BOROX Catalysis: Self-assembled AMINO-BOROX and IMINO-BOROX Chiral Brønsted Acids in a Five Component Catalyst Assembly/Catalytic Asymmetric Aziridination

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Supporting Information

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A. General Information

All reactions were carried out in flame-dried glassware under an atmosphere of nitrogen unless otherwise indicated. Toluene was distilled from sodium under nitrogen. $CHCl_3$ was treated with potassium hydroxide and then distilled from calcium hydride under nitrogen. Hexanes and ethyl acetate were ACS grade and used as purchased.

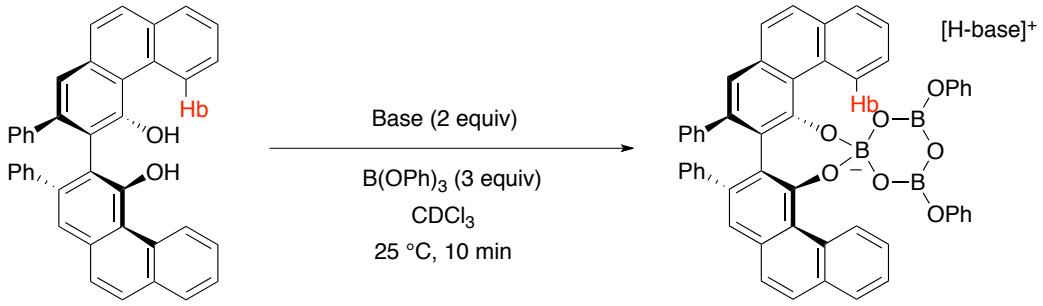
IR spectra were recorded in KBr matrix (for solids) and on NaCl disc (for liquids). ^1H NMR and ^{13}C NMR were recorded using $CDCl_3$ as solvent (unless otherwise noted) with the residual solvent peak as the internal standard (^1H NMR : 7.24 ppm, ^{13}C NMR : 77 ppm). Chemical shifts were reported in parts per million. Low-resolution Mass Spectrometry and High Resolution Mass Spectrometry were performed. Analytical thin-layer chromatography (TLC) was performed on Silicycle silica gel plates with F-254 indicator. Visualization was by short wave (254 nm) and long wave (365 nm) ultraviolet light, or by staining with phosphomolybdic acid in ethanol or with potassium permanganate. Column chromatography was performed with silica gel 60 (230 – 450 mesh). Chiral HPLC data for the aziridines were obtained using a CHIRALCEL OD-H column.

Optical rotations were obtained at a wavelength of 589 nm (sodium D line) using a 1.0 decimeter cell with a total volume of 1.0 mL. Specific rotations are reported in degrees per decimeter at 20 °C and the concentrations are given in gram per 100 mL in ethyl acetate unless otherwise noted.

All reagents were purified by simple distillation or crystallization with simple solvents unless otherwise indicated. Ethyl diazoacetate **2** and triphenylborate **8** obtained from Aldrich Chemical Co., Inc. and used as received. VAPOL and VANOL were made according to published procedure.[1] Imine **1a** and bis-(3,5-di-methyl-4-methoxyphenyl)methanamine **6** (MEDAM amine) was made according to the published procedure.[2] Imine 1a′ was made according to the published procedure.[4]

B. NMR analysis of a mixture of VAPOL, and $B(OPh)_3$ and different bases:

As shown in Table 1 of the manuscript, a mixture of (*S*)-VAPOL and $B(OPh)_3$ gives different yields of unreacted VAPOL **3**, mesoborate B1 **10** and pyroborate B2 **11** employing different bases. Also, it was evident from the ^1H NMR and ^{11}B NMR that no boroxinate B3 **9** was formed unless a base was added (characteristic peaks i.e δ 10.2-10.4 and δ 5.5-5.7 were missing in ^1H NMR and ^{11}B NMR respectively). The amount of B3 **9** differs with respect to different bases depending upon the strength of the bases. The analysis was carried out by mixing (*S*)-VAPOL (0.1 mmol) with $B(OPh)_3$ (0.3 mmol, 3 equiv) and base (0.2 mmol, 50 mol % catalyst loading) at room temperature in $CDCl_3$. The yields of boroxinate B3 **9** were determined by integration against an internal standard (Ph_3CH). In most of the cases, an additional peak at δ 1.2-2.4 in ^{11}B NMR was also observed (for example; see Figure 3). This peak is tentatively assigned to be of the tetraphenoxy borate salt of the base involved (unpublished results by Gupta, A. K. and Wulff, W. D.).



(*S*)-VAPOL **3**
(1 equiv)
δ = 9.77 ppm
(Hb)

B3 **9** BOROX catalyst
δ = 10.2-10.4 ppm
(Hb)

Procedure: To a 10 mL flame-dried single-necked round bottom flask, equipped with a stir bar and a rubber septum and filled with argon was added (*S*)-VAPOL **3** (54 mg, 0.10 mmol, 1.0 equiv), $B(OPh)_3$ (87 mg, 0.30 mmol, 3.0 equiv), base (0.20 mmol, 2.0 equiv), Ph_3CH (12.2 mg, 0.500 mmol) and $CDCl_3$ (1 mL). The resultant mixture was stirred for 10 min at room temperature. The resulting solution was then directly transferred to a quartz NMR tube (freshly flame-dried) and was subjected to NMR analysis.

^{1}H and ^{11}B NMR spectra for AMINO-BOROX catalyst **9d** is shown as an example:

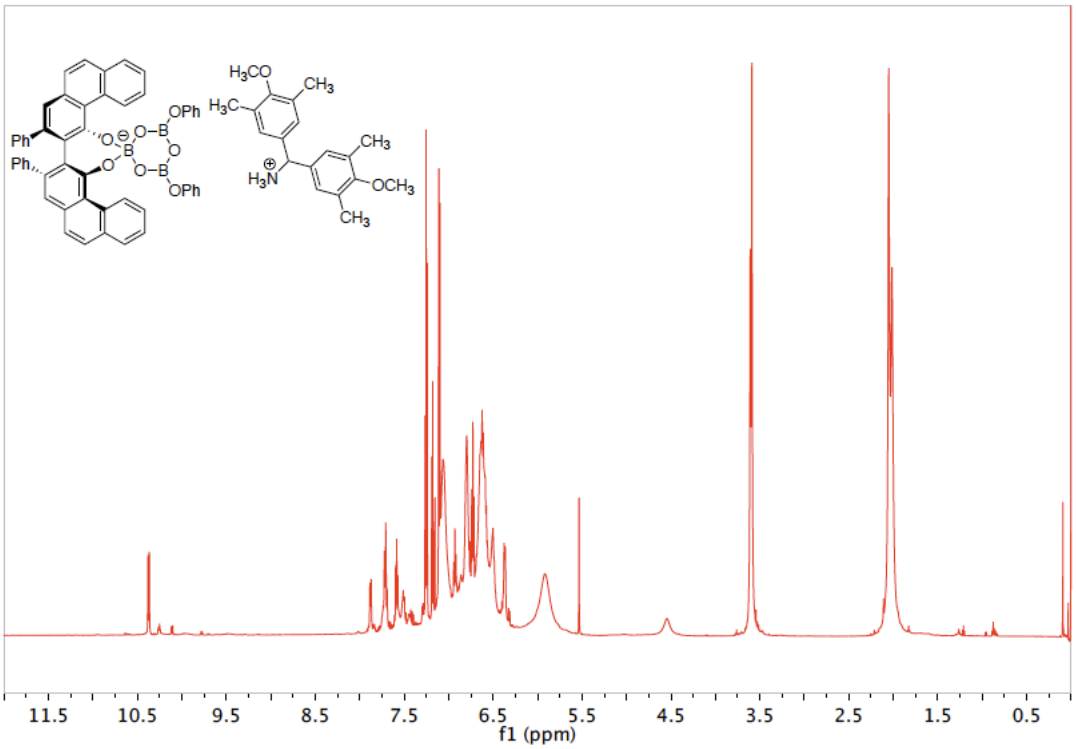


Figure 1: ^{1}H NMR of AMINO-BOROX catalyst **9d**.

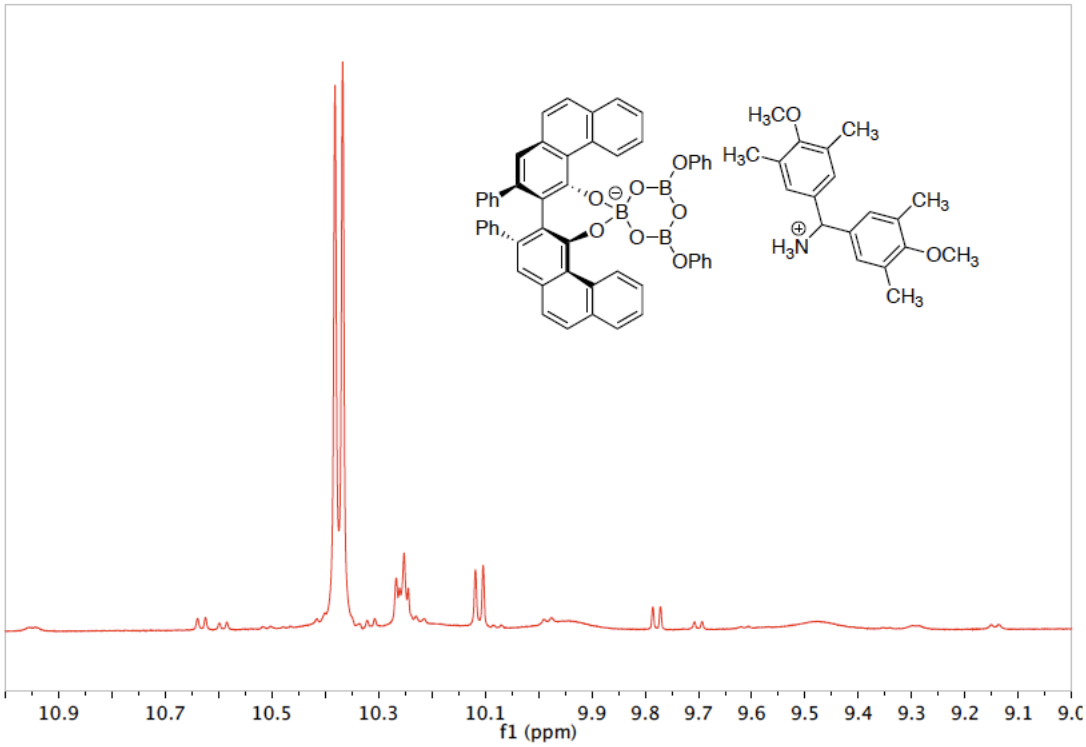


Figure 2: ^{1}H NMR of the bay region of AMINO-BOROX catalyst **9d**.

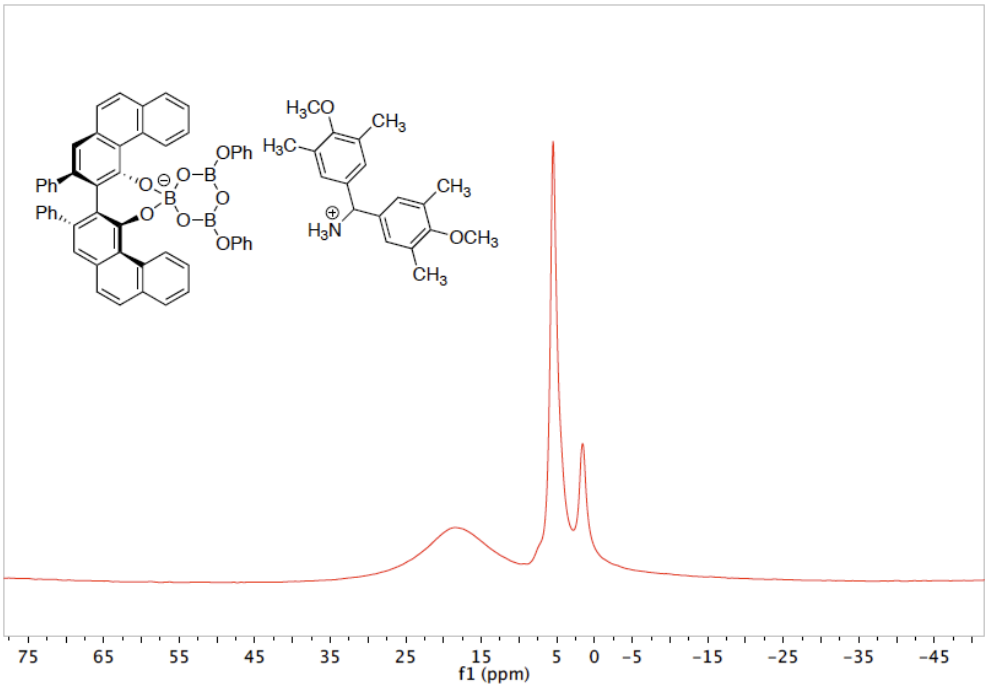
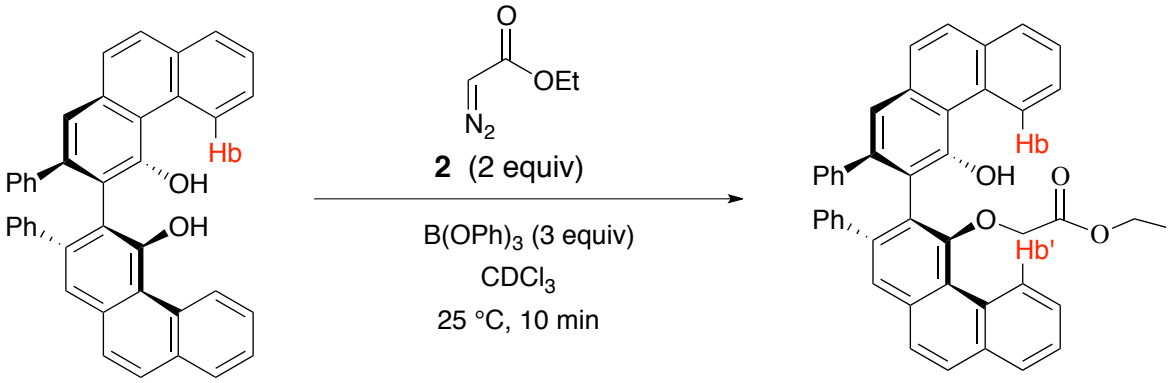


Figure 3: ^{11}B NMR of AMINO-BOROX catalyst **9d**.

Entry 6 of Table 1 in the manuscript:



(*S*)-VAPOL **3**
(1 equiv)
δ = 9.77 ppm
(Hb)

mono-alkylated (*S*)-VAPOL derivative **12**
δ = 9.56 ppm and 9.83 ppm
(Hb and Hb')

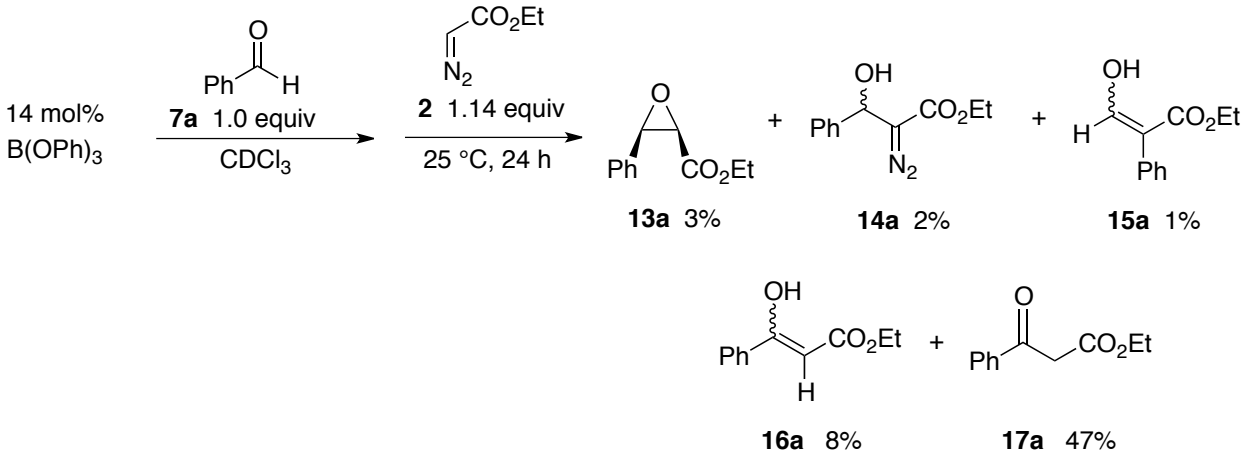
Procedure: To a 10 mL flame-dried round bottom flask, equipped with a stir bar and a rubber septum and filled with argon was added (*S*)-VAPOL **3** (54 mg, 0.10 mmol, 1.0 equiv), $B(OPh)_3$

(87 mg, 0.30 mmol, 3.0 equiv), ethyl diazoacetate **2** (0.20 mmol, 2.0 equiv.), Ph_3CH (12.2 mg, 0.500 mmol) and $CDCl_3$ (1 mL). The resultant mixture was stirred for 10 min at room temperature. The resulting solution was then directly transferred to a quartz NMR tube (freshly flame-dried) and was subjected to NMR analysis. The reaction furnished the mono-alkylated adduct **12** in 80 % yield as determined by integration against an internal standard (Ph_3CH) and with the aid of the spectral data previously published for this compound.[3,4]

C. NMR analysis of a mixture of PhCHO 7a and EDA 2 in different reaction conditions:

As discussed in the manuscript, benzaldehyde and ethyl diazoacetate react with each other in presence of Lewis acids and Brønsted acids resulting in the formation of several products. It was thought to examine the possibility of these products under the reaction conditions of a possible **m**ulti**c**omponent **az**iridination (MCAZ).

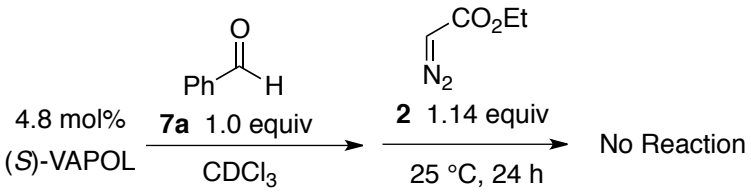
(a) with $B(OPh)_3$:



Procedure: To a 10 mL flame-dried single-necked round bottom flask, equipped with a stir bar and a rubber septum and filled with argon was added $B(OPh)_3$ (22 mg, 0.075 mmol, 0.14 equiv), benzaldehyde **7a** (52.0 µL, 0.525 mmol, 1.00 equiv), ethyl diazoacetate **2** (62.0 µL, 0.600 mmoL, 1.14 equiv), Ph_3CH (12.2 mg, 0.500 mmol) and $CDCl_3$ (1 mL). The resultant mixture was stirred for 24 h at room temperature. The resulting solution was then directly transferred to a NMR tube and was then subjected to NMR analysis. Several products were observed as shown in the reaction. The presence of each product was confirmed by characteristic peaks (δ 3.83 **13a**[5], δ 5.91 **14a**[6], δ 12.20 **15a**[7], δ 12.61 **16a**[8], δ 3.98 **17a**[7]) in the ^1H NMR previously published for these

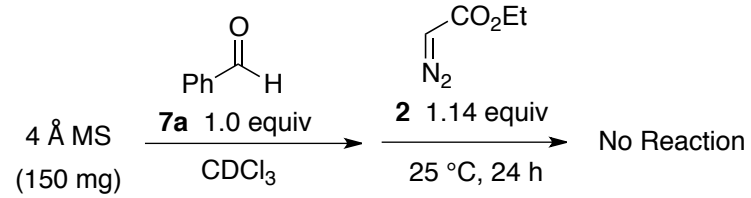
compounds and the amount of each was quantified by integration against an internal standard (Ph_3CH). There was also 5 % of unreacted benzaldehyde **7a**.

(b) with (*S*)-VAPOL:



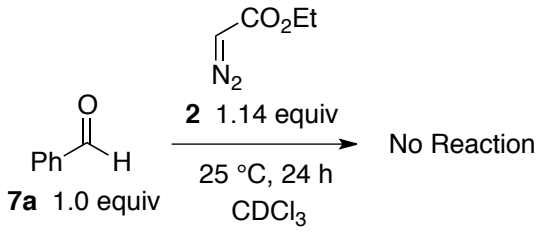
Procedure: To a 10 mL flame-dried single-necked round bottom flask, equipped with a stir barand a rubber septum and filled with argon was added (*S*)-VAPOL **3** (14 mg, 0.025 mmol, 0.048 equiv), benzaldehyde **7a** (52.0 μL, 0.525 mmol, 1.00 equiv), ethyl diazoacetate **2** (62.0 μL, 0.600 mmoL, 1.14 equiv), Ph_3CH (12.2 mg, 0.500 mmol) and $CDCl_3$ (1 mL). The resultant mixture was stirred for 24 h at room temperature. The resulting solution was then directly transferred to a NMR tube and was then subjected to NMR analysis. The crude NMR revealed the presence of unreacted starting materials.

(c) with 4 Å Molecular Seives :



Procedure: To a 10 mL flame-dried single-necked round bottom flask, equipped with a stir bar and a rubber septum and filled with argon was added 4 Å Molecular Seives (150 mg, freshly flame-dried), benzaldehyde **7a** (52.0 μL, 0.525 mmol, 1.00 equiv.), ethyl diazoacetate **2** (62.0 μL, 0.600 mmoL, 1.14 equiv), Ph_3CH (12.2 mg, 0.500 mmol) and $CDCl_3$ (1 mL). The resultant mixture was stirred for 24 h at room temperature. The resulting solution was then directly transferred to a NMR tube utilizing a filter syringe (Corning® syringe filters, Aldrich) to remove the 4Å Molecular Sieves. It was then subjected to NMR analysis. The crude NMR revealed the presence of unreacted starting materials.

(d) without any catalyst/additive:

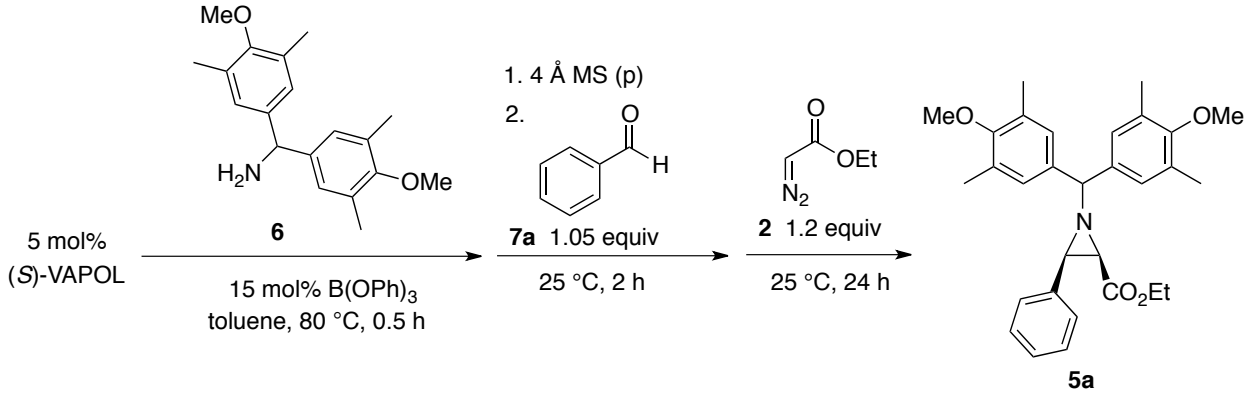


Procedure: To a 10 mL flame-dried single-necked round bottom flask, equipped with a stir bar and a rubber septum and filled with argon was added benzaldehyde **7a** (52.0 μL, 0.525 mmol, 1.00 equiv.), ethyl diazoacetate **2** (62.0 μL, 0.600 mmoL, 1.14 equiv), Ph_3CH (12.2 mg, 0.500 mmol) and $CDCl_3$ (1 mL). The resultant mixture was stirred for 24 h at room temperature. The resulting solution was then directly transferred to a NMR tube and was then subjected to NMR analysis. The crude NMR revealed the presence of unreacted starting materials.

D. Different protocols for MCAZ: Procedures (I, IIA-B, IIIA-C)

As shown in Table 2 of the manuscript, the present work represents a true multi-component aziridination reaction.

Procedure I: Catalyst @ 80 °C, 0.5 h and EDA 2 added after 2 h after the addition of aldehyde 7a.

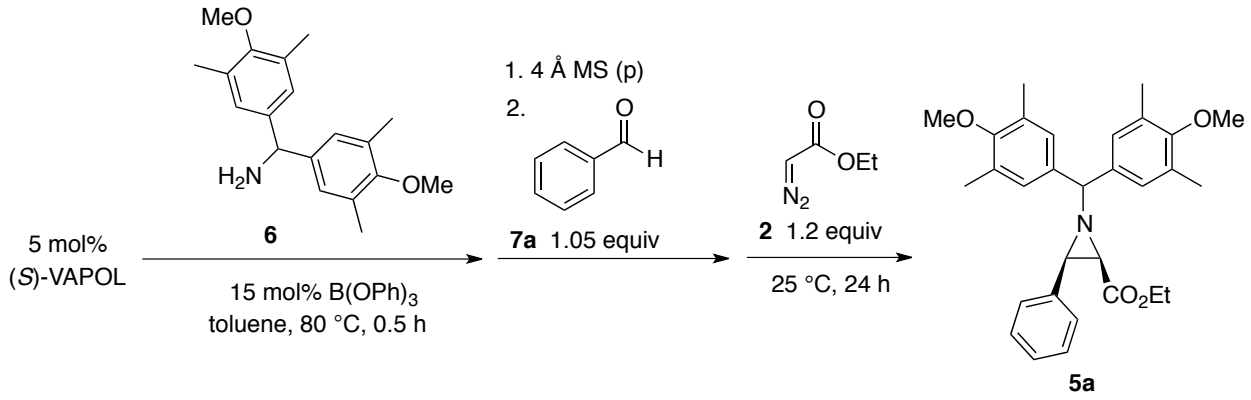


(2*R*,3*R*)-ethyl-1-(bis(4-methoxy-3,5-dimethylphenyl)methyl)-3-phenylaziridine-2-carboxylate 5a: To a 10 mL flame-dried home-made Schlenk flask, prepared from a single-necked 25 mL pear-shaped flask that had its 14/20 glass joint replaced with a high vacuum threaded Teflon valve, equipped with a stir bar and filled with argon was added (*S)*-VAPOL (14

mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol) and amine **6** (149.7 mg, 0.5000 mmol). Under an argon flow through the side-arm of the Schlenk flask, dry toluene (2 mL) was added. The flask was sealed by closing the Teflon valve, and then placed in an oil bath (80 ºC) for 0.5 h. The flask was then allowed to cool to room temperature and open to argon through side-arm of the Schlenk flask. To the flask containing the catalyst was added the 4Å Molecular Sieves (150 mg, freshly flame-dried) and aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv). The resulting mixture was allowed to stir for 2 h at ambient temperature. Thereafter, ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv) was added. The resulting mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The reaction mixture was then filtered through a Celite pad to a 100 mL round bottom flask. The reaction flask was rinsed with EtOAc (3 mL × 3) and the rinse was filtered through the same Celite pad. The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude aziridine as an off-white solid.

The *cis/trans* ratio was determined by comparing the ^{1}H NMR integration of the ring methine protons for each aziridine in the crude reaction mixture. The *cis* (J = 7-8 Hz) and the *trans* (J = 2-3 Hz) coupling constants were used to differentiate the two isomers. The yields of the acyclic enamine side products **18a** and **19a** were determined by ^{1}H NMR analysis of the crude reaction mixture by integration of the *N*-H proton relative to the that of the *cis*-aziridine methine protons with the aid of the isolated yield of the *cis*-aziridine. Purification of the crude aziridine by silica gel chromatography (30 mm × 300 mm column, 9:1 hexanes/EtOAc as eluent, gravity column) afforded pure cis-aziridine **5a** as a white solid (mp 107-108 ºC on 99.8% ee material) in 92 % isolated yield (218 mg, 0.460 mmol); *cis/trans*: >50:1. Enamine side products: <1 % yield of **18a** and <1% yield of **19a.** The optical purity of **5a** was determined to be 95 % *ee* by HPLC analysis (CHIRALCEL OD-H column, 99:1 hexane/2-propanol at 226nm, flow-rate: 0.7 mL/min): retention times; R_t = 9.26 min (major enantiomer, **5a**) and R_t = 12.52 min (minor enantiomer, *ent*-**5a**).

Procedure IIA: Catalyst @ 80 °C, 0.5 h and EDA 2 added immediately after the addition of the aldehyde 7a.

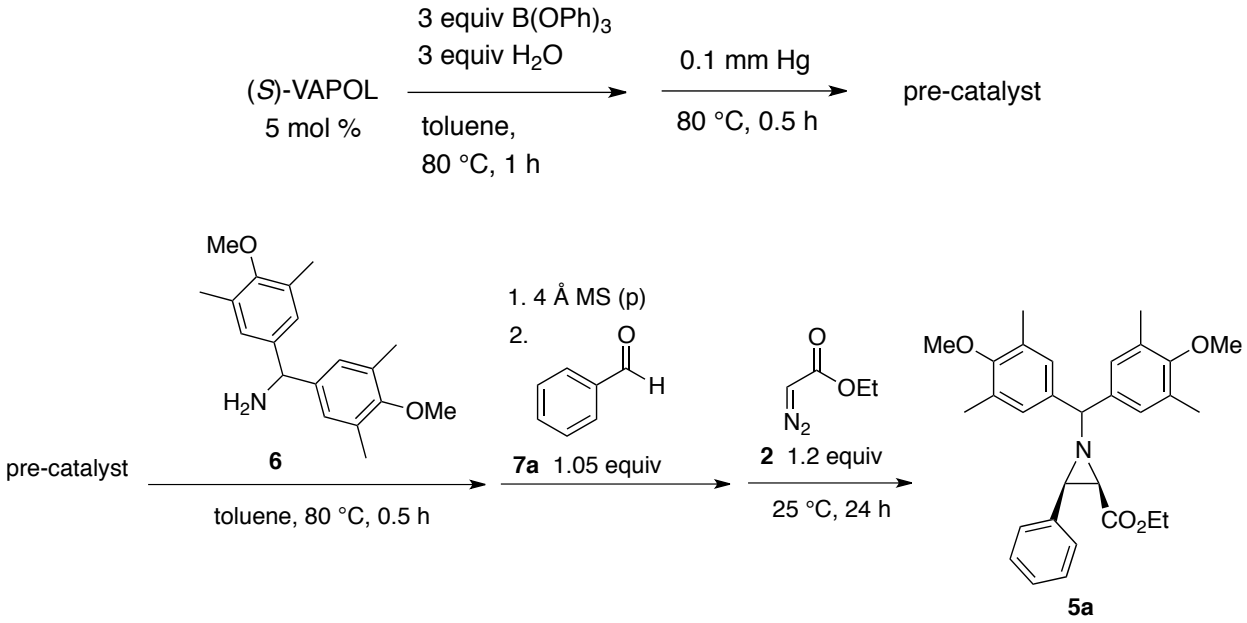


(2*R*,3*R*)-ethyl-1-(bis(4-methoxy-3,5-dimethylphenyl)methyl)-3-phenylaziridine-2-carboxylate 5a: To a 10 mL flame-dried home-made Schlenk flask, prepared from a single-necked 25 mL pear-shaped flask that had its 14/20 glass joint replaced with a high vacuum threaded Teflon valve, equipped with a stir bar and filled with argon was added (*S)*-VAPOL (14 mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol) and amine **6** (149.7 mg, 0.5000 mmol). Under an argon flow through the side-arm of the Schlenk flask, dry toluene (2 mL) was added. The flask was sealed by closing the Teflon valve, and then placed in an oil bath (80 ºC) for 0.5 h. The flask was then allowed to cool to room temperature and open to argon through side-arm of the Schlenk flask. To the flask containing the catalyst was added the 4Å Molecular Sieves (150 mg, freshly flame-dried) and aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv). To this solution was rapidly added ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv). The resulting mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The reaction mixture was then filtered through a Celite pad to a 100 mL round bottom flask. The reaction flask was rinsed with EtOAc (3 mL × 3) and the rinse was filtered through the same Celite pad. The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude aziridine as an off-white solid.

The *cis/trans* ratio was determined by comparing the ^{1}H NMR integration of the ring methine protons for each aziridine in the crude reaction mixture. The *cis* (J = 7-8 Hz) and the *trans* (J = 2-3 Hz) coupling constants were used to differentiate the two isomers. The yields of

the acyclic enamine side products **18a** and **19a** were determined by ^{1}H NMR analysis of the crude reaction mixture by integration of the *N*-H proton relative to the that of the *cis*-aziridine methine protons with the aid of the isolated yield of the *cis*-aziridine. Purification of the crude aziridine by silica gel chromatography (30 mm × 300 mm column, 9:1 hexanes/EtOAc as eluent, gravity column) afforded pure cis-aziridine **5a** as a white solid (mp 107-108 ºC on 99.8% ee material) in 97 % isolated yield (230 mg, 0.485 mmol); *cis/trans*: >50:1. Enamine side products: <1 % yield of **18a** and <1% yield of **19a.** The optical purity of **5a** was determined to be 98 % *ee* by HPLC analysis (CHIRALCEL OD-H column, 99:1 hexane/2-propanol at 226nm, flow-rate: 0.7 mL/min): retention times; R_t = 9.26 min (major enantiomer, **5a**) and R_t = 12.52 min (minor enantiomer, *ent*-**5a**).

Procedure IIB: Pre-catalyst followed by the addition of amine 6 and stirring @ 80 °C, 0.5 h and then EDA 2 added immediately after the addition of the aldehyde 7a.



(2*R*,3*R*)-ethyl-1-(bis(4-methoxy-3,5-dimethylphenyl)methyl)-3-phenylaziridine-2-carboxylate 5a: To a 10 mL flame-dried home-made Schlenk flask, prepared from a single-necked 25 mL pear-shaped flask that had its 14/20 glass joint replaced with a high vacuum threaded Teflon valve, equipped with a stir bar and filled with argon was added (*S)*-VAPOL (14 mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol). Under an argon flow through the side-arm of

the Schlenk flask, dry toluene (2 mL) was added through the top of the Teflon valve to dissolve the two reagents and this was followed by the addition of water (1.4 μL, 0.075 mmol). The flask was sealed by closing the Teflon valve, and then placed in an 80 ºC (oil bath) for 1 h. After 1 h, a vacuum (0.5 mm Hg) was carefully applied by slightly opening the Teflon valve to remove the volatiles. After the volatiles are removed completely, a full vacuum is applied and is maintained for a period of 30 min at a temperature of 80 ºC (oil bath). The flask was then allowed to cool to room temperature and opened to argon through the side-arm of the Schlenk flask. To the flask containing the pre-catalyst was added the amine **6** (149.7 mg, 0.5000 mmol) and then dry toluene (1 mL) under an argon flow through side-arm of the Schlenk flask. The flask was sealed by closing the Teflon valve, and then placed in an oil bath (80 ºC) for 0.5 h. The flask was then allowed to cool to room temperature and open to argon through side-arm of the Schlenk flask. To the flask containing the precatalyst was added the 4Å Molecular Sieves (150 mg, freshly flame-dried) and aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv). To this solution was rapidly added ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv). The resulting mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The reaction mixture was then filtered through a Celite pad to a 100 mL round bottom flask. The reaction flask was rinsed with EtOAc (3 mL × 3) and the rinse was filtered through the same Celite pad. The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude aziridine as an off-white solid.

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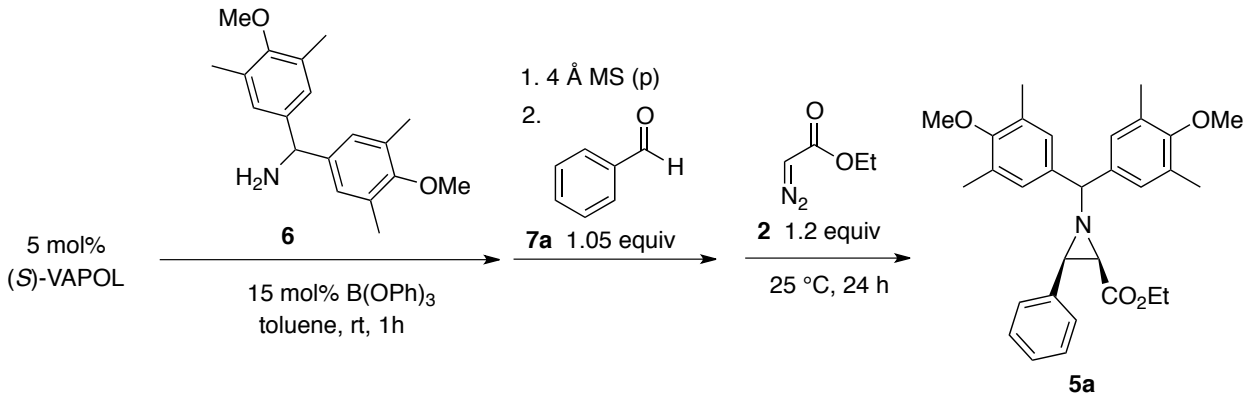
0.7 mL/min): retention times; R_t = 9.26 min (major enantiomer, **5a**) and R_t = 12.52 min (minor enantiomer, *ent*-**5a**).

Procedure IIIA: Catalyst @ 25 °C, 1 h and EDA 2 added immediately after the addition of the aldehyde 7a.



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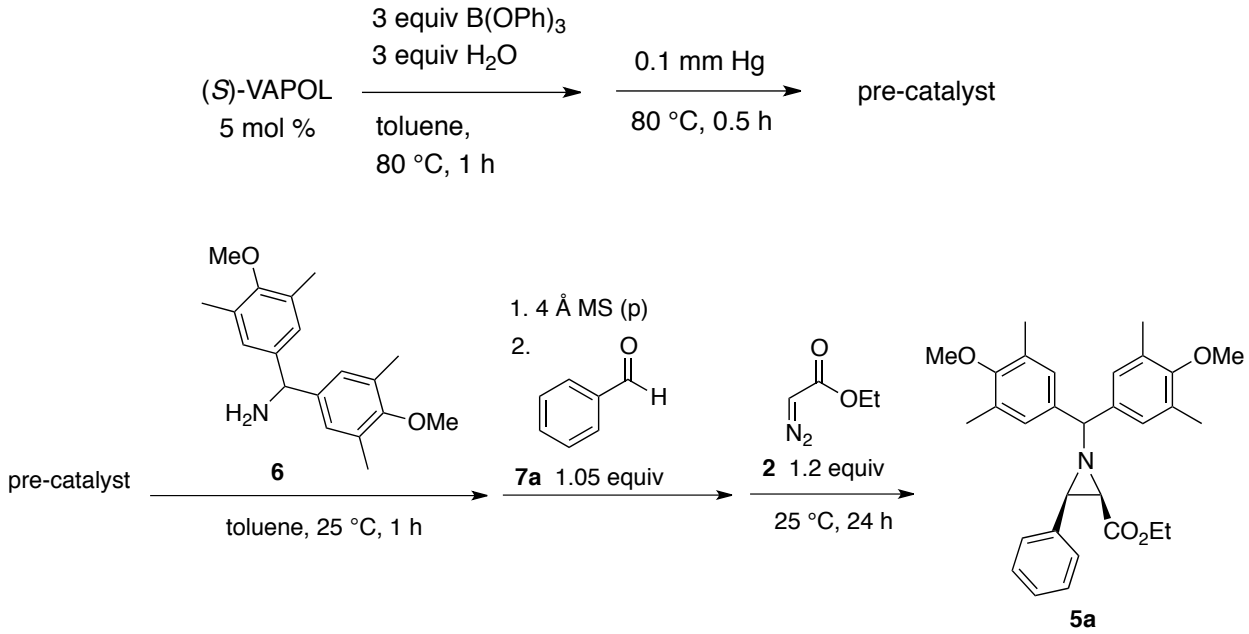
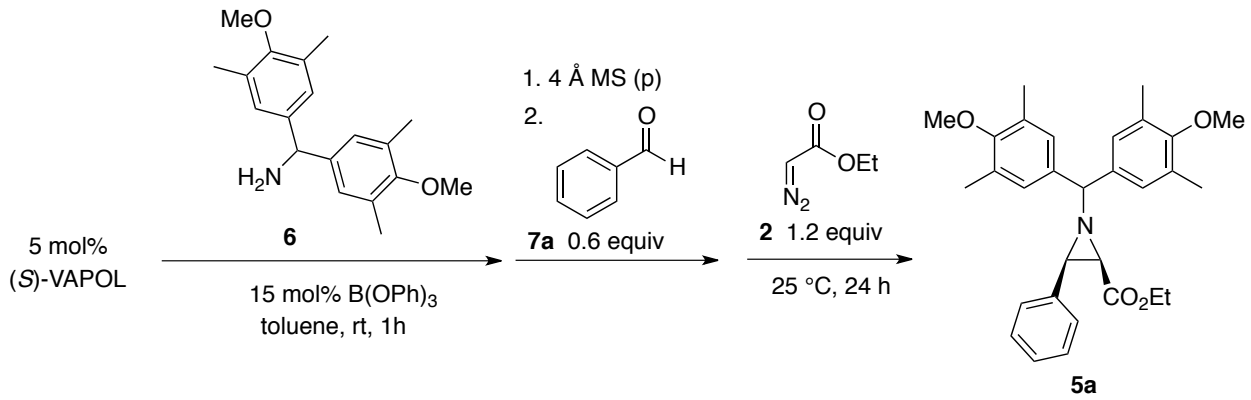


(2*R*,3*R*)-ethyl-1-(bis(4-methoxy-3,5-dimethylphenyl)methyl)-3-phenylaziridine-2-carboxylate 5a: To a 10 mL flame-dried home-made Schlenk flask, prepared from a single-necked 25 mL pear-shaped flask that had its 14/20 glass joint replaced with a high vacuum threaded Teflon valve, equipped with a stir bar and filled with argon was added (*S)*-VAPOL (14 mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol). Under an argon flow through the side-arm of the Schlenk flask, dry toluene (2 mL) was added through the top of the Teflon valve to dissolve the two reagents and this was followed by the addition of water (1.4 μL, 0.075 mmol). The flask

was sealed by closing the Teflon valve, and then placed in an 80 ºC (oil bath) for 1 h. After 1 h, a vacuum (0.5 mm Hg) was carefully applied by slightly opening the Teflon valve to remove the volatiles. After the volatiles are removed completely, a full vacuum is applied and is maintained for a period of 30 min at a temperature of 80 ºC (oil bath). The flask was then allowed to cool to room temperature and opened to argon through the side-arm of the Schlenk flask. To the flask containing the pre-catalyst was added the amine **6** (149.7 mg, 0.5000 mmol) and then dry toluene (1 mL) under an argon flow through side-arm of the Schlenk flask. The flask was sealed by closing the Teflon valve, and then the resulting mixture was allowed to stir at room temperature for 1 h. The flask was then open to argon through side-arm of the Schlenk flask. To the flask containing the catalyst was added the 4Å Molecular Sieves (150 mg, freshly flame-dried) and aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv). To this solution was rapidly added ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv). The resulting mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The reaction mixture was then filtered through a Celite pad to a 100 mL round bottom flask. The reaction flask was rinsed with EtOAc (3 mL × 3) and the rinse was filtered through the same Celite pad. The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude aziridine as an off-white solid.

The *cis/trans* ratio was determined by comparing the ^{1}H NMR integration of the ring methine protons for each aziridine in the crude reaction mixture. The *cis* (J = 7-8 Hz) and the *trans* (J = 2-3 Hz) coupling constants were used to differentiate the two isomers. The yields of the acyclic enamine side products **18a** and **19a** were determined by ^{1}H NMR analysis of the crude reaction mixture by integration of the *N*-H proton relative to the that of the *cis*-aziridine methine protons with the aid of the isolated yield of the *cis*-aziridine. Purification of the crude aziridine by silica gel chromatography (30 mm × 300 mm column, 9:1 hexanes/EtOAc as eluent, gravity column) afforded pure cis-aziridine **5a** as a white solid (mp 107-108 ºC on 99.8% ee material) in 94 % isolated yield (223 mg, 0.470 mmol); *cis/trans*: >50:1. Enamine side products: <1 % yield of **18a** and <1% yield of **19a.** The optical purity of **5a** was determined to be 98 % *ee* by HPLC analysis (CHIRALCEL OD-H column, 99:1 hexane/2-propanol at 226nm, flow-rate: 0.7 mL/min): retention times; R_t = 9.26 min (major enantiomer, **5a**) and R_t = 12.52 min (minor enantiomer, *ent*-**5a**).

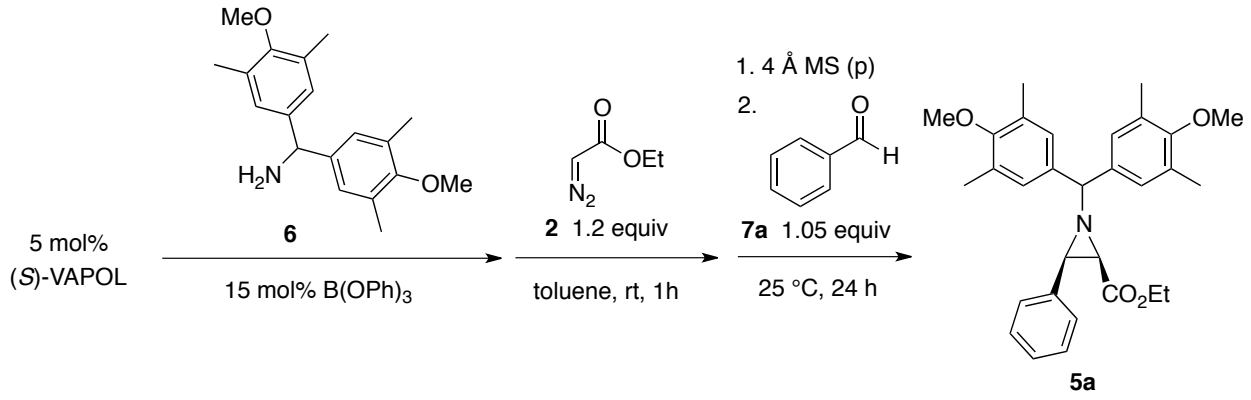
Procedure IIIC: Catalyst @ 25 °C, 1 h and EDA 2 added immediately after the addition of the aldehyde 7a (0.6 equiv with respect to amine 6).



(2*R*,3*R*)-ethyl-1-(bis(4-methoxy-3,5-dimethylphenyl)methyl)-3-phenylaziridine-2-carboxylate 5a: The procedure is exactly similar to procedure IIIA except that 0.6 equiv of benzaldehyde **7a** was added. No aziridine **5a** was observed from crude NMR analysis.

E. Different order of addition of reagents in MCAZ: Procedures (IV-VII)

Procedure IV: Catalyst + EDA 2 @ 25 °C, 1 h and then addition of the aldehyde 7a.

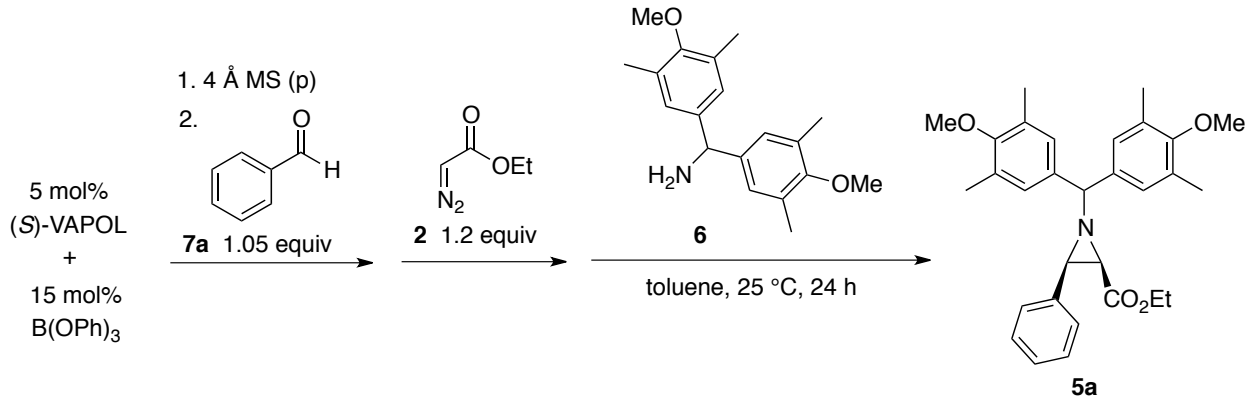


(2*R*,3*R*)-ethyl-1-(bis(4-methoxy-3,5-dimethylphenyl)methyl)-3-phenylaziridine-2-carboxylate 5a: To a 10 mL flame-dried single-necked round bottom flask equipped with a stir bar and filled with argon was added in the following order (*S)*-VAPOL (14 mg, 0.025 mmol),

$B(OPh)_3$ (22 mg, 0.075 mmol), amine **6** (149.7 mg, 0.5000 mmol) and ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv). Dry toluene (1 mL) was added under an argon atmosphere to dissolve the reagents. The flask was fitted with a rubber septum and a nitrogen balloon. The reaction mixture was stirred at room temperature for 1 h. Thereafter, 4Å Molecular Sieves (150 mg, freshly flame-dried) was added followed by the addition of the aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv). The resulting mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The reaction mixture was then filtered through a Celite pad to a 100 mL round bottom flask. The reaction flask was rinsed with EtOAc (3 mL × 3) and the rinse was filtered through the same Celite pad. The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude aziridine as an off-white solid.

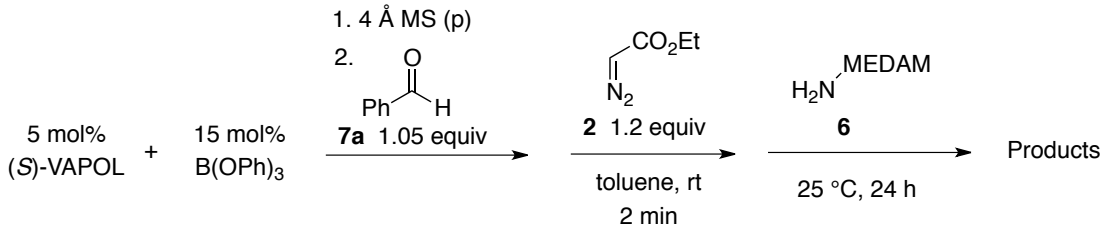
The *cis/trans* ratio was determined by comparing the ^{1}H NMR integration of the ring methine protons for each aziridine in the crude reaction mixture. The *cis* (J = 7-8 Hz) and the *trans* (J = 2-3 Hz) coupling constants were used to differentiate the two isomers. The yields of the acyclic enamine side products **18a** and **19a** were determined by ^{1}H NMR analysis of the crude reaction mixture by integration of the *N*-H proton relative to the that of the *cis*-aziridine methine protons with the aid of the isolated yield of the *cis*-aziridine. Purification of the crude aziridine by silica gel chromatography (30 mm × 300 mm column, 9:1 hexanes/EtOAc as eluent, gravity column) afforded pure cis-aziridine **5a** as a white solid (mp 107-108 ºC on 99.8% ee material) in 94 % isolated yield (223 mg, 0.47 mmol); *cis/trans*: >50:1. Enamine side products: <1 % yield of **18a** and <1 % yield of **19a.** The optical purity of **5a** was determined to be 98 % *ee* by HPLC analysis (CHIRALCEL OD-H column, 99:1 hexane/2-propanol at 226nm, flow-rate: 0.7 mL/min): retention times; R_t = 9.26 min (major enantiomer, **5a**) and R_t = 12.52 min (minor enantiomer, *ent*-**5a**).

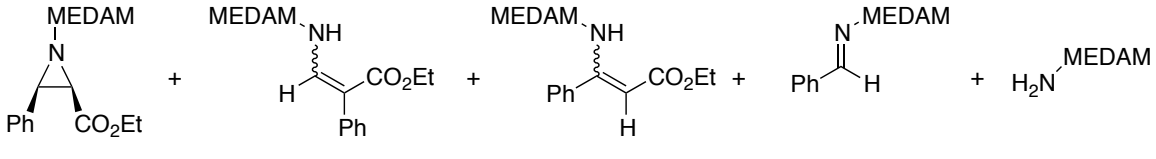
Procedure V: Amine 6 added at the end prior to the addition of toluene.

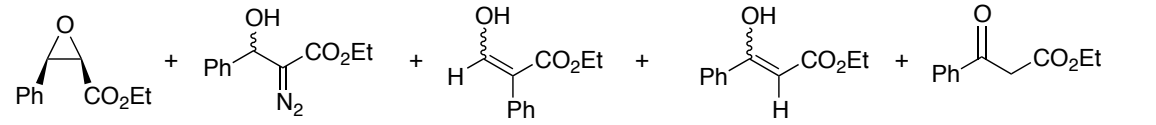


(2*R*,3*R*)-ethyl-1-(bis(4-methoxy-3,5-dimethylphenyl)methyl)-3-phenylaziridine-2-carboxylate 5a: To a 10 mL flame-dried single-necked round bottom flask equipped with a stir bar and filled with argon was added in following order (*S)*-VAPOL (14 mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol), 4Å Molecular Sieves (150 mg, freshly flame-dried), aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv), ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv) and amine **6** (149.7 mg, 0.5000 mmol). Dry toluene (1 mL) was added under an argon atmosphere to dissolve the reagents. The flask was fitted with a rubber septum and a nitrogen balloon. The reaction mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The reaction mixture was then filtered through a Celite pad to a 100 mL round bottom flask. The reaction flask was rinsed with EtOAc (3 mL × 3) and the rinse was filtered through the same Celite pad. The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude aziridine as an off-white solid. Purification of the crude aziridine by silica gel chromatography (30 mm × 300 mm column, 9:1 hexanes/EtOAc as eluent, gravity column) afforded pure cis-aziridine **5a** as a white solid (mp 107-108 ºC on 99.8% ee material) in 85 % isolated yield (201 mg, 0.430 mmol); *cis/trans*: >50:1. Enamine side products: 2 % yield of **18a** and 1 % yield of **19a.** The optical purity of **5a** was determined to be 98 % *ee* by HPLC analysis (CHIRALCEL OD-H column, 99:1 hexane/2-propanol at 226nm, flow-rate: 0.7 mL/min): retention times; R_t = 9.26 min (major enantiomer, **5a**) and R_t = 12.52 min (minor enantiomer, *ent*-**5a**). A repeat of this reaction also gave **5a** in 85 % yield. This is the ^{1}H NMR yield detemined by integration against an internal standard (Ph_3CH).

Procedure VI: Amine 6 added at the end after 2 min stirring of a mixture of VAPOL 3, $B(OPh)_3$, aldehyde 7a and EDA 2 in toluene.



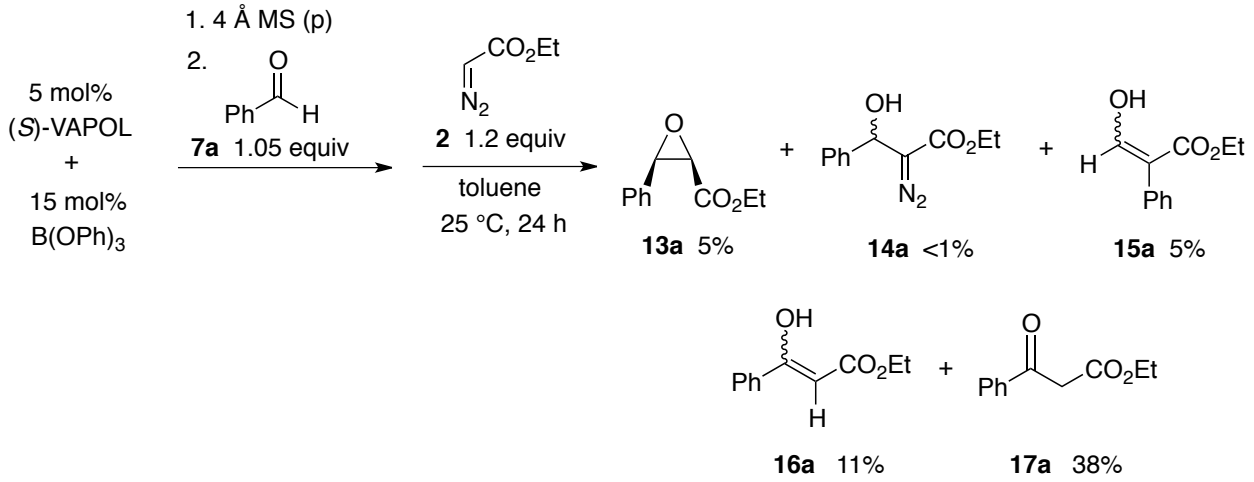




To a 10 mL flame-dried single-necked round bottom flask equipped with a stir bar and filled with argon was added in the following order (*S)*-VAPOL (14 mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol), 4Å Molecular Sieves (150 mg, freshly flame-dried), aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv), ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv). Dry toluene (1 mL) was added under an argon atmosphere to dissolve the reagents. The flask was fitted with a rubber septum and a nitrogen balloon. The mixture was stirred for 2 min followed by the addition of amine **6** (149.7 mg, 0.5000 mmol). The reaction mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The reaction mixture was then filtered through a Celite pad to a 100 mL round bottom flask. The reaction flask was rinsed with EtOAc (3 mL × 3) and the rinse was filtered through the same Celite pad. The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude mixture. An internal standard Ph_3CH (12.2 mg, 0.500 mmol) was added and subjected to NMR analysis. The crude NMR revealed the presence of several products as

shown in the reaction scheme. The presence of each product was confirmed by characteristic peaks (as discussed in section **C**) in the ^{1}H NMR previously published for these compounds and the amount of each was quantified by integration against an internal standard (Ph_3CH).

Procedure VII: Same as Procedure VI except that amine 6 is not added.

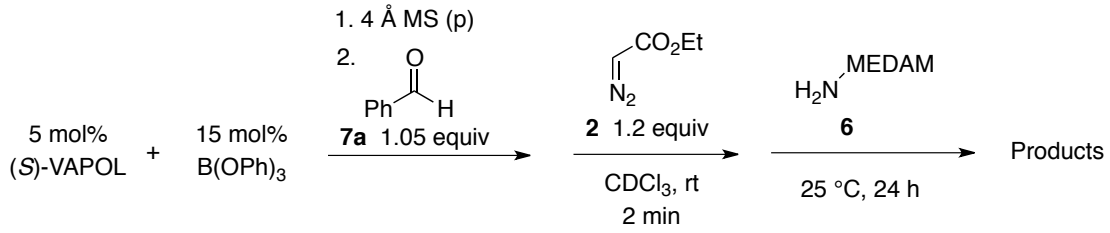


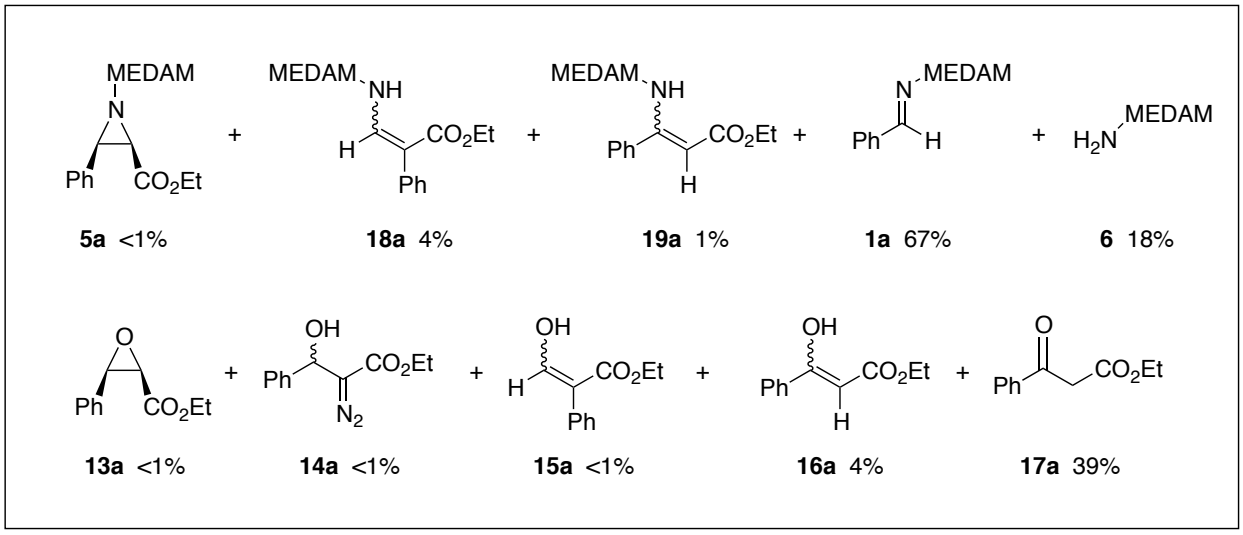
To a 10 mL flame-dried single-necked round bottom flask equipped with a stir bar and filled with argon was added in the following order (*S)*-VAPOL (14 mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol), 4Å Molecular Sieves (150 mg, freshly flame-dried), aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv), ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv). Dry toluene (1 mL) was added under an argon atmosphere to dissolve the reagents. The flask was fitted with a rubber septum and a nitrogen balloon. The resulting mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The reaction mixture was then filtered through a Celite pad to a 100 mL round bottom flask. The reaction flask was rinsed with EtOAc (3 mL × 3) and the rinse was filtered through the same Celite pad. The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude mixture. An internal standard Ph_3CH (12.2 mg, 0.500 mmol) was added and subjected to NMR analysis. The crude NMR revealed the presence of several products as shown in the reaction scheme. The crude NMR revealed the presence of several products as shown in the reaction scheme. The presence of each product was confirmed by characteristic peaks (as discussed in section **C**) in the ^{1}H NMR previously published for these compounds.

There was also mono-alkylated (*S*)-VAPOL derivative **12** in 37% yield (with respect to (*S*)-VAPOL).

Procedure VI in $CDCl_3$: Amine 6 added at the end after 2 min stirring of a mixture of VAPOL 3, $B(OPh)_3$, aldehyde 7a and EDA 2 in $CDCl_3$.

This reaction was run in $CDCl_3$ because the crude reaction mixture in toluene was stripped of volatiles before the ^1H NMR was taken and some of the products many have been lost**.**



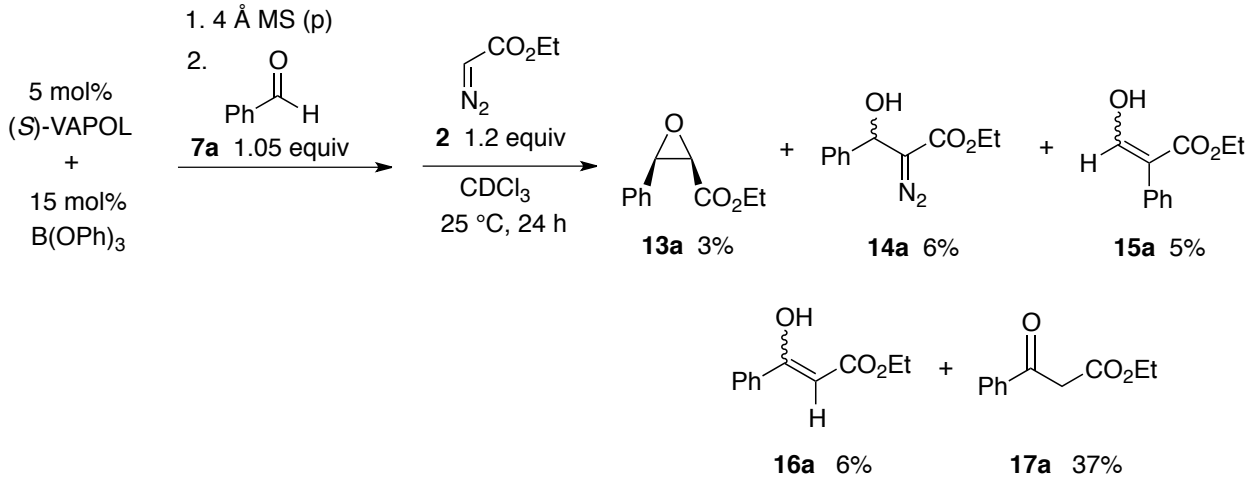


To a 10 mL flame-dried single-necked round bottom flask equipped with a stir bar and filled with argon was added (*S)*-VAPOL in the following order (14 mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol), 4Å Molecular Sieves (150 mg, freshly flame-dried), aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv), ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv). Dry toluene (1 mL) was added under an argon atmosphere to dissolve the reagents. The flask was fitted with a rubber septum and a nitrogen balloon. The mixture was stirred for 2 min followed by the addition of amine **6** (149.7 mg, 0.5000 mmol). The reaction mixture was stirred for 24 h at room temperature. After 24 h, an internal standard Ph_3CH (12.2 mg, 0.500 mmol) was added. The resulting solution was then directly transferred to a NMR tube utilizing a filter syringe

(Corning® syringe filters, Aldrich) to remove the 4Å Molecular Sieves. It was then subjected to NMR analysis. The crude NMR revealed the presence of several products as shown in the reaction scheme. The presence of each product was confirmed by characteristic peaks (as discussed in section **C**) in the ^{1}H NMR previously published for these compounds. There was also mono-alkylated (*S*)-VAPOL derivative **12** in 28% yield (with respect to (*S*)-VAPOL).

Procedure VII in $CDCl_3$: Same as Procedure VI except that amine 6 is not added (in $CDCl_3$).

This reaction was run in $CDCl_3$ because the crude reaction mixture in toluene was stripped of volatiles before the ^{1}H NMR was taken and some of the products many have been lost**.**

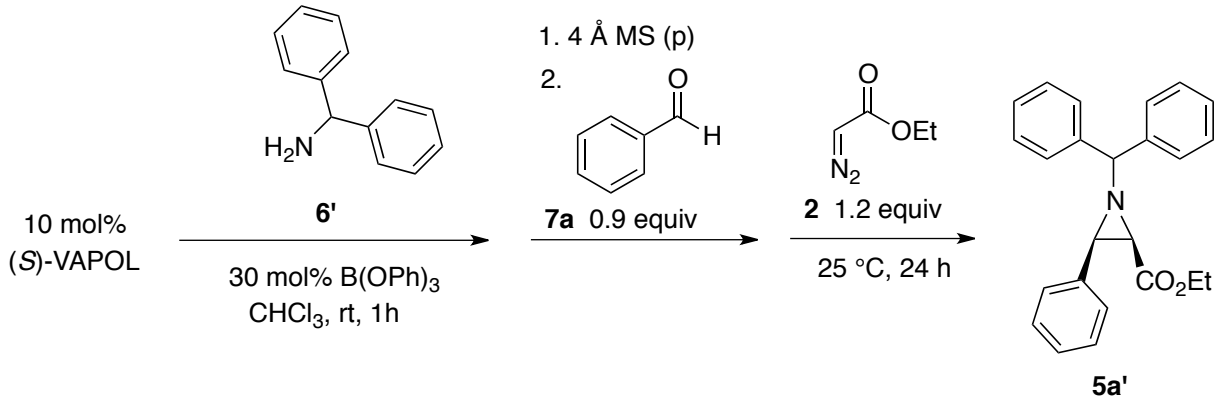


To a 10 mL flame-dried single-necked round bottom flask equipped with a stir bar and filled with argon was added in the following order (*S)*-VAPOL (14 mg, 0.025 mmol), $B(OPh)_3$ (22 mg, 0.075 mmol), 4Å Molecular Sieves (150 mg, freshly flame-dried), aldehyde **7a** (52.0 μL, 0.525 mmoL, 1.05 equiv), ethyl diazoacetate (EDA) **2** (62 μL, 0.60 mmoL, 1.2 equiv). Dry toluene (1 mL) was added under an argon atmosphere to dissolve the reagents. The flask was fitted with a rubber septum and a nitrogen balloon. The resulting mixture was stirred for 24 h at room temperature. After 24 h, an internal standard Ph_3CH (12.2 mg, 0.5000 mmol) was added. The resulting solution was then directly transferred to a NMR tube utilizing a filter syringe (Corning® syringe filters, Aldrich) to remove the 4Å Molecular Sieves. It was then subjected to NMR analysis. The crude NMR revealed the presence of several products as shown in the reaction scheme. The presence of each product was confirmed by characteristic peaks (as

discussed in section **C**) in the ^{1}H NMR previously published for these compounds. There was also 26% of unreacted benzaldehyde **7a**. There was also mono-alkylated (*S*)-VAPOL derivative **12** in 11% yield (with respect to (*S*)-VAPOL).

F. Mechanistic Study of multi-component aziridination reaction

a) MCAZ with 0.9 equivalents of benzaldehyde 7a and amine 6′:

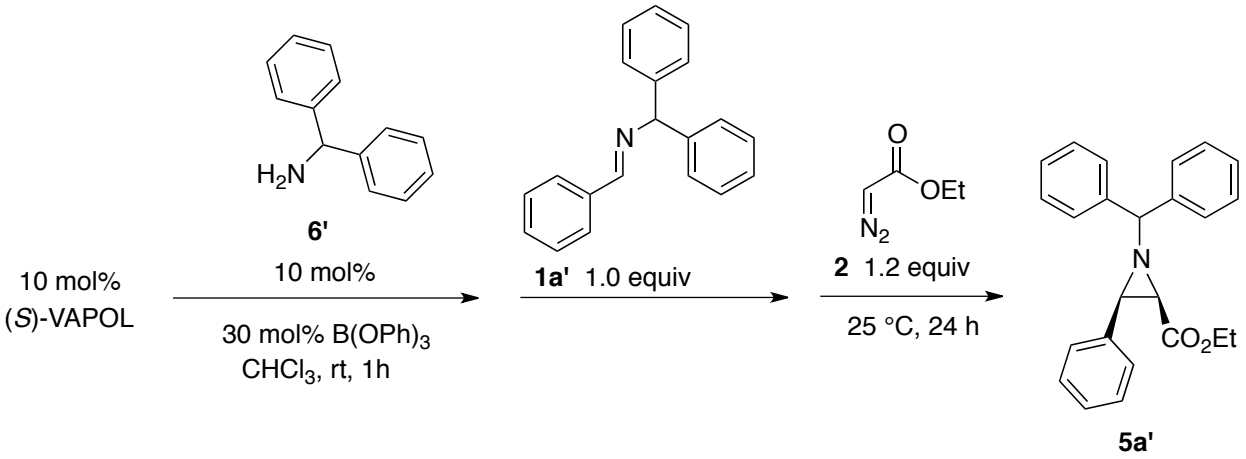


(2*R*,3*R*)-ethyl 1-benzhydryl-3-phenylaziridine-2-carboxylate 5a′: Aldehyde **7a** (46.0 µL, 0.450 mmol, 0.900 equiv) was reacted according to the general Procedure IIIA described above with (*S*)-VAPOL as ligand. Purification of the crude aziridine by silica gel chromatography (30 mm × 300 mm column, 19:1 hexanes/EtOAc as eluent, gravity column) afforded pure cis-aziridine **5a′** as a white solid (mp. 127.5-128.5 °C) in 73 % isolated yield (117 mg, 0.323 mmol); *cis/trans*: 25:1. Enamine side products: 8 % yield of enamines. The optical purity of **5a′** was determined to be 89% *ee* by HPLC analysis (CHIRALCEL OD-H column, 90:10 hexane/2-propanol at 226 nm, flow-rate: 0.7 mL/min): retention times; R_t = 9.01 min (major enantiomer, **5a′**) and R_t = 4.67 min (minor enantiomer, *ent*-**5a′**). There was 8% of unreacted imine **1a′** was also observed. Same procedure was followed to do MCAZ for 0.6-1.0 equivalents of benzaldehyde **7a** and the results are presented in Table 5 of the manuscript.

Spectral data for **5a′**: R_f = 0.3 (1:9 EtOAc/hexanes); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 0.95 (t, 3H, *J* = 7.3 Hz), 2.64 (d, 1H, *J* = 6.8 Hz), 3.19 (d, 1H, *J* = 6.8 Hz), 3.91 (q, 2H, *J* = 7.1 Hz), 3.93 (s, 1H), 7.16-7.38 (m, 11H), 7.47 (d, 2H, *J* = 7.1 Hz), 7.58 (d, 2H, *J* = 7.6 Hz); ^{13}C NMR ($CDCl_3$,

125 MHz) δ 13.93, 46.36, 48.01, 60.57, 77.68, 127.18, 127.31, 127.39, 127.52, 127.76, 127.78, 128.48, 135.00, 142.37, 142.49, 167.75 (one sp^2 carbon not located); $[\alpha]^{20}_D$ = + 33.4 (*c* 1.0, CH_2Cl_2) on 91% *ee* material (HPLC). These spectral data match those previously reported for this compound.[4]

b) Aziridination with preformed imine 1a′ with added bases illustrated by utilizing amine 6′ as the base: Imine **1a′** was prepared according to the published procedure.[4]



(2*R*,3*R*)-ethyl 1-benzhydryl-3-phenylaziridine-2-carboxylate 5a′: To a 10 mL flame-dried single-necked round bottom flask equipped with a stir bar and filled with argon was added (*S*)-VAPOL (54 mg, 0.10 mmol), $B(OPh)_3$ (87 mg, 0.30 mmol) and amine **6′** (17.2 μL, 0.10 mmol). Dry toluene (2 mL) was added under an argon atmosphere to dissolve the reagents. The flask was fitted with a rubber septum and a nitrogen balloon. The reaction mixture was stirred at room temperature for 1 h. Thereafter, imine **1a′** (271 mg, 1.00 mmoL) was added to the catalyst solution and stirred for 5 min. To this solution was rapidly added ethyl diazoacetate (EDA) **2** (124 μL, 1.20 mmoL, 1.2 equiv). The resulting mixture was stirred for 24 h at room temperature. The reaction was dilluted by addition of hexane (6 mL). The resulting solution was then concentrated *in vacuo* followed by exposure to high vacuum (0.05 mm Hg) for 1 h to afford the crude aziridine as an off-white solid. Purification of the crude aziridine by silica gel chromatography (30 mm × 300 mm column, 19:1 hexanes/EtOAc as eluent, gravity column) afforded pure cis-aziridine **5a′** as a white solid (mp. 127.5-128.5 °C) in 80 % isolated yield (286 mg, 0.800 mmol); *cis/trans*: 27:1. Enamine side products: 10 % yield of enamines. The optical purity of **5a′** was determined to be 89% *ee* by HPLC analysis (CHIRALCEL OD-H column,

90:10 hexane/2-propanol at 226 nm, flow-rate: 0.7 mL/min): retention times; R_t = 9.01 min (major enantiomer, **5a′**) and R_t = 4.67 min (minor enantiomer, *ent*-**5a′**). Same procedure was followed to do MCAZ for other bases.

G. DFT calclulations of IMINO-BOROX 9a and AMINO-BOROX 9d:

All quantum mechanical calculations were performed using the GAUSSIAN 03.[9] The B3LYP[10,11] and BHandHLYP[12-14] density functional were used along with 3-21G* and 6-31G* basis sets. The calculated distances (d_1-d_5 and d_1'-d_4') for both IMINO-BOROX **9a** and AMINO-BOROX **9d** are presented in Table 1.

Table 1: Calculated distances in Angstrom

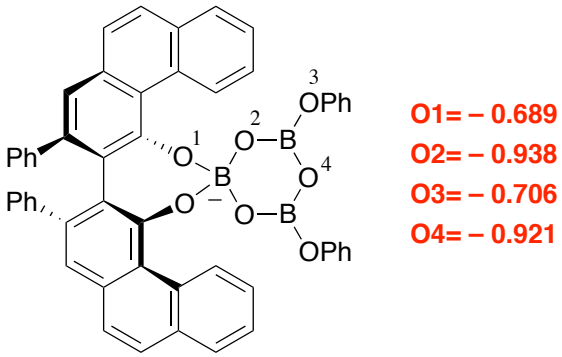
A) IMINO-BOROX **9a**

Methods	d_1 (Å)	d_2 (Å)	d_3 (Å)	d_4 (Å)	d_5 (Å)
X-ray Crystals	2.02	4.42	3.49	5.52	4.78
B3LYP/3-21g*	1.53	3.89	3.52	4.42	4.19
B3LYP/6-31g*	1.73	3.92	5.56	4.66	4.02
BHandHLYP/6-31g*	1.73	3.84	3.52	4.55	3.88

B) AMINO-BOROX **9d**

Methods	d_1' (Å)	d_2' (Å)	d_3' (Å)	d_4' (Å)
X-ray Crystals	-	-	-	-
B3LYP/3-21g*	1.60	1.86	3.15	4.05
B3LYP/6-31g*	1.75	1.96	3.21	4.18
BHandHLYP/6-31g*	1.74	1.99	3.16	4.13

a) NBO analysis on (*S*)-VAPOL-BOROX anion: NBO analysis was performed at the B3LYP/6-31G* level of theory as shown in Figure 4.



B3 **9** BOROX anion

Figure 4: Natural charges on the oxygen atoms of the boroxinate anion

b) Coordinates of IMINO-BOROX 9a:

B3LYP/3-21G*

Energy = -3796.83103601 hartrees
Number of Imaginary frequencies = none

Zero-point correction=	1.249090 (Hartree/Particle)
Thermal correction to Energy=	1.326418
Thermal correction to Enthalpy=	1.327362
Thermal correction to Gibbs Free Energy=	1.125838
Sum of electronic and zero-point Energies=	-3795.581946
Sum of electronic and thermal Energies=	-3795.504618
Sum of electronic and thermal Enthalpies=	-3795.503674
Sum of electronic and thermal Free Energies=	-3795.705198

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	832.340	302.009	424.143

Standard orientation:

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.309357	1.003946	-0.477093

2	6	0	-1.440386	1.706267	-0.913874
3	6	0	-2.636115	1.421926	-0.251971
4	6	0	-2.667754	0.297649	0.731746
5	6	0	-1.835606	0.365934	1.859922
6	8	0	-0.858421	1.335012	1.900117
7	5	0	0.200342	1.436692	0.863026
8	8	0	1.344403	0.473067	1.169940
9	5	0	2.647966	0.894871	1.438071
10	8	0	2.977588	2.246052	1.435037
11	5	0	1.986605	3.223585	1.119119
12	8	0	0.705606	2.811167	0.856186
13	8	0	3.567952	-0.118925	1.709242
14	6	0	4.924642	-0.043202	2.058128
15	6	0	5.661116	1.144476	2.056397
16	1	0	5.174451	2.070898	1.791487
17	6	0	7.011663	1.107318	2.408218
18	1	0	7.582425	2.028799	2.406209
19	6	0	7.627515	-0.095717	2.760106
20	1	0	8.676171	-0.113930	3.031672
21	6	0	6.879296	-1.276245	2.762178
22	1	0	7.344304	-2.215509	3.038524
23	6	0	5.530094	-1.252275	2.413035
24	1	0	4.926546	-2.150328	2.419568
25	8	0	2.418951	4.536789	1.112818
26	6	0	1.729635	5.705011	0.761090
27	6	0	2.399736	6.905454	1.006378
28	1	0	3.384875	6.864224	1.451882
29	6	0	1.797065	8.116898	0.673089
30	1	0	2.320296	9.046575	0.865636
31	6	0	0.526217	8.132861	0.091173
32	1	0	0.058148	9.074461	-0.170883
33	6	0	-0.134277	6.926263	-0.150706
34	1	0	-1.117352	6.923991	-0.607220
35	6	0	0.457696	5.707340	0.183773
36	1	0	-0.050334	4.772073	0.005588
37	6	0	-1.355550	2.685052	-1.946315
38	6	0	-0.151176	2.986620	-2.724204
39	6	0	1.079548	2.294912	-2.578151
40	1	0	1.131601	1.493104	-1.863306
41	6	0	2.187580	2.619754	-3.341986
42	1	0	3.106937	2.062661	-3.206286
43	6	0	2.127736	3.655192	-4.292587
44	1	0	3.003668	3.909197	-4.878146
45	6	0	0.942957	4.340546	-4.471708
46	1	0	0.872703	5.137954	-5.204303
47	6	0	-0.207132	4.024487	-3.710869

48	6	0	-1.431012	4.738571	-3.939090
49	1	0	-1.435002	5.521616	-4.689942
50	6	0	-2.554238	4.437975	-3.241229
51	1	0	-3.481180	4.972378	-3.419161
52	6	0	-2.555673	3.408008	-2.239326
53	6	0	-3.735526	3.158344	-1.510469
54	1	0	-4.605415	3.775166	-1.705379
55	6	0	-3.803121	2.185302	-0.527663
56	6	0	-5.062918	2.054340	0.259959
57	6	0	-6.299488	1.943346	-0.394761
58	1	0	-6.318309	1.859044	-1.474844
59	6	0	-7.488688	1.906039	0.334724
60	1	0	-8.436039	1.813896	-0.184580
61	6	0	-7.458525	1.977237	1.729333
62	1	0	-8.381773	1.949503	2.297004
63	6	0	-6.231390	2.085826	2.389712
64	1	0	-6.200260	2.147385	3.471535
65	6	0	-5.042124	2.125497	1.662245
66	1	0	-4.093209	2.222840	2.173785
67	6	0	-3.583459	-0.780747	0.586513
68	6	0	-4.396480	-1.001567	-0.646285
69	6	0	-5.732971	-1.424026	-0.537284
70	1	0	-6.190330	-1.476801	0.443214
71	6	0	-6.480922	-1.729335	-1.674147
72	1	0	-7.513010	-2.044542	-1.570021
73	6	0	-5.908907	-1.612626	-2.943665
74	1	0	-6.490583	-1.845609	-3.828358
75	6	0	-4.585447	-1.179085	-3.065636
76	1	0	-4.135382	-1.076275	-4.046480
77	6	0	-3.836213	-0.874068	-1.928661
78	1	0	-2.814743	-0.533167	-2.030836
79	6	0	-3.678272	-1.713425	1.610793
80	1	0	-4.338922	-2.565500	1.496819
81	6	0	-2.948355	-1.583821	2.808331
82	6	0	-3.137338	-2.545797	3.859335
83	1	0	-3.842089	-3.352286	3.687441
84	6	0	-2.468061	-2.446152	5.034714
85	1	0	-2.622163	-3.172367	5.825841
86	6	0	-1.557153	-1.362762	5.274860
87	6	0	-0.919994	-1.243493	6.532635
88	1	0	-1.127752	-1.994202	7.288353
89	6	0	-0.067522	-0.191054	6.805643
90	1	0	0.404797	-0.103801	7.777649
91	6	0	0.163275	0.781942	5.814579
92	1	0	0.810129	1.625516	6.028325
93	6	0	-0.442830	0.688340	4.572755

94	1	0	-0.287319	1.448143	3.825493
95	6	0	-1.312992	-0.388944	4.251878
96	6	0	-2.004181	-0.523510	2.967295
97	6	0	0.789518	-1.886731	-1.182388
98	1	0	0.107585	-1.029060	-1.228602
99	7	0	1.113998	-1.972081	0.292021
100	1	0	1.205849	-0.994002	0.749676
101	6	0	1.284812	-3.089915	0.917487
102	1	0	1.170326	-3.996792	0.328167
103	6	0	1.611078	-3.258460	2.318815
104	6	0	1.918038	-4.562621	2.759250
105	1	0	1.896913	-5.384871	2.051942
106	6	0	2.247213	-4.790571	4.090613
107	1	0	2.488643	-5.791520	4.426544
108	6	0	2.251631	-3.723830	4.995967
109	1	0	2.493349	-3.902730	6.037138
110	6	0	1.930987	-2.430089	4.570578
111	1	0	1.894391	-1.613161	5.278606
112	6	0	1.619553	-2.189351	3.236709
113	1	0	1.358127	-1.191862	2.914022
114	6	0	0.098142	-3.162268	-1.646635
115	6	0	0.790231	-4.170847	-2.326941
116	1	0	1.834306	-4.024645	-2.577169
117	6	0	0.142939	-5.350172	-2.708191
118	6	0	0.872827	-6.457670	-3.440339
119	1	0	1.950340	-6.400991	-3.260231
120	1	0	0.709519	-6.384030	-4.523640
121	1	0	0.496724	-7.430045	-3.112559
122	6	0	-1.214370	-5.510951	-2.392776
123	8	0	-1.858099	-6.712497	-2.749803
124	6	0	-2.553196	-6.656003	-4.054942
125	1	0	-2.992798	-7.645147	-4.189444
126	1	0	-1.850283	-6.445141	-4.868221
127	1	0	-3.339771	-5.894411	-4.049503
128	6	0	-1.921841	-4.522316	-1.692046
129	6	0	-3.379591	-4.732108	-1.338794
130	1	0	-3.597059	-4.318220	-0.349907
131	1	0	-3.609665	-5.799835	-1.347511
132	1	0	-4.031746	-4.218456	-2.056199
133	6	0	-1.250173	-3.353928	-1.321728
134	1	0	-1.785887	-2.591252	-0.766541
135	6	0	2.051926	-1.544656	-1.978363
136	6	0	3.334291	-1.550270	-1.420623
137	1	0	3.474530	-1.738149	-0.364201
138	6	0	4.457378	-1.246655	-2.200752
139	6	0	5.848470	-1.221271	-1.600170

140	1	0	6.449510	-0.457187	-2.099468
141	1	0	6.353319	-2.187717	-1.734769
142	1	0	5.808218	-1.010554	-0.528477
143	6	0	4.278412	-0.926456	-3.553142
144	8	0	5.400562	-0.585359	-4.338168
145	6	0	6.058498	-1.746167	-4.974274
146	1	0	6.900449	-1.331444	-5.530294
147	1	0	5.374765	-2.260297	-5.659105
148	1	0	6.421612	-2.456671	-4.223982
149	6	0	2.996470	-0.878538	-4.123741
150	6	0	2.815365	-0.440044	-5.563217
151	1	0	2.076042	0.366248	-5.617838
152	1	0	2.468411	-1.269386	-6.191872
153	1	0	3.766261	-0.071004	-5.951409
154	6	0	1.895040	-1.188739	-3.323405
155	1	0	0.900389	-1.145438	-3.754264

B3LYP/6-31G*

Energy = -3817.70063424 hartrees
Number of Imaginary frequencies = none

Zero-point correction= 1.242009 (Hartree/Particle)
Thermal correction to Energy= 1.320573
Thermal correction to Enthalpy= 1.321517
Thermal correction to Gibbs Free Energy= 1.115078
Sum of electronic and zero-point Energies= -3816.458625
Sum of electronic and thermal Energies= -3816.380061
Sum of electronic and thermal Enthalpies= -3816.379117
Sum of electronic and thermal Free Energies= -3816.585556

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	828.672	306.363	434.487

Standard orientation:

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.471533	0.966556	-0.650731

2	6	0	-1.640664	1.341962	-1.248481
3	6	0	-2.825135	0.896240	-0.645352
4	6	0	-2.734807	-0.059523	0.501976
5	6	0	-2.028419	0.334274	1.656014
6	8	0	-1.283477	1.455927	1.603722
7	5	0	-0.182450	1.618179	0.642063
8	8	0	1.057067	0.922399	1.140121
9	5	0	2.220389	1.602242	1.349959
10	8	0	2.331575	2.952492	1.180209
11	5	0	1.204150	3.668240	0.761162
12	8	0	0.042493	3.045807	0.507141
13	8	0	3.286258	0.822324	1.770386
14	6	0	4.588519	1.211557	1.985927
15	6	0	5.227498	2.202507	1.233318
16	1	0	4.676839	2.747619	0.476977
17	6	0	6.569955	2.490437	1.484996
18	1	0	7.061151	3.265385	0.902323
19	6	0	7.280527	1.799951	2.468801
20	1	0	8.325043	2.032541	2.655930
21	6	0	6.634271	0.809793	3.211364
22	1	0	7.173087	0.265314	3.982699
23	6	0	5.292489	0.513724	2.972812
24	1	0	4.772907	-0.249147	3.544939
25	8	0	1.418017	5.020623	0.662579
26	6	0	0.535461	6.005333	0.285253
27	6	0	0.818949	7.292351	0.754036
28	1	0	1.682647	7.432634	1.396959
29	6	0	0.000873	8.360938	0.392146
30	1	0	0.227543	9.357692	0.762425
31	6	0	-1.100945	8.153769	-0.440759
32	1	0	-1.739505	8.986348	-0.723440
33	6	0	-1.372542	6.866761	-0.907621
34	1	0	-2.224908	6.691935	-1.559173
35	6	0	-0.561969	5.786664	-0.553696
36	1	0	-0.779503	4.789575	-0.913146
37	6	0	-1.634640	2.125769	-2.443564
38	6	0	-0.438239	2.564682	-3.167531
39	6	0	0.890571	2.231799	-2.797426
40	1	0	1.047274	1.601572	-1.936859
41	6	0	1.983816	2.687429	-3.516068
42	1	0	2.983345	2.410438	-3.191599
43	6	0	1.813504	3.498561	-4.650779
44	1	0	2.675810	3.859752	-5.204981
45	6	0	0.534528	3.828785	-5.050896
46	1	0	0.375793	4.449412	-5.930119
47	6	0	-0.598997	3.377249	-4.336967

48	6	0	-1.909008	3.735272	-4.794482
49	1	0	-1.994417	4.353899	-5.684882
50	6	0	-3.016093	3.311404	-4.134645
51	1	0	-4.009411	3.583395	-4.483439
52	6	0	-2.915289	2.502353	-2.954585
53	6	0	-4.094155	2.128847	-2.282220
54	1	0	-5.041159	2.507224	-2.657227
55	6	0	-4.083244	1.348953	-1.137390
56	6	0	-5.379650	1.098460	-0.445717
57	6	0	-6.508619	0.689554	-1.174283
58	1	0	-6.404816	0.472809	-2.233746
59	6	0	-7.746545	0.531866	-0.551384
60	1	0	-8.604928	0.207766	-1.134674
61	6	0	-7.881214	0.781591	0.815240
62	1	0	-8.845419	0.660131	1.302332
63	6	0	-6.767477	1.191490	1.551515
64	1	0	-6.862186	1.398716	2.614375
65	6	0	-5.530294	1.348792	0.928465
66	1	0	-4.675783	1.687866	1.504955
67	6	0	-3.403288	-1.318042	0.481203
68	6	0	-4.039602	-1.899043	-0.737462
69	6	0	-5.262321	-2.586076	-0.634083
70	1	0	-5.779961	-2.602664	0.320206
71	6	0	-5.836041	-3.209729	-1.741107
72	1	0	-6.786901	-3.725645	-1.634097
73	6	0	-5.202604	-3.157395	-2.984235
74	1	0	-5.651840	-3.636967	-3.850161
75	6	0	-3.991981	-2.471963	-3.106586
76	1	0	-3.489501	-2.418941	-4.069120
77	6	0	-3.418118	-1.850518	-1.997586
78	1	0	-2.476688	-1.323724	-2.109580
79	6	0	-3.422446	-2.073933	1.646372
80	1	0	-3.894470	-3.052625	1.641747
81	6	0	-2.860683	-1.613634	2.851622
82	6	0	-2.990371	-2.413248	4.035832
83	1	0	-3.510859	-3.364762	3.955384
84	6	0	-2.497446	-1.992300	5.228026
85	1	0	-2.612509	-2.599931	6.122805
86	6	0	-1.839139	-0.724104	5.345059
87	6	0	-1.391319	-0.284406	6.611867
88	1	0	-1.553115	-0.933962	7.469691
89	6	0	-0.779235	0.943915	6.770837
90	1	0	-0.450082	1.273637	7.753026
91	6	0	-0.604462	1.768946	5.646028
92	1	0	-0.142388	2.746631	5.756960
93	6	0	-1.029235	1.361614	4.391141

94	1	0	-0.905955	2.021384	3.546377
95	6	0	-1.653039	0.101615	4.188060
96	6	0	-2.154601	-0.373370	2.895610
97	6	0	1.321110	-1.999160	-0.806672
98	1	0	0.504749	-1.328280	-1.096707
99	7	0	1.420029	-1.780568	0.667480
100	1	0	1.297431	-0.776931	0.947088
101	6	0	1.674146	-2.706439	1.533265
102	1	0	1.789031	-3.708821	1.125271
103	6	0	1.830883	-2.558271	2.963013
104	6	0	2.234425	-3.706705	3.675995
105	1	0	2.393833	-4.640316	3.142299
106	6	0	2.435043	-3.645324	5.049614
107	1	0	2.750914	-4.530390	5.593482
108	6	0	2.219742	-2.440369	5.724601
109	1	0	2.366794	-2.390886	6.799993
110	6	0	1.803525	-1.299665	5.029217
111	1	0	1.608449	-0.374493	5.560562
112	6	0	1.610327	-1.349302	3.653984
113	1	0	1.277371	-0.464588	3.125044
114	6	0	0.926993	-3.435121	-1.137648
115	6	0	1.860355	-4.381662	-1.574509
116	1	0	2.897867	-4.090856	-1.710955
117	6	0	1.481388	-5.697490	-1.859183
118	6	0	2.491060	-6.721828	-2.318393
119	1	0	3.507092	-6.319702	-2.261026
120	1	0	2.314724	-7.029749	-3.356537
121	1	0	2.439188	-7.629979	-1.708866
122	6	0	0.132266	-6.052628	-1.696791
123	8	0	-0.228150	-7.366517	-1.936435
124	6	0	-0.801985	-7.610978	-3.221071
125	1	0	-0.991763	-8.685518	-3.273418
126	1	0	-0.114224	-7.323654	-4.027067
127	1	0	-1.747189	-7.070112	-3.351620
128	6	0	-0.826704	-5.133555	-1.235868
129	6	0	-2.265702	-5.539953	-1.030216
130	1	0	-2.731627	-4.933969	-0.248193
131	1	0	-2.338082	-6.595432	-0.753091
132	1	0	-2.861167	-5.388376	-1.939464
133	6	0	-0.405395	-3.827978	-0.964547
134	1	0	-1.135664	-3.108767	-0.601003
135	6	0	2.593180	-1.517909	-1.501924
136	6	0	3.840102	-1.478435	-0.871345
137	1	0	3.931860	-1.713685	0.184330
138	6	0	4.995480	-1.100056	-1.565050
139	6	0	6.332999	-1.019547	-0.869924

140	1	0	6.798916	-0.042124	-1.028458
141	1	0	7.035588	-1.772903	-1.248371
142	1	0	6.222847	-1.170697	0.207495
143	6	0	4.876442	-0.770003	-2.923951
144	8	0	6.011207	-0.356691	-3.601257
145	6	0	6.667063	-1.378490	-4.349059
146	1	0	7.551617	-0.916539	-4.793917
147	1	0	6.024695	-1.771444	-5.147765
148	1	0	6.978866	-2.210594	-3.703825
149	6	0	3.633169	-0.770887	-3.580433
150	6	0	3.513591	-0.360413	-5.028384
151	1	0	2.554003	0.131161	-5.212665
152	1	0	3.577339	-1.227044	-5.700318
153	1	0	4.314365	0.330692	-5.303906
154	6	0	2.503643	-1.143565	-2.846479
155	1	0	1.533346	-1.137141	-3.337553

BHandHLYP/6-31G*

Energy = -3815.48426974 hartrees
Number of Imaginary frequencies = none

Zero-point correction= 1.289748 (Hartree/Particle)
Thermal correction to Energy= 1.365579
Thermal correction to Enthalpy= 1.366523
Thermal correction to Gibbs Free Energy= 1.167169
Sum of electronic and zero-point Energies= -3814.194522
Sum of electronic and thermal Energies= -3814.118690
Sum of electronic and thermal Enthalpies= -3814.117746
Sum of electronic and thermal Free Energies= -3814.317101

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	856.914	294.506	419.577

Standard orientation:

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.426816	0.996368	-0.603016
2	6	0	-1.575398	1.426778	-1.170917
3	6	0	-2.759192	1.018511	-0.571327
4	6	0	-2.688145	0.051512	0.559472

5	6	0	-1.949865	0.406335	1.688948
6	8	0	-1.188863	1.502464	1.631713
7	5	0	-0.088760	1.614634	0.682185
8	8	0	1.099626	0.852299	1.160975
9	5	0	2.297623	1.446734	1.347587
10	8	0	2.485910	2.778885	1.191457
11	5	0	1.406686	3.559841	0.806532
12	8	0	0.218664	3.014475	0.559300
13	8	0	3.316710	0.604476	1.721194
14	6	0	4.633429	0.901198	1.908772
15	6	0	5.306129	1.868707	1.175305
16	1	0	4.773781	2.467842	0.459924
17	6	0	6.660801	2.063675	1.393598
18	1	0	7.178372	2.820523	0.826387
19	6	0	7.350032	1.303120	2.325011
20	1	0	8.403442	1.463338	2.486178
21	6	0	6.669158	0.337264	3.049442
22	1	0	7.190450	-0.260370	3.780141
23	6	0	5.314866	0.134591	2.843801
24	1	0	4.768805	-0.607762	3.402128
25	8	0	1.678957	4.891530	0.727195
26	6	0	0.803102	5.873946	0.371375
27	6	0	0.837186	7.048808	1.106774
28	1	0	1.516926	7.119648	1.939541
29	6	0	0.007626	8.102027	0.760808
30	1	0	0.037180	9.012869	1.337498
31	6	0	-0.854839	7.988212	-0.318443
32	1	0	-1.501781	8.807729	-0.586522
33	6	0	-0.876461	6.811307	-1.050580
34	1	0	-1.540907	6.708454	-1.893561
35	6	0	-0.049343	5.752002	-0.715331
36	1	0	-0.068010	4.839422	-1.282426
37	6	0	-1.552720	2.239399	-2.333461
38	6	0	-0.350406	2.649725	-3.051876
39	6	0	0.957631	2.244489	-2.713150
40	1	0	1.095642	1.577230	-1.889116
41	6	0	2.053853	2.679453	-3.418283
42	1	0	3.035370	2.345784	-3.122198
43	6	0	1.908952	3.540386	-4.508246
44	1	0	2.774063	3.884399	-5.051763
45	6	0	0.651868	3.938488	-4.876313
46	1	0	0.512909	4.597090	-5.719684
47	6	0	-0.484902	3.507462	-4.172836
48	6	0	-1.778130	3.939157	-4.600169
49	1	0	-1.843305	4.591119	-5.457190
50	6	0	-2.885430	3.538418	-3.953672

51	1	0	-3.861864	3.862285	-4.277569
52	6	0	-2.807132	2.682336	-2.811295
53	6	0	-3.987465	2.334868	-2.146458
54	1	0	-4.915588	2.754943	-2.498507
55	6	0	-3.993948	1.526448	-1.036286
56	6	0	-5.288196	1.296105	-0.347050
57	6	0	-6.417861	0.928466	-1.074486
58	1	0	-6.322544	0.733163	-2.130195
59	6	0	-7.647599	0.782862	-0.454361
60	1	0	-8.507762	0.490696	-1.035622
61	6	0	-7.770301	1.003993	0.907895
62	1	0	-8.726933	0.892058	1.392866
63	6	0	-6.654017	1.373558	1.642743
64	1	0	-6.739869	1.557666	2.701692
65	6	0	-5.425313	1.519046	1.021804
66	1	0	-4.567655	1.823768	1.597129
67	6	0	-3.392312	-1.174645	0.540774
68	6	0	-4.085234	-1.709852	-0.660083
69	6	0	-5.326596	-2.331920	-0.527738
70	1	0	-5.812566	-2.334815	0.433633
71	6	0	-5.958892	-2.906745	-1.616720
72	1	0	-6.923101	-3.372289	-1.488998
73	6	0	-5.364330	-2.868613	-2.868191
74	1	0	-5.858133	-3.309531	-3.719397
75	6	0	-4.133771	-2.247428	-3.017552
76	1	0	-3.661876	-2.206432	-3.986277
77	6	0	-3.502034	-1.674523	-1.926161
78	1	0	-2.547877	-1.194615	-2.058727
79	6	0	-3.402134	-1.942405	1.684012
80	1	0	-3.908191	-2.894177	1.681405
81	6	0	-2.787882	-1.523509	2.868018
82	6	0	-2.904789	-2.337348	4.038162
83	1	0	-3.453298	-3.262859	3.959455
84	6	0	-2.365524	-1.955528	5.207708
85	1	0	-2.469316	-2.568073	6.089743
86	6	0	-1.663013	-0.716168	5.320889
87	6	0	-1.162875	-0.319503	6.571840
88	1	0	-1.320108	-0.971996	7.417049
89	6	0	-0.503618	0.871460	6.728592
90	1	0	-0.133400	1.169992	7.696399
91	6	0	-0.331804	1.701326	5.617876
92	1	0	0.169807	2.649516	5.727482
93	6	0	-0.810117	1.335710	4.381875
94	1	0	-0.688507	1.999666	3.551454
95	6	0	-1.486888	0.112685	4.183816
96	6	0	-2.049398	-0.319674	2.907633

97	6	0	1.168302	-1.996489	-0.846020
98	1	0	0.378941	-1.290109	-1.086221
99	7	0	1.322632	-1.840355	0.617806
100	1	0	1.249609	-0.858256	0.934366
101	6	0	1.564830	-2.793408	1.434097
102	1	0	1.628080	-3.778776	0.998238
103	6	0	1.773389	-2.693280	2.857244
104	6	0	2.152237	-3.864806	3.519937
105	1	0	2.255856	-4.783032	2.963596
106	6	0	2.399197	-3.846749	4.877715
107	1	0	2.695710	-4.749127	5.385495
108	6	0	2.255578	-2.659751	5.581980
109	1	0	2.440160	-2.642927	6.643823
110	6	0	1.865105	-1.494478	4.934638
111	1	0	1.728360	-0.582890	5.489643
112	6	0	1.624785	-1.503388	3.575557
113	1	0	1.314626	-0.599706	3.083347
114	6	0	0.706399	-3.394616	-1.207968
115	6	0	1.570811	-4.351344	-1.723028
116	1	0	2.603070	-4.098944	-1.901221
117	6	0	1.125675	-5.629954	-2.031483
118	6	0	2.060328	-6.671438	-2.576393
119	1	0	3.086675	-6.318104	-2.552480
120	1	0	1.822564	-6.924285	-3.607863
121	1	0	1.996398	-7.592321	-2.003837
122	6	0	-0.215758	-5.935609	-1.813858
123	8	0	-0.641906	-7.207324	-2.088360
124	6	0	-1.267563	-7.371969	-3.343312
125	1	0	-1.513287	-8.423580	-3.431985
126	1	0	-0.601392	-7.088135	-4.156046
127	1	0	-2.179344	-6.783354	-3.413492
128	6	0	-1.104162	-5.005417	-1.276060
129	6	0	-2.540519	-5.357960	-1.016948
130	1	0	-2.930715	-4.782791	-0.183551
131	1	0	-2.646772	-6.414900	-0.795918
132	1	0	-3.167376	-5.126897	-1.876441
133	6	0	-0.620136	-3.738537	-0.981178
134	1	0	-1.295149	-3.011000	-0.557901
135	6	0	2.428167	-1.547399	-1.562715
136	6	0	3.682653	-1.552855	-0.970491
137	1	0	3.797521	-1.809164	0.069122
138	6	0	4.819221	-1.192690	-1.684696
139	6	0	6.171786	-1.164503	-1.033001
140	1	0	6.654624	-0.203958	-1.183746
141	1	0	6.833164	-1.923537	-1.447290
142	1	0	6.090337	-1.334906	0.035502

143	6	0	4.673087	-0.832391	-3.020957
144	8	0	5.787587	-0.443636	-3.717139
145	6	0	6.392425	-1.457186	-4.487920
146	1	0	7.270862	-1.018353	-4.946449
147	1	0	5.723964	-1.817240	-5.267742
148	1	0	6.694399	-2.299309	-3.867375
149	6	0	3.423400	-0.790975	-3.637903
150	6	0	3.276923	-0.350801	-5.066159
151	1	0	2.326502	0.151368	-5.215459
152	1	0	3.315416	-1.198270	-5.749964
153	1	0	4.072294	0.332602	-5.342991
154	6	0	2.313323	-1.149182	-2.887465
155	1	0	1.338166	-1.109020	-3.347681

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c) Coordinates of AMINO-BOROX 9d:

B3LYP/3-21G*

Energy = -3529.17572942 hartrees
Number of Imaginary frequencies = none

Zero-point correction= 1.163496 (Hartree/Particle)
Thermal correction to Energy= 1.235231
Thermal correction to Enthalpy= 1.236175
Thermal correction to Gibbs Free Energy= 1.046771
Sum of electronic and zero-point Energies= -3528.012234
Sum of electronic and thermal Energies= -3527.940499
Sum of electronic and thermal Enthalpies= -3527.939554
Sum of electronic and thermal Free Energies= -3528.128958

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	775.119	280.763	398.634

Standard orientation:

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.270858	-0.275466	0.413774
2	6	0	-2.606721	0.172147	0.410310
3	6	0	-2.822061	1.446874	-0.118308
4	6	0	-1.623326	2.275141	-0.451275
5	6	0	-0.746386	1.785901	-1.429146
6	8	0	-0.980249	0.508842	-1.902561
7	5	0	-0.726922	-0.623134	-0.957108
8	8	0	0.769295	-0.784038	-0.747067
9	5	0	1.489959	-1.807247	-1.348231
10	8	0	0.837664	-2.787609	-2.098503
11	5	0	-0.584866	-2.837771	-2.133237
12	8	0	-1.301426	-1.837054	-1.516638
13	8	0	2.870651	-1.827749	-1.124481
14	6	0	3.864683	-2.651153	-1.682583
15	6	0	3.635691	-3.521437	-2.750906
16	1	0	2.641343	-3.611775	-3.160659
17	6	0	4.696783	-4.279293	-3.249683
18	1	0	4.518570	-4.954508	-4.078698
19	6	0	5.972878	-4.180022	-2.690929
20	1	0	6.789839	-4.772089	-3.085516
21	6	0	6.186166	-3.315790	-1.613955
22	1	0	7.169412	-3.234656	-1.165463
23	6	0	5.134568	-2.553672	-1.106950
24	1	0	5.277393	-1.884393	-0.268623
25	8	0	-1.142339	-3.918391	-2.790546
26	6	0	-2.488419	-4.282623	-2.937252
27	6	0	-2.737010	-5.366823	-3.781527
28	1	0	-1.897164	-5.844916	-4.268069

29	6	0	-4.044340	-5.808558	-3.975664
30	1	0	-4.233704	-6.650096	-4.632189
31	6	0	-5.105381	-5.171364	-3.325811
32	1	0	-6.121858	-5.516128	-3.474933
33	6	0	-4.844950	-4.088816	-2.482729
34	1	0	-5.657608	-3.588490	-1.968684
35	6	0	-3.539871	-3.635429	-2.283926
36	1	0	-3.332320	-2.795765	-1.638577
37	6	0	-3.669367	-0.648877	0.879859
38	6	0	-3.508410	-1.947240	1.543414
39	6	0	-2.253478	-2.504427	1.907903
40	1	0	-1.360098	-1.950501	1.674860
41	6	0	-2.165659	-3.723222	2.563024
42	1	0	-1.199421	-4.116234	2.857360
43	6	0	-3.328070	-4.453527	2.873637
44	1	0	-3.248565	-5.411550	3.374486
45	6	0	-4.564842	-3.938544	2.544234
46	1	0	-5.472316	-4.481299	2.787975
47	6	0	-4.683969	-2.686509	1.897300
48	6	0	-5.987276	-2.147873	1.628391
49	1	0	-6.852900	-2.742017	1.901768
50	6	0	-6.134391	-0.919536	1.073701
51	1	0	-7.119325	-0.503287	0.892406
52	6	0	-4.993256	-0.130911	0.699277
53	6	0	-5.195742	1.129633	0.101859
54	1	0	-6.212241	1.462369	-0.074871
55	6	0	-4.141469	1.932566	-0.299879
56	6	0	-4.430672	3.215946	-1.000685
57	6	0	-5.297090	4.161041	-0.430915
58	1	0	-5.687646	3.987013	0.564722
59	6	0	-5.626791	5.327453	-1.123373

60	1	0	-6.292753	6.052824	-0.669715
61	6	0	-5.094580	5.563818	-2.392902
62	1	0	-5.351972	6.468656	-2.931722
63	6	0	-4.229897	4.627476	-2.966952
64	1	0	-3.819414	4.801430	-3.955039
65	6	0	-3.899954	3.460894	-2.277443
66	1	0	-3.243400	2.726319	-2.726758
67	6	0	-1.343957	3.499494	0.212497
68	6	0	-2.168210	4.025999	1.340469
69	6	0	-2.512187	5.387587	1.376168
70	1	0	-2.252514	6.019328	0.535247
71	6	0	-3.214161	5.916497	2.459500
72	1	0	-3.479730	6.967467	2.466626
73	6	0	-3.586860	5.092895	3.524304
74	1	0	-4.134204	5.502662	4.365385
75	6	0	-3.256823	3.735384	3.495232
76	1	0	-3.547159	3.087975	4.314770
77	6	0	-2.553995	3.205326	2.413086
78	1	0	-2.312806	2.150557	2.392186
79	6	0	-0.196984	4.198697	-0.146638
80	1	0	0.057239	5.109391	0.383864
81	6	0	0.657343	3.760293	-1.181303
82	6	0	1.828537	4.527406	-1.511184
83	1	0	2.001056	5.450160	-0.967951
84	6	0	2.691192	4.112617	-2.472469
85	1	0	3.572390	4.697036	-2.715878
86	6	0	2.453189	2.904463	-3.212509
87	6	0	3.347739	2.513673	-4.237670
88	1	0	4.216520	3.134941	-4.430537
89	6	0	3.115211	1.380037	-4.991371
90	1	0	3.806648	1.090086	-5.773727

91	6	0	1.962042	0.612231	-4.746034
92	1	0	1.760452	-0.263696	-5.351841
93	6	0	1.073861	0.965241	-3.744940
94	1	0	0.180354	0.388345	-3.572857
95	6	0	1.296688	2.108157	-2.931489
96	6	0	0.393702	2.528799	-1.859964
97	6	0	1.964793	0.876280	2.308508
98	1	0	1.596128	1.581678	3.059265
99	7	0	1.027627	1.015349	1.104862
100	1	0	0.043060	0.704266	1.298506
101	6	0	3.377836	1.278354	1.909307
102	6	0	4.177916	1.914804	2.865972
103	1	0	3.787075	2.090925	3.863482
104	6	0	5.475760	2.327224	2.562544
105	6	0	6.358236	3.000922	3.593456
106	1	0	6.074659	2.700258	4.606285
107	1	0	6.274242	4.093991	3.529993
108	1	0	7.402255	2.734110	3.412644
109	6	0	5.969728	2.103585	1.267787
110	8	0	7.284511	2.508888	0.958396
111	6	0	7.373888	3.883003	0.418098
112	1	0	8.436012	4.052538	0.236534
113	1	0	6.996177	4.617374	1.137884
114	1	0	6.814385	3.974026	-0.518998
115	6	0	5.195260	1.453397	0.298570
116	6	0	5.753640	1.208362	-1.088990
117	1	0	5.518456	0.195537	-1.429734
118	1	0	6.837271	1.340973	-1.075568
119	1	0	5.312767	1.906701	-1.811268
120	6	0	3.900411	1.035805	0.634587
121	1	0	3.329606	0.505002	-0.118738

122	6	0	1.800926	-0.539036	2.843663
123	6	0	2.316691	-1.635879	2.148443
124	1	0	2.911582	-1.490378	1.256031
125	6	0	2.019680	-2.940466	2.553012
126	6	0	2.511090	-4.134488	1.761118
127	1	0	1.757670	-4.926392	1.779015
128	1	0	3.439879	-4.536367	2.186731
129	1	0	2.716011	-3.848690	0.726935
130	6	0	1.199083	-3.127468	3.673371
131	8	0	0.778928	-4.426329	4.024430
132	6	0	1.716142	-5.179025	4.886206
133	1	0	1.241416	-6.147152	5.049357
134	1	0	1.864217	-4.668270	5.843669
135	1	0	2.683785	-5.316346	4.393879
136	6	0	0.689353	-2.043676	4.399593
137	6	0	-0.249331	-2.297478	5.559467
138	1	0	-0.514247	-1.359228	6.054965
139	1	0	0.201302	-2.965214	6.301036
140	1	0	-1.166330	-2.771649	5.193299
141	6	0	0.998026	-0.750688	3.969855
142	1	0	0.582210	0.096747	4.506649
143	1	0	1.022149	1.977474	0.727411
144	1	0	1.245416	0.318081	0.313630

B3LYP/6-31G*

Energy = -3548.55770299 hartrees
Number of Imaginary frequencies = none

Zero-point correction= 1.157089 (Hartree/Particle)
Thermal correction to Energy= 1.229949
Thermal correction to Enthalpy= 1.230893

Thermal correction to Gibbs Free Energy= 1.038082
Sum of electronic and zero-point Energies= -3547.400614
Sum of electronic and thermal Energies= -3547.327754
Sum of electronic and thermal Enthalpies= -3547.326810
Sum of electronic and thermal Free Energies= -3547.519621

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	771.805	284.757	405.806

Standard orientation:

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.299161	-0.375441	0.322761
2	6	0	-2.583140	0.103558	0.404865
3	6	0	-2.799481	1.399342	-0.085137
4	6	0	-1.604634	2.193214	-0.511903
5	6	0	-0.799535	1.668896	-1.541545
6	8	0	-1.088854	0.422630	-1.976470
7	5	0	-0.793379	-0.691850	-1.053078
8	8	0	0.686766	-0.826822	-0.876784
9	5	0	1.375413	-1.825821	-1.491178
10	8	0	0.742143	-2.840153	-2.158712
11	5	0	-0.654716	-2.871129	-2.162499
12	8	0	-1.380393	-1.888213	-1.597160
13	8	0	2.754782	-1.773126	-1.369063
14	6	0	3.689654	-2.585339	-1.971646
15	6	0	3.502757	-3.168253	-3.229405
16	1	0	2.567142	-3.030250	-3.756060
17	6	0	4.526226	-3.937833	-3.783671

18	1	0	4.374198	-4.392980	-4.758908
19	6	0	5.732268	-4.126356	-3.106090
20	1	0	6.521842	-4.727285	-3.548166
21	6	0	5.913432	-3.532564	-1.856133
22	1	0	6.847742	-3.665118	-1.316828
23	6	0	4.897833	-2.762955	-1.288651
24	1	0	5.029904	-2.290490	-0.319648
25	8	0	-1.191711	-3.967196	-2.790463
26	6	0	-2.531122	-4.263620	-2.910377
27	6	0	-2.954441	-4.796185	-4.130858
28	1	0	-2.229103	-4.912554	-4.930466
29	6	0	-4.287911	-5.167471	-4.299261
30	1	0	-4.612346	-5.579232	-5.251650
31	6	0	-5.200419	-5.012316	-3.253622
32	1	0	-6.239721	-5.300458	-3.386129
33	6	0	-4.765202	-4.485720	-2.035935
34	1	0	-5.464177	-4.360516	-1.213115
35	6	0	-3.433140	-4.112541	-1.853714
36	1	0	-3.097814	-3.701961	-0.908908
37	6	0	-3.616613	-0.673729	1.006674
38	6	0	-3.437526	-1.978782	1.649790
39	6	0	-2.185166	-2.624144	1.823459
40	1	0	-1.294047	-2.140901	1.455836
41	6	0	-2.079424	-3.850729	2.460293
42	1	0	-1.100893	-4.307362	2.581162
43	6	0	-3.220296	-4.505626	2.955024
44	1	0	-3.130603	-5.471256	3.445448
45	6	0	-4.454419	-3.904462	2.811079
46	1	0	-5.350789	-4.387764	3.193622
47	6	0	-4.589828	-2.648265	2.177021
48	6	0	-5.885423	-2.041890	2.083059

49	1	0	-6.738741	-2.581574	2.487212
50	6	0	-6.042608	-0.817807	1.519997
51	1	0	-7.024447	-0.354565	1.461324
52	6	0	-4.924997	-0.097943	0.981242
53	6	0	-5.145068	1.164120	0.397119
54	1	0	-6.165703	1.531879	0.336614
55	6	0	-4.118867	1.927337	-0.136036
56	6	0	-4.456891	3.220449	-0.793677
57	6	0	-5.303662	4.142933	-0.157899
58	1	0	-5.646475	3.938050	0.852422
59	6	0	-5.682671	5.324500	-0.794517
60	1	0	-6.333019	6.027956	-0.280637
61	6	0	-5.223834	5.606079	-2.082377
62	1	0	-5.519435	6.525997	-2.580288
63	6	0	-4.384371	4.695389	-2.727732
64	1	0	-4.029938	4.899209	-3.734886
65	6	0	-4.004697	3.514739	-2.090750
66	1	0	-3.370700	2.801663	-2.608030
67	6	0	-1.246241	3.424444	0.108256
68	6	0	-1.945234	3.995892	1.296899
69	6	0	-2.230895	5.370854	1.346388
70	1	0	-2.019935	5.986144	0.476718
71	6	0	-2.809434	5.945361	2.477332
72	1	0	-3.029686	7.009696	2.486356
73	6	0	-3.114819	5.156780	3.587673
74	1	0	-3.567626	5.602540	4.469368
75	6	0	-2.839420	3.788463	3.553435
76	1	0	-3.074468	3.162936	4.410761
77	6	0	-2.262065	3.214852	2.421172
78	1	0	-2.061319	2.148065	2.409440
79	6	0	-0.129680	4.101216	-0.372582

80	1	0	0.183990	5.020447	0.114823
81	6	0	0.623129	3.638515	-1.472082
82	6	0	1.758307	4.396578	-1.916748
83	1	0	1.987147	5.326363	-1.401523
84	6	0	2.527504	3.966831	-2.949150
85	1	0	3.386517	4.546840	-3.279113
86	6	0	2.214085	2.756110	-3.651168
87	6	0	3.007994	2.358958	-4.751295
88	1	0	3.860961	2.976856	-5.023510
89	6	0	2.706377	1.224954	-5.478525
90	1	0	3.324352	0.931442	-6.322750
91	6	0	1.580082	0.463684	-5.122478
92	1	0	1.316108	-0.416619	-5.702741
93	6	0	0.790613	0.822985	-4.042663
94	1	0	-0.080836	0.234711	-3.798219
95	6	0	1.086787	1.966666	-3.256702
96	6	0	0.293168	2.400929	-2.105644
97	6	0	1.943912	0.859495	2.293184
98	1	0	1.526625	1.560664	3.022259
99	7	0	1.036897	0.977930	1.086935
100	1	0	0.064879	0.662901	1.267243
101	6	0	3.347584	1.321451	1.937575
102	6	0	4.089669	1.993451	2.915787
103	1	0	3.648064	2.176214	3.893527
104	6	0	5.391389	2.431958	2.671672
105	6	0	6.198753	3.132530	3.737107
106	1	0	5.660600	3.144416	4.689639
107	1	0	6.419107	4.171908	3.464817
108	1	0	7.163095	2.636463	3.888884
109	6	0	5.944224	2.195861	1.400335
110	8	0	7.247713	2.599797	1.173390

111	6	0	7.382310	3.847341	0.492569
112	1	0	8.454359	4.044973	0.421555
113	1	0	6.898916	4.660991	1.049178
114	1	0	6.954773	3.805572	-0.516889
115	6	0	5.235249	1.510710	0.402036
116	6	0	5.851109	1.231290	-0.947827
117	1	0	5.480335	0.287449	-1.358911
118	1	0	6.940615	1.177993	-0.876516
119	1	0	5.599389	2.016829	-1.672589
120	6	0	3.933728	1.078675	0.691977
121	1	0	3.401850	0.534549	-0.084914
122	6	0	1.814110	-0.544123	2.866166
123	6	0	2.454880	-1.639870	2.281509
124	1	0	3.093981	-1.497403	1.415347
125	6	0	2.271710	-2.935672	2.774476
126	6	0	2.940804	-4.116317	2.112522
127	1	0	2.295869	-4.999113	2.143424
128	1	0	3.881758	-4.381627	2.612838
129	1	0	3.180611	-3.894899	1.068617
130	6	0	1.426858	-3.108475	3.884658
131	8	0	1.160388	-4.382284	4.353846
132	6	0	2.121543	-4.910029	5.268197
133	1	0	1.752890	-5.893705	5.567452
134	1	0	2.218874	-4.272379	6.156561
135	1	0	3.107867	-5.020820	4.801137
136	6	0	0.761441	-2.029750	4.489402
137	6	0	-0.193040	-2.261863	5.634425
138	1	0	-0.590766	-1.313236	6.007518
139	1	0	0.286341	-2.780845	6.471889
140	1	0	-1.036124	-2.882960	5.311888
141	6	0	0.974745	-0.752280	3.965390

142	1	0	0.460763	0.092930	4.420150
143	1	0	0.998836	1.938312	0.721936
144	1	0	1.282024	0.332998	0.297092

BHandHLYP/6-31G*

Energy = -3546.50524236 hartrees
Number of Imaginary frequencies = none

Zero-point correction= 1.201484 (Hartree/Particle)
Thermal correction to Energy= 1.271915
Thermal correction to Enthalpy= 1.272859
Thermal correction to Gibbs Free Energy= 1.085723
Sum of electronic and zero-point Energies= -3545.303758
Sum of electronic and thermal Energies= -3545.233327
Sum of electronic and thermal Enthalpies= -3545.232383
Sum of electronic and thermal Free Energies= -3545.419519

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	798.139	273.863	393.861

Standard orientation:

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.312046	-0.357533	0.320089
2	6	0	-2.588411	0.103865	0.355173
3	6	0	-2.799521	1.387441	-0.132138
4	6	0	-1.601125	2.181685	-0.524377
5	6	0	-0.768361	1.651930	-1.509730
6	8	0	-1.047239	0.418036	-1.947022
7	5	0	-0.764539	-0.679992	-1.019290

8	8	0	0.697647	-0.792277	-0.806044
9	5	0	1.416367	-1.755001	-1.418608
10	8	0	0.819712	-2.767311	-2.099805
11	5	0	-0.563061	-2.838914	-2.117691
12	8	0	-1.310898	-1.881169	-1.565580
13	8	0	2.780376	-1.674395	-1.282534
14	6	0	3.731017	-2.457864	-1.868211
15	6	0	3.578917	-3.021249	-3.127505
16	1	0	2.660401	-2.887193	-3.667873
17	6	0	4.614707	-3.767419	-3.665484
18	1	0	4.490008	-4.208216	-4.641490
19	6	0	5.799136	-3.950816	-2.969319
20	1	0	6.598050	-4.533007	-3.398279
21	6	0	5.945509	-3.375414	-1.717579
22	1	0	6.862148	-3.503635	-1.164596
23	6	0	4.916523	-2.629774	-1.166822
24	1	0	5.021331	-2.170305	-0.197639
25	8	0	-1.066652	-3.940864	-2.737077
26	6	0	-2.387346	-4.257481	-2.865593
27	6	0	-2.801139	-4.762827	-4.088346
28	1	0	-2.081331	-4.846973	-4.885402
29	6	0	-4.119114	-5.149579	-4.262783
30	1	0	-4.436065	-5.540240	-5.216663
31	6	0	-5.025547	-5.036030	-3.220207
32	1	0	-6.051989	-5.335418	-3.357032
33	6	0	-4.599616	-4.535377	-1.999808
34	1	0	-5.293078	-4.441223	-1.179640
35	6	0	-3.282940	-4.147967	-1.812568
36	1	0	-2.955797	-3.756951	-0.866030
37	6	0	-3.629428	-0.683700	0.903979
38	6	0	-3.458141	-1.988660	1.535610

39	6	0	-2.211712	-2.611794	1.756699
40	1	0	-1.318234	-2.116472	1.439955
41	6	0	-2.116940	-3.836839	2.373728
42	1	0	-1.145869	-4.277282	2.532615
43	6	0	-3.262239	-4.512529	2.801251
44	1	0	-3.180505	-5.476881	3.276052
45	6	0	-4.487388	-3.931381	2.611955
46	1	0	-5.385536	-4.429476	2.943037
47	6	0	-4.609850	-2.675130	1.995872
48	6	0	-5.905331	-2.087947	1.856064
49	1	0	-6.759441	-2.642302	2.212354
50	6	0	-6.055181	-0.869603	1.311297
51	1	0	-7.031966	-0.422269	1.217671
52	6	0	-4.929012	-0.130711	0.831731
53	6	0	-5.141053	1.127876	0.258787
54	1	0	-6.154211	1.484368	0.167796
55	6	0	-4.111462	1.899483	-0.222761
56	6	0	-4.434640	3.196085	-0.866652
57	6	0	-5.292430	4.098212	-0.241409
58	1	0	-5.660335	3.875664	0.746942
59	6	0	-5.650160	5.284292	-0.860245
60	1	0	-6.309818	5.972286	-0.355834
61	6	0	-5.156716	5.589126	-2.118654
62	1	0	-5.434936	6.511734	-2.602503
63	6	0	-4.305115	4.697593	-2.753040
64	1	0	-3.923976	4.920184	-3.736805
65	6	0	-3.947828	3.512110	-2.133598
66	1	0	-3.301675	2.815802	-2.640995
67	6	0	-1.265550	3.408281	0.092571
68	6	0	-2.016739	3.997123	1.231745
69	6	0	-2.307510	5.360202	1.237553

70	1	0	-2.058840	5.954007	0.373558
71	6	0	-2.941395	5.949631	2.317933
72	1	0	-3.165319	7.004022	2.294725
73	6	0	-3.297130	5.186536	3.418304
74	1	0	-3.792634	5.643212	4.259861
75	6	0	-3.016639	3.829106	3.425612
76	1	0	-3.291141	3.224280	4.274972
77	6	0	-2.383860	3.240959	2.343572
78	1	0	-2.182823	2.182985	2.361635
79	6	0	-0.133611	4.068787	-0.338764
80	1	0	0.158850	4.986186	0.146110
81	6	0	0.661777	3.588597	-1.387872
82	6	0	1.824233	4.325951	-1.779036
83	1	0	2.035053	5.251839	-1.267657
84	6	0	2.633944	3.875981	-2.752482
85	1	0	3.510285	4.435133	-3.041578
86	6	0	2.343488	2.663046	-3.451730
87	6	0	3.189062	2.243980	-4.491981
88	1	0	4.058854	2.840621	-4.719885
89	6	0	2.915050	1.114114	-5.215326
90	1	0	3.570785	0.801885	-6.011716
91	6	0	1.764414	0.380165	-4.918544
92	1	0	1.521495	-0.495307	-5.499072
93	6	0	0.926386	0.762739	-3.899315
94	1	0	0.038578	0.196991	-3.703823
95	6	0	1.196254	1.903822	-3.115560
96	6	0	0.351834	2.361749	-2.018236
97	6	0	1.880569	0.868069	2.342180
98	1	0	1.484097	1.550487	3.087141
99	7	0	0.974046	1.012501	1.160678
100	1	0	0.016067	0.703134	1.347838

101	6	0	3.275818	1.320511	1.979508
102	6	0	4.040940	1.942720	2.958375
103	1	0	3.626634	2.091916	3.944125
104	6	0	5.331476	2.372779	2.701311
105	6	0	6.168680	3.021958	3.764826
106	1	0	5.655025	3.010231	4.721204
107	1	0	6.396493	4.057765	3.522084
108	1	0	7.119329	2.508381	3.877203
109	6	0	5.849058	2.179703	1.420138
110	8	0	7.134137	2.584609	1.176607
111	6	0	7.256267	3.845223	0.554252
112	1	0	8.317300	4.044282	0.460782
113	1	0	6.794644	4.627942	1.153855
114	1	0	6.802774	3.846260	-0.434511
115	6	0	5.116585	1.545455	0.422549
116	6	0	5.693129	1.313404	-0.944644
117	1	0	5.320115	0.385874	-1.367885
118	1	0	6.775969	1.266553	-0.906024
119	1	0	5.413488	2.112420	-1.630045
120	6	0	3.826019	1.119489	0.722566
121	1	0	3.277177	0.613486	-0.056417
122	6	0	1.743232	-0.540793	2.875855
123	6	0	2.373134	-1.613920	2.263538
124	1	0	3.016927	-1.449330	1.415628
125	6	0	2.169303	-2.914018	2.705252
126	6	0	2.828478	-4.073537	2.014571
127	1	0	2.175528	-4.940162	2.003227
128	1	0	3.750430	-4.365566	2.515904
129	1	0	3.084559	-3.819006	0.991131
130	6	0	1.316989	-3.114220	3.789912
131	8	0	1.041543	-4.388018	4.209577

132	6	0	1.968881	-4.942176	5.118178
133	1	0	1.596361	-5.925128	5.380542
134	1	0	2.049061	-4.335258	6.018182
135	1	0	2.955265	-5.040722	4.670803
136	6	0	0.664565	-2.058453	4.421627
137	6	0	-0.298009	-2.321029	5.542527
138	1	0	-0.699125	-1.390010	5.931254
139	1	0	0.171507	-2.853865	6.365605
140	1	0	-1.128029	-2.930944	5.195568
141	6	0	0.896116	-0.774712	3.950060
142	1	0	0.390773	0.053142	4.425304
143	1	0	0.937910	1.968328	0.810969
144	1	0	1.214804	0.384189	0.373231

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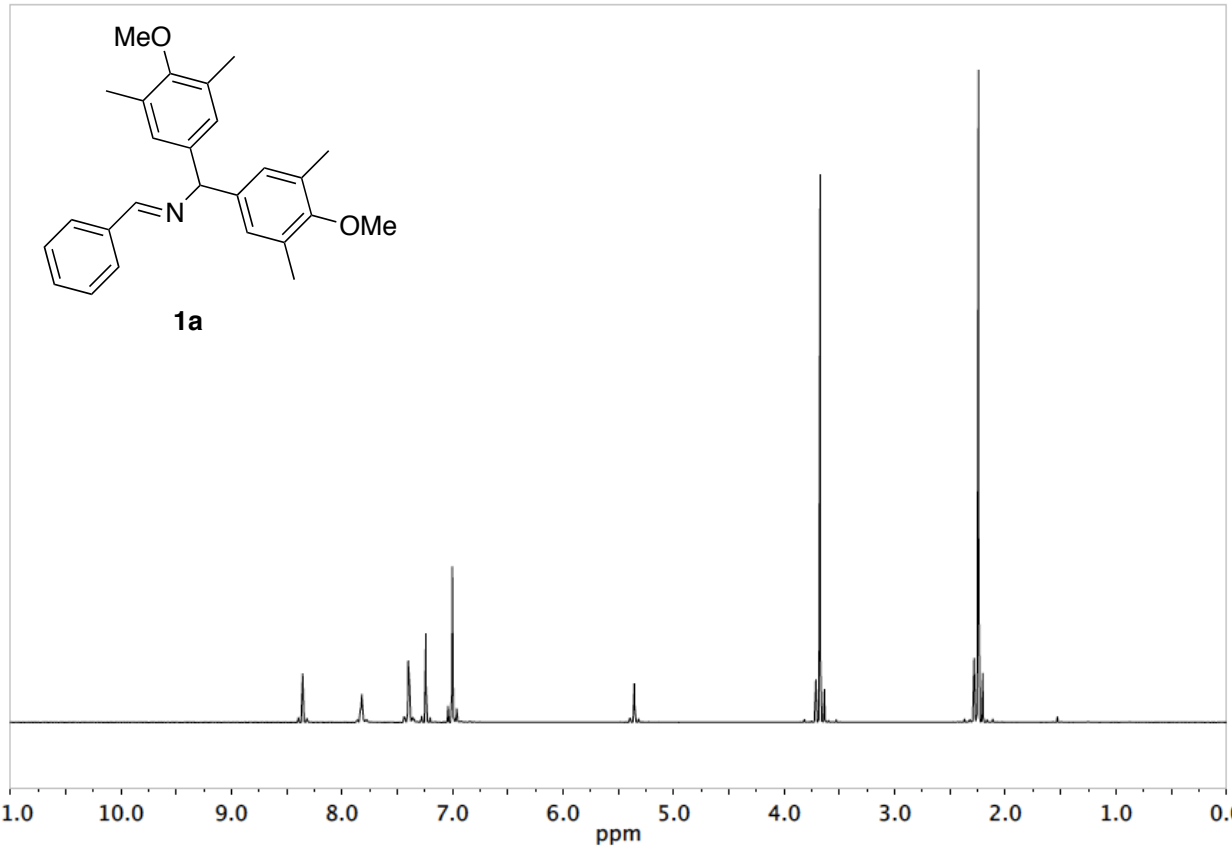
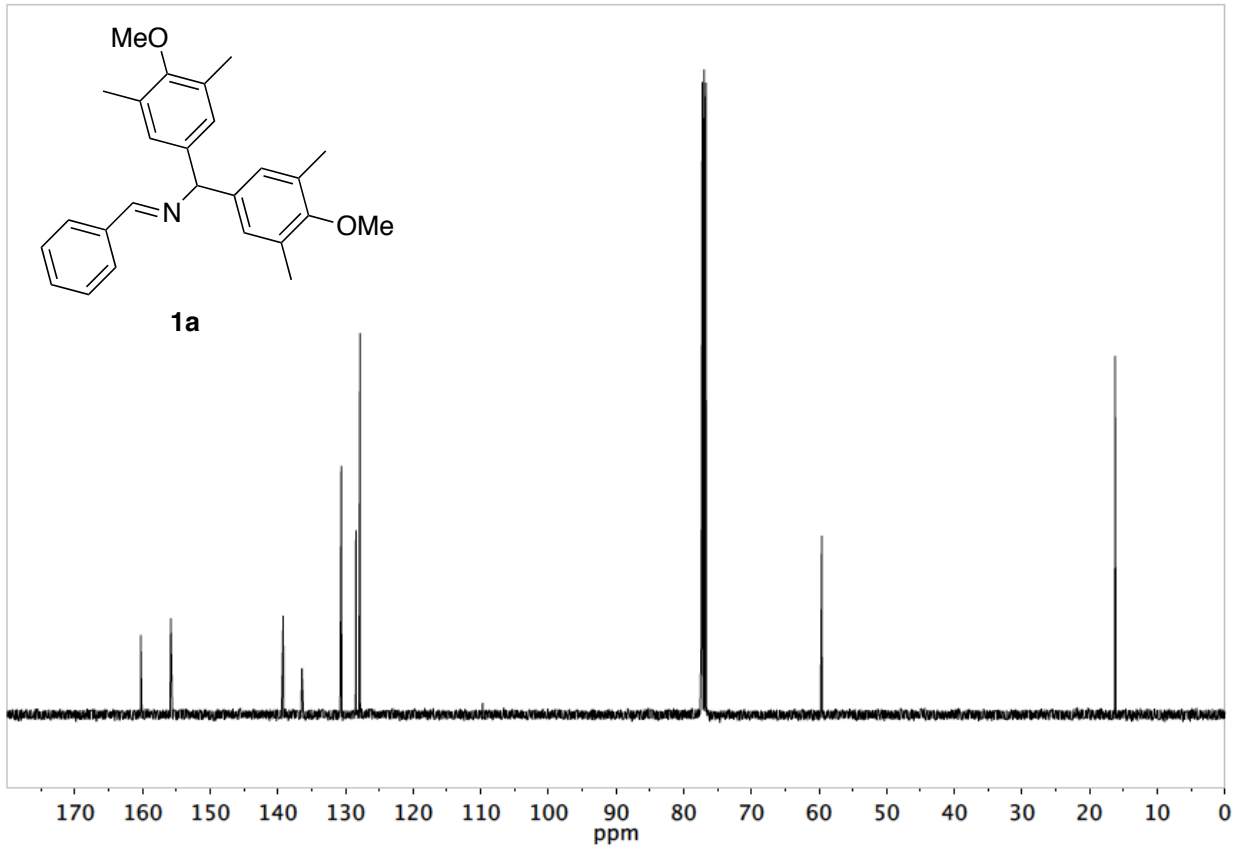
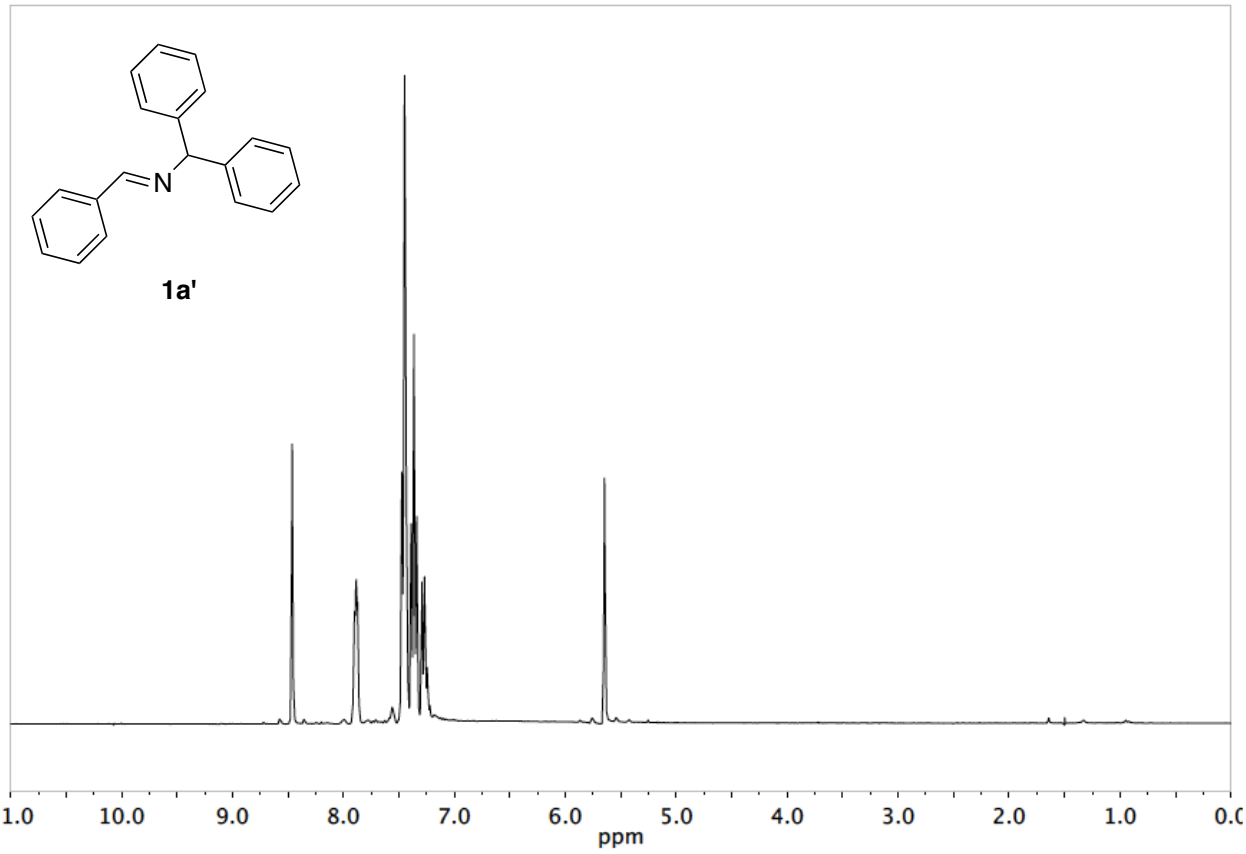
I. ^{1}H and ^{13}C NMR of **1a**, **1a′**, **5a**, **5a′**, **6** and **12**:



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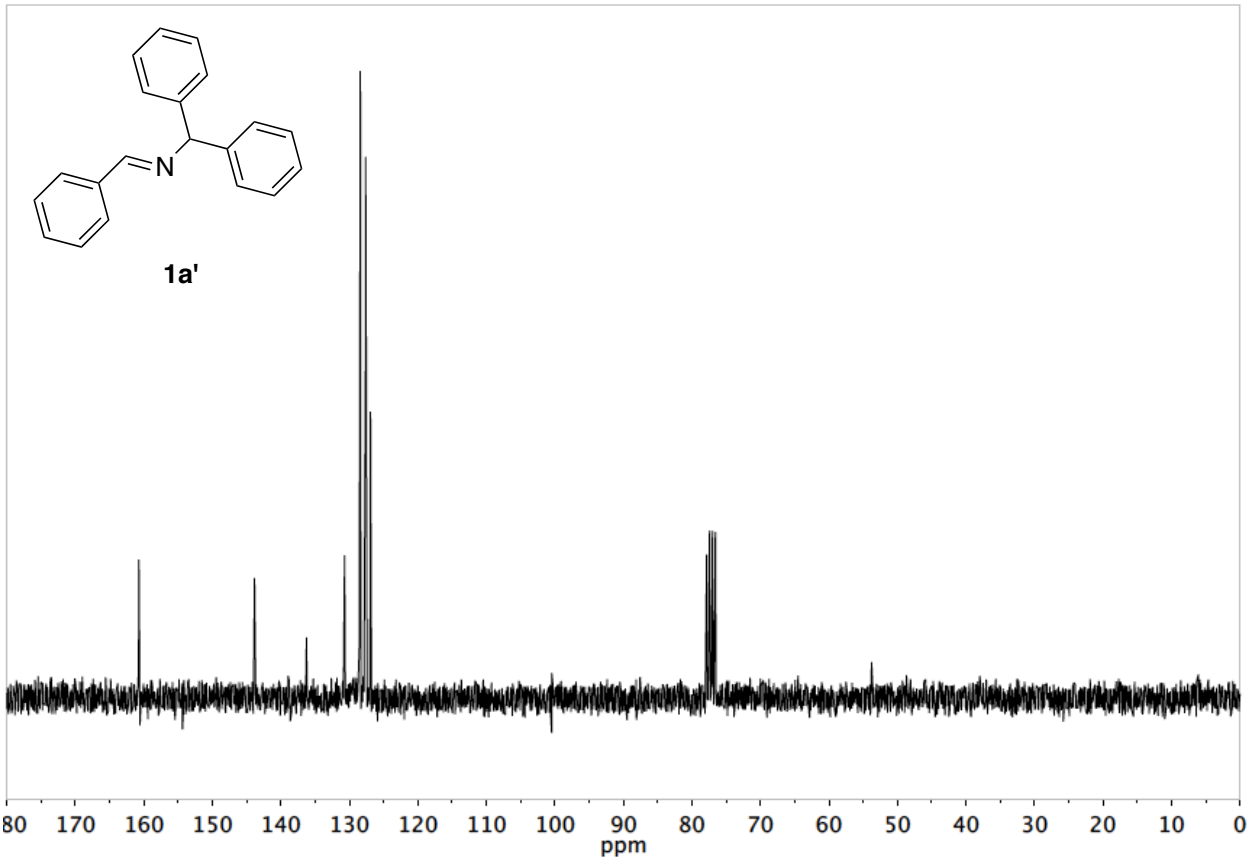
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm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130
120
110
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80
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60
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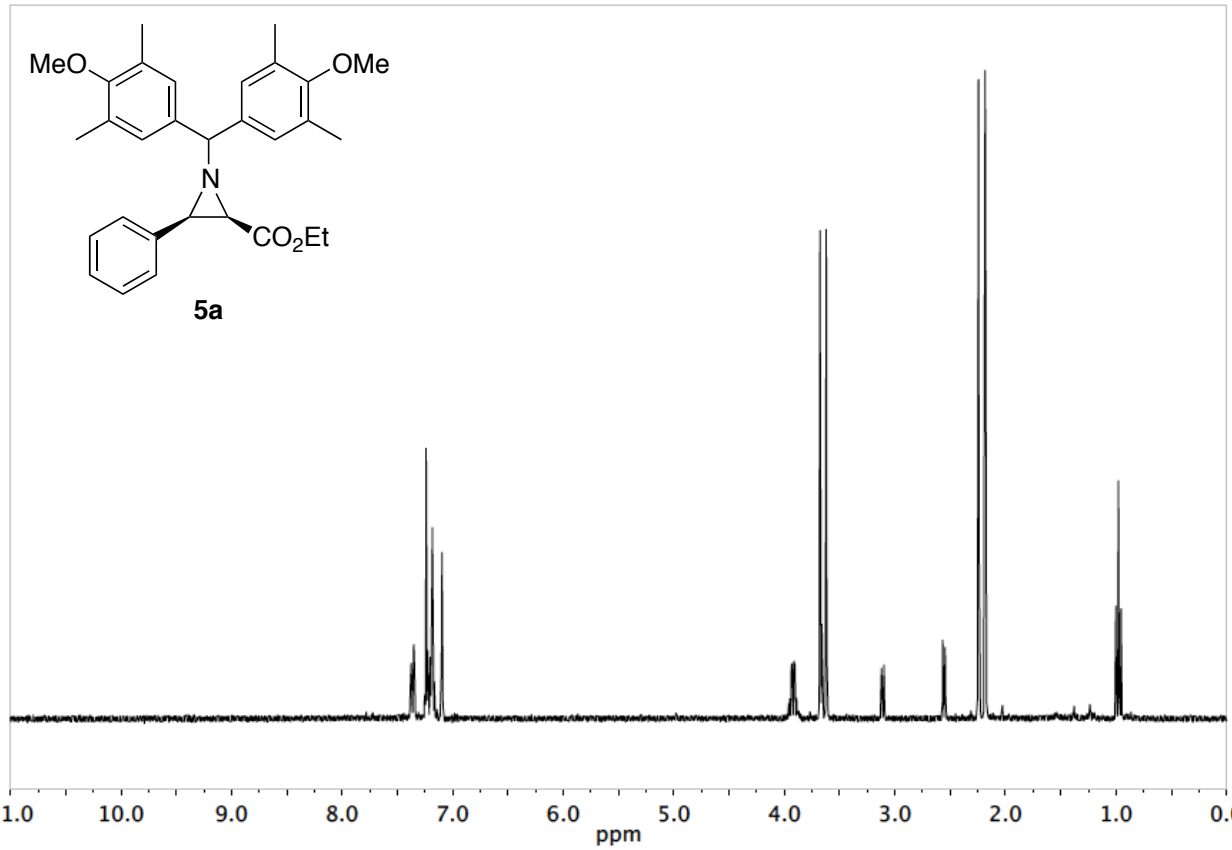
40
30
20
10
0
ppm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CO2Et
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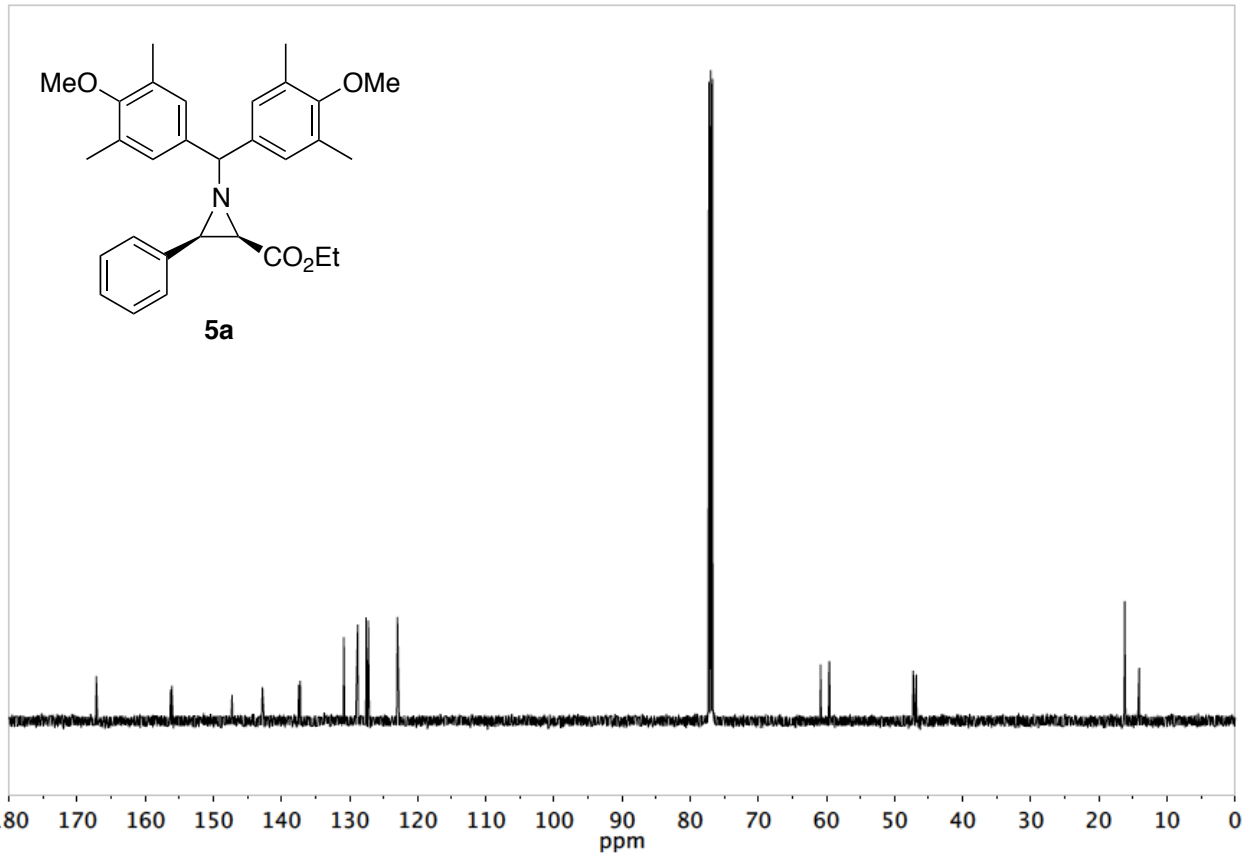
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm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50
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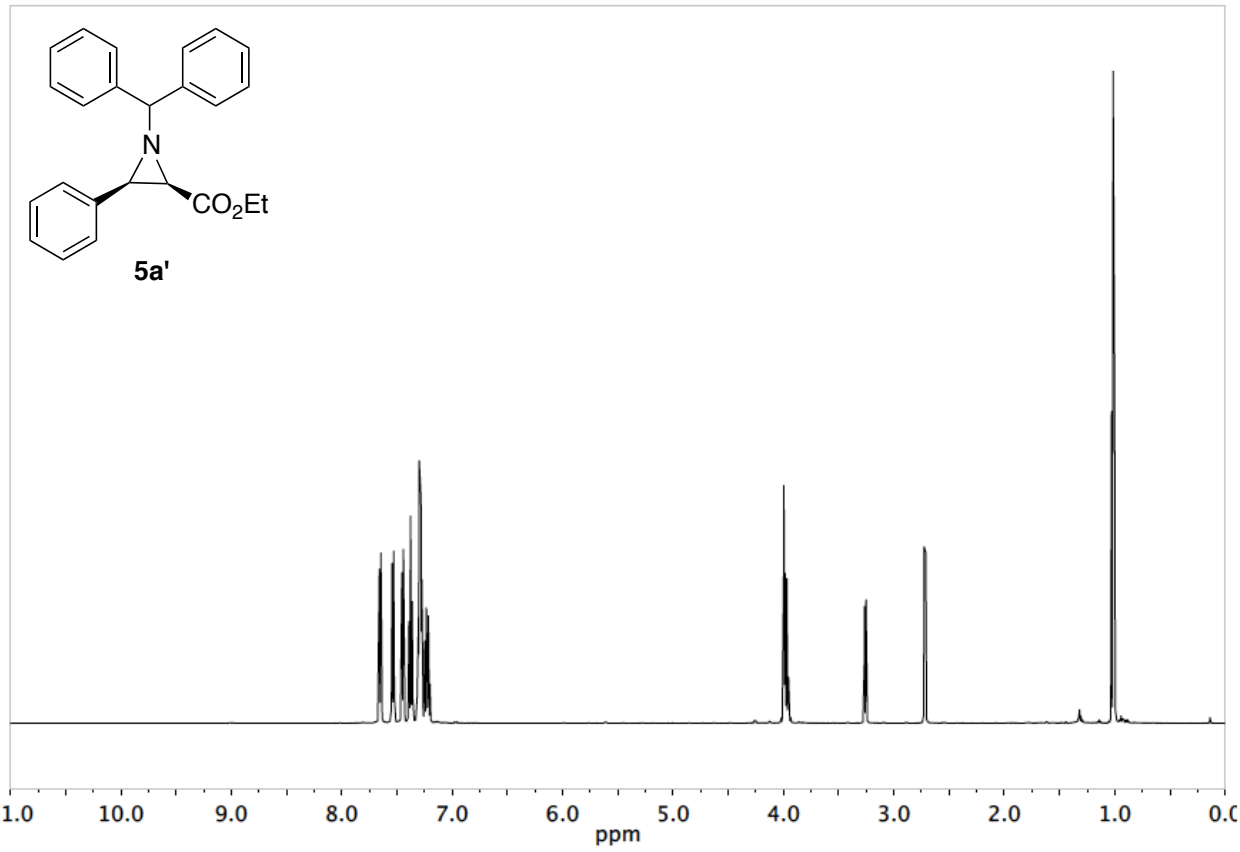
0
ppm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8.0
7.0
6.0
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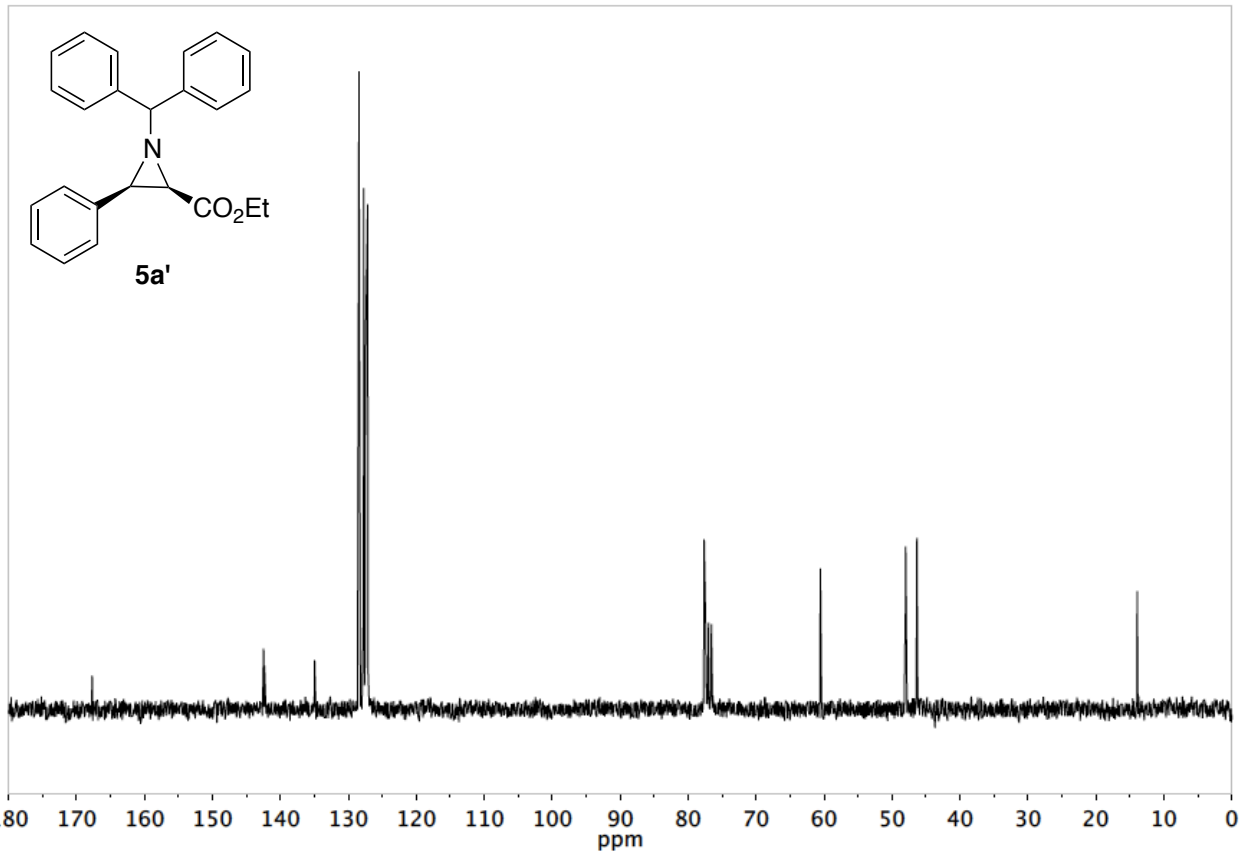
3.0
2.0
1.0
0.0
ppm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CO2Et
5a'
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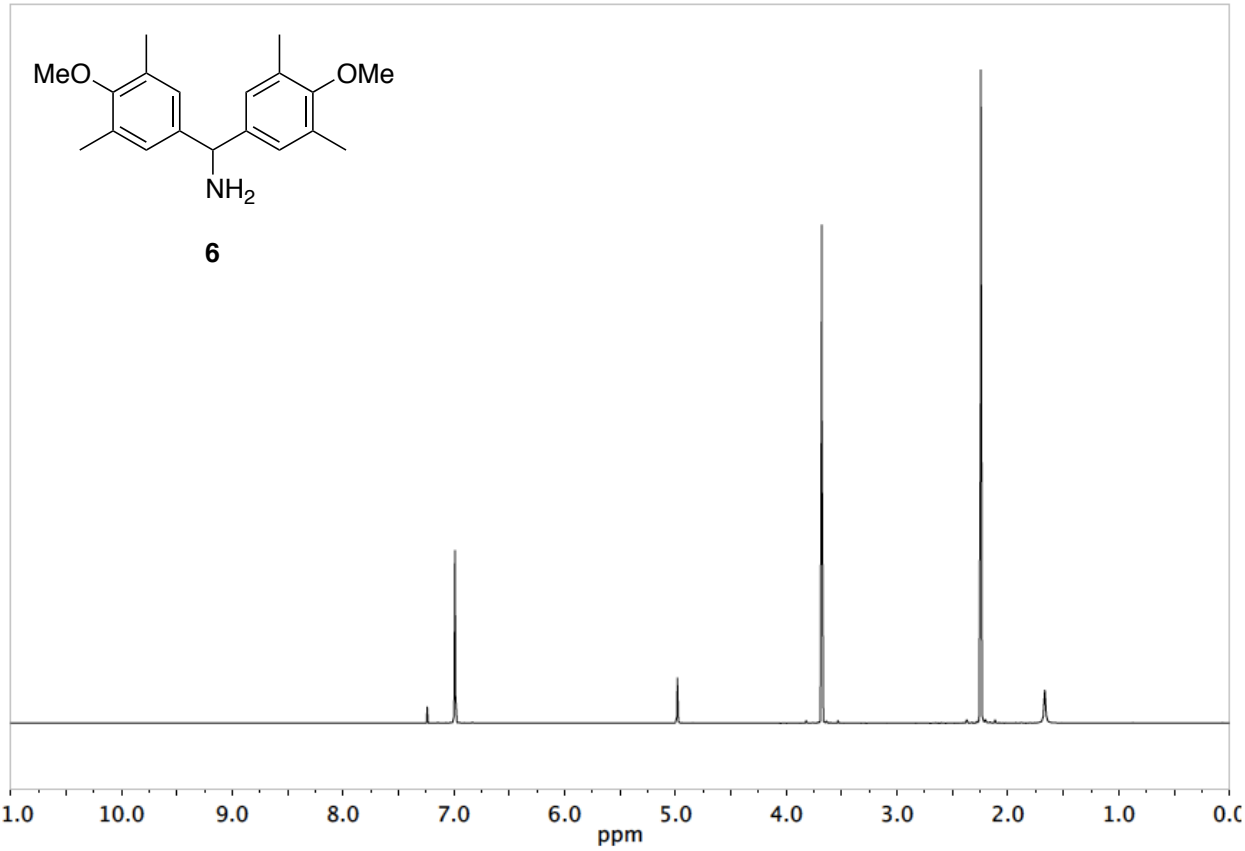
ppm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OMe
NH2
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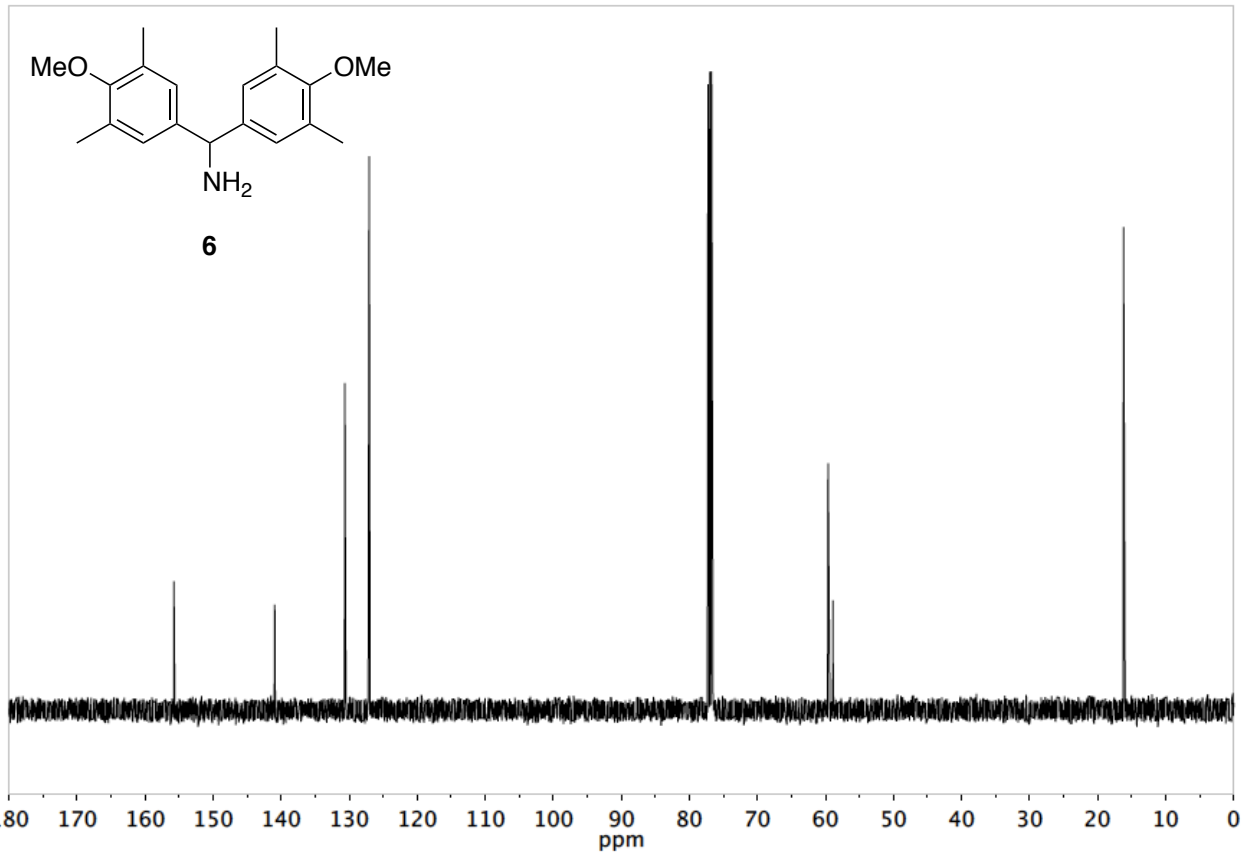
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm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NH2
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0
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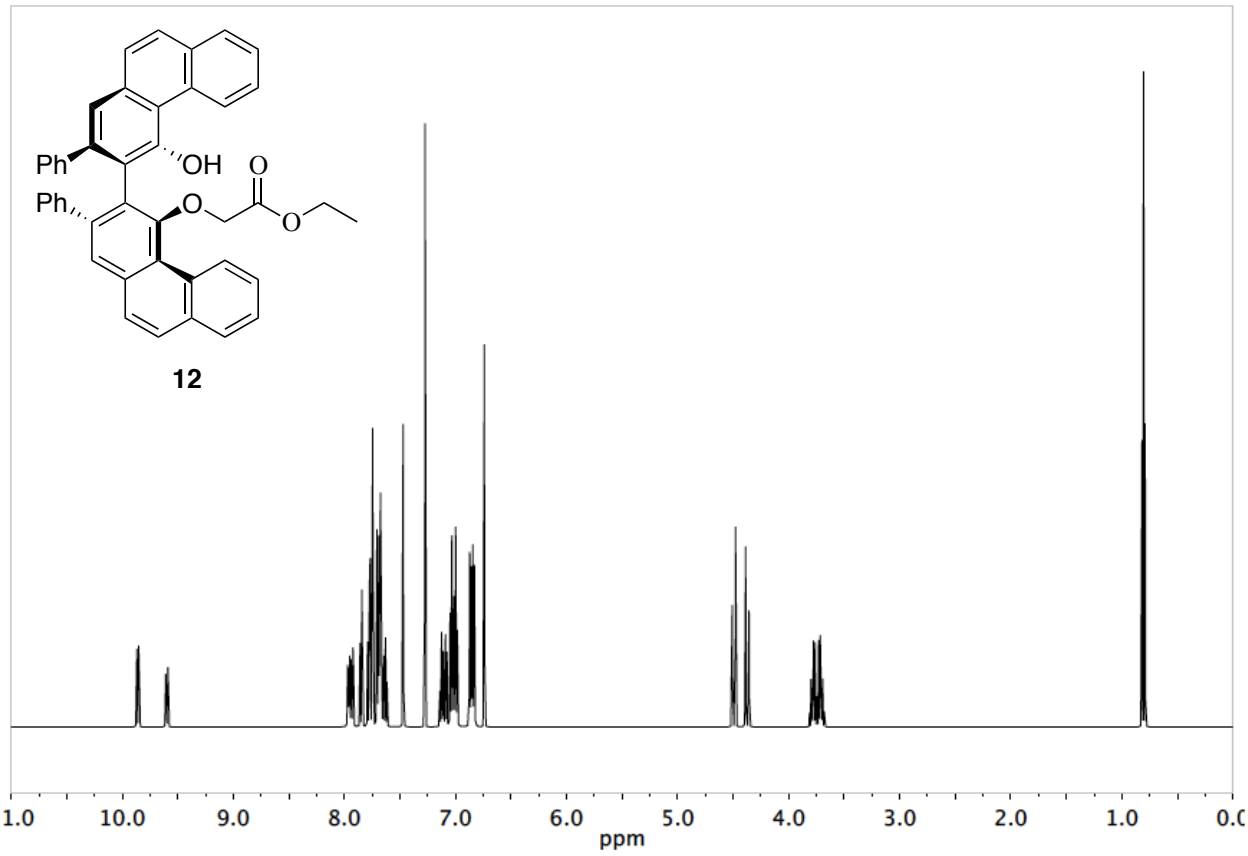
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1.0
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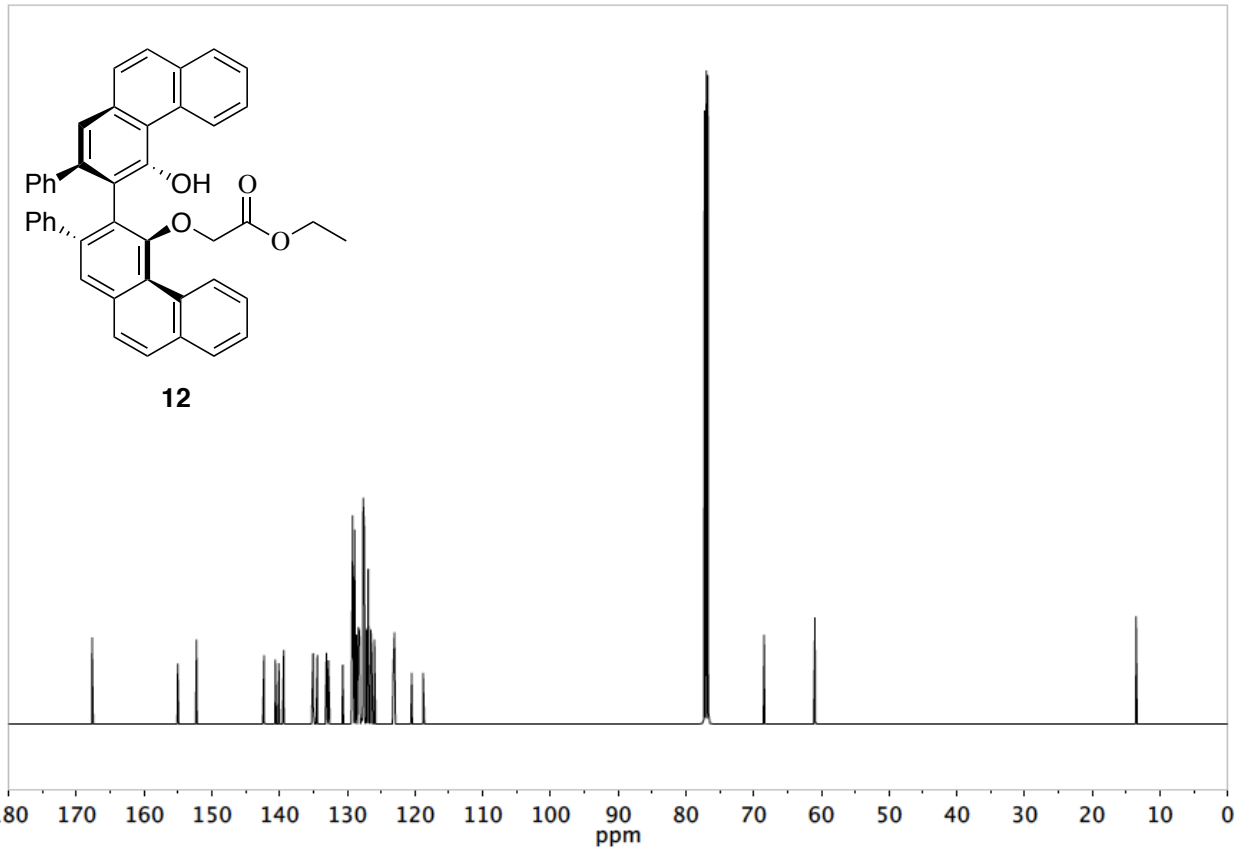
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30
20
10
0
ppm