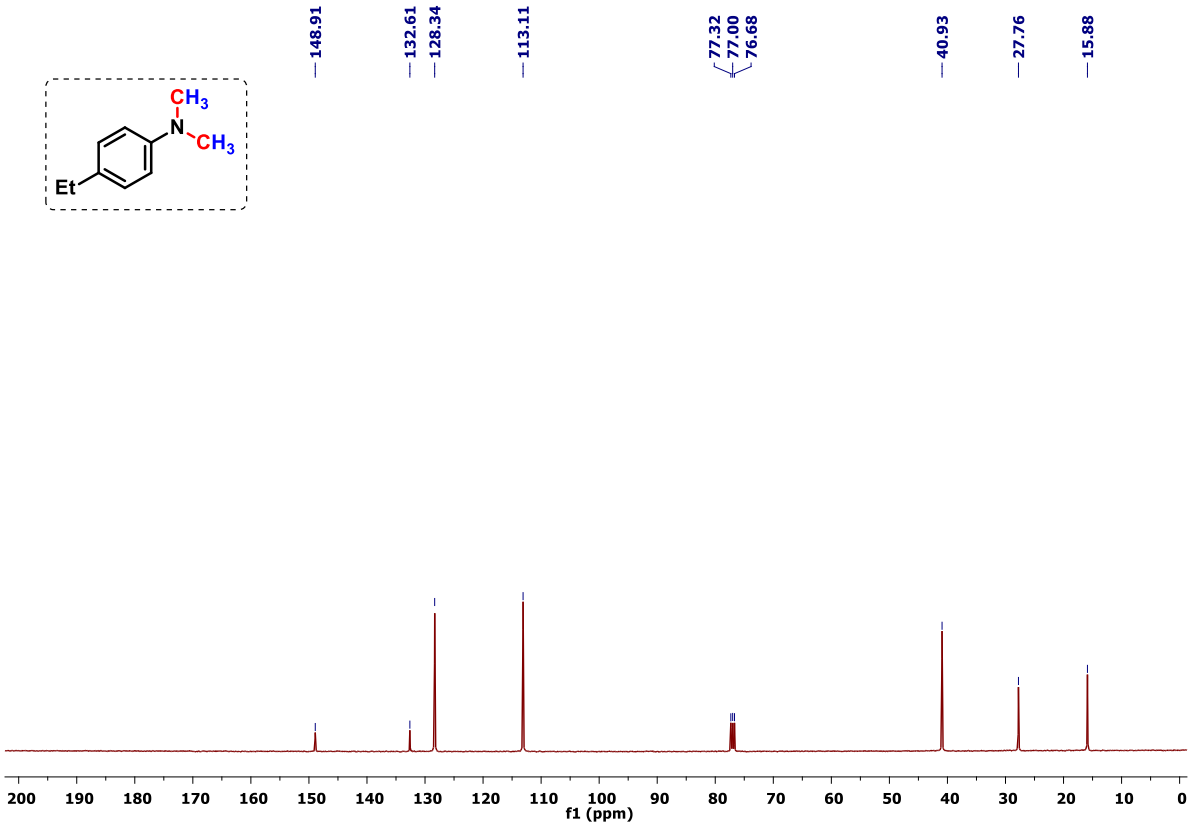


Figure S64. $^{13}C\{^{1}H\}$ NMR spectrum of **5d** in $CDCl_3$.

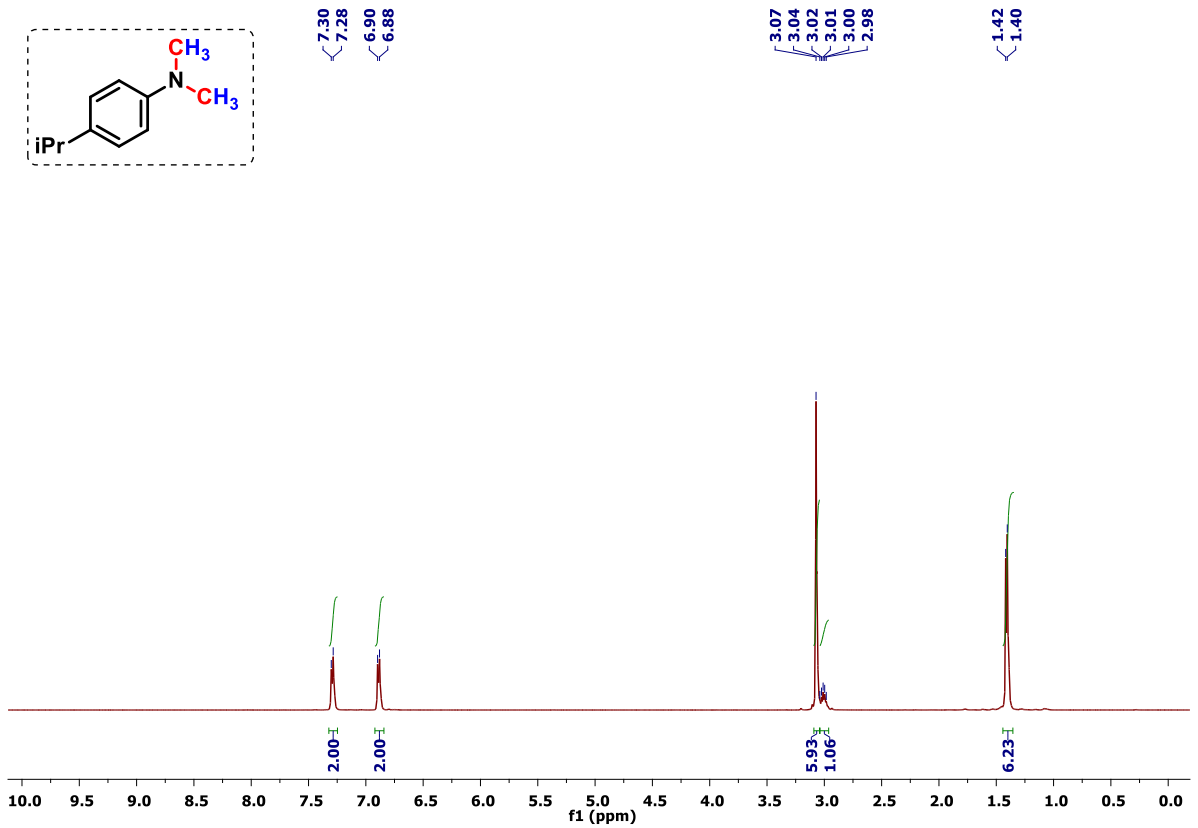


Figure S65. ^{1}H NMR spectrum of **5e** in $CDCl_3$.

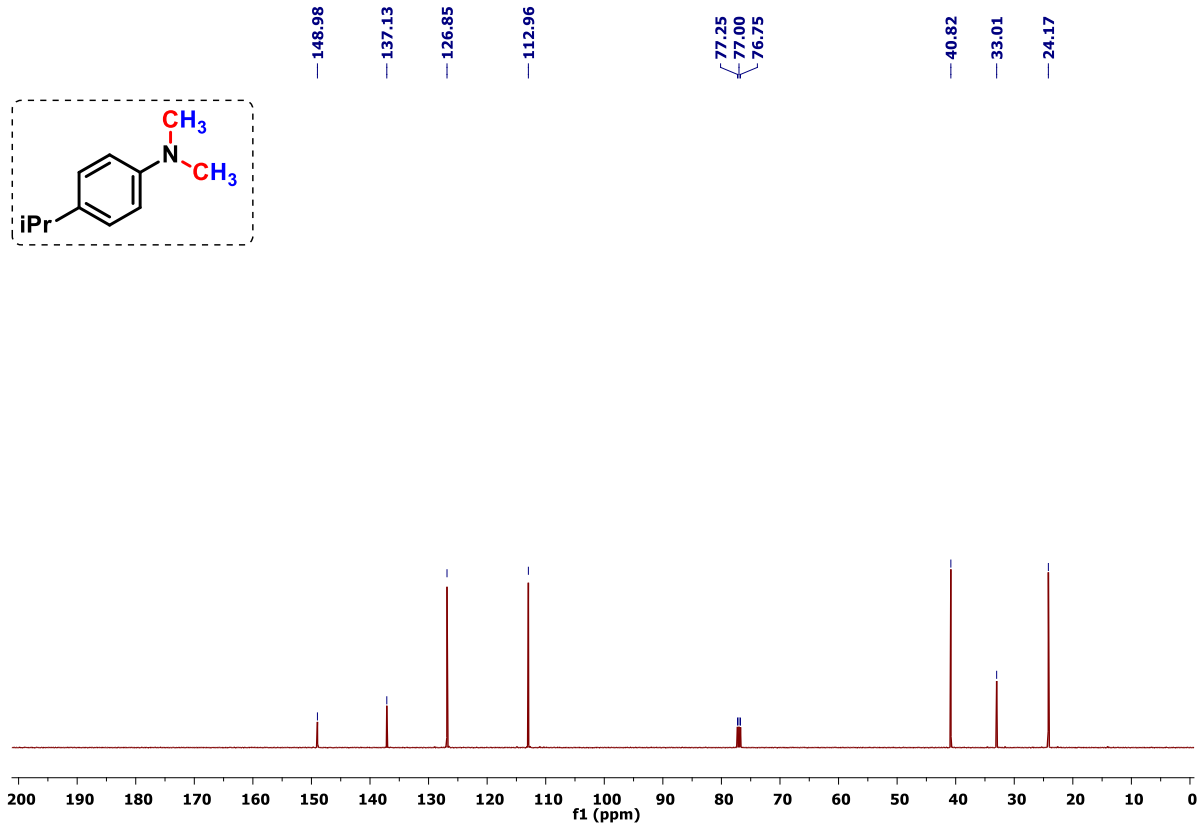


Figure S66. $^{13}C\{^{1}H\}$ NMR spectrum of **5e** in $CDCl_3$.

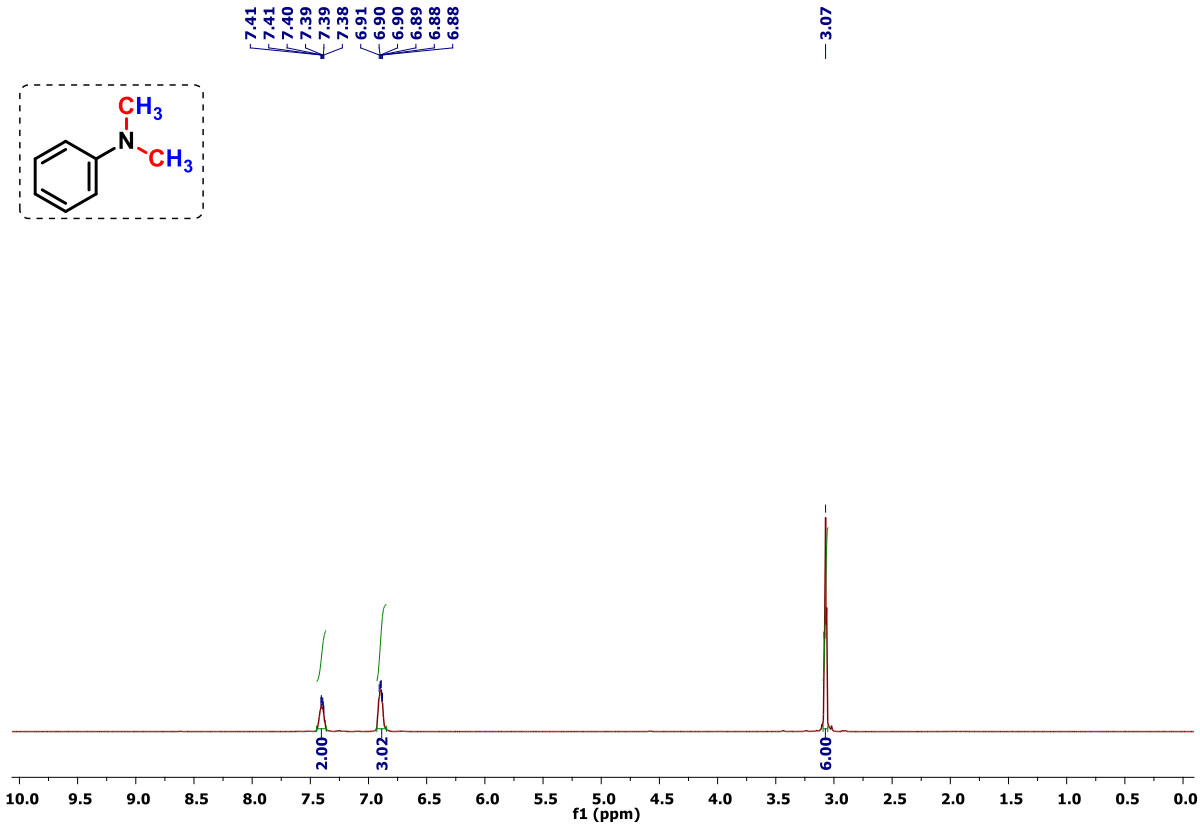


Figure S67. ^{1}H NMR spectrum of **5f** in $CDCl_3$.

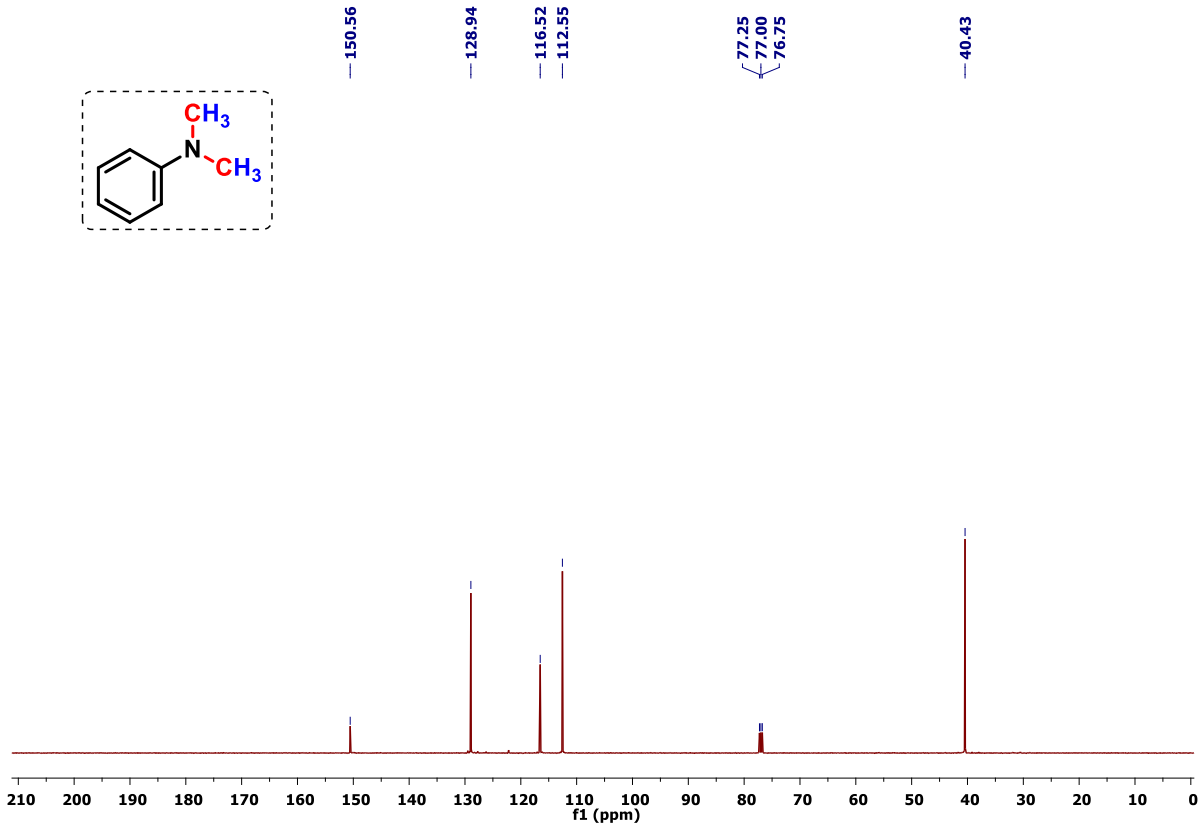


Figure S68. $^{13}C\{^{1}H\}$ NMR spectrum of **5f** in $CDCl_3$.

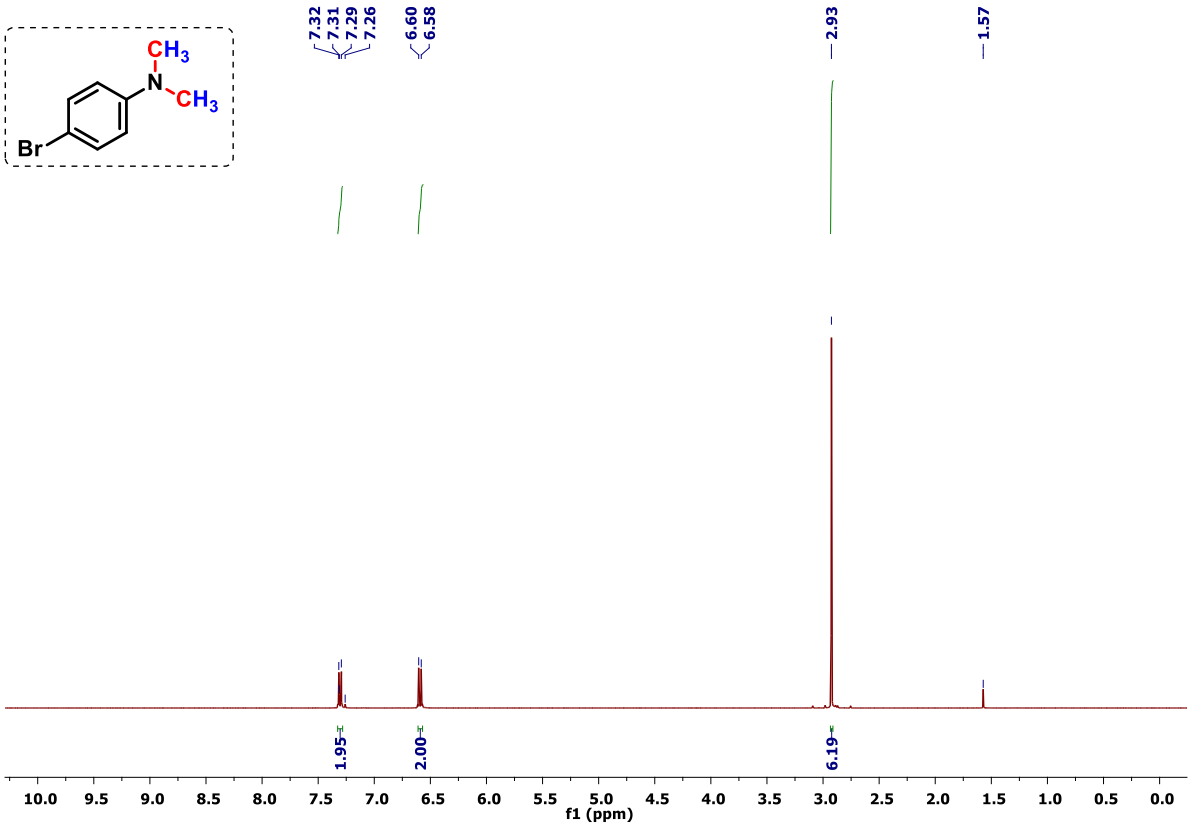


Figure S69. ^{1}H NMR spectrum of **5g** in $CDCl_3$.

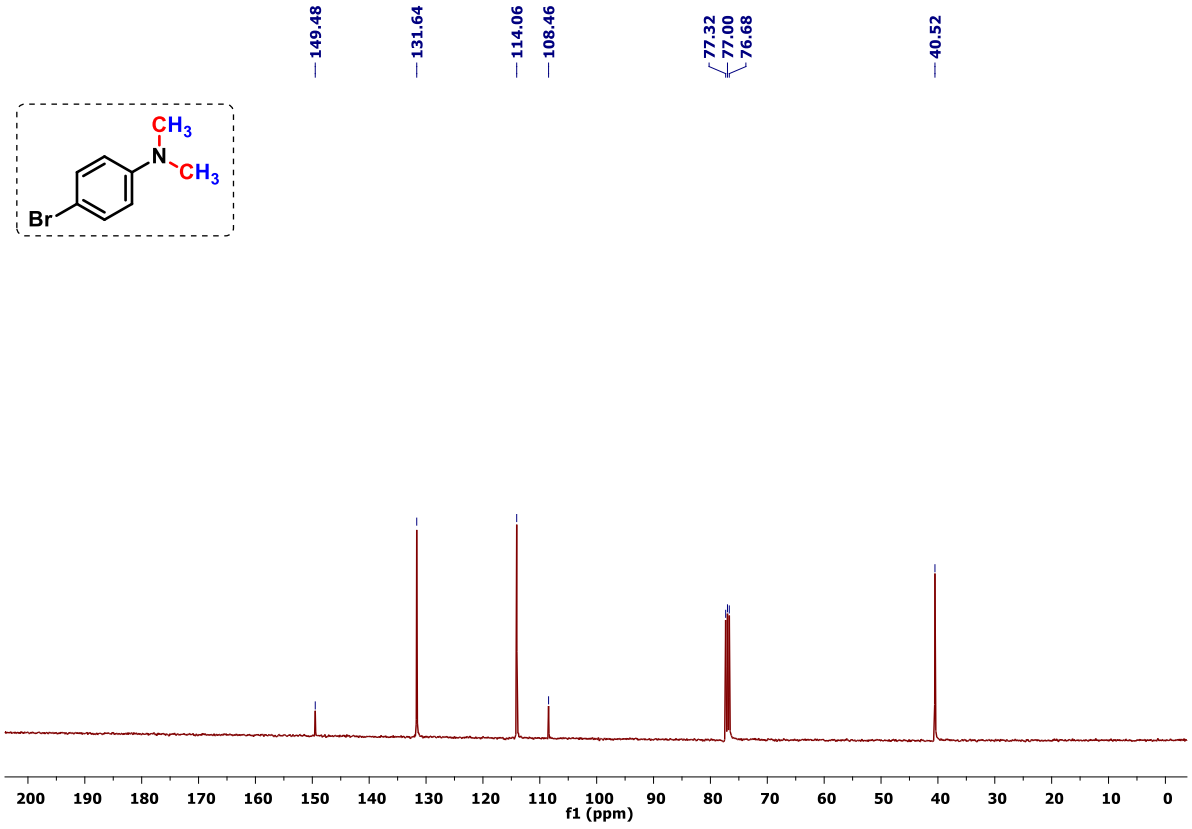


Figure S70. $^{13}C\{^{1}H\}$ NMR spectrum of **5g** in $CDCl_3$.

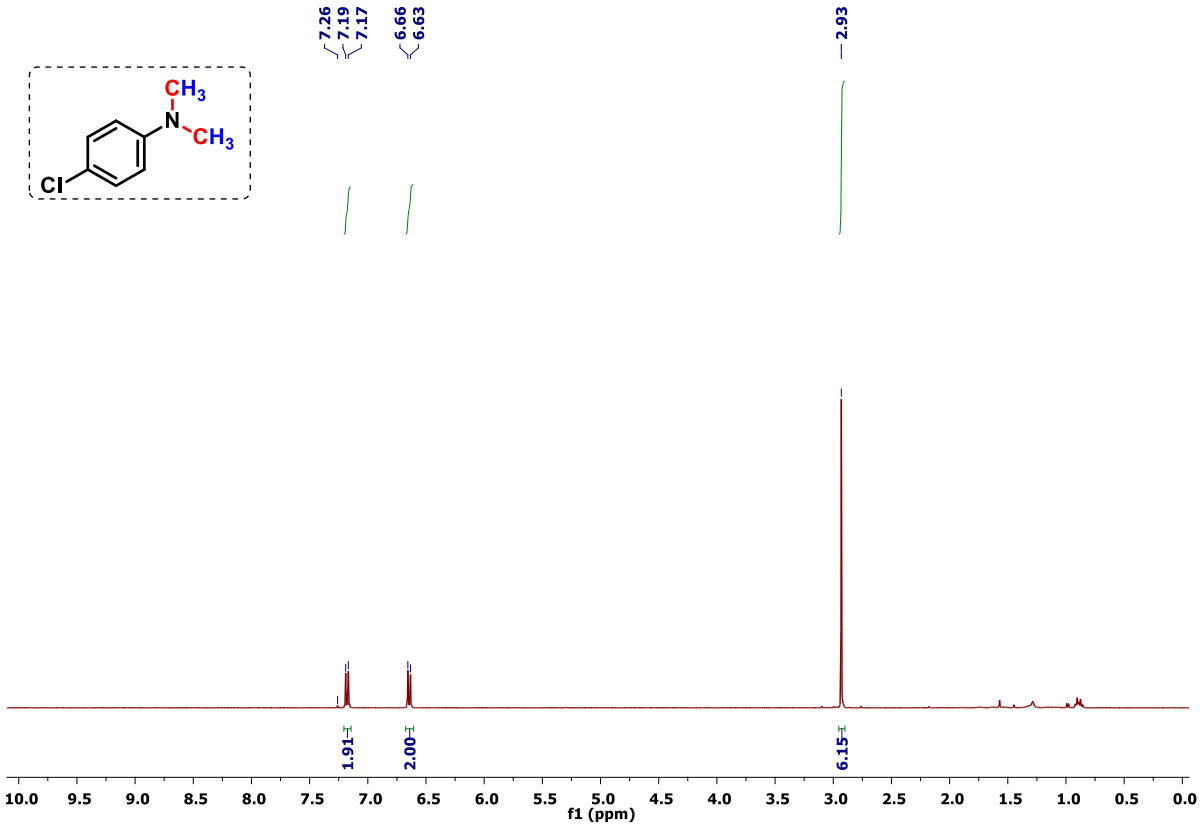


Figure S71. ^{1}H NMR spectrum of **5h** in $CDCl_3$.

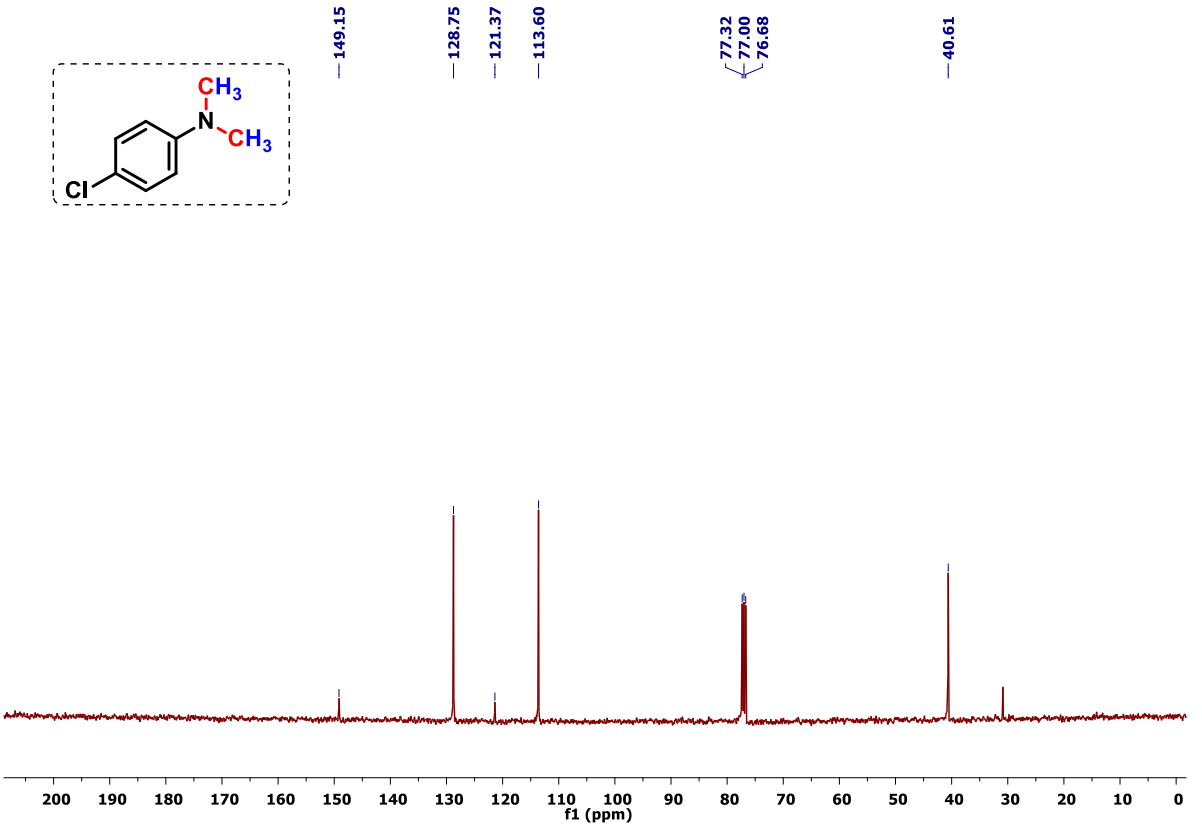


Figure S72. $^{13}C\{^{1}H\}$ NMR spectrum of **5h** in $CDCl_3$.

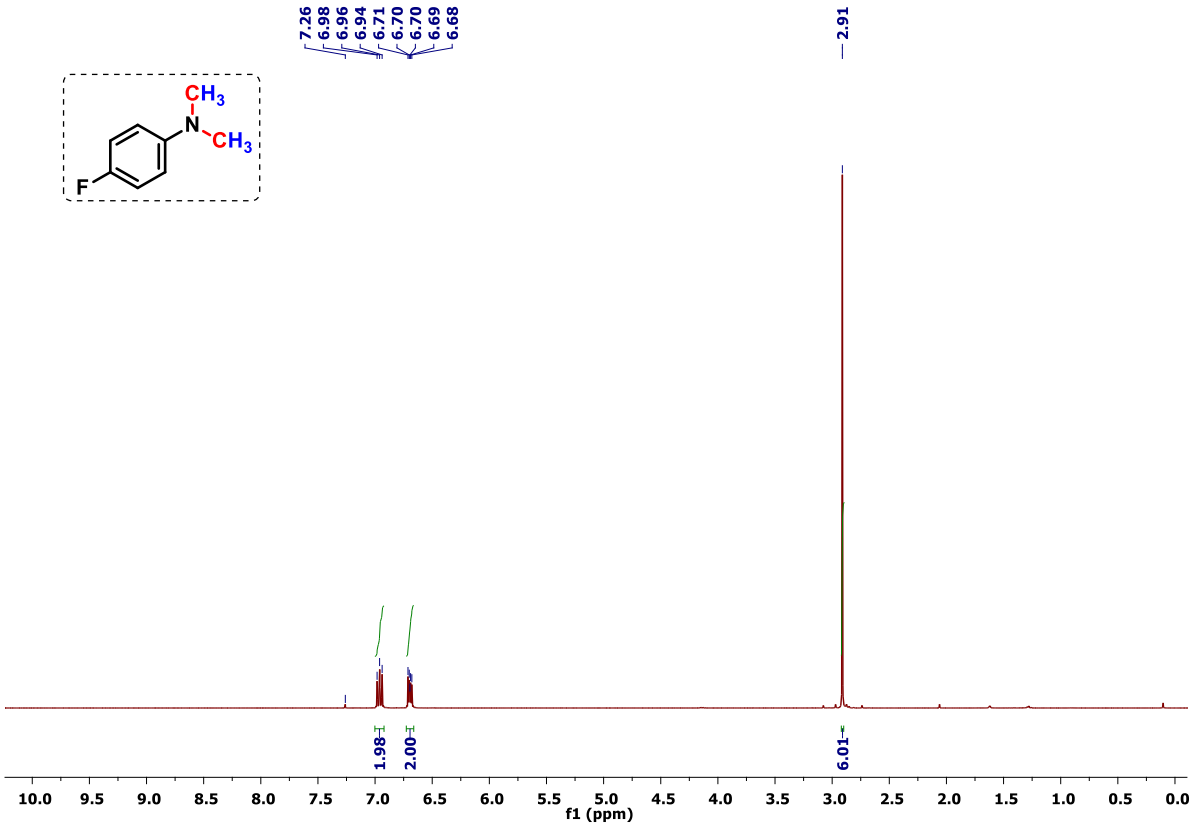


Figure S73. ^{1}H NMR spectrum of **5i** in $CDCl_3$.

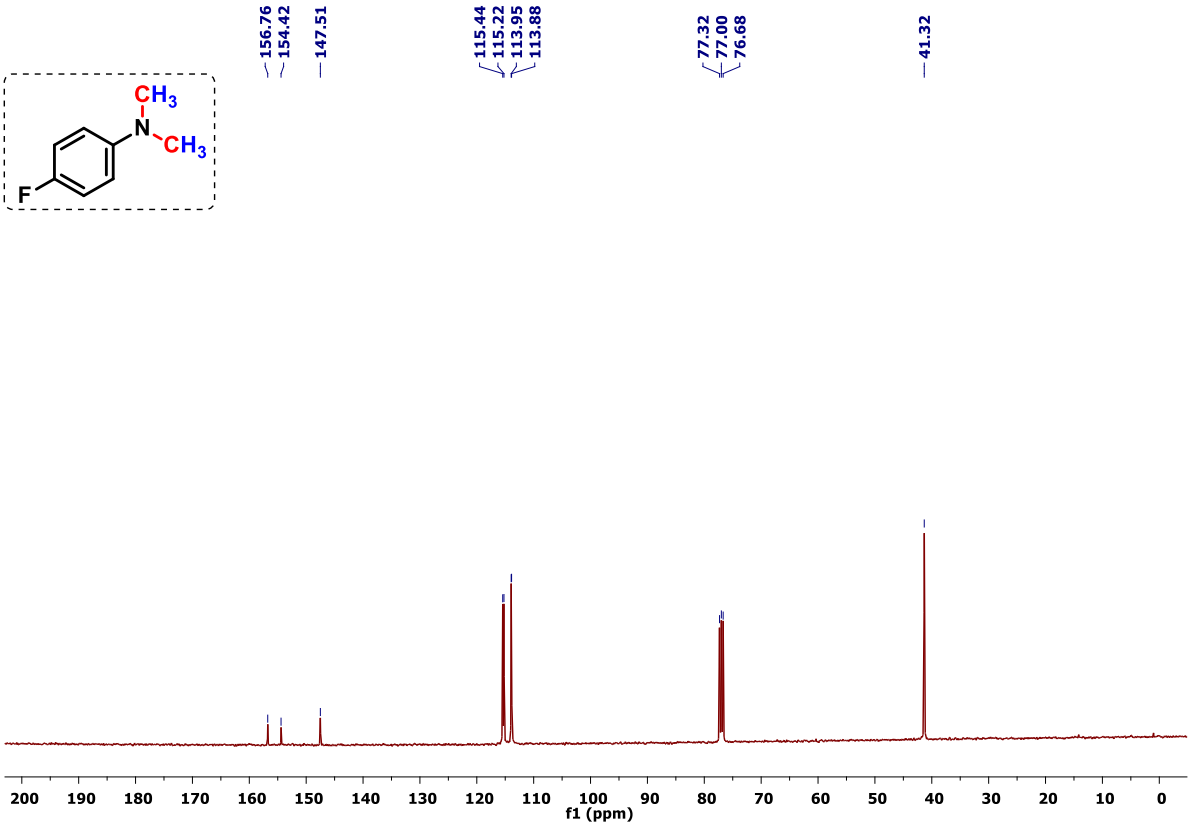


Figure S74. $^{13}C\{^{1}H\}$ NMR spectrum of **5i** in $CDCl_3$.

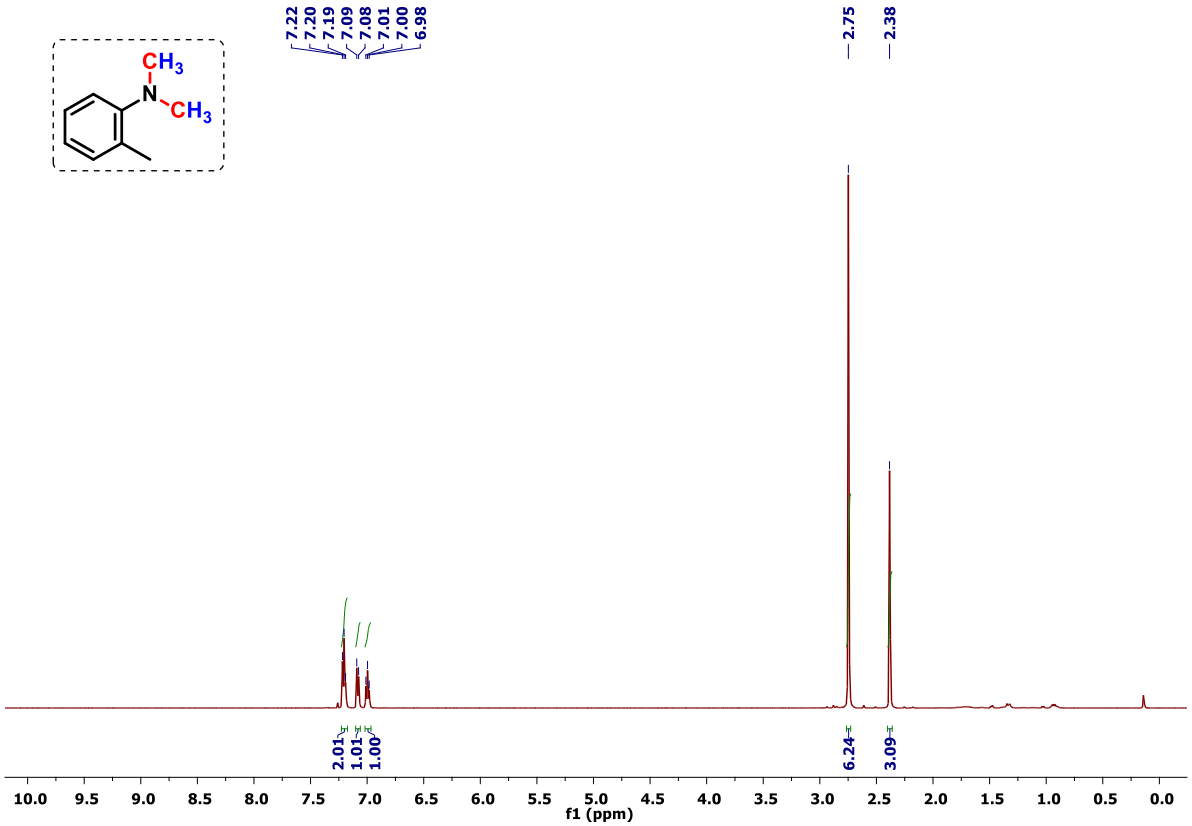


Figure S75. ^{1}H NMR spectrum of **5j** in $CDCl_3$.

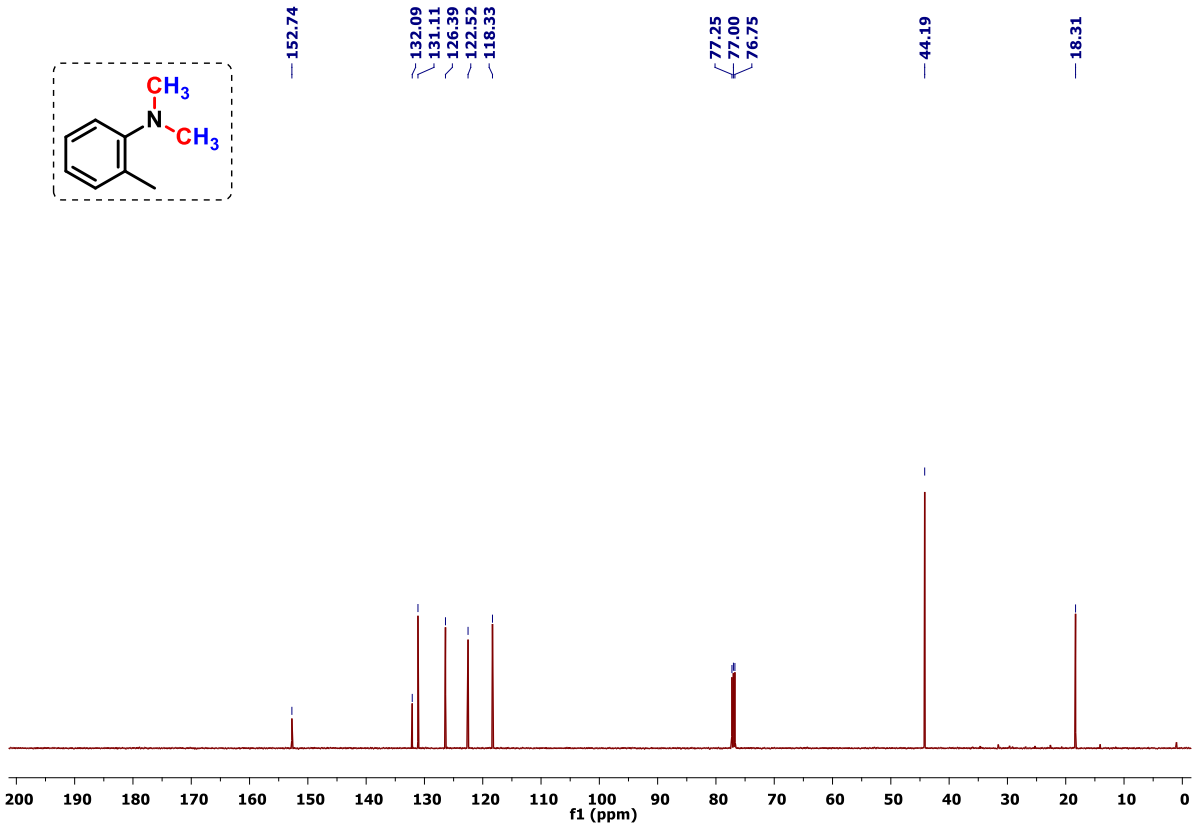


Figure S76. $^{13}C\{^{1}H\}$ NMR spectrum of **5j** in $CDCl_3$.

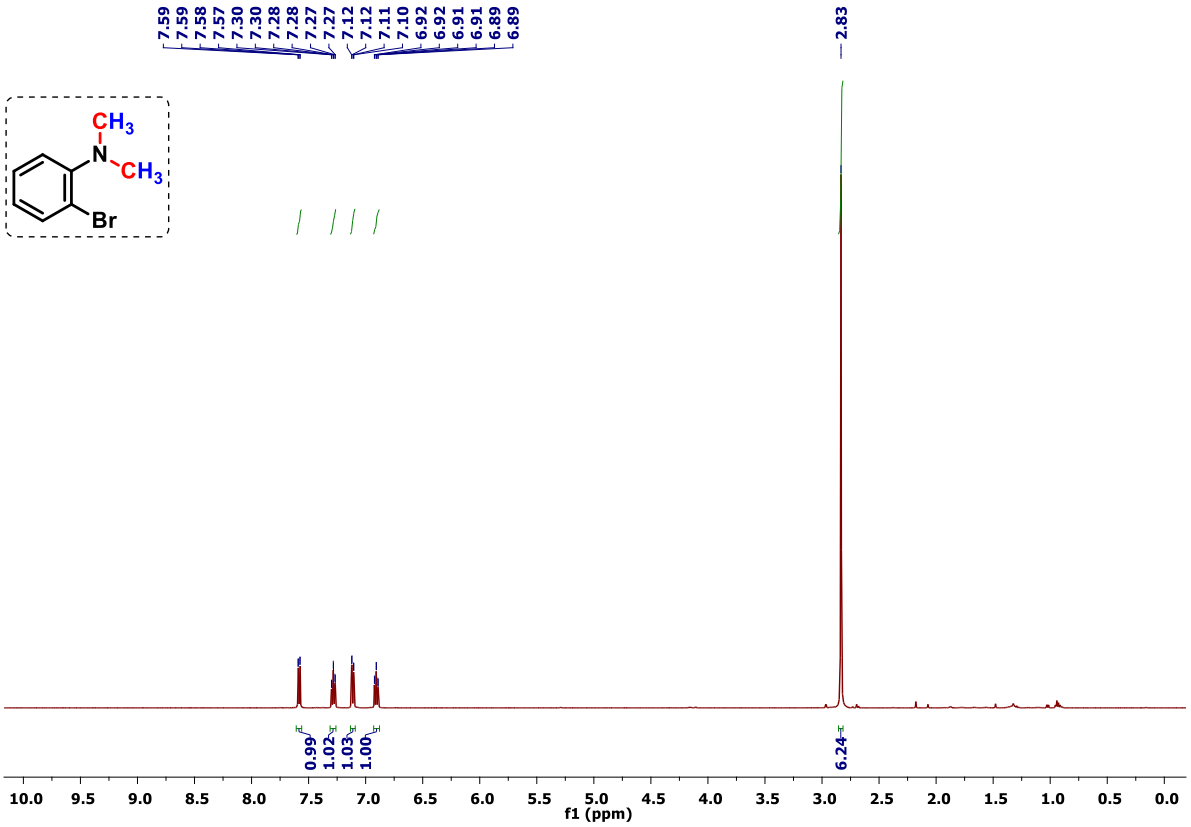


Figure S77. ^{1}H NMR spectrum of **5k** in $CDCl_3$.

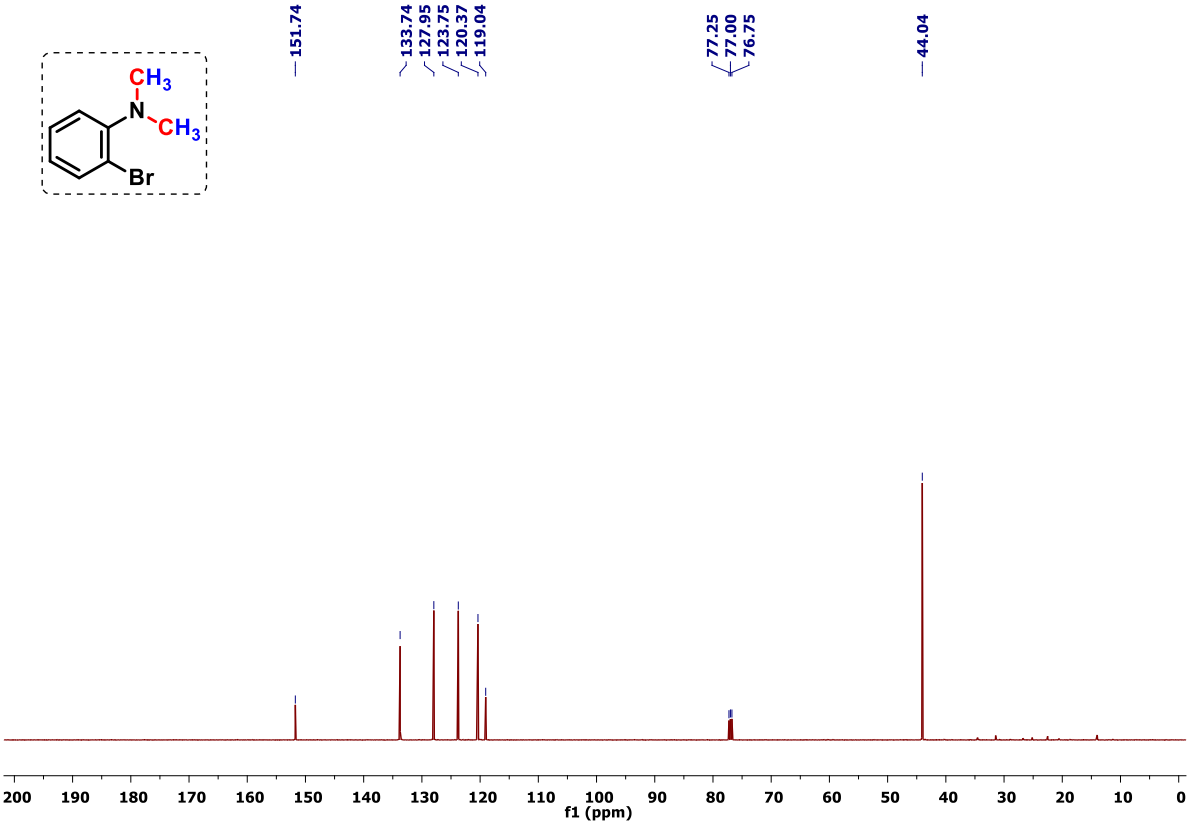


Figure S78. $^{13}C\{^{1}H\}$ NMR spectrum of **5k** in $CDCl_3$.

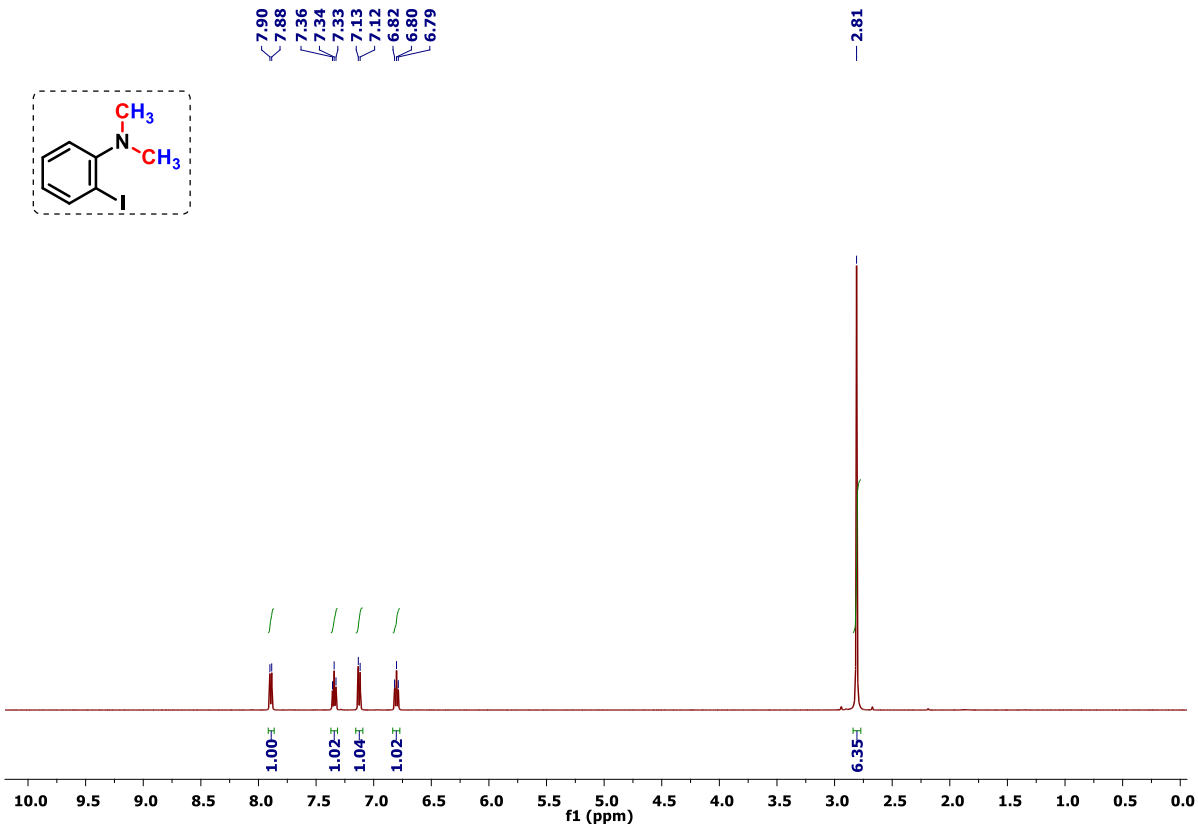


Figure S79. ^{1}H NMR spectrum of **5l** in $CDCl_3$.

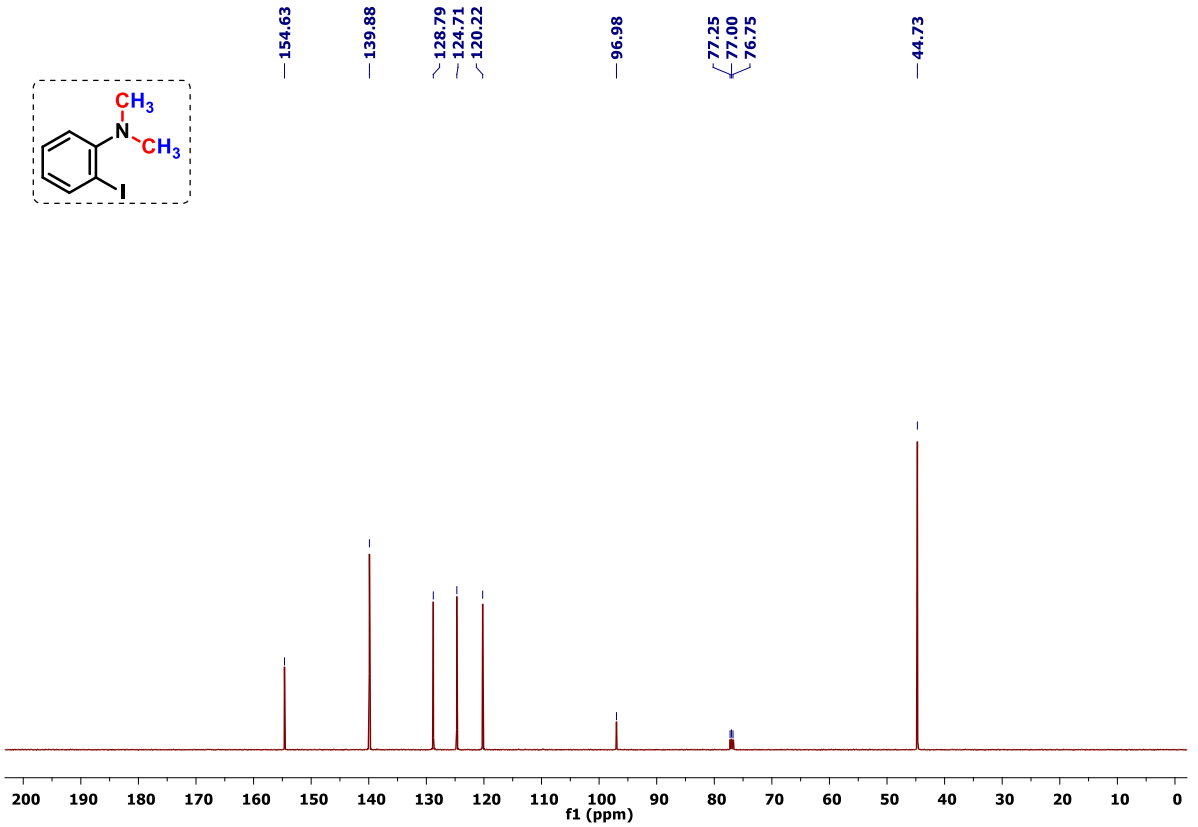


Figure S80. $^{13}C\{^{1}H\}$ NMR spectrum of **5l** in $CDCl_3$.

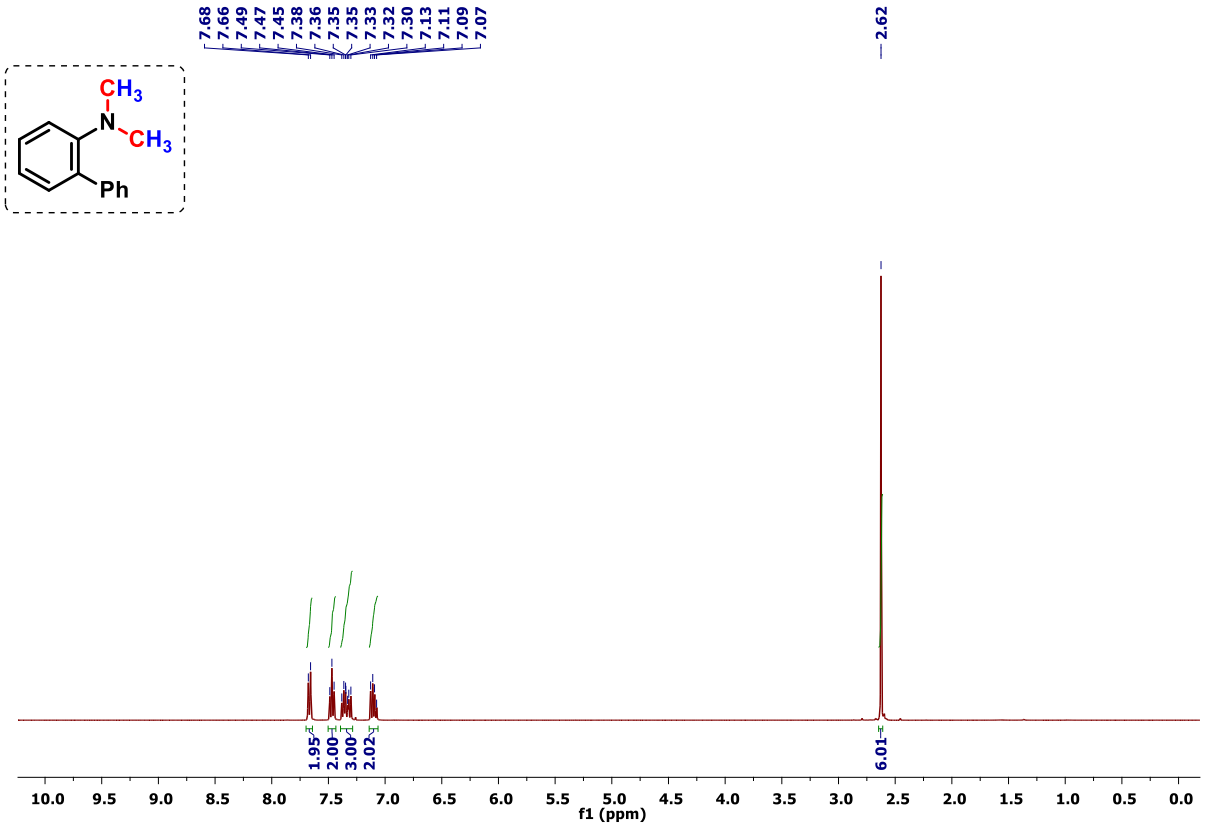


Figure S81. ^{1}H NMR spectrum of **5m** in $CDCl_3$.

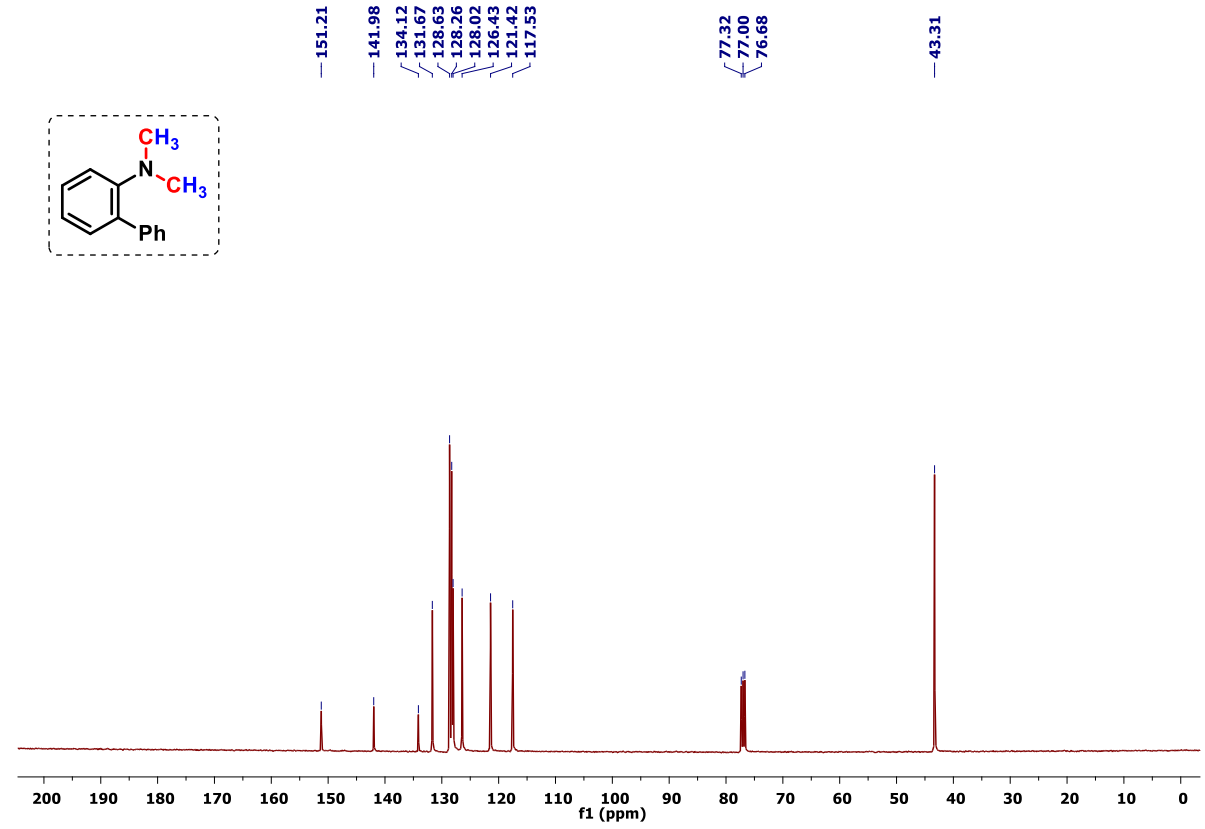


Figure S82. $^{13}C\{^{1}H\}$ NMR spectrum of **5m** in $CDCl_3$.

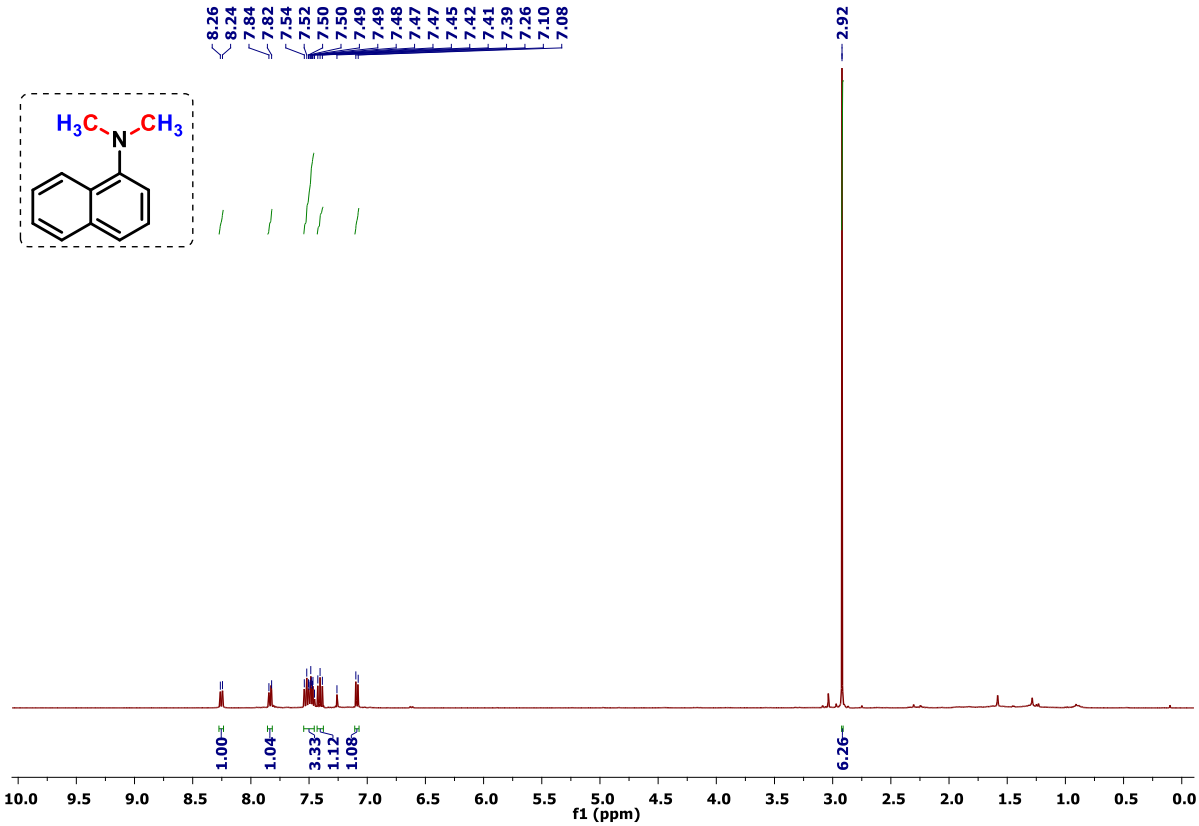


Figure S83. ^{1}H NMR spectrum of **5n** in $CDCl_3$.

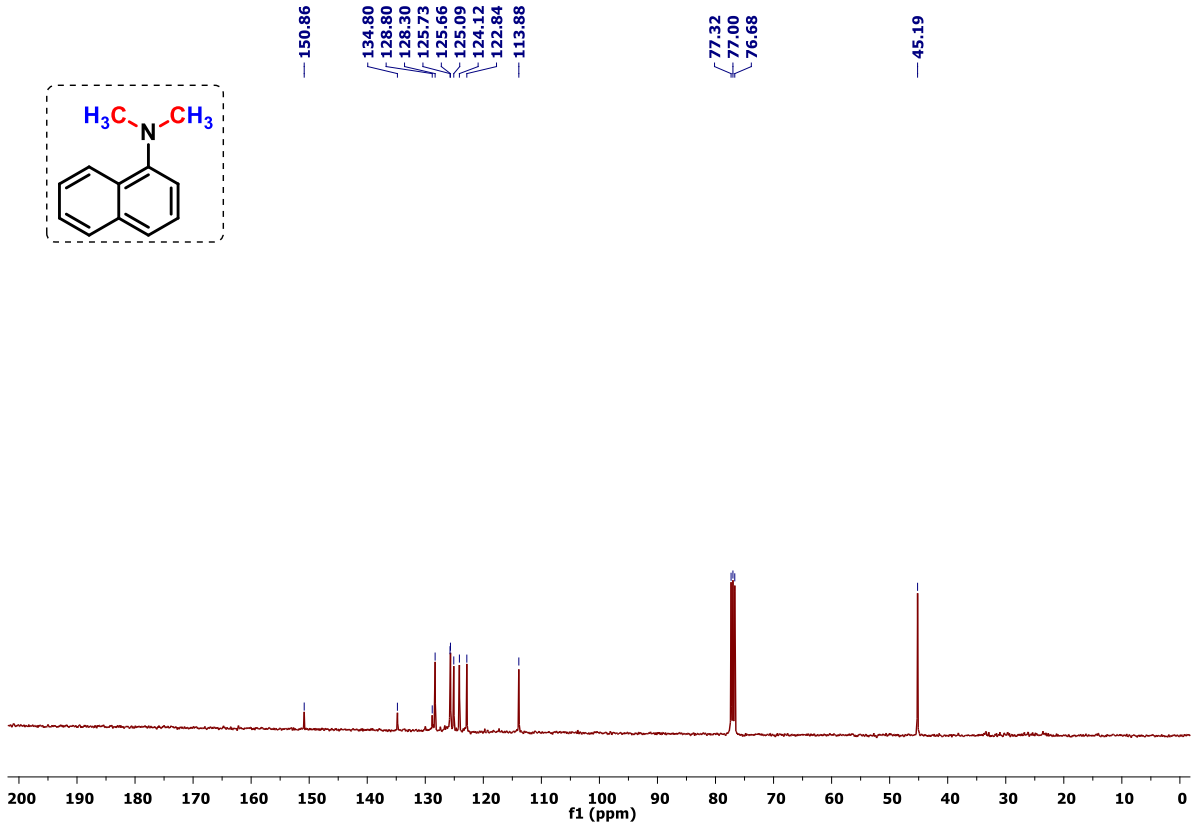


Figure S84. $^{13}C\{^{1}H\}$ NMR spectrum of **5n** in $CDCl_3$.

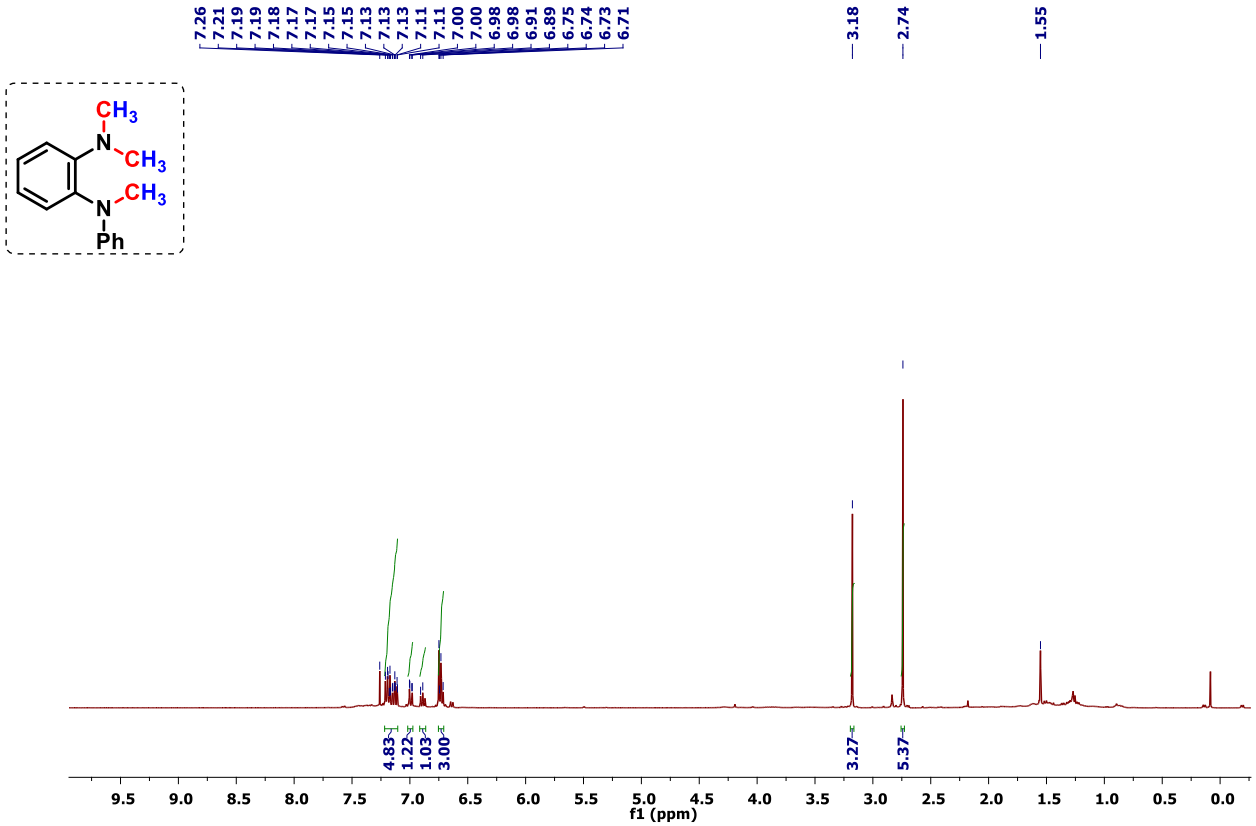


Figure S85. ^{1}H NMR spectrum of **5q** in $CDCl_3$.

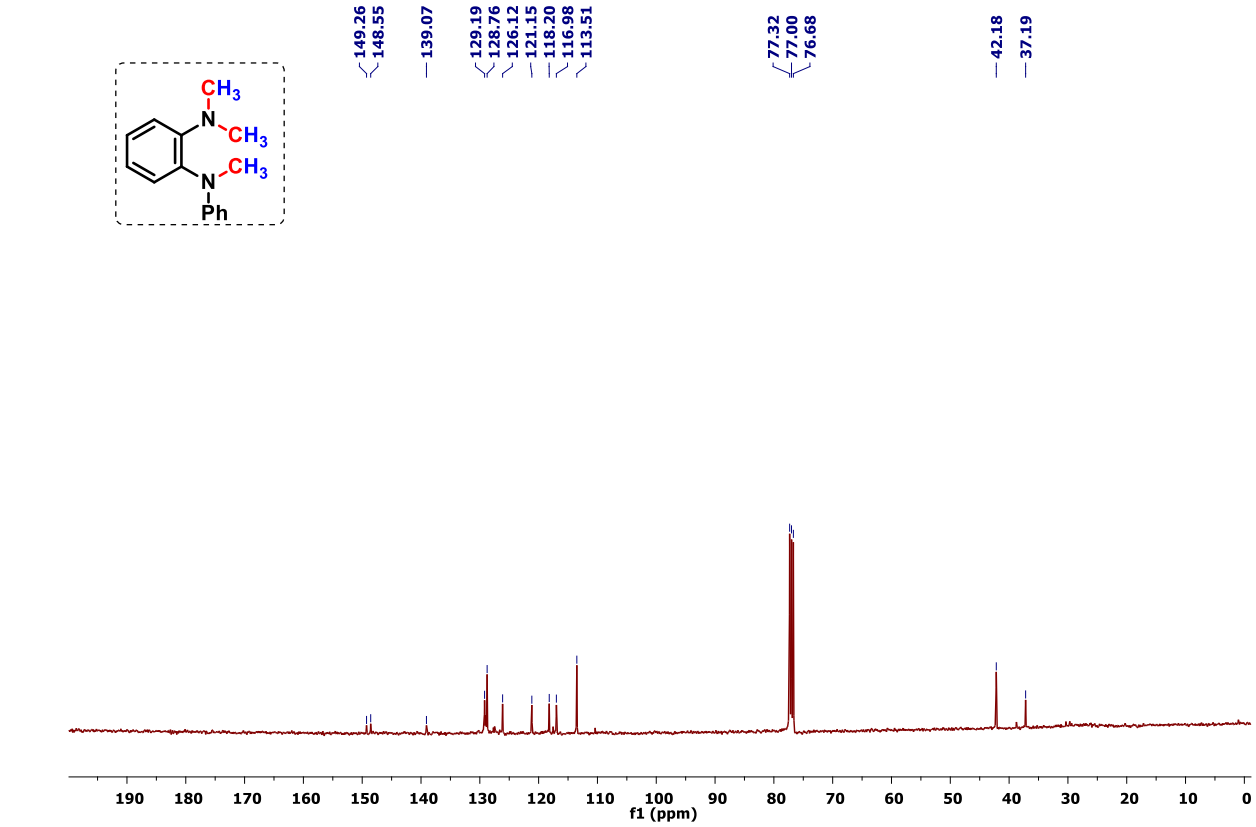


Figure S86. $^{13}C\{^{1}H\}$ NMR spectrum of **5q** in $CDCl_3$.

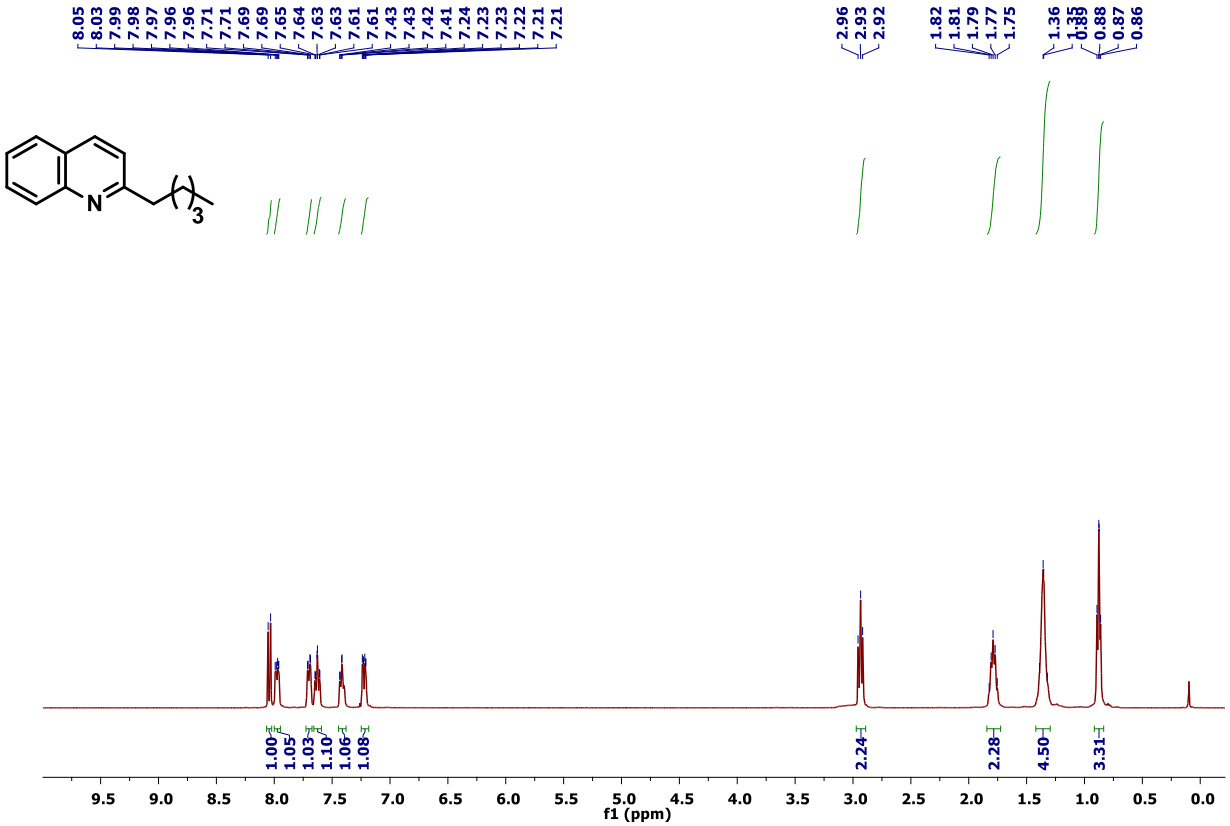


Figure S87. ^{1}H NMR spectrum of **6'** in $CDCl_3$.

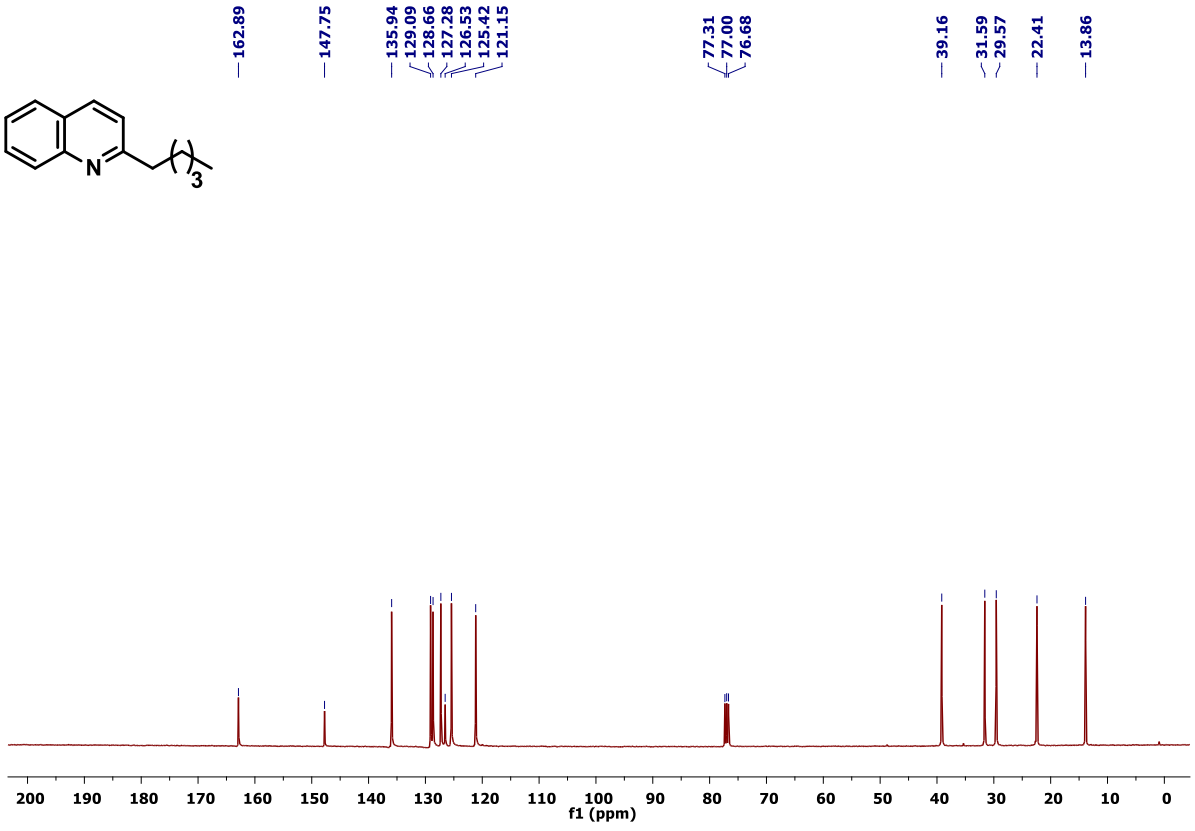


Figure S88. $^{13}C\{^{1}H\}$ NMR spectrum of **6'** in $CDCl_3$.

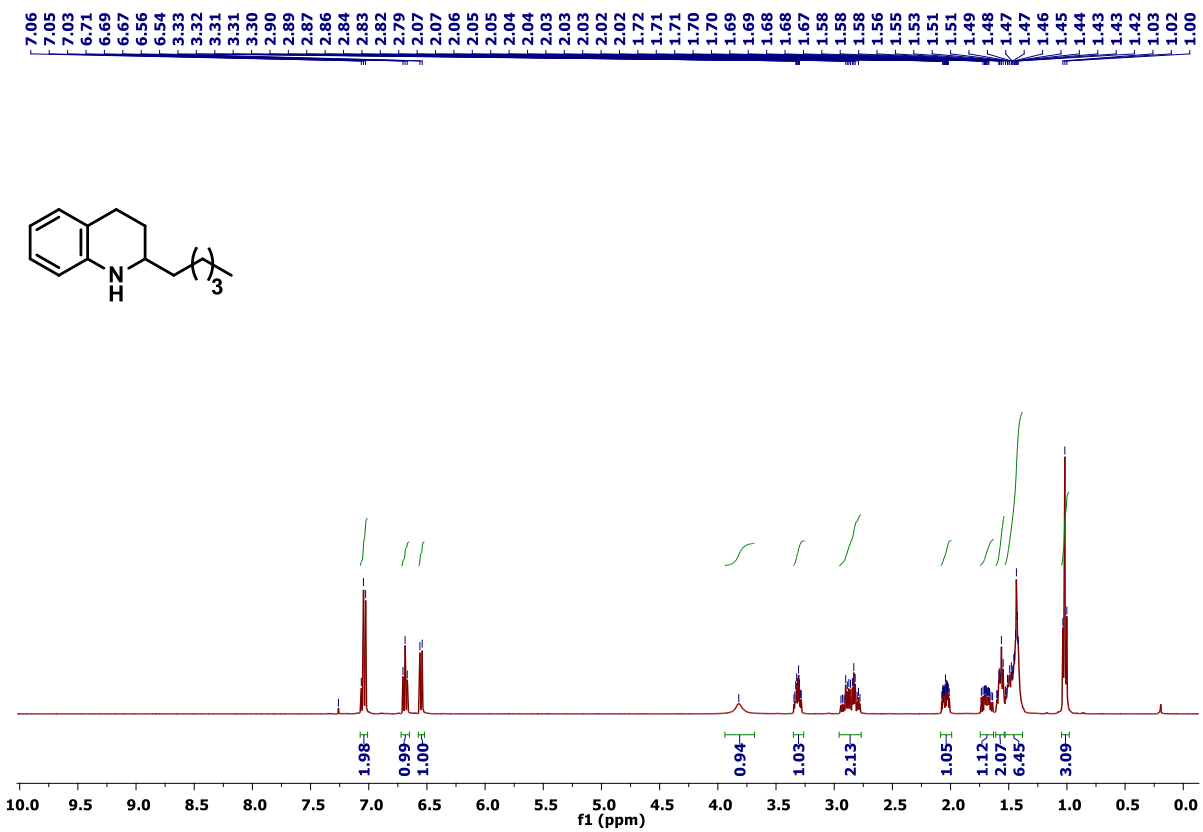


Figure S89. ^{1}H NMR spectrum of **6** in $CDCl_3$.

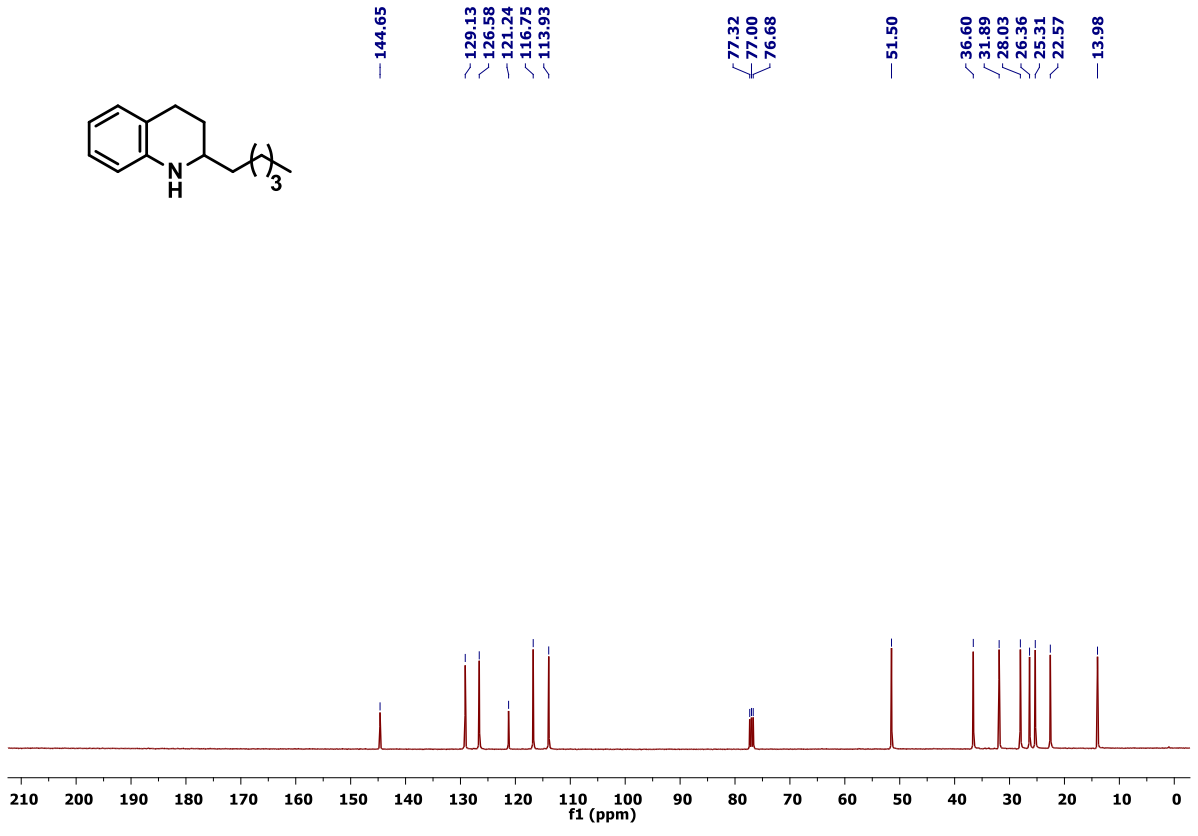


Figure S90. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$.

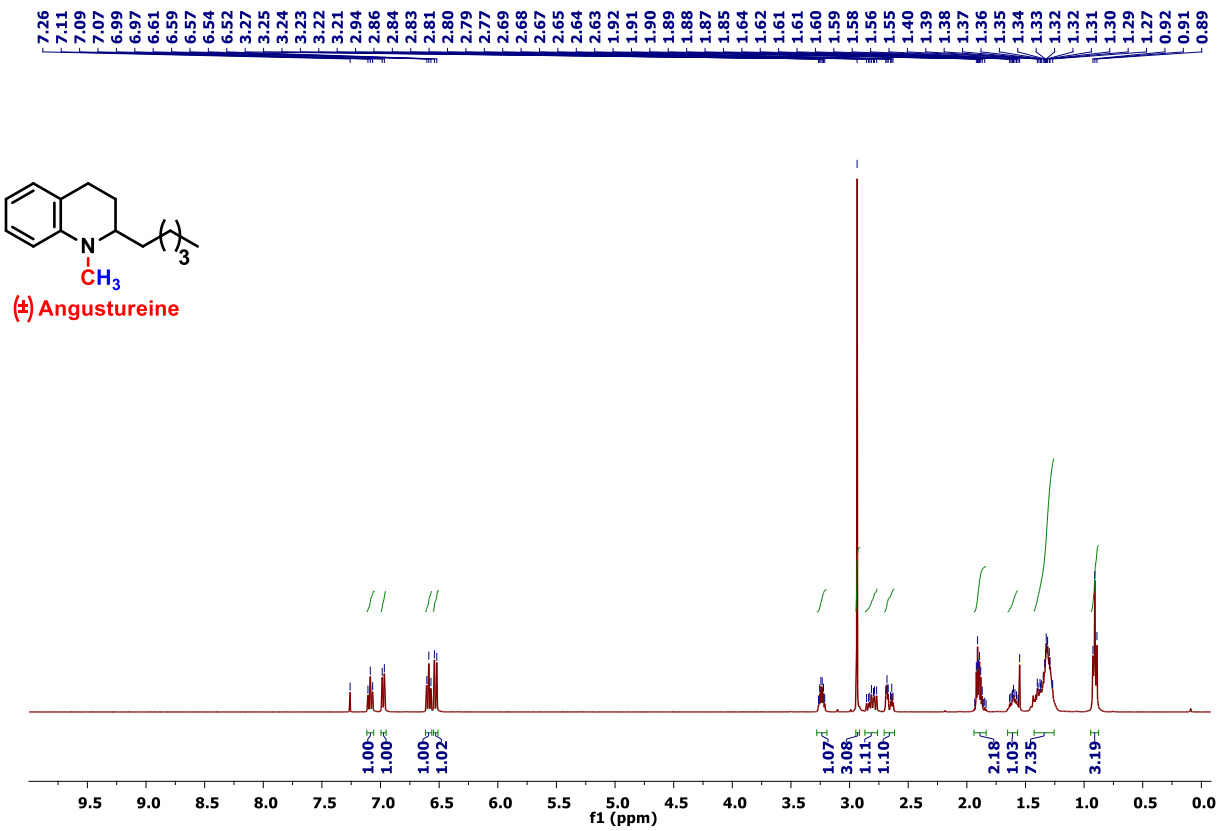


Figure S91. ^{1}H NMR spectrum of **7** in $CDCl_3$.

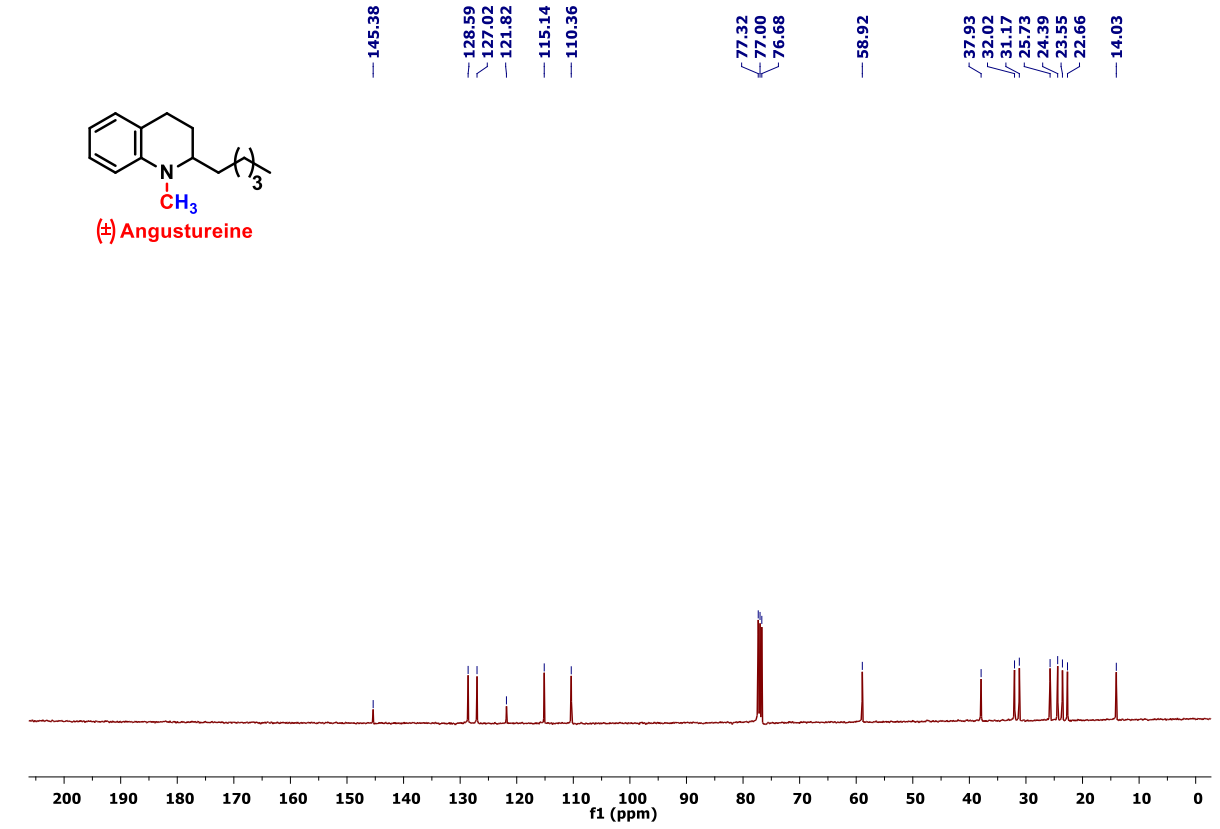


Figure S92. $^{13}C\{^{1}H\}$ NMR spectrum of **7** in $CDCl_3$.

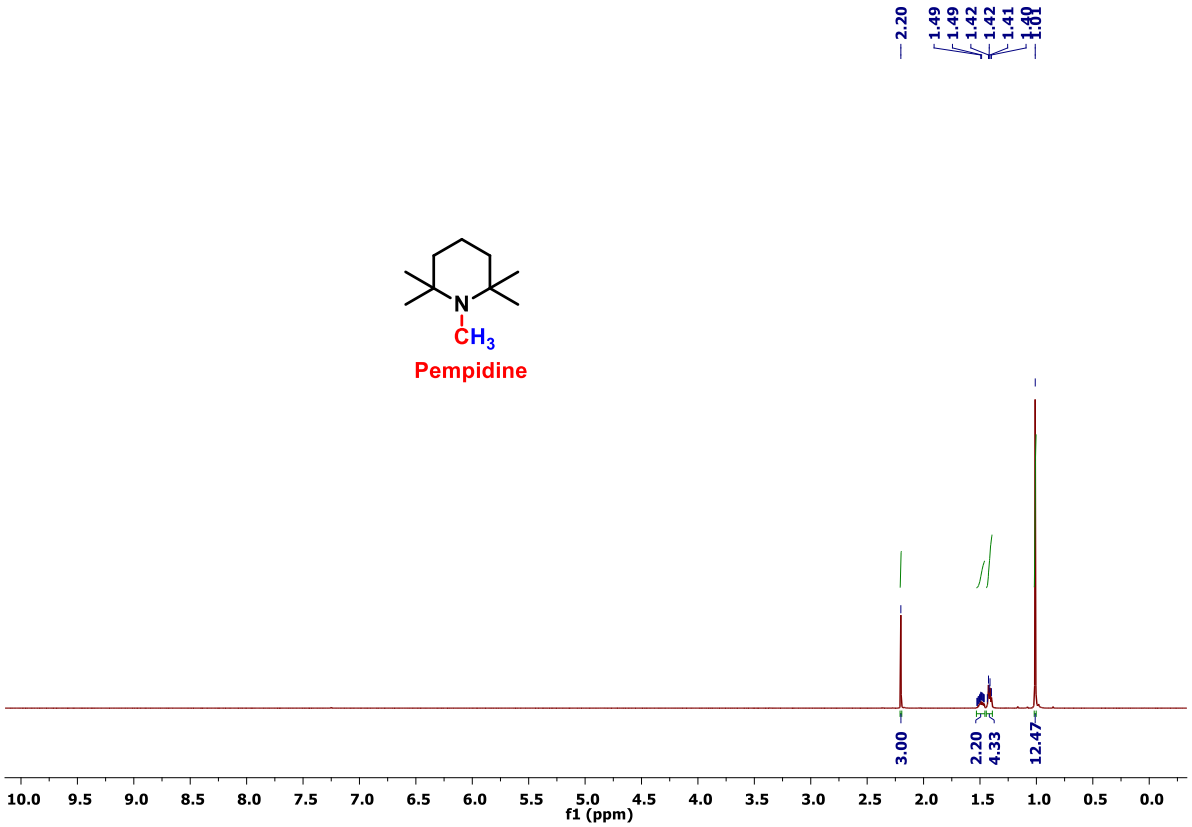


Figure S93. ^{1}H NMR spectrum of **9** in $CDCl_3$.

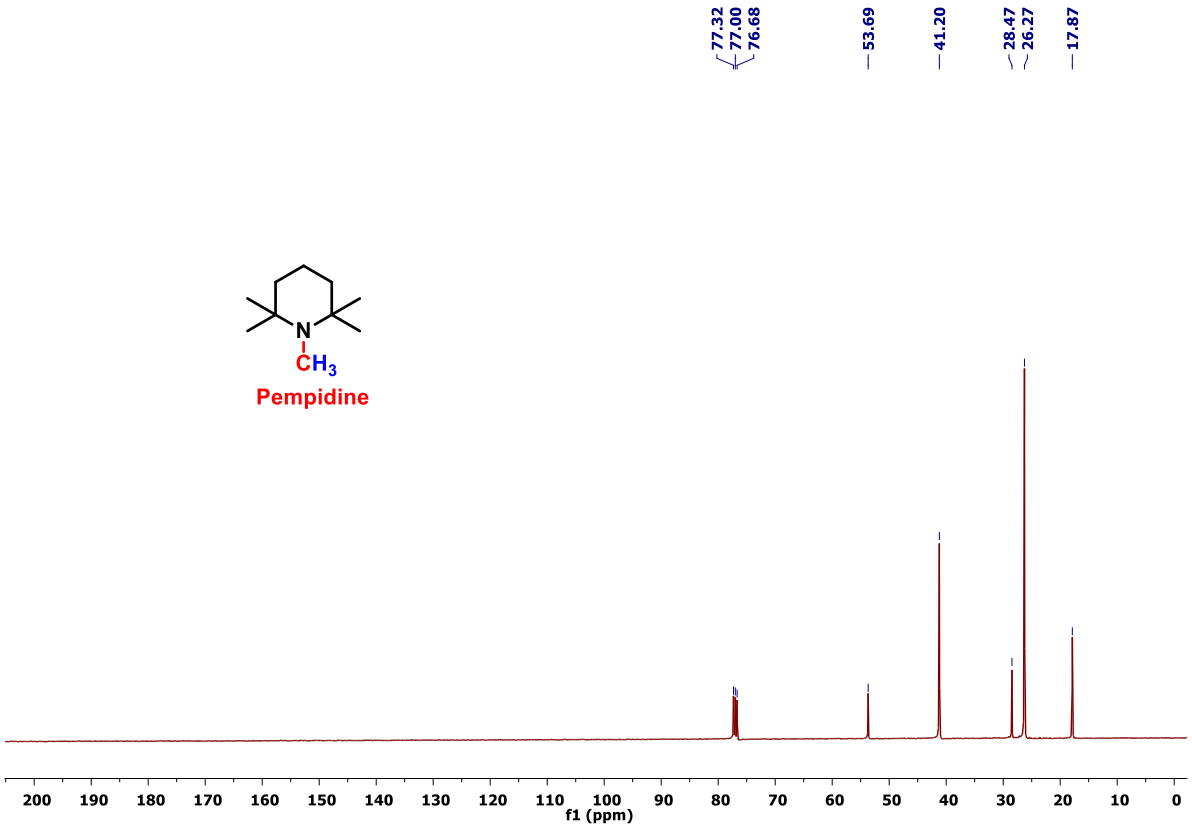


Figure S94. $^{13}C\{^{1}H\}$ NMR spectrum of **9** in $CDCl_3$.

VI) Computational Study

Computational details:

Theoretical calculations were performed with the Gaussian16 program suite[S23]. All theoretical calculations were carried out using the density functional theory (DFT) method with Becke's three-parameter hybrid exchange functionals and the Lee-Yang-Parr correlation functional (B3LYP) employing the 6-31G(d) basis set[S24-S25] for all atoms. The single point energy calculation of each optimized geometries were carried out by m062x method[S26] with 6-31+g(d) basis set considering SMD solvent model[S27] for THF.

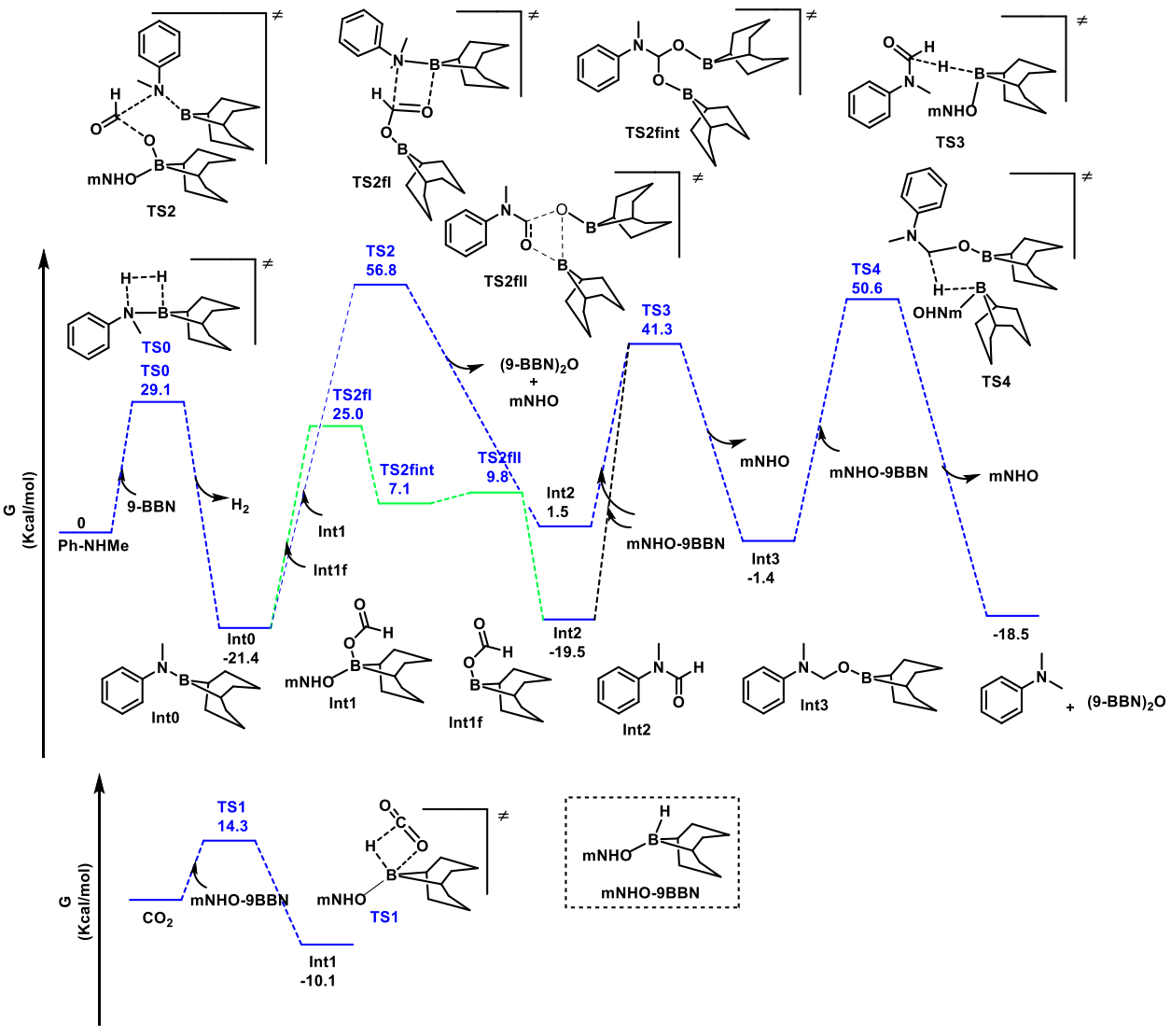


Figure S95: Computed Gibbs free energy profile for catalytic N-methylation of amines using *mNHO* as a catalyst. (f= catalyst free)

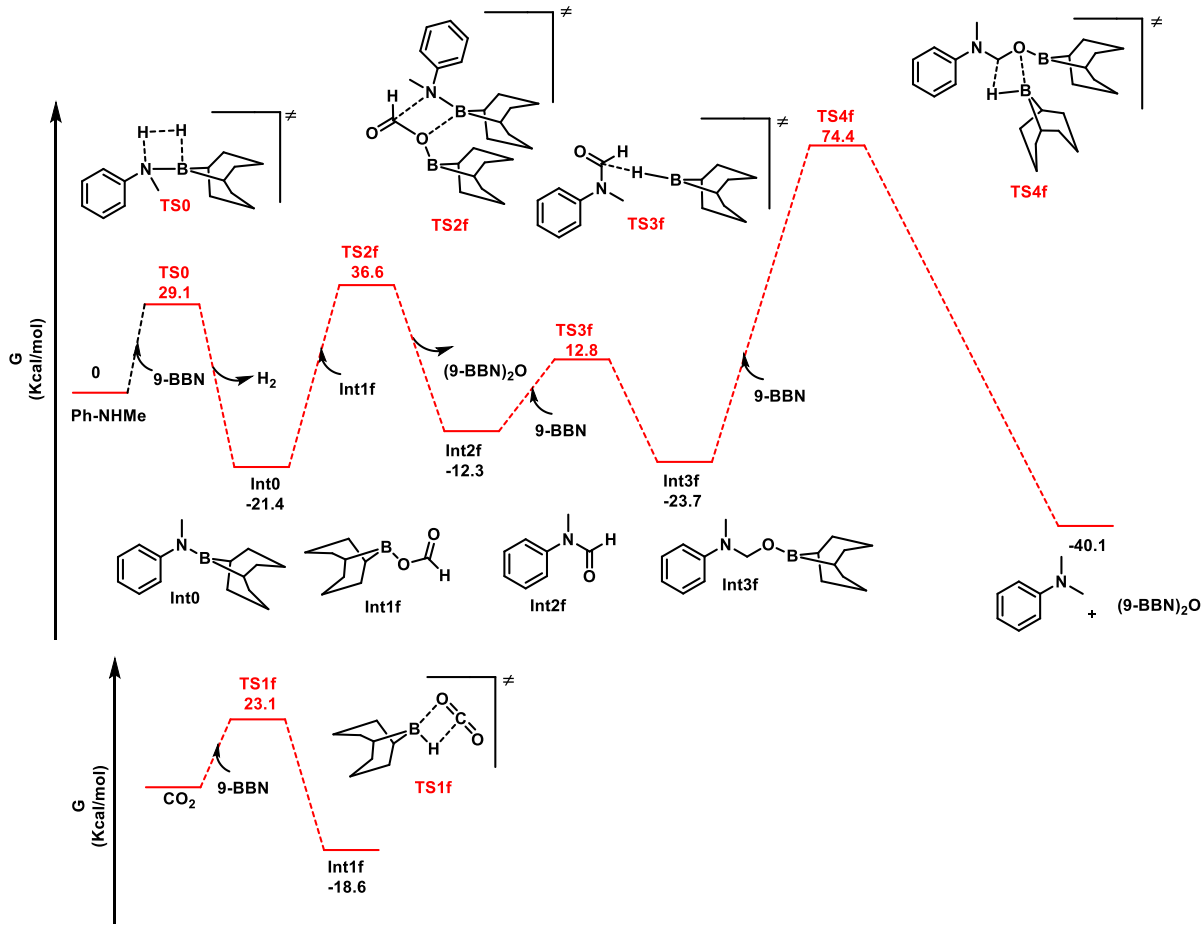


Figure S96: Computed Gibbs free energy profile for uncatalysed pathway for N-methylation of amines.

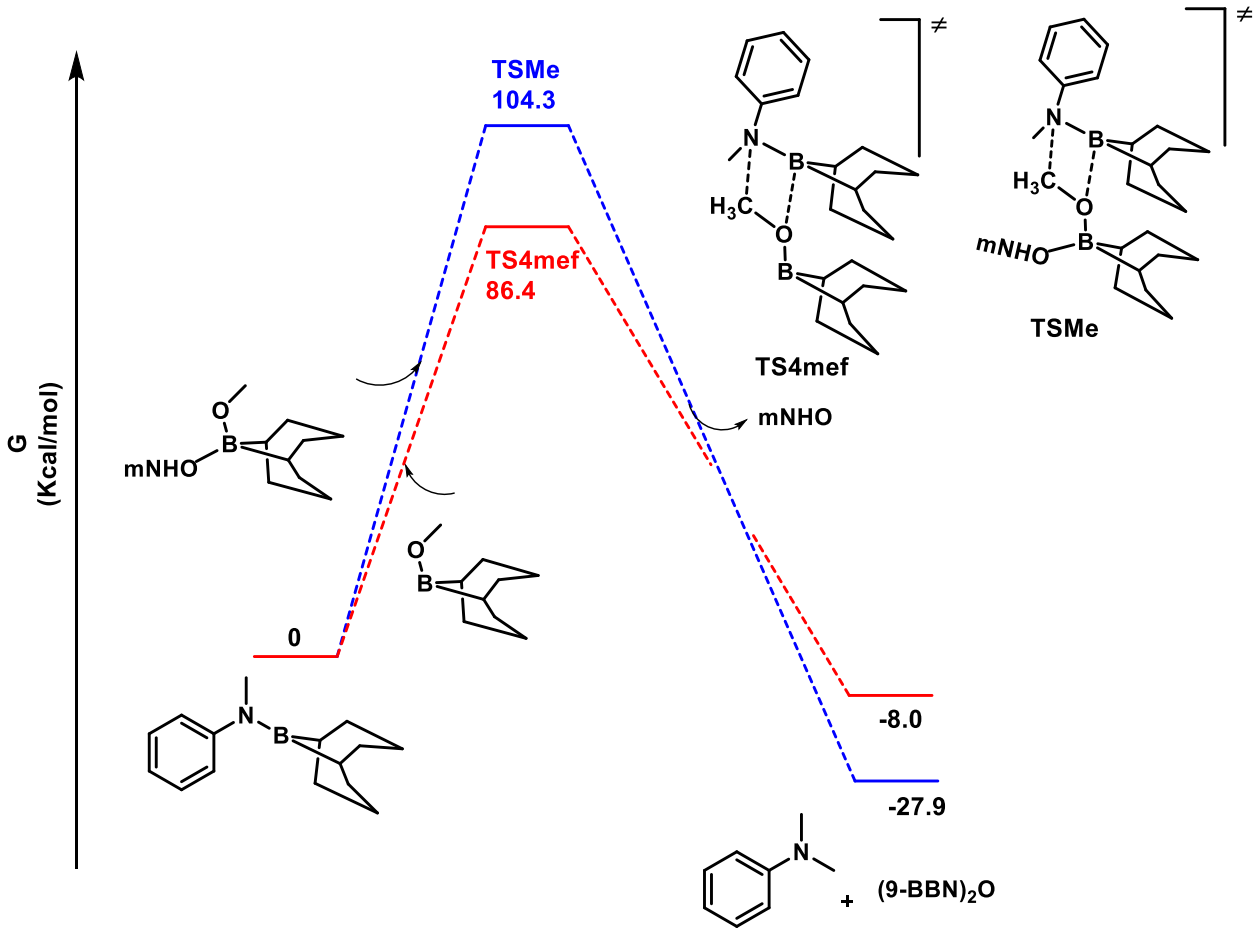


Figure S97: Computed Gibbs free energy profile for catalysed and uncatalysed pathway for N-methylation of amines through methyl transfer.

Table S3 Energies, enthalpies, and free energies (in Hartree) of the structures calculated with M06-2X/6-311+G(d)//B3LYP/6-31G(d).

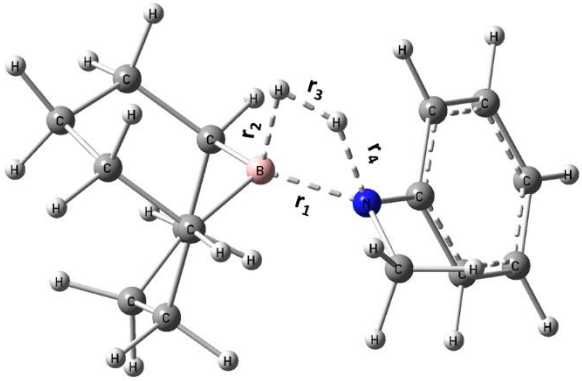
Structure	**ZPE**	**ΔE**	**ΔH**	**ΔG**	**E**	**H**	**G**	**IR Freq**	**Intensity**
mNHO	0.76181	0.80284	0.80378	0.68880	-1660.6344	-1660.6334	-1660.7484		
9-BBN	0.2193	0.2269	0.2279	0.18760	-338.5012	-338.5003	-338.5406		
CO_2	0.01159	0.01424	0.01518	-0.00912	-188.5667	-188.5657	-188.5900		
9BBN-formate (Int1f)	0.23631	0.24743	0.24837	0.19903	-527.1004	-527.0995	-527.1488		
9BBN-OMe	0.25486	0.26576	0.26670	0.21792	-453.05605	-453.05510	-453.10388		
N-MeAniline	0.14588	0.15308	0.15403	0.11459	-326.7565	-326.7555	-326.7950		
AniFormBBN (Int3f)	0.38216	0.39985	0.40080	0.33431	-778.6328	-778.6319	-778.6984		
N-methylaniline-BBN (Int0)	0.34826	0.36366	0.36460	0.30441	-664.1342	-664.1332	-664.1934		
N-methyl N-formyl aniline (Int2f)	0.15606	0.16494	0.16588	0.12179	-440.0856	-440.0846	-440.1287		
BOB dimer	0.42863	0.44634	0.44729	0.38105	-751.1705	-751.1695	-751.2358		
N,N- dimethyl aniline	0.17427	0.18290	0.18384	0.14078	-366.0322	-366.0313	-366.0744		
TS0	0.36408	0.37936	0.38031	0.32189	-665.2206	-665.2196	-665.2780	-1442.73	1841.6838
TS1f	0.23253	0.24300	0.24395	0.19669	-527.0404	-527.0395	-527.0867	-478.60	354.3011
TS2f(formyl)	0.58795	0.61366	0.61460	0.53381	-1191.1791	-1191.1782	-1191.2590	-236.14	43.3361
TS2fI	0.58781	0.61364	0.61458	0.53134	-1191.1973	-1191.1963	-1191.2796	-70.29	8.0403
TS2fII	0.58707	0.61331	0.61425	0.53072	-1191.2171	-1191.2162	-1191.2997	-149.64	121.6595
TS2fInt	0.58856	0.61535	0.61629	0.52905	-1191.2330	-1191.2321	-1191.3193		
TS3f	0.37759	0.39451	0.39545	0.33255	-778.57655	-778.57561	-778.63851	-577.83	1247.0993
TS4f	0.59606	0.62332	0.62426	0.53445	-1117.0279	-1117.0269	-1117.1167	-482.00	42.7812
TS4Mef	0.60416	0.62987	0.63081	0.55091	-1117.0806	-1117.0797	-1117.1596	-493.68	433.1766
mNHO	0.76181	0.80284	0.80378	0.68880	-1660.6344	-1660.6334	-1660.7484		
mNHO-9BBN	0.98602	1.03526	1.03621	0.90374	-1999.1597	-1999.1587	-1999.2912		
mNHO-BBN formate(Int1)	1.00235	1.0549	1.05585	0.91662	-2187.7572	-2187.7563	-2187.8955		
mNHO-BBNOMe	1.01953	1.07165	1.07260	0.93517	-2113.6842	-2113.6833	-2113.8207		
TS1	0.99969	1.05231	1.05326	0.91320	-2187.6979	-2187.6970	-2187.8370	-47.79	6.1878
TS2	1.35472	1.42132	1.42226	1.25685	-2851.7840	-2851.7830	-2851.9484	-250.17	41.6267
TS3	1.14394	1.20255	1.20350	1.05043	-2439.1884	-2439.1875	-2439.3405	-130.12	97.7184

TS4	1.36412	1.43355	1.43449	1.25437	-2777.7260	-2777.7251	-2777.9052	-349.31	1806.1306
TS4Me	1.37003	1.43692	1.43786	1.27100	-2777.6820	-2777.6811	-2777.8479	-571.37	508.0835
H_2	0.01014	0.01250	0.01345	-0.00134	-1.1629	-1.16203	-1.17682		

Table S4 Energies, enthalpies, and free energies (in Hartree) of the structures calculated with M06-2X/6-311+G(d)-SMD(THF)//B3LYP/6-31G(d).

Structure	**ZPE**	**ΔE**	**ΔH**	**ΔG**	**E**	**H**	**G**	**IR Freq**	**Intensity**
9-BBN	0.21946	0.22711	0.22806	0.18754	-338.3438	-338.3429	-338.3834		
9BBN-formate (Int1f)	0.23659	0.24769	0.24864	0.19960	-526.8915	-526.8906	-526.9396		
BBN-OMe	0.25540	0.26614	0.26709	0.21936	-452.8597	-452.8588	-452.9065		
N-Me Aniline	0.14651	0.15370	0.15465	0.11529	-326.6251	-326.6241	-326.6635		
N-methyl N-formyl aniline(Int2f)	0.15681	0.16567	0.16662	0.12258	-439.9207	-439.9197	-439.9637		
N-methyl aniline-9BBN(Int0)	0.34895	0.36434	0.36528	0.30599	-663.8583	-663.8573	-663.9166		
N-methyl aniline-OBBN (Int3f)	0.38307	0.40056	0.40151	0.33472	-778.3191	-778.3182	-778.3850		
N,N-dimethylaniline	0.1748	0.1826	0.1835	0.1425	-365.8812	-365.8802	-365.9213		
CO_2	0.01165	0.01426	0.01521	-0.00905	-188.5032	-188.5022	-188.5265		
H_2	0.0101	0.0124	0.0134	-0.0013	-1.1505	-1.1496	-1.1644		
TS0	0.36458	0.37988	0.38082	0.32273	-664.94353	-664.94258	-665.0006	-1612.06	4045.8267
TS1f	0.23256	0.24301	0.24395	0.19694	-526.8270	-526.8261	-526.8731	-575.54	841.9556
TS2f	0.58894	0.61461	0.61556	0.53601	-1190.7193	-1190.7184	-1190.7979	-271.76	133.1852
TS2fI	0.58887	0.61465	0.61560	0.53388	-1190.7357	-1190.7347	-1190.8165	133.1852	10.3273
TS2fII	0.58762	0.61396	0.61490	0.53210	-1190.7475	-1190.7465	-1190.8293	-170.48	245.8732
TS2fInt	0.58960	0.61631	0.61725	0.53127	-1190.7599	-1190.7589	-1190.8449		
TS3f	0.37872	0.39552	0.39646	0.33441	-778.2657	-778.2647	-778.3268	-648.30	2430.6904
TS4f	0.5971	0.62445	0.6253	0.5378	-	-	-	-455.71	134.7

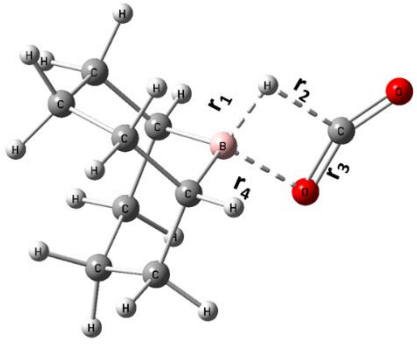
	6		9	5	1116.56335	1116.56240	1116.64994		440
mNHO-9BBN	0.98800	1.03721	1.03816	0.90516	-1998.3899	-1998.3890	-1998.5220		
mNHO-9BBNformate (Int1)	1.00321	1.05436	1.05530	0.92048	-2186.9307	-2186.9298	-2187.0646		
mNHO-BBNOMe	1.02155	1.07360	1.07454	0.93714	-2112.8778	-2112.8769	-2113.0143		
TS1	1.00110	1.05221	1.05315	0.91729	-2186.8908	-2186.8899	-2187.0258	-62.18 -52.57	3.0635 14.7477
TS2	1.35719	1.42311	1.42405	1.26139	-2850.7290	-2850.7281	-2850.8907	-282.58 -43.38	133.3135 2.2251
TS3	1.14560	1.20361	1.20455	1.05299	-2438.2692	-2438.2683	-2438.4199	-153.46 -26.93	252.1692 7.3460
TS4	1.36570	1.43538	1.43632	1.25642	-2776.6474	-2776.6465	-2776.8264	-463.24	4557.6735
TS4Me	1.37236	1.43853	1.43947	1.27613	-2776.6301	-2776.6292	-2776.7925	-668.82 -4.57	1073.3551 4.2711



r_1 = 1.626 Å
r_2 = 1.405 Å
r_3 = 0.987 Å
r_4 = 1.386 Å

$\Delta G_1^{\neq}$ = 29.10 Kcal/mol

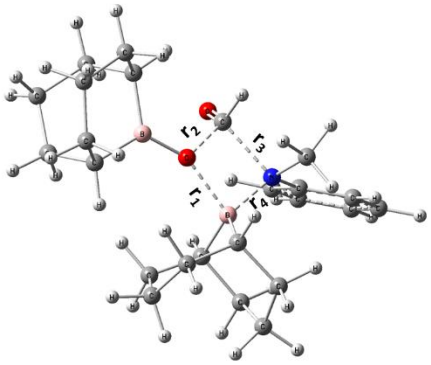
TS0



r_1 = 1.294 Å
r_2 = 1.577 Å
r_3 = 1.231 Å
r_4 = 1.708 Å

$\Delta G_2^{\neq}$ = 23.12 Kcal/mol

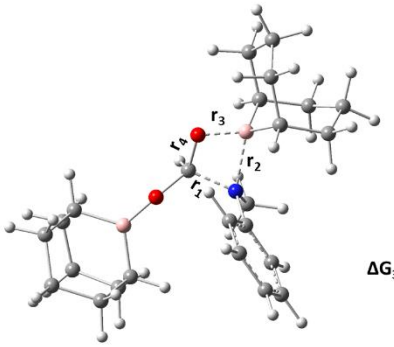
TS1f



r_1 = 1.818 Å
r_2 = 1.570 Å
r_3 = 1.912 Å
r_4 = 1.585 Å

$\Delta G_3^{\neq}$ = 36.63 Kcal/mol

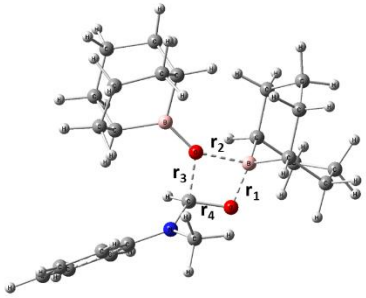
TS2f



r_1 = 1.556 Å
r_2 = 1.906 Å
r_3 = 1.491 Å
r_4 = 1.361 Å

$\Delta G_{3I'}^{\neq}$ = 25.00 Kcal/mol

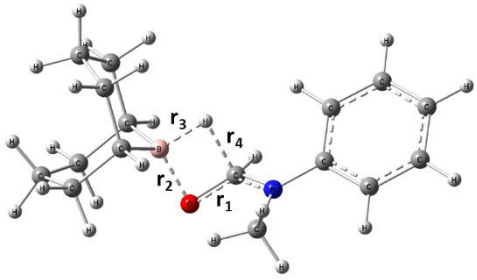
TS2fI



r_1 = 1.481 Å
r_2 = 1.824 Å
r_3 = 1.626 Å
r_4 = 1.348 Å

$\Delta G_{3II'}^{\neq}$ = 9.77 Kcal/mol

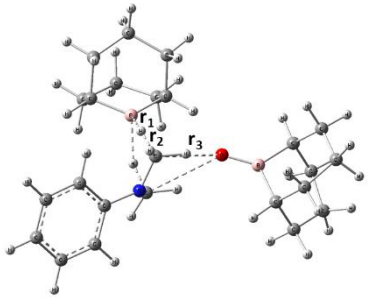
TS2fII



r_1 = 1.321 Å
r_2 = 1.545 Å
r_3 = 1.332 Å
r_4 = 1.551 Å

$\Delta G_4^{\neq}$ = 12.83 Kcal/mol

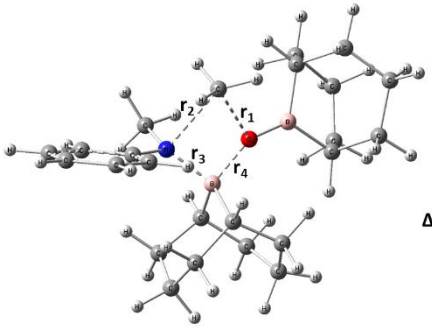
TS3f



r_1 = 1.19 Å
r_2 = 1.68 Å
r_3 = 2.92 Å

$\Delta G_4^{\neq}$ = 74.40 Kcal/mol

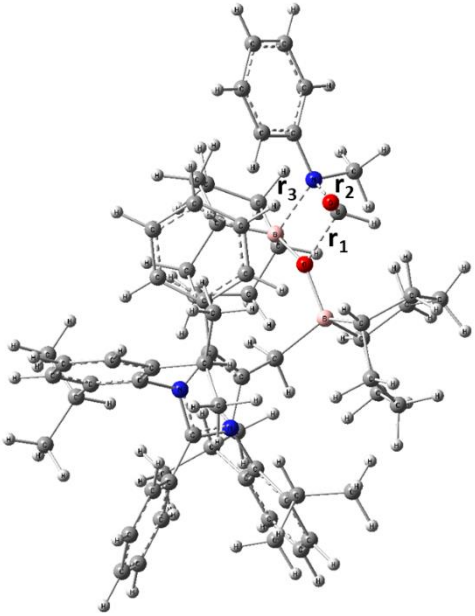
TS4f



r_1 = 2.061 Å
r_2 = 2.275 Å
r_3 = 1.605 Å
r_4 = 1.596 Å

$\Delta G_{mef}^{\neq}$ = 86.40 Kcal/mol

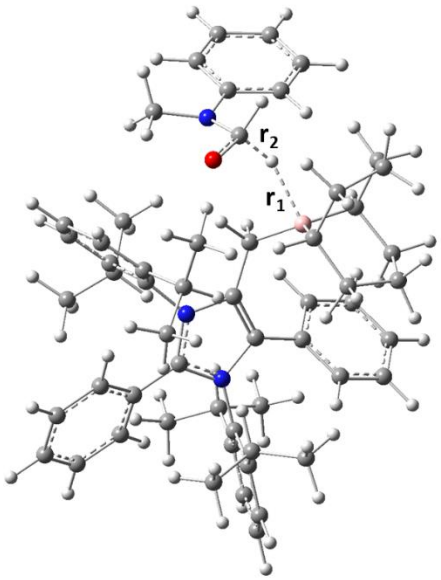
TSmef



r_1 = 1.808 Å
r_2 = 1.597 Å
r_3 = 1.863 Å

$\Delta G_{3'}^{\neq}$ = 56.80 Kcal/mol

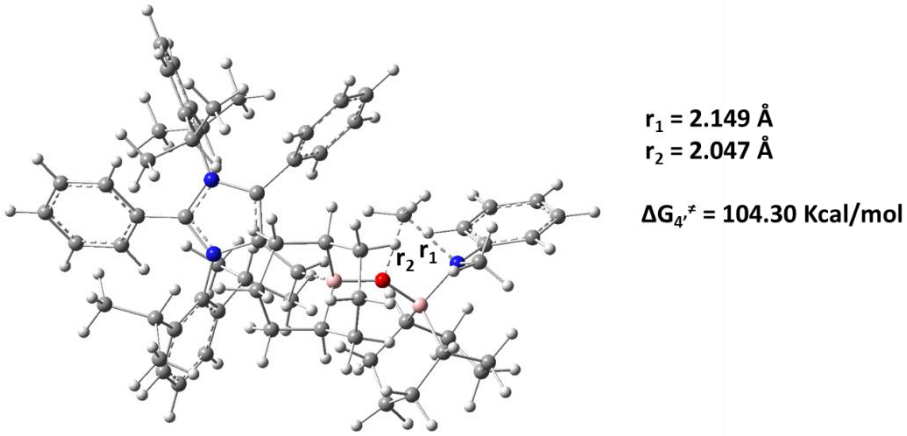
TS2



r_1 = 1.836 Å
r_2 = 1.192 Å

$\Delta G_{4'}^{\neq}$ = 41.80 Kcal/mol

TS3



TS4me

Figure S98 Optimized structures of the transition states involved in the potential energy surface of catalytic N-methylation of amines by the mNHO catalyst.

Co-ordinates:

9BBN

0 1

C	-0.00004200	-1.30476700	0.70759800
C	-1.31216000	-1.29521400	-0.13643900
C	0.00006100	1.30476700	0.70759800
C	-1.31201000	1.29534500	-0.13650600
C	1.57594700	-0.00005900	-0.93353200
C	1.31212800	1.29520400	-0.13654600
C	1.31197700	-1.29533600	-0.13661300
C	-1.57606100	0.00005900	-0.93339000
H	-0.00003400	-2.22923500	1.29980900
H	-2.15374900	-1.46018300	0.55275100
H	-1.31753600	-2.15474500	-0.82293900
H	0.00013400	2.22923600	1.29980900
H	-1.31723500	2.15483600	-0.82305800
H	-2.15360700	1.46047100	0.55263500
H	2.62066300	-0.00011100	-1.27273500
H	0.97498900	0.00000500	-1.84732300
H	2.15377600	1.46015400	0.55257700
H	1.31746200	2.15474400	-0.82303600
H	1.31716200	-2.15483500	-0.82315500
H	2.15363400	-1.46044200	0.55246200
H	-2.62081100	0.00011100	-1.27249000
H	-0.97519700	-0.00000500	-1.84724300
B	0.00008500	0.00000000	1.58470100
H	0.00087900	-0.00000100	2.78541000

9BBNformate

0 1

C	0.18325100	0.15847900	1.09640200
C	-0.22568800	1.64258200	0.83050600
C	-0.67765900	-0.48815600	-1.29681300
C	-1.07391300	1.00402600	-1.54265200
C	-2.15897800	-0.99188300	0.79979900
C	-1.79619000	-1.35774700	-0.65584900
C	-0.94159400	-0.72637400	1.71150200
C	-1.29484300	1.84748200	-0.26661100
H	1.02270500	0.17555500	1.79960400

H	0.68750100	2.18430700	0.54833400
H	-0.57369800	2.10171800	1.76707200
H	-0.41824800	-0.92721200	-2.26914900
H	-1.97591500	1.04801100	-2.17018900
H	-0.27275800	1.46780300	-2.13674400
H	-2.75220400	-1.80875900	1.23215100
H	-2.81981600	-0.12034400	0.80634900
H	-1.45887700	-2.40448300	-0.68202700
H	-2.70326400	-1.32036400	-1.27663500
H	-1.28754800	-0.28013500	2.65513200
H	-0.49216400	-1.69240700	1.98663000
H	-1.31235300	2.90923500	-0.54658100
H	-2.28764300	1.63995700	0.14278100
B	0.54254600	-0.42601900	-0.31446600
O	1.79782700	-0.85523700	-0.75373400
C	2.98965700	-0.52018800	-0.20089000
H	3.74146200	-1.28688600	-0.44274600
O	3.22290100	0.48458400	0.41698200

9BBNOMe

0 1

C	0.35816600	-0.00007300	1.14585300
C	-0.45866000	1.31085900	1.35194500
C	-0.33438600	0.00002900	-1.38413400
C	-1.14326900	1.30967500	-1.15531900
C	-1.56582300	-1.57548200	0.30683200
C	-1.14343000	-1.30953100	-1.15540000
C	-0.45875100	-1.31095400	1.35184500
C	-1.56567300	1.57557600	0.30692200
H	1.16484800	-0.00012400	1.89230100
H	0.25064600	2.15208900	1.33006800
H	-0.90308700	1.32190100	2.35843400
H	0.01738800	0.00004200	-2.42452500
H	-2.03813600	1.32078200	-1.79558400
H	-0.51999000	2.14896800	-1.49814200
H	-1.89214200	-2.62046600	0.39747800
H	-2.44822600	-0.97615500	0.54941400
H	-0.52026100	-2.14887100	-1.49830500
H	-2.03831500	-1.32047400	-1.79564300
H	-0.90315400	-1.32206600	2.35834500
H	0.25047900	-2.15224600	1.32986200
H	-1.89188400	2.62058900	0.39761700

H	-2.44814800	0.97633000	0.54944100
B	0.86069400	-0.00003800	-0.35449800
O	2.14669600	-0.00002900	-0.79921000
C	3.26631700	-0.00005000	0.08277900
H	4.16909900	0.00029900	-0.53403300
H	3.27327800	0.89093500	0.72100700
H	3.27362700	-0.89139900	0.72049900

N-methylanilineformateBBN

0 1

C	2.38585500	0.85621500	0.76647500
C	3.48429100	0.10717900	1.58102900
C	2.20131200	-1.21562100	-0.82815500
C	3.29842800	-1.94530900	-0.00028300
C	3.55191300	0.89401100	-1.58592300
C	2.74214800	-0.35300500	-2.00394200
C	2.92837900	1.70073200	-0.42553000
C	4.22044300	-1.02165200	0.82578300
H	1.90293900	1.55924500	1.46010400
H	3.00193300	-0.32379400	2.47127400
H	4.22341200	0.82787300	1.96139600
H	1.53738500	-1.98091400	-1.25171600
H	3.91568700	-2.57508700	-0.65833800
H	2.79037700	-2.63861200	0.68647700
H	3.66006100	1.55614200	-2.45568400
H	4.57125100	0.59956900	-1.31961800
H	1.87771300	-0.02604100	-2.60068200
H	3.35460400	-0.96999500	-2.67841200
H	3.66308000	2.43375200	-0.06039100
H	2.08960100	2.29234200	-0.82354400
H	4.77237100	-1.62990000	1.55514800
H	4.98516900	-0.58772600	0.17507100
B	1.43051100	-0.25466700	0.16006900
O	0.10638800	-0.46205100	0.40044300
N	-1.79328600	0.98057700	0.59536500
C	-2.94321100	0.26865500	0.21979800
C	-4.07542900	0.94888300	-0.27036700
C	-3.01009200	-1.13546600	0.33057800
C	-5.23460100	0.25145200	-0.60653400
H	-4.06088800	2.02796500	-0.37595300
C	-4.17934900	-1.81655600	0.00103400
H	-2.13372900	-1.69961900	0.62728700

C	-5.30361800	-1.13437300	-0.46711300
H	-6.09340600	0.80576400	-0.97712300
H	-4.19957700	-2.89959900	0.09424100
H	-6.20905100	-1.67342800	-0.73003700
C	-1.56803500	2.31295000	0.05376900
H	-2.25065600	3.05497900	0.49007400
H	-0.54679400	2.62492600	0.28401200
H	-1.69342500	2.33384100	-1.03681800
C	-0.72488000	0.32866500	1.27457500
H	-1.13244000	-0.36488100	2.01447700
H	-0.11760500	1.07833600	1.78614200

N-methylanilineBBN

0 1

C	-0.78859500	-1.09376100	0.17033800
C	-1.52077600	-1.29972600	1.52714100
C	-2.08718100	1.14780100	-0.17453600
C	-2.81151500	0.92383400	1.18483100
C	-2.85681500	-1.01870300	-1.43462400
C	-2.81159300	0.52421400	-1.40303000
C	-1.52440100	-1.70135000	-1.05768000
C	-2.85404300	-0.53719000	1.68211900
H	0.17995300	-1.60356000	0.24856600
H	-0.83634300	-0.97455000	2.32518400
H	-1.69729900	-2.37167500	1.70351400
H	-2.06768600	2.23344600	-0.34246500
H	-3.83842600	1.31654600	1.13440300
H	-2.29430700	1.53501300	1.93987000
H	-3.15166000	-1.34387300	-2.44189400
H	-3.65190000	-1.37518800	-0.77286400
H	-2.29332000	0.87744100	-2.30736000
H	-3.83785000	0.91536300	-1.47444500
H	-1.70336500	-2.77571200	-0.89928800
H	-0.84169700	-1.63621700	-1.91841300
H	-3.14677400	-0.54242400	2.74114100
H	-3.64940500	-1.07853100	1.16100300
B	-0.65282200	0.47032800	-0.07111700
N	0.58606800	1.14133100	-0.17207900
C	1.84329500	0.44709200	-0.07071000

C	2.50041600	0.35476400	1.16126800
C	2.43673100	-0.10996400	-1.20872600
C	3.73047900	-0.29770100	1.25567000
H	2.03460100	0.78847900	2.04219500
C	3.66620400	-0.76381600	-1.11277100
H	1.92267600	-0.03322200	-2.16303500
C	4.31657100	-0.85821600	0.11900500
H	4.22867500	-0.37151800	2.21878300
H	4.11455400	-1.20103500	-2.00105100
H	5.27328000	-1.36797900	0.19335100
C	0.75959200	2.58108200	-0.38745200
H	1.30810700	2.77330900	-1.31896800
H	-0.21194100	3.07202900	-0.44661300
H	1.33154600	3.03273600	0.43346900

BOB dimer

0 1

C	2.23960400	0.80423700	-1.05056500
C	3.08217800	1.83109200	-0.23927600
C	2.20658500	-0.78933900	1.03526800
C	3.04858700	0.25366800	1.82797700
C	3.85407200	-1.25994700	-0.94824900
C	3.04614100	-1.83158900	0.23873500
C	3.07786600	-0.25404900	-1.82819500
C	3.85731800	1.24685400	0.96318500
H	1.64351700	1.36384700	-1.78458100
H	2.39469000	2.60657500	0.13028000
H	3.78813400	2.35001800	-0.90466300
H	1.58823300	-1.33946600	1.75805200
H	3.73211800	-0.26065800	2.51976300
H	2.35553700	0.82572600	2.46297100
H	4.19050900	-2.09363200	-1.57930200
H	4.77009700	-0.79204100	-0.57625000
H	2.35206100	-2.59442000	-0.14431100
H	3.72984300	-2.36302800	0.91741400
H	3.78227700	0.24813300	-2.50791300
H	2.38674400	-0.81494100	-2.47487900
H	4.19489000	2.07507100	1.60079000
H	4.77308300	0.76433700	0.60955700
B	1.34599600	0.01261700	-0.01775300
O	-0.00005400	0.01801200	-0.03678500

C	-2.21894600	1.03848600	0.80179700
C	-3.10059000	1.82854700	-0.20897300
C	-2.22706800	-1.01743200	-0.83098000
C	-3.10615300	-0.20664700	-1.82720000
C	-3.80808300	-0.99564500	1.25973700
C	-3.02874400	-1.83680500	0.22377600
C	-3.01853700	0.19819300	1.84207900
C	-3.90375900	0.96180200	-1.20500700
H	-1.60975500	1.76554700	1.35639700
H	-2.43570800	2.49317700	-0.78047300
H	-3.79286000	2.49115900	0.33152300
H	-1.62229300	-1.72510300	-1.41477900
H	-3.80200300	-0.87941900	-2.35026100
H	-2.44062000	0.19786600	-2.60429000
H	-4.11652000	-1.65074400	2.08564000
H	-4.73977800	-0.63593600	0.81373000
H	-2.31358400	-2.47856600	0.75974300
H	-3.72546400	-2.52222900	-0.28137800
H	-3.70803400	0.84802700	2.40128400
H	-2.30040600	-0.18364100	2.58311700
H	-4.27320900	1.60633700	-2.01402700
H	-4.80080500	0.57315400	-0.71406800
B	-1.34661400	0.01782400	-0.02814200

CO_2

0 1

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16914800
O	0.00000000	0.00000000	-1.16914800

mNHO

0 1

C	0.90698600	-3.12854800	0.34640100
H	1.97303600	-3.30512800	0.30765100
H	0.26129400	-3.97037100	0.54529600
C	0.39961100	-1.86271200	0.25683500
C	-0.94080200	-1.33836200	0.29970700
C	0.44407400	0.43560800	-0.06085600
C	0.93903400	1.78669900	-0.32069100
C	2.17866900	2.21713600	0.20682400

C	0.22007400	2.71205600	-1.11287800
C	2.66254000	3.49903100	-0.03791400
H	2.76598100	1.54762600	0.81823700
C	0.70596700	3.99551600	-1.34338300
H	-0.72293700	2.42716400	-1.55625500
C	1.93114300	4.40260200	-0.81089300
H	3.61737800	3.79329800	0.38969800
H	0.12429700	4.67697700	-1.95858400
H	2.31014500	5.40314600	-0.99851100
C	-1.98099200	0.93956400	0.04668700
C	-2.22778100	1.76644900	1.16330500
C	-2.80959800	0.93973300	-1.09629200
C	-3.32852600	2.62989200	1.09544100
C	-3.89580600	1.82337900	-1.10289800
C	-4.15380200	2.66335600	-0.02383900
H	-3.54261000	3.28251600	1.93690500
H	-4.54955700	1.85177500	-1.96974100
H	-5.00248900	3.34156600	-0.05361700
C	-2.17765800	-2.09428600	0.45137400
C	-3.31511200	-1.62629600	1.15002900
C	-2.26101500	-3.39100500	-0.11123900
C	-4.46321900	-2.40560300	1.26881500
H	-3.30131100	-0.64749000	1.61144500
C	-3.40865400	-4.16746400	0.01849600
H	-1.42052000	-3.77094900	-0.68068700
C	-4.52222700	-3.68424100	0.70976200
H	-5.31519800	-2.01159700	1.81784700
H	-3.43570100	-5.15514000	-0.43579400
H	-5.41617300	-4.29280600	0.81475000
C	2.64035400	-0.81309100	-0.05099800
C	3.43172300	-0.94136700	1.11397100
C	3.20114900	-0.86311900	-1.34421400
C	4.81466800	-1.08227300	0.94929600
C	4.59095100	-1.00196300	-1.44932100
C	5.39252300	-1.10673900	-0.31720400
H	5.44762800	-1.17776500	1.82729500
H	5.04920200	-1.03852100	-2.43354600
H	6.46892800	-1.21638800	-0.42137800
N	1.21544500	-0.70115800	0.09157400
N	-0.84490500	0.04170700	0.08269300
C	2.83925900	-0.93467700	2.52316000
H	1.76050700	-0.77678000	2.43251200
C	3.04200800	-2.29215100	3.22577700
H	2.58386400	-2.27267100	4.22191200

H	2.57521500	-3.09720300	2.65215000
H	4.10682500	-2.52267300	3.35313400
C	3.40865600	0.20717800	3.38948100
H	4.48931200	0.10040800	3.53984600
H	3.22916600	1.19141600	2.94355200
H	2.93652700	0.19820300	4.37894900
C	2.34778200	-0.81729900	-2.60787700
H	1.32516000	-0.56178400	-2.31656200
C	2.81927900	0.26383500	-3.59764100
H	2.13712200	0.31155900	-4.45463300
H	2.84359300	1.25187900	-3.12593500
H	3.82074400	0.05127100	-3.98979100
C	2.29216400	-2.20820400	-3.27205600
H	1.89027200	-2.95147000	-2.57559100
H	1.64882700	-2.18154500	-4.16008200
H	3.28915300	-2.53721700	-3.58964600
C	-2.57196400	0.04263600	-2.31176800
H	-1.72537300	-0.61342400	-2.09204300
C	-3.78925400	-0.86123900	-2.59367100
H	-4.66355400	-0.27216700	-2.89605600
H	-3.55858400	-1.55198300	-3.41290900
H	-4.06235900	-1.45233300	-1.71607500
C	-2.21382500	0.86047000	-3.56987800
H	-1.30193600	1.45067200	-3.43149500
H	-2.04880800	0.18693500	-4.41889900
H	-3.02170100	1.54886000	-3.84511900
C	-1.37068400	1.75248700	2.42894300
H	-0.55953500	1.03290600	2.28629200
C	-2.17783200	1.28757500	3.65830500
H	-1.53283800	1.26897800	4.54455100
H	-3.01404700	1.96405400	3.87065700
H	-2.58440400	0.28081500	3.51924400
C	-0.72872900	3.12873100	2.69632400
H	-0.13912200	3.47201700	1.84180800
H	-1.48960400	3.88867500	2.91078200
H	-0.06640700	3.07108500	3.56803700

mNHO-9BBN

0 1

C	3.88471200	-1.71146700	0.28045700
C	2.19055000	0.23145700	-0.89263800
C	4.65780300	-1.95584300	-1.03826500
C	4.63063500	0.77907500	0.25847300
C	5.37849500	0.54042300	-1.07612800
C	5.88435100	-0.93384000	1.78127300
C	5.50175500	0.53999400	1.51527600
C	4.74123100	-1.94749000	1.55085200
C	5.76525600	-0.92752500	-1.36167800
H	3.08799600	-2.47075300	0.31558500
H	2.35876000	1.27287700	-1.18835100
H	2.40914600	-0.38390600	-1.77144500
H	3.93113400	-1.94880200	-1.86674600
H	5.10240600	-2.96596300	-1.05708600
H	4.36335300	1.85117700	0.26534900
H	6.29043200	1.15908000	-1.13929200
H	4.73049700	0.89287600	-1.89485300
H	6.24553500	-1.02899800	2.81679000
H	6.74253700	-1.20545700	1.15647500
H	4.93153500	0.90678800	2.38167400
H	6.42795000	1.14060800	1.48380900
H	5.17349400	-2.96354300	1.55687100
H	4.06044600	-1.90158100	2.41353700
H	6.05265400	-1.02576700	-2.41999900
H	6.66949800	-1.17886900	-0.79721400
C	0.77417800	0.06822900	-0.52486000
C	0.01614000	-1.07292100	-0.31302000
C	-1.33301300	0.69671600	0.09177600
C	-2.53572900	1.52008300	0.32577400
C	-2.45817400	2.81754200	0.87259600
C	-3.81452400	1.03833700	-0.02379500
C	-3.60433400	3.58412500	1.06900200
H	-1.50464300	3.23906400	1.14834700
C	-4.95689500	1.80861200	0.17739900
H	-3.92519500	0.05653400	-0.45723900
C	-4.86167700	3.08713000	0.72688000
H	-3.50606000	4.57762800	1.49699400
H	-5.92428500	1.40358600	-0.10579700
H	-5.75304400	3.68811500	0.88242300
C	-2.32350000	-1.56767300	0.49941200
C	-2.59662800	-1.67405900	1.88093000

C	-3.02099800	-2.31939800	-0.47304100
C	-3.63053800	-2.53639400	2.26758700
C	-4.04296800	-3.16249900	-0.02029900
C	-4.35229200	-3.26859200	1.33188800
H	-3.86842300	-2.63558600	3.32243500
H	-4.60334000	-3.74812200	-0.74274500
H	-5.15129900	-3.92950200	1.65666100
C	0.40375100	-2.48131900	-0.52173400
C	0.22233700	-3.46994700	0.45810700
C	0.99300200	-2.85054100	-1.74308300
C	0.61912000	-4.78534500	0.22315500
H	-0.21429900	-3.20811200	1.41415600
C	1.39914100	-4.16325100	-1.97286700
H	1.13400100	-2.10120600	-2.51508900
C	1.21223300	-5.13701500	-0.99062000
H	0.47854500	-5.53321000	0.99872100
H	1.86219600	-4.42365500	-2.92040300
H	1.53204600	-6.16032100	-1.16660900
C	0.24204000	2.53370100	-0.52114600
C	0.93353800	3.29573900	0.44990000
C	-0.15975100	3.06187400	-1.76450600
C	1.14367100	4.64843300	0.15281500
C	0.09075900	4.41902500	-2.00334700
C	0.71941500	5.20929300	-1.04934900
H	1.66579900	5.27133100	0.87024900
H	-0.20560500	4.85607500	-2.95231000
H	0.90102400	6.26199300	-1.24922600
H	2.71395700	-0.01609000	1.43574200
B	3.30093900	-0.17858000	0.35929700
N	-0.08509800	1.14374100	-0.24648700
N	-1.27138100	-0.66048100	0.07059000
C	1.46714600	2.70295000	1.75694600
H	1.76744900	1.66954400	1.55538800
C	2.72805300	3.42495000	2.26511600
H	3.18283700	2.82942300	3.06292500
H	3.47525300	3.54099300	1.47533500
H	2.50199500	4.41486000	2.68223400
C	0.41989700	2.66981800	2.88973200
H	0.04450500	3.67549100	3.12046200
H	-0.43791900	2.03282500	2.65579000
H	0.88306900	2.27116400	3.79939200
C	-0.80204500	2.21929300	-2.86427400
H	-0.99985600	1.21927400	-2.46657300
C	-2.15097900	2.79616300	-3.33406000

H	-2.60578300	2.13109100	-4.07757500
H	-2.85223600	2.90729700	-2.50073600
H	-2.02910800	3.77812200	-3.80513400
C	0.17082900	2.04445900	-4.04858900
H	1.11303300	1.59222600	-3.72258700
H	-0.27433800	1.39856900	-4.81477600
H	0.40413000	3.00759400	-4.51702600
C	-2.72716600	-2.26123000	-1.97346200
H	-1.84345900	-1.63561800	-2.12781500
C	-2.40466900	-3.66139200	-2.53465900
H	-3.28712400	-4.31156000	-2.51414400
H	-2.08229200	-3.57919700	-3.57879800
H	-1.60733400	-4.14968400	-1.96977400
C	-3.88660800	-1.63154000	-2.77407300
H	-4.08004800	-0.59468600	-2.48141400
H	-3.64493000	-1.63388800	-3.84315200
H	-4.81606600	-2.19782700	-2.64321900
C	-1.83316800	-0.90988400	2.96279400
H	-1.04736700	-0.31824000	2.48475000
C	-1.13130900	-1.85989800	3.95453200
H	-0.57539000	-1.27604700	4.69633500
H	-1.85102300	-2.48586800	4.49437000
H	-0.41712400	-2.52003100	3.45285600
C	-2.75834200	0.06304000	3.72267300
H	-3.26309500	0.75753100	3.04508100
H	-3.52819400	-0.47954900	4.28386800
H	-2.17604000	0.64960400	4.44221600

mNHO-BBNformate

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C	3.83701200	-1.57005200	-0.17112800
C	2.00661600	0.39670100	-1.05642300
C	4.44998900	-1.63793800	-1.59425400
C	4.47187200	0.93852000	-0.00475100
C	5.08210800	0.87621000	-1.43002900
C	5.98190700	-0.84442900	1.16580800
C	5.49465900	0.62282900	1.11209100
C	4.88726900	-1.91107400	0.91985200
C	5.48076600	-0.53394800	-1.91895500
H	3.08197000	-2.36701900	-0.11949000
H	2.12177900	1.46935700	-1.24663800

H	2.19006500	-0.10096300	-2.01485300
H	3.63551400	-1.58420400	-2.33118800
H	4.92328500	-2.61961600	-1.75953800
H	4.16172300	1.98678400	0.14119900
H	5.96326700	1.53449900	-1.50176700
H	4.34780100	1.29439100	-2.13489400
H	6.45219700	-1.03118000	2.14244900
H	6.78578400	-0.97980100	0.43486700
H	5.03317700	0.88077900	2.07577100
H	6.37668900	1.27913300	1.02983900
H	5.38377500	-2.86595800	0.68039200
H	4.35506800	-2.09980300	1.86132700
H	5.64912700	-0.50382900	-3.00576000
H	6.44961100	-0.80643000	-1.48820700
C	0.59685500	0.15009900	-0.65759200
C	-0.07732400	-1.03433100	-0.44791800
C	-1.53473800	0.63603700	-0.00766000
C	-2.80013000	1.36943700	0.21615000
C	-2.82679500	2.71856000	0.62618100
C	-4.04490100	0.74554000	-0.01423100
C	-4.03009800	3.39721400	0.80486500
H	-1.91086100	3.25345300	0.80986000
C	-5.24456000	1.42809700	0.16722100
H	-4.08882300	-0.28188800	-0.33558600
C	-5.24897200	2.75991000	0.57969400
H	-4.00410700	4.43409700	1.12734600
H	-6.17957700	0.90847700	-0.02202400
H	-6.18543400	3.29175500	0.72136900
C	-2.32604300	-1.70106500	0.46724100
C	-2.46966800	-1.83330700	1.86580500
C	-3.05083500	-2.48959100	-0.45448200
C	-3.43527100	-2.73967000	2.32430300
C	-3.99418800	-3.38084900	0.07005600
C	-4.19810000	-3.49628000	1.44211000
H	-3.57890100	-2.85775400	3.39390100
H	-4.57686200	-3.99539100	-0.60973400
H	-4.94186200	-4.19075300	1.82355800
C	0.39394800	-2.41380300	-0.68166000
C	0.39407100	-3.39094700	0.32483900
C	0.87852800	-2.75712900	-1.95451000
C	0.86259900	-4.67736500	0.06224500
H	0.04991600	-3.13741200	1.32005200
C	1.35645200	-4.04066000	-2.21308200
H	0.88027100	-2.01119800	-2.74345800

C	1.34724200	-5.00627200	-1.20531100
H	0.86309700	-5.41935100	0.85586900
H	1.73520800	-4.28482800	-3.20155900
H	1.72122400	-6.00687000	-1.40399100
C	-0.06454500	2.57668800	-0.61274600
C	0.46404500	3.39070000	0.41583500
C	-0.37037000	3.07170900	-1.89798800
C	0.63938200	4.74892200	0.11617000
C	-0.16269700	4.43561700	-2.13405500
C	0.32847100	5.27000000	-1.13582000
H	1.03530800	5.40697600	0.88322200
H	-0.38903100	4.84617700	-3.11377900
H	0.47896300	6.32743800	-1.33654800
B	3.19483100	-0.08055100	0.07259100
N	-0.32472700	1.16644500	-0.36279800
N	-1.37752600	-0.71551100	-0.03054100
C	0.83753200	2.88261800	1.80925700
H	0.83116200	1.79200700	1.80080500
C	2.26440200	3.31208000	2.20225700
H	2.54688700	2.79756700	3.12588200
H	2.99213700	3.04887200	1.43192000
H	2.33121800	4.39155400	2.38699600
C	-0.14037100	3.35013400	2.90840400
H	-0.19427100	4.44525600	2.96165100
H	-1.15493500	2.96685200	2.76797300
H	0.21466100	2.98057500	3.87610000
C	-0.90166700	2.19413800	-3.02932500
H	-1.01814600	1.17371300	-2.65183300
C	-2.28809300	2.66147900	-3.51408100
H	-2.66710000	1.98247800	-4.28694700
H	-3.01257700	2.68408200	-2.69345700
H	-2.24368500	3.66591100	-3.95048100
C	0.10140200	2.12701800	-4.19840000
H	1.07697900	1.76046900	-3.86326700
H	-0.26987000	1.45199700	-4.97858700
H	0.25102500	3.11215700	-4.65496000
C	-2.86049800	-2.42384600	-1.97111800
H	-2.03134700	-1.74252300	-2.18435500
C	-2.48160400	-3.80620500	-2.54136200
H	-3.31517100	-4.51299900	-2.45584400
H	-2.23444200	-3.71717600	-3.60546000
H	-1.61843300	-4.23336900	-2.02562900
C	-4.10566100	-1.88048900	-2.70302500
H	-4.34871100	-0.85578000	-2.40559500

H	-3.93063800	-1.87906800	-3.78509200
H	-4.98543600	-2.50559200	-2.51084500
C	-1.62257400	-1.06997800	2.88359600
H	-0.81385200	-0.54860600	2.36406400
C	-0.93936500	-2.01487800	3.89400200
H	-0.19736700	-1.44846900	4.46286700
H	-1.66082400	-2.45613400	4.59240800
H	-0.41249000	-2.83578400	3.39597600
C	-2.45454000	-0.01518300	3.64094600
H	-2.93253600	0.69768600	2.96253800
H	-3.24365000	-0.49025300	4.23697800
H	-1.80521000	0.54278300	4.32383600
O	2.36768900	0.05588400	1.38833500
C	2.53730800	-0.18761800	2.65527800
H	3.52198500	-0.58955600	2.94726100
O	1.67255200	0.01641600	3.50262800

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C	3.98875800	-1.67884500	0.08746200
C	2.08758100	0.24029800	-0.82960600
C	4.53883000	-1.83182600	-1.35292900
C	4.60213400	0.84478400	0.04619900
C	5.13387800	0.69936500	-1.39978800
C	6.18708100	-0.84240400	1.24887200
C	5.67793900	0.61147400	1.13422600
C	5.07998200	-1.91761500	1.16738000
C	5.52629700	-0.73619000	-1.81485600
H	3.25653700	-2.49369100	0.21272400
H	2.24031200	1.29417900	-1.08352700
H	2.28925600	-0.32980500	-1.74128000
H	3.68786400	-1.84634700	-2.05107400
H	5.02547500	-2.81397400	-1.47772500
H	4.27772200	1.89563900	0.15150100
H	6.00130300	1.35962800	-1.56813700
H	4.35734400	1.06084000	-2.09188000
H	6.72690600	-0.95917200	2.20076200
H	6.93741000	-1.03105900	0.47307900

H	5.23030500	0.89590300	2.09469100
H	6.54567800	1.27660700	0.98382700
H	5.55799900	-2.90142200	1.02110100
H	4.58441000	-1.97072200	2.14567400
H	5.62791500	-0.78147900	-2.91005200
H	6.52440900	-0.96407600	-1.42752200
C	0.67121600	0.06579000	-0.46729700
C	-0.09745600	-1.07410400	-0.28003100
C	-1.45848600	0.69825800	0.06431700
C	-2.66856300	1.52384000	0.24759700
C	-2.61155400	2.80755000	0.82692800
C	-3.92838400	1.05940500	-0.18382000
C	-3.76142000	3.57884000	0.97762000
H	-1.67081100	3.21354800	1.16326500
C	-5.07473300	1.83477000	-0.02923800
H	-4.02100000	0.08825300	-0.64523200
C	-5.00100600	3.09959000	0.55452300
H	-3.68048900	4.56161800	1.43304700
H	-6.02774900	1.44488000	-0.37539800
H	-5.89552300	3.70416100	0.67398900
C	-2.48708700	-1.56008400	0.39630100
C	-2.87529000	-1.66501000	1.75035300
C	-3.11343700	-2.30159700	-0.63187500
C	-3.94143600	-2.52299900	2.04970900
C	-4.17291700	-3.14006000	-0.26499400
C	-4.58900600	-3.24998800	1.05776100
H	-4.26546900	-2.62113900	3.08141300
H	-4.67917200	-3.71753300	-1.03249200
H	-5.41497000	-3.90728200	1.31548300
C	0.29772400	-2.48550400	-0.44833200
C	0.05029500	-3.46107700	0.53144700
C	0.95838000	-2.87484600	-1.62587300
C	0.45117700	-4.78201600	0.33775900
H	-0.44684500	-3.18532800	1.45352200
C	1.36731100	-4.19346500	-1.81440900
H	1.15034800	-2.13815800	-2.39849300
C	1.11403700	-5.15335400	-0.83349700
H	0.25637600	-5.51922100	1.11182800
H	1.88523700	-4.46842000	-2.72873300
H	1.43542300	-6.18114500	-0.97746500
C	0.12507700	2.53475000	-0.50830300
C	0.77813000	3.31779100	0.47204000
C	-0.24619500	3.04273600	-1.77042000
C	0.97541700	4.67069300	0.16528100

C	-0.00866700	4.40037400	-2.01768700
C	0.57825000	5.21182700	-1.05437800
H	1.46771100	5.30778900	0.89169800
H	-0.28199100	4.82164200	-2.98060500
H	0.74913300	6.26498600	-1.26139700
B	3.34832500	-0.17947400	0.32359500
N	-0.19956400	1.14447300	-0.22535700
N	-1.39930500	-0.65889200	0.05006600
C	1.29290900	2.75088300	1.79606900
H	1.58215800	1.70759000	1.63501600
C	2.57807800	3.44908800	2.27713000
H	3.02551000	2.84740700	3.07375100
H	3.31742700	3.52811500	1.47505300
H	2.38832100	4.45297700	2.67926700
C	0.24540800	2.78653600	2.92880700
H	-0.11503100	3.80723200	3.11508200
H	-0.62291600	2.15206000	2.72473000
H	0.70225700	2.42196300	3.85567600
C	-0.83891900	2.17893000	-2.88172200
H	-1.03955400	1.18127600	-2.47933600
C	-2.17622700	2.73335100	-3.40843500
H	-2.59636700	2.05232300	-4.15797900
H	-2.90862900	2.84893100	-2.60299300
H	-2.04799600	3.70948700	-3.88973900
C	0.17821700	2.00153400	-4.02803700
H	1.11367500	1.56577900	-3.66270900
H	-0.23106900	1.34064400	-4.80149000
H	0.41609900	2.96186500	-4.49985700
C	-2.71246700	-2.23293800	-2.10705000
H	-1.81244000	-1.61791800	-2.19311900
C	-2.37015700	-3.63099600	-2.66148800
H	-3.26070900	-4.26807000	-2.71450800
H	-1.97105000	-3.54107600	-3.67810400
H	-1.62333900	-4.13839100	-2.04655400
C	-3.80489200	-1.57798800	-2.97873000
H	-4.00448700	-0.54194500	-2.68719900
H	-3.48916400	-1.57144300	-4.02832100
H	-4.74861900	-2.13260000	-2.91980000
C	-2.20711800	-0.90276500	2.89471400
H	-1.39114700	-0.30051000	2.48522400
C	-1.58075400	-1.85655500	3.93219800
H	-1.08983700	-1.27634000	4.72121200
H	-2.33804600	-2.49104500	4.40674100
H	-0.82513200	-2.50926200	3.48419300

C	-3.19616400	0.05822600	3.58647800
H	-3.65490300	0.75132900	2.87584100
H	-4.00069200	-0.49335200	4.08695100
H	-2.67433200	0.64655400	4.34971600
O	2.85806800	0.06801000	1.71483700
C	2.14662500	-0.87459700	2.45572900
H	2.21511800	-1.89429400	2.05133000
H	2.52114700	-0.90438900	3.49279100
H	1.06824800	-0.62354400	2.51826800

N-methyl N-formylaniline

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C	2.95662800	0.18818900	-0.07351500
C	2.34683500	-1.03760700	-0.34452700
C	0.95958900	-1.16620900	-0.29309100
C	0.16016600	-0.06436200	0.04480900
C	0.77728800	1.16019000	0.34574000
C	2.16382900	1.28430200	0.26939300
H	4.03743900	0.28535200	-0.11847800
H	2.95151200	-1.90123900	-0.60791300
H	0.49712200	-2.11932300	-0.52818800
H	0.17563500	2.00409700	0.66775100
H	2.62533200	2.23970600	0.50382300
N	-1.25315600	-0.19332000	0.09978500
C	-2.08403300	0.80085600	-0.36829800
H	-1.52474200	1.65382400	-0.78863800
O	-3.30157300	0.75823000	-0.34269100
C	-1.86323100	-1.43817500	0.56392700
H	-1.32418400	-1.80845200	1.43980400
H	-2.89928700	-1.21923300	0.82334500
H	-1.85656800	-2.21043700	-0.21510000

N-Methylaniline

0 1

N	1.79277500	-0.60911600	0.15224500
C	0.44360800	-0.27351900	0.06136100
C	0.00088900	1.06180400	0.05778400
C	-0.52280600	-1.29839800	0.00653000
C	-1.36388300	1.35103600	0.01156300
H	0.71815800	1.87504800	0.09310200

C	-1.87844900	-0.99587800	-0.04422500
H	-0.19596900	-2.33673300	0.01059400
C	-2.31473300	0.33294000	-0.04090900
H	-1.68122800	2.39110000	0.01131000
H	-2.60159000	-1.80670000	-0.08744900
H	-3.37455300	0.56664500	-0.08041200
C	2.83569900	0.36447100	-0.10896300
H	2.83839200	1.14123000	0.66446100
H	3.80400700	-0.14140100	-0.06904800
H	2.73959700	0.86136700	-1.08870900
H	2.00181200	-1.54148300	-0.17841400

TS0

0 1

C	-0.89210200	-1.20604200	-0.00122000
C	-0.84568800	-0.92373800	1.52592800
C	-2.09657600	1.08542100	-0.36817100
C	-2.05255500	1.34329700	1.16428600
C	-3.48203900	-1.13538600	-0.38908200
C	-3.36379200	0.33271500	-0.85335300
C	-2.16925000	-1.94381700	-0.48292100
C	-1.89439600	0.08409900	2.04399800
H	-0.04430500	-1.86707600	-0.22070400
H	0.15699000	-0.54277200	1.76530000
H	-0.94903400	-1.86590900	2.08444200
H	-2.11476800	2.07022200	-0.85583300
H	-2.95377500	1.89079200	1.47854400
H	-1.20835100	2.01701400	1.37110100
H	-4.25217400	-1.63665100	-0.99131700
H	-3.85714400	-1.16433700	0.63852000
H	-3.35969700	0.35277800	-1.95321400
H	-4.26865100	0.87802300	-0.54603200
H	-2.29245300	-2.88736000	0.06940700
H	-2.01019600	-2.23004000	-1.53331900
H	-1.61774900	0.39489600	3.06088200
H	-2.86312100	-0.41377100	2.14856400
B	-0.81099500	0.20607000	-0.74366300
N	0.62657100	0.96095300	-0.84214000
C	1.83909400	0.34390900	-0.41890200
C	2.66248900	0.94598500	0.54602100
C	2.25525700	-0.87101500	-0.98914700
C	3.85931700	0.34273200	0.93500400

H	2.36244200	1.88404500	1.00238400
C	3.44461800	-1.47500300	-0.58621700
H	1.65266000	-1.33403600	-1.76483300
C	4.25594400	-0.87258800	0.37741800
H	4.47937200	0.82702500	1.68507100
H	3.74538200	-2.41449600	-1.04256300
H	5.18674500	-1.34124300	0.68373700
C	0.63305100	2.42447700	-0.92660600
H	1.60720400	2.77405300	-1.28295000
H	-0.12903500	2.74957800	-1.64075300
H	0.41646800	2.91035100	0.03381700
H	-0.03815900	0.38852400	-1.91607400
H	-0.89989100	-0.04690500	-2.12309800

TS1

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C	4.31252700	-1.86168800	-0.93341700
C	1.99885700	-0.39367400	-0.95966900
C	5.63753500	-1.43865100	-0.23989000
C	3.05883700	-1.71551200	1.34330300
C	4.36917800	-1.20448700	2.01167200
C	3.88833000	-4.04460300	0.43761000
C	2.91849300	-3.27200600	1.36037500
C	4.08351500	-3.40532700	-0.95290400
C	5.67398300	-1.61062500	1.29518700
H	4.36894200	-1.52540100	-1.97806000
H	2.52240400	0.59393500	-1.13514100
H	1.95279700	-0.77344100	-1.99007300
H	5.80313200	-0.38165900	-0.47681000
H	6.48089900	-1.98916900	-0.68406800
H	2.21400900	-1.31708400	1.92595100
H	4.40796700	-1.54928000	3.05662800
H	4.32375500	-0.10878800	2.05245200
H	3.51016400	-5.06862000	0.31069500
H	4.86036200	-4.15163300	0.92660800
H	1.89080900	-3.52240000	1.06808500
H	3.03398800	-3.63608800	2.39274100
H	4.92603900	-3.89589700	-1.46284800
H	3.19613700	-3.61945400	-1.56673300
H	6.49586600	-1.00334700	1.69692600
H	5.92523100	-2.64447900	1.55288300
C	0.59958200	-0.20800400	-0.47034200

C	-0.40193000	-1.14575500	-0.31786200
C	-1.30767500	0.87426500	0.10958800
C	-2.29589200	1.94431800	0.37091100
C	-1.96223000	3.10915600	1.08862500
C	-3.61192800	1.82670400	-0.11749600
C	-2.91168100	4.10249100	1.31657200
H	-0.96163100	3.25289200	1.46546200
C	-4.55619300	2.82437200	0.11206400
H	-3.90596000	0.95688400	-0.68472200
C	-4.21308400	3.96761600	0.83360900
H	-2.62363900	4.98811900	1.87522200
H	-5.56090200	2.70494300	-0.28296200
H	-4.94906800	4.74645700	1.01170400
C	-2.85309600	-1.09271000	0.32391700
C	-3.27859300	-1.19166700	1.66719100
C	-3.61902000	-1.59519600	-0.75350600
C	-4.52274600	-1.78873200	1.90674900
C	-4.85355400	-2.17928000	-0.44500300
C	-5.30709800	-2.27325200	0.86652500
H	-4.87914500	-1.87377100	2.92885500
H	-5.46921700	-2.56780800	-1.25043500
H	-6.27026700	-2.72957500	1.07766300
C	-0.34614800	-2.60445100	-0.54618000
C	-0.83820500	-3.52711700	0.39189200
C	0.22313900	-3.09843800	-1.73247100
C	-0.76362200	-4.89819000	0.15068200
H	-1.27405400	-3.17349900	1.31809200
C	0.30587000	-4.47040000	-1.96829400
H	0.59076900	-2.40501300	-2.48056300
C	-0.18789400	-5.37599300	-1.02805300
H	-1.14686500	-5.59351600	0.89221700
H	0.75070500	-4.82884200	-2.89218900
H	-0.12403600	-6.44480100	-1.21151100
C	0.64090200	2.34790100	-0.30449700
C	1.39341200	2.86997600	0.77202400
C	0.41132700	3.05725400	-1.49562000
C	1.81624700	4.19658800	0.65295500
C	0.86049400	4.38129700	-1.54988000
C	1.53268100	4.95338400	-0.48034000
H	2.42024700	4.63451200	1.43726600
H	0.70793100	4.95616300	-2.45830300
H	1.88956800	5.97698400	-0.54602400
B	3.06180400	-1.26266000	-0.17251500
N	0.01347100	1.03235700	-0.17590300

N	-1.57444300	-0.45776100	0.03985000
C	1.80604900	2.04174800	1.99488700
H	1.98903400	1.02048600	1.64183100
C	3.12016400	2.54241900	2.62795800
H	3.49550300	1.78781000	3.32833000
H	3.88646900	2.74573400	1.87299400
H	2.95619500	3.46038800	3.20674600
C	0.72138900	1.95919400	3.08889900
H	0.48356100	2.95636100	3.48006500
H	-0.21004100	1.50599100	2.73552800
H	1.08594200	1.35441400	3.92758900
C	-0.19298200	2.42701600	-2.74561300
H	-0.47816700	1.39439400	-2.51215100
C	-1.46062500	3.15301800	-3.23292200
H	-1.86360800	2.65494700	-4.12320700
H	-2.24298500	3.17046900	-2.46619600
H	-1.24211200	4.19055200	-3.51004000
C	0.87963400	2.36378800	-3.85680000
H	1.83001200	1.98792700	-3.46610800
H	0.53469200	1.72817000	-4.68220800
H	1.07065700	3.36284800	-4.26605100
C	-3.18602500	-1.53580600	-2.22026200
H	-2.16891900	-1.13638500	-2.26722200
C	-3.16161300	-2.94295100	-2.85259400
H	-4.17359600	-3.35245100	-2.95110300
H	-2.72996100	-2.89193500	-3.85844200
H	-2.56758800	-3.64394400	-2.26149200
C	-4.08443500	-0.60405300	-3.06112600
H	-4.04511400	0.43441900	-2.71846800
H	-3.75668300	-0.61749600	-4.10666300
H	-5.13087900	-0.92930400	-3.03670100
C	-2.46802500	-0.68592900	2.86005000
H	-1.52286400	-0.27836200	2.49075600
C	-2.11271200	-1.82051800	3.84287400
H	-1.51089600	-1.42230500	4.66726900
H	-3.01042500	-2.27508100	4.27675400
H	-1.53248300	-2.61539400	3.36329000
C	-3.20653700	0.44525400	3.60508000
H	-3.46990100	1.26881400	2.93614800
H	-4.12969800	0.07659600	4.06722800
H	-2.57223800	0.84405500	4.40469100
C	4.25487300	2.23928700	-0.72020500
O	4.75483300	3.30826100	-0.33486300
H	4.44919200	1.33574100	-0.05114500

O	3.52852800	1.98100900	-1.72434000

TS1f

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C	-0.20317900	0.08827300	1.31747700
C	-1.17609900	1.30096200	1.30232900
C	-0.20318800	0.08829000	-1.31747800
C	-1.17609700	1.30098700	-1.30231000
C	-1.64834600	-1.65594400	-0.00000400
C	-0.89045300	-1.30613200	-1.30147900
C	-0.89043400	-1.30615400	1.30146600
C	-1.99037900	1.47933300	0.00001000
H	0.38970100	0.15390500	2.24083100
H	-0.57748800	2.20881100	1.46829500
H	-1.87032000	1.23850100	2.15271800
H	0.38968900	0.15392700	-2.24083400
H	-1.87031700	1.23854900	-2.15270200
H	-0.57748000	2.20883400	-1.46825400
H	-1.86782300	-2.73202400	-0.00001200
H	-2.62493300	-1.16263700	0.00000800
H	-0.10904100	-2.06164700	-1.46537100
H	-1.57937700	-1.39531200	-2.15404700
H	-1.57934400	-1.39535600	2.15404300
H	-0.10901500	-2.06166700	1.46532900
H	-2.43846600	2.48195600	0.00002000
H	-2.83615800	0.78552100	0.00000300
B	0.66362100	0.19233300	-0.00000200
C	2.67341300	0.09180100	-0.00000400
O	1.96495500	-0.91511000	-0.00001600
H	1.51761000	1.16540600	-0.00000300
O	3.71669800	0.63049400	0.00000800

TS2

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C	-1.40694100	-1.92622800	-2.39494300
C	-0.27115100	-1.43934500	0.15235700
C	-0.09161200	-2.71017000	-2.61985100
C	-1.97110200	-3.48568700	-0.41311000
C	-0.75779200	-4.39550900	-0.75270200
C	-3.17972000	-3.86133900	-2.70145000
C	-3.23268200	-3.97654800	-1.16126000

C	-2.53516300	-2.56339200	-3.25678500
C	-0.13031300	-4.17952200	-2.14979700
H	-1.24551800	-0.93081700	-2.83243300
H	-0.69834900	-1.15053900	1.11582000
H	0.22686200	-2.38931600	0.33805200
H	0.72769100	-2.18619500	-2.11044500
H	0.16618200	-2.69816800	-3.69184700
H	-2.17747200	-3.64478600	0.65760900
H	-1.04689900	-5.45536400	-0.66165900
H	0.02631200	-4.25730000	0.00401100
H	-4.19914200	-3.95853000	-3.10358700
H	-2.64196700	-4.73105200	-3.09403800
H	-4.09086400	-3.41227700	-0.78597200
H	-3.44419700	-5.02757100	-0.90436400
H	-2.13559800	-2.78822000	-4.25982900
H	-3.30267900	-1.80654700	-3.43455000
H	0.88733100	-4.59713400	-2.15316400
H	-0.67974800	-4.76610800	-2.89274200
C	0.85607500	-0.46795600	-0.06405300
C	0.89985500	0.90952200	-0.22933300
C	3.03323200	0.23442300	0.11496600
C	4.49406200	0.26664500	0.34297400
C	5.10125600	-0.58276500	1.28701200
C	5.32067700	1.16126400	-0.36339900
C	6.47456500	-0.53537900	1.51603600
H	4.50576300	-1.28862500	1.84528300
C	6.69321300	1.20685300	-0.12983900
H	4.89873100	1.82281000	-1.10476900
C	7.27952900	0.36008400	0.81124700
H	6.91180000	-1.20222000	2.25348900
H	7.30403900	1.90460600	-0.69529000
H	8.35023100	0.39552400	0.99093300
C	2.72115800	2.68783600	-0.15222500
C	3.07698900	3.32244200	1.05910100
C	2.81282100	3.33315400	-1.40560800
C	3.54814400	4.63874400	0.97881400
C	3.29912500	4.64615500	-1.41613300
C	3.66386600	5.29527400	-0.24131800
H	3.82908000	5.15580900	1.89139500
H	3.38746000	5.16895600	-2.36342500
H	4.03495800	6.31591400	-0.27667800
C	-0.15259500	1.89919000	-0.54867800
C	-0.27422500	3.10243000	0.17009800
C	-1.00338800	1.68678100	-1.64142000

C	-1.18104600	4.08160800	-0.22528600
H	0.34258000	3.27702500	1.04094600
C	-1.91093400	2.66838800	-2.03972100
H	-0.95453400	0.75415100	-2.18561400
C	-1.99017000	3.87537100	-1.34540800
H	-1.25621000	5.00381400	0.34447500
H	-2.56815600	2.46273100	-2.87644400
H	-2.69062600	4.64381300	-1.66206300
C	2.72006600	-2.21880000	0.28788100
C	2.51396500	-2.88756600	1.52043800
C	3.45377200	-2.80984800	-0.77186700
C	3.05426200	-4.17165000	1.65996000
C	3.95544100	-4.10211700	-0.56482800
C	3.76290000	-4.78004600	0.63104500
H	2.91230900	-4.70417700	2.59463100
H	4.51764000	-4.57948500	-1.36100100
H	4.16631400	-5.78023900	0.76294100
B	-1.67417800	-1.88597500	-0.76362600
N	2.21701300	-0.85490700	0.13524000
N	2.24732000	1.31236500	-0.10891100
C	1.76134100	-2.29608400	2.71693900
H	1.24533100	-1.38988600	2.39199200
C	0.69097600	-3.27204200	3.24638500
H	0.07892300	-2.77678400	4.00627300
H	0.02693500	-3.61681200	2.44992200
H	1.14516500	-4.15241000	3.71510700
C	2.70753900	-1.90167200	3.87181400
H	3.29974600	-2.75899800	4.21318900
H	3.40119200	-1.10191100	3.59308500
H	2.11962100	-1.54296200	4.72429400
C	3.80463000	-2.13059600	-2.09973700
H	3.29843000	-1.16039400	-2.14286300
C	5.32804200	-1.89297800	-2.21653800
H	5.54573000	-1.30873000	-3.11844800
H	5.74406500	-1.36486100	-1.35788400
H	5.85796900	-2.84800800	-2.31032200
C	3.35146900	-2.94313800	-3.32968400
H	2.28384000	-3.15543900	-3.31628800
H	3.57668100	-2.37891300	-4.24227800
H	3.88946900	-3.89559400	-3.39644300
C	2.42426600	2.68018000	-2.73389700
H	1.92786200	1.72960400	-2.52100500
C	1.42444200	3.55026800	-3.52156900
H	1.89346200	4.47274000	-3.88362200

H	1.06551200	2.99959500	-4.39801900
H	0.55820500	3.82051600	-2.91384800
C	3.65507500	2.37394600	-3.61369300
H	4.33943600	1.66085400	-3.14230800
H	3.33167800	1.93922700	-4.56618900
H	4.22072000	3.28583900	-3.83877900
C	2.98912400	2.66103700	2.43672700
H	2.63241900	1.63425400	2.30952200
C	1.98774500	3.37514100	3.36881900
H	1.97648900	2.88182000	4.34727400
H	2.26579700	4.42307500	3.52845000
H	0.96641000	3.35231200	2.97817200
C	4.37275800	2.59489700	3.11741200
H	5.11948800	2.11121100	2.48277400
H	4.73934100	3.59782400	3.36503000
H	4.30188900	2.03123300	4.05477700
O	-2.86878100	-0.94176100	-0.31818800
C	-4.16866300	-0.53871700	-1.50863100
H	-4.36159100	-1.56827700	-1.81581200
O	-3.89216700	0.34465100	-2.29690700
C	-3.32296600	0.88236800	1.63347300
C	-4.48741500	1.36345600	2.54403600
C	-4.01520300	-1.57476800	2.06242800
C	-5.17021800	-1.09322100	2.98363500
C	-2.03624400	-0.51726600	3.43526200
C	-2.71219900	-1.79403700	2.88272500
C	-2.02920400	0.68802700	2.46731000
C	-5.01388500	0.32914100	3.56029500
H	-3.10193100	1.70241100	0.93878300
H	-5.32365600	1.68232400	1.91621300
H	-4.17317200	2.26576100	3.09359900
H	-4.29610700	-2.57108300	1.68927200
H	-5.29674700	-1.80256800	3.81733500
H	-6.11698200	-1.12997100	2.43212800
H	-0.99918400	-0.75499000	3.71741000
H	-2.51952600	-0.22690100	4.37233800
H	-2.00161500	-2.32600300	2.24441700
H	-2.91684500	-2.47363000	3.72597000
H	-1.82532200	1.60204900	3.04974000
H	-1.18749800	0.59499200	1.77458100
H	-5.98804800	0.66772200	3.94169400
H	-4.36092900	0.30043100	4.43787400
B	-3.68143100	-0.51417700	0.86949300
N	-5.13946500	-0.27754500	-0.26706400

C	-5.87719100	0.97425200	-0.38690100
C	-7.26952700	1.03643200	-0.21604000
C	-5.19628600	2.16341700	-0.69091800
C	-7.95267900	2.24949600	-0.32692600
H	-7.84837900	0.15165400	0.01277700
C	-5.88659600	3.36710500	-0.80722800
H	-4.13060700	2.14217500	-0.83849400
C	-7.26858400	3.42464600	-0.62517500
H	-9.02958400	2.26291200	-0.17940000
H	-5.32938400	4.27141900	-1.03946800
H	-7.80111300	4.36792500	-0.71252700
C	-6.05162200	-1.44698400	-0.23252700
H	-6.65872000	-1.48743600	-1.14473300
H	-5.45971400	-2.35405800	-0.15630600
H	-6.70732000	-1.40513900	0.63367500

TS4Me

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C	1.69417900	1.83033600	-2.55732100
C	0.27400400	1.47174000	-0.10850500
C	0.43803700	2.66207700	-2.91382000
C	2.13869000	3.32671000	-0.50175400
C	1.04063400	4.32425600	-0.98574300
C	3.59130500	3.68809500	-2.60816200
C	3.51798800	3.72408400	-1.06899200
C	2.94131700	2.44448100	-3.26702000
C	0.51270300	4.12687200	-2.43077700
H	1.55735000	0.84098400	-3.01904600
H	0.61291800	1.33187900	0.92557700
H	-0.20187900	2.45205200	-0.10031400
H	-0.44993100	2.17419700	-2.48605200
H	0.27802400	2.67050300	-4.00539100
H	2.20486500	3.46825400	0.58988300
H	1.41714000	5.35608300	-0.89750300
H	0.18233500	4.28805900	-0.29993500
H	4.64444700	3.73116200	-2.91483200
H	3.13306900	4.60195800	-3.00616500
H	4.27614100	3.05017200	-0.66384000
H	3.78589300	4.74063400	-0.73467400
H	2.66482800	2.70391900	-4.30358400
H	3.71540000	1.68163200	-3.35618000
H	-0.47861600	4.59768500	-2.51840500

H	1.15065800	4.67773500	-3.12830800
C	-0.88716700	0.52355700	-0.23013700
C	-1.04145200	-0.81396200	-0.54617800
C	-3.02173400	-0.12779200	0.30816400
C	-4.40233100	-0.13087400	0.83612100
C	-4.75416600	0.69699100	1.91778500
C	-5.39857000	-0.96851700	0.29936800
C	-6.04521400	0.68925500	2.43930400
H	-4.01836400	1.35080500	2.35796400
C	-6.68871500	-0.97522700	0.82468600
H	-5.17509000	-1.61789800	-0.53266600
C	-7.02114700	-0.14707700	1.89696000
H	-6.28238200	1.33868800	3.27686800
H	-7.43588700	-1.62984300	0.38552700
H	-8.02809300	-0.15315300	2.30423700
C	-2.85734500	-2.56368800	-0.18867100
C	-2.87761900	-3.27379400	1.03254300
C	-3.31469600	-3.12520400	-1.40229100
C	-3.40232600	-4.57235800	1.01242200
C	-3.83080400	-4.42592000	-1.35209300
C	-3.88023300	-5.14333800	-0.16138800
H	-3.43553100	-5.14274900	1.93570500
H	-4.19724800	-4.88414400	-2.26551700
H	-4.28612300	-6.15117900	-0.15035200
C	-0.17422300	-1.74648800	-1.30063000
C	0.16180200	-3.02422900	-0.82488100
C	0.23835500	-1.38292700	-2.59227700
C	0.88052200	-3.91417500	-1.62289400
H	-0.13788300	-3.32617500	0.17078300
C	0.97570900	-2.26513000	-3.38224900
H	-0.03148800	-0.40764700	-2.97797700
C	1.29033600	-3.53826500	-2.90422400
H	1.12792700	-4.89904400	-1.23655800
H	1.29153000	-1.95748800	-4.37496200
H	1.85394900	-4.23132900	-3.52287500
C	-2.62185500	2.31373400	0.42126400
C	-2.30697300	3.05034300	1.58773800
C	-3.42103000	2.85872600	-0.61425300
C	-2.85869500	4.33232600	1.70919700
C	-3.92958700	4.15060200	-0.43152100
C	-3.66560100	4.87987500	0.71996300
H	-2.64071400	4.91509900	2.59826700
H	-4.54537400	4.58885500	-1.21059300
H	-4.07704500	5.87807300	0.84138700

B	1.76761300	1.75841900	-0.90837000
N	-2.16664200	0.92966600	0.26725900
N	-2.35418000	-1.19734700	-0.18285600
C	-1.39192900	2.56530900	2.71491200
H	-0.96355600	1.60149200	2.42718200
C	-0.22841100	3.55867800	2.92207000
H	0.46710900	3.17311800	3.67271900
H	0.32994900	3.72736700	1.99862300
H	-0.59341700	4.52792700	3.27966000
C	-2.13301200	2.36419500	4.05435900
H	-2.62361300	3.28707700	4.38483300
H	-2.89281900	1.57757400	4.00574300
H	-1.41511500	2.07467400	4.82967800
C	-3.78081300	2.13803000	-1.91520000
H	-3.27526100	1.16678400	-1.93279300
C	-5.30062500	1.88966300	-2.02307400
H	-5.52300500	1.30962800	-2.92648600
H	-5.69660400	1.34762800	-1.16085800
H	-5.84568300	2.83735900	-2.10059000
C	-3.30176700	2.91933800	-3.15584600
H	-2.23041400	3.12407600	-3.12080000
H	-3.51011000	2.33906800	-4.06242200
H	-3.82795800	3.87581800	-3.25133500
C	-3.28085800	-2.40201900	-2.75028300
H	-2.73329000	-1.46336300	-2.62461000
C	-2.53475800	-3.23477900	-3.81247900
H	-3.10552500	-4.12857800	-4.09019200
H	-2.39606200	-2.63972600	-4.72193700
H	-1.55151000	-3.55360500	-3.46083100
C	-4.69195400	-2.05331900	-3.26973600
H	-5.22380800	-1.36095300	-2.61030800
H	-4.61712100	-1.57793200	-4.25440400
H	-5.30771300	-2.95332400	-3.38235600
C	-2.37199300	-2.70940300	2.36114800
H	-1.97854500	-1.70285100	2.18911900
C	-1.21610800	-3.54923200	2.94243300
H	-0.86895400	-3.10317300	3.88056500
H	-1.53323100	-4.57584600	3.15826900
H	-0.35791900	-3.59498500	2.26550400
C	-3.51098800	-2.59884400	3.39649600
H	-4.35075500	-2.00823300	3.02075100
H	-3.89210600	-3.58922500	3.67145100
H	-3.13946000	-2.12327600	4.31129400
O	2.83170500	0.69722300	-0.37972000

C	4.21489800	0.28915800	-1.39244300
C	2.54502000	-1.19399900	1.63896200
C	3.54516500	-2.09672200	2.41871700
C	4.14959400	0.80815800	1.95929400
C	5.03851700	-0.03026900	2.92143100
C	2.05165200	0.60419200	3.48410000
C	3.02807100	1.54130100	2.74685100
C	1.52290000	-0.56385300	2.62114400
C	4.43328600	-1.35793500	3.43991400
H	1.96125300	-1.85805300	0.98589900
H	4.20359500	-2.61546800	1.71224200
H	2.99298600	-2.89263300	2.94559600
H	4.78380200	1.59698300	1.53033000
H	5.32223900	0.58629400	3.78985400
H	5.97678300	-0.26474100	2.41391500
H	1.19742300	1.18388400	3.86124800
H	2.53867800	0.21144300	4.38088300
H	2.46808300	2.17317100	2.05056700
H	3.47589100	2.22748700	3.48309600
H	1.12446500	-1.34435200	3.29155700
H	0.66003300	-0.21577100	2.04124000
H	5.25115700	-2.02611100	3.74463200
H	3.85657000	-1.18176100	4.35336500
B	3.40123600	-0.06636300	0.80869000
N	4.46790700	-0.90685100	-0.33992900
C	3.74963500	-2.06322900	-0.92438800
C	5.88481500	-1.18353800	-0.12360100
C	6.39118300	-2.49112200	-0.18314500
C	6.78440000	-0.13507400	0.13595500
C	7.75051700	-2.74520200	0.01311400
H	5.73958600	-3.33370900	-0.37584600
C	8.14127700	-0.39705400	0.31399200
H	6.42149100	0.87907200	0.17698600
C	8.63718100	-1.70020400	0.25703600
H	8.10800200	-3.77090500	-0.03124700
H	8.81450700	0.43449400	0.50544000
H	9.69595100	-1.89635100	0.40380200
H	2.74192500	-1.73802800	-1.16343100
H	4.24966400	-2.39401100	-1.84137800
H	3.68921200	-2.89517200	-0.22511800
O	5.07771100	1.13248400	-1.54552800
H	3.64523900	-0.13819800	-2.22933300

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C	2.92361800	-1.75027000	0.48282000
C	3.53302900	-2.26733300	-0.85557700
C	3.07790300	0.70443300	-0.39471400
C	3.68084300	0.16428600	-1.73154300
C	4.87937800	-0.19609300	1.28035500
C	4.13358200	1.02388800	0.70262400
C	3.96735800	-1.40118700	1.58484100
C	4.34414000	-1.22656100	-1.65477500
H	2.31075600	-2.56934800	0.87404200
H	2.69752100	-2.62422000	-1.47322100
H	4.16282900	-3.14698100	-0.65797200
H	2.57267100	1.64146300	-0.63823200
H	4.40562200	0.89329700	-2.12224300
H	2.86797900	0.12497200	-2.47140000
H	5.39213700	0.10446300	2.20394400
H	5.67417000	-0.50130200	0.59375700
H	3.61528700	1.54083000	1.52426400
H	4.86558400	1.74555600	0.31181300
H	4.58953900	-2.28336500	1.79493500
H	3.41638500	-1.19753900	2.51605000
H	4.49442000	-1.60232200	-2.67568000
H	5.34789400	-1.13303700	-1.22986700
B	2.11715500	-0.43016500	0.13358500
O	0.73296000	-0.34265000	0.24155300
C	-0.01016000	-1.70417800	0.48827400
H	0.20760800	-1.99036600	1.52399300
O	-0.09506200	-2.46270800	-0.44264800
C	-1.13858100	1.14336600	-1.23010700
C	-2.51654600	1.87157900	-1.19016600
C	-0.63006900	1.96729600	1.18069900
C	-2.04432900	2.62271300	1.23870400
C	0.38478100	3.24526900	-0.87732600
C	0.45003000	2.93584300	0.63735400
C	-0.00673600	2.05036900	-1.77601200
C	-2.64635700	2.98872400	-0.13263600
H	-1.24116300	0.31771200	-1.94400900
H	-3.29767000	1.12554700	-1.00585000
H	-2.73284600	2.29193000	-2.18353600
H	-0.34542500	1.74419100	2.21857300
H	-2.00493200	3.52337200	1.86905800
H	-2.73760100	1.93634200	1.74584200
H	1.36075600	3.63206700	-1.20261300

H	-0.31581100	4.06764800	-1.04949700
H	1.42879900	2.50359600	0.87418600
H	0.40804200	3.88447100	1.19368600
H	-0.29215400	2.43646700	-2.76583400
H	0.87375900	1.42107800	-1.94896400
H	-3.70940100	3.23223100	-0.00046000
H	-2.18260500	3.90906800	-0.49903200
B	-0.78086900	0.66412800	0.25524300
N	-1.51402100	-0.59152900	0.88754900
C	-2.74478200	-1.10452700	0.31511000
C	-3.94213700	-1.10053300	1.04966400
C	-2.75980300	-1.63472500	-0.98545200
C	-5.12114000	-1.59972300	0.49571900
H	-3.97506400	-0.69448900	2.05357700
C	-3.94284000	-2.13539200	-1.52781200
H	-1.84679300	-1.68444600	-1.55816400
C	-5.13052400	-2.12036500	-0.79707000
H	-6.03460400	-1.57525600	1.08405000
H	-3.92711300	-2.54521200	-2.53416600
H	-6.04883700	-2.50946900	-1.22779300
C	-1.51860100	-0.60501400	2.36630400
H	-1.85396100	-1.58241000	2.72653300
H	-0.50423600	-0.42467500	2.72652600
H	-2.16034800	0.17069300	2.78981800

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C	3.22174900	0.26812300	-0.93903000
C	4.15552900	0.97667600	0.07218300
C	2.94079400	-1.70158500	0.74987100
C	3.93627900	-1.01602500	1.71937100
C	4.53692700	-1.97481800	-1.30755800
C	3.61769500	-2.66295500	-0.27468900
C	3.93937700	-0.69394100	-1.93386700
C	4.85886900	0.04752000	1.08318300
H	2.75397600	1.04964200	-1.55115700
H	3.55079600	1.70999100	0.62751000
H	4.91907500	1.56531000	-0.45876200
H	2.27406100	-2.33635300	1.35629800
H	4.55813100	-1.77170500	2.22367500
H	3.35931800	-0.53325200	2.52125300
H	4.76293200	-2.68961400	-2.11085300

H	5.50199500	-1.74637600	-0.84467500
H	2.81611700	-3.18679600	-0.81270300
H	4.19024700	-3.43753800	0.25759100
H	4.73070400	-0.15513000	-2.47686400
H	3.19931800	-0.99053200	-2.69014700
H	5.30208400	0.65738100	1.88295500
H	5.70549700	-0.44491100	0.59558000
B	2.16474700	-0.64519700	-0.17730900
N	0.76285300	0.24349900	0.76050500
C	0.47935400	1.59521300	0.29811700
C	0.37655800	2.66578800	1.19681300
C	0.32231100	1.85124000	-1.07518400
C	0.13086300	3.96121800	0.73339100
H	0.48644600	2.51554900	2.26321800
C	0.06843700	3.14442100	-1.52426100
H	0.39375100	1.03851100	-1.78476100
C	-0.02683700	4.20973900	-0.62682200
H	0.06145800	4.77349000	1.45181000
H	-0.05145800	3.31668300	-2.59040600
H	-0.22047400	5.21689000	-0.98469100
C	0.65216400	0.06685700	2.22045500
H	-0.34768400	0.33687200	2.58282200
H	0.85593400	-0.97572600	2.46326200
H	1.39622200	0.68020600	2.72927900
C	0.04030300	-0.88895500	-0.02611900
H	-0.10940200	-1.69333800	0.71078300
O	0.99999700	-1.16068000	-0.95315400
C	-3.41243900	-1.85010600	-0.68750500
C	-4.06037100	-2.44909100	0.59626400
C	-3.30032400	0.49211100	0.48480800
C	-3.94599700	-0.13051200	1.75858500
C	-5.19964300	-0.01524200	-1.25450600
C	-4.32336100	1.04759500	-0.55449700
C	-4.43261000	-1.27371100	-1.71834300
C	-4.75138600	-1.42762500	1.52609400
H	-2.84991200	-2.64908900	-1.18843800
H	-3.26818500	-2.96054000	1.16405700
H	-4.78051500	-3.23371700	0.32150200
H	-2.66487500	1.32962800	0.80081300
H	-4.58901500	0.61176000	2.25395700
H	-3.13708400	-0.34532100	2.47477900
H	-5.68045600	0.44537400	-2.12790700
H	-6.02121700	-0.30770800	-0.59421100
H	-3.75148100	1.59370300	-1.31859900

H	-4.97271100	1.79505200	-0.07531400
H	-5.15355300	-2.05342000	-2.00508700
H	-3.87551100	-1.02939400	-2.63447300
H	-4.94145300	-1.90492700	2.49686700
H	-5.73928500	-1.17848100	1.12864400
B	-2.49707400	-0.64588600	-0.25029500
O	-1.16094400	-0.55342700	-0.58980200

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C	2.85419000	-0.97430000	1.22604300
C	3.74492900	-2.23615700	1.00468600
C	2.69998300	-0.64329600	-1.36330500
C	3.59742000	-1.90224900	-1.57104600
C	4.33845000	0.82749700	0.04828500
C	3.48583800	0.68336400	-1.23322600
C	3.64710700	0.34867300	1.34566600
C	4.47457800	-2.29158000	-0.35789100
H	2.31359700	-1.12802100	2.17254600
H	3.09607300	-3.11888800	1.08987800
H	4.48635200	-2.32233300	1.81331800
H	2.05478800	-0.56534400	-2.25277400
H	4.24277000	-1.76638800	-2.45192800
H	2.93230100	-2.74474400	-1.80495700
H	4.62421400	1.88202800	0.16676700
H	5.28207700	0.28866300	-0.08075300
H	2.75892700	1.50654500	-1.26301200
H	4.13627300	0.83153500	-2.10888600
H	4.40394300	0.27028400	2.14128000
H	2.94761500	1.12708500	1.68098900
H	4.85778500	-3.30973600	-0.51192000
H	5.36149300	-1.65150000	-0.32530300
B	1.88777900	-0.96946400	-0.03404900
N	-1.31283000	-1.79127300	0.58863900
C	-2.65997200	-1.81440800	0.14771600
C	-2.98582600	-2.22765200	-1.15669100
C	-3.70264200	-1.47494800	1.02464400
C	-4.31362500	-2.25669600	-1.57697200
H	-2.20510300	-2.56109700	-1.83294200
C	-5.03052600	-1.52803300	0.59981400
H	-3.47873200	-1.15971500	2.03795000

C	-5.34612700	-1.90852600	-0.70381200
H	-4.54099000	-2.57972100	-2.58934800
H	-5.82020300	-1.25993200	1.29664200
H	-6.38057300	-1.94500500	-1.03237000
C	-1.01197400	-1.99683100	2.00383700
H	-1.64199400	-2.79958900	2.39572000
H	0.03350900	-2.29178100	2.08890900
H	-1.17621800	-1.09067900	2.60204200
C	-0.27702400	-1.40079800	-0.25092700
H	-0.62822800	-1.25601300	-1.27403400
O	0.88761500	-2.06086300	-0.08924800
C	0.56588400	2.62347100	0.37003500
C	0.54358500	3.58020100	-0.85662200
C	-1.69647000	1.56992900	-0.41934500
C	-1.66697900	2.50053200	-1.66838800
C	-1.68026200	3.37060200	1.49296000
C	-2.40879000	2.18390400	0.82404800
C	-0.15484600	3.18281900	1.63520000
C	-0.83783400	3.79180600	-1.51307200
H	1.61470200	2.45824100	0.64078500
H	1.22767500	3.16739100	-1.61199600
H	0.96486600	4.55655200	-0.57521600
H	-2.26073600	0.67380500	-0.70068500
H	-2.69530400	2.76241800	-1.95741500
H	-1.25997600	1.91993600	-2.51020100
H	-2.11196700	3.53372000	2.48974900
H	-1.88459400	4.28967500	0.93645100
H	-2.52722300	1.38093500	1.56628400
H	-3.43000800	2.48937800	0.55335900
H	0.30173200	4.13929700	1.92901800
H	0.04159800	2.49003000	2.46725300
H	-0.69336400	4.24136400	-2.50464600
H	-1.41135600	4.52851200	-0.94300400
B	-0.19673300	1.29221900	-0.00316000
O	0.37794200	0.04764800	0.09152300

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C	-2.56022400	0.16995900	1.01761000
C	-3.65161500	1.26044900	1.23469200
C	-3.85528600	-0.65364600	-1.10588300
C	-4.93546600	0.44132000	-0.86809600

C	-4.06972200	-1.97503800	1.14421800
C	-4.14176100	-2.01026700	-0.39832000
C	-2.86212800	-1.19378900	1.70799400
C	-5.02082600	0.97739900	0.57801500
H	-1.62609600	0.55115500	1.43928000
H	-3.25457300	2.20472100	0.83401600
H	-3.79827700	1.43082100	2.31178600
H	-3.80389200	-0.84467400	-2.18644200
H	-5.92469300	0.07089300	-1.17641600
H	-4.71003400	1.28270700	-1.54100500
H	-4.03098000	-3.00642200	1.52060000
H	-4.99749300	-1.55642500	1.54540900
H	-3.40462800	-2.73916300	-0.76718700
H	-5.12466300	-2.39739700	-0.70633600
H	-3.00512600	-1.04106200	2.78821700
H	-1.96142600	-1.81771300	1.61056200
H	-5.61200300	1.90340800	0.57851200
H	-5.58615500	0.27429600	1.19679300
B	-2.48990000	-0.10629500	-0.53354500
N	-0.20373000	1.93903200	-0.70165700
C	1.00707200	2.45198000	-0.11644500
C	1.97470700	3.13512200	-0.86805800
C	1.21318100	2.29163000	1.26207800
C	3.12200700	3.64359900	-0.25359000
H	1.83616500	3.27739700	-1.93531200
C	2.36471100	2.78926600	1.86933300
H	0.45481500	1.78296400	1.84638000
C	3.32481100	3.46932900	1.11490900
H	3.85837300	4.17444000	-0.85152800
H	2.50391500	2.66058600	2.93959700
H	4.21668500	3.86633000	1.59183900
C	-0.74722500	2.75328700	-1.79427300
H	-0.18471600	2.66148400	-2.73993700
H	-1.77710400	2.45283800	-1.99321100
H	-0.74076500	3.80121000	-1.48672300
C	-0.15658100	0.52440300	-1.07502000
H	0.44309700	0.37701800	-1.98487400
O	-1.44228400	0.06071000	-1.41021500
C	1.90165200	-1.87421400	1.17236800
C	1.77418800	-3.38765500	0.83222500
C	2.38789000	-1.35513500	-1.35029700
C	2.25833300	-2.87664100	-1.66685000
C	4.36012700	-1.44732800	0.38088100
C	3.82449700	-0.89237100	-0.95730600

C	3.34079700	-1.40859100	1.54058700
C	2.47742300	-3.82831400	-0.47015600
H	1.25237300	-1.66900400	2.03419900
H	0.70215200	-3.62122400	0.74889100
H	2.14839100	-3.99590200	1.66901500
H	2.11976200	-0.81566900	-2.26829400
H	2.95362500	-3.14724900	-2.47505400
H	1.24930200	-3.04689700	-2.07091700
H	5.24722200	-0.86803800	0.67035600
H	4.71764900	-2.47121700	0.23717100
H	3.81563600	0.20592900	-0.90372200
H	4.52851400	-1.14994200	-1.76239800
H	3.72636200	-2.00402400	2.38158600
H	3.26999400	-0.37480500	1.90807500
H	2.11831600	-4.82883000	-0.74659900
H	3.54935600	-3.94632800	-0.28722000
B	1.45934300	-1.06505600	-0.10496300
O	0.37058800	-0.23336100	-0.02086800

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C	2.99197300	-2.63756400	0.92550100
C	1.50980500	-0.23970800	0.15830100
C	4.33201200	-2.72913900	1.71261900
C	2.04121500	-1.08047000	2.76928000
C	3.36647100	-1.19179400	3.56411400
C	1.39265700	-3.61371100	2.77308300
C	0.98784400	-2.17004700	3.13637500
C	2.00169900	-3.76385200	1.36101600
C	4.24645500	-2.41200300	3.22109700
H	3.22376800	-2.81201700	-0.13584700
H	1.88457900	0.75451800	0.46733200
H	1.89053300	-0.41286000	-0.85769400
H	5.05048800	-2.03420100	1.26458400
H	4.76547000	-3.73315000	1.58271900
H	1.60525800	-0.11350700	3.03152700
H	3.15931300	-1.19546600	4.64649200
H	3.92502600	-0.27010700	3.36382300
H	0.50964100	-4.26530800	2.84797200
H	2.09292400	-3.98991900	3.52393800
H	0.04476200	-1.92884100	2.61909000
H	0.75774100	-2.12081100	4.21250600

H	2.50797700	-4.73947000	1.29259400
H	1.18471100	-3.80279700	0.63654800
H	5.26290000	-2.23456500	3.59934700
H	3.88983800	-3.29402900	3.76324900
C	0.01836300	-0.14212700	0.07324800
C	-0.93936400	-1.08398400	-0.24184700
C	-2.00676900	0.89770400	-0.03686500
C	-3.05303800	1.94175400	-0.10451800
C	-2.96943500	3.13506100	0.63980000
C	-4.16772600	1.78346900	-0.95352100
C	-3.96056700	4.10955900	0.55034000
H	-2.12792500	3.31791100	1.28664400
C	-5.15490500	2.76144400	-1.04053400
H	-4.27252800	0.89572400	-1.55592800
C	-5.06124400	3.93092200	-0.28646600
H	-3.86293500	5.01436000	1.14299800
H	-5.99688700	2.60443100	-1.70850700
H	-5.83155200	4.69369100	-0.35461600
C	-3.45931300	-1.11056600	-0.42471600
C	-4.23523200	-1.30245800	0.73934100
C	-3.86861300	-1.56700100	-1.69816400
C	-5.46948900	-1.94756100	0.58969300
C	-5.11375000	-2.20235600	-1.77878500
C	-5.90996000	-2.38858500	-0.65310200
H	-6.09230700	-2.10667000	1.46482300
H	-5.46284700	-2.55889400	-2.74300900
H	-6.87261100	-2.88403000	-0.74452500
C	-0.75443700	-2.49482100	-0.63944900
C	-1.48643300	-3.54923400	-0.07039000
C	0.18735100	-2.79160700	-1.63998500
C	-1.28152100	-4.86257400	-0.49240100
H	-2.21150400	-3.34705700	0.70908400
C	0.39498900	-4.10570600	-2.05562900
H	0.75987600	-1.98884100	-2.09228900
C	-0.34045100	-5.14565500	-1.48436600
H	-1.85148300	-5.66663500	-0.03540300
H	1.13278600	-4.31412400	-2.82495100
H	-0.17719700	-6.17071600	-1.80500400
C	-0.04202700	2.38844500	0.29244600
C	0.27128800	2.93872900	1.55432600
C	0.19165800	3.06676600	-0.92201100
C	0.77208700	4.24627900	1.56197600
C	0.70560400	4.36561900	-0.84409400
C	0.97815700	4.95683400	0.38425000

H	1.02594300	4.70617500	2.51068700
H	0.90076400	4.91566700	-1.75974600
H	1.37510700	5.96751600	0.42422000
B	2.28656100	-1.22689400	1.20360000
N	-0.67741900	1.07684000	0.20234800
N	-2.18227100	-0.42701000	-0.28971700
C	0.09907900	2.20096900	2.88466400
H	-0.00150400	1.13400500	2.66204400
C	1.34104300	2.36956000	3.78459100
H	1.25833900	1.69205100	4.64283300
H	2.25930500	2.14374600	3.23275400
H	1.40177600	3.38814100	4.18830500
C	-1.16421900	2.62959200	3.66381800
H	-1.17640100	3.71347500	3.83356000
H	-2.09674600	2.35539900	3.15969200
H	-1.16801100	2.14294900	4.64580300
C	-0.06232500	2.44918600	-2.29605900
H	-0.50965000	1.45922400	-2.15764800
C	-1.05373600	3.28139200	-3.13280400
H	-1.25258100	2.78180300	-4.08837500
H	-2.00761700	3.41865400	-2.61280600
H	-0.65019100	4.27437900	-3.36056500
C	1.26128700	2.23742900	-3.05912000
H	1.97302000	1.64669000	-2.47467000
H	1.07281100	1.71908300	-4.00695400
H	1.73936100	3.19497900	-3.29445400
C	-3.04267500	-1.40227600	-2.97603400
H	-2.06940300	-0.98197800	-2.70628700
C	-2.78710500	-2.76237400	-3.65714800
H	-3.71423000	-3.18439900	-4.06220500
H	-2.09243500	-2.63422200	-4.49463400
H	-2.35632800	-3.48915600	-2.96503000
C	-3.70151400	-0.43524400	-3.98297900
H	-3.79800400	0.58019700	-3.58692700
H	-3.09325400	-0.37746500	-4.89266600
H	-4.70016000	-0.78164800	-4.27333500
C	-3.80414600	-0.85138900	2.13531900
H	-2.81879000	-0.38152700	2.06424000
C	-3.65988800	-2.04330900	3.10333600
H	-3.32987200	-1.68776000	4.08559900
H	-4.61146900	-2.56906400	3.24161100
H	-2.92084100	-2.76935000	2.74927200
C	-4.77608900	0.19694300	2.71464300
H	-4.88706200	1.05791600	2.04896900

H	-5.77131100	-0.23179000	2.88001600
H	-4.40627500	0.55716700	3.68120100
C	4.22525500	0.90250900	0.88967700
H	5.22714900	0.62431500	1.30428300
N	4.46710000	1.39481700	-0.54560500
C	5.25242600	0.70089000	-1.44726100
C	5.52517100	-0.68054200	-1.28694300
C	5.80316200	1.32620200	-2.59624200
C	6.29180000	-1.38067000	-2.21298300
H	5.11787800	-1.20844800	-0.43741700
C	6.56492100	0.60909700	-3.51625700
H	5.63595800	2.38266000	-2.76903900
C	6.82300000	-0.75113600	-3.34142600
H	6.47552500	-2.44015900	-2.04440200
H	6.96711200	1.13146600	-4.38249300
H	7.42235300	-1.30355500	-4.05997600
C	4.33449000	2.83114600	-0.70278000
H	3.83361500	3.08885000	-1.64519000
H	3.73286900	3.17425000	0.13906700
H	5.30950800	3.34833000	-0.68816100
O	3.48702600	1.70381500	1.58416700
H	3.72333000	-0.17200400	0.76294300

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C	-1.97532900	-0.51030000	1.10007800
C	-2.38350700	0.76202300	1.88516000
C	-2.30102000	0.81071400	-1.15481700
C	-2.70473000	2.06865400	-0.34571600
C	-4.14233600	-0.85878300	-0.33200200
C	-3.47351700	-0.13957300	-1.52681700
C	-3.15545800	-1.44298400	0.70568700
C	-3.21225000	1.79633300	1.08897300
H	-1.30479600	-1.09434800	1.74857800
H	-1.45816900	1.24825300	2.22921800
H	-2.93852100	0.49182500	2.79666800
H	-1.85553600	1.15389200	-2.10211600
H	-3.46666100	2.65172500	-0.88546100
H	-1.81892600	2.71936700	-0.28238900
H	-4.76972300	-1.67423900	-0.71800200
H	-4.83556300	-0.17433200	0.16685900
H	-3.07165100	-0.90041800	-2.21057300
H	-4.24525000	0.40323600	-2.09380300
H	-3.71836900	-1.74753900	1.60141000

H	-2.72139200	-2.36421200	0.29124300
H	-3.22399100	2.74340200	1.64629100
H	-4.25729800	1.47354500	1.05049200
B	-1.29663500	-0.06797600	-0.27951000
C	0.53160700	-0.47195500	-0.86896800
H	0.81617300	0.24724800	-1.64224700
N	1.59894000	-0.99438100	-0.18572800
C	2.81036600	-0.25961300	-0.08751500
C	2.82351600	1.13693900	-0.24020300
C	4.01709900	-0.92657200	0.17587500
C	4.02613100	1.83869700	-0.16408100
H	1.89852000	1.68373700	-0.38676300
C	5.21008700	-0.21165600	0.26165100
H	4.03066100	-2.00326000	0.30198000
C	5.22564800	1.17261400	0.08563900
H	4.01573300	2.91851300	-0.28422700
H	6.13419400	-0.74681800	0.46235100
H	6.15832000	1.72495900	0.15114800
C	1.44002700	-2.23800200	0.57052400
H	1.72355500	-2.08581300	1.61684200
H	0.39722900	-2.54111300	0.50636400
H	2.05935100	-3.03374500	0.14298500
O	-0.56212300	-1.19437300	-1.04083100
H	-0.17831800	0.60245600	-0.00336900

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C	-1.22197200	0.02572100	2.81797600
C	-0.62015800	0.76839700	0.06910200
C	0.12850500	0.60293100	3.31735500
C	-1.91956700	2.38460500	2.03935300
C	-0.55193700	2.94155100	2.47603000
C	-2.75191000	1.46307900	4.35969000
C	-2.97498300	2.43081200	3.17791600
C	-2.29931600	0.05407900	3.93029600
C	0.17576300	2.12552900	3.56038600
H	-1.02618500	-1.03733000	2.62154300
H	-1.20500600	0.13483800	-0.60652800
H	-0.61773800	1.76761100	-0.37409000
H	0.89762900	0.36413700	2.57142800
H	0.44319000	0.08976500	4.24368100
H	-2.27748000	3.06316600	1.25177400
H	-0.65131000	3.98211800	2.82719600
H	0.08551300	2.98446400	1.58302800

H	-3.68798500	1.38185600	4.93183200
H	-2.02672900	1.88281900	5.06464500
H	-3.94725800	2.19007400	2.74074300
H	-3.06480900	3.45585000	3.57557600
H	-1.94886000	-0.49386000	4.82199400
H	-3.17961700	-0.49301700	3.57104400
H	1.22737400	2.44767600	3.62235500
H	-0.24808600	2.36066900	4.54064400
C	0.77457300	0.25859000	0.02382000
C	1.28131700	-1.00785500	0.27496200
C	3.04368900	0.26947800	-0.32682900
C	4.40794300	0.65317900	-0.75740600
C	4.61616600	1.47562400	-1.88350900
C	5.54848400	0.18113300	-0.07701000
C	5.90226000	1.80934000	-2.30259100
H	3.77744300	1.86429500	-2.43948700
C	6.83176200	0.52077100	-0.49933900
H	5.44460200	-0.45095100	0.79093300
C	7.01931100	1.33702700	-1.61447600
H	6.02405600	2.44352300	-3.17596800
H	7.68683900	0.14466400	0.05495100
H	8.02077200	1.60143800	-1.94156300
C	3.56664100	-2.08280400	0.35001500
C	4.00925100	-2.85735200	-0.74120700
C	3.97158700	-2.34021700	1.68226500
C	4.91631800	-3.89115300	-0.47281100
C	4.88462300	-3.38246300	1.88068500
C	5.35988100	-4.14653500	0.81851100
H	5.27874900	-4.50265700	-1.29353700
H	5.22508900	-3.60272800	2.88719700
H	6.06870500	-4.94942000	1.00192700
C	0.56732200	-2.30189000	0.41709700
C	-0.01748800	-2.86202800	-0.73132400
C	0.45798000	-2.99466500	1.62996200
C	-0.68287600	-4.08684400	-0.67135200
H	0.04242100	-2.32568500	-1.67427700
C	-0.20377500	-4.22149800	1.69040800
H	0.86304500	-2.55943800	2.53413800
C	-0.77152900	-4.77291800	0.54102300
H	-1.13878200	-4.49818700	-1.56745600
H	-0.28568200	-4.74016700	2.64152600
H	-1.29247300	-5.72492400	0.59183800
C	1.81205900	2.31907000	-1.04470800
C	1.32648800	2.31687000	-2.37801000

C	2.25289900	3.49994000	-0.40411800
C	1.26986100	3.54304700	-3.04902000
C	2.18337000	4.69025300	-1.14282900
C	1.69426200	4.72013300	-2.44227300
H	0.89391600	3.57175000	-4.06713500
H	2.51511400	5.61414500	-0.68125300
H	1.64366300	5.66095900	-2.98343100
B	-1.76800300	0.84871400	1.48142300
N	1.90289300	1.02575800	-0.37524500
N	2.67294700	-0.96188600	0.09862100
C	0.91731400	1.05543100	-3.14718500
H	0.96692500	0.20029300	-2.46747500
C	-0.53034100	1.13739200	-3.66636300
H	-0.80692800	0.19273600	-4.14903000
H	-1.23924300	1.32851400	-2.85990800
H	-0.64478000	1.93099000	-4.41373700
C	1.87462200	0.76466400	-4.32381700
H	1.87876700	1.58840600	-5.04679000
H	2.90598700	0.60108300	-3.99573800
H	1.54634600	-0.13677900	-4.85441900
C	2.82707900	3.56628500	1.01357200
H	2.54257900	2.64858200	1.53955800
C	4.36886600	3.67004000	1.01208800
H	4.73336900	3.74217200	2.04369600
H	4.85581900	2.81657700	0.53984700
H	4.69091200	4.57515600	0.48319700
C	2.27473300	4.76318600	1.81744800
H	1.19006200	4.84892300	1.74612600
H	2.53612600	4.64446400	2.87444400
H	2.71879200	5.70714700	1.48065300
C	3.47821100	-1.54235000	2.89332200
H	2.55860500	-1.02393600	2.61042300
C	3.14051600	-2.45373700	4.09178600
H	4.04485700	-2.83679000	4.57843700
H	2.58557100	-1.88114600	4.84256800
H	2.53186100	-3.31395100	3.79724200
C	4.47990100	-0.46051300	3.35214100
H	4.62764000	0.31994200	2.60043700
H	4.10499500	0.02684100	4.25889400
H	5.45745900	-0.89972900	3.58608100
C	3.55949500	-2.63098100	-2.18235600
H	2.83423700	-1.81093100	-2.19224400
C	2.85177200	-3.87725900	-2.75179100
H	2.47246600	-3.66545700	-3.75835500

H	3.54056700	-4.72596400	-2.83227400
H	2.01014100	-4.18345900	-2.12434600
C	4.73716500	-2.22393600	-3.09142800
H	5.25050700	-1.33262600	-2.72052300
H	5.47504600	-3.03111400	-3.16706600
H	4.37381200	-2.01336600	-4.10391900
O	-3.07407700	0.29637900	0.96370200
C	-3.01659200	-1.74955000	0.91117800
H	-3.19921400	-1.88839700	1.96786000
C	-4.02606800	0.89490200	-1.49344300
C	-5.29778500	0.83709600	-2.38895500
C	-5.44084800	1.65140200	0.52736800
C	-6.73763700	1.39265100	-0.29081400
C	-4.29911900	3.44682500	-1.01218400
C	-4.97739200	3.11970700	0.33544800
C	-3.40117100	2.31571000	-1.54386300
C	-6.57063900	1.51215400	-1.81942000
H	-3.28286700	0.22611900	-1.96356000
H	-5.53620000	-0.20836400	-2.59951900
H	-5.07683000	1.28795500	-3.37136700
H	-5.72475100	1.56740700	1.58776400
H	-7.52614100	2.09504100	0.02553800
H	-7.12544700	0.39216100	-0.06225600
H	-3.69382000	4.35839100	-0.89759000
H	-5.05076900	3.69670400	-1.76740700
H	-4.27993700	3.37353400	1.13564100
H	-5.83668500	3.79765600	0.47095700
H	-3.11806500	2.56423400	-2.58020100
H	-2.47390000	2.31738600	-0.96399900
H	-7.45225000	1.07577500	-2.31111700
H	-6.58680300	2.57107300	-2.09529000
B	-4.31169900	0.51371700	0.08500700
N	-4.95147800	-0.98034500	0.37644300
C	-5.48155200	-1.89625200	-0.56410400
C	-6.72856100	-2.53333100	-0.39395800
C	-4.70524700	-2.29487300	-1.67590700
C	-7.18676900	-3.48544100	-1.30466100
H	-7.36430200	-2.26916100	0.44258000
C	-5.16796200	-3.24668600	-2.58055000
H	-3.73764700	-1.83343000	-1.83198800
C	-6.41328000	-3.85328400	-2.40478700
H	-8.16189000	-3.94038300	-1.14733700
H	-4.54476400	-3.51816900	-3.42968500
H	-6.77145400	-4.59849100	-3.10979700

C	-5.59642100	-1.06211000	1.69457500
H	-5.62729000	-2.10255300	2.04314200
H	-5.01329600	-0.46779100	2.39579400
H	-6.62211300	-0.67325300	1.69291800
H	-1.98488900	-1.53138400	0.68742500
H	-3.38525400	-2.56443800	0.29167700

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C	-1.40720100	-2.23620000	-2.02839100
C	-0.50812700	-0.81429700	0.33324100
C	-0.09724500	-2.75259300	-2.67933600
C	-0.88150000	-3.63483800	0.10490500
C	0.43963500	-4.10943900	-0.55334200
C	-2.60069300	-4.54414400	-1.65541900
C	-2.08741200	-4.56304300	-0.19455500
C	-2.62117300	-3.15376600	-2.33647300
C	0.45663000	-4.06630200	-2.09350900
H	-1.62500900	-1.26186500	-2.49485300
H	-1.15100700	0.03721600	0.07845200
H	0.67091200	-1.97848200	-2.55644900
H	-0.22526500	-2.87319800	-3.76780900
H	-0.72624500	-3.66888000	1.19789300
H	0.70114700	-5.12897700	-0.22511300
H	1.25216800	-3.46125400	-0.18938800
H	-3.61772600	-4.96107700	-1.67740100
H	-2.00028300	-5.23406100	-2.25798000
H	-2.90807800	-4.24827000	0.46546300
H	-1.86116800	-5.60679900	0.08140800
H	-2.72933200	-3.30309700	-3.42337800
H	-3.53058200	-2.62650000	-2.01877400
H	1.49060400	-4.21279700	-2.44516200
H	-0.10152200	-4.91847000	-2.49200400
C	0.89079300	-0.36279000	0.10076900
C	1.47524600	0.19943100	-1.01976200
C	3.07396100	0.08528600	0.57611600
C	4.33436100	0.33454300	1.31144400
C	4.30553000	0.81948200	2.63478600
C	5.59535600	0.14476100	0.71205700
C	5.48373200	1.09174000	3.32614200
H	3.36347500	0.99061300	3.13301800
C	6.77002900	0.41627100	1.41020500

H	5.67192300	-0.21664900	-0.30156500
C	6.72400500	0.88969100	2.72119300
H	5.42419900	1.46788900	4.34329000
H	7.72532800	0.25194200	0.92016900
H	7.64162200	1.10055400	3.26275400
C	3.82504400	0.87026100	-1.67173100
C	4.14159200	2.24076600	-1.69776300
C	4.43827000	-0.07996200	-2.52396300
C	5.14700700	2.65034400	-2.58413700
C	5.44148300	0.39163700	-3.37786100
C	5.79995100	1.73804100	-3.40383900
H	5.41764900	3.70090800	-2.62921200
H	5.94401400	-0.30407100	-4.04198100
H	6.58167400	2.07647200	-4.07840700
C	0.81150100	0.77391900	-2.21429300
C	-0.24997500	1.67282500	-2.00353300
C	1.19621300	0.49725800	-3.53451900
C	-0.91343100	2.26438300	-3.07728000
H	-0.55941300	1.91981500	-0.99319000
C	0.53895100	1.09619800	-4.60812200
H	1.99673400	-0.20217400	-3.73058000
C	-0.51884500	1.97824500	-4.38509500
H	-1.73686400	2.94460600	-2.88264500
H	0.84977900	0.86132800	-5.62240000
H	-1.03517500	2.43627700	-5.22408800
C	1.66742300	-0.70137500	2.49331200
C	0.94768700	0.23770200	3.27502800
C	2.20051400	-1.88728900	3.04191700
C	0.80075000	-0.03992200	4.63895400
C	2.02210900	-2.09920200	4.41602400
C	1.33691900	-1.18927600	5.21013700
H	0.25644800	0.66165500	5.26310000
H	2.42802300	-2.99960300	4.86616100
H	1.21256400	-1.37794600	6.27293500
B	-1.25148500	-2.13904500	-0.41162800
N	1.89737900	-0.38653700	1.08724000
N	2.83196600	0.40357300	-0.71988000
C	0.34285800	1.53760900	2.73595700
H	0.43312100	1.54133200	1.64646400
C	-1.15813000	1.64939200	3.07160600
H	-1.59124000	2.52511500	2.57915300
H	-1.72169100	0.77485000	2.73780000
H	-1.32271400	1.76481800	4.14887000
C	1.08853500	2.78375300	3.26021200

H	1.05586400	2.83621400	4.35466400
H	2.14003100	2.80050600	2.95390500
H	0.61303700	3.69070100	2.87067300
C	2.95706600	-2.94621800	2.24345100
H	2.91490200	-2.67560900	1.18339300
C	4.44150000	-3.02778300	2.65754400
H	4.96097100	-3.77018500	2.04034600
H	4.95734500	-2.07064900	2.54756700
H	4.53891200	-3.34285200	3.70309700
C	2.29959600	-4.33329700	2.39193400
H	1.23487900	-4.30476400	2.14924500
H	2.78238000	-5.04918400	1.71790800
H	2.40796900	-4.71723700	3.41281800
C	4.05282300	-1.56482900	-2.55388600
H	3.05257900	-1.66486800	-2.12044400
C	3.98147100	-2.12498000	-3.98987000
H	4.97850700	-2.24334900	-4.42930400
H	3.51253800	-3.11419600	-3.97246600
H	3.39618800	-1.48779300	-4.66001500
C	5.00166600	-2.45306600	-1.72007600
H	4.96746300	-2.21885000	-0.65257200
H	4.71684500	-3.50482500	-1.83417800
H	6.03953400	-2.34812900	-2.05910600
C	3.43865400	3.27974200	-0.82912300
H	2.70880800	2.76315200	-0.19787700
C	2.65597400	4.28773100	-1.69489800
H	2.12027700	4.99653100	-1.05338500
H	3.32774600	4.86539800	-2.34040900
H	1.92226800	3.78389600	-2.33092200
C	4.42486900	4.00662400	0.10649300
H	4.97481400	3.30367300	0.74004400
H	5.15682800	4.59304900	-0.46089200
H	3.88093200	4.70070600	0.75719000
O	-4.76792000	1.09676000	1.20496300
C	-3.96263100	2.94119500	-0.49557300
C	-5.05321700	3.49698600	-1.44911600
C	-5.45236800	3.58875200	1.55984900
C	-6.52789100	4.15001800	0.59322200
C	-3.43519500	5.10803200	0.87782800
C	-4.38251700	4.62085800	1.99764600
C	-2.91110600	3.99060600	-0.05368500
C	-6.02068600	4.52473700	-0.81859400
H	-3.42659300	2.14737700	-1.04321800
H	-5.64395700	2.63948900	-1.80692700

H	-4.60635000	3.94743000	-2.35373200
H	-5.97187500	3.24790000	2.46761500
H	-7.03732500	5.02870200	1.02565900
H	-7.30547600	3.37821600	0.48655500
H	-2.57709800	5.62769300	1.33140700
H	-3.94287400	5.86952700	0.27726300
H	-3.77386000	4.15105300	2.78700400
H	-4.84553600	5.50525100	2.46889500
H	-2.42110800	4.46660500	-0.92304100
H	-2.10815700	3.45122800	0.47726300
H	-6.88495000	4.65537500	-1.48671700
H	-5.53636100	5.50664300	-0.78525400
B	-4.71574400	2.34556800	0.82057400
N	-4.65588500	-1.74338000	0.99653800
C	-5.81839700	-2.08380100	0.22833800
C	-6.19650500	-3.42308600	0.08777900
C	-6.57935900	-1.06225600	-0.35009000
C	-7.33753400	-3.74215300	-0.64864400
H	-5.59067200	-4.20382400	0.53939900
C	-7.71217300	-1.39476200	-1.09401100
H	-6.27471300	-0.03429700	-0.16743700
C	-8.09357700	-2.72992300	-1.24488400
H	-7.62879200	-4.78261900	-0.76580200
H	-8.30757300	-0.60457800	-1.54392500
H	-8.97939600	-2.98224500	-1.82189700
C	-4.72131000	-1.86392300	2.45713900
H	-3.73683500	-2.13905100	2.84951700
H	-5.03485000	-0.89925200	2.87021300
H	-5.43634500	-2.64296600	2.72605500
C	-3.70770700	-0.95680700	0.47937800
H	-2.46170800	-1.89180300	0.04615700
H	-3.82915600	-0.59172600	-0.52914700
H	-3.08636900	-0.39464100	1.15365300
H	-0.62924600	-0.97531600	1.40950000

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C	-0.43152500	-2.36813900	0.05706200
C	-0.54624800	-3.15074900	1.40927500
C	-3.07502600	-2.05873500	0.06174000
C	-3.13329400	-2.84815100	1.41727600
C	-1.94865900	-3.89286600	-1.46199800

C	-3.14956400	-2.94736200	-1.23066500
C	-0.56208300	-3.24722200	-1.23363200
C	-1.93000200	-3.77560500	1.70253700
H	0.52506900	-1.81057600	0.03286700
H	-0.28322300	-2.45409400	2.21650600
H	0.22370100	-3.93358800	1.42882600
H	-3.90967800	-1.35008600	0.04091500
H	-4.06523100	-3.42952400	1.44348900
H	-3.21543600	-2.10821800	2.22540800
H	-1.99942900	-4.26665700	-2.49289100
H	-2.05330400	-4.77709000	-0.82739700
H	-3.24290000	-2.27042300	-2.09145200
H	-4.08100000	-3.52938800	-1.20151500
H	0.20872400	-4.02893900	-1.20560900
H	-0.31078600	-2.61191500	-2.09361800
H	-1.96763700	-4.07175000	2.75889300
H	-2.04344900	-4.70444500	1.13676500
B	-1.65281800	-1.46896300	0.02832000
O	1.52256100	-0.08301100	-0.01035500
C	3.39587200	1.74357500	-0.10083300
C	4.20951500	2.01095800	1.19270500
C	4.03901100	-0.79208200	0.03765100
C	4.84800200	-0.50565400	1.33011000
C	5.29787800	0.78996300	-1.62482900
C	4.85002900	-0.64802600	-1.27723900
C	4.21150600	1.86917900	-1.41462200
C	5.29592400	0.96143300	1.51950900
H	2.58835500	2.49197800	-0.14233500
H	3.49572800	2.04141400	2.03116200
H	4.67980200	3.00860100	1.16631500
H	3.68558800	-1.83338300	0.09422100
H	5.73703000	-1.15590800	1.39306800
H	4.21342400	-0.78649400	2.18526000
H	5.62902600	0.81694500	-2.67345800
H	6.18578900	1.04740400	-1.03835900
H	4.21669500	-1.02066100	-2.09750400
H	5.73931800	-1.30091000	-1.26764000
H	4.68241100	2.86358700	-1.49545600
H	3.49869300	1.80941900	-2.25218700
H	5.62662800	1.10226000	2.55915100
H	6.18403100	1.15374900	0.90888900
B	2.79896100	0.24263100	-0.02183200
N	-1.39774500	1.65161200	-0.06610600
C	-2.63129600	2.36329900	-0.07090300

C	-3.63435200	2.11385900	-1.01834100
C	-2.83513300	3.36231300	0.89421800
C	-4.81935000	2.85167200	-0.99362400
H	-3.50424700	1.33991000	-1.76731200
C	-4.02542700	4.08354900	0.91851200
H	-2.04463500	3.58968300	1.60317400
C	-5.02455900	3.83411300	-0.02596000
H	-5.58799400	2.64583600	-1.73359000
H	-4.16460400	4.85690000	1.66879100
H	-5.94864800	4.40432800	-0.01047200
C	-0.98572400	0.97691800	1.11453500
H	-1.45193400	-0.11498800	1.01878100
H	0.09508600	0.76571600	1.09267600
H	-1.38233100	1.40727700	2.03330800
C	-0.98093000	0.89148900	-1.17969700
H	-1.47030700	-0.19219500	-1.03140800
H	-1.31758400	1.28022300	-2.14022200
H	0.09486200	0.65409200	-1.09962500

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C	2.82551800	-1.88980600	0.15500000
C	3.67958900	-2.21183700	-1.10323800
C	3.12745200	0.66740000	-0.24334900
C	3.90071100	0.32514400	-1.55625200
C	4.63256900	-0.56403500	1.51360200
C	4.02723900	0.76640100	1.01971400
C	3.64880800	-1.74823200	1.47078800
C	4.57816300	-1.05838900	-1.59790900
H	2.15188300	-2.74019600	0.31499500
H	2.99002500	-2.48605400	-1.91684400
H	4.29679100	-3.10515700	-0.92434600
H	2.68328500	1.65131000	-0.40234400
H	4.65725400	1.10169800	-1.74250800
H	3.19040500	0.39705900	-2.39394000
H	4.98828700	-0.43390000	2.54461500
H	5.52414800	-0.80882400	0.92889100
H	3.41665400	1.19200800	1.82924400
H	4.83682600	1.49067800	0.84525700
H	4.19668700	-2.68263500	1.66429600

H	2.93601100	-1.64403400	2.30371400
H	4.89435900	-1.26957200	-2.62840600
H	5.50145200	-1.03147100	-1.01201500
B	2.06051400	-0.50066300	-0.05860800
O	0.69825000	-0.42989900	-0.11980500
C	-0.24055700	-2.20463500	-0.61206900
H	-0.19559400	-2.82313600	0.27561400
C	-1.01994700	1.28427700	-1.23755800
C	-2.35058600	2.06871000	-1.04740100
C	-0.46964800	1.59409000	1.27732000
C	-1.88627400	2.18839200	1.50288100
C	0.52192300	3.25774500	-0.50837800
C	0.56251700	2.69854800	0.93622300
C	0.15174100	2.23207500	-1.60137600
C	-2.47977100	2.88296400	0.26203200
H	-1.15077900	0.63725700	-2.12002800
H	-3.18487700	1.36183500	-1.08619300
H	-2.50102100	2.74801400	-1.90111600
H	-0.14719900	1.16898900	2.23992300
H	-1.86166300	2.91118500	2.33294000
H	-2.56980500	1.38873900	1.82166400
H	1.49940400	3.70068000	-0.74794500
H	-0.18466200	4.09189300	-0.55780600
H	1.56004200	2.29561700	1.13445900
H	0.44842500	3.53895600	1.63894700
H	-0.08977000	2.78227200	-2.52376900
H	1.02824100	1.61913500	-1.84423500
H	-3.54268100	3.09579800	0.44223000
H	-2.00675200	3.86275300	0.14409800
B	-0.60724200	0.46164000	0.10430500
N	-1.53090400	-0.76108300	0.58262500
C	-2.86054000	-1.04909600	0.19144400
C	-3.85760900	-1.40261500	1.12734000
C	-3.22049100	-1.09094200	-1.17508200
C	-5.14133400	-1.75866700	0.71820500
H	-3.64442800	-1.37651400	2.18881500
C	-4.50506600	-1.45181300	-1.57517500
H	-2.49452700	-0.81652000	-1.92939500
C	-5.47766500	-1.79195000	-0.63480400
H	-5.88400900	-2.00980200	1.47119200
H	-4.74175800	-1.46741200	-2.63590000
H	-6.47761300	-2.07543800	-0.95006600
C	-1.20858200	-1.21055000	1.94407100
H	-1.53995400	-2.24446700	2.09746800

H	-0.12862200	-1.16320100	2.08262400
H	-1.67447900	-0.58512700	2.71579300
H	0.63075100	-2.27669100	-1.24845600
H	-1.17572100	-2.23290000	-1.15608200

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