Electronic Supplementary Material (ESI) for ChemComm.

Solvent Free Zinc (NSNO) Complex- Catalyzed Dihydroboration of Nitriles

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I. Experimental

General considerations

All experiments were carried out under dinitrogen, using a MBraun glovebox unless otherwise stated. Diethyl ether, toluene and THF were dried on columns of activated alumina using a J. C. Meyer (formerly Glass Contour) solvent purification system. Anhydrous C_6D_6 and THF-d_8 were dried with activated alumina (ca. 10 wt %) overnight, followed by filtration. $CDCl_3$ was stored over activated 4 Å molecular sieves (heated at 250 °C for 24 h under vacuum). Anhydrous methanol and ethanol were purchased from Aldrich and used as obtained. Other chemicals were used as obtained commercially: 2-chloromethylpyridine (Alfa Aesar), 2-amino benzenethiol (Alfa Aesar), diethylzinc (Aldrich), salicylaldehyde (Aldrich), sodium borohydride (Aldrich). All reagents were purchased from commercial suppliers. ^{1}H and ^{11}B NMR spectra were recorded on a 300 MHz Bruker Avance or Avance II instrument at room temperature (21−25 °C). ^{1}H NMR spectra were referenced respectively to solvent residual protons (C_6D_6, δ 7.15; $CDCl_3$, δ 7.26; THF-d_8, δ 1.72 and 3.58). Mass spectra were recorded on an AB Sciex Q1MS mass spectrometer with electrospray ionization (ESIMS) in positive mode (ion spray voltage, 5000.0 V; TEM, 400 °C; declustering potential, 11.00 V; focusing potential, 300.0 V) with samples prepared to ca. 0.05 mg/mL in acetonitrile or dichloromethane. For electron impact (EI), solid samples were prepared by drying products under vacuum, and spectra obtained using a Kratos Concept S1 instrument (Hres 7000−10000). X-ray diffraction data were collected on a Bruker Smart or Kappa diffractometer equipped with an ApexII CCD detector and a sealed-tube Mo K source (λ = 0.71073 Å).

Synthesis of H_2L

Precursor **1** was obtained through the literature procedure.[1] To an ethanolic solution of **1** (2.00 g, 9.24 mmol) was added salicylaldehyde (1.129 g, 9.24 mmol) and the mixture was refluxed for 2 h. Then, the solution was cooled down to 0-5 ˚C and $NaBH_4$ (0.70 g, 18.48 mmol) was added pinch wise and the mixture was heated to 50 ˚C for 2 h. Finally, the solvent was removed under vacuum and H_2L was extracted with ethyl acetate and kept in the freezer. After 4-6 h, colourless crystals of H_2L appeared and were filtered and dried (2.41 g, 81%). The same crystal was used for X-ray crystallography. ^{1}H NMR (300 MHz, CDCl3): δ 9.09 (b, 1H, OH), 8.50 (d, 1H, N-adjacent H in Py ring), 7.62 (t, 1H, aromatic), 7.39 (d, 1H, aromatic), 7.21 (ov mult, 4H, aromatic), 7.12 (d, 1H, aromatic), 6.90 (m, 2H, aromatic), 6.84 (d, 1H, aromatic), 6.70 (t, 1H, aromatic), 5.91 (brt, 1H, NH), 4.39 (d, 2H, N-CH_2), 3.99 (s, 2H, S-CH_2).

Synthesis of Zn-1

3 mL of 1 M solution of diethylzinc in hexane (3.00 mmol) was added to a solution of H_2L (0.96 g, 3 mmol in 5 mL of THF) dropwise at RT. The final solution turned yellow after 5 min and **Zn-1** precipitated out after 2 h. The precipitate was filtered, washed with diethyl ether (3 × 3 mL), and dried under vacuum (2.08 g, 89%). Suitable crystals for crystallography were grown by ether layering of a THF solution of **Zn-1** at RT. ^{1}H NMR (300 MHz, CDCl3): δ 8.80 (d, 1H, N-adjacent H in Py ring), 7.72 (t, 1H, aromatic), 7.64 (d, 1H, aromatic), 7.38 (ov mult, 2H, aromatic), 7.21 (d, 1H, aromatic), 7.02 (ov mult, 2H, aromatic), 6.84 (d, 1H, aromatic), 6.66 (d, 1H, aromatic), 6.58 (t, 1H, aromatic), 6.39 (t,

1H, aromatic), 4.43, 4.32 (d, 14 Hz, 1H), 4.16, 3.94 (d, 14.5 Hz, 1H). EI-MS [M/2] 384.02, Calc'd 384.03 (Figure S5).

Synthesis of O-borylated HL (HL-Bpin)

0.1 g of **H_2L** (0.31 mmol) was dissolved in 5 mL of THF in a vial and 44 µL of HBpin (0.31 mmol) was added and the solution was stirred at room temperature for 5 h. Then the solvent was evaporated under vacuum and the residue dissolved in C_6D_6. ^{1}H NMR (300 MHz, C_6D_6): δ 8.30 (d, 1H, N-adjacent H in Py ring), 7.40 (d, 1H, aromatic), 7.28 (d, 1H, aromatic), 7.23 (d, 1H, aromatic), 6.97 (ov mult, 2H, aromatic), 6.83 (ov mult, 2H, aromatic), 6.51 (ov mult, 2H, aromatic), 5.90 (t, 1H, NH), 4.30 (d, 2H, N-CH_2), 3.91 (s, 1H, S-CH_2), 1.00 (s, 12H, Bpin CH_3) (Figure S20). ^{11}B NMR 21.8 ppm (Figure S19). ESI-MS $[NaM]^+$ 471.18, Calc'd 471.18.

Catalysis protocols

A catalyst stock solution was prepared by dissolving 15 mg (0.020 mmol) of **Zn-1** in 4 mL of THF. Ten small vials were charged with 20 µL of the catalyst stock solution (0.7 mg, 0.001 mmol, 1 mol%). Then, THF was evaporated under vacuum and nitrile substrates (0.1 mmol: isobutyronitrile 6.9 mg or 8.9 µL, acetonitrile 4.1 mg or 5.2 µL, 2-chlorobenzonitrile 13.7 mg, 2-bromobenzonitrile 18.2 mg, 3-chlorobenzonitrile 13.7 mg, 3-bromobenzonitrile 18.2 mg, 4-fluorobenzonitrile 12.1 mg, 4-bromobenzonitrile 18.2 mg, 2-thiophenecarbonitrile 10.9 mg or 9.3 µL, 4-methoxybenzonitrile 13.3 mg) were added to the vials, and subsequently after putting a tiny magnetic stir bar in the vials, HBpin (29 µL, 0.2 mmol) was added to the vials. The vials were capped and the stir bars started stirring very gently. After 6-12 h, the reaction mixtures were dissolved in C_6D_6 and transferred to NMR tubes and a ^{1}H NMR spectrum was taken at room temperature. Concentration of the di-hydroborated products were calculated based on integrals of the characteristic product signal in the reaction mixture and the known [HBpin] as well.

II. Spectroscopic Data

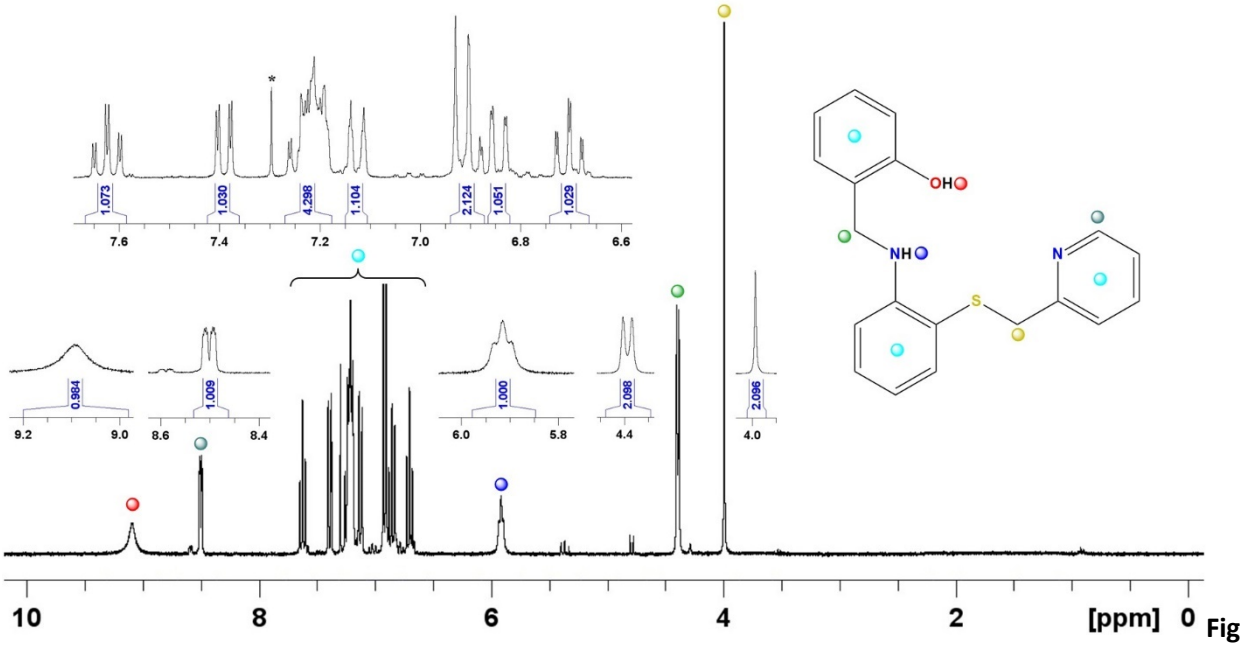

Figure S1. ^{1}H NMR spectrum of **H_2L**. * indicates protic impurity in $CDCl_3$.

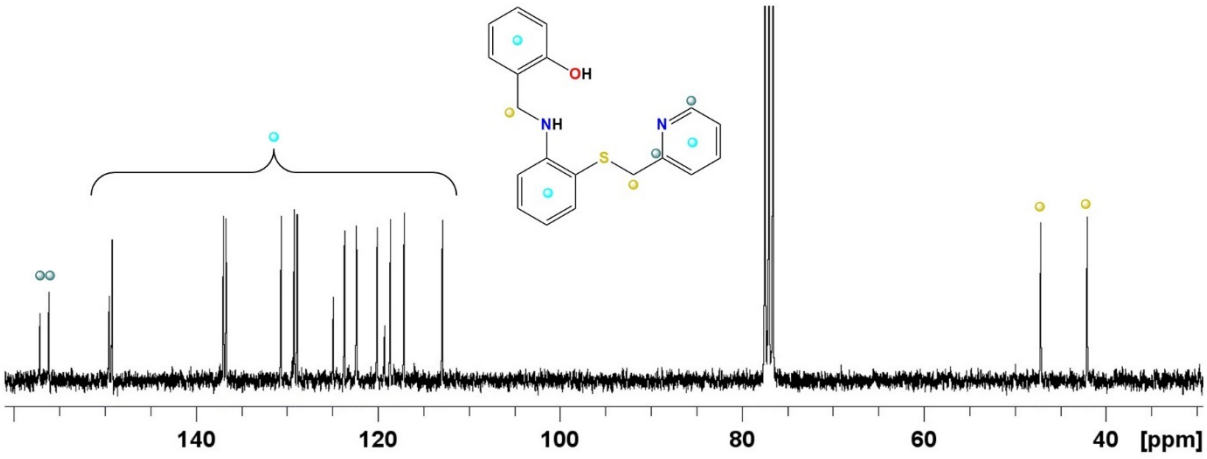

Figure S2. ^{13}C NMR spectrum of **H_2L**. * indicates protic impurity in $CDCl_3$.

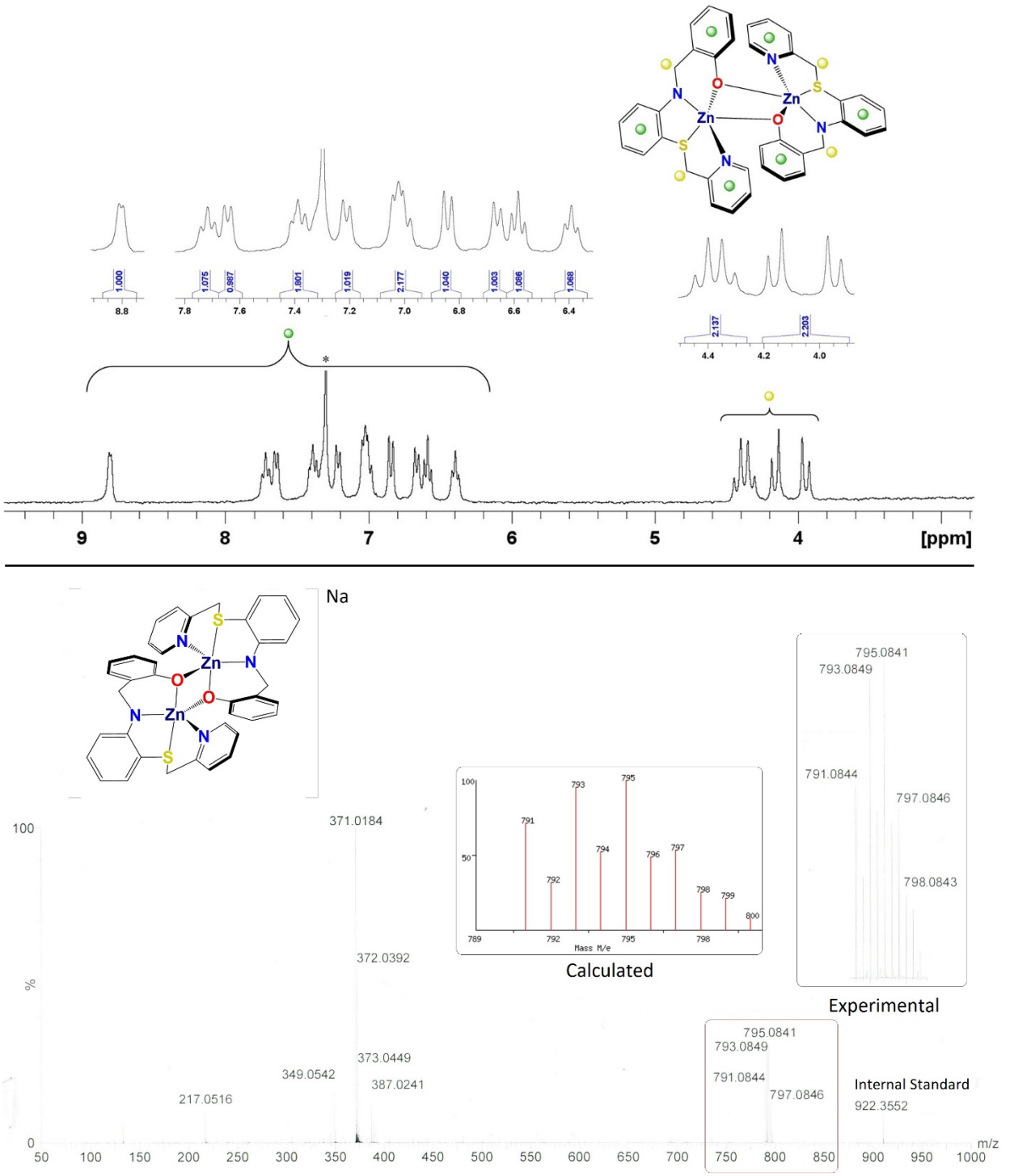

Figure S3. ^{1}H NMR spectrum of **Zn-1**. * indicates protic impurity in $CDCl_3$ (top). ESI-MS spectrum of **Zn-1** (bottom).

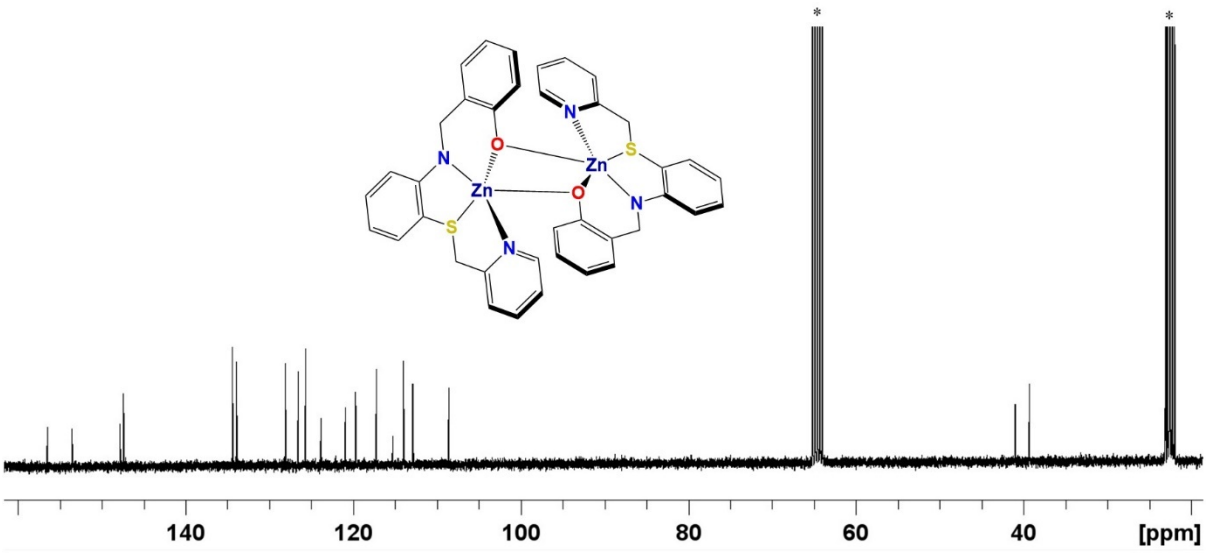

Figure S4. ^{13}C NMR spectrum of **Zn-1**. * indicates protic impurity in THF-d_8.

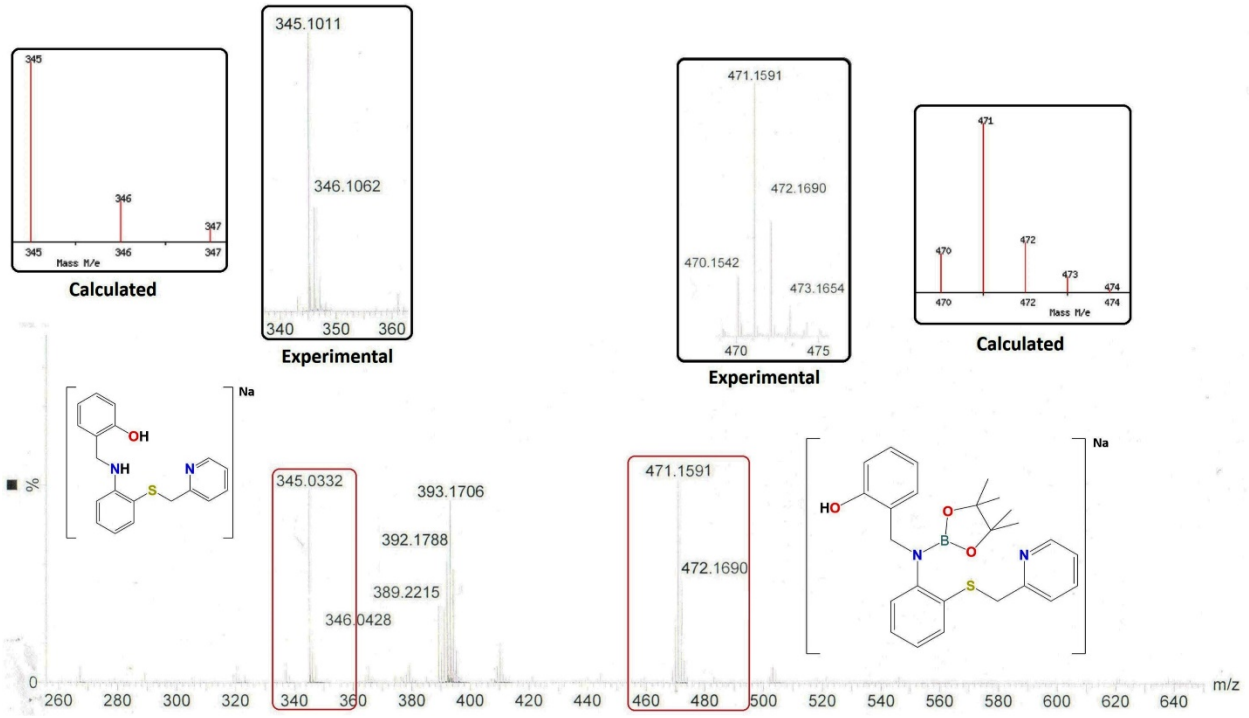

Figure S5. ESI-MS spectrum of the evaporated filtrate of the stoichiometric reaction mixture of **Zn-1** and HBpin after 12 h.

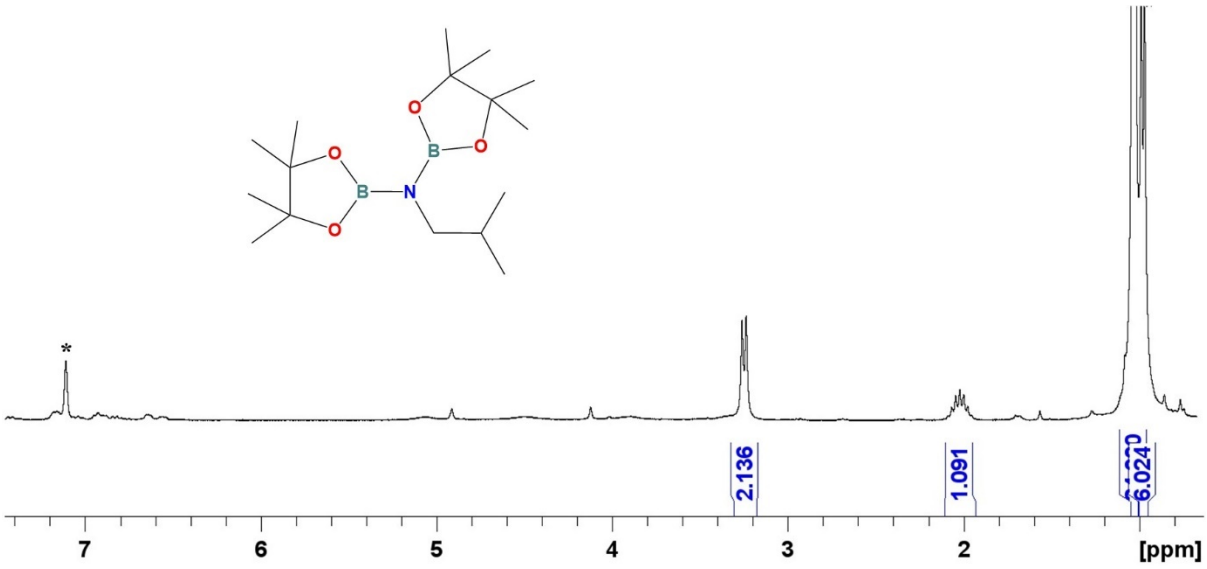

Figure S6. ^{1}H NMR spectrum of isobutyronitrile hydroboration product. * indicates protic impurity in C_6D_6.

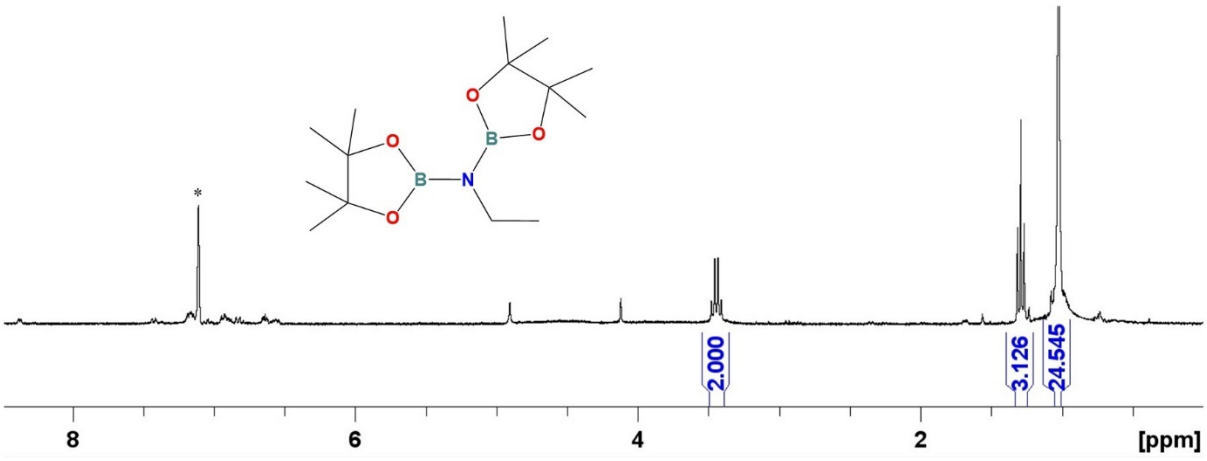

Figure S7. ^{1}H NMR spectrum of acetonitrile hydroboration product. * indicates protic impurity in C_6D_6.

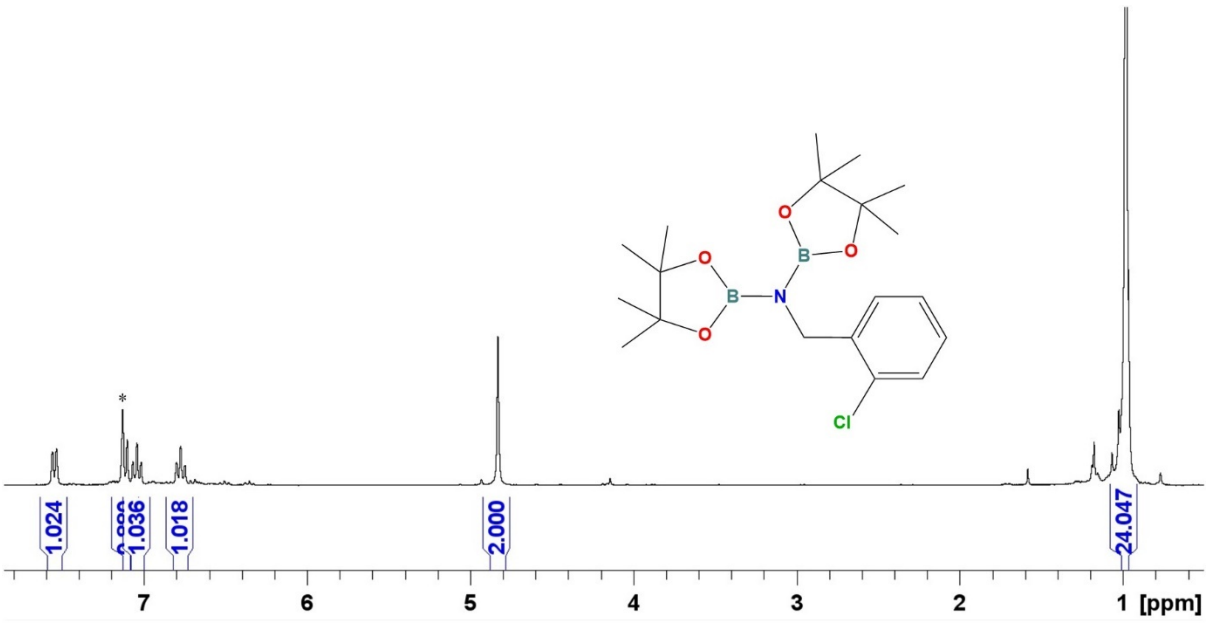

Figure S8. ^{1}H NMR spectrum of 2-chloro-benzonitrile hydroboration product. * indicates protic impurity in C_6D_6.

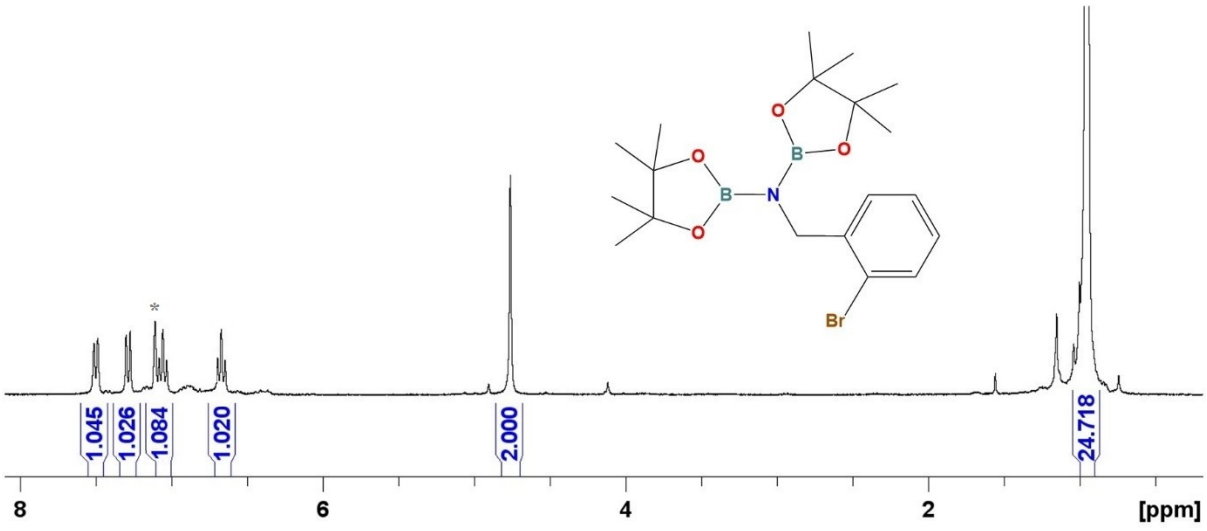

Figure S9. ^{1}H NMR spectrum of 2-bromo-benzonitrile hydroboration product. * indicates protic impurity in C_6D_6.

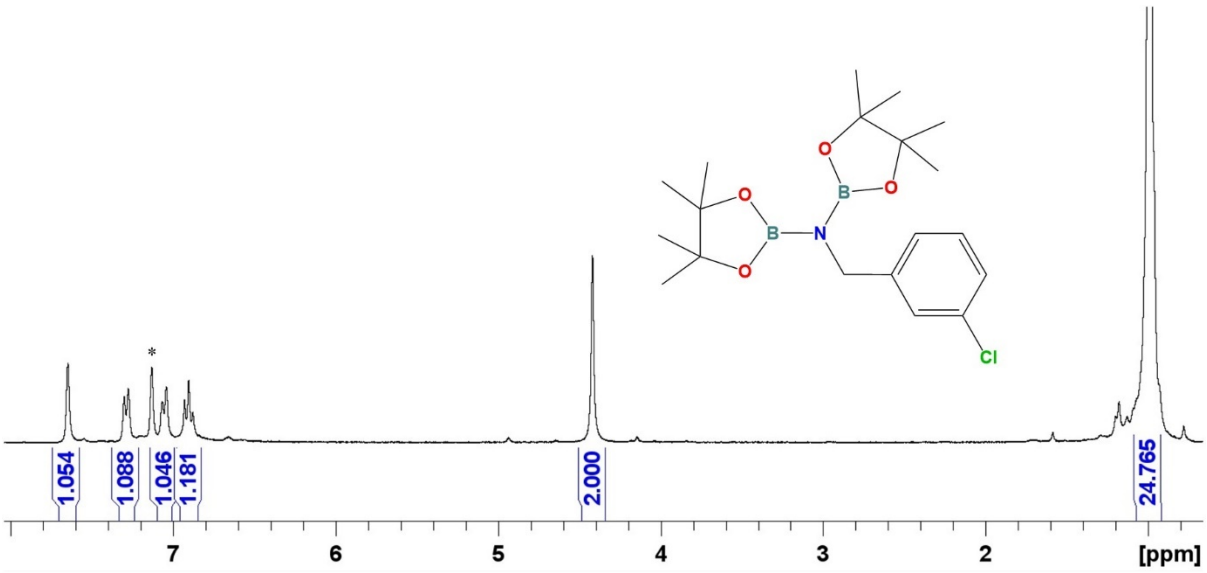

Figure S10. ^{1}H NMR spectrum of 3-chloro-benzonitrile hydroboration product. * indicates protic impurity in C_6D_6.

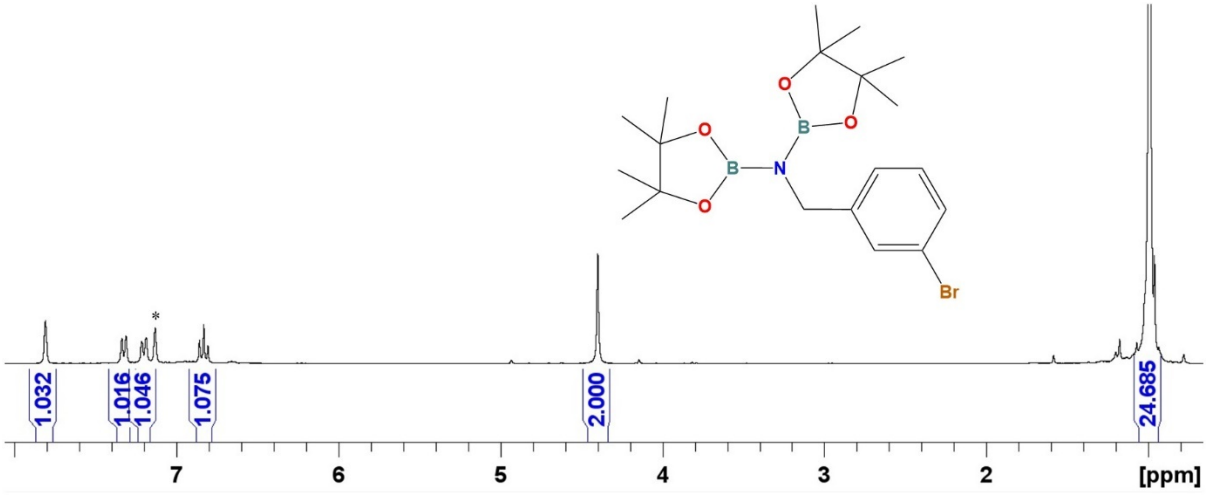

Figure S11. ^{1}H NMR spectrum of 3-bromo-benzonitrile hydroboration product. * indicates protic impurity in C_6D_6.

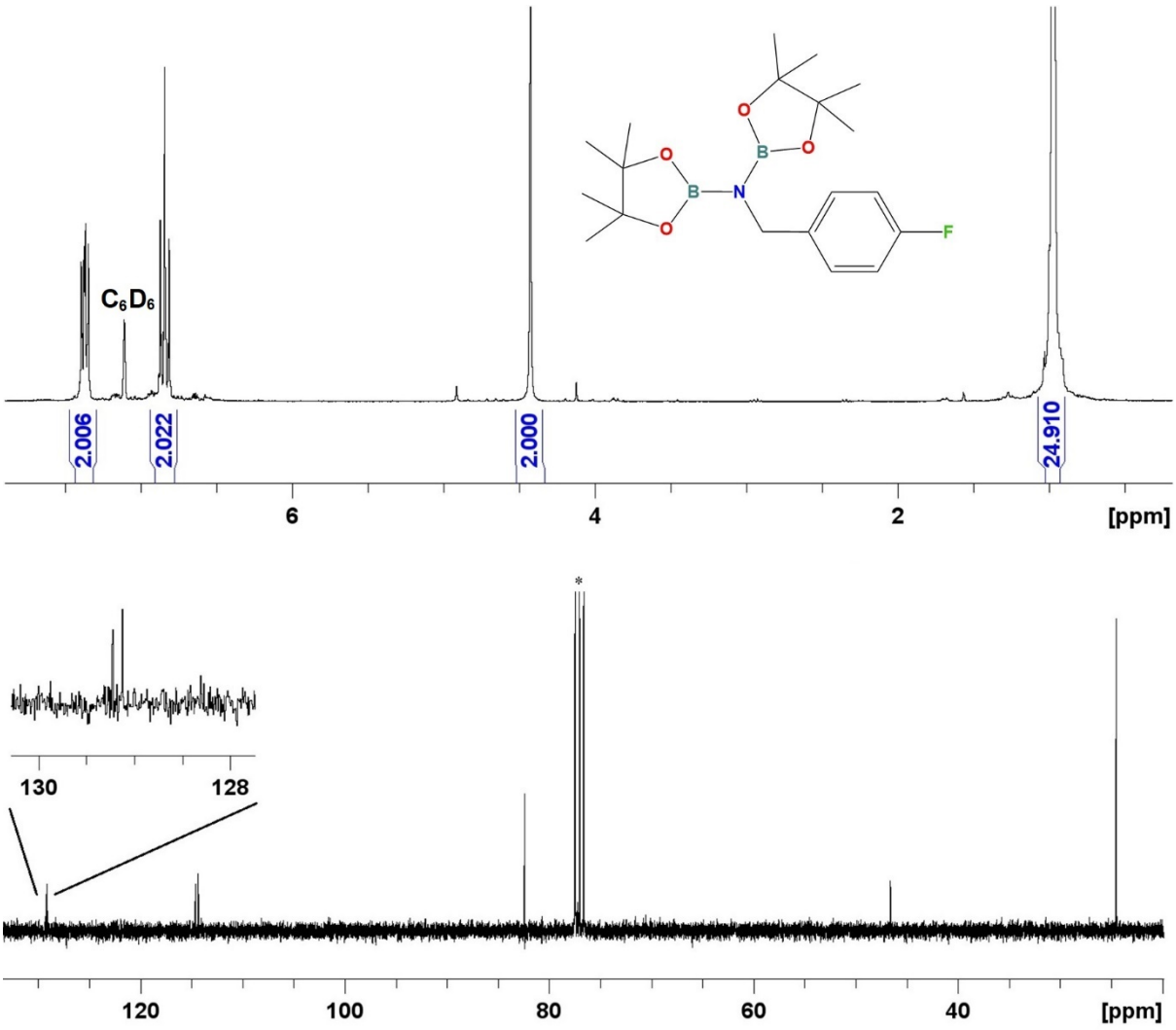

Figure S12. ^{1}H and ^{13}C NMR spectra of 4-fluoro-benzonitrile hydroboration product. * indicates protic impurity in $CDCl_3$.

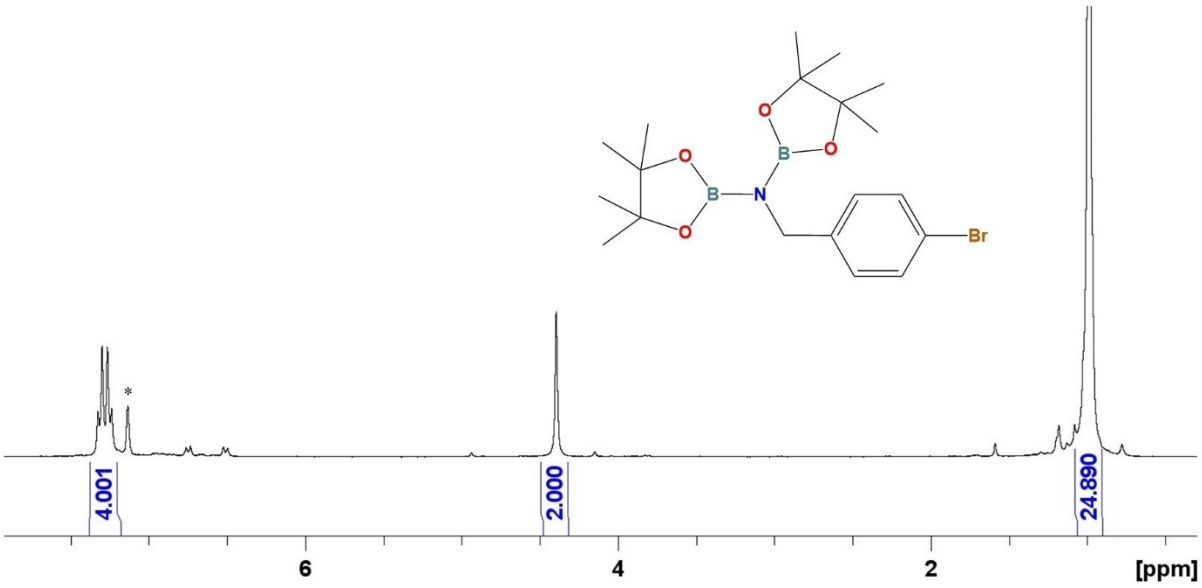

Figure S13. ^{1}H NMR spectrum of 4-bromo-benzonitrile hydroboration product. * indicates protic impurity in C_6D_6.

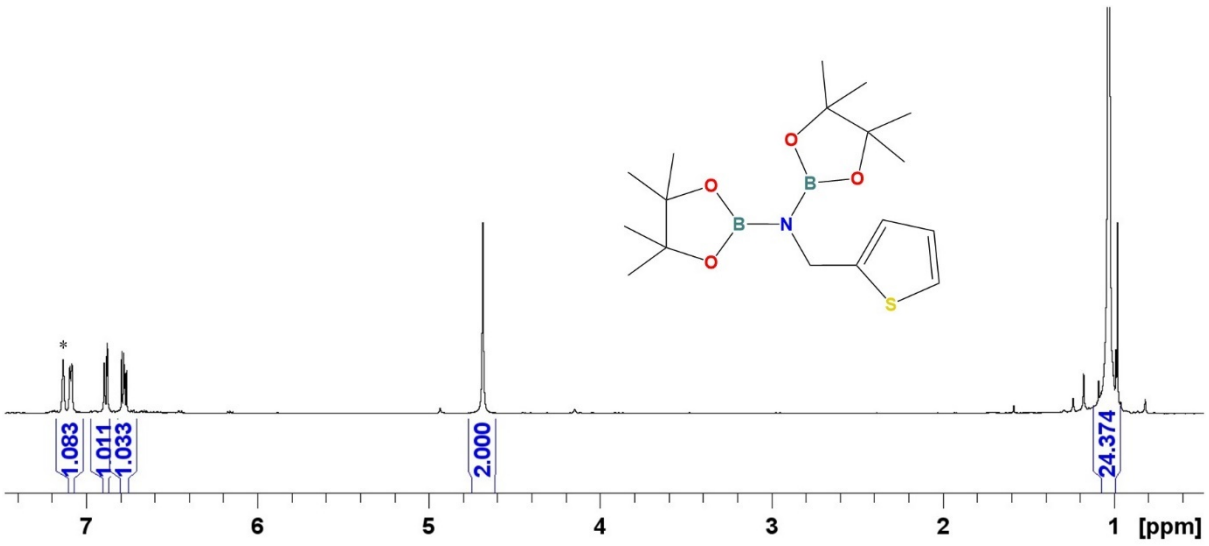

Figure S14. ^{1}H NMR spectrum of 2-cyano-thiophene hydroboration product. * indicates protic impurity in C_6D_6.

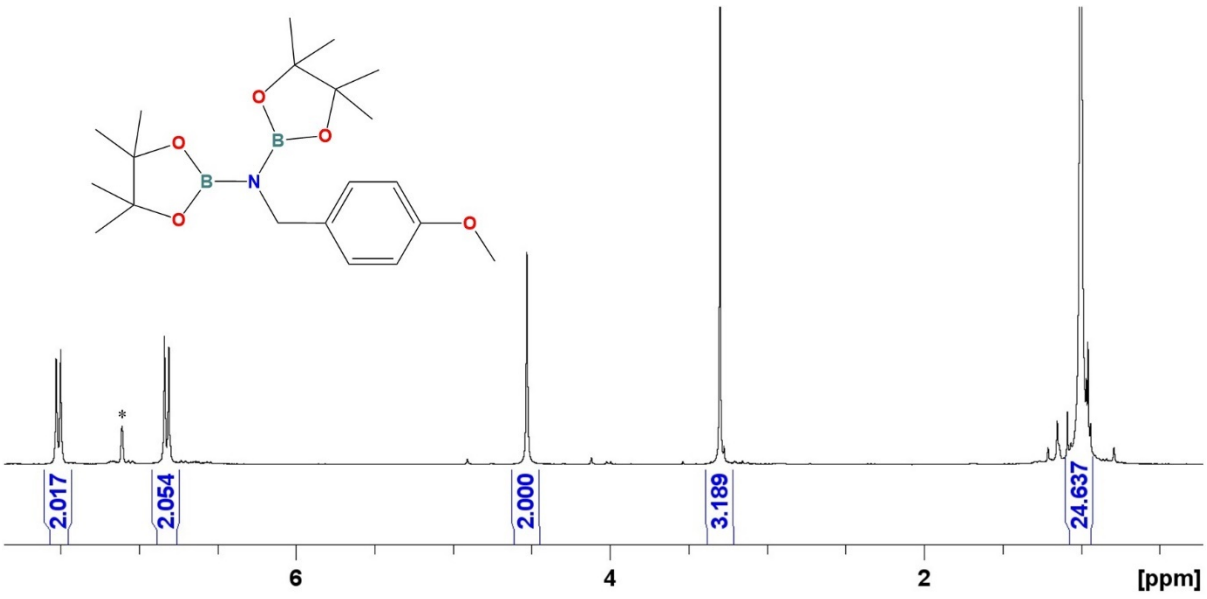

Figure S15. ^{1}H NMR spectrum of 4-methoxy-benzonitrile hydroboration product. * indicates protic impurity in C_6D_6.

III. Mechanistic Studies

A small vial was charged with 4-fluorobenzonitrile (12 mg, 0.1 mmol), **Zn-1** (38.5 mg, 0.05 mmol) and 1 mL of C_6D_6. The vial was capped and the mixture was stirred for 2 h at room temperature and then transferred to an NMR tube and ^{19}F and ^{1}H NMR spectra were recorded (Figure S16).

A small vial was charged with **Zn-1** (38.5 mg, 0.05 mmol), HBpin (15 µL, 0.1 mmol) and 1 mL of C_6D_6. The vial was capped and the mixture was stirred for almost 2 h and then transferred to an NMR tube and ^{1}H and ^{11}B NMR spectra were recorded. Then 2.6 µL of acetonitrile (0.05 mmol) was added to the same NMR tube. The NMR tube was well shaken, left in the glovebox for 8 h, at room temperature. ^{1}H and ^{11}B NMR spectra were then recorded (Figure S17).

Through the same procedure, **Zn-1** (38.5 mg, 0.05 mmol) and 2 equiv of HBpin (15 µL, 0.1 mmol) were treated together and after 12 h, ^{1}H and ^{11}B NMR spectra were recorded for comparison (Figures S17 and S18).

In an attempt to recover a zinc complex after the catalytic reaction, 15 mg (0.020 mmol) of **Zn-1**, acetonitrile (20.8 µL, 0.4 mmol) and HBpin (116 µL, 0.8 mmol) were added to a vial with a magnetic stir bar and the vial was capped. After 12 h, any remaining acetonitrile was evaporated under vacuum and 5 mL of hexane was added. After all the product was dissolved in hexane, the mixture was filtered and the residue was collected as a pale green-white powder and dried under vacuum. The filtrate was then subsjected to ESI-MS analysis (Fig. S5). The residue showed no solubility in available solvents and a reaction run using the residue (5 mg), acetonitrile (5.2 µL, 0.1 mmol) and HBpin (29 µL, 0.2 mmol) showed no hydroboration product after 24 h. Also, addition of HCl to this residue resulted in gas bubble formation

as the residue dissolved. Finally, the filtrate from above was evaporated and the resulting residue also showed no nitrile hydroboration activity.

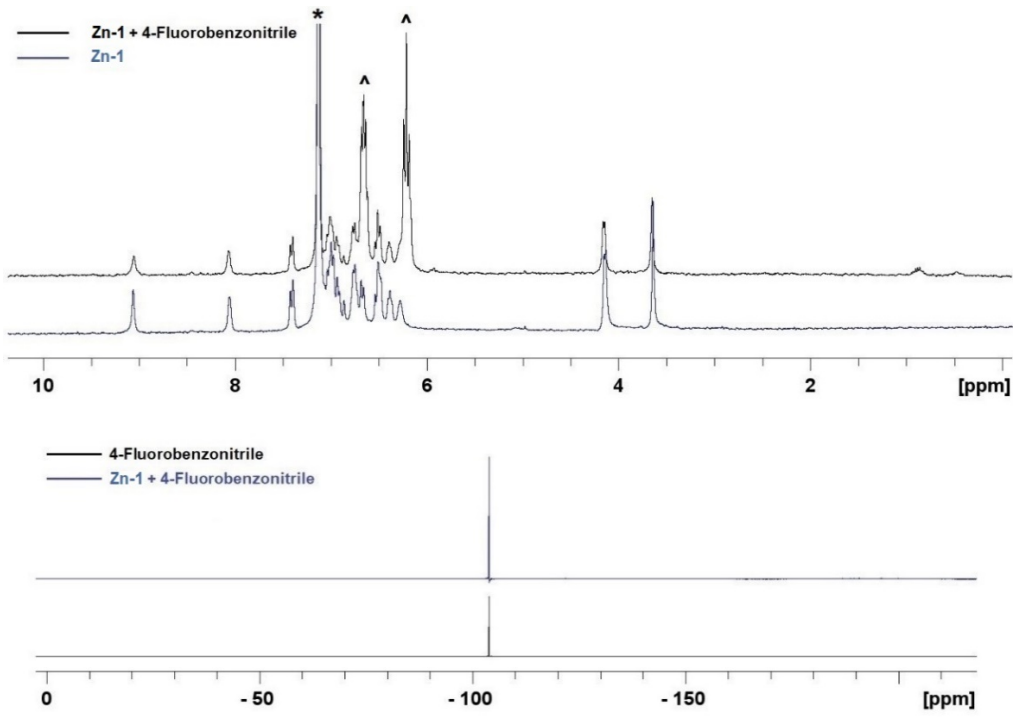

Figure S16. Stacked plot of ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of **Zn-1** in C_6D_6 (black) and reaction of **Zn-1** dimer with two equiv of 4-fluorobenzonitrile (blue). * Indicates C_6D_6 and **^** indicates 4-fluorobenzonitrile.

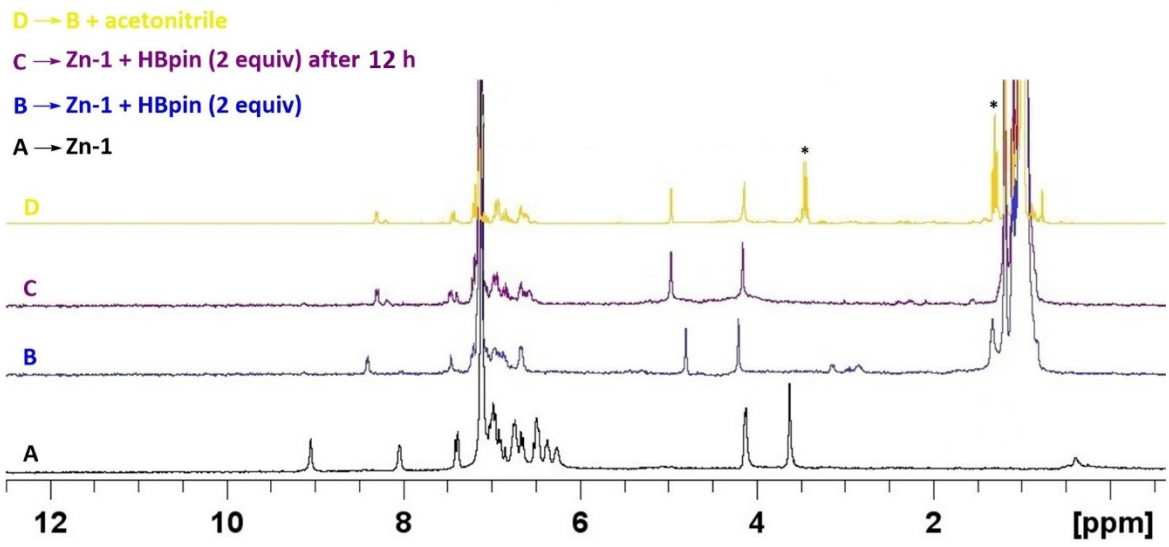

Figure S17. Stacked plot of $^{1}H\{^{11}B\}$ NMR spectra (in C_6D_6) of **Zn-1** (**A**), reaction of **Zn-1** dimer with two equiv of HBpin (**B**), B after 12 h (**C**), and subsequent addition of one equiv of acetonitrile to B (**D**).* indicates diborylamine product of acetonitrile hydroboration.

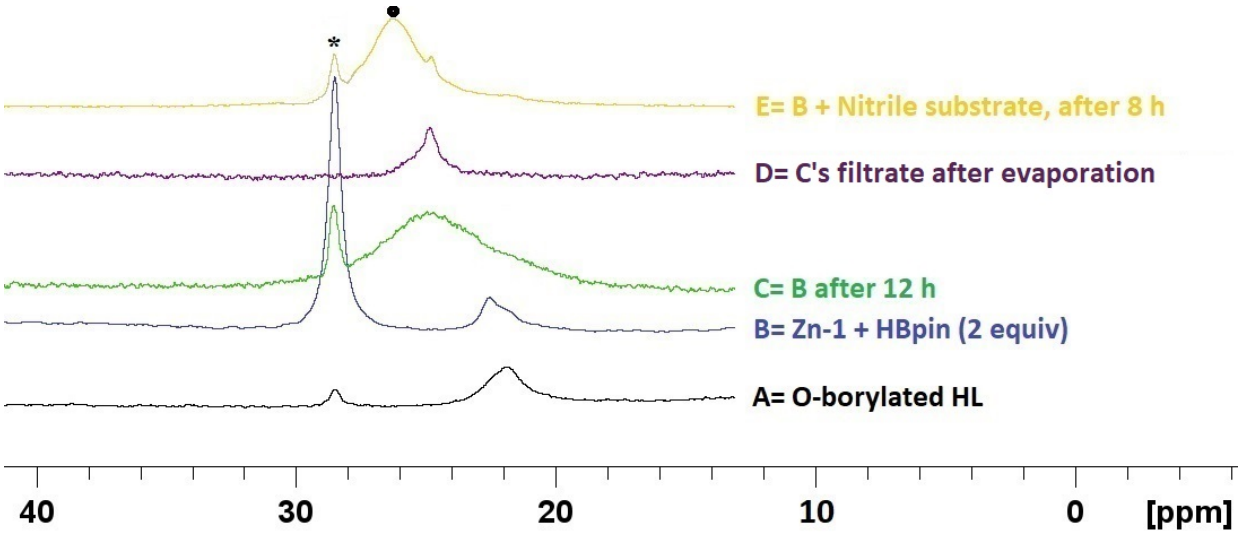

Figure S18. $^{11}B\{^{1}H\}$ NMR spectra (in C_6D_6) of O-borylated HL (**A**), stoichiometric reaction of **Zn-1** dimer with 2 equiv of HBpin (**B**), **B** after 12 h (**C**), **C**'s filtrate after solvent evaporation (**D**), and subsequent reaction of **B** with acetonitrile (**E**). * indicates HBpin and ● indicates product of acetonitrile dihydroboration.

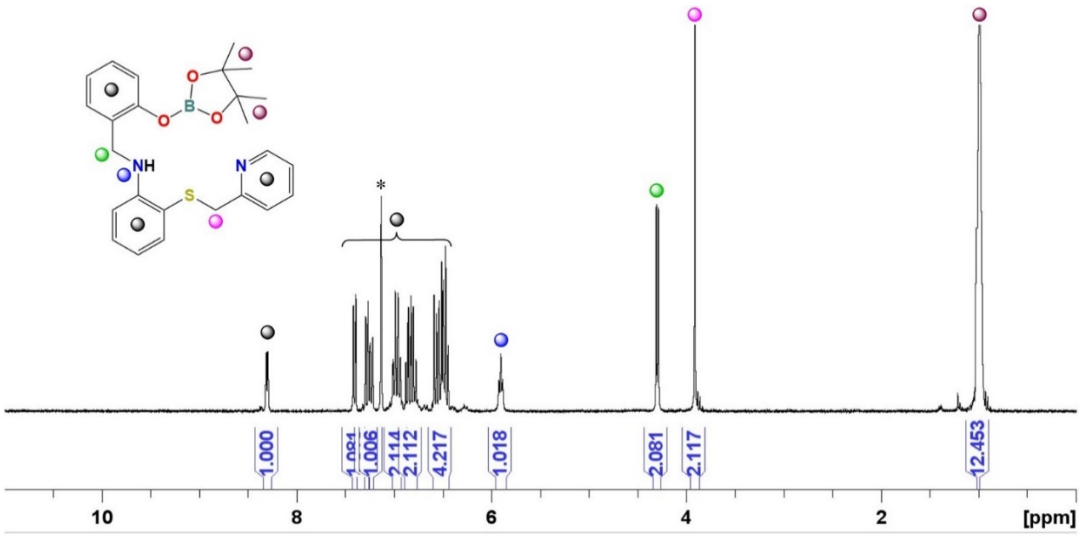

Figure S19. ^{1}H NMR spectrum of O-borylated HL (**HL-Bpin**). * indicates protic impurity in C_6D_6.

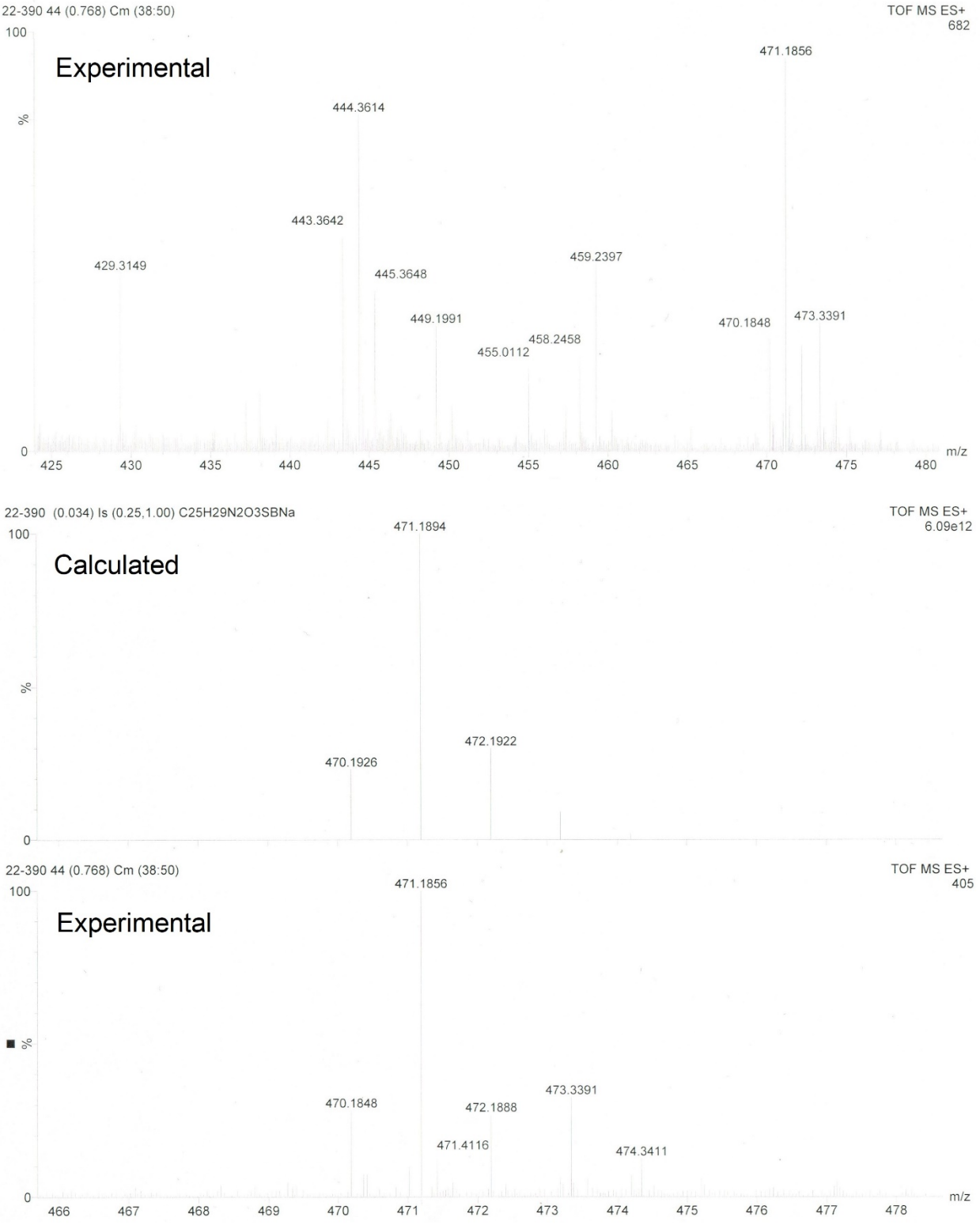

Figure S20. ESI-MS spectrum of O-borylated HL (**HL-Bpin**) $[NaM]^+$.

IV. Kinetic Studies

All kinetic reactions were set up in a nitrogen-filled glovebox and performed the same way with appropriate amounts of **Zn-1**, 2-fluorobenzonitrile, HBpin, and N-(4-fluorobenzyl)-4,4,5,5-tetramethyl-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine (abbreviated as 4-F-C_6H_4)$CH_2N(Bpin)_2$) – See **Table S1**.

General Procedure for Reaction A.

Note: All employed concentrations of **Zn-1** in the kinetic study are calculated for a monomer form of the zinc complex (Mm: 385.79 g/mol) not the dimeric form. This consideration is only for the kinetic study (Other **Zn-1** concentrations in other sections are stated for the dimeric form having Mm: 771.58 g/mol).

Product isolation: A vial was charged with 7 mg of **Zn-1** (0.01 mmol, 1 mol%). Then, 4-fluorobenzonitrile (121 mg, 1 mmol) and HBpin (290 µL, 2 mmol) were added to the vial. After 10 h, the product (g) was extracted into 10 mL of pentane and filtered. Then, the solution was concentrated to 2 mL and kept at -30 ˚C overnight, so crystals of (4-F-C_6H_4)$CH_2N(Bpin)_2$ (*g)* were formed (several crystals were separated for crystallography) and then filtered and dried under vacuum. Product *g* was then used in the kinetic study for reaction F (Table S1).

A catalyst stock solution was prepared by dissolving 15 mg (0.040 mM as a monomer) of **Zn-1** in 4 mL of THF. 10 small vials were charged with 20 µL of the catalyst stock solution (0.7 mg, 0.002 mM, 2 mol%). Then, THF was evaporated under vacuum and 4-fluorobenzonitrile (17 mg, 0.1 mM) was added to the vials and subsequently after putting a tiny magnetic stir bar in the vials, HBpin (29 µL, 0.2 mM) was added, the vials were capped and the stir bars started stirring very gently. Every 45 min (Reactions A, C, D, E and F) or 40 min (Reaction B) the reaction mixture of one of the vials was immediately dissolved in C_6D_6 and transferred to an NMR tube and ^1H and ^{11}B NMR spectra were taken at room temperature. The concentration of (4-F-C_6H_4)$CH_2N(Bpin)_2$ product was calculated based on integrals of the known [HBpin] and the characteristic signal of (4-F-C_6H_4)$CH_2N(Bpin)_2$. All the other 5 reactions (B-F) were carried out through the same procedure, but reaction F in which (4-F-C_6H_4)$CH_2N(Bpin)_2$ (12 mg, 0.032 mM) was added to the vials before adding HBpin. The outlier results (compared to the uniform progression of the catalytic yield vs. time) were repeated several times and for the cases in which the results of all the repetitions were close, the average was considered, otherwise the best matching one was selected.

Table S1. Concentrations of Reagents for Reactions A-F for VTNA*.

	[Zn-1]	**[4-Fluorobenzonitrile]**	**[HBpin]**	**(4-F-C_6H_4)$CH_2N(Bpin)_2$**
Reaction A	0.002	0.1	0.2	-
Reaction B	0.002	0.15	0.2	-
Reaction C	0.002	0.1	0.3	-

Reaction D	0.006	0.1	0.2	-
Reaction E	0.002	0.068	0.136	-
Reaction F	0.002	0.068	0.136	0.032

*All the amounts are in mM.

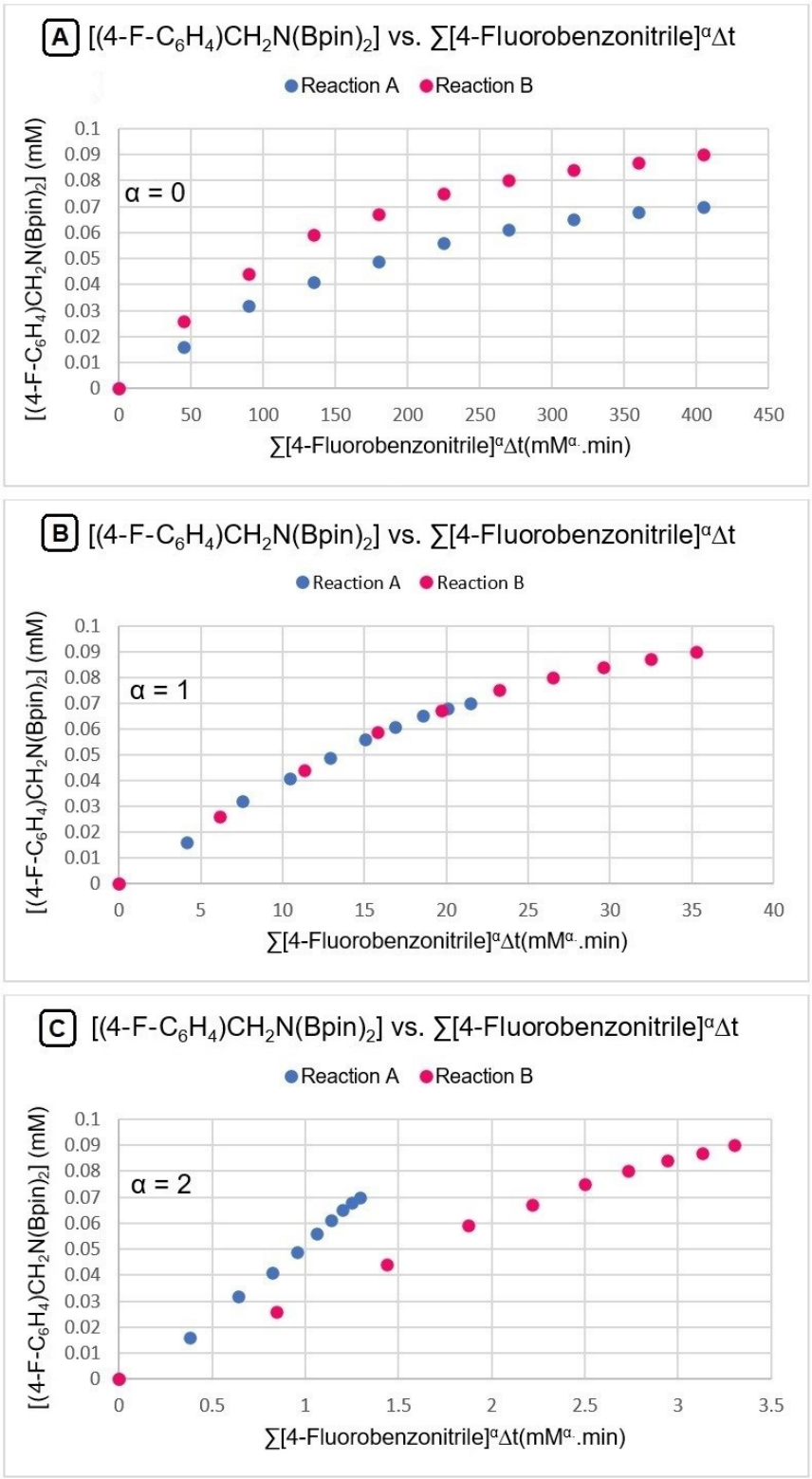

Figure S21. VTNA of rate order of [4-Fluorobenzonitrile].

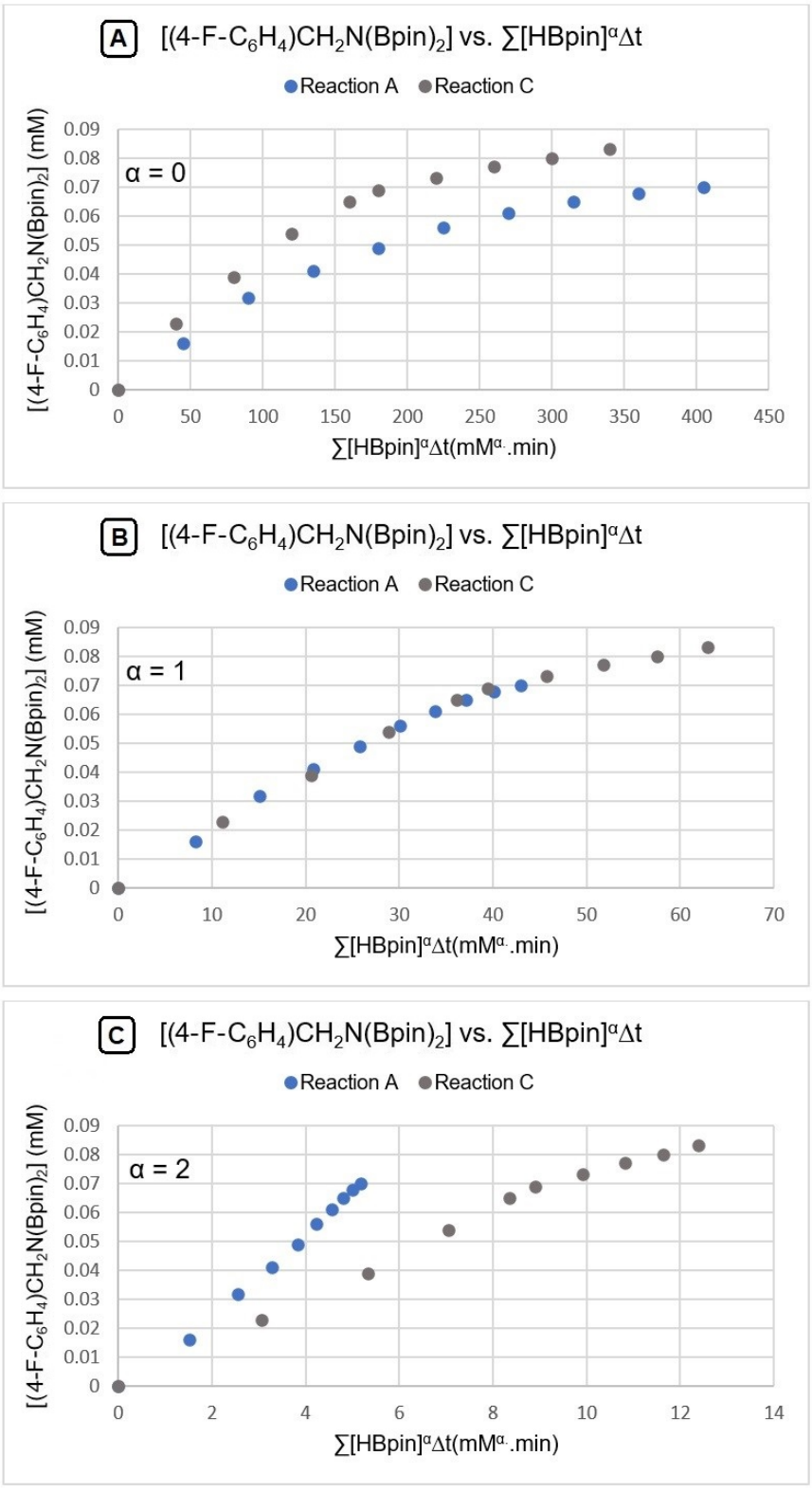

Figure S22. VTNA of rate order of [HBpin].

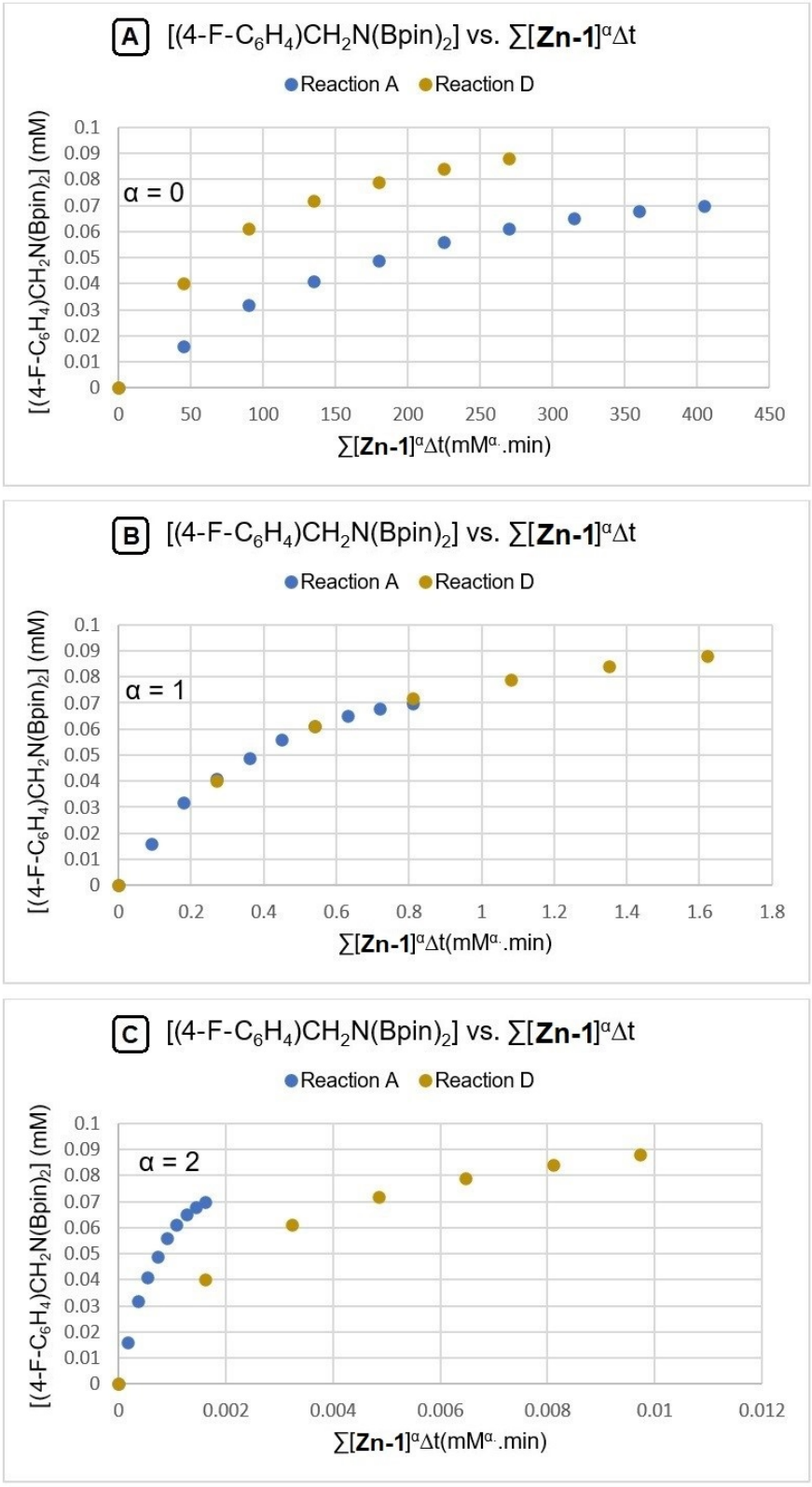

Figure S23. VTNA of rate order of [**Zn-1**].

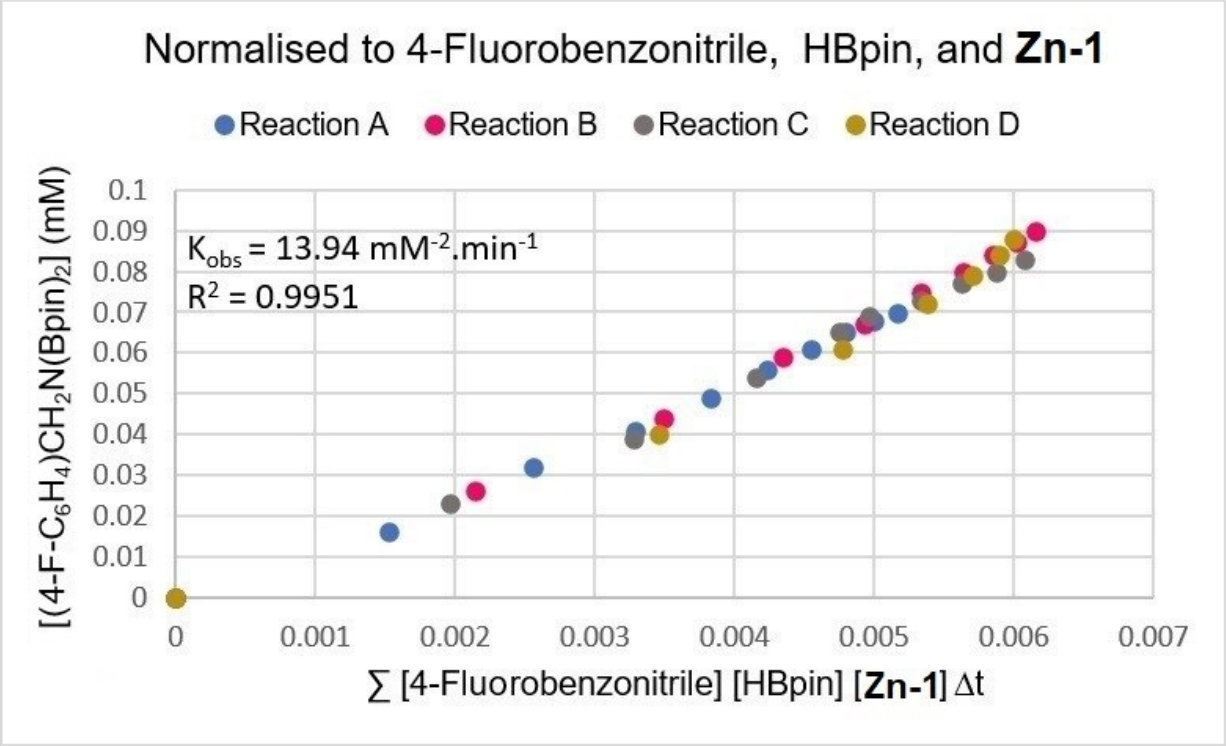

Figure S24. VTNA of $(4\text{-F-}C_6H_4)CH_2N(Bpin)_2$ vs. Σ [4-Fluorobenzonitrile][HBpin][**Zn-1**] Δt to give k_{obs}.

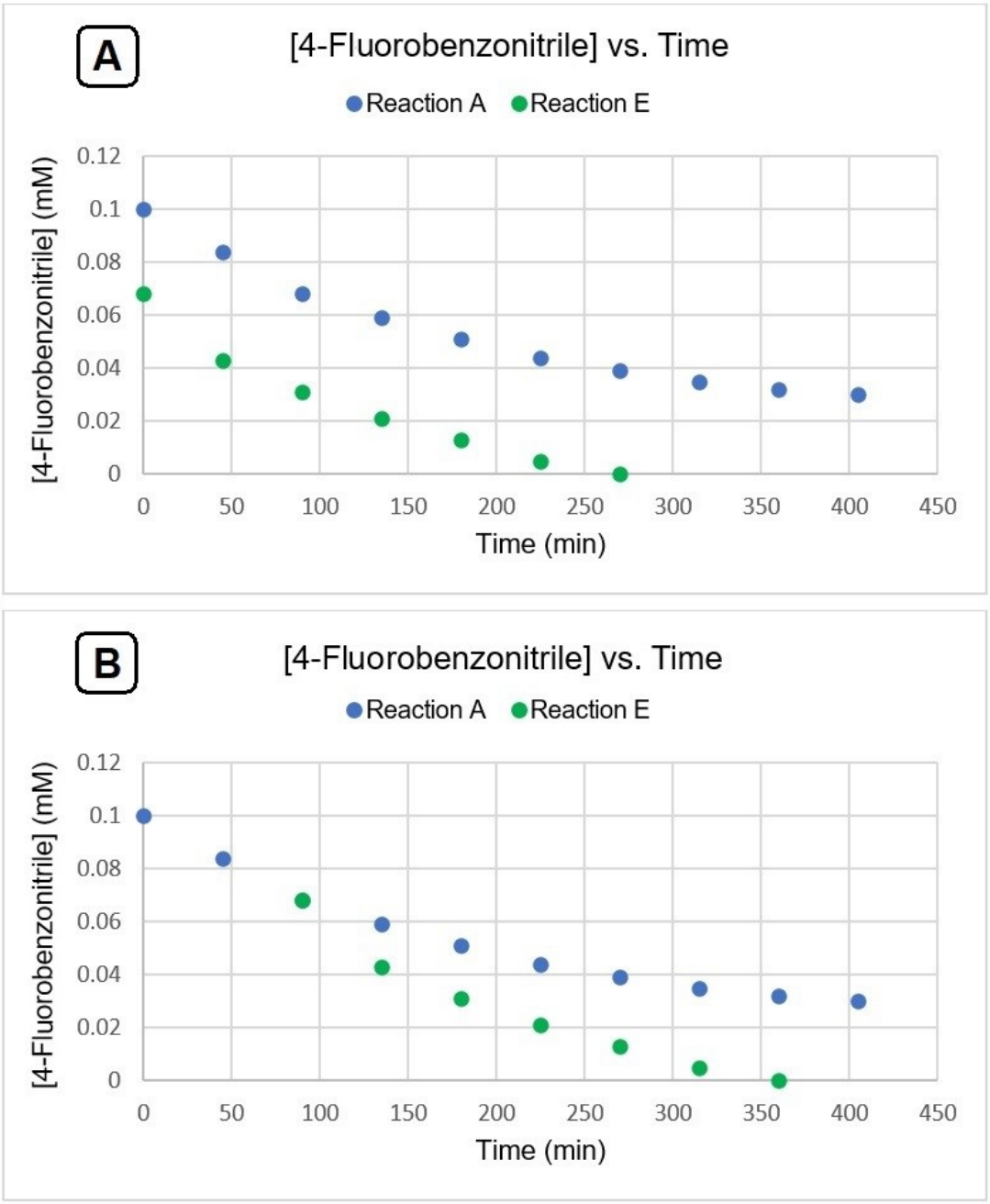

Figure S25. VTNA of [4-Fluorobenzonitrile] vs. Time to find out if the catalytic system suffers either product inhibition or catalyst deactivation. Top: before time adjustment. Bottom: after time adjustment

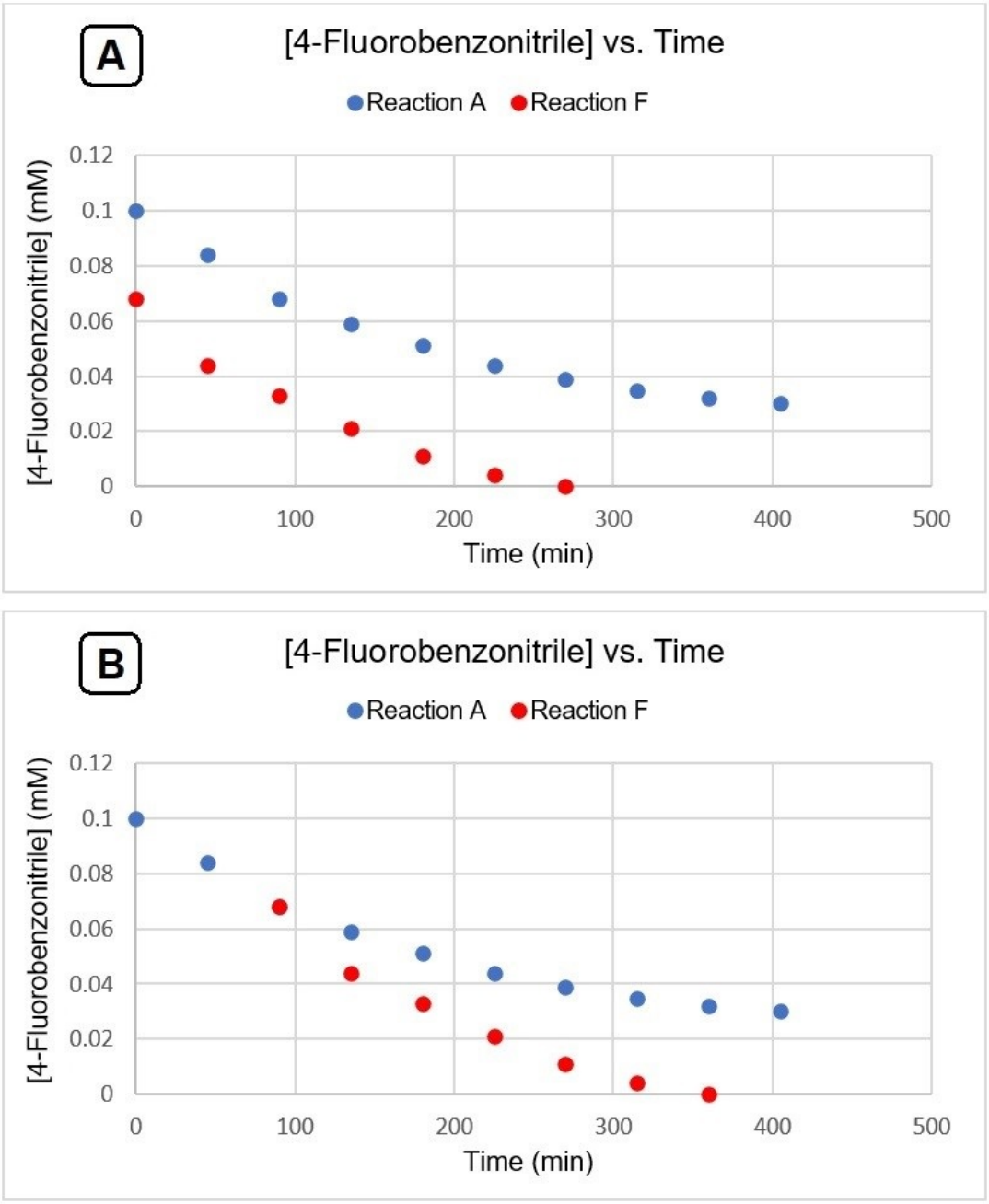

Figure S26. VTNA of [4-Fluorobenzonitrile] vs. Time to find out if the catalytic system suffers product inhibition. Top: before time adjustment. Bottom: after time adjustment

V. Crystallographic Details

Crystallographic data for all compounds were collected from a single crystal mounted on a MiTeGen dual thickness MicroMount using Parabar oil. Data were collected on a Bruker ApexII single crystal diffractometer equipped with a graphite monochromator. The instrument was equipped with a sealed tube Mo Kα source ($\lambda =$ 0.71073 Å), an ApexII CCD detector and a dry compressed air-cooling system operating at 203 K. Raw data collection and processing were performed with the Apex3 software package from Bruker.[2] Initial unit cell parameters were determined from 36 data frames from select ω scans. Semi-empirical absorption corrections based on equivalent reflections were applied.[3] Systematic absences in the diffraction data-set and unit-cell parameters were consistent with the assigned space group. The initial structural solutions were determined using ShelxT direct methods,[4] and refined with full-matrix least-squares procedures based on F^2 using ShelXL or ShelXle.[5] Hydrogen atoms were placed geometrically and refined using a riding model. Additional crystallographic information is given in Table S2.

Table S2: X-ray crystallographic data collection and refinement details.

	g (K0991)	**H_2L (S0769)**	**Zn-1 (K0572)**
empirical formula	$C_{19}H_{30}B_2FNO_4$	$C_{19}H_{18}N_2OS$	$C_{54}H_{64}N_4O_6S_2Zn_2$
formula weight (g · mol^{-1})	377.06	322.41	1059.95
crystal system	triclinic	monoclininc	triclinic
space group	$P\bar{1}$	$P\,2_1/n$	$P\bar{1}$
a (A)	6.5967(4)	8.4071(19)	9.9532(13)
b (A)	12.0859(6)	17.688(4)	10.9777(14)
c (A)	14.3335(7)	11.345(2)	12.1123(16)
α (deg)	105.426(1)	90	88.174(2)
β (deg)	97.881(1)	103.767(7)	83.185(2)
γ (deg)	103.322(1)	90	80.990(2)
V (A^3)	1047.7(1)	1638.6(6)	1297.7(3)
Z	2	4	1
T (K)	203(2)	203(2)	203(2)
ρ_{calcd} (g · cm^{-3})	1.195	1.307	1.356
μ (mm^{-1})	0.086	0.203	1.057
2^{θ}_{max} (deg)	50.042	50.484	50.484
total/unique reflections	15994/3664	12506/3740	31432/8030
Reflections [$I_o \geq 2\sigma(I_o)$]	2901	2679	5376
R_1, wR_2 [$I_o \geq 2\sigma(I_o)$]	0.0391, 0.1000	0.0418, 0.0844	0.0487, 0.1327
goodness of fit	1.036	1.015	1.014
CCDC number	2128270	2129544	2129545

Table S3. Bond lengths for product ***g***.

Atom1	Atom2	Length/Å
F1	C17	1.365(2)
O1	C2	1.458(2)
O1	B1	1.371(2)
O2	B1	1.366(2)
O2	C1A	1.444(3)
O3	C7	1.466(2)
O3	B2	1.371(2)
O4	C8	1.457(2)
O4	B2	1.375(2)
N1	C13	1.478(2)
N1	B1	1.423(2)
N1	B2	1.429(2)
C2	C1A	1.643(5)
C2	C3A	1.338(6)
C2	C4A	1.655(7)
C6	H6A	0.97
C6	H6B	0.97
C6	H6C	0.97
C6	C1A	1.404(5)
C7	C8	1.550(2)
C7	C11	1.522(2)
C7	C12	1.515(2)
C8	C9	1.520(2)
C8	C10	1.516(2)
C9	H9A	0.97
C9	H9B	0.97
C9	H9C	0.97
C10	H10A	0.97
C10	H10B	0.97
C10	H10C	0.97
C11	H11A	0.97
C11	H11B	0.97
C11	H11C	0.97
C12	H12A	0.97
C12	H12B	0.97
C12	H12C	0.97
C13	H13A	0.98
C13	H13B	0.98
C13	C14	1.511(2)
C14	C15	1.385(2)
C14	C19	1.382(3)
C15	H15	0.94

C15	C16	1.387(2)
C16	H16	0.94
C16	C17	1.355(3)
C17	C18	1.364(3)
C18	H18	0.94
C18	C19	1.385(3)
C19	H19	0.94
C1A	C5A	1.501(8)
C3A	H3A1	0.97
C3A	H3A2	0.97
C3A	H3A3	0.97
C4A	H4AA	0.97
C4A	H4AB	0.97
C4A	H4AC	0.97
C5A	H5AA	0.97
C5A	H5AB	0.97
C5A	H5AC	0.97

Table S4. Bond lengths for **H_2L**.

Atom1	**Atom2**	**Length/Å**
S1	C6	1.827(2)
S1	C7	1.774(2)
O1	H1A	0.83
O1	C19	1.358(2)
N1	C1	1.335(3)
N1	C5	1.336(2)
N2	H2A	0.87
N2	C12	1.360(2)
N2	C13	1.446(2)
C1	H1	0.94
C1	C2	1.371(3)
C2	H2	0.94
C2	C3	1.362(3)
C3	H3	0.94
C3	C4	1.381(3)
C4	H4	0.94
C4	C5	1.380(2)
C5	C6	1.498(3)
C6	H6A	0.98
C6	H6AB	0.98
C7	C8	1.382(3)
C7	C12	1.409(2)
C8	H8	0.94

C8	C9	1.375(3)
C9	H9	0.94
C9	C10	1.379(3)
C10	H10	0.94
C10	C11	1.374(3)
C11	H11	0.94
C11	C12	1.399(3)
C13	H13A	0.98
C13	H13B	0.98
C13	C14	1.507(2)
C14	C15	1.383(2)
C14	C19	1.401(2)
C15	H15	0.94
C15	C16	1.389(3)
C16	H16	0.94
C16	C17	1.381(3)
C17	H17	0.94
C17	C18	1.380(2)
C18	H18	0.94
C18	C19	1.384(3)

Table S5. Bond lengths for **Zn-1.**

Atom1	**Atom2**	**Length/Å**
Zn1	S1	2.5784(8)
Zn1	N1	1.940(2)
Zn1	O1	2.059(2)
Zn1	N2	2.056(2)
Zn1	O1	1.964(2)
C1	O1	1.342(3)
C1	C2	1.404(3)
C1	C6	1.391(3)
S1	C13	1.764(3)
S1	C14	1.844(3)
N1	C8	1.359(3)
N1	C7	1.468(3)
O1	Zn1	1.964(2)
C2	H2	0.94
C2	C3	1.377(5)
N2	C15	1.342(4)
N2	C19	1.338(4)
C6	C5	1.397(4)
C6	C7	1.516(3)
C5	H5	0.94

C5	C4	1.395(5)
C4	H4	0.94
C4	C3	1.353(5)
C3	H3	0.94
C9	H9	0.94
C9	C8	1.409(4)
C9	C10	1.390(5)
C8	C13	1.432(4)
C7	H7A	0.98
C7	H7AB	0.98
C10	H10	0.94
C10	C11	1.383(6)
C11	H11	0.94
C11	C12	1.368(6)
C12	H12	0.94
C12	C13	1.392(4)
C14	H14A	0.98
C14	H14B	0.98
C14	C15	1.495(4)
C15	C16	1.387(4)
C16	H16	0.94
C16	C17	1.373(5)
C17	H17	0.939
C17	C18	1.374(5)
C18	H18	0.94
C18	C19	1.380(4)
C19	H19	0.94
Zn1	S1	2.5784(8)
Zn1	N1	1.940(2)
Zn1	O1	2.059(2)
Zn1	N2	2.056(2)
C1	O1	1.342(3)
C1	C2	1.404(3)
C1	C6	1.391(3)
S1	C13	1.764(3)
S1	C14	1.844(3)
N1	C8	1.359(3)
N1	C7	1.468(3)
C2	H2	0.94
C2	C3	1.377(5)
N2	C15	1.342(4)
N2	C19	1.338(4)
C6	C5	1.397(4)
C6	C7	1.516(3)
C5	H5	0.94

C5	C4	1.395(5)
C4	H4	0.94
C4	C3	1.353(5)
C3	H3	0.94
C9	H9	0.94
C9	C8	1.409(4)
C9	C10	1.390(5)
C8	C13	1.432(4)
C7	H7A	0.98
C7	H7AB	0.98
C10	H10	0.94
C10	C11	1.383(6)
C11	H11	0.94
C11	C12	1.368(6)
C12	H12	0.94
C12	C13	1.392(4)
C14	H14A	0.98
C14	H14B	0.98
C14	C15	1.495(4)
C15	C16	1.387(4)
C16	H16	0.94
C16	C17	1.373(5)
C17	H17	0.939
C17	C18	1.374(5)
C18	H18	0.94
C18	C19	1.380(4)
C19	H19	0.94
O1_1	C1_1	1.48(1)
O1_1	C4_1	1.45(1)
C1_1	H1A_1	0.98
C1_1	H1AB_1	0.98
C1_1	C2_1	1.39(1)
C2_1	H2A_1	0.98
C2_1	H2B_1	0.98
C2_1	C3_1	1.34(1)
C3_1	H3A_1	0.979
C3_1	H3B_1	0.98
C3_1	C4_1	1.40(1)
C4_1	H4A_1	0.98
C4_1	H4AB_1	0.98
O1_3	C1_3	1.48(1)
O1_3	C4_3	1.45(2)
C1_3	H1A_3	0.98
C1_3	H1AB_3	0.98
C1_3	C2_3	1.38(1)

C2_3	H2A_3	0.98
C2_3	H2B_3	0.98
C2_3	C3_3	1.34(2)
C3_3	H3A_3	0.98
C3_3	H3B_3	0.98
C3_3	C4_3	1.40(1)
C4_3	H4A_3	0.98
C4_3	H4AB_3	0.98

VI. References

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