

Supporting Information

for

Reactions of saturated NHC-boranes with electron deficient alkyne and alkene. Borirane formation, their reactivities, and coupling of tetracyanoethylene

P. R. Amrutha,^{ab‡} Gargi Kundu,^{ab‡} Vemuri Lakshmi Ganesh,^{cd} Rajesh G. Gonnade,^{*be}
Gopinadhanpillai Gopakumar,^{*cd} and Sakya S. Sen^{*ab}

^a *Inorganic Chemistry and Catalysis Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008, India.*

^b *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.*

^c *Fuel Chemistry Division, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu.*

^d *Homi Bhabha National Institute, Training School Complex, Anushakthinagar, Mumbai, Maharashtra 400094, India.*

^e *Physical and Material Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008, India.*

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S1. EXPERIMENTAL SECTION

All air- and moisture-sensitive reactions were carried out under an inert atmosphere of argon using standard Schlenk techniques or in a MBRAUN glove-box equipped with a -35 °C freezer. The solvents, toluene, acetonitrile, and tetrahydrofuran (THF) were purified by MBRAUN solvent purification system MB SPS-800. Other chemicals were purchased from Sigma Aldrich and TCI Chemicals, and were used without further purification. All the reaction glass wares were oven dried overnight at 180 °C. AlCl_3 and $\text{B}(\text{C}_6\text{F}_5)_3$ was sublimised before performing the reactions. The starting materials, 5-SIDipp· BH_3 and 6-SIDipp· BH_3 were synthesized by using the literature procedure.^{S1} The ^1H , ^{13}C , and ^{11}B NMR spectra were recorded in CDCl_3 , THF-d^8 using a Bruker Avance DPX 400, and a Bruker Avance DPX 500 spectrometer. Chemical shifts (δ) are given in ppm. NMR spectra were referenced to external SiMe_4 (^1H and ^{13}C), $\text{BF}_3\cdot\text{OEt}_2$ (^{11}B). High resolution mass spectra (HRMS) were obtained using a Q Exactive Thermo Scientific. Melting points were measured in a sealed glass tube on a Stuart SMP-30 melting point apparatus and were uncorrected. The IR data were recorded using a Bruker Alpha II FTIR Spectrophotometer. Absorbance data were measured with the help of a Shimadzu UV-VIS-IR (UV-3600 Plus) spectrometer for checking the bulk purity, Powder X-ray diffraction was done in CSIR-NCL, Pune for compound **8**.

S2. Synthesis and spectroscopic characterization of 1-8

Compound 1. To a solution of 5-SIDipp· BH_3 (1.5 g, 3.7 mmol) in 30 ml acetonitrile, 2 equivalents of dimethyl acetylenedicarboxylate (DMAD) (0.91 ml, 7.4 mmol) was added at room temperature. The reaction mixture was heated up to 80 °C and stirred for 2 days. The reaction mixture was then dried completely, and subjected to ethyl acetate/ hexane column chromatography in silica to yield **1** (1.25 g, 63%). Single crystals suitable for single crystal X-ray analysis were grown in the concentrated toluene solution at 4 °C in a freezer.

^1H NMR (500 MHz, 298 K, CDCl_3): δ = 0.86 (1 H, BH), δ = 1.24 - 1.30 (m, 12 H, $\text{CH}(\text{CH}_3)_2$) 1.30 (d, J = 6.75 Hz, 6 H, $\text{CH}(\text{CH}_3)_2$), 1.38 (d, J = 6.75 Hz, 6 H, $\text{CH}(\text{CH}_3)_2$), 1.62 (s, 2 H, CHCO_2Me), 3.21 (sept, J = 5 Hz, 2 H, $\text{CH}(\text{CH}_3)_2$), 3.25 (s, 3 H, CO_2CH_3), 3.40 (sept, J = 5 Hz, 2 H, $\text{CH}(\text{CH}_3)_2$), 3.50 (s, 3 H, CO_2CH_3), 4.02 - 4.12 (m, 4 H, $\text{NCH}_2\text{CH}_2\text{N}$), 7.25 – 7.29 (m, 4 H, Ar-H), 7.41 (t, J = 7.75 Hz, 2 H, Ar-H) ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, 298 K, CDCl_3): δ = 22.5 ($\text{CH}(\text{CH}_3)_2$), 23.7 ($\text{CH}(\text{CH}_3)_2$), 26.1 (CHCO_2Me), 26.45 (CHCO_2Me), 28.4 ($\text{CH}(\text{CH}_3)_2$), 28.5 ($\text{CH}(\text{CH}_3)_2$), 49.9 (CO_2CH_3), 50.3 (CO_2CH_3), 53 (CH_2CH_2), 124.8 (Ar-C), 129.4 (Ar-C), 134.4 (Ar-C), 146.3 (Ar-C), 177.8 (CO_2Me), 177.9 (CO_2Me) ppm.

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, 298 K, CDCl_3): δ = -26.1 (d, J_{BH} = 120.16 Hz, 1 B, BH) ppm.

HRMS (CH_3CN): m/z Calcd. for $\text{C}_{33}\text{H}_{47}\text{BN}_2\text{O}_4$ $[\text{M}+\text{H}]^+$ 547.3702, found 547.3694.

Melting Point: 225-230 °C (Decomposed to brown liquid).

Figure S1. ^1H NMR spectrum of **1** in CDCl_3 .

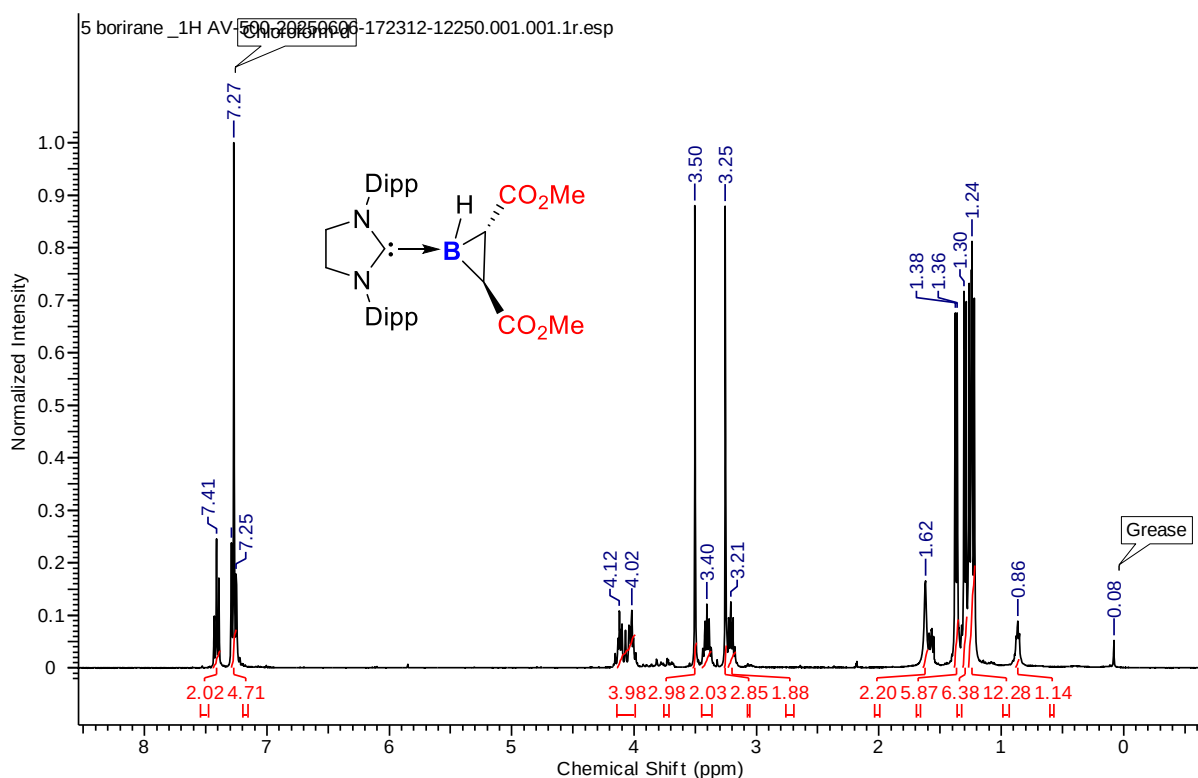


Figure S2. Enlarged ^1H NMR spectrum of **1** in CDCl_3 from 0 to 4 ppm.

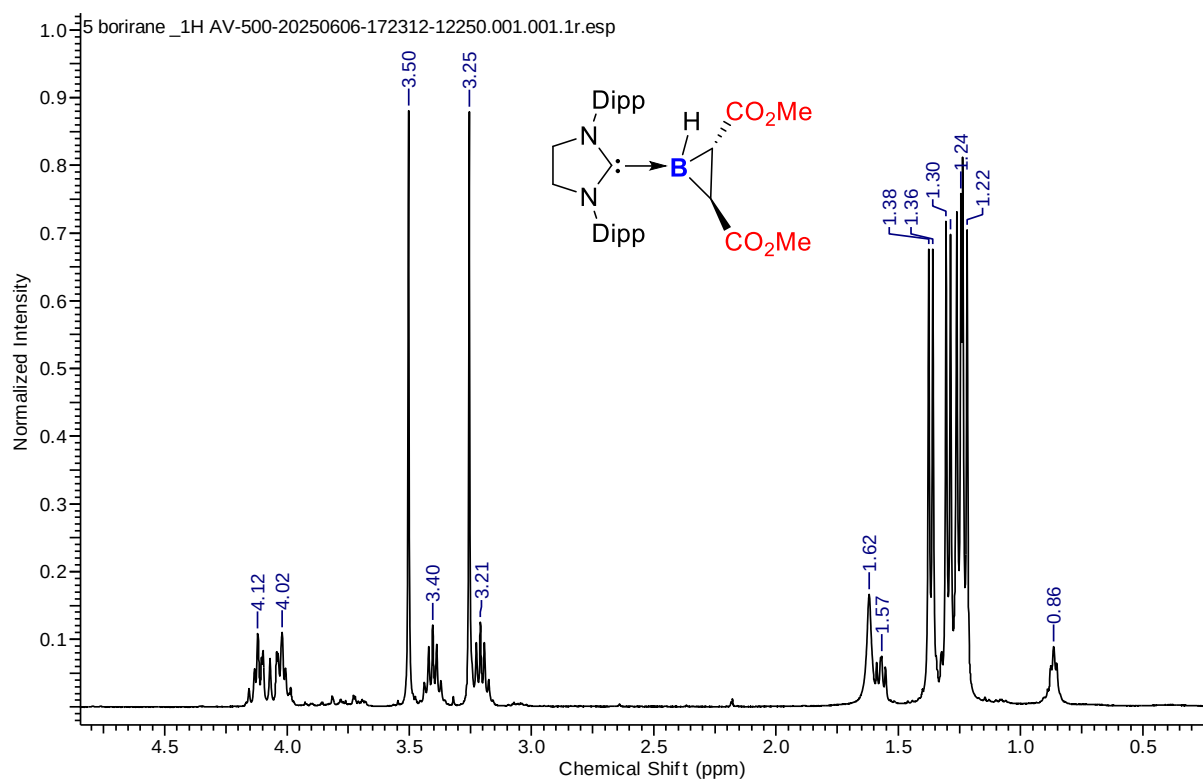


Figure S3. ^{13}C NMR spectrum of **1** in CDCl_3 .

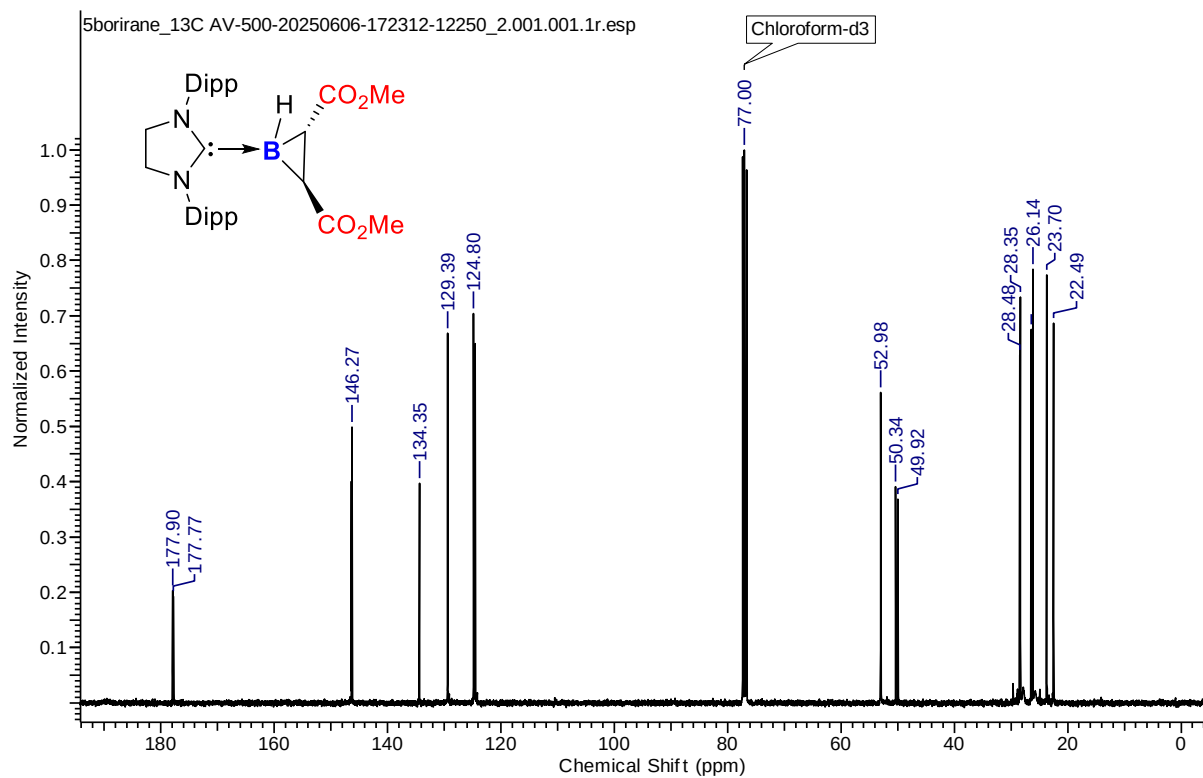


Figure S4. ^{11}B NMR spectrum of **1** in CDCl_3 .

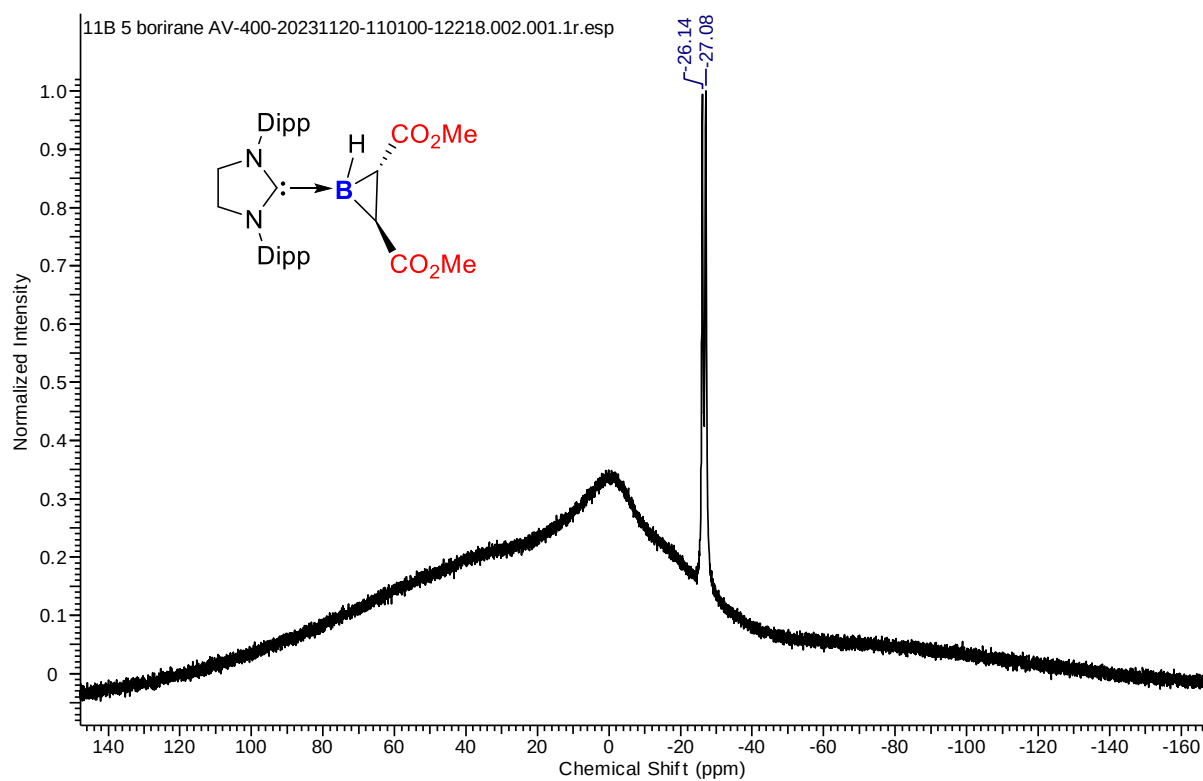
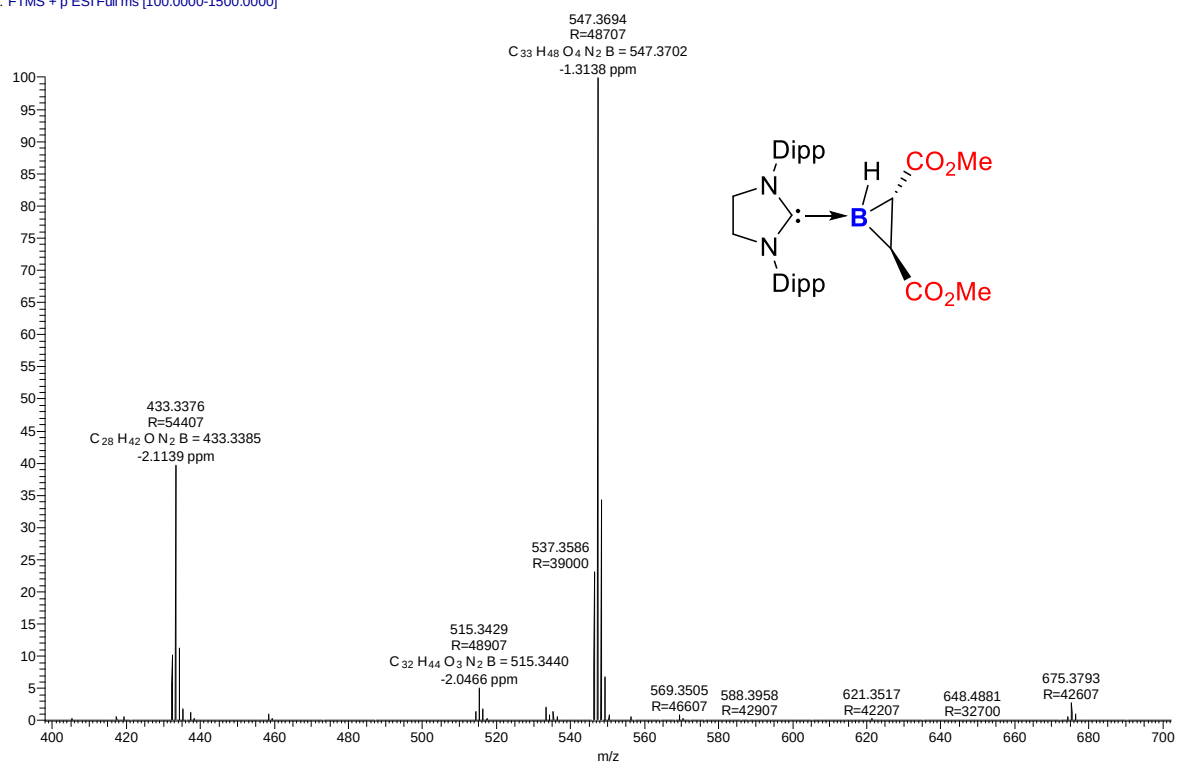


Figure S5. HR-MS spectrum of **1** in CH_3CN .

OM-4 #424 RT: 1.89 AV: 1 NL: 3.44E9

T: FTMS + p ESI Full ms [100.0000-1500.0000]



Compound 2. 2.5 equivalents of dimethyl acetylenedicarboxylate (DMAD) (1.1 ml, 9 mmol) were added to 30 ml acetonitrile solution of 6-SIDipp·BH₃ (1.5 g, 3.6 mmol). Heated the reaction at 80 °C for 3 days and carried out the ethyl acetate/hexane column chromatography in silica to yield **2** (1.2 g, 2.1 mmol, 60%). Single crystals for the X-ray analysis were grown in concentrated toluene at 4 °C in a freezer.

¹H NMR (500 MHz, 298 K, CDCl₃): δ = 0.70 (1 H, BH), 1.20 (d, J = 6.75 Hz, 6 H, CH(CH₃)₂), 1.23 (d, J = 6.63 Hz, 6 H, CH(CH₃)₂), 1.27 (d, J = 6.88 Hz, 6 H, CH(CH₃)₂), 1.35 (d, J = 6.63 Hz, 6 H, CH(CH₃)₂), 1.6 (s, 2 H, CHCO₂CH₃), 2.36 (quintet, J = 5.13 Hz, 2 H, NCH₂CH₂CH₂N), 3.18 (s, 3 H, CO₂CH₃), 3.23 (quintet, J = 6.75 Hz, 2 H, CH(CH₃)₂), 3.35 (quintet, J = 6.75 Hz, 2 H, CH(CH₃)₂), 3.46 (s, 3 H, CO₂CH₃), 3.61 - 3.65 (m, 4 H, NCH₂CH₂CH₂N), 7.21 - 7.25 (m, 4 H, Ar-H), 7.35 (t, J = 7.63 Hz, 2 H, Ar-H) ppm.

¹³C{¹H} NMR (125 MHz, 298 K, CDCl₃): δ = 19.9 (CH₂CH₂CH₂), 22.8 (CH(CH₃)₂), 24 (CH(CH₃)₂), 26.3 (CHCO₂CH₃), 26.5 (CHCO₂CH₃), 28.2 (CH(CH₃)₂), 28.6 (CH(CH₃)₂), 49.7 (CO₂Me), 50.3 (CO₂Me), 51.3 (CH₂CH₂CH₂), 124.6 (Ar-C), 124.9 (Ar-C), 128.6 (Ar-C), 141.2 (Ar-C), 144.6 (Ar-C), 144.8 (Ar-C), 177.9 (CO₂Me), 178.4 (CO₂Me) ppm.

¹¹B{¹H} NMR (128 MHz, 298 K, CDCl₃): δ = -23 (d, J_{BH} = 116.52 Hz, 1 B, BH) ppm.

HRMS (CH₃CN): m/z Calcd. for C₃₄H₄₉BN₂O₄ [M+H]⁺ 561.3858, found 561.3855.

Melting Point: 208-212 °C (Decomposed to brown liquid).

Figure S6. ^1H NMR spectrum of **2** in CDCl_3 .

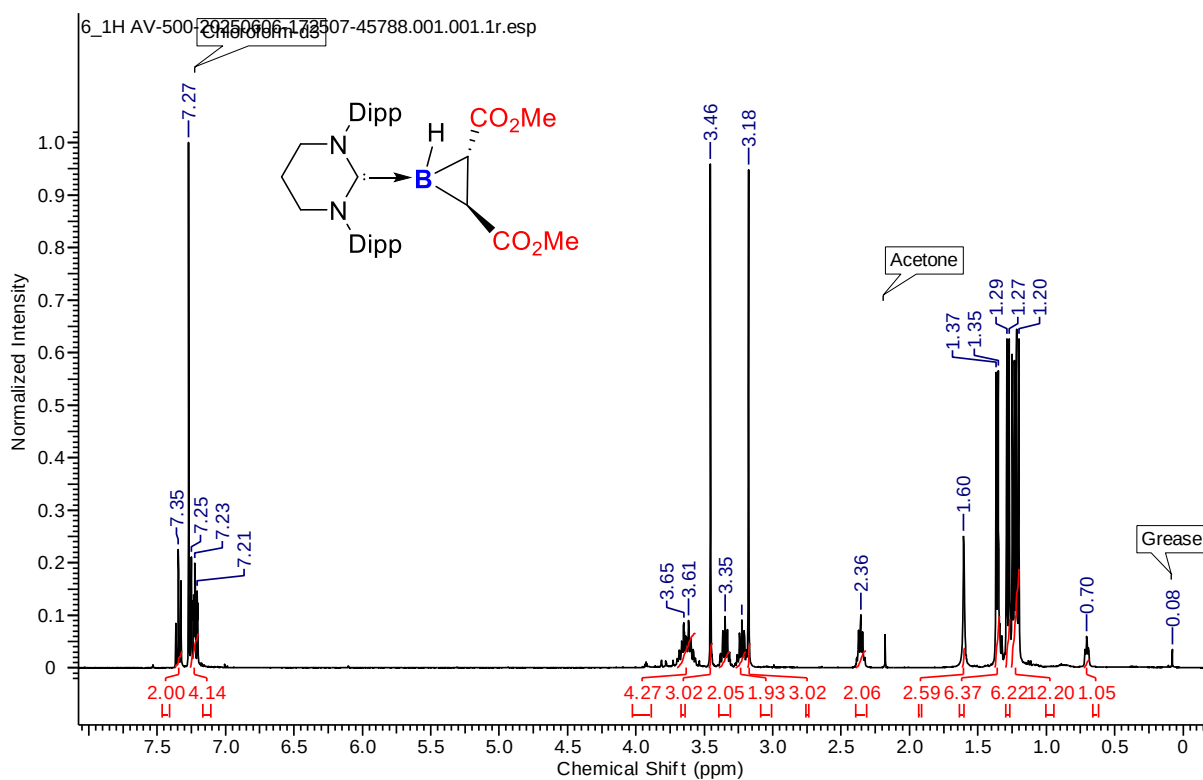


Figure S7. Enlarged ^1H NMR spectrum of **2** in CDCl_3 from 0 to 4 ppm.

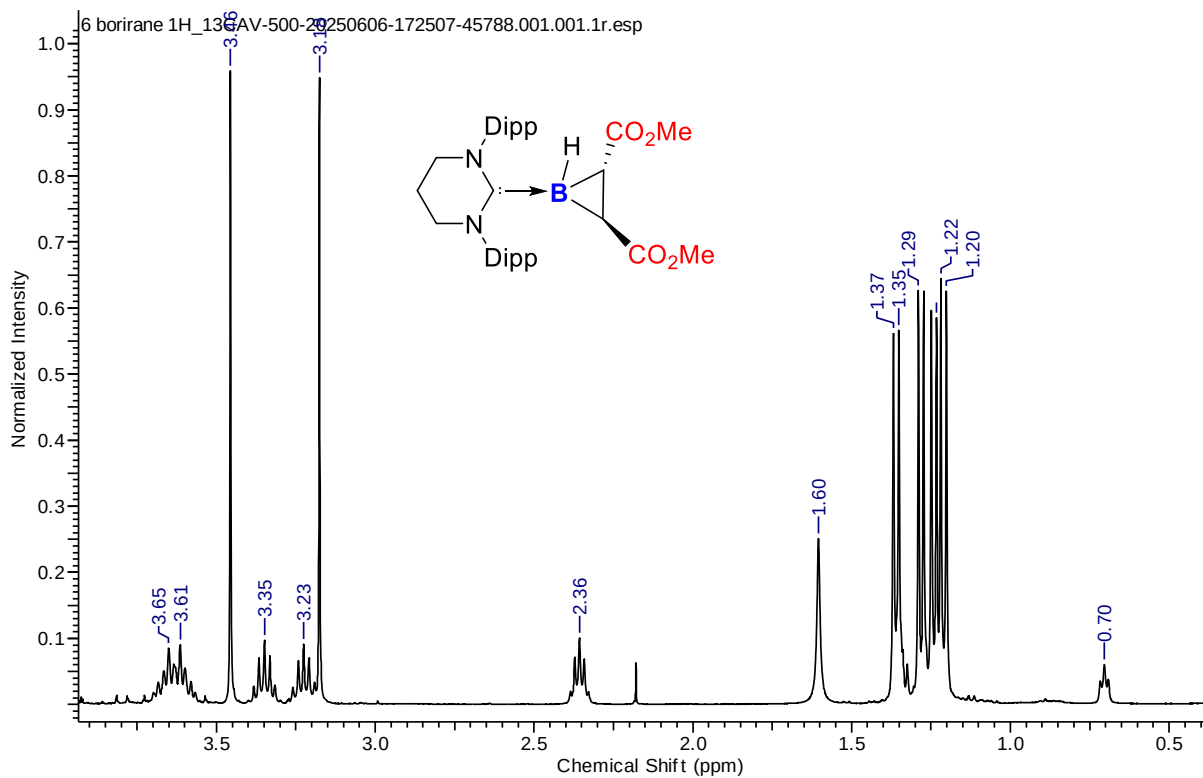


Figure S8. ^{13}C NMR spectrum of **2** in CDCl_3 .

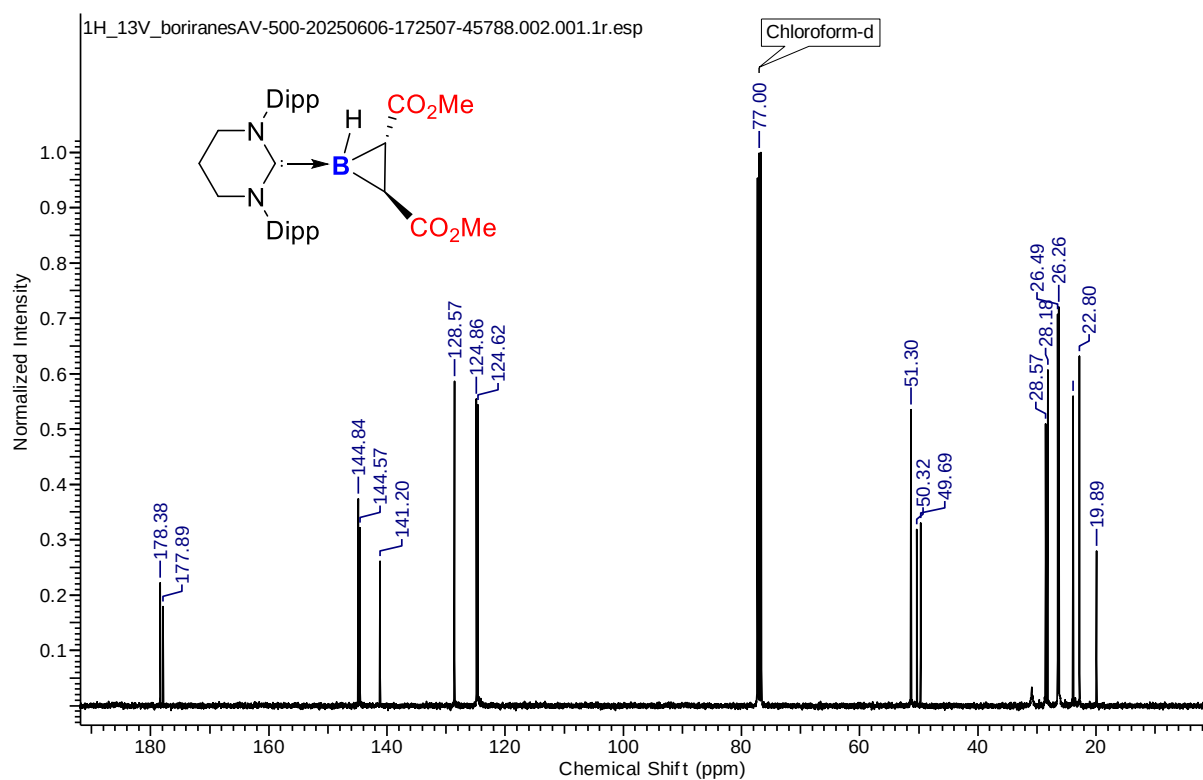


Figure S9. ^{11}B NMR spectrum of **2** in CDCl_3 .

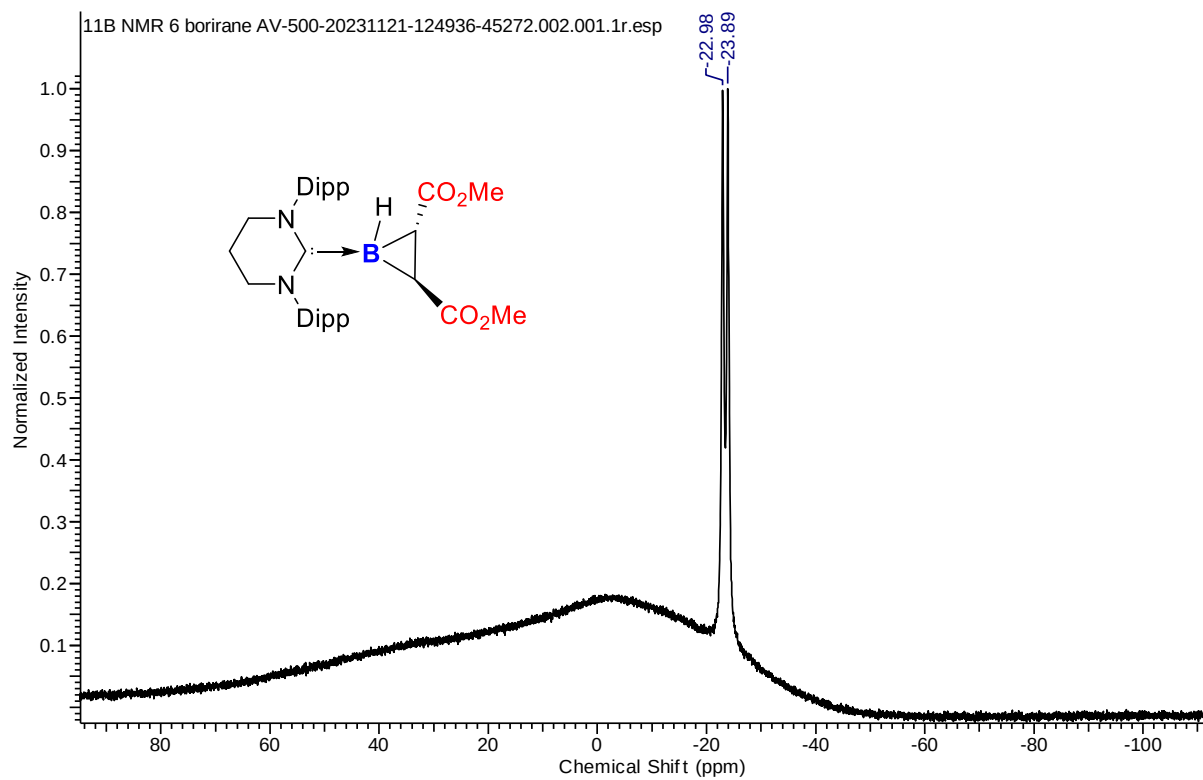
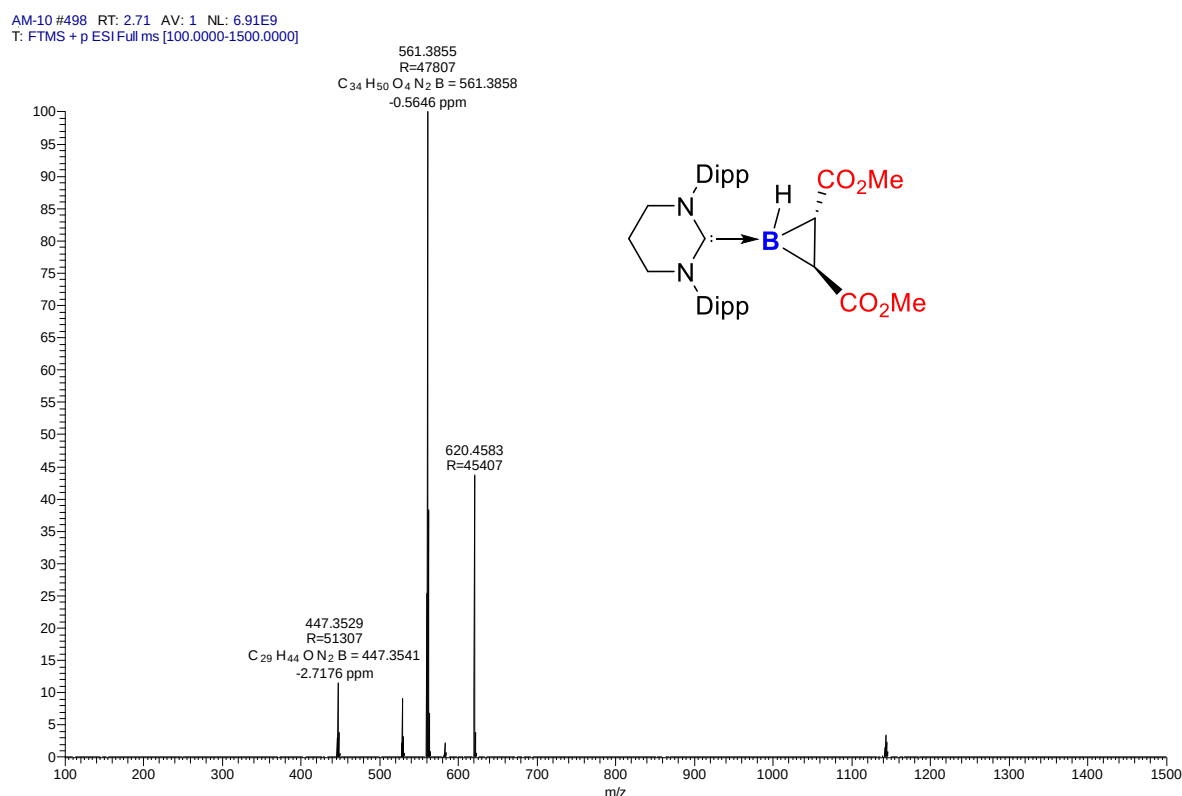


Figure S10. HR-MS spectra of **2** in CH₃CN.



Compound 3. To a 10 ml toluene/ thf solution of **1** (0.20 g, 0.37 mmol), 1.2 equivalent of HCl (4.0 M in Dioxane) (0.1 ml, 0.44 mmol) or Me₃SiCl (60 μ l, 0.44 mmol) was added under -30 °C. The reaction mixture was brought slowly to 30–35 °C, and run for another 12 hrs, and subsequently a cannula filtration was carried out to yield the compound **3** (0.13 g, 61%). Single crystals suitable for X-ray diffraction studies were grown in concentrated toluene at room temperature.

¹H NMR (400 MHz, 298 K, CDCl₃): δ = 0.85 (1 H, BH), 1.21 (d, J = 1.63 Hz, 1 H, CO₂MeCHCH₂CO₂Me), 1.28 (d, J = 6.25 Hz, 12 H, CH(CH₃)₂), 1.44 (d, J = 6.63 Hz, 6 H, CH(CH₃)₂), 1.49 (d, J = 6.63 Hz, 6 H, CH(CH₃)₂), 1.89 (dt, J = 4 Hz, J = 12.36 Hz, 1 H, CO₂MeCHCH₂CO₂CH₃), 2.43 (dd, J = 12.1 Hz, 1 H, CO₂MeCHCH₂CO₂Me), 3.23 (quintet, J = 6.75 Hz, 2 H, CH(CH₃)₂), 3.32 (quintet, J = 6.75 Hz, 2 H, CH(CH₃)₂), 3.44 (s, 6 H, CO₂CH₃), 4.05 - 4.13 (m, 4 H, NCH₂CH₂N), 7.25 (m, 4 H, Ar-H), 7.38 (t, J = 7.75 Hz, 2 H, Ar-H) ppm.

¹³C{¹H} NMR (101 MHz, 298 K, CDCl₃): δ = 22.9 (CH(CH₃)₂), 23.2 (CH(CH₃)₂), 26.3 (CHCO₂Me), 26.8 (CH(CH₃)₂), 28.8 (CH(CH₃)₂), 33.4 (CH₂CO₂Me), 50.7(CHCO₂CH₃),

53 (CH₂CH₂), 124.6 (Ar-C), 124.7 (Ar-C), 129.9 (Ar-C), 133.8 (Ar-C), 146.5 (Ar-C), 175.2 (CO₂Me), 179.3 (CO₂Me) ppm.

¹¹B{¹H} NMR (128 MHz, 298 K, CDCl₃): δ = -10.8 (s, 1 B, BH) ppm.

HRMS (CH₃CN): *m/z* Calcd. for C₃₃H₄₈BClN₂O₄ [M-H]⁺ 581.3312, found 581.3312.

Figure S11. ¹H NMR spectrum of **3** in CDCl₃.

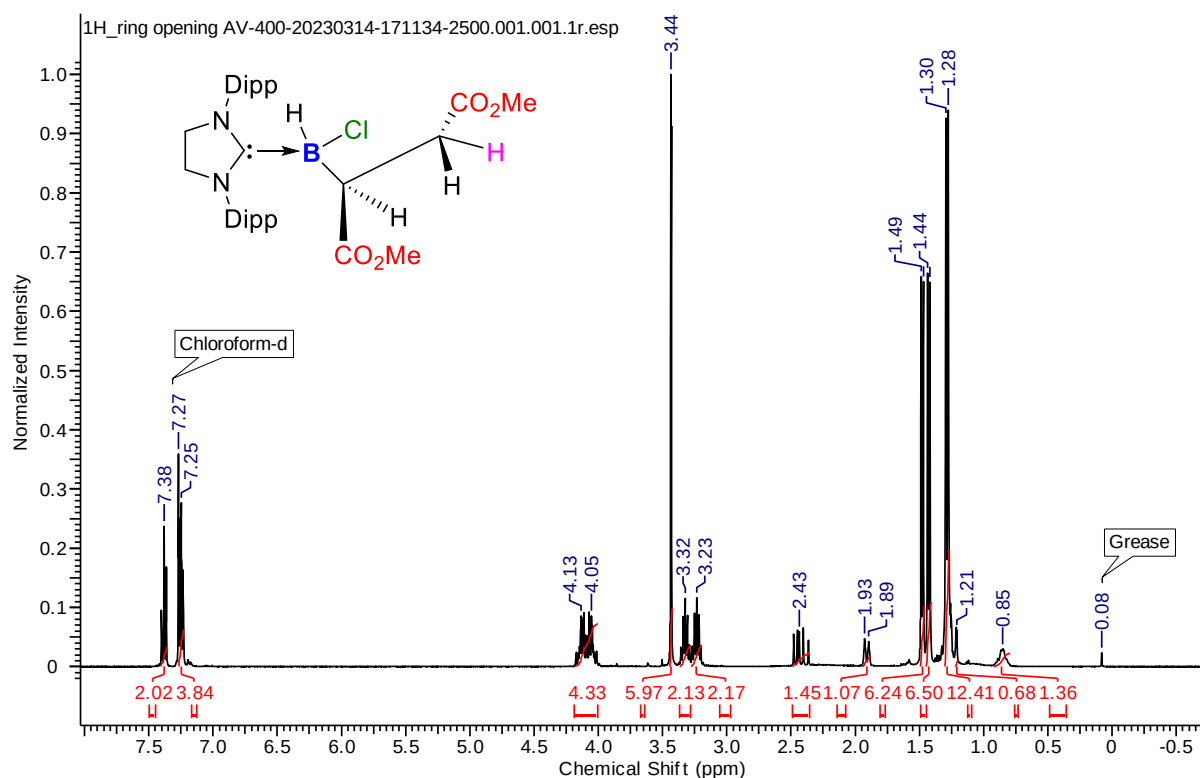


Figure S12. Enlarged ^1H NMR spectrum of **3** in CDCl_3 from 0 to 4 ppm.

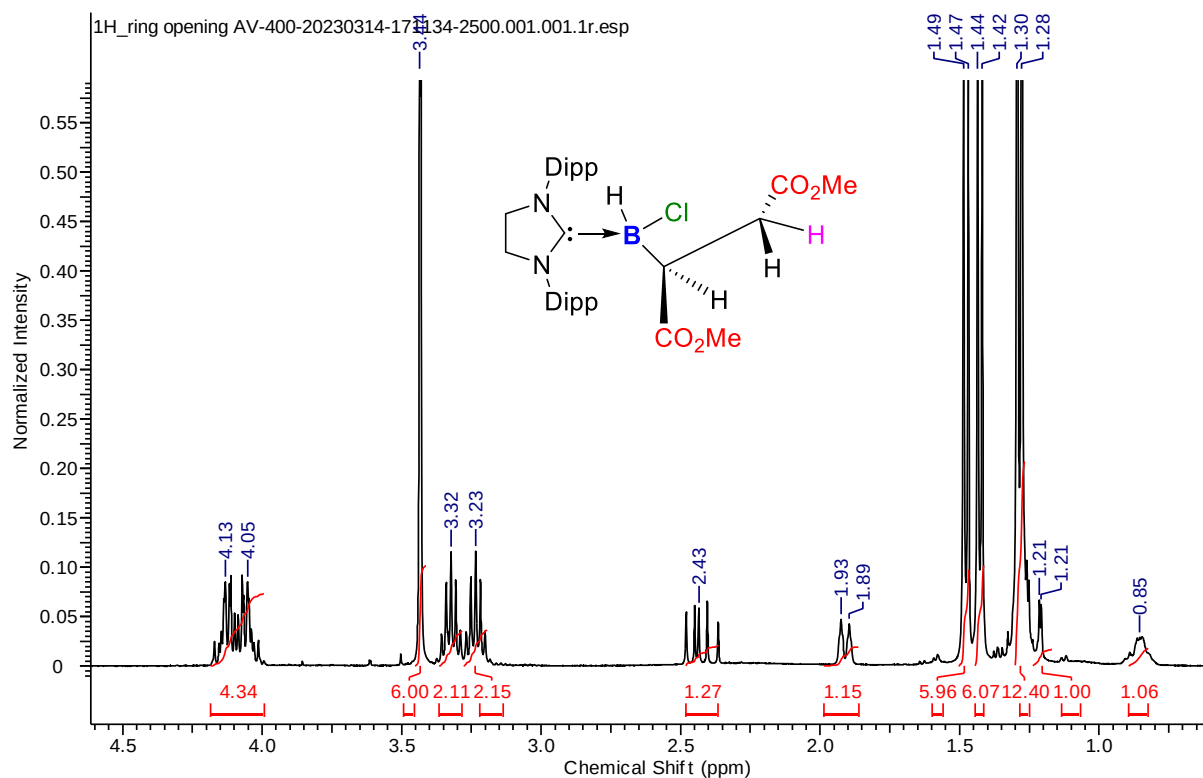


Figure S13. ^{13}C NMR spectrum of **3** in CDCl_3 .

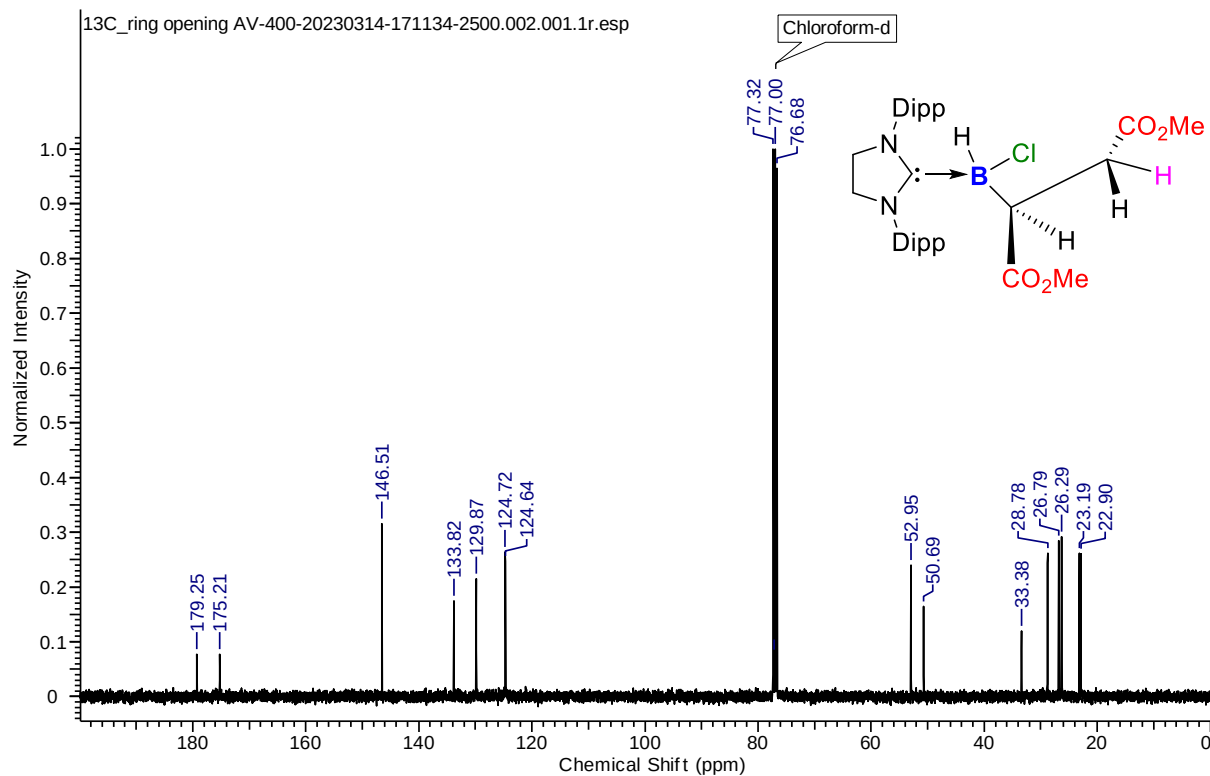


Figure S14. ^{11}B NMR spectrum of **3** in CDCl_3 .

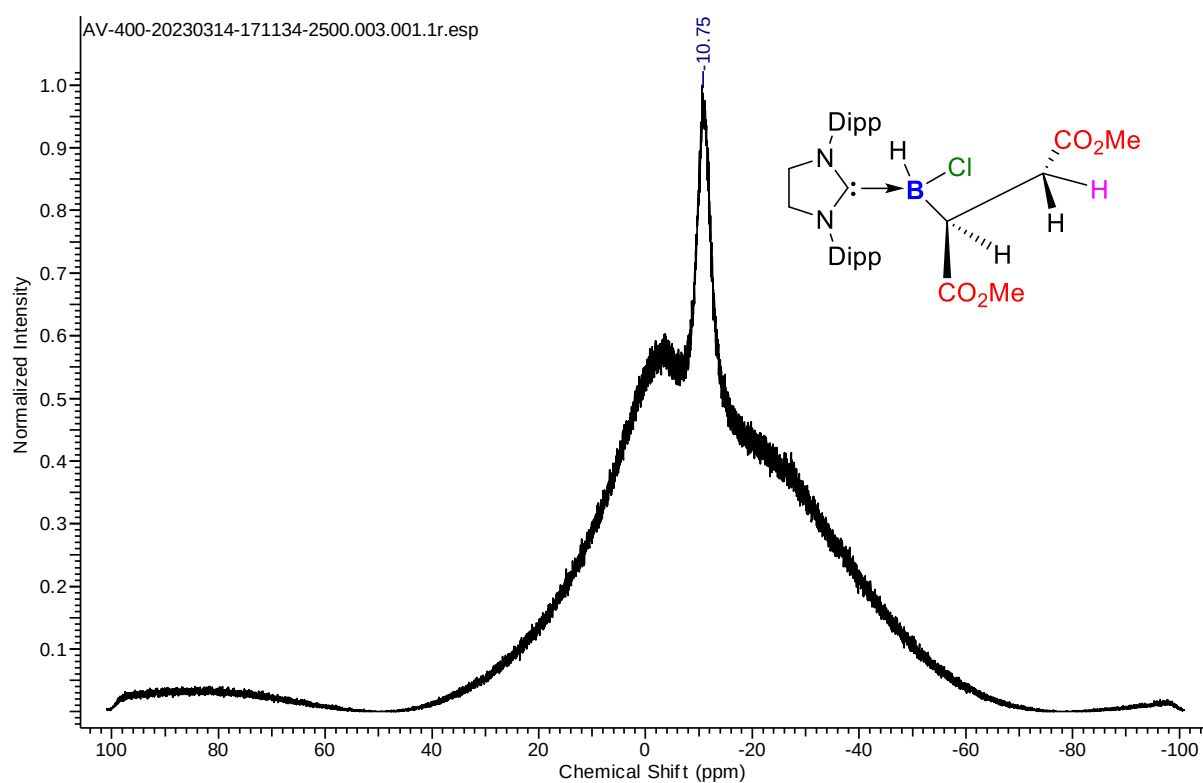


Figure S15. HR-MS spectrum of **3** in CH_3CN .

AM-12 #438 RT: 2.35 AV: 1 NL: 3.09E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

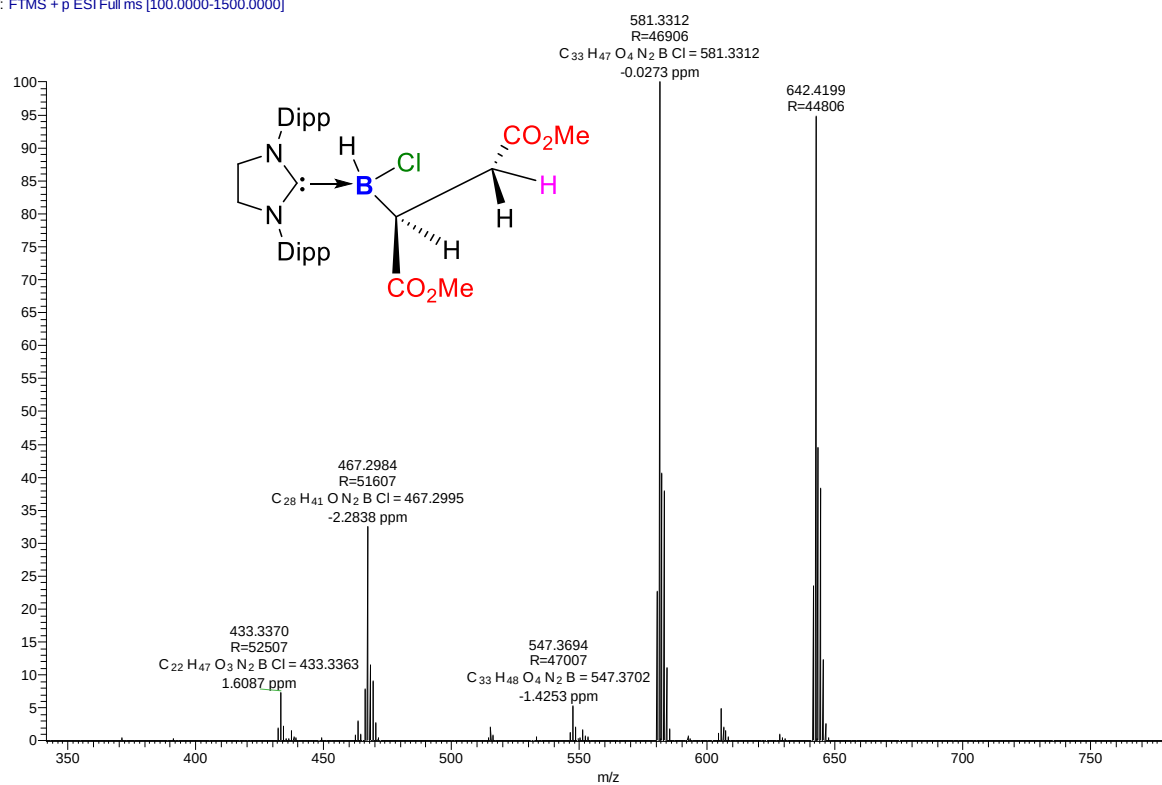
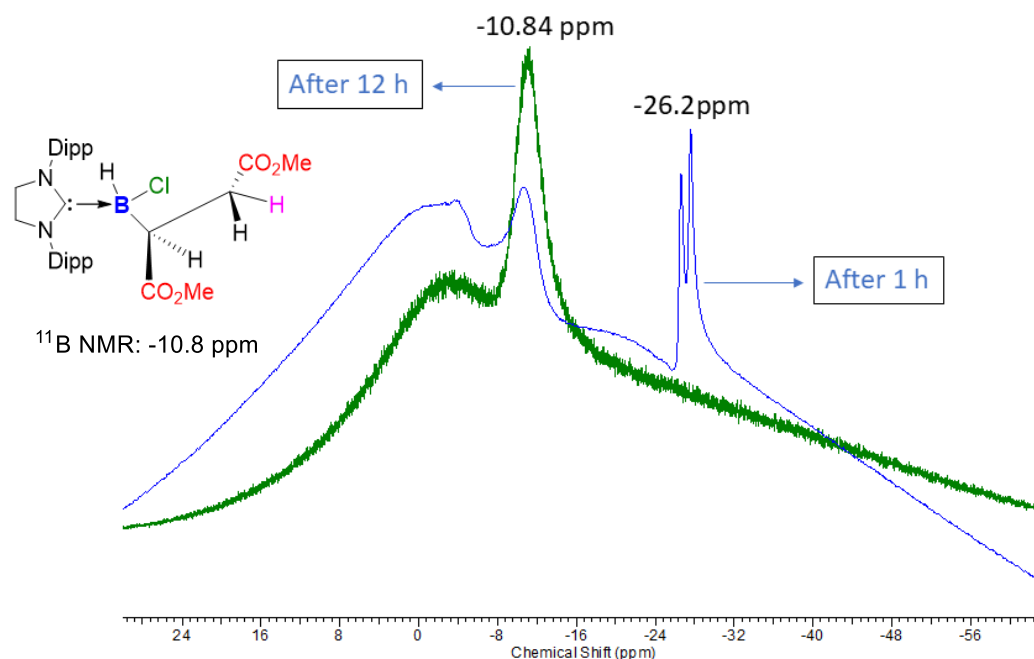


Figure S16. Time dependent ^{11}B NMR spectrum of NMR tube reactions of **1** with HCl after 1 h and 12 h in toluene.



For a note: Time-dependent ^{11}B NMR spectra of the reaction of compound **1** with HCl in toluene, recorded after 1 h and 12 h, confirm the selective formation of the ring-opened product in toluene. The spectrum shows two resonances at $\delta = 10.8$ ppm and $\delta = 26.2$ ppm, corresponding to compound **3** and **1**, respectively. These observations demonstrate that in toluene, the reaction proceeds selectively to afford only the ring-opened product.

Compound 4. To a 10 ml acetonitrile solution of **1** (0.20 g, 0.37 mmol), 1.2 equivalent of HCl (4.0 M in Dioxane) (0.1 ml, 0.44 mmol) was added under -30 $^{\circ}\text{C}$. The reaction mixture was brought slowly to 30 – 35 $^{\circ}\text{C}$, and run for another 12 hrs, and subsequently a cannula filtration was carried out to yield mixture of **3** and **4**. Column chromatography was carried out to yield compound **4** (0.06 g, 0.11 mmol, 30%). Crystals suitable for X-ray diffraction studies were grown in concentrated toluene at room temperature.

^1H NMR (400 MHz, 298 K, CDCl_3): δ = 0.89 (1 H, BH), 1.27 (m, 1 H, $\text{CO}_2\text{MeCHCH}_2\text{CO}$), 1.31 (t, J = 7.5 Hz, 12 H, $\text{CH}(\text{CH}_3)_2$), 1.42 (t, J = 6.18 Hz, 12 H, $\text{CH}(\text{CH}_3)_2$), 1.83 (m, 1 H, $\text{CO}_2\text{MeCHCH}_2\text{CO}$), 2.28 - 2.33 (dd, J = 6.13 Hz, J = 6.13 Hz, 1 H, $\text{CO}_2\text{MeCHCH}_2\text{CO}$), 3.14 (quintet, J = 6.63 Hz, 4 H, $\text{CH}(\text{CH}_3)_2$), 3.33 (s, 3 H,

CO₂CH₃), 4.12 (s, 4 H, NCH₂CH₂N), 7.25 – 7.28 (m, 4 H, Ar-H), 7.42 (t, *J* = 7.63 Hz, 2 H, Ar-H) ppm.

There are a few additional peaks presumably originating during the separation of **3** and **4**.

¹³C{¹H} NMR (125 MHz, 298 K, CDCl₃): δ = 22.8 (CH(CH₃)₂), 23.1(CH(CH₃)₂), 26.3 (CHCO₂Me), 28.9 (CH(CH₃)₂), 29 (CH(CH₃)₂), 32.9 (CH₂CO₂Me), 50.7 (CO₂CH₃), 53.2 (CH₂CH₂), 124.5 (Ar-C), 124.7 (Ar-C), 130 (Ar-C), 133.2 (Ar-C), 145.7 (Ar-C), 146.3 (Ar-C), 179.13 (CO₂Me), 180.6 (CO₂B) ppm.

¹¹B{¹H} NMR (128 MHz, 298 K, CDCl₃): δ = -4.3 (s, 1 B, BH) ppm.

HRMS (CH₃CN): *m/z* Calcd. for C₃₃H₄₇BN₂O₄ [M+H]⁺ 533.3545, found 533.3539.

Figure S17. ¹H NMR spectrum of **4** in CDCl₃.

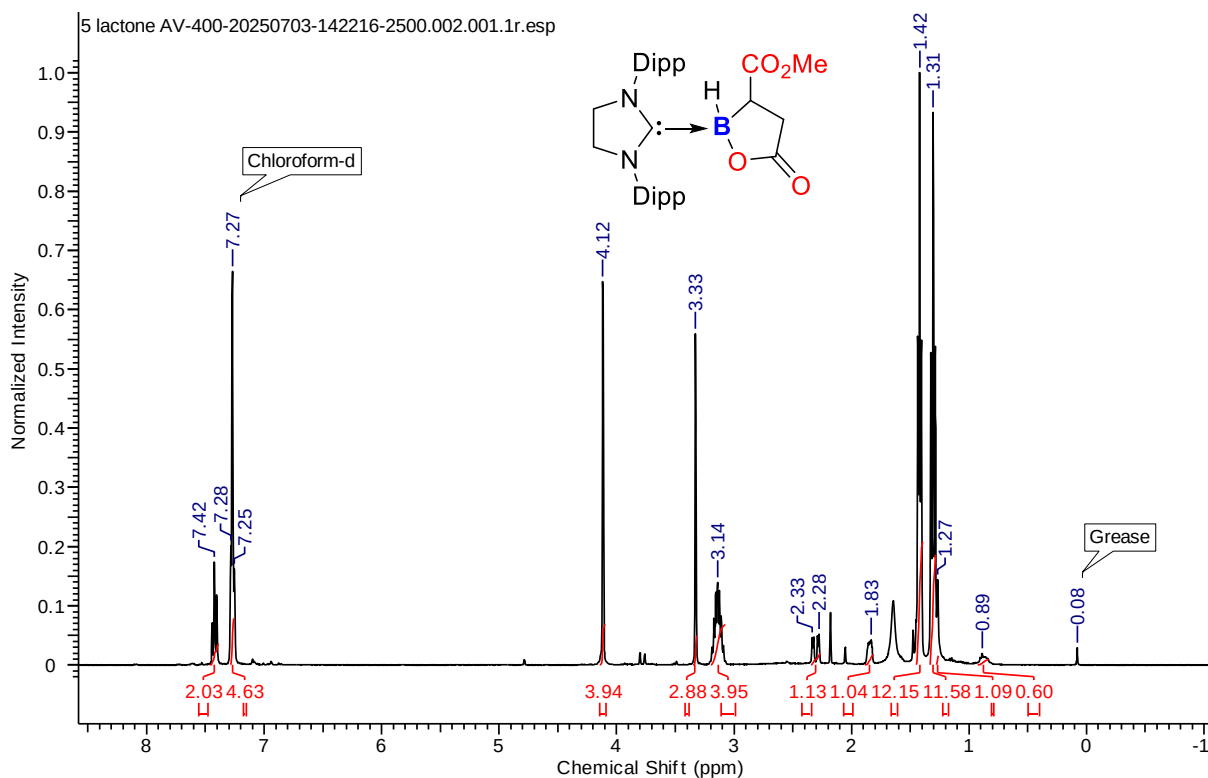


Figure S18. ^{13}C NMR spectrum of **4** in CDCl_3 .

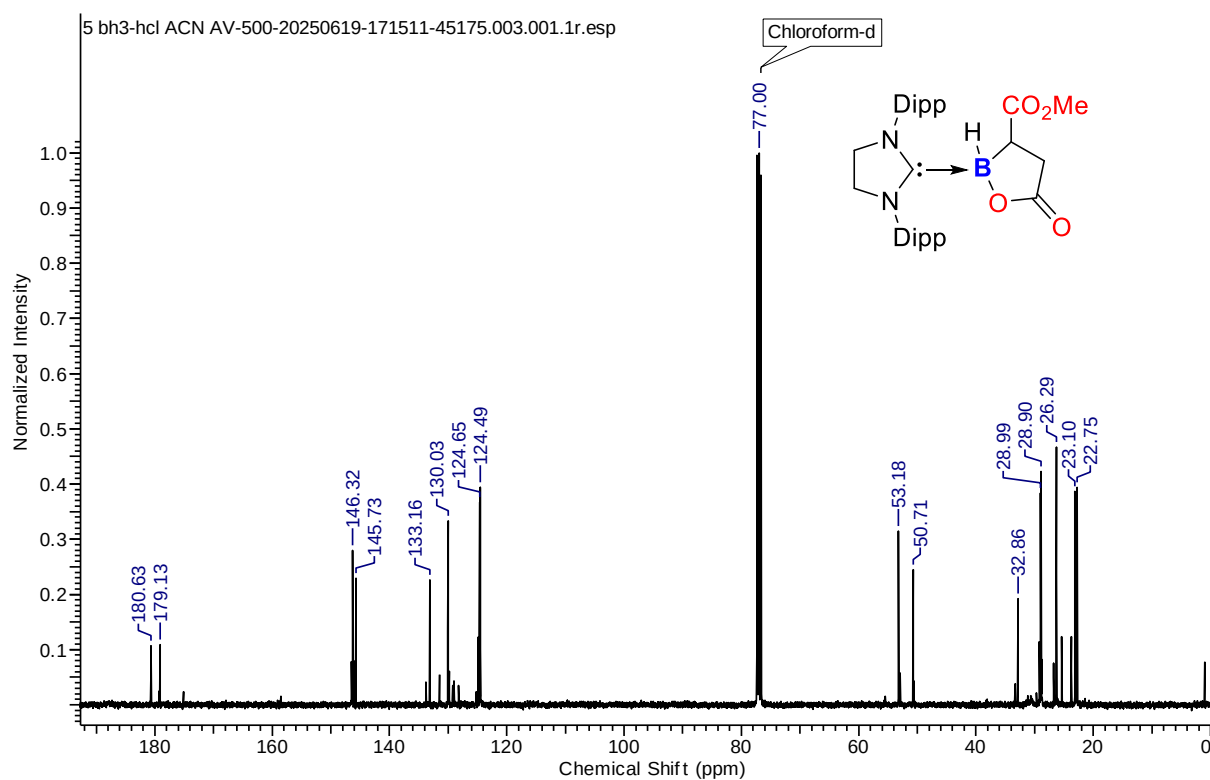


Figure S19. ^{11}B NMR spectrum of **4** in CDCl_3 .

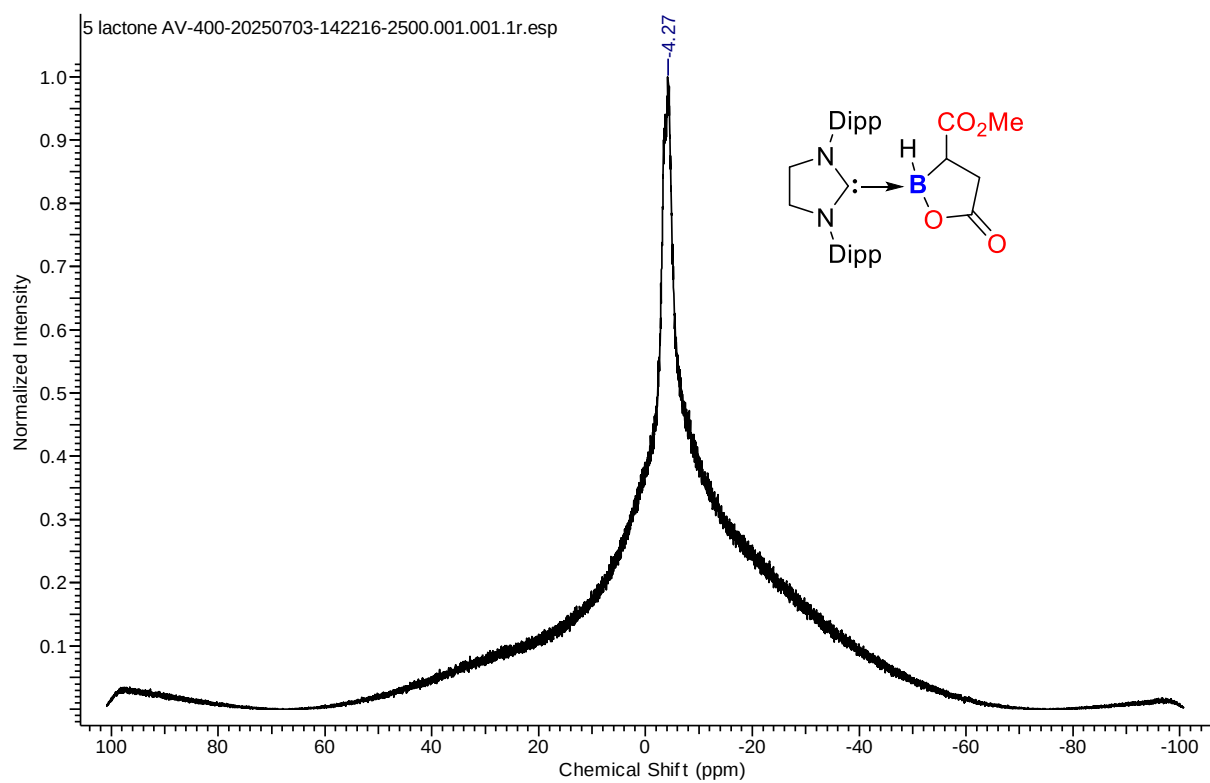


Figure S20. HR-MS spectrum of **4** in CH₃CN.

AM-28 #376 RT: 2.02 AV: 1 NL: 1.94E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

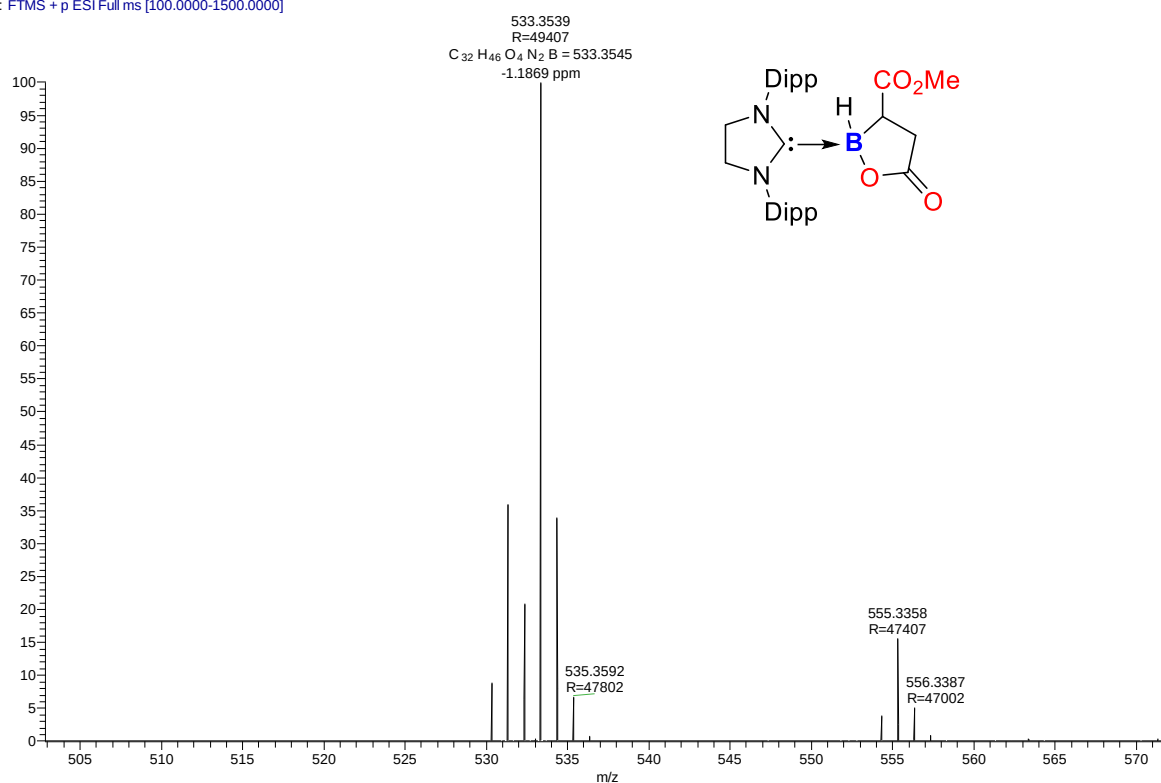
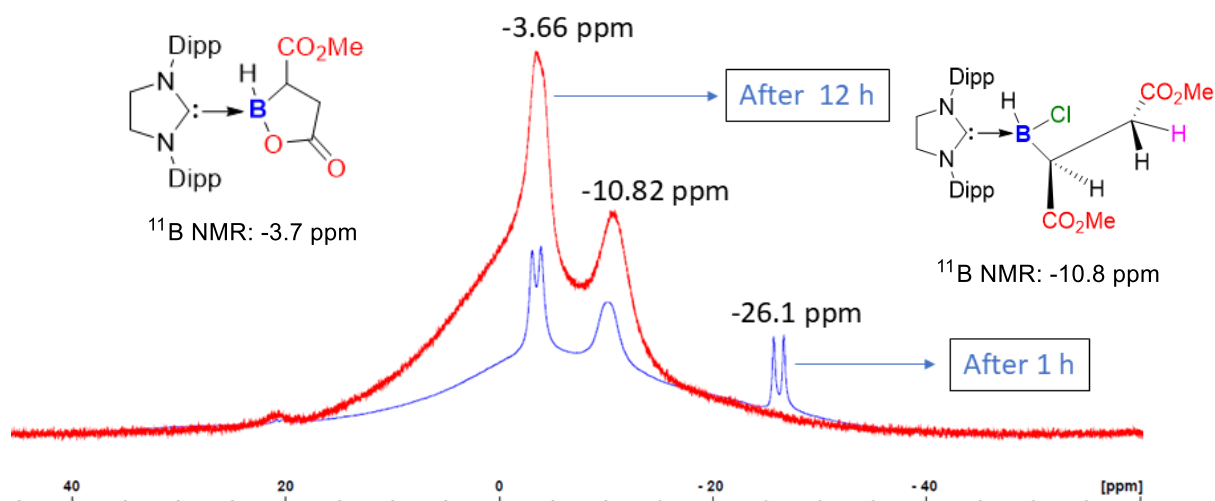


Figure S21. Time dependent ¹¹B NMR spectrum of NMR tube reactions after 1 h and 12 h in acetonitrile.



For a note: Time-dependent ¹¹B NMR spectra of the reaction of compound **1** with HCl in acetonitrile, recorded after 1 h and 12 h, confirm the mixture product formation. The spectrum shows three resonances at $\delta = -3.7$ ppm, $\delta = 10.8$ ppm and $\delta = 26.1$ ppm,

corresponding to compound **4**, **3** and **1**, respectively. These observations demonstrate that in acetonitrile, the reaction proceeds to afford mixture of products from the beginning.

Compound 5. 1.2 equivalent of HCl (4.0 M in dioxane) (0.1 ml, 0.428 mmol) or Me₃SiCl (55 μ l, 0.428 mmol) was added to the 10 ml toluene solution of **2** (0.2 g, 0.357 mmol) at -30 °C. The reaction mixture was brought to 30–35 °C, and stirred for 12 hrs, and subjected to a cannula filtration to yield **5** (0.12, 64 %). Colourless crystals were grown in concentrated toluene at room temperature in 3-4 days.

¹H NMR (400 MHz, 298 K, CDCl₃): δ = 0.92 (1 H, BH), 1.04 (dd, J = 10.26 Hz, J = 10.26 Hz 1 H, CO₂MeCHCH₂CO), 1.22 - 1.28 (m, 12 H, CH(CH₃)₂), 1.40 (d, J = 5.88 Hz, 12H, CH(CH₃)₂), 1.75 (m, 1 H, CO₂MeCHCH₂CO), 2.01 – 2.06 (dd, J = 4.88 Hz, J = 4.88 Hz, 1 H, CO₂MeCHCH₂CO), 2.34 (s, 2 H, NCH₂CH₂CH₂N), 3.06 (quintet, J = 6.63 Hz, 2 H, CH(CH₃)₂), 3.17 (quintet, J = 6.63 Hz, 2 H, CH(CH₃)₂), 3.29 (s, 3 H, CO₂CH₃), 3.62 (sept, 4 H, NCH₂CH₂CH₂N), 7.20 (m, 4 H, Ar-H), 7.32 (t, J = 7.63 Hz, 2 H, Ar-H) ppm.

¹³C{¹H} NMR (125 MHz, 298 K, CDCl₃): δ = 19.9 (CH₂CH₂CH₂), 22.6 (CH(CH₃)₂), 23.2 (CH(CH₃)₂), 26.4 (CHCO₂Me), 26.6 CH(CH₃)₂), 28.8 CH(CH₃)₂), 28.9 (CH(CH₃)₂), 32.7(CH₂CO₂Me), 50.6 (CHCO₂CH₃), 51.8 (CH₂CH₂CH₂), 124.4 (Ar-C), 124.7 (Ar-C), 129.3 (Ar-C), 139.9 (Ar-C), 144.4 (Ar-C), 145.3 (Ar-C), 179.2 (CO₂Me), 180.8 (CO₂Me) ppm.

¹¹B{¹H} NMR (128 MHz, 298 K, CDCl₃): δ = -2.5 (s, 1 B, BH) ppm.

HRMS (CH₃CN): m/z Calcd. for C₃₃H₄₇BN₂O₄ [M-1]⁺ 545.3545, found 545.3547.

Figure S22. ^1H NMR spectrum of **5** in CDCl_3 .

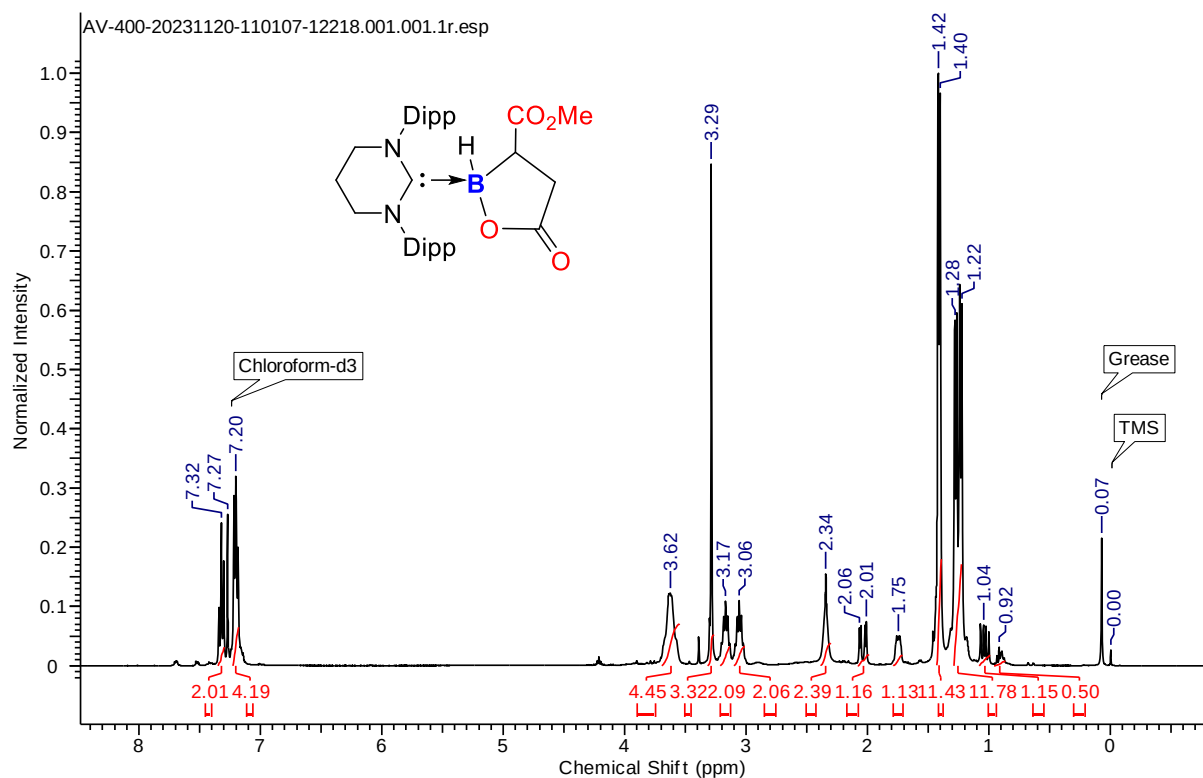


Figure S23. Enlarged ^1H NMR spectrum of **5** in CDCl_3 from 0 to 4 ppm.

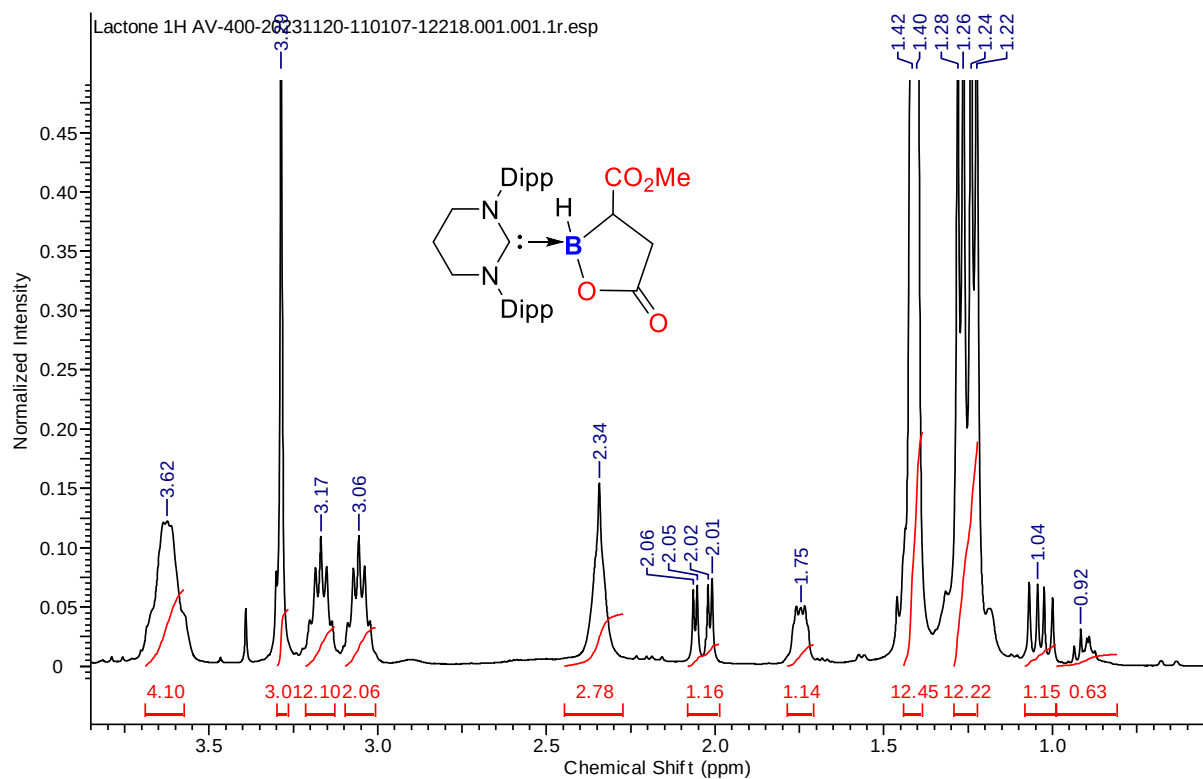


Figure S24. ^{13}C NMR spectrum of **5** in CDCl_3 .

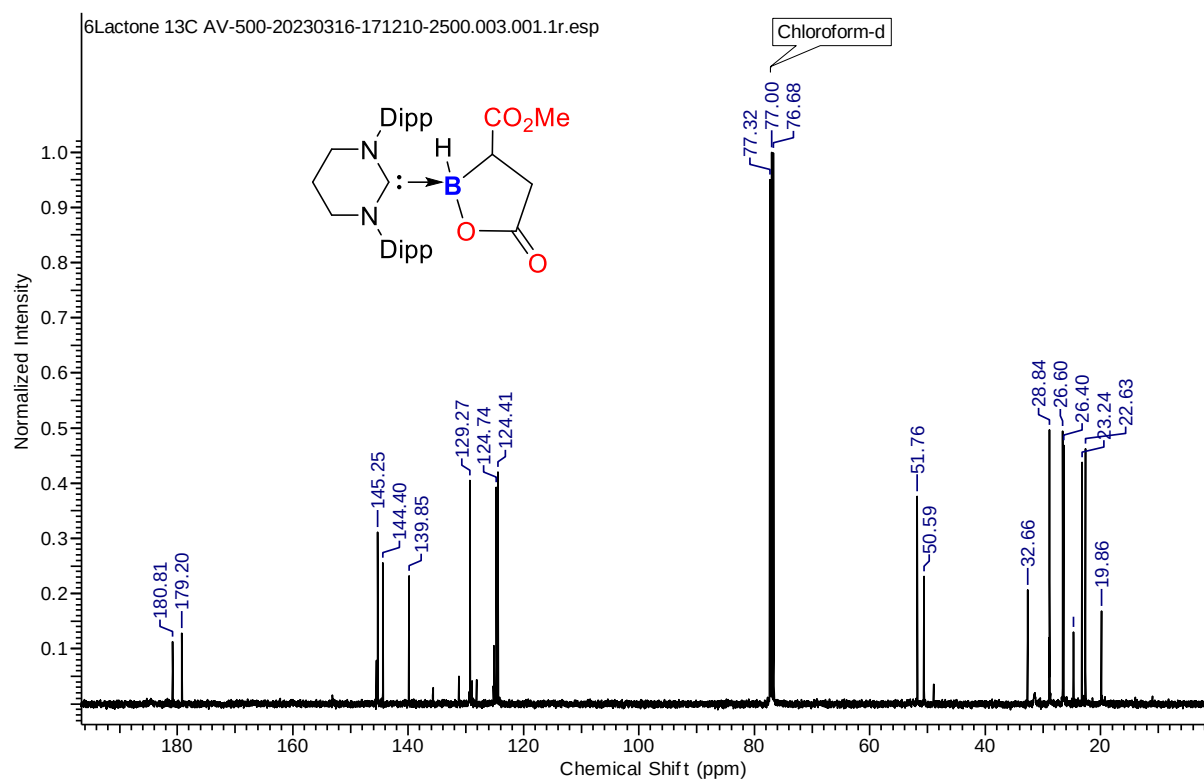


Figure S25. ^{11}B NMR spectrum of **5** in CDCl_3 .

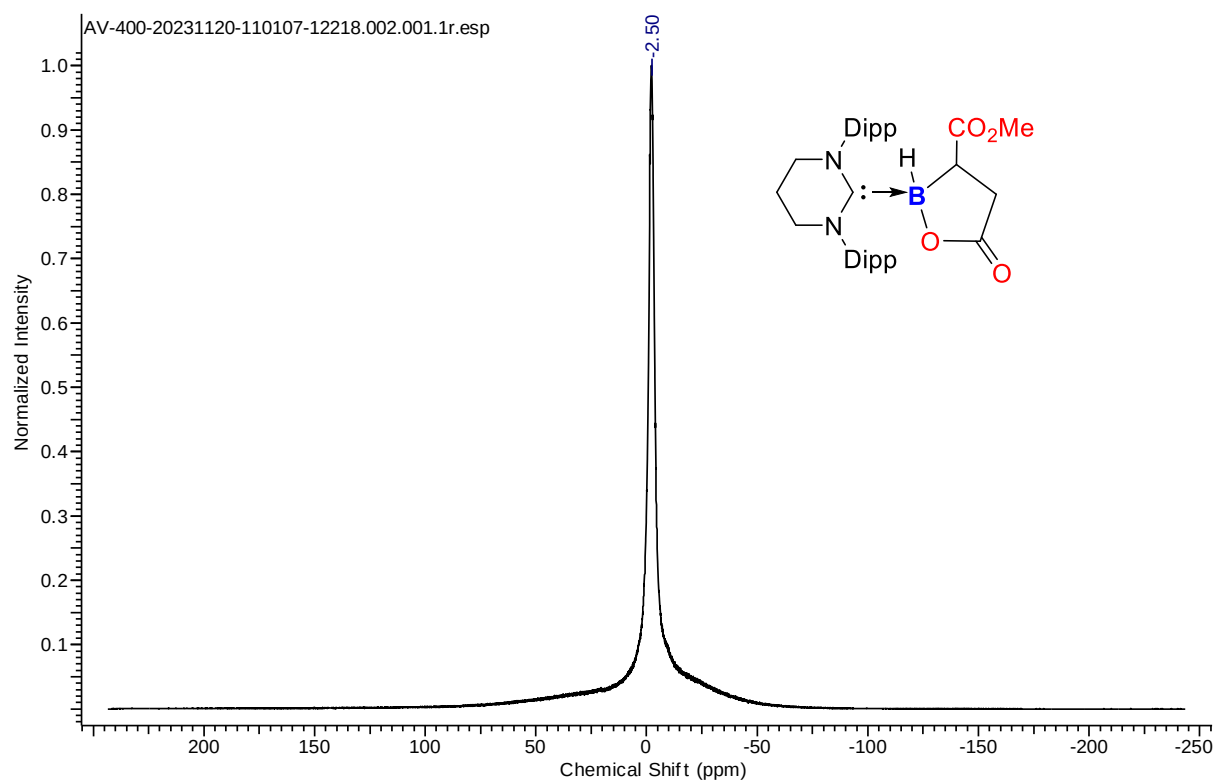
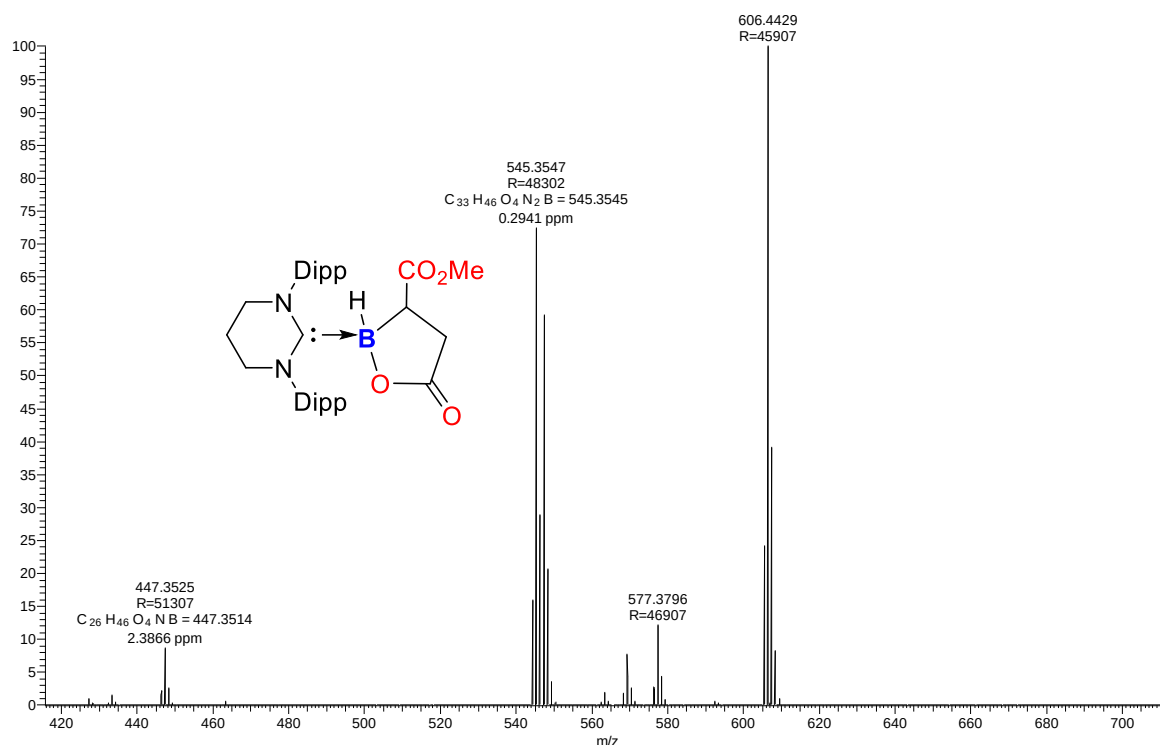


Figure S26. HR-MS spectrum of **5** in CH₃CN.

AM-11 #427 RT: 2.28 AV: 1 NL: 3.43E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



Compound 6. 10 ml of acetonitrile was added at -78 °C to a mixture of **1** (0.2 g, 0.37 mmol) and freshly sublimised AlCl₃ (0.06 g, 0.44 mmol). The reaction mixture was warmed up to room temperature and allowed to run for another 12 h. After the reaction, cannula filtration was carried out to yield **6**. A few tiny colourless crystals suitable for analysis were grown in toluene at 4 °C.

¹H NMR (400 MHz, 298 K, CDCl₃): δ = 0.90 (1 H, BH), 1.27 (t, J = 5.88 Hz, 12 H, CH(CH₃)₂), 1.41 (dd, J = 6 Hz, J = 6.25 Hz, 12 H, CH(CH₃)₂), 1.86 (m, 2 H, MeCO₂HCCHCO₂Me), 2 (s, 3 H, NCCH₃), 3.13-3.22 (m, 4 H, CH(CH₃)₂), 3.32 (s, 3 H, CO₂CH₃), 3.42 (s, 3 H, CO₂CH₃), 3.75 (s, 1 H, N-H), 4.12 (m, 4 H, NCH₂CH₂N), 7.24 (m, 4 H, Ar-H), 7.38 (m, 2 H, Ar-H) ppm.

For a note: The ¹H NMR spectrum was recorded from the crystals. Moreover, after crystallization, there is a solubility issue and the compound is sparingly soluble in CDCl₃, C₇D₈, and THF-d₈. The turbid solution in CDCl₃ gave not so clean ¹³C spectra with peaks of **6** along with some unidentified peaks which presumably generated due to the decomposition with time in deuterated solvents. However, we could able to detect the CN as well as CH₃ peaks which are characteristics for compound **6**.

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, 298 K, CDCl_3): δ = 0.9, 22.5, 22.8, 26.4, 29, 51.3, 53.5, 54.3, 57.9, 116.4, 124.6, 130.8, 131.2, 132.1, 145.5, 146.2, 167.70 176.8, 177.3 ppm.

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, 298 K, CDCl_3): δ = -5.7 (s, 1 B, BH) ppm.

Figure S27. ^1H NMR spectrum of **6** in CDCl_3 .

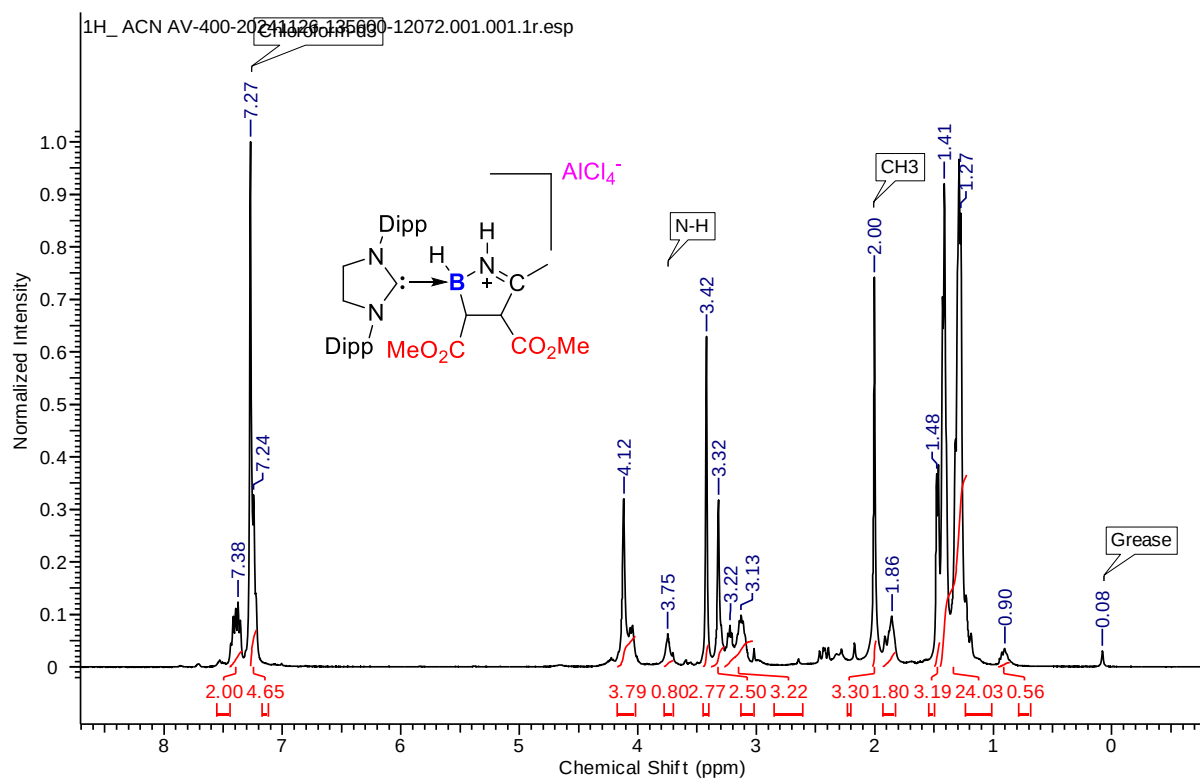


Figure S28. ^{13}C NMR spectrum of **6** in CDCl_3 .

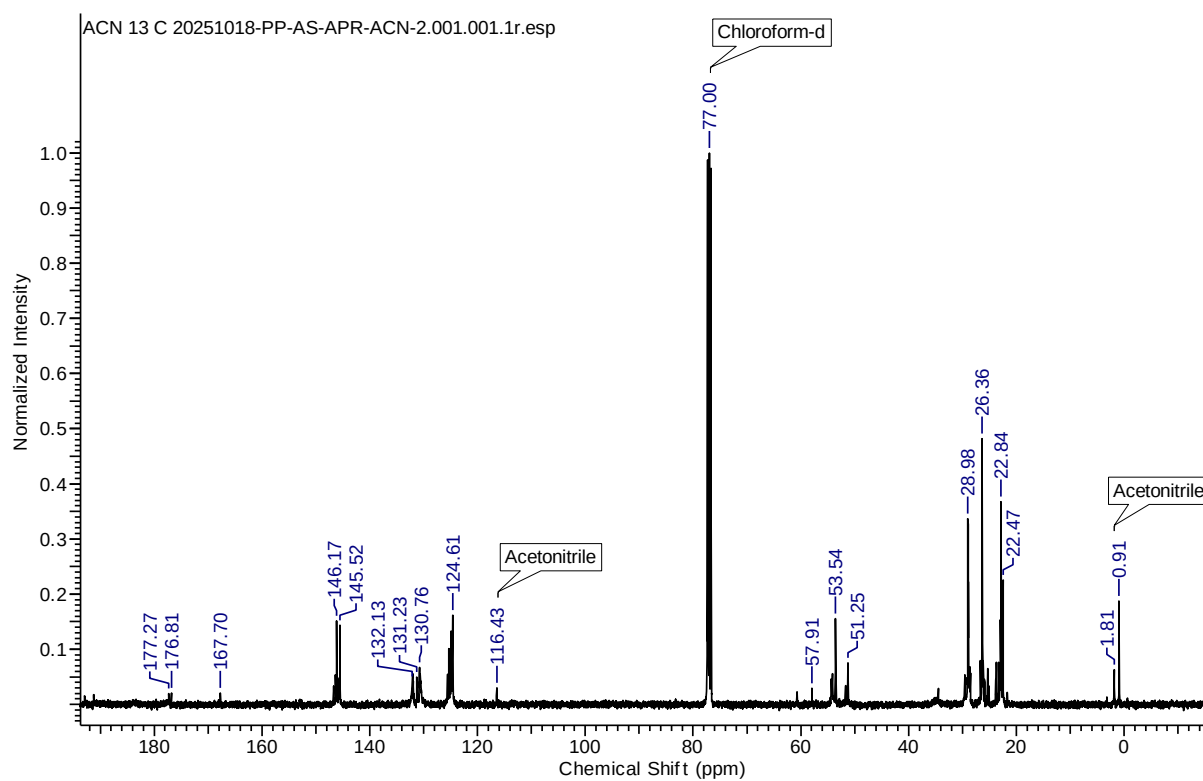
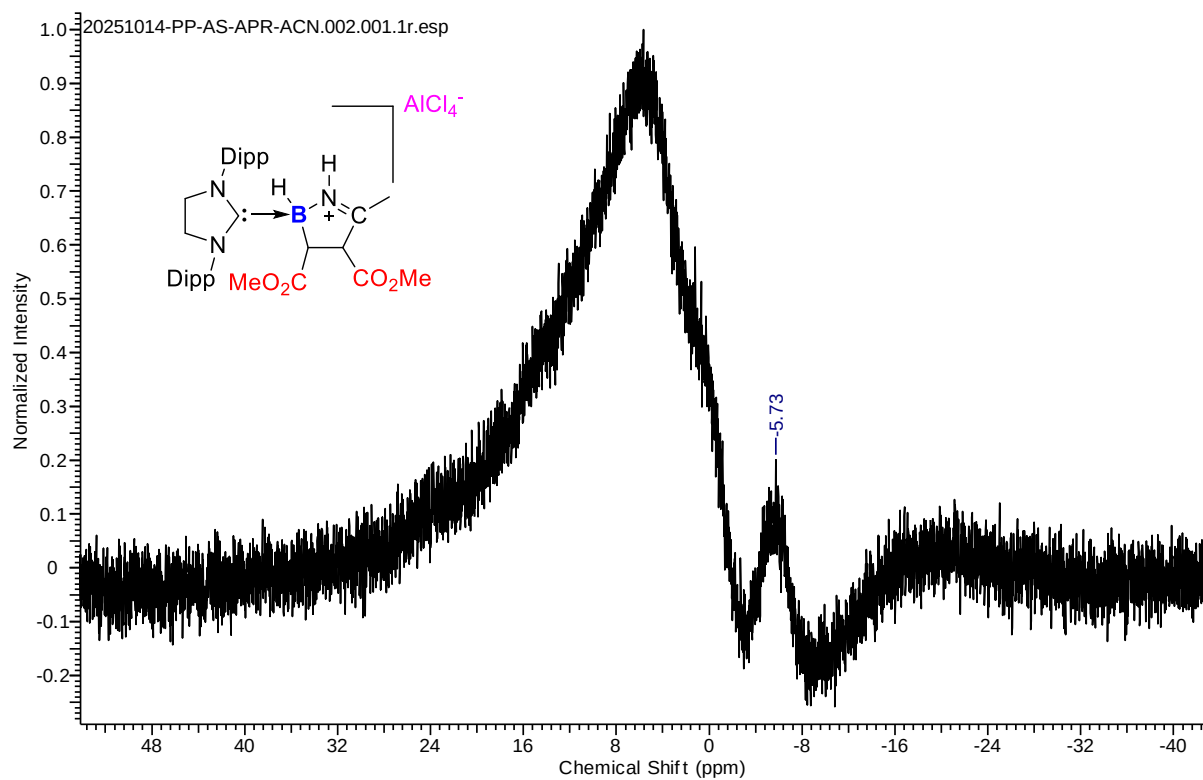


Figure S29. ^{11}B NMR spectrum of **6** in CDCl_3 .



Compound 7. To a mixture of **1** (0.20 g, 0.37 mmol) and freshly sublimed $\text{B}(\text{C}_6\text{F}_5)_3$ (0.48 g, 0.92 mmol), tetrahydrofuran (10 ml) was added at $-78\text{ }^\circ\text{C}$. The slightly turbid reaction mixture was then slowly brought to room temperature, and run for further 24 hrs to yield **7** (0.19 g, 0.18 mmol, 48%). Colourless crystals of **7** were grown in THF solution at $4\text{ }^\circ\text{C}$ in a freezer.

For a note: Upon the generation of the crystals of **7**, the compound is sparingly soluble in most common organic solvents, which impedes NMR characterization. More over compound starts decomposing over time. The extra peak generation around -20 ppm suggests some unknown compound formation, which we could not identify.

^1H NMR (400 MHz, 298 K, THF- d_8): $\delta = 0.82$ (1 H, BH), $\delta = 1.26 - 1.36$ (m, 24 H, $\text{CH}(\text{CH}_3)_2$), 1.59 (s, 2 H, CHCO_2CH_3), 3.11 (s, 3 H, CO_2CH_3), 3.25 (quintet, $J = 7.7\text{ Hz}$, 2 H, $\text{CH}(\text{CH}_3)_2$), 3.37 (m, 2 H, $\text{CH}(\text{CH}_3)_2$), 3.44 (s, 3 H, CO_2CH_3), 4.17 (m, 4 H, $\text{NCH}_2\text{CH}_2\text{N}$), 7.28 (m, 4 H, Ar-H), 7.36 (t, $J = 7.75\text{ Hz}$, 2H, Ar-H) ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, 298 K, THF- d_8): $\delta = 23.1, 24.3, 26.5, 26.7, 27.7, 29.3, 29.4, 49.4, 50.3, 54.2, 71.4, 125.3, 125.5, 130, 136, 147.3, 147.5, 177, 178.6\text{ ppm}$.

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, 298 K, THF- d_8): $\delta = -3.1$ (s, 1 B, $(\text{C}_6\text{F}_5)_3\text{BO}_2\text{CCH}_3$), -26.3 (d, 1 B, $J_{\text{BH}} = 154.2\text{ Hz B-H}$) ppm.

Figure S30. ^1H NMR spectrum of **7** in THF- d_8 .

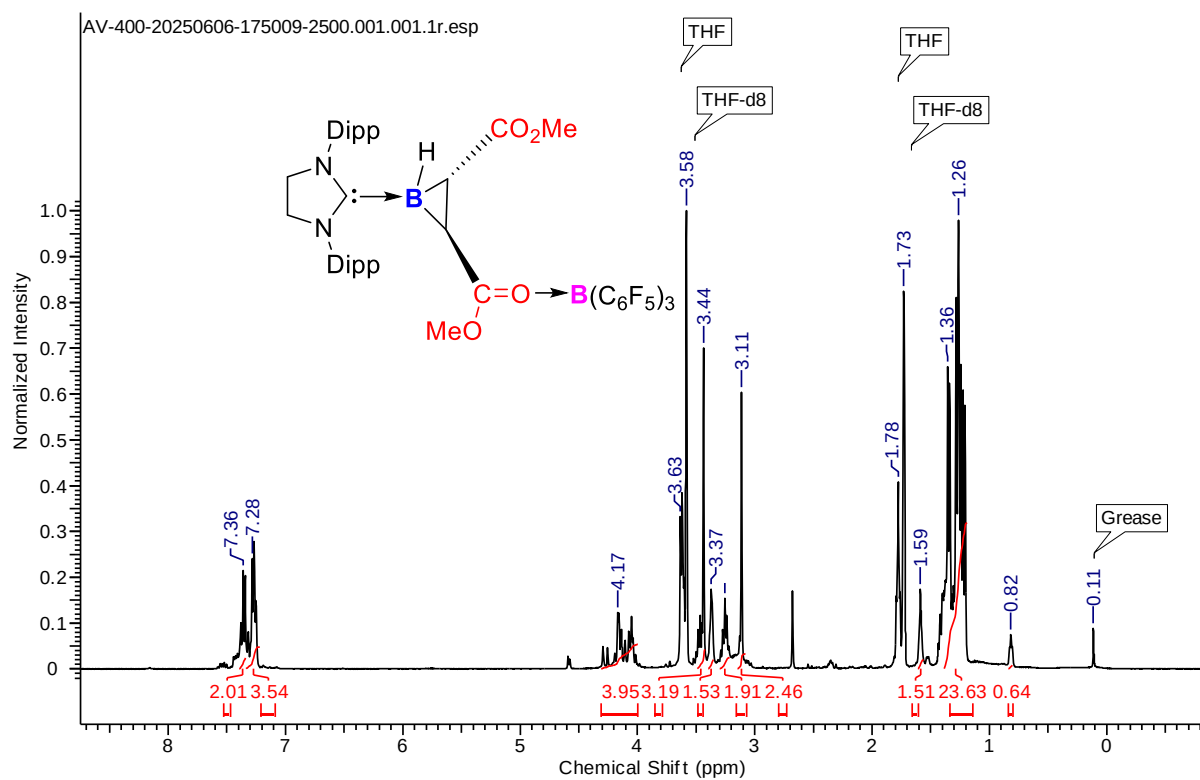


Figure S31. ^{13}C NMR spectrum of **7** in THF- d_8 .

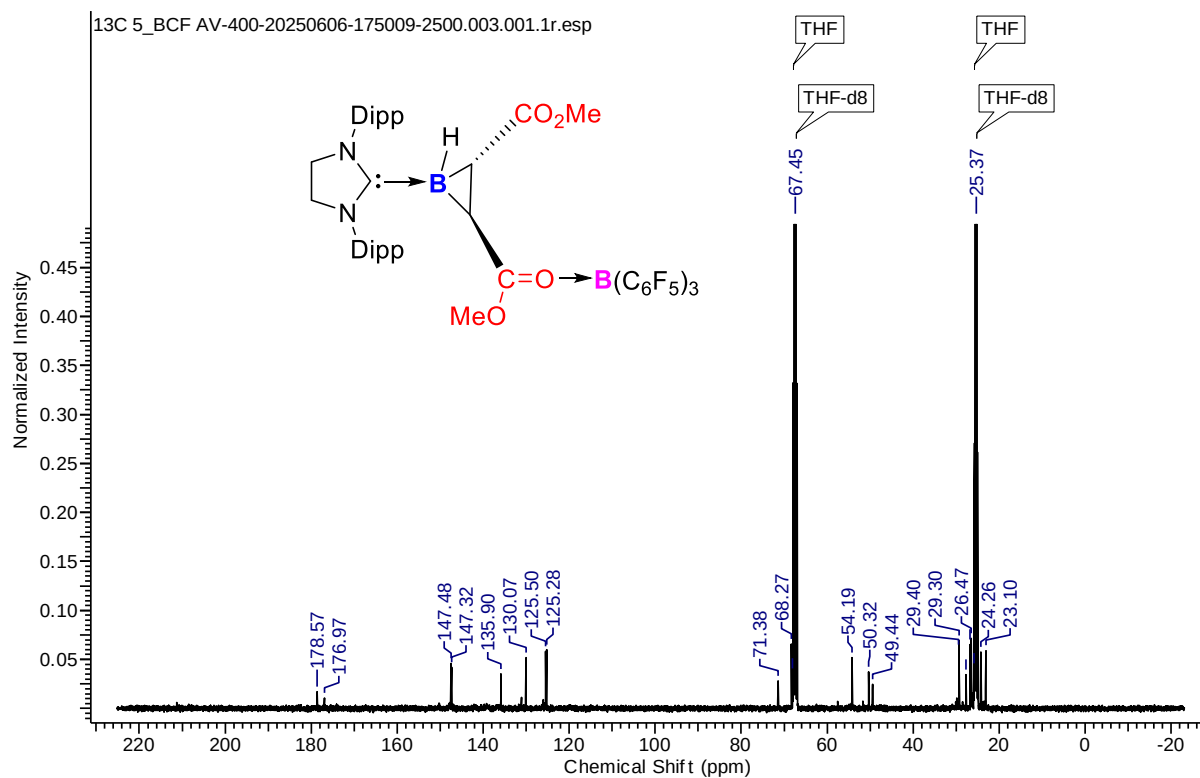
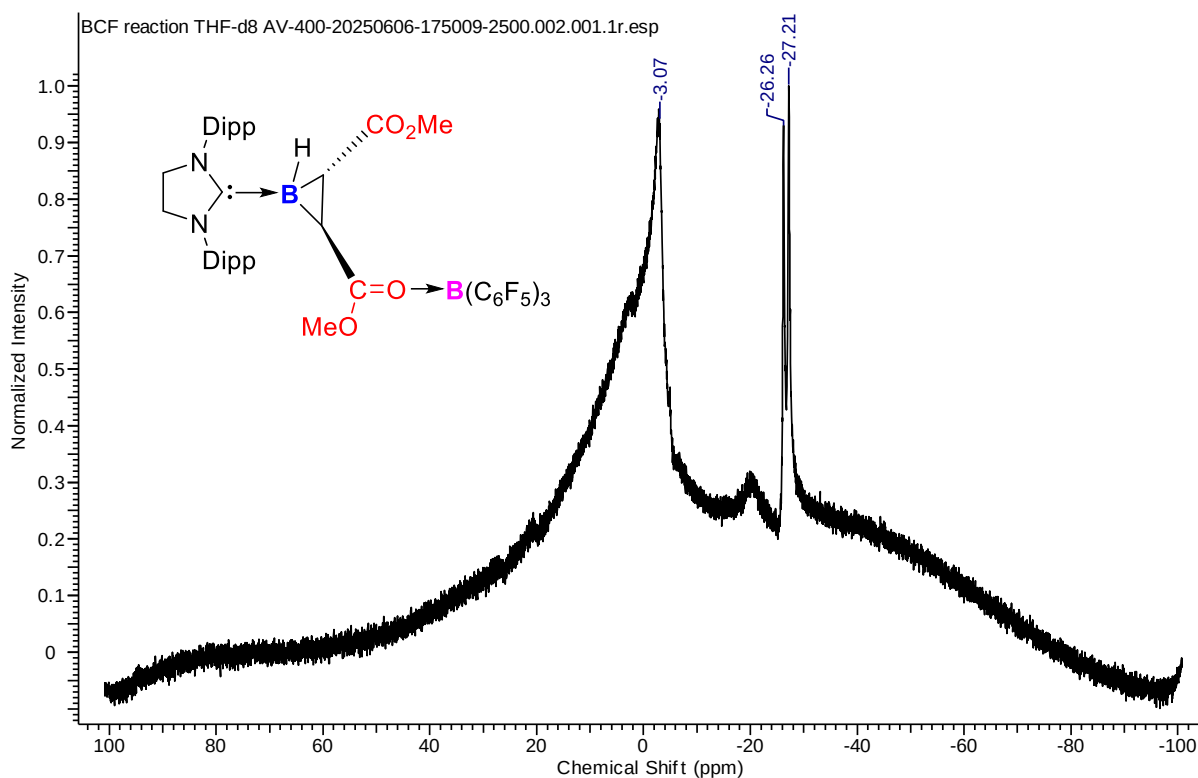


Figure S32. ^{11}B NMR spectrum of **7** in THF- d_8 .



Compound 8. 10 ml of THF was added to a mixture of 6-SiDipp- BH_3 (0.2 g, 0.48 mmol) and TCNE (0.122 g, 0.96 mmol) at 30–35 °C. The reaction was run for another 10 h at room temperature and then the cannula filtration was carried out. Few crystals of **8** suitable for single crystal X-ray analysis was grown in concentrated THF solution at room temperature in 2-3 days. However, the yield was not sufficient enough that allows the complete spectroscopic characterization of **8**. Moreover, the presence of several $\text{C}\equiv\text{N}$ groups resulted in diminished solubility of **8** in majority of the deuterated solvents like CDCl_3 , CD_3CN , THF- d_8 leading to poor NMR data. Hence, we refrain from providing the ^1H NMR.

$^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, 298 K, CDCl_3): δ = -5.8 (br, BH_2NC) ppm, -20.1 (br, BHNHC) ppm.

ESI-MS (CH_3CN): m/z Calcd. for $\text{C}_{68}\text{H}_{85}\text{B}_2\text{N}_{12}$ $[\text{M}+\text{H}]^+$ 1091.7201, found 1091.7197.

IR (cm^{-1}): 610, 767, 802, 1100, 1307, 1448, 1535, 1661 ($\text{C}=\text{C}$), 2183 ($\text{C}\equiv\text{N}$).

UV-Vis in 10 μM THF (nm): 390, 537.

Figure S33. ^{11}B NMR spectrum of **8** in CDCl_3 .

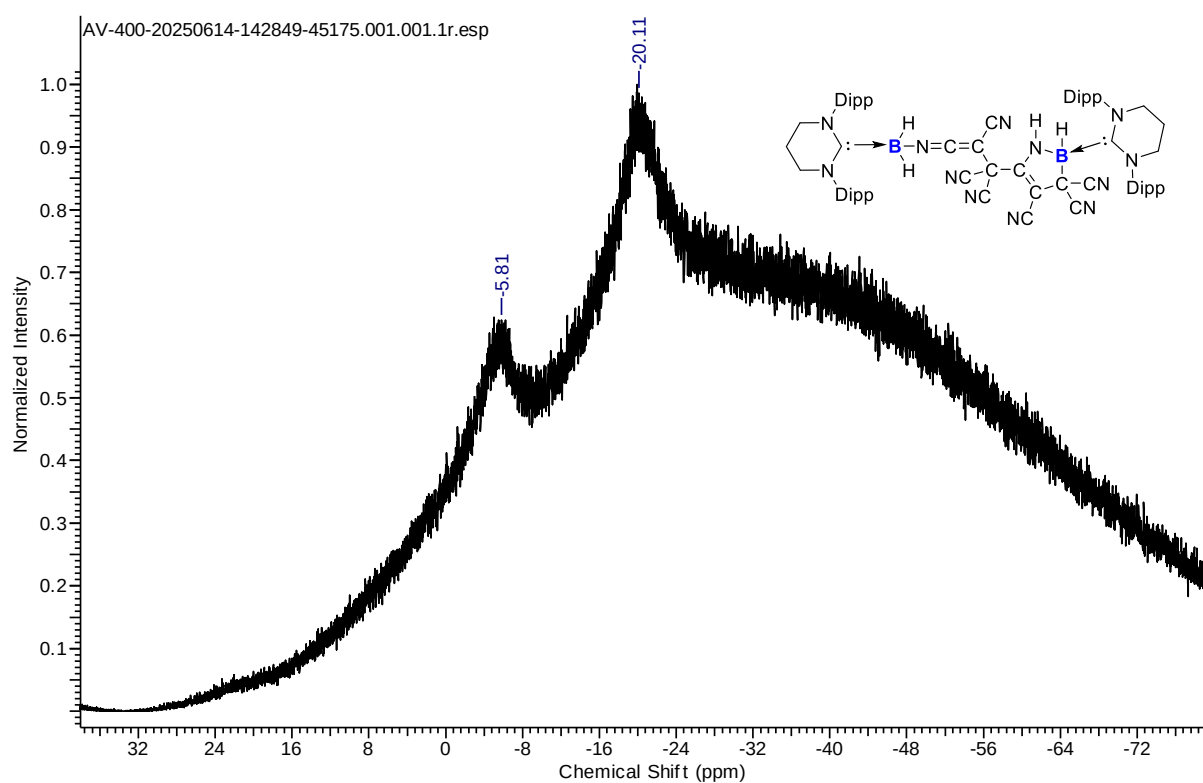


Figure S34. ESI-MS spectrum of **8** in CH_3CN .

APR-2 #544 RT: 2.89 AV: 1 NL: 1.12E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

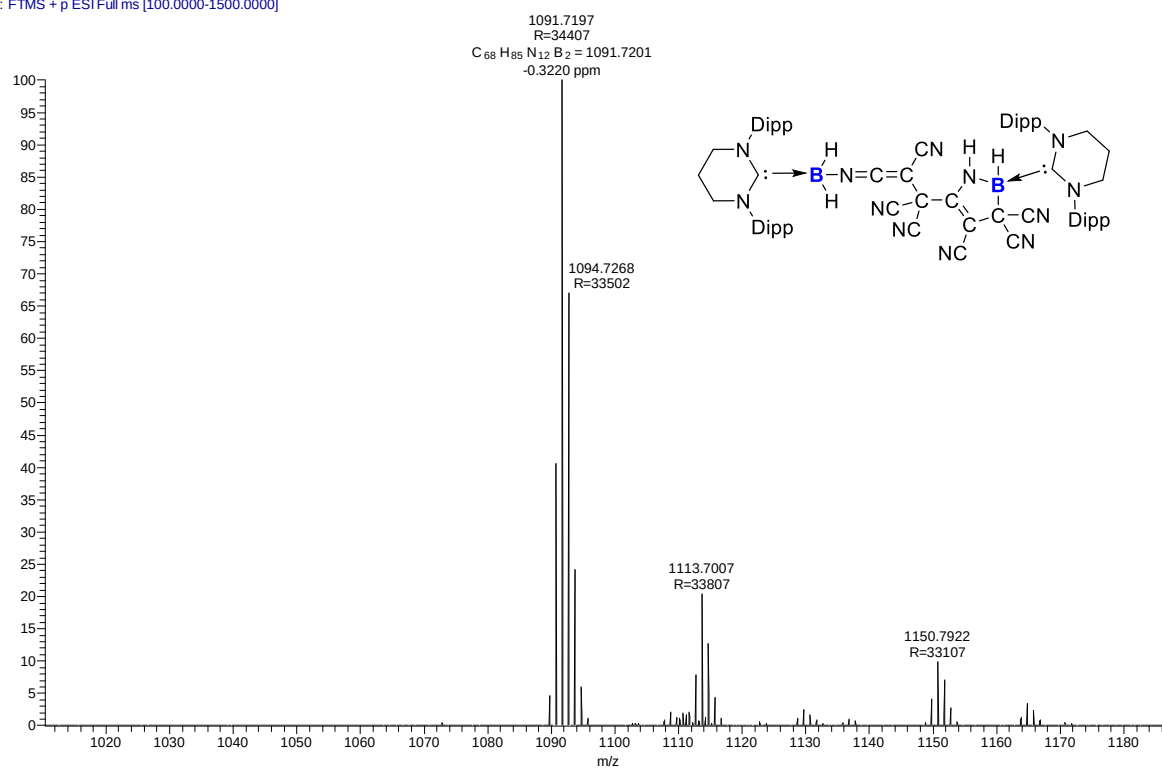


Figure S35. SC-XRD and PXRD pattern of **8**. (Crystal = Simulated pattern for **8** from the cif file).

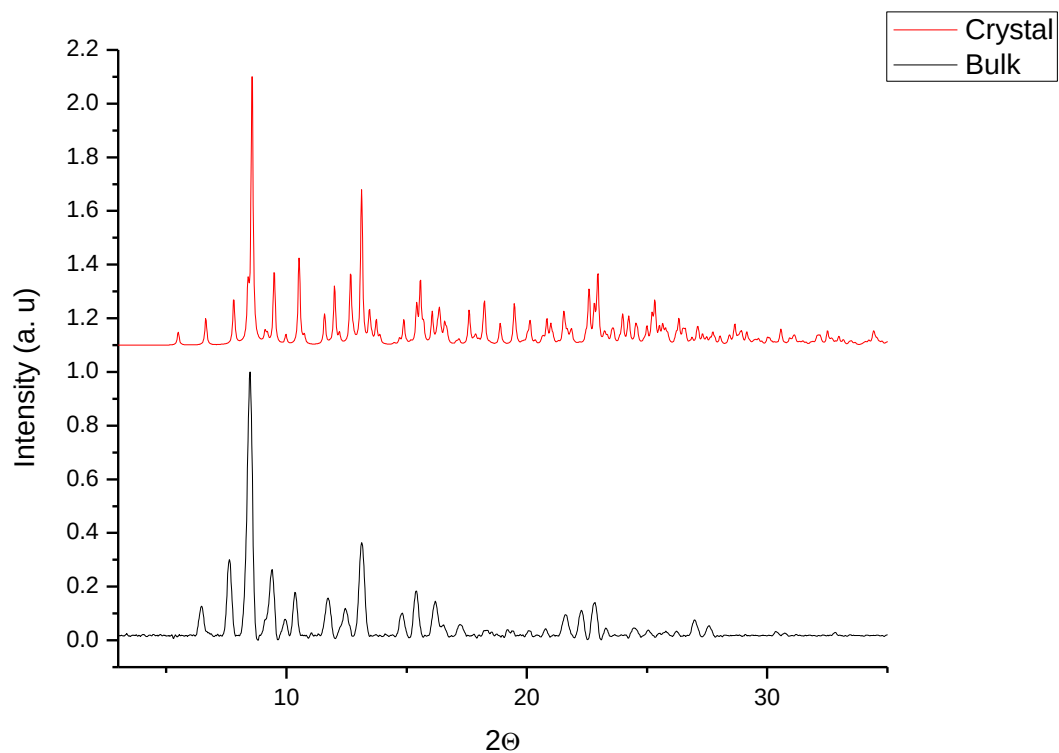


Figure S36. IR Spectrum of compound **8** in comparison with starting material.

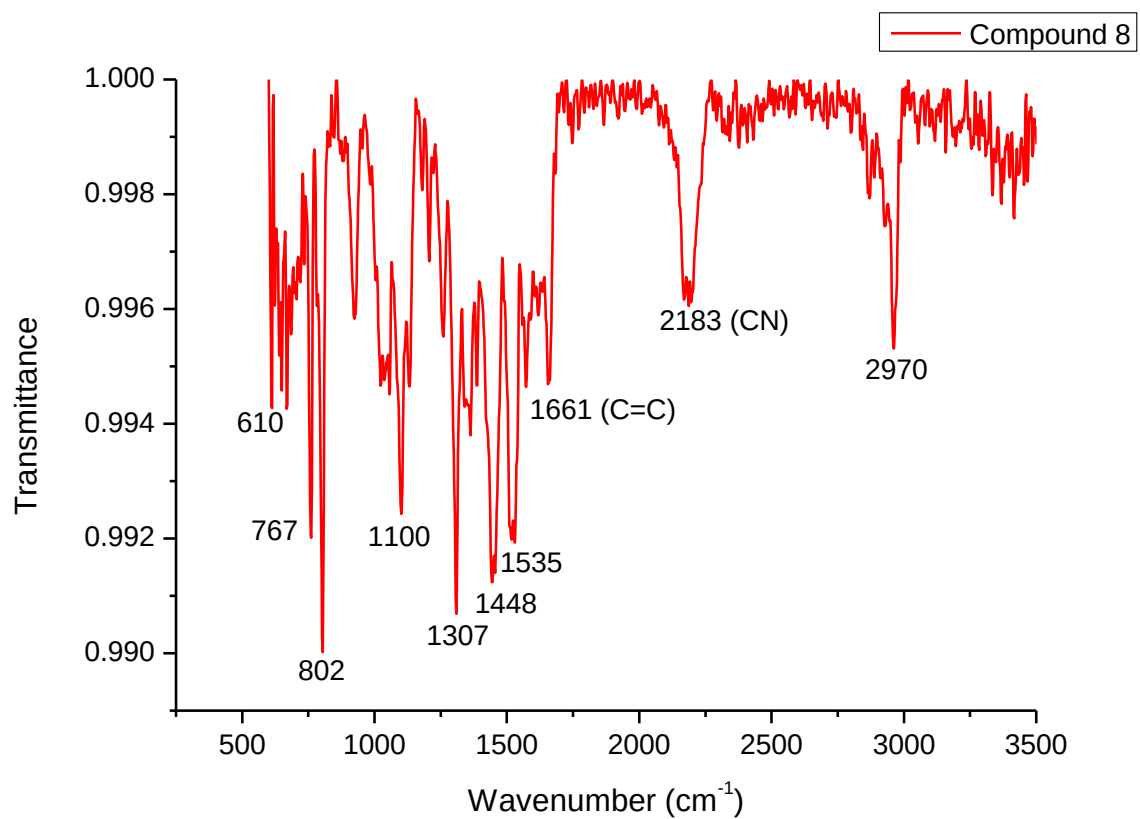
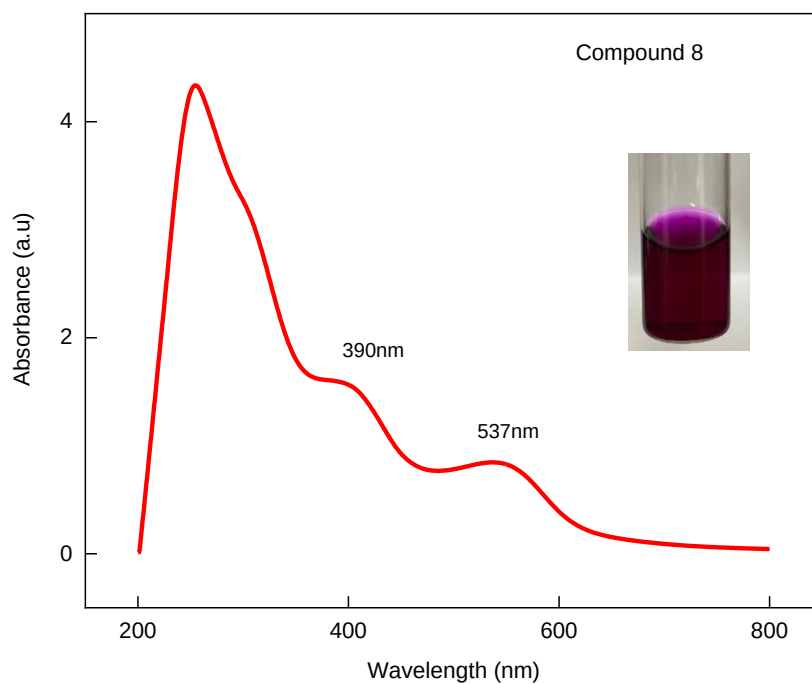
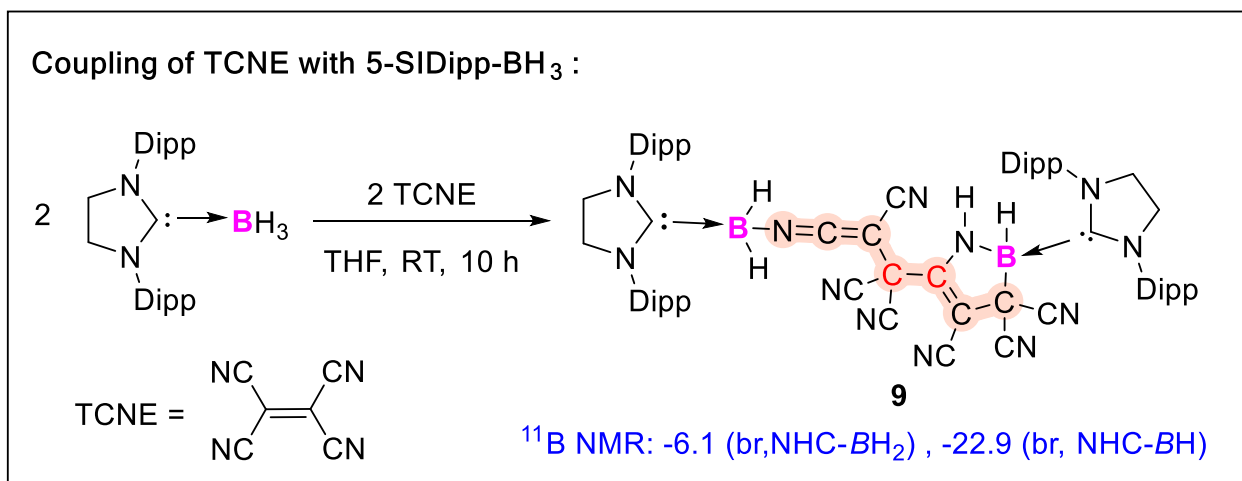


Figure S37. UV-Vis absorption spectrum of compound **8** in THF.



Scheme S1. Reaction of 5-SIDipp·BH₃ with TCNE.



Compound 9. 10 ml of THF was added to a mixture of 5-SiDipp·BH₃ (0.2 g, 0.49 mmol) and TCNE (0.126 g, 0.99 mmol) at room temperature. The reaction was run for another 10 h at room temperature and then the cannula filtration was carried out. Even after repeated trials we could not able to isolate crystals to confirms the exact structure of the compound.

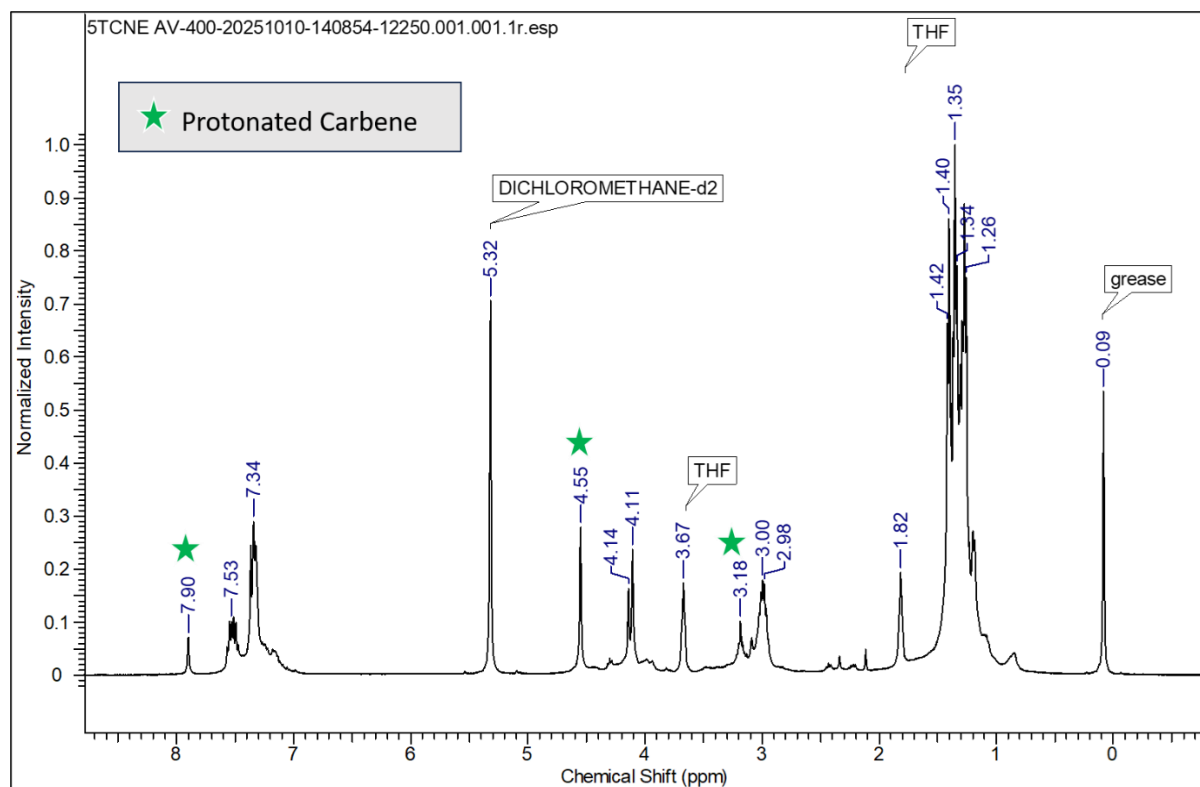
¹¹B{¹H} NMR (128 MHz, 298 K, CDCl₃): δ = -5.8 (br, BH₂NC) ppm, -20.1 (br, BH₂NHC) ppm.

ESI-MS (CH₃CN): *m/z* Calcd. for C₆₈H₈₅B₂N₁₂ [M+1]⁺ 1063.6888, found 1063.6892

IR (cm⁻¹): 762, 802, 1105, 1317, 1453, 1529, 1661 (C=C), 2202 (C≡N), 2970

UV-Vis in 10 μ M THF (nm): 402, 551.

Figure S38. ¹H NMR spectrum of **9** in CD₂Cl₂.



Note: In deuterated solvent compound **9** decomposes to form [NHC-H]⁺.

Figure S39. ^{11}B NMR spectrum of **9** in CDCl_3 .

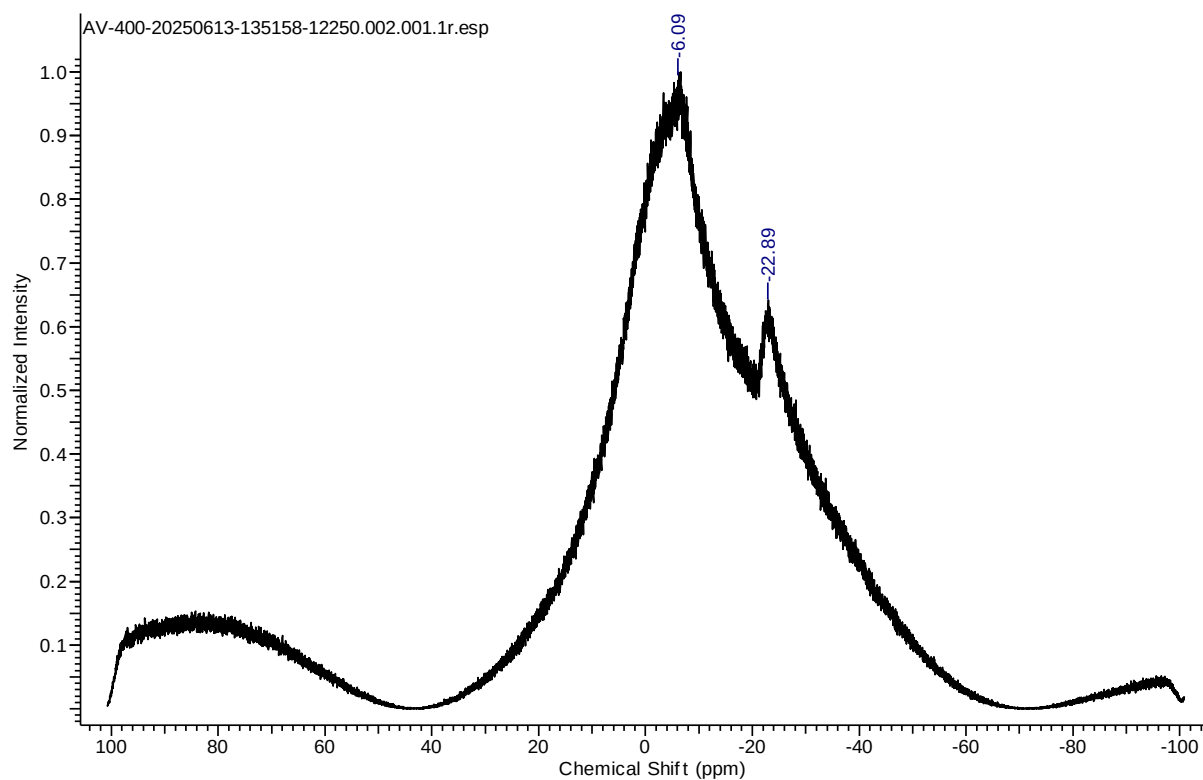


Figure S40. ESI-MS spectrum of **9** in CH_3CN .

APR-5 #708 RT: 3.78 AV: 1 NL: 1.34E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

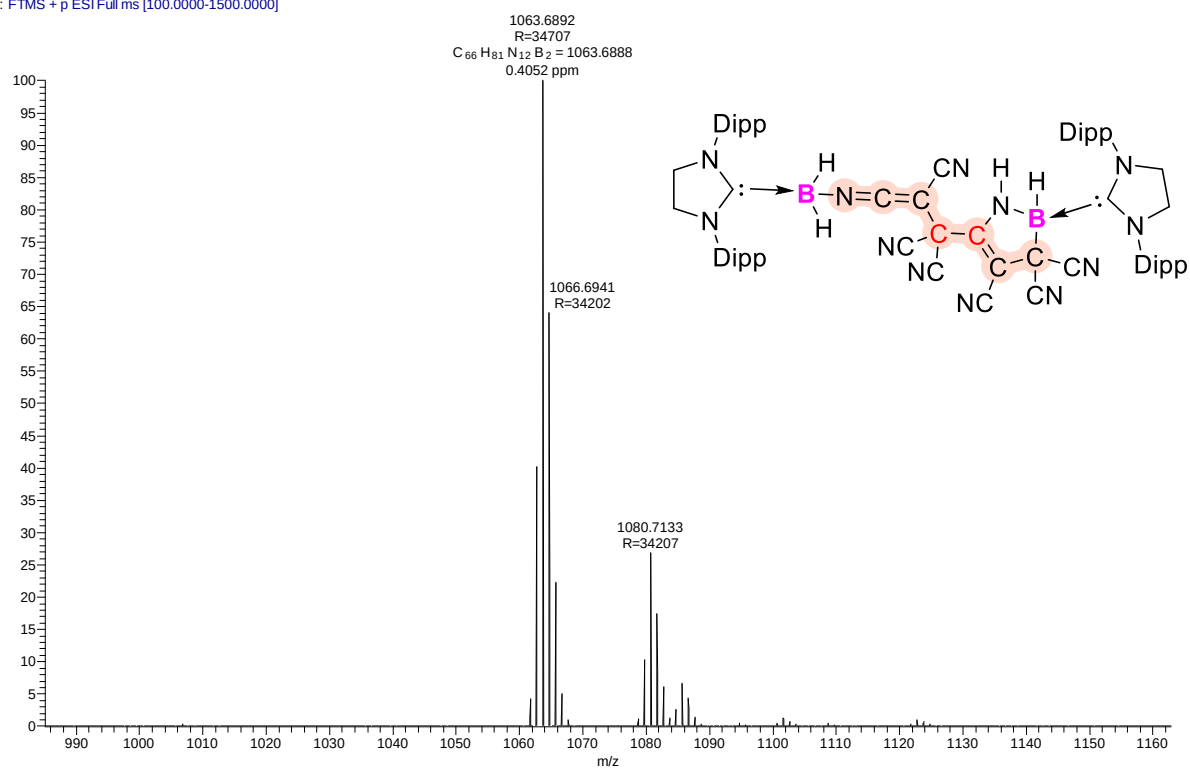


Figure S41. IR spectrum of **9**.

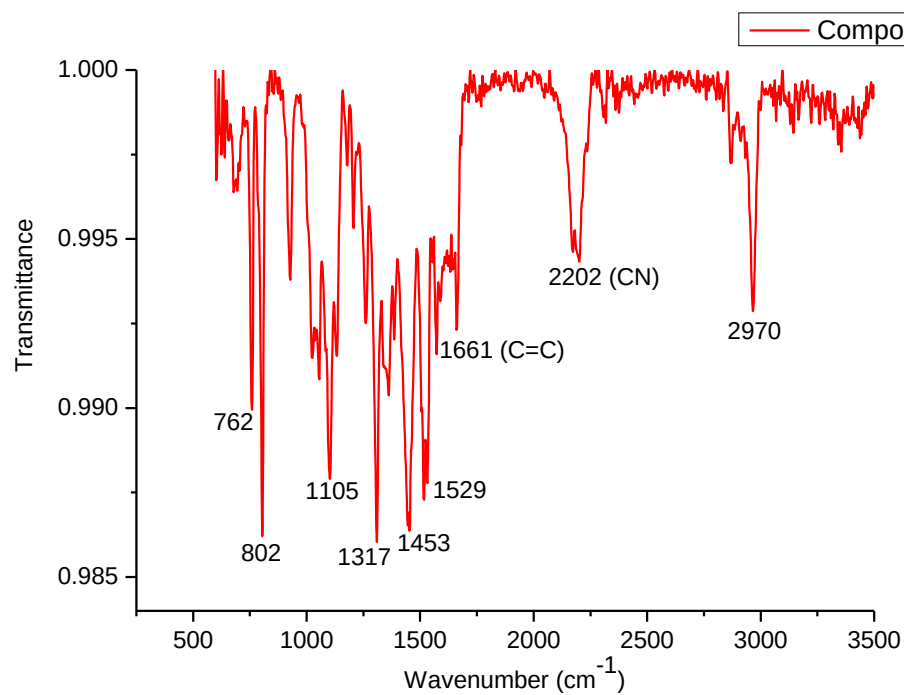
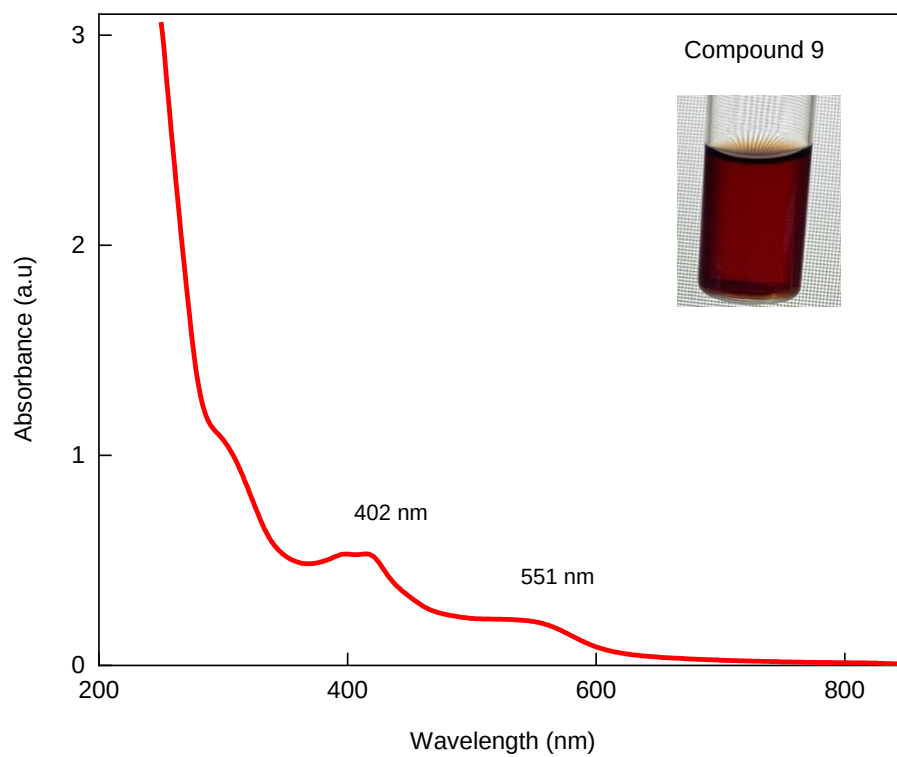


Figure S42. UV-Vis absorption spectrum of compound **9** in THF.



S2. Crystallographic data for the structural analysis of 1- 8

Single crystals of **1-8** were mounted on a Bruker SMART APEX II single crystal X-ray CCD diffractometer having graphite monochromatised (Mo-K α = 0.71073 Å) radiation at low temperature 100 K. The X-ray generator was operated at 50 kV and 30 mA. The X-ray data acquisition was monitored by APEX2 program suit. The data were corrected for Lorentz-polarization and absorption effects using SAINT and SADABS programs which are an integral part of APEX2 package.^{S2} The structures were solved by direct methods and refined by full matrix least squares, based on F^2 , using SHELXL Crystal structures were refined using Olex2-1.0 software. Anisotropic refinement was performed for all non-H atom. The C-H hydrogen atoms were calculated using the riding model.^{S3} The structures were examined using the ADSYM subroutine of PLATON to assure that no additional symmetry could be applied to the models. The molecular weight of each structure mentioned herein has been calculated considering the solvent molecules trapped in the crystal. Crystallographic information is available at www.ccdc.cam.ac.uk/data or as part of Supporting Information.

Identification code	1	2	3	4
Empirical formula	C ₃₆ H ₅₀ N ₂ O ₆ B	C ₃₄ H ₄₉ BN ₂ O ₄	C ₃₃ H ₄₈ N ₂ O ₄ B Cl	C ₃₂ H ₄₅ BN ₂ O ₄
Formula weight	617.59	560.56	582.99	532.51
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	orthorhombic	monoclinic	monoclinic
Space group	<i>P2₁/c</i>	<i>Pbca</i>	<i>P2₁/c</i>	<i>P2₁/c</i>
a/Å	10.3991(7)	18.2979(8)	20.6370(18)	9.2071(6)
b/Å	19.8483(16)	17.8752(8)	10.0008(9)	10.1666(6)
c/Å	17.3803(14)	19.8239(8)	16.7544(13)	32.2381(17)
α/°	90	90	90	90
β/°	102.656(3)	90	109.428(3)	91.399(2)
γ/°	90	90	90	90
Volume/Å³	3500.2(5)	6484.0(5)	3261.0(5)	3016.7(3)
Z	4	8	4	4
$\rho_{\text{calc}}/\text{cm}^3$	1.172	1.148	1.187	1.172
μ/mm^{-1}	0.078	0.074	0.155	0.076
F(000)	1332.0	2432.0	1256.0	1152.0
Crystal size/mm³	0.12 × 0.11 × 0.1	0.2 × 0.13 × 0.05	0.2 × 0.13 × 0.1	0.2 × 0.12 × 0.1

Radiation	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)
2θ range for data collection/°	4.676 to 62.606	5 to 52	5.842 to 56	4.738 to 55.052
Index ranges	-12 $\leq$ h $\leq$ 15, -28 $\leq$ k $\leq$ 28, -25 $\leq$ l $\leq$ 25	-22 $\leq$ h $\leq$ 22, -22 $\leq$ k $\leq$ 22, -24 $\leq$ l $\leq$ 24	-27 $\leq$ h $\leq$ 27, - 13 $\leq$ k $\leq$ 13, - 22 $\leq$ l $\leq$ 22	-11 $\leq$ h $\leq$ 11, - 13 $\leq$ k $\leq$ 13, - 41 $\leq$ l $\leq$ 41
Reflections collected	131473	331220	83384	149855
Independent reflections	11392 [R_{int} = 0.0748, R_{sigma} = 0.0342]	6362 [R_{int} = 0.11891, R_{sigma} = 0.0295]	7831 [R_{int} = 0.06295, R_{sigma} = 0.0234]	6931 [R_{int} = 0.1152, R_{sigma} = 0.0368]
Data/restraints/parameters	11392/0/417	6362/0/393	7831/0/380	6931/0/365
Goodness-of-fit on F^2	1.120	1.091	1.135	1.066
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0552, wR_2 = 0.1467	R_1 = 0.0425, wR_2 = 0.1040	R_1 = 0.0461, wR_2 = 0.1267	R_1 = 0.0482, wR_2 = 0.1083
Final R indexes [all data]	R_1 = 0.0662, wR_2 = 0.1540	R_1 = 0.0584, wR_2 = 0.1207	R_1 = 0.0496, wR_2 = 0.1298	R_1 = 0.0733, wR_2 = 0.1233
Largest diff. peak/hole / e $\text{\AA}^{-3}$	0.49/-0.27	0.50/-0.48	1.00/-0.37	0.33/-0.31
CCDC No	2493687	2493697	2493688	2493691

Identification code	5	6	7	8
Empirical formula	C ₃₃ H ₄₇ BN ₂ O ₄	C _{45.5} H ₆₃ AlBCl ₄ N ₃ O ₄	C _{57.05} H ₅₉ B ₂ F ₁₅ N ₂ O _{5.55}	C ₇₆ H ₁₀₀ N ₁₂ O ₂ B ₂
Formula weight	546.53	895.58	1168.08	1235.29
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	<i>Cc</i>	<i>P2₁/n</i>	<i>P2₁/c</i>	<i>P2₁/n</i>
a/$\text{\AA}$	16.7284(18)	14.5696(10)	13.2296(6)	11.4137(6)
b/$\text{\AA}$	9.7573(10)	21.6410(14)	21.9553(10)	22.3005(13)
c/$\text{\AA}$	18.4994(16)	15.5770(11)	19.6771(9)	28.7746(17)
α/°	90	90	90	90
β/°	92.683(3)	98.076(2)	103.710(2)	95.381(2)
γ/°	90	90	90	90
Volume/$\text{\AA}^3$	3016.2(5)	4862.7(6)	5552.6(4)	7291.8(7)
Z	4	4	4	4
ρ_{calc}/cm³	1.204	1.223	1.397	1.125
μ/mm⁻¹	0.078	0.304	0.122	0.069
F(000)	1184.0	1900.0	2419.0	2664.0
Crystal size/mm³	0.2 $\times$ 0.12 $\times$ 0.1	0.12 $\times$ 0.08 $\times$ 0.03	0.22 $\times$ 0.13 $\times$ 0.08	0.23 $\times$ 0.15 $\times$ 0.1

Radiation	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)
2θ range for data collection/$^\circ$	5.266 to 62.07	4.048 to 56.622	4.648 to 50.998	4.63 to 51
Index ranges	-24 $\leq$ h $\leq$ 24, -14 $\leq$ k $\leq$ 14, -26 $\leq$ l $\leq$ 26	-18 $\leq$ h $\leq$ 19, - 28 $\leq$ k $\leq$ 28, - 20 $\leq$ l $\leq$ 20	-16 $\leq$ h $\leq$ 16, - 26 $\leq$ k $\leq$ 26, - 23 $\leq$ l $\leq$ 23	-13 $\leq$ h $\leq$ 13, -27 $\leq$ k $\leq$ 27, -34 $\leq$ l $\leq$ 34
Reflections collected	122470	93554	25883 2	219277
Independent reflections	9605 [R_{int} = 0.0697, R_{sigma} = 0.0326]	12077 [R_{int} = 0.1472, R_{sigma} = 0.0916]	10304 [R_{int} = 0.0803, R_{sigma} = 0.0251]	13537 [R_{int} = 0.1825, R_{sigma} = 0.0672]
Data/restraints/parameters	9605/2/374	12077/321/70 8	10304/96/746	13537/13/85 8
Goodness-of-fit on F^2	1.041	1.116	1.158	1.101
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0434, wR_2 = 0.1119	R_1 = 0.1101, wR_2 = 0.2199	R_1 = 0.0706, wR_2 = 0.1773	R_1 = 0.0650, wR_2 = 0.1561
Final R indexes [all data]	R_1 = 0.0492, wR_2 = 0.1161	R_1 = 0.1781, wR_2 = 0.2504	R_1 = 0.0754, wR_2 = 0.1806	R_1 = 0.1250, wR_2 = 0.2060
Largest diff. peak/hole / e $\text{\AA}^{-3}$	0.54/-0.26	0.45/-0.42	0.88/-0.84	0.69/-0.50
CCDC No	2493693	2493694	2493695	2493696

S3. (a) Theoretical details

Geometry optimizations for all reactants, intermediates, and transition states were carried out using density functional theory (DFT) with the B3LYP^{S4-S6} functional in conjunction with the def2-SVP basis set.^{S7} Harmonic vibrational frequency analyses at the same level were performed to confirm the nature of the stationary points: minima were characterized by the absence of imaginary frequencies, whereas transition states exhibited a single imaginary frequency corresponding to the reaction coordinate. Transition state geometries were located using the Nudged Elastic Band (NEB)^{S8} method, and their connectivity to adjacent intermediates was verified through intrinsic reaction coordinate (IRC)^{S9} calculations. The resolution-of-identity (RI)^{S10-S12} approximation was employed to accelerate the evaluation of two-electron integrals. Dispersion interactions were included using Grimme's D3 correction with Becke–Johnson damping (D3BJ),^{S13-S15} and this computational setup is hereafter referred to

as RI-B3LYP-D3BJ/def2-SVP. Solvent effects (toluene) were incorporated through single-point energy calculations using the conductor-like polarizable continuum model (CPCM),^{S16} designated as RI-B3LYP-D3BJ-CPCM/def2-SVP. To refine the computed energetics, single-point energy corrections were carried out using the larger def2-TZVP basis set (RI-B3LYP-D3BJ-CPCM/def2-TZVP//RI-B3LYP-D3BJ/def2-SVP). The reported Gibbs free energies (ΔG) include zero-point energy and thermal corrections. All DFT calculations were carried out using the ORCA quantum chemistry package, version 4.2.1.^{S17}

Electronic structure analyses were performed using Natural Bond Orbital (NBO) analysis with the NBO 6.0 program.^{S18-S20} Additionally, Quantum Theory of Atoms in Molecules (QTAIM) analyses were carried out using AIMAll (version 19.10.12),^{S21} based on wavefunction files generated from ORCA. Energy Decomposition analysis^{S22-S24} was conducted on key transition states to partition the interaction energies into steric, electrostatic, orbital, and dispersion components using the B3LYP exchange-correlation functional. In this step, the molecular orbitals (MOs) were expanded in terms of Slater-type orbitals (STOs), with all electrons included in the calculation. A triple- ζ basis set with two sets of polarization functions (TZ2P) was employed for all atoms, and D3BJ dispersion corrections were incorporated. This computational setup is hereafter referred to as RI-B3LYP-D3BJ/TZ2P. All EDA calculations were carried out using the Amsterdam Density Functional (ADF) package.^{S25}

(b) Preliminary Mechanistic Studies

To rationalize the divergent product formation, we undertook a detailed mechanistic investigation supported by density functional theory (DFT) calculations. All reported Gibbs free energy values have been corrected for solvent effects using appropriate methodologies (see Figure S55 and Tables S1-S10). The sequence begins with protonation of the carboxylate oxygen by HCl, followed by nucleophilic attack of chloride at boron through TS1 to give the transient enol intermediate (**Int-1**). Tautomerization via TS2 converts **Int-1** to the keto intermediate (**Int-2**). A subsequent σ C–C bond rotation generates two rotameric species (**Int-3** and **Int-4**) through TS3 and TS4, positioning the acetyl oxygen for intramolecular nucleophilic attack on boron. This step, proceeding via TS5, promotes lactonization with chloride departure to yield

Int-5. Finally, chloride induces nucleophilic dealkylation of the acetyl methyl group through TS6, leading to the borolactone product (**5**) (cf. Figure S55 for full mechanism).

Preliminary calculations indicated that the nucleophilic attack of HCl on boron in both pathways proceeds via a high-energy transition state (TS1; ca. 30.7 kcal/mol; see Figure S55). This high-energy barrier prompted us to explore alternate pathways in which the participation of additional HCl molecules, through hydrogen-bonding interactions, lowers the barriers for the proton-transfer and chloride attack steps (cf. Figure 7 of manuscript). For both pathways, the first transition state (TS1) corresponds to a concerted event involving protonation of the carboxylate oxygen by HCl, concomitant with nucleophilic chloride attack at the boron center, followed by tautomerization to yield the keto intermediate (**Int-2**).

Table S1: Relative energies (kcal/mol) of Pathway A (5-borirane) at the RI-B3LYP-D3BJ/def2-SVP-CPCM level of theory.

Species	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP}	ΔG_{B3LYP}
			+	+	+	+
			$E_{sol(Toluene)}$	$E_{sol(Toluene)}$	$E_{sol(Acetonitrile)}$	$E_{sol(Acetonitrile)}$
React	0.0	0.0	0.0	0.0	0.0	0.0
RC	-11.3	0.1	-10.5	0.8	-8.6	2.7
TS1	20.0	32.3	18.4	30.7	18.4	30.7
Int-1	-23.3	-8.5	-22.7	-7.9	-21.3	-6.5
TS2	13.1	25.5	11.2	23.6	10.8	23.2
Int-2	-41.1	-27.7	-43.2	-29.7	-44.0	-30.5
TS3	-35.1	-20.8	-37.1	-22.8	-37.9	-23.6
Int-3	-36.0	-22.2	-37.9	-24.0	-38.4	-24.6
TS4	-32.9	-18.4	-34.1	-19.6	-34.0	-19.5
Int-4	-37.4	-22.7	-38.0	-23.4	-37.7	-23.0
TS5	-17.6	-3.8	-20.3	-6.5	-21.5	-7.7
Int-5	-34.1	-18.6	-36.2	-20.6	-36.4	-20.9
TS6	-13.2	1.5	-14.6	0.0	-14.4	0.3
Prdt	-29.4	-29.9	-31.1	-31.6	-32.8	-33.3

Table S2: Relative energies (kcal/mol) of Pathway A (5-borirane) at the RI-B3LYP-D3BJ/def2-SVP//RI-B3LYP-D3BJ/def2-TZVP-CPCM level of theory.

Species	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP}	ΔG_{B3LYP}
			+	+	+	+
			$E_{sol(Toluene)}$	$E_{sol(Toluene)}$	$E_{sol(Acetonitrile)}$	$E_{sol(Acetonitrile)}$
React	0.0	0.0	0.0	0.0	0.0	0.0
RC	-5.9	5.4	-8.6	2.7	-5.3	6.1
TS1	24.5	36.8	18.4	30.7	22.8	35.1
Int-1	-16.4	-1.6	-21.3	-6.5	-15.9	-1.1

TS2	16.8	29.2	10.8	23.2	14.6	27.0
Int-2	-36.6	-23.2	-44.0	-30.5	-39.0	-25.6
TS3	-31.3	-17.0	-37.9	-23.6	-33.7	-19.4
Int-3	-31.1	-17.2	-38.4	-24.6	-33.3	-19.5
TS4	-27.6	-13.0	-34.0	-19.5	-29.0	-14.4
Int-4	-31.6	-16.9	-37.7	-23.0	-32.3	-17.7
TS5	-12.8	1.0	-21.5	-7.7	-16.3	-2.5
Int-5	-29.4	-13.8	-36.4	-20.9	-32.4	-16.8
TS6	-10.8	3.9	-14.4	0.3	-13.0	1.6
Prdt	-31.2	-31.8	-32.8	-33.3	-33.4	-34.0

Table S3: Relative energies (kcal/mol) of Pathway A (5-borirane) - new_mechansim at the RI-B3LYP-D3BJ/def2-SVP-CPCM level of theory.

Species	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP}	ΔG_{B3LYP}
			+	+	+	+
			$E_{sol}(Toluene)$	$E_{sol}(Toluene)$	$E_{sol}(Acetonitrile)$	$E_{sol}(Acetonitrile)$
React	0.0	0.0	0.0	0.0	0.0	0.0
RC	-39.8	-5.8	-40.6	-6.6	-37.3	-3.3
TS1	-7.9	26.5	-9.0	25.4	-5.8	28.6
Int-2	-41.1	-27.7	-43.2	-29.7	-44.0	-30.5
TS3	-35.1	-20.8	-37.1	-22.8	-37.9	-23.6
Int-3	-36.0	-22.2	-37.9	-24.0	-38.4	-24.6
TS4	-32.9	-18.4	-34.1	-19.6	-34.0	-19.5
Int-4	-37.4	-22.7	-38.0	-23.4	-37.7	-23.0
TS5	-17.6	-3.8	-20.3	-6.5	-21.5	-7.7
Int-5	-34.1	-18.6	-36.2	-20.6	-36.4	-20.9
TS6	-13.2	1.5	-14.6	0.0	-14.4	0.3
Prdt	-29.4	-29.9	-31.1	-31.6	-32.8	-33.3

Table S4: Relative energies (kcal/mol) of Pathway A (5-borirane) - new_mechansim at the RI-B3LYP-D3BJ/def2-SVP//RI-B3LYP-D3BJ/def2-TZVP-CPCM level of theory.

Species	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP}	ΔG_{B3LYP}
			+	+	+	+
			$E_{sol}(Toluene)$	$E_{sol}(Toluene)$	$E_{sol}(Acetonitrile)$	$E_{sol}(Acetonitrile)$
React	0.0	0.0	0.0	0.0	0.0	0.0
RC	-26.6	7.4	-27.9	6.1	-25.0	9.0
TS1	5.7	40.1	4.4	38.8	7.2	41.6
Int-2	-36.6	-23.2	-44.0	-30.5	-39.0	-25.6
TS3	-31.3	-17.0	-37.9	-23.6	-33.7	-19.4

Table S5: Relative energies (kcal/mol) of Pathway A (5-borirane) at the RI-DLPNO-CCSD(T)/cc-pVDZ-CPCM level of theory.

Species	$\Delta E_{\text{[DLPNO-CCSD(T)]}}$	$\Delta E_{\text{[DLPNO-CCSD(T)]}}$ + $\Delta G_{\text{corr (DFT)}}$	$\Delta E_{\text{[DLPNO-CCSD(T)]}}$ + $\Delta E_{\text{sol (Toluene, DFT)}}$	$\Delta E_{\text{[DLPNO-CCSD(T)]}}$ + $\Delta G_{\text{corr (DFT)}}$ + $\Delta E_{\text{sol (Toluene, DFT)}}$	$\Delta E_{\text{[DLPNO-CCSD(T)]}}$ + $\Delta G_{\text{corr (DFT)}}$ + $\Delta E_{\text{sol (Acetonitrile, DFT)}}$	$\Delta E_{\text{[DLPNO-CCSD(T)]}}$ + $\Delta G_{\text{corr (DFT)}}$ + $\Delta E_{\text{sol (Acetonitrile, DFT)}}$
React	0.0	0.0	0.0	0.0	0.0	0.0
TS1	34.5	46.8	33.0	45.3	32.9	45.2
Int-1	-16.1	-1.3	-15.5	-0.7	-14.1	0.8
TS2	21.8	34.2	19.9	32.3	19.5	31.9
Int-2	-38.5	-25.0	-40.5	-27.1	-41.3	-27.8
TS3	-32.8	-18.4	-34.8	-20.5	-35.6	-21.3
Int-3	-33.1	-19.2	-34.9	-21.1	-35.5	-21.6
TS4	-29.0	-14.4	-30.2	-15.7	-30.1	-15.5
Int-4	-34.8	-20.2	-35.5	-20.8	-35.1	-20.5
TS5	-10.0	3.8	-12.7	1.1	-13.9	-0.1
Int-5	-24.9	-9.3	-26.9	-11.4	-27.2	-11.6
TS6	-2.9	11.8	-4.3	10.3	-4.1	10.6
Prdt	-31.0	-31.6	-32.7	-33.2	-34.4	-35.0
Int-3	-31.1	-17.2	-38.4	-24.6	-33.3	-19.5
TS4	-27.6	-13.0	-34.0	-19.5	-29.0	-14.4
Int-4	-31.6	-16.9	-37.7	-23.0	-32.3	-17.7
TS5	-12.8	1.0	-21.5	-7.7	-16.3	-2.5
Int-5	-29.4	-13.8	-36.4	-20.9	-32.4	-16.8
TS6	-10.8	3.9	-14.4	0.3	-13.0	1.6
Prdt	-31.2	-31.8	-32.8	-33.3	-33.4	-34.0

Table S6: Relative energies (kcal/mol) of Pathway B (6-borirane) at the RI-B3LYP-D3BJ/def2-SVP-CPCM level of theory.

Species	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP} + $E_{\text{sol(Toluene)}}$	ΔG_{B3LYP} + $E_{\text{sol(Toluene)}}$
React	0.0	0.0	0.0	0.0
RC	-24.5	-12.1	-23.0	-10.6
TS1	9.2	21.9	8.5	21.2
Int-1	-32.2	-16.3	-30.8	-14.9
TS2	4.1	17.4	3.1	16.5
Int-2	-50.5	-36.0	-51.8	-37.2

TS3	-44.6	-28.9	-45.8	-30.1
Int-3	-45.9	-30.6	-46.5	-31.2
TS4	-41.9	-25.6	-42.2	-25.8
Int-4	-46.1	-30.8	-46.6	-31.2
TS5	-28.3	-13.2	-29.5	-14.4
Int-5	-45.7	-29.1	-46.7	-30.1
TS6	-22.7	-7.2	-23.2	-7.6
Prdt	-39.3	-39.1	-40.3	-40.1

Table S7: Relative energies (kcal/mol) of Pathway B (6-borirane) at the RI-B3LYP-D3BJ/def2-SVP//RI-B3LYP-D3BJ/def2-TZVP-CPCM level of theory.

Species	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP} + $E_{sol}(\text{Toluene})$	ΔG_{B3LYP} + $E_{sol}(\text{Toluene})$
React	0.0	0.0	0.0	0.0
RC	-17.6	-5.2	-16.1	-3.7
TS1	14.3	27.1	13.5	26.2
Int-1	-24.4	-8.5	-23.0	-7.1
TS2	8.8	22.1	7.6	20.9
Int-2	-45.1	-30.5	-46.5	-31.9
TS3	-39.5	-23.8	-40.9	-25.2
Int-3	-40.0	-24.6	-40.9	-25.6
TS4	-35.9	-19.5	-36.3	-20.0
Int-4	-39.8	-24.5	-40.3	-25.0
TS5	-22.4	-7.4	-24.2	-9.1
Int-5	-39.9	-23.3	-41.8	-25.2
TS6	-19.7	-4.1	-20.8	-5.3
Prdt	-40.1	-39.9	-41.5	-41.3

Table S8: Relative energies (kcal/mol) of Pathway B (6-borirane) - new_mechanism at the RI-B3LYP-D3BJ/def2-SVP-CPCM level of theory.

Species	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP} + $E_{sol}(\text{Toluene})$	ΔG_{B3LYP} + $E_{sol}(\text{Toluene})$
React	0.0	0.0	0.0	0.0
RC	-41.4	-6.0	-41.7	-6.3
TS1	-16.8	17.8	-17.1	17.5
Int-2	-50.5	-36.0	-51.8	-37.2

TS3	-44.6	-28.9	-45.8	-30.1
Int-3	-45.9	-30.6	-46.5	-31.2
TS4	-41.9	-25.6	-42.2	-25.8
Int-4	-46.1	-30.8	-46.6	-31.2
TS5	-28.3	-13.2	-29.5	-14.4
Int-5	-45.7	-29.1	-46.7	-30.1
TS6	-22.7	-7.2	-23.2	-7.6
Prdt	-39.3	-39.1	-40.3	-40.1

Table S9: Relative energies (kcal/mol) of Pathway B (6-borirane) - new_mechansim at the RI-B3LYP-D3BJ/def2-SVP//RI-B3LYP-D3BJ/def2-TZVP-CPCM level of theory.

Species	ΔE_{B3LYP}	ΔG_{B3LYP}	ΔE_{B3LYP} + $E_{sol}(\text{Toluene})$	ΔG_{B3LYP} + $E_{sol}(\text{Toluene})$
React	0.0	0.0	0.0	0.0
RC	-27.6	7.8	-28.1	7.4
TS1	-2.5	32.1	-3.1	31.5
Int-2	-45.1	-30.5	-46.5	-31.9
TS3	-39.5	-23.8	-40.9	-25.2
Int-3	-40.0	-24.6	-40.9	-25.6
TS4	-35.9	-19.5	-36.3	-20.2
Int-4	-39.8	-24.5	-40.3	-25.0
TS5	-22.4	-7.4	-24.2	-9.1
Int-5	-39.9	-23.3	-41.8	-25.5
TS6	-19.7	-4.1	-20.8	-5.3
Prdt	-40.1	-39.9	-41.5	-41.3

Table S10: Relative energies (kcal/mol) of Pathway B (6-borirane) at the RI-DLPNO-CCSD(T)/cc-pVDZ-CPCM level of theory.

Species	$\Delta E_{[DLPNO-CCSD(T)]}$	$\Delta E_{[DLPNO-CCSD(T)]}$ + $\Delta G_{corr}(\text{DFT})$	$\Delta E_{[DLPNO-CCSD(T)]}$ + $\Delta E_{sol}(\text{Toluene, DFT})$	$\Delta E_{[DLPNO-CCSD(T)]}$ + $\Delta G_{corr}(\text{DFT})$ + $\Delta E_{sol}(\text{Toluene, DFT})$
React	0.0	0.0	0.0	0.0
TS1	25.0	37.7	24.3	37.0
Int-1	-24.0	-8.1	-22.6	-6.7

TS2	14.6	28.0	13.6	27.0
Int-2	-46.5	-31.9	-47.8	-33.2
TS3	-40.6	-24.9	-41.9	-26.1
Int-3	-41.7	-26.4	-42.3	-27.0
TS4	-36.4	-20.0	-36.7	-20.3
Int-4	-41.7	-26.4	-42.2	-26.8
TS5	-18.8	-3.7	-19.9	-4.8
Int-5	-35.4	-18.8	-36.4	-19.8
TS6	-11.8	3.7	-12.3	3.3
Prdt	-40.6	-40.4	-41.6	-41.4

Table S11: Energy Decomposition Analysis (kcal/mol) of key transition states at the RI-B3LYP-D3BJ/def-TZ2P level of theory.

Transition states		Pauli Repulsion ΔE_{Pauli}	Electrostatic Attraction ΔV_{elst}	Orbital Interaction ΔE_{oi}	Dispersion Interaction ΔE_{disp}	Binding Energy
TS1	Pathway A	120.0	-155.2	-83.6	-8.9	-127.7
	Pathway B	116.2	-151.5	-81.0	-9.4	-124.9
TS5	Pathway A	66.2	-99.6	-43.8	-9.9	-87.2
	Pathway B	71.2	-103.8	-45.9	-10.7	-89.3
TS6	Pathway A	51.2	-108.8	-44.3	-6.8	-108.7
	Pathway B	51.4	-109.5	-45.1	-6.7	-109.9

Table S12: NBO analysis of TS1 at the RI-B3LYP-D3BJ/def2-SVP level of theory.

Pathway	Cl	B	C
A	-0.45	0.37	-0.52
B	-0.46	0.40	-0.51

Table S13: NBO analysis of TS1 -new_mechanism at the RI-B3LYP-D3BJ/def2-SVP level of theory.

Pathway	Cl	B	C
A	-0.46	0.44	-0.61
B	-0.46	0.47	-0.67

Table S14: NBO analysis of TS5 at the RI-B3LYP-D3BJ/def2-SVP level of theory.

Pathway	Cl	B	O
A	-0.63	0.53	-0.61
B	-0.62	0.56	-0.61

Table S15: NBO analysis of TS6 at RI-B3LYP-D3BJ/def2-SVP level of theory.

Pathway	Cl	C	O
A	-0.64	-0.30	-0.56
B	-0.63	-0.30	-0.57

Table S16: HOMO, LUMO, and HOMO-LUMO gap of key transition states at the RI-B3LYP-D3BJ/def2-SVP level of theory.

Transition states		HOMO (eV)	LUMO (eV)	HOMO-LUMO Gap (eV)
TS1	Pathway A	-5.8	-4.0	1.8
	Pathway B	-3.9	-1.2	2.7
TS1-new mechanism	Pathway A	-4.9	-1.6	3.5
	Pathway B	-5.0	-1.6	3.4
TS5	Pathway A	-5.0	-0.9	4.1
	Pathway B	-5.1	-1.0	4.1
TS6	Pathway A	-5.7	-1.4	4.3
	Pathway B	-5.7	-1.2	4.5

Table S17: QTAIM analysis of the electron density of TS5 in Pathway A at the RI-B3LYP-D3BJ/def2-SVP level of theory.

BCP	Atoms	ρ	$\nabla^2(\rho)$	Ellipticity (ϵ)	K
77	Cl41 - H46	0.021849	0.047903	0.039576	0.001422
75	Cl41 - H77	0.021756	0.04856	0.043981	0.00136
106	Cl41 - H80	0.00748	0.027829	1.081995	-0.00125

Table S18: QTAIM analysis of the electron density of TS5 in Pathway B at the RI-B3LYP-D3BJ/def2-SVP level of theory.

BCP	Atoms	ρ	$\nabla^2(\rho)$	Ellipticity (ϵ)	K
61	Cl34 - H47	0.021531	0.048758	0.055285	0.001266
99	Cl34 - H58	0.008039	0.028953	0.673145	-0.001181
58	Cl34 - H78	0.022476	0.051008	0.044865	0.001352
60	Cl34 - H91	0.011456	0.030164	0.063289	-0.000191

Table S19: Gross population of relevant fragment orbitals shown in Figure 3.

Borirane	σ	$p(B)$	π	π^*
1	0.54 (−1.46)	0.67 (+0.67)	1.66 (−0.34)	1.12 (+1.12)
2	0.54 (−1.46)	0.63 (+0.63)	1.67 (−0.33)	1.13 (+1.13)

The difference between integer gross population in the isolated fragment and the gross population in the compound is given in parenthesis.

Figure S43. QTAIM-derived molecular graphs of TS5 in (a) Pathway A and (b) Pathway B.

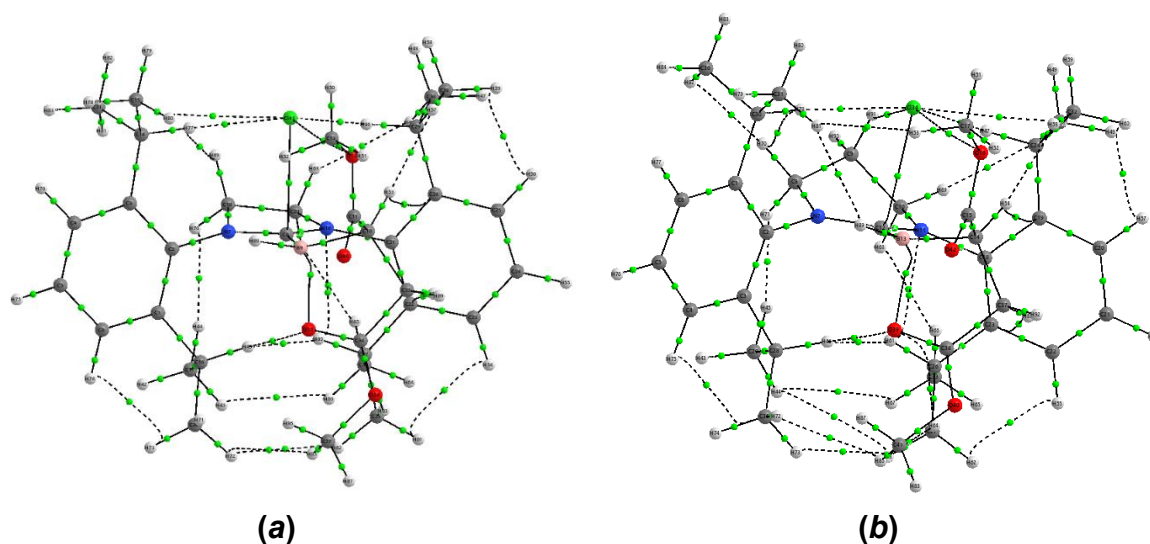
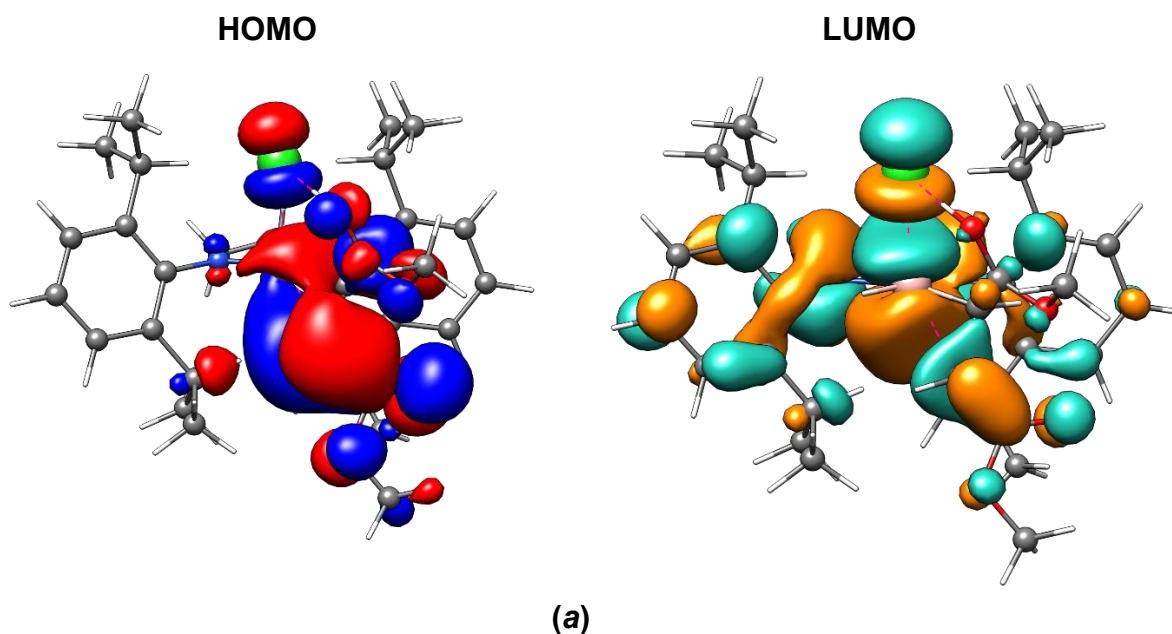


Figure S44. HOMO and LUMO of TS1 in (a) Pathway A and (b) Pathway B at the RI-B3LYP-D3BJ/def2-SVP level of theory. For color code, see Figure S47.



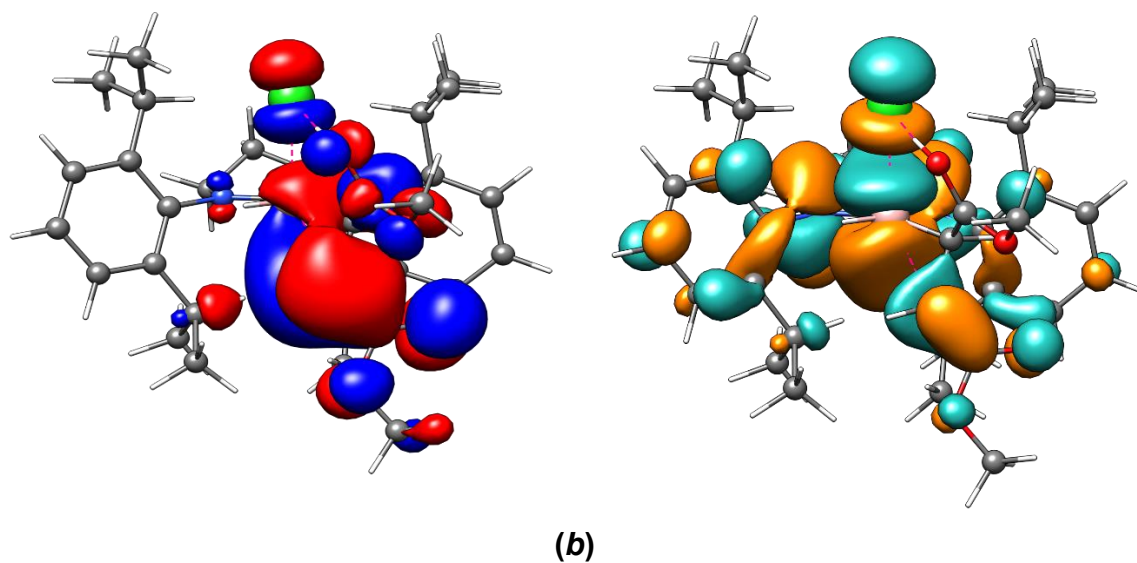
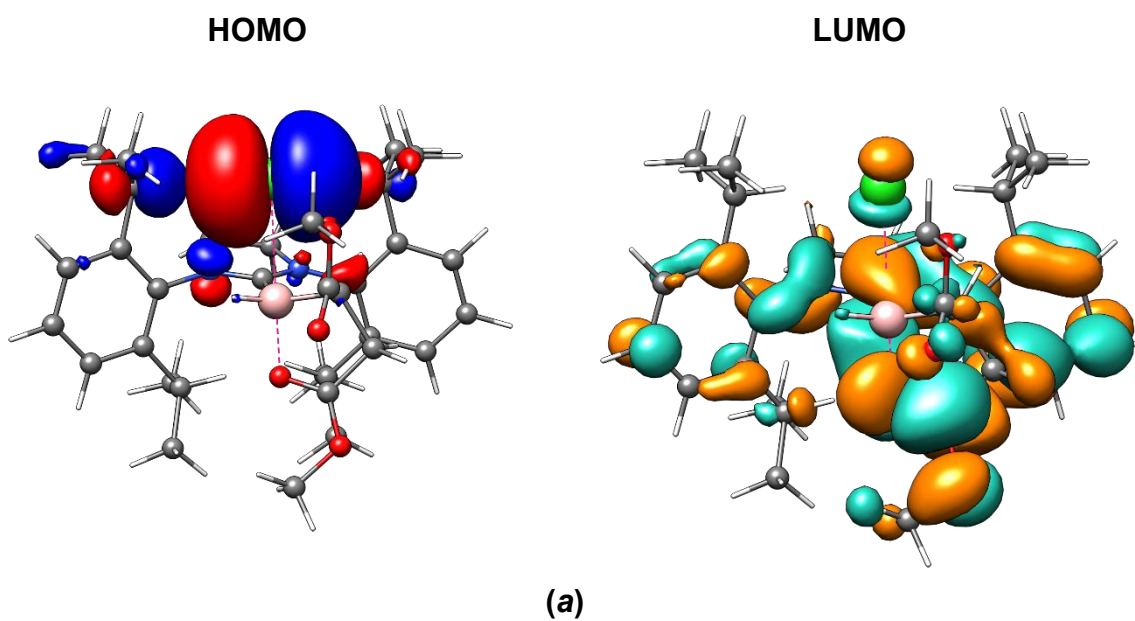


Figure S45. HOMO and LUMO of TS5 in (a) Pathway A and (b) Pathway B at the RI-B3LYP-D3BJ/def2-SVP level of theory. For color code, see Figure S47.



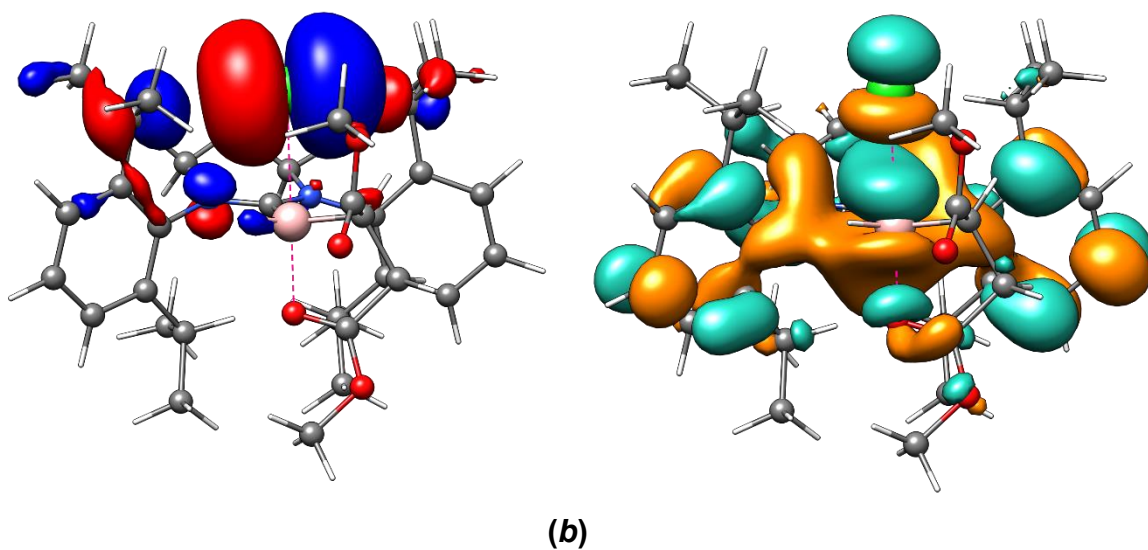
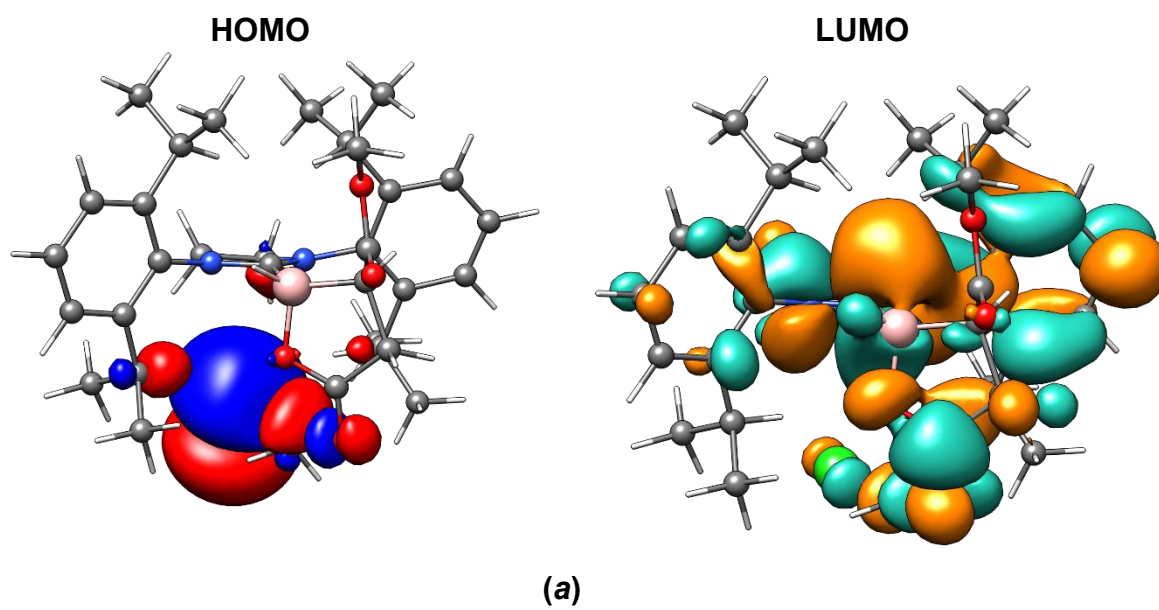


Figure S46. HOMO and LUMO of TS6 in (a) Pathway A and (b) Pathway B at the RI-B3LYP-D3BJ/def2-SVP level of theory. For color code, see Figure S47.



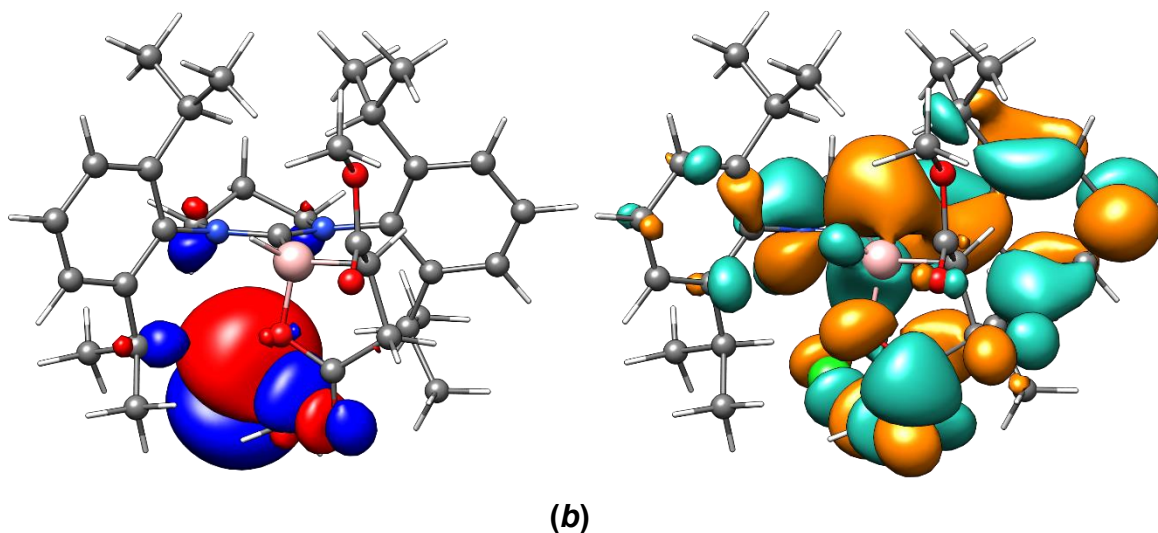
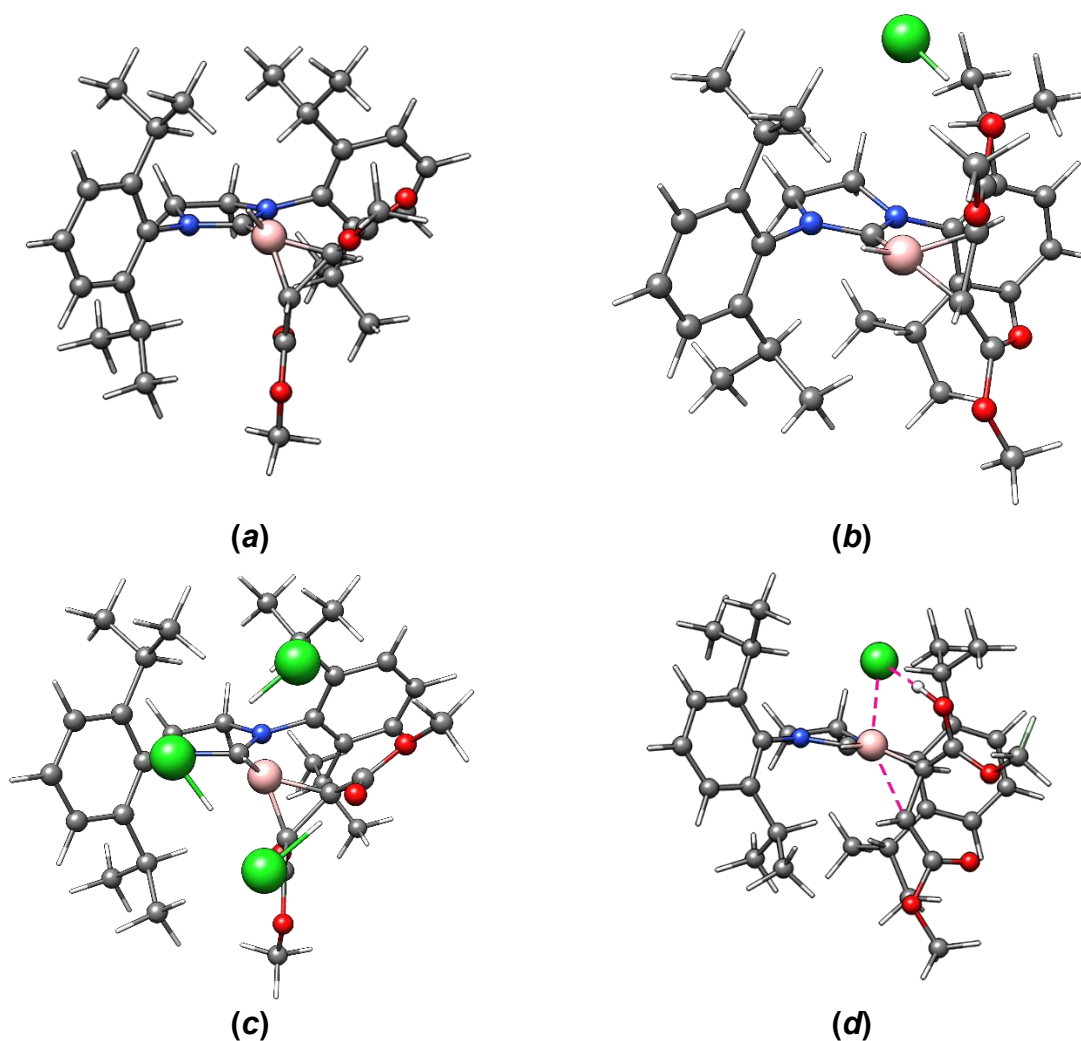
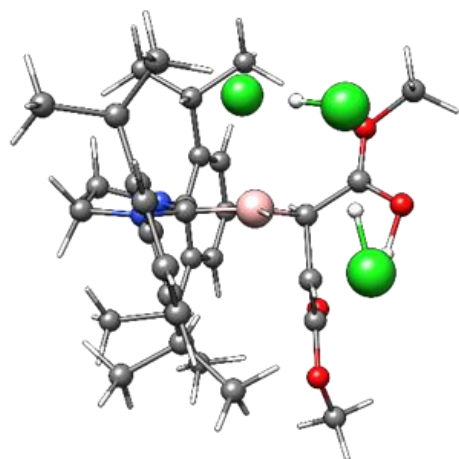
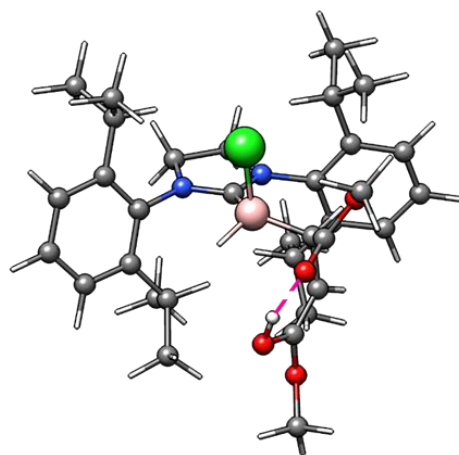


Figure S47. Optimized geometries of Pathway A at the RI-B3LYP-D3BJ/def2-SVP level of theory. (a) 1, (b) RC, (c) RC-new mechanism, (d) TS1, (e) TS-1 new-mechanism and (f) Int-1. Colour code: red is oxygen, peach is boron, blue is nitrogen, grey is carbon, white is hydrogen, and the large green ball is a chlorine atom.



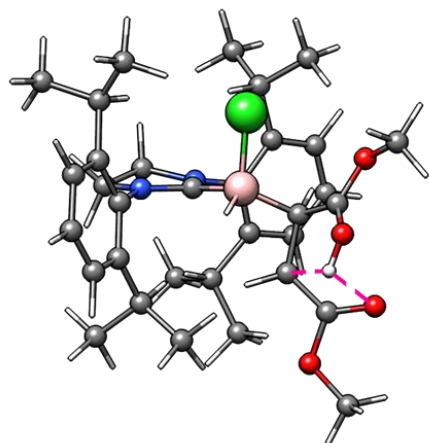


(e)

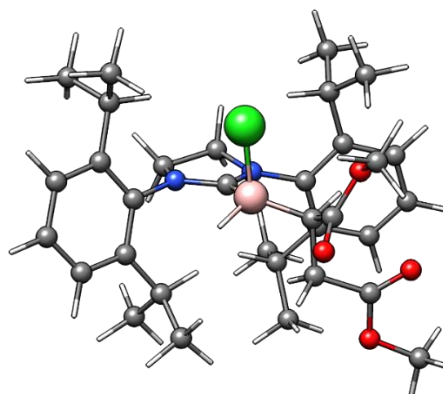


(f)

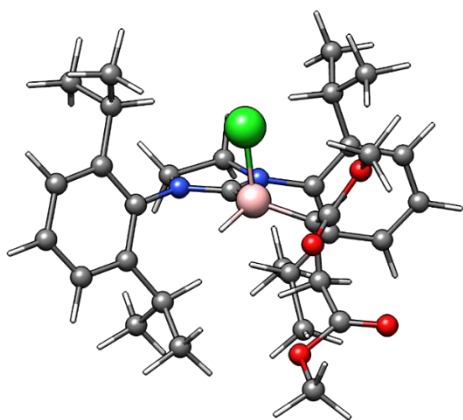
Figure S48. Optimized geometries of Pathway A at the RI-B3LYP-D3BJ/def2-SVP level of theory. (a) TS-2, (b) Int-2, (c) TS3, (d) Int-3, and (e) TS4. For color code, see Figure S47.



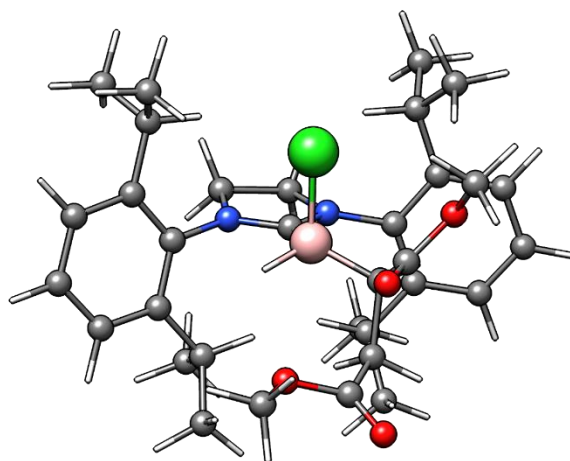
(a)



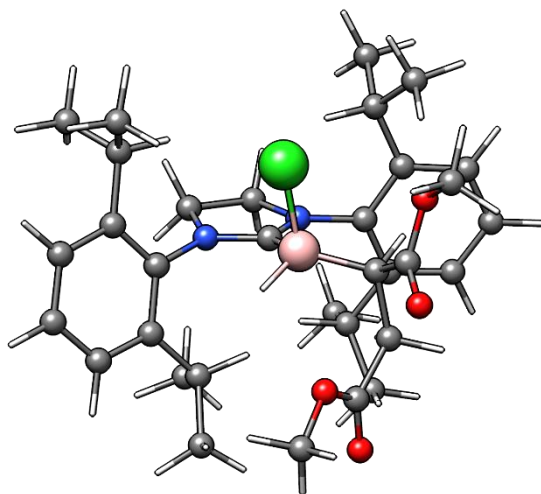
(b)



(c)

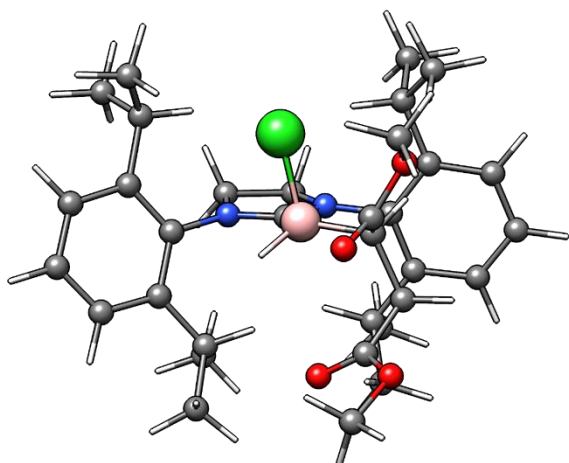


(d)

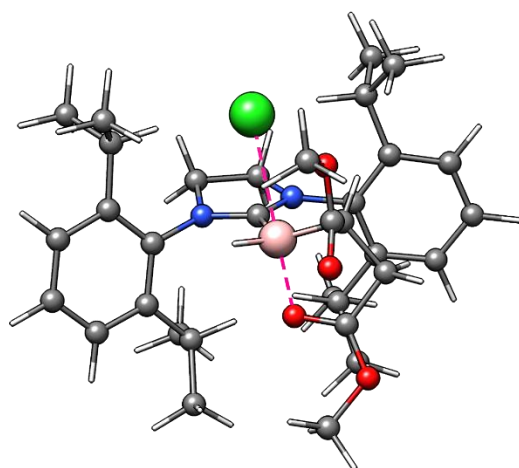


(e)

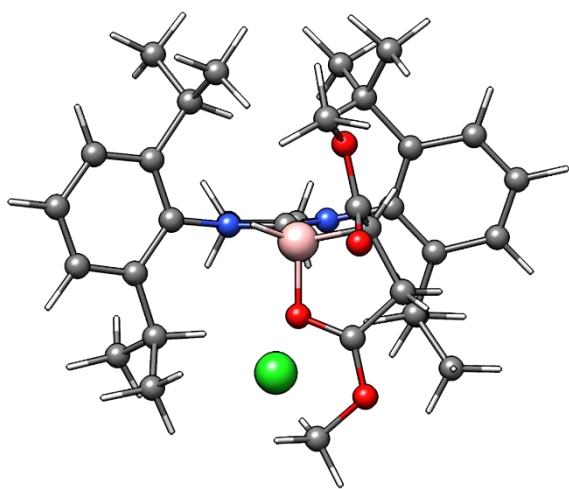
Figure S49. Optimized geometries of Pathway A at the RI-B3LYP-D3BJ/def2-SVP level of theory. (a) Int-4, (b) TS5, (c) Int-5, and (d) TS6. For color code, see Figure S47.



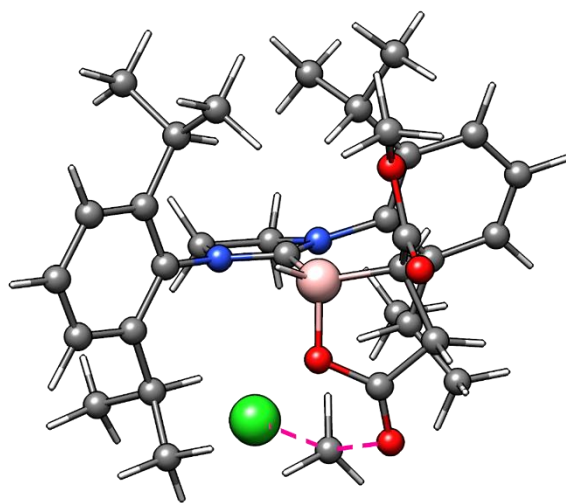
(a)



(b)



(c)



(d)

Figure S50. Optimized geometries of Pathway A at the RI-B3LYP-D3BJ/def2-SVP level of theory. (a) 5-boralactone (4) (Prdt), (b) mecl (Prdt). For color code, see Figure S47.

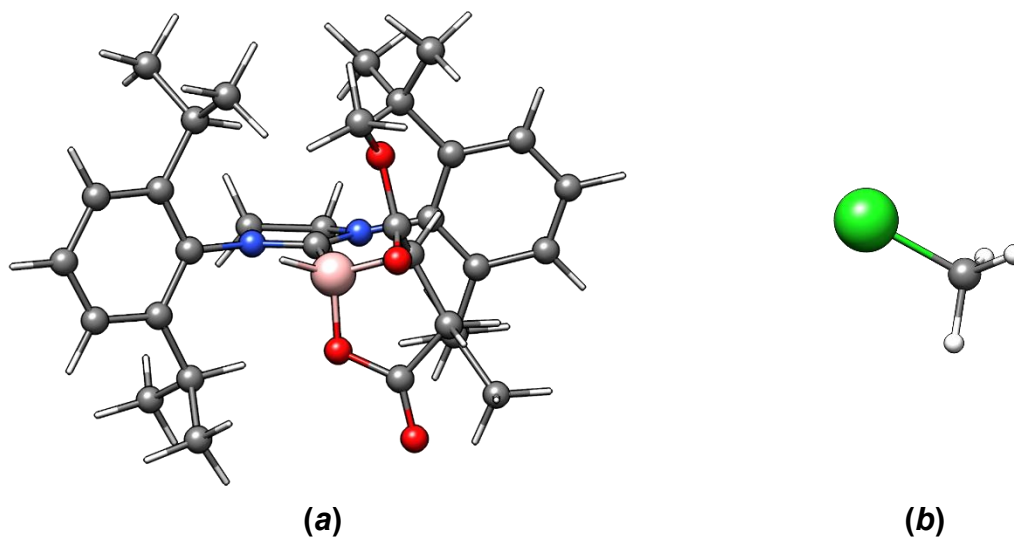


Figure S51. Optimized geometries of Pathway B at the RI-B3LYP-D3BJ/def2-SVP level of theory. (a) 2, (b) RC, (c) RC-new_mechanism, (d) TS1, (e) TS-1-new_mechanism and (f) TS2. For color code, see Figure S47.

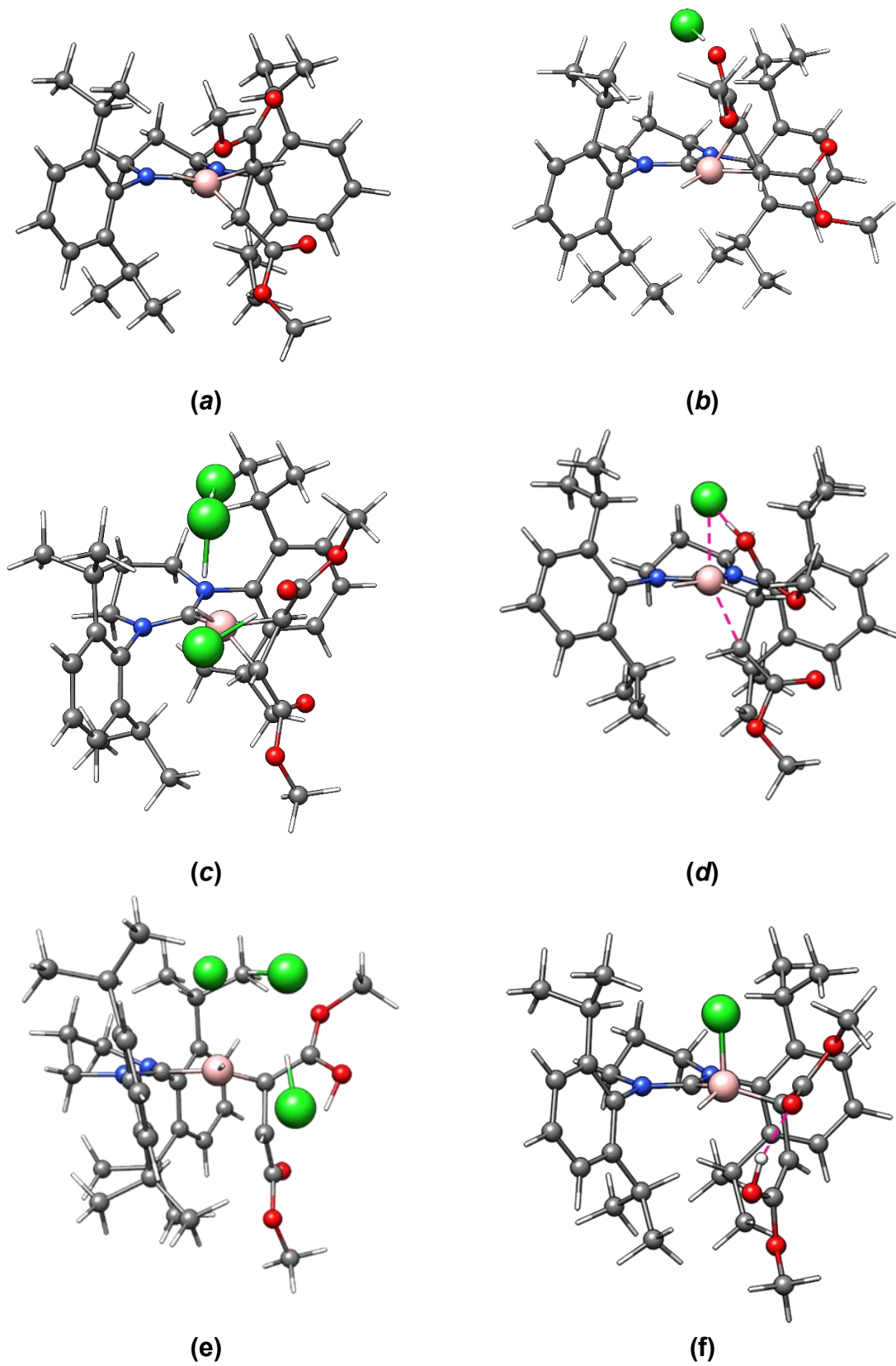


Figure S52. Optimized geometries of Pathway B at the RI-B3LYP-D3BJ/def2-SVP level of theory. (a) TS2 (b) Int-2, (c) TS3, (d) Int-3, and (e) TS4. For color code, see Figure S47.

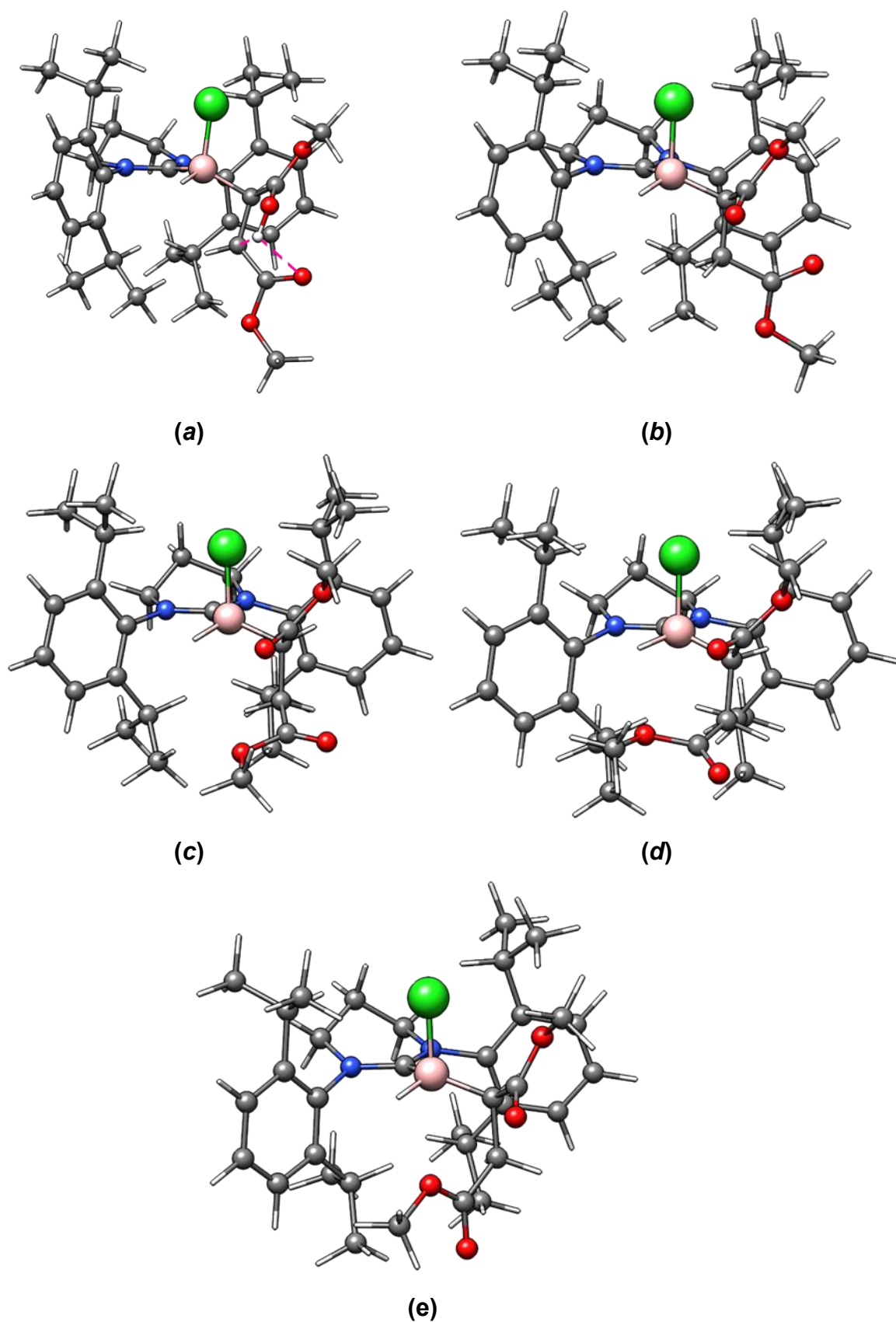


Figure S53. Optimized geometries of Pathway B at the RI-B3LYP-D3BJ/def2-SVP level of theory. (a) Int-4, (b) TS5, (c) Int-5, and (d) TS6. For color code, see Figure S47.

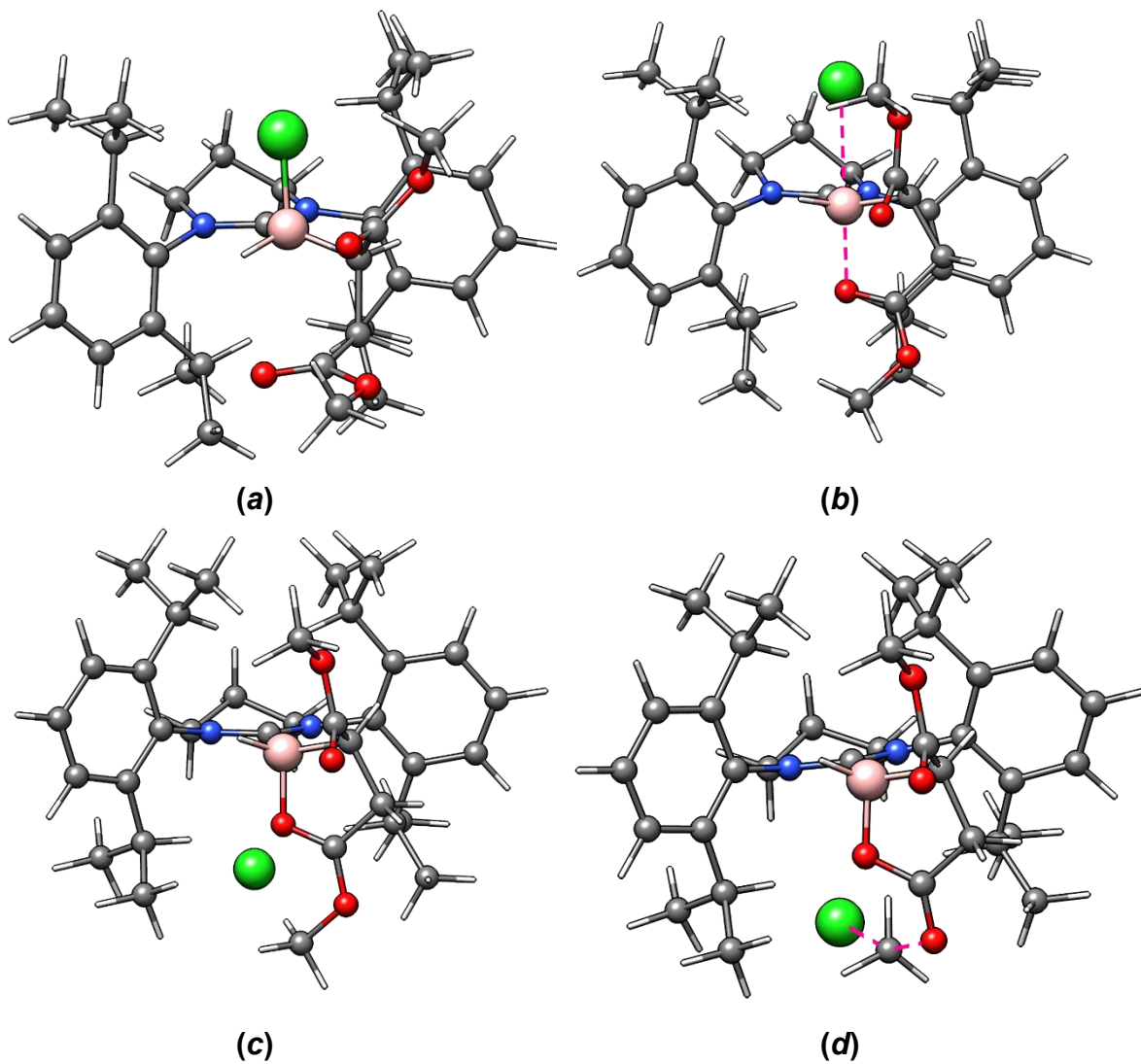


Figure S54. Optimized geometries of Pathway B at the RI-B3LYP-D3BJ/def2-SVP level of theory. (a) 6-boralactone (5) (Prdt), (b) mecl (Prdt). For color code, see Figure S47.

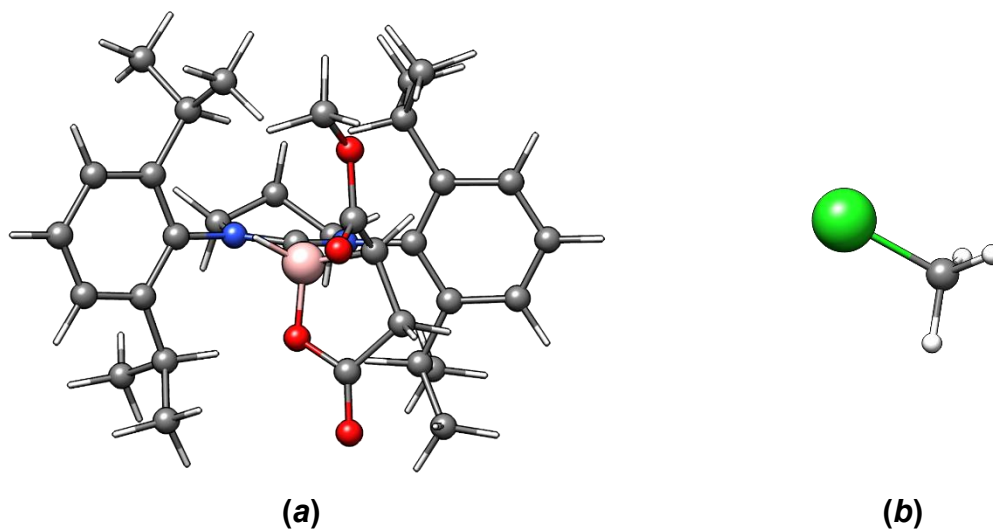


Figure S55. Full energy landscape of the reactions of boriranes, **1** and **2**, with HCl at RI-B3LYP-D3BJ/def2-SVP-CPCM level of theory.

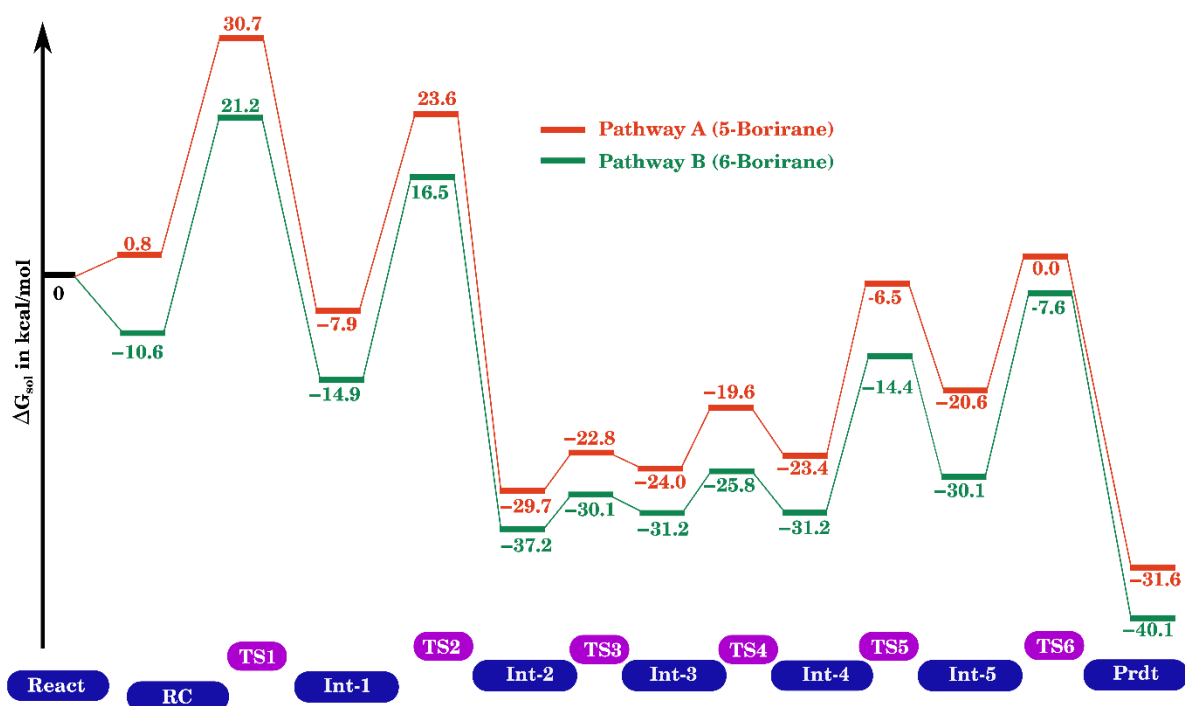


Figure S56. Full energy landscape of the reactions of boriranes, **1** and **2**, with **3** HCl at RI-B3LYP-D3BJ/def2-SVP-CPCM level of theory.

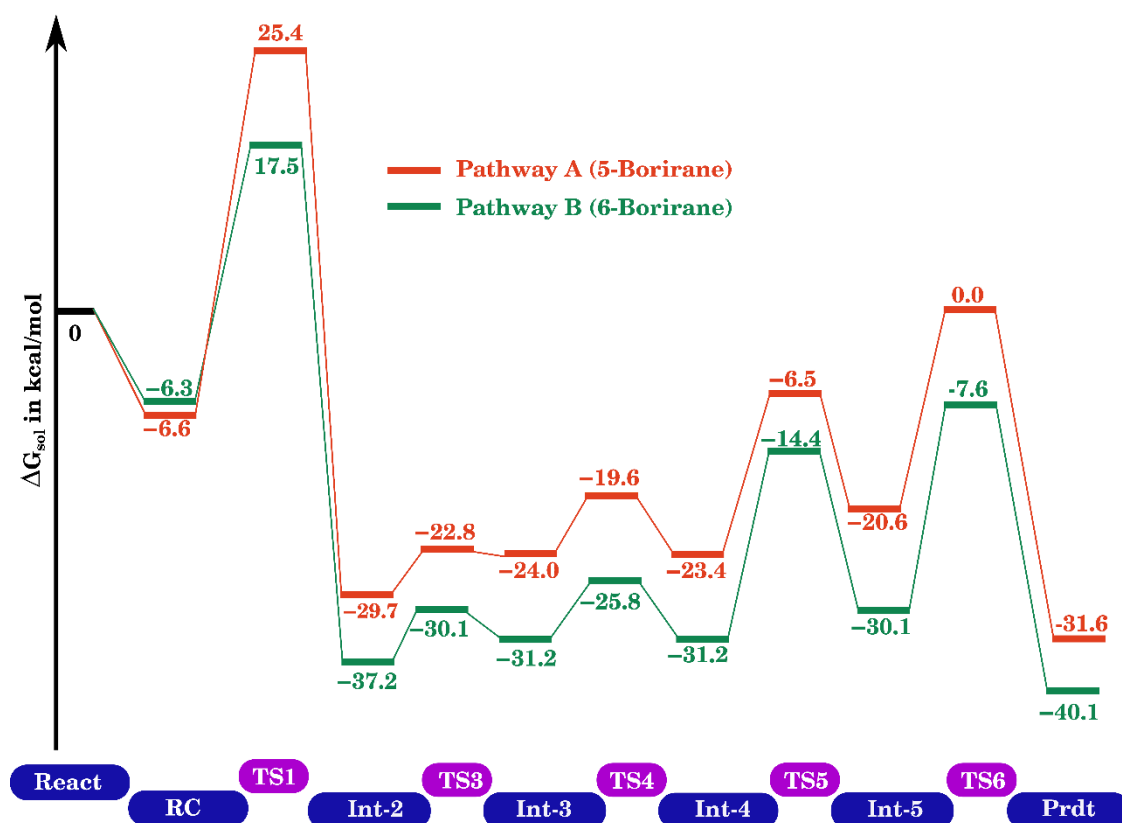
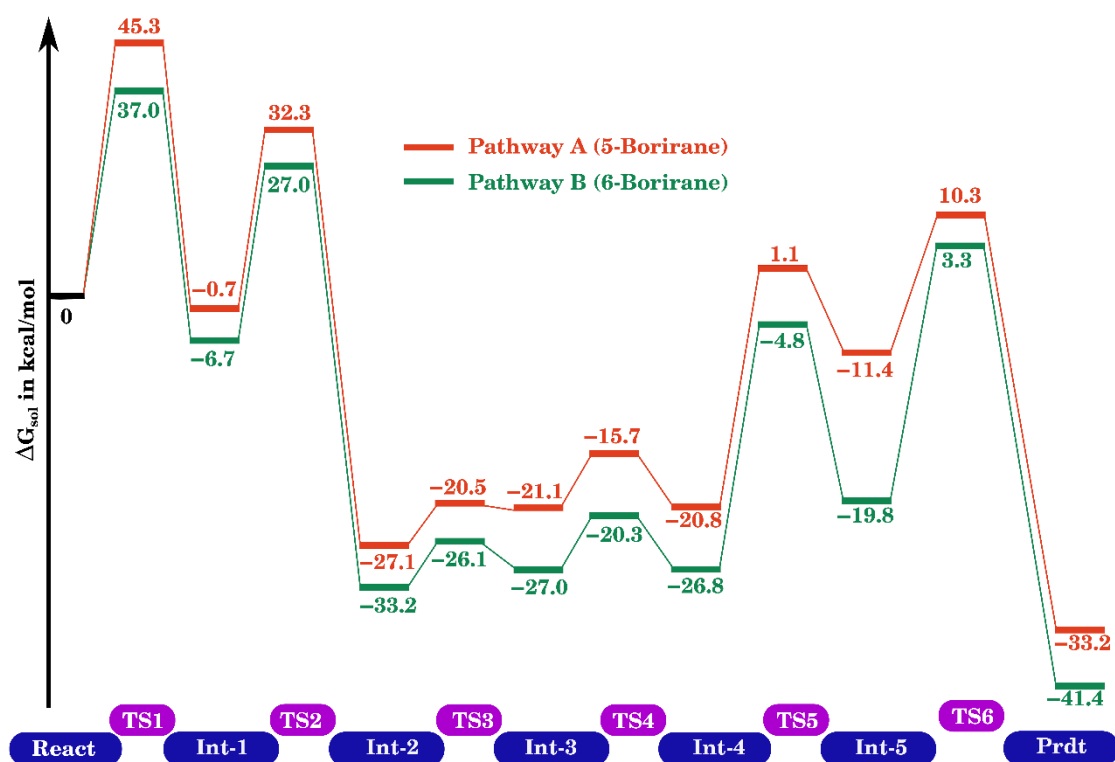


Figure S57. Full energy landscape of the reactions of boriranes, **1** and **2** with HCl at DLPNO-CCSD(T)-cc-PVDZ level of theory.



S4. References

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Coordinates of Optimized Geometries

Reactant (1) (Pathway A)

```
C -2.39833032389603 1.46142567652367 1.62057897389318
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C -3.85606110026227 -0.2008310308112 1.95946751070438
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B 0.29277993348954 0.50356638479772 3.80907914876737
C 0.33865486874518 -0.76723722027286 4.80653711758512
C 0.72022148840980 -2.09319418354292 4.31441183750099
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RC (PATHWAY A)

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H -1.38006009719849 -5.36958528437021 -2.28342147956027
H 1.18275517902573 0.22972207082203 -1.70599718027676
H -0.91665563972322 3.51600241000672 -1.85314171158308

RC-New_mechanism (Pathway A)

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C -2.51343037880733 1.64771776724122 0.86511569806327
C -3.90376714430450 1.78203259092667 0.78187237834707
C -4.75859090568966 0.78699770414044 1.253444983083470
C -4.23115925115210 -0.36636181497095 1.82273262242055
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C 1.2625588461724 0.33733932715996 2.80175524393664
C 2.73393593088982 0.63859894536154 0.15755863957400
C 3.11026122657853 1.99060713472781 -0.00065232761569
C 4.31089189860794 2.6548634240232 -0.66348419589505
C 5.10421348212156 1.23812737651814 -1.16645812530921
C 4.70306948338411 -0.08638041953845 -1.01853277809477
C 3.51470300888978 -0.41594625024254 -0.35287000691645
C 2.25146242654629 3.14515613191975 0.49426607871757
C 1.75960279216506 4.01252148494294 -0.67327995120682
C 3.11715144577999 -1.87310316568630 -0.19135119962610
C 3.95179787874874 -2.55231182276545 0.90770816837050
B 0.03488414881476 0.08488387484090 -1.08160477502803
C -1.41878399953087 -0.48979592373769 -1.59596270505129
C -1.94199822371795 0.16335558020647 -2.75278356425590
O -3.11582165686249 0.73928540331948 -2.59799935399145
C -3.66378149446936 1.48788444406165 -3.69686673182597
C -1.61402972107327 2.80271083228896 0.43761724523903
C -1.18626432573174 3.6220025122735 1.66879234254007
C -2.32634075994458 -1.84000355337831 2.56295953368747
C -2.99539092352199 -3.10188116681008 1.99975633251851
C -2.24526162434725 3.72189378097039 -0.61221431044906
C -2.49803388389226 -1.77209000212002 4.09094431526542
O -0.18747275243380 -1.37782806418867 -1.6913835119568
O -0.18816976259719 -2.582522710247168 -0.84308023508522
O -0.43441108465602 -2.625461410337624 0.34931435682537
O 0.15373173403595 -3.68574943202786 -1.53307153040775
C 0.24634987734398 -4.89537694031592 -0.78661093995092
C 3.21807261788601 -2.63690245360294 -1.52006246833458
C 2.98150842365492 3.98888118623737 1.55066681948463
O -1.40481207306916 0.27850407807089 -3.89925338454344

CI -0.46888271418726 3.54871361229310 -3.71140061147818
CI 1.10063359262293 -0.69360346318428 -4.77209085614719
H 5.02220011588336 -2.56113723656291 0.64432496166027
H 3.62966170286286 -3.59689702858563 1.05110855240340
H 3.85275493967315 -2.03033589154668 1.87334407672067
H 2.07068708233185 -1.89737710346275 0.13807859627631
H -0.71066610796250 2.38560054788810 -0.2639243900959
H -2.06848680518907 4.05392868467203 2.16826757338361
H -0.52159276051131 4.44817331449450 1.37370690994421
H -0.65307507500418 3.01066393738692 2.41085806176499
H -3.88858683168494 0.81594116971987 -4.53772067268419
H -2.95153190639157 2.25679243081955 -4.02384483394451
H -4.58390884071857 1.93914960577212 -3.30839957872367
H -2.16378143127446 -0.70536757381831 -0.83158455137489
H -4.90501115377814 -1.13765007829687 2.20021678707801
H -5.84128233109715 0.917065520951171 1.18034084683834
H -4.32892702081207 2.68662119919312 0.34803740011239
H -2.61741370629258 3.14663044517194 -1.47012232050902
H -1.49220891410057 4.42649759366452 -0.99140193846526
H -3.07752512733755 4.31228988059466 -0.19584828817718
H -1.26302807526736 -1.92987770848980 2.31764860566286
H -4.06149444931943 -3.16312204941902 2.27265463176317
H -2.48989536703021 -3.99934695127195 2.40137824237040
H -2.90960490619332 -3.13482010370169 0.90529581381873
H -3.56455468851494 -1.72790223297015 4.36641853271250
H -2.01495735907641 -0.88099559212215 4.52242298698085
H -2.06349804463999 -2.66396803274302 4.57127802861500
H -0.07952299983251 -0.57358115856600 3.37845259265256
H -0.22895829444785 1.19840402578019 3.38624718424197
H 2.07464785807343 1.3868401203855 2.70789280375297
H 2.21353818129669 -0.38558204093843 2.79809856869370
H 2.66347565942346 -2.12843768795583 -2.32233827957748
H 2.81115029990978 -3.65263079079421 -1.41194857100439
H 4.26617131950481 -2.73804593993823 -1.84448900653454
H 5.32200244133585 -0.88418632815422 -1.43238069398009
H 6.03082218543659 1.47243193093767 -1.69568751476944
H 4.61619332943050 3.30358417638939 -0.81025728451098
H 1.35767779920260 2.72510910542164 0.97349473617319
H 2.60067512035714 4.47851952360655 -1.20990454410132
H 1.10818031916734 4.82172369419563 -0.30593586036593
H 1.19410027186464 3.41990544542195 -1.40255942287083
H 3.33137358831154 3.37258194339213 2.39487824145124
H 2.31519245782252 4.77107566020721 1.94944623018467
H 3.86415150883240 4.49010394769098 1.12228002600000
H 0.19753070207444 -1.55364949135022 -2.69608537516042
H -0.72834804517166 -5.16412331939039 -0.35100281499537
H 0.97571578799856 -4.79676846760376 0.03241047851448
H 0.57248390421024 -5.66677251030100 -1.49514771056259
H 0.60959065558305 0.88138297565911 -1.77160937547802
H -0.43752323664670 -1.03098663144582 -4.12912913164615
H 1.99389968162718 0.77495793813745 -4.16999738048890
CI 2.58482274665159 1.96054118008125 -3.72402512309272
H 0.68510136841974 2.903677474233922 -3.78945890843945

TS1 (Pathway A)

C -2.85842061162062 1.52619240150847 1.05944310748121
C -1.91159953047739 0.51721824290963 1.33227530673953
C -2.29032532022170 -0.80847895607203 1.66015061050381
C -3.66048301384698 -1.09432974677076 1.68910560398117
C -4.61335867284641 -0.11325188402240 1.42273869289877
C -4.21620365863871 1.18350796823508 1.11203815021891
N -0.51504743665037 0.85682649291571 1.35769274690748
C 0.40858632495063 0.69859551059490 0.39285417274500
N 1.63041855340147 0.94036238575490 0.90071126876098
C 1.56583930856902 1.24923880739257 2.33975437480999
C 0.07628636169380 1.52382564663332 2.53214386736292
C 2.89910910846312 0.716653004455170 0.26741170823825
C 3.32748661029246 -0.60977550167086 0.02189071142076
C 4.61328714994273 -0.78883266721985 -0.50324335104808
C 5.44328248116085 0.29857746895577 -0.77406133206438
C 4.99178850412010 1.59500430704672 -0.54229837291037
C 3.71043471839398 1.83245932687233 -0.02570149679170
C 2.45206209512950 -1.82017458348196 0.31744474447106
C 2.71754128052984 -2.37108580330878 1.72801708793915
C 3.24319261375411 3.26395852369335 0.19782564716265
C 3.35310496329091 4.10590443204391 -1.08216639404929
B 0.19983871657560 0.48920382611066 -1.17492572536611
C -1.1006207356527 -0.18840561457980 -1.76322592525055
C -1.48430406044421 0.18570469493455 -3.1471636085447
O -2.30956292448411 -0.57484565315570 -3.80093883581375
C -2.61500734451575 -0.28911809859043 -5.17249401859929
C -1.26696430458968 -1.9017042894369 1.97022126789006
C -1.84456568717997 -3.31915089911527 1.88220605978778
C -2.45655399118945 2.95758491392190 0.73894824934906
C -2.78051820235783 -3.89438644907149 1.91506780906293
C -0.62068190195046 -1.726601877667245 3.35678074812097
C -3.10005624737034 3.46234649316211 -0.55992022485684
C 4.00958485298748 3.92734954504117 1.35502935314486
C 2.58587322330993 -2.93045721338657 -0.73380231451437
C -0.58261376699367 -1.60412541936799 -1.72911766728061
C -1.45312464238031 -2.67842659301694 -1.42996657001688
O -2.63789651783186 -2.62128256807413 -1.09162856141392
O -0.81162515061131 -3.90711763052190 -1.53089146189579
C -1.62501959208247 -5.053822189030650 -1.39310652320916
O -1.00284475178108 1.19213733513936 -3.78718534196805
CI 0.12374474711783 2.74289191962990 -1.64284199142049
H 3.76018945762903 -2.71624354882709 1.82513227726047
H 2.05391089418807 -3.22537987378176 1.93726169868450
H 2.54527539182795 -1.61318767993899 2.50721081788690

H 1.40333931299207 -1.50114810455178 0.27016041775970
H -1.37264523552159 2.97756452058967 0.56713337690177
H -3.86665444531969 3.94207750986625 2.09813566217072
H -2.42846857203328 4.91770880197103 1.70553436389546
H -2.3068806567822 3.553556174735905 2.8497624543225
H -1.70938567161150 -0.38471414801272 -5.78914193270514
H -3.01976954281265 0.72801329345578 -5.27448122231985
H -3.36077117701809 -1.03538971875213 -5.46782837716720
H -2.00626197849835 -0.12153810782639 -1.13989391350033
H -3.99145530992377 -2.10834001396050 1.90558909344964
H -5.67575139155321 -0.36842143966578 1.44849043646132
H -4.96991051570750 1.94520291713995 0.90146430426663
H -2.86273350716421 2.79390353509046 -1.39939314464326
H -2.70615828524953 4.45862558891496 -0.81414168616332
H -4.19573151867859 3.54272925270532 -0.47162741086955
H -0.48083346966570 -1.82410716021302 1.20246219010128
H -2.49481395595950 -3.54158116822360 2.74524695794662
H -1.02113951951696 -4.05039712488357 1.89731269596898
H -2.41575073560762 -3.45525945911033 0.95626033979378
H -1.39347714029616 -1.69834231016094 4.14255851850932
H -0.01708313435373 -0.81653652297633 3.4443598896840
H 0.04596190592132 -2.57649605833415 3.57068604098460
H -0.33856386663944 1.12414897240389 3.46450467331152
H -0.14920336126371 2.60233996650642 2.48382277080808
H 2.19635795613102 2.11217694279200 2.58359940193505
H 1.92428359561171 0.38209648651017 2.91941209568760
H 2.55415437690127 -2.15591538630668 -1.75197977659829
H 1.74434404868629 -3.63317623822611 -0.64433669013568
H 3.52622110723427 -3.49566673236485 -0.62229413971219
H 4.96963003320488 -1.80020060427523 -0.70507941944347
H 6.44484947991448 0.13259228563133 -1.17912789991596
H 5.64026261515755 2.44221772146569 -0.77534381833434
H 2.17475526604931 3.229421787942777 0.455030470990609
H 4.40151011498825 4.22982786566406 -1.39879190463646
H 2.93616052178998 5.11123644786883 -0.90926799024825
H 2.78413455081055 3.64366700850042 -1.89998735080407
H 3.94564392314722 3.34146829298422 2.28624443087224
H 3.61332741935044 4.93582156320301 1.55681928695962
H 5.07964255067035 4.03100099024900 1.11147872594667
H 0.34773419694348 -1.82454196263874 -2.24819658619351
H -2.57201994577164 -4.94707364827294 -1.94592025548199
H -1.87551506311699 -5.25890733088089 -0.33792603058913
H -1.04783513606061 -5.90110767939890 -1.79247620884711
H 1.22084480812714 0.30520766499985 -1.77858934670535
H -0.50066319230777 1.81411958542127 -3.13681186015244

TS1-New_mechanism (Pathway A)

C -2.30191591995060 -0.94915772836081 1.72821188567991
C -2.01557738703594 0.40492482868658 1.42123549166149
C -3.03188604390808 1.35756119005375 1.19898970352834
C -4.36322364481046 0.92501423023583 1.27067690157424
C -4.66935670822155 -0.40210363522007 1.55360058117237
C -3.64946015037354 -1.32496367232627 1.77798056312355
N -0.64195836519749 0.82835451423797 1.41453005368464
C 0.26542547773164 0.70956788238062 0.42995556115554
N 1.48973460291778 1.00267239834107 0.90128181509449
C 1.44419761044238 1.33324508206305 2.33666841523826
C -0.05265880974673 1.53520979319545 2.56678116763197
C 2.74047546399425 0.86487356799548 0.20502960763130
C 3.46894697296841 2.02848539233094 -0.12327088386736
C 4.70508146699499 1.86834837777930 -0.76466803535416
C 5.19319089432148 0.60457632986853 -1.08141433046396
C 4.45380108042403 -0.53082551602888 -0.75482110291987
C 3.22064758347118 -0.43192466338814 -0.10021376265208
C 2.97471731928450 3.43082115149879 0.20205082523710
C 3.06175175110306 4.73256160575871 -1.008339508955377
C 2.46044994661223 -1.69658702722615 0.27918179481371
C 2.82002020986722 -2.15254299232650 1.70346013426460
B 0.04463773624456 0.45907059920416 -1.12013150570860
C -1.26686827136303 -0.14343319908620 -1.77398257306278
C -1.52714040507670 0.38778614839617 -3.10958553467636
O -2.2303111187439 1.44628381669334 -3.29189652385451
C -2.25211504610821 2.08713415788944 -4.58910280616118
C -2.73260404616000 2.82180330351500 0.92048300681814
C -3.07406322919941 3.68982436944530 2.14358349454487
C -1.20376608122990 -1.97446251025518 2.00968931819763
C -1.68797227726176 -3.42670465296027 1.92300131774085
C -3.44883265754231 3.33331729390534 -0.33728683340322
C -0.54596227139629 -1.76504536149849 3.38598587710457
C -0.60083563023436 -1.48926102597066 -1.77236917876776
C -1.33562118848652 -2.65073583033161 -1.38437800854632
O -5.2016002778316 -2.70687924658510 -1.06888702632255
O -0.55673093182361 -3.78707338634463 -1.42757064935477
C -1.23707532281024 -5.02680779203302 -1.33637975889025
C 2.65752033106618 -2.84562523486383 -0.71772838933300
C 3.74695234458667 4.02564465245145 1.3936219652893459
O -0.99681937612692 -0.19376233023159 -4.12670951677412
Cl -0.15544625910355 2.97712917086469 -1.37201448595427
Cl 2.29575591825928 -0.86379062628502 -4.15081208555211
H 3.89151246924600 -2.40173395178544 1.77337223222893
H 2.24212115451031 -3.04998254477425 1.97727270019763
H 2.61064151769580 -1.37606038126049 2.45403805528774
H 1.38805155767176 -1.46510113030842 0.26272247076403
H -1.65859789552819 2.91732386284669 0.71717881962544
H -4.15402596263016 3.66023851901241 2.36365432233334
H -2.79524833603119 4.74059622793194 1.96225277027903
H -2.54689160678677 3.34681117021252 3.04843150018323
H -2.67748589561133 1.40294575348038 -5.33588286509259
H -1.22594596405294 2.37106110703449 -4.85979153902167
H -2.88432555676265 2.97156155531345 -4.46008901957303

H -2.15221743784077 -0.06830980519478 -1.13225453564629
H -3.91040945291421 -2.36185882732357 1.98181718551480
H -5.71225204229233 -0.72624609878356 1.59471313598479
H -5.16831890699099 1.64196497168834 1.09743765918864
H -3.21667202139641 2.70079709548256 -1.20486894974624
H -3.10770434172134 4.35343224553198 -0.57226091059018
H -4.54258903513254 3.36402473206019 -0.20187813841816
H -0.43228788842606 -1.84156973218775 1.23476085324548
H -2.31353259859458 -3.69197491175436 2.79159675163624
H -0.81913043478267 -4.10323548211795 1.92855689613735
H -2.26192021828649 -3.60014809638258 1.00529358661903
H -1.30374840655174 -1.80818227898681 4.18525940972248
H -0.01848562849405 -0.80909183818365 3.47298193463658
H 0.19184907056017 -2.55993100690281 3.57623112130631
H -0.42195087803079 1.12345631611915 3.51313102951271
H -0.33231636523638 2.60020399361845 2.51505646070233
H 2.03145502912222 2.23272728282807 2.54925067333915
H 1.86364897566962 0.49783041212807 2.92124237341879
H 2.55263626455562 -2.49474787856312 -1.75372513456859
H 1.89323841322722 -3.61771033859874 -0.55110722188856
H 3.65034429760923 -3.31345083054798 -0.61295497898757
H 4.84053444658526 -1.51530109297741 -1.01888223190415
H 6.15236932162274 0.50131673994176 -1.59488612162645
H 5.28446700516045 2.75344423004259 -1.03359909363488
H 1.90924525520835 3.35650707477328 0.46008797013164
H 4.10672121407402 4.62572957271979 -1.25139947692790
H 2.53451764176927 5.31462265761387 -0.79004652917936
H 2.60011668699326 3.92453641030960 -1.89692621509141
H 3.71289504676745 3.37841213187895 2.28465085669068
H 3.33740945692123 5.01109885082387 1.6964645157209
H 4.81058073476266 4.1635683475094 1.13916301030914
H 0.40993811632655 -1.611322507246 2.15819426642333
H -2.13941277304374 -0.50633041675614 -1.96786510270613
H -1.54455950033100 -5.25044269283328 -0.30230313039975
H -0.52968733024078 -5.79639029977160 -1.67661368041994
H 1.03893777319352 0.48424100208096 -1.77471068537750
H -0.56142459960677 -1.01830450393653 -3.74271825867711
H 2.02795060917469 0.41740328940199 -4.02818361537235
Cl 1.37264154095144 2.52929929301336 -4.12267986166987
H 0.72050093047458 2.74814047084791 -2.8801752279355

Int-1 (Pathway A)

C -2.21212352157343 -0.78857160912094 2.33055833081505
C -1.40592094626342 0.36238122341331 2.16875710842479
C -1.91126180172534 1.66652076886676 2.34705103592348
C -3.27615720896646 1.80308469055761 2.63368998964980
C -4.10052691332564 0.68580838945662 2.75445484112065
C -3.56941858739096 -0.59601540938594 2.617806962594566
N -0.01598061435868 0.17722727163024 1.85983701648171
C 0.55095570403120 0.11999049041292 0.64454408394926
N 1.81926345118230 -0.30266862517420 0.76617226667631
C 2.22425179447625 -0.47634106772390 2.17057003475253
C 0.94533184773046 -0.11269627039522 2.93815644266362
C 2.70252753381077 -0.69359554611554 -0.29663002678904
C 3.82891222054697 0.10310777232095 -0.57998089487527
C 4.73132875287766 -0.35779498022939 -1.54981838169578
C 4.50912336461792 -1.55387921629562 -2.22393904043197
C 3.37116084703869 -2.31271723516189 -1.94725316972483
C 2.44466706333178 -1.90716113026775 -0.9802082921989
C 4.09595906319489 1.42536621353592 0.12548376686816
C 4.31774453535654 2.57177525509832 -0.87225266874625
C 1.21464696049945 -2.75930055742121 -0.68276659669895
C 1.44165593918356 -3.67053488636895 0.53586470298617
B -0.00450404619702 0.66891892276808 -0.78537434385592
Cl 0.78207880901745 2.45335481661963 -0.77314107963263
C -1.01443627351186 2.89347027893216 2.280375225070380
C -0.69890255358041 3.39436858557322 3.70109532901377
C -1.63381381472201 -2.19971963959861 2.30444570160590
C -2.43360670767080 -3.20004860186689 1.45906089316773
C -1.59902770729322 4.01703151756631 1.41431068741553
C -1.49730062611251 -3.29189652385451 3.74591523995157
C -1.62577157192035 0.76794360265390 -1.01070603381070
C -1.81404587796998 1.61599584280097 -2.23017933730878
O -2.20183592182988 2.86586642085847 -1.955751278362319
C -2.17267415277087 3.79774325428936 -0.30657511909038
C -2.24000149331775 -0.61218042849473 -1.11641564266683
C -2.01366165383662 -1.51826306380814 -2.09212777282914
O -2.49151100317888 -2.78550700278766 -1.95008745356411
C -2.91878992103842 -3.45611428740165 -3.12567759880490
O -1.59782418813635 1.25859057929688 -3.38117742531132
C 0.74581359768939 -3.59100655186417 -1.88183915120177
C 5.28530095577363 1.30757647333220 1.09438545946252
O -1.31984190584085 -1.33772417051803 -3.2216257127809
H -1.27482261640398 -0.35813711376185 -3.40291318353559
H -2.10000791504263 1.29891965128988 -0.18061390091250
H 2.26778766821947 -4.37535065905041 0.34676283367211
H 0.53408272379827 -4.25705068764711 0.74948151987803
H 1.69291459460758 -3.10291095576388 1.44330254328621
H 0.38466347785095 -2.07822670909171 -0.44603659113557
H -0.07046740562803 2.59628986358686 1.80530602396664
H -1.61455511290350 3.73014138319549 4.21559200309577
H 0.00057711436794 4.24534140095956 3.66500270959139
H -0.24536675311483 2.604477530726860 4.32173373085839
H -2.80924005094815 3.4577180767332 -3.86654432456237
H -1.14150332188275 3.91590138625553 -3.40249196303185
H -2.54273693644940 4.7469486164699 -2.62955435294088
H -4.22037495072115 -1.46438659067324 2.73675878550331
H -5.16458522843352 0.81412573817510 2.96873038457378
H -3.69846325724994 2.801586752520061 2.76088650910805

H -1.83046765268455 3.66163772295041 0.40090066756949
H -0.86449430200856 4.83239683048758 1.32064514365607
H -2.51318559916527 4.44416792739107 1.85908365841459
H -0.62866737864356 -2.14373655807241 1.86408353694032
H -3.46048147998754 -3.32292660276758 1.83970429331017
H -1.95283126007758 -4.19054277539456 1.50988191809602
H -2.48699262534483 -2.91016587636458 0.40261910098861
H -2.49143198813364 -2.88949262889620 4.19410699764688
H -0.95749973707950 -2.02933315293502 4.40194154273984
H -0.96367852001801 -3.69414237892581 3.75626250476182
H 0.57692286733920 -0.92876728619099 3.57312843906874
H 1.06749576369929 0.78131687740202 3.56871300261747
H 3.06054116939260 0.19383547241461 2.41100958930109
H 2.55950555648739 -1.50948595504516 2.34417354625246
H 0.60550530768378 -2.95924647491627 -2.76963588615612
H -0.22644387791018 -4.04749707394543 -1.64785471588762
H 1.45149981248040 -4.40311625393288 -2.12242872941791
H 3.20005644310295 -3.23709220896087 -2.49910343009831
H 5.21972174398227 -1.895413687093528 -2.9809452598536
H 5.61448522425443 0.23939446188186 -1.78600060146425
H 3.19342539906397 1.68472185827448 0.69715611971426
H 5.23840355921026 2.42798447915498 -1.46069589644064
H 4.41582661865648 3.52774579719813 -0.33256301161354
H 3.46530402577263 2.65555234158225 -1.55973613604303
H 5.14852594427093 0.49228986624483 1.82288542192368
H 5.42817623243314 2.24708806809503 1.65295983264909
H 6.21884936788787 1.09850474306046 0.54676769611693
H -2.92135743453794 -0.91572055952760 -0.32437976510381
H -3.3522064938276 -4.41803229073426 -2.79587315223055
H -2.08446357471896 -3.63669718647956 -3.82118725483495
H -3.70212121725978 -2.88161954183095 -3.65139726630714
H 0.52936825034154 0.05918190810817 -1.67865284492046

TS2 (Pathway A)

H -1.54344096313058 -0.21741380552206 -3.36281906626544
O -3.48121131012330 -0.82449114059868 -2.76915706809851
C -1.74276257369022 -0.92413597290742 -1.16062954751870
C 3.93340623701421 0.26080834693448 -0.42739825248532
C 2.84729822059284 -0.61150901204062 -0.21173794896784
C 2.70354840126503 -1.82604361414629 -0.91881921660185
C 3.69121738882894 -1.25263733109404 -1.85656540593518
C 4.77794652376051 -1.30917860470516 -2.08257575785124
C 4.89488398062010 -0.11431505727053 -1.37538279399607
N 1.89568617296424 -0.28653428341089 0.81362751655100
C 0.63596480353664 0.14498484408066 0.64232797668615
N 0.00379979891298 0.15582986025579 1.826931128248236
C 0.94616738014038 -0.10126335392284 2.93289829540683
C 2.15019345921048 -0.69637832241062 2.20408971337249
C -1.39438121106073 0.37183191013769 2.09294418211213
C -1.87895714489910 1.68508482294117 2.26329215640484
C -3.25002001631620 1.85026153966926 2.50311121786628
C -4.10268936570808 0.75149114645717 2.58047708888703
C -3.59412232557345 -0.53948815800552 2.45490601525310
C -2.623150332671168 -0.762314109540499 2.22122070052642
C -0.96071678528677 2.89735747188743 2.25306540790227
C -1.50200977170141 4.04489893275727 1.39016106064722
C -1.69047433633971 -2.18708489959034 2.22992507521230
C -1.51476406839268 -2.67001104408877 3.68458588720896
B 0.14476918974508 0.70129796873747 -0.80399818291379
C -1.49471729851999 0.54435258796588 -1.06293161644082
C -1.67626497382810 1.26900273307278 -2.304225037011236
O -1.45137269547715 0.75873285338218 -3.47238634653828
C 1.53541824698353 -2.7757827940260 -0.69315244348916
C 0.82050878006244 -3.14079297397472 -2.002475738818158
C 4.09440576973922 1.56012390086809 0.34827380789621
C 5.22024090179496 1.44239077510018 1.39036372692209
C 1.98036605200915 -4.03482517851442 0.06947466826932
C 4.32840624667119 2.76265508587969 -0.57687496377588
CI 0.75934020319404 2.52989396185678 -0.76082354155633
C -2.55771003081439 -3.19320911944622 1.46189356177337
C -0.68723953343105 3.36764711512228 3.69277831778804
C -2.75653052730052 -1.44631983474673 -1.96226876882184
O -2.90131124226101 -2.83037277318989 -1.84548524894864
C -3.85804409917443 -3.41601249662095 -2.70237232563275
O -1.97743361901887 2.53138457052418 -2.26449833770637
C -1.93229708745865 3.31007700948754 -3.46906234789298
H -2.04319406297700 1.10009981829124 -0.28349192809341
H 2.71099303855220 -4.61622586321942 -0.51635797708883
H 1.11519056990448 -4.68637096995256 0.27380024429672
H 2.45521621599984 -3.78397080239768 1.03199274505484
H 0.79523183123261 -2.26081278164489 -0.06721348795762
H -0.00449471907335 2.59634857551441 1.80610865631306
H -1.61596752500926 3.70393445765266 4.18257318650317
H 0.02333912811625 4.21039128152151 3.69812640077031
H -0.26508873640931 2.559397214414884 4.31167417222358
H -2.55716361819665 2.84904388782182 -4.24589661339881
H -0.89216946812617 3.38715558072678 -3.81680484783525
H -2.31525873063258 4.29912382691048 -3.19430086388604
H -4.26808461298886 -1.39351588001888 2.53597820470250
H -5.17167802879528 0.90121963118953 2.75174889405576
H -3.65403846273378 2.85664158743873 2.62663760983132
H -1.72222863998065 3.70138406891060 0.36988174473483
H -0.74956969894460 4.84586025924422 1.31714106022853
H -2.41581829354477 4.48560128051290 1.82123209715708
H -0.69941872417989 -2.17363856392229 1.75075256976156
H -3.52866836995912 -2.364651150013843 1.96047288334716
H -2.05288727452710 -4.17306124859084 1.44041828806346
H -2.74176819921582 -2.88390694632909 0.42567690848558
H -2.496736688656709 -2.76465877185867 4.17558104303691

H -0.91724690019380 -1.97742051526443 4.29699054989591
H -1.02875629225129 -3.65896222439832 3.70975630791141
H 0.50605832417057 -0.77538205734605 3.67509992910650
H 1.18583829280480 0.85470751433686 3.42854930025449
H 3.11109915979640 -0.30180991504322 2.5579835838308
H 2.18525265449612 -1.79793855301361 2.26015265242685
H 0.54796620351571 -2.23459192592246 -2.56050634849691
H -0.11742119216467 -3.67679675929430 -1.79197686939015
H 1.45031620748405 -3.78060110132359 -2.64223614108506
H 3.60357625141598 -3.08275466343045 -2.42188338458065
H 5.53716820664890 -1.58369082412457 -2.81939048291075
H 5.74601681128599 0.54309572159850 -1.56456438049888
H 3.14844412086929 1.74779965207547 0.87635757679967
H 5.29245802287731 2.68920055802021 -1.10603927886765
H 4.34529394323477 3.69437165815338 0.01145127667483
H 3.52195503810887 2.84395355220769 -1.31839599083455
H 5.06163778870601 0.59443057732795 2.07599640436150
H 5.29080302530708 2.36185852887301 1.99418326280156
H 6.19545777074959 1.28579823821242 0.90083520562760
H -1.13890937950851 -1.59902133492178 -0.56304214170875
H -3.86295274557851 -4.492680893903342 -2.47583686006780
H -3.60420453811085 -3.26445369759316 -3.76612228201478
H -4.86540423498607 -2.99717100788832 -2.54258004796512
H 0.76278508664018 0.15146974470772 -1.68118409196860

Int-2 (Pathway A)

H -1.41455575203825 -1.19259578827775 -2.45949765715597
O -0.03917198200801 0.02378012749583 -1.49875567017045
C -1.75764580911319 -0.79785984160758 -1.48929205963888
C 4.14363733568879 0.22867167836056 -0.29971741963402
C 3.02464311191601 -0.61157601996295 -0.13807785084996
C 2.89524808581289 -1.83507049012651 -0.83338629060610
C 3.93320983797154 -2.20792000109514 -1.69530498971914
C 5.05640988276592 -1.39819556179378 -1.86174061656508
C 5.15682156115217 -0.19216101103087 -1.17223894975375
N 2.01778526033925 -0.25059089422309 0.81787851812542
C 0.75249131553312 0.11295723658854 0.54742791314552
N 0.04574853281389 0.12018614865604 1.69197594926099
C 0.92483608181476 -0.03674990093156 2.86503019931889
C 2.20519269359708 -0.58857191953696 2.23771680691693
C -1.38192922954885 0.19182741672871 1.83551130746991
C -2.01985545794675 1.44741272244821 1.88725669572424
C -3.41860401158684 1.46367036163019 1.96519860664929
C -4.1508849841803 0.27943403258876 2.00540118425593
C -3.49607564286534 -0.95127352919082 2.00932292834732
C -2.09959234109538 -1.02394694810129 1.93501841126539
C -1.22746965018742 2.74572798117744 1.89933381083836
C -1.80712678264680 3.82061119240260 0.97125734167704
C -1.39994847488549 -2.37473752216372 2.05373971495600
C -1.35544767168199 -2.81715624700775 3.52964214751564
B 0.32938504155678 0.62769217334895 -0.94610962466502
C -1.25633444105999 0.6324131206701 -1.31456262751444
C -1.45594938839442 1.39596511237338 -2.59555485357391
O -1.31269161571438 0.94915715971093 -3.71118519234279
C 1.68820914885470 -2.74864862661838 -0.66621970356762
C 1.06685374771146 -3.14649251589904 -2.01236337815072
C 4.28012228434722 1.54603189666987 0.44899439731917
C 5.34831545116592 1.44647893015607 1.55165437156010
C 2.03769534383143 -3.98687804790063 0.17571884474974
C 4.57635067600793 2.71763755682087 -0.497983030391778
CI 1.03819980449832 2.42519650321210 -0.87168019187502
C -2.02542355216592 -3.49047410527693 1.20471633089225
C -1.10278922656125 3.26544515748229 3.34309983900039
C -3.26344820229736 -0.89878707472054 -1.45877233174937
C -3.66876060889605 -2.18836815576007 -1.37941857392933
C -5.07648916487764 -2.39897586373831 -1.32905294022002
O -1.79204938594107 2.68265197136423 -2.36775147011052
C -1.85665275046541 3.52536466789324 -3.51082208084157
H -1.84616867629629 1.14072345492859 -0.54718450584840
H 2.79700144569886 -4.60695610915169 -0.32787885902677
H 1.14360335830429 -4.6113231777888 0.33738502905366
H 2.44198777576098 3.70662860963075 1.16164641237082
H 0.91509647591132 -2.19391216463692 -0.1191823030222
H -0.21741364298672 2.52863418140927 1.52734825125695
H -2.09222855609455 3.52029685689573 3.75774949253376
H -0.47806575247644 4.17283280267639 3.37464945832478
H -0.65040240294249 2.51433415126611 0.41100297311804
H -0.87169738236351 3.59111830790482 -3.9923581162944
H -2.16362048550605 4.51450045363679 -3.14691541753698
H -2.58460563019925 3.14327542380101 -4.24277988620049
H -4.07902662644834 -1.87248727122565 2.06660978418918
H -5.24225600856366 0.31577776685851 2.03966083927651
H -3.94186559941298 2.42097638672693 1.97729108601458
H -1.90554959152650 3.4562243792325 0.05931741836019
H -1.13179641316337 4.69042205018387 0.9039853434851
H -2.79155815137640 4.17561158555040 1.31866389445328
H -0.36364762210104 -2.24766028395630 1.70680715410003
H -3.02894517504158 -3.76014980152620 1.57118721473228
H -1.40392441864469 -4.39805299748414 1.26800669483236
H -2.12932542363129 -3.21002912794889 0.14920360798054
H -2.37374810846605 -3.01852084143955 3.89941054514551
H -0.92143497818936 -2.04776810374214 4.18604705022449
H -0.76489448264911 -3.74085653385368 3.64314555035642
H 0.47683692263785 -0.70498404517258 3.60869498729003
H 1.07992309760537 0.95042147722271 3.33219960572279
H 3.11582598609895 -0.1229554872658 2.63527633758078
H 2.30140957359549 -1.68292431805120 2.34609306695391
H 0.84937705734561 -2.25752550238039 -2.62123381035328
H 0.12340368740527 -3.69117112659922 -1.84951898527337

H	1.73447631217888	-3.80566206208245	-2.58996645204301	H	-2.27924125969456	-4.22015767164457	-1.67942928516328
H	3.85959532487948	-3.14632286996980	-2.24887311409172	H	-3.81762181757449	-4.68117813958836	-0.90203871590409
H	5.85540125891961	-1.70748108290686	-2.54027864836813	H	-2.27587318876325	-4.87914117780193	-0.03369718617749
H	6.03472219561652	0.44061117699351	-1.31809908078261	H	-2.42248113942988	4.14771779951670	-2.5579929406663
H	3.30795381137352	1.75899570097292	0.91651056153485	H	0.7811428818278	5.31417818065668	1.30571976358509
H	5.56268762352212	2.61455167842852	-0.97905280590509	H	-0.93853719655194	5.73060254400425	1.65868297486723
H	4.58034871986066	3.66570928471667	0.06387947709414	H	-0.04195694303306	6.64785703512743	0.40826648106260
H	3.80557134057584	2.78724516168965	-1.27759526166426	H	-2.01305439184974	1.32992963271330	-0.00748252843005
H	5.14750216014508	0.61775327306991	2.24993758283446				
H	5.39509257127841	2.38102195094052	2.13420689746132				
H	6.34692320566552	1.27054000724402	1.11903187216974				
H	-1.35365837468523	-1.47680434536112	-0.72617966171991				
H	-5.22462742020516	-3.48517177362394	-1.27556846866755				
H	-5.56758756100779	-1.98947876887783	-2.22493084381519				
H	-5.51156723011990	-1.90967530068826	-0.44359047593486				
H	0.97746225259975	0.01518918156281	-1.76474225293751				

TS3 (Pathway A)

C	-5.15839811562620	1.96788622805734	-3.78852018533322
C	-3.77998062679835	1.70460749423181	-3.92077064671913
C	-9.2724891959246	2.51833400509405	-4.70275044351893
C	-3.48398378859502	3.65019051453587	-5.31129126598910
C	-4.83625432365852	3.95398230048700	-5.15844406769300
C	-5.66439032683448	3.11439290417161	-4.41551023217707
N	-3.20835271256997	0.55104324919018	-3.28687306364867
C	-2.71309419253357	0.45683642012254	-2.04119685006662
B	-2.96711435401763	1.41523543733158	-0.74514847512973
C	-3.36481914281865	2.97855187390563	-0.99538059614511
C	-2.14135848705260	3.74694749505554	-1.57605682375396
C	-1.69746177521392	4.93066921963784	-0.74723917542475
O	-2.28296313524387	5.98430684238504	-0.68648325185620
C	-1.46847661986856	2.15526841728179	-4.96335583466002
C	-1.31236035273260	1.58208554302143	-6.38488339719553
C	-6.08729545271110	1.02792775872641	-3.03569800551064
C	-7.02631388591780	1.75827065570194	-2.06669315946281
C	-3.04466887030886	-0.71034490911443	-4.03191960263976
N	-2.04576781746259	-0.70302333137938	-1.92222188243851
C	-2.00979580322292	-1.45522461938165	-3.18668790474944
C	-1.19982384328245	-1.09983495442417	-0.83269054993753
C	0.06545171088424	-0.48599593579260	-0.69516619412594
C	0.9050777298494	-0.94570601982241	0.32624278700666
C	0.50609118534873	-1.97543859986599	1.17751506395866
C	-0.74762825485586	-2.56243322991749	1.02439967501497
C	-1.62760230530193	-2.13716075816891	0.01967989620113
C	0.54376386162441	0.62258477964424	-1.62320848368052
C	1.10012785823766	1.83090554542797	-0.85825150839088
C	-2.98333420698829	-2.80948690899792	-0.13859789668827
C	-2.83049869861247	-4.22374756268891	-0.72514071360180
CI	-4.43388546385797	0.45437699314192	0.07806386265557
C	-0.48600887364667	3.31747893616742	-4.75913662023884
C	-6.87877730578379	0.16268642151702	-4.03294901625185
C	-3.76776203584483	-2.84744545166783	1.180544830642794
C	1.56688251939343	0.08894231189293	-2.64037469845155
C	-3.82726876755505	3.50510168377510	0.33597618435539
O	-3.11872507712371	3.79159008999515	1.27415463850869
O	-5.17444845410277	3.58118467790765	0.39806311565191
C	-5.72307918458942	3.87032263906442	1.67902537535230
O	-0.55077054272404	4.68078096806358	-0.08584139792124
C	-0.16805974423889	5.65959034695672	0.87613794630608
H	-1.28368275380008	3.07582233083682	-1.70767564353004
H	-4.20900831869404	3.07692236944988	-1.68368130854716
H	2.47837060178595	-0.26702971195322	-2.13333401126885
H	1.86113096854825	0.88195285041617	-3.34742328583495
H	1.16331455086901	-0.75546334566117	-3.22182146819159
H	-0.32192654635133	0.98500265859746	-2.19390802567006
H	-5.46825641850306	0.36070265265920	-2.42176788292674
H	-7.53908458380990	0.78440281774550	-4.66012933571920
H	-7.50864874272244	-0.565794880453883	-3.49706979741956
H	-6.21146602652886	-0.39445327027674	-4.71063776879871
H	-5.33126237113157	4.82148807930934	2.06957551725646
H	-5.47466554580025	3.06779426744957	2.391712150014585
H	-6.81047069446683	3.92987807299494	1.54168887159325
H	-2.84961833389401	4.30524866534333	-5.91194628069117
H	-5.24958798590222	4.84878321680976	-5.63029492309735
H	-6.72440299868113	3.35420616783413	-4.31493208652794
H	-6.46542180208986	2.37609273598698	-1.35184181860450
H	-7.60265992363017	1.02098263989277	-1.48603437975786
H	-7.74940591499668	2.39754704861675	-2.60000686745708
H	-1.18435200717208	1.36856012051853	-4.24921227718859
H	-0.67027238950410	4.13716347252549	-5.47143252163181
H	0.54588274948738	2.96803216590928	-4.92369024117424
H	-0.54554885443313	3.73032428648759	-3.74435103908331
H	-1.52814305967195	2.35491677946997	-7.14016947393656
H	-2.00237601802746	0.74496606288524	-6.57297998353100
H	-0.28321314525355	1.22455968304747	-6.5512997408865
H	-2.71587786514452	-0.51941473610817	-5.06033284884498
H	-4.01414897973578	-1.23494690255559	-4.06922129762055
H	-2.26622314806779	-2.50935363404265	-3.02188073690933
H	-0.99306478899829	-1.41080914965398	-3.61292093688744
H	0.37328441932183	2.21791736732128	-0.13155131635729
H	1.33325559204864	2.64921023273633	-1.55747522636145
H	2.03068330726001	1.57950914821398	-0.32439114102894
H	1.88713032910336	-0.48760568773213	0.45947657348706
H	1.17669401103956	-2.31844953542384	1.96943428729013
H	-1.05438540969123	-3.36265859217891	1.70097241383977
H	-3.57298022580522	-2.19888436882355	-0.83747537253966
H	-3.27693241010108	-3.49091404213394	1.92878355918430
H	-4.77745647268260	-3.25375157851136	1.00768374619581
H	-3.87407759262878	-1.83629151596835	1.59615602920522

Int-3 (Pathway A)

C	-3.17420501424445	5.99047228115730	3.62421195055498
C	-3.89919693135761	4.83843339169379	3.23667759316859
C	-5.25877743731089	4.66376442456758	3.56600450745933
C	-5.87005078213673	5.64622958188387	4.35708211707804
C	-5.16386040032228	6.76644812746058	4.78835983627024
C	-3.83223107081481	6.94142300600796	4.41345475189358
N	-3.23215586493273	3.84327946875860	2.44313354053728
C	-2.51410049432136	2.79669416271942	2.88272303492576
B	-2.50819473885559	2.06986532931174	4.34655839580997
C	-2.73182341608828	3.00035652949610	5.67502787380653
C	-1.40822709597245	3.66295017613616	6.14001067209652
C	-0.52952302908692	2.82813993199674	7.05203741140926
O	0.02773056875649	1.78210629966856	6.40944976966940
C	0.64993706494760	0.80421252435956	7.23657408767912
C	-6.06904577237778	3.48266186454829	3.05669011824867
C	-6.89382058234002	2.81500520096037	4.16460295497498
C	-1.74848042716805	6.25499881543493	3.15487866228837
C	-1.74559318319886	7.261624848980475	1.98817831614072
C	-3.14725809227303	4.00360470735745	0.98002672893787
N	-1.87749914086772	2.23006999386214	1.84662373933474
C	-2.28429371609350	2.80727089036175	0.55392932284529
C	-0.83049840690642	1.25063553413552	1.916961577370803
C	-1.09084808789276	-0.07171494724914	1.51341337452444
C	-0.02002122995415	-0.97816497479978	1.51158758505440
C	1.25271085919183	-0.58618561842451	1.91439324634910
C	1.48214307626169	0.72488816001909	2.33573697219379
C	0.45201504484244	1.67063559615958	2.34453886776201
C	-2.47618730828330	-0.53339105498233	1.08629127182586
C	-2.52946191971275	-0.78925180340007	-0.42951859372239
C	0.71618469636216	3.10441721303682	2.78952841008613
C	1.79271292654957	3.22258556842812	3.87353860027937
C	-6.96084939943575	3.91636809282654	1.87994635888424
C	-0.81506908351553	6.75413146796959	4.26700303467820
CI	-3.98860465603900	0.84114357862669	4.06624053614133
C	1.04704674601929	4.01236913162607	1.59283333595797
C	-2.93597941559922	-1.76955522741438	1.87255882047298
C	-3.33843476769439	2.14185321112981	6.75034759696507
O	-2.74487098466695	1.35024021201328	7.44749626145142
O	-4.67585274817871	2.31681468094668	8.64238493206717
C	-5.36433513262706	1.39564541069327	7.68279697840480
O	-0.30927249276671	3.08609001467427	8.20921652182253
H	-0.81167410294733	3.93375448092847	5.25649031703398
H	-3.45353990646523	3.79816004383254	5.46511513400858
H	1.97349584761197	3.67948491544196	1.09739340590256
H	1.19306537454491	5.05363665494843	1.92342354268309
H	0.24862978403858	4.00968221227469	0.83646815976975
H	-0.21232875258787	3.47919001563450	3.24130527717818
H	-5.36287333572614	2.72430774905429	2.69445024193302
H	-7.70182588308084	4.66755200698758	2.1999420199679
H	-7.51034984043769	3.05223303632950	1.47252122332078
H	-6.37368315722624	4.36443518323086	1.06175571483851
H	-4.98123527827203	1.43900716499334	8.71342905651961
H	-5.24142776431527	0.36937649345116	7.30357968647967
H	-6.42270563189885	1.68564665653319	7.65357354701673
H	-3.29461867139671	7.83389946243132	4.73932714053589
H	-5.65639756780164	7.5105658111163	5.41392636630207
H	-6.91653151075628	5.52597342366616	4.64264617424493
H	-6.25434047885882	2.56211293099462	5.02032125577872
H	-7.34445372187954	1.88420097951235	3.78596742985008
H	-7.71531729021832	3.46430869608479	4.51066741892998
H	-1.33410737688980	5.30697492636734	

TS4 (Pathway A)

C	-3.09178401089745	6.00297236203825	3.68328678373667
C	-3.81669456325648	4.84900023493104	3.29776576153608
C	-5.18159702952117	4.68041155649296	3.61264584500541
C	-5.79744429162911	5.66696757505987	4.39445028404211
C	-5.09011729358825	6.78582425921524	4.82982444170975
C	-3.75576445024405	6.95732870327769	4.46428590510101
N	-3.14761785491191	3.84710801361756	2.51397049071685
C	-2.50381893190100	2.74868519129996	2.94700260945656
B	-2.59846533646362	1.96287902068888	4.38865243351407
C	-3.01413618757480	2.85431466158240	5.70037421650338
C	-1.92321309466527	3.84738481416269	6.11068385125570
C	-0.51740572345097	3.40416933021307	6.46302280257024
O	-0.37338625773393	2.08931390452349	6.62645278454025
C	0.83161093879352	1.58069388190343	7.18515183220949
C	-5.99079514282529	3.50301997062083	3.08973261847922
C	-6.84070892309417	2.82969123931012	4.17497098412610
C	-1.67211048430877	6.28057453510771	3.19471163939680
C	-1.71773183083936	7.29322620476414	2.03197370868551
C	-3.01322823258943	4.03941349636942	1.05807974698153
N	-1.85838169295647	2.18482547225809	1.91047987532643
C	-2.20511492628385	2.81122341087019	0.624782229851245
C	-0.86809446485128	1.14629429370059	1.96055863145167
C	-1.17535458411215	-0.12851082212891	1.44816677788083
C	-0.14821210613620	-1.0838382378593	1.40542776034594
C	1.12891975891000	-0.78521993141759	1.86673721407146
C	1.40620304374503	0.47873990564120	2.39034611212674
C	0.42206934836039	1.4717938299495	2.44767432988504
C	-2.55991970968506	-0.49472209795434	0.93296069471865
C	-2.56287441437340	-0.6205428722284	-0.60050912948026
C	0.74421941516864	2.85188456416125	3.01375074746546
C	1.94264263676120	2.85649659171755	3.96814460765605
C	-6.85947898350038	3.95029273644095	1.90025900682424
C	-0.70142504614405	6.79051942976495	4.27181624166981
CI	-3.97958757402522	0.68667801614258	3.93259081426166
C	0.96910875280627	3.89194652906873	1.90226649366586
C	-3.09621627357344	-1.77652844185012	1.58683023317352
C	-3.48752516657239	2.04040070900465	6.87817729459671
O	-2.85795977908547	1.754483344325621	7.86957458946309
O	-4.78808562367326	1.68502857238131	6.73588967224529
C	-5.31801238504600	0.82334229213814	7.73314097456405
O	0.38406372500573	4.20707040545237	6.60029757246368
H	-1.80043858854150	4.58642433764342	5.31202168516623
H	-3.88761008883153	3.45796031121262	5.42014137451903
H	1.81617244482819	3.59597143062736	1.26251951213082
H	1.20118666496971	4.87532581934686	2.34069050549036
H	0.09072120117501	4.01528526054544	1.25473108082796
H	-0.12776590828955	3.71191910395451	3.60364334713661
H	-5.28668245184219	2.74082416731514	2.73199723140798
H	-7.60436627139351	4.70058032214276	2.21323892334899
H	-7.40304243514255	3.09125482768089	1.47469264192498
H	-6.25534858374597	4.40418034790777	1.09779329471083
H	-5.24754572232039	1.28009487746716	8.73269171227200
H	-4.77306021331056	-0.13353742076914	7.75115885164752
H	-6.36847831730759	0.65185647172061	7.46407084154606
H	-3.21913054196332	7.85084012618891	4.78886545503831
H	-5.58614557570777	7.53845999781951	5.44787789184766
H	-6.84786645007311	5.55247057100433	4.66799110673706
H	-6.122173084597107	2.514017733637	5.02574614136836
H	-7.32177611895533	1.92948950459557	3.76112715754098
H	-7.64171469975945	3.494441194820540	4.53935007511272
H	-1.25889129769110	5.33804697546198	2.80894330583392
H	-1.03649120102407	7.74947307171255	4.69794337502166
H	0.28597977304798	6.9698596506527	3.81694684598990
H	-0.55344830598223	6.08082251940619	5.09721968714526
H	-2.03125530813135	8.28404094245232	2.39848914533373
H	-2.43163590535957	6.99975464328029	1.24734577063047
H	-0.72223924008413	7.40216830087454	1.57197674063731
H	-2.50079416492325	4.98725553714464	0.84459544081775
H	-4.01065312736969	4.07956923253347	0.59732483958252
H	-2.81077788577973	2.11585744746157	0.01725156421231
H	-1.29564256719798	3.05958917102321	0.06004215649725
H	1.86648246193772	2.05122610955440	4.70991720057484
H	1.97992187591322	3.80745326789154	4.51797035779798
H	2.89487689451095	2.73455014292837	3.42638172810132
H	2.40910163745741	0.69241963445287	2.76007859690250
H	1.91595730410020	-1.54264709380947	1.82801356900182
H	-0.36056675469482	-2.07947724202264	1.01064984870777
H	-3.24700251457404	0.31006275217469	1.22916074875201
H	-2.49946679901214	-2.65969524639718	1.30663299871892
H	-4.13244857862340	-1.96025978181075	1.25983576597528
H	-3.09876956161986	-1.67977019084873	2.680912778800301
H	-2.18378558690291	0.28945110702970	-1.09242038605979
H	-3.58212472008439	-0.81346766271707	-0.97337464001743
H	-1.92306570568725	-1.45640681813399	-0.92815228147011
H	-2.24553383660326	4.43660146477605	6.98764161423418
H	1.13865422554741	0.71406334449246	6.58268479561971
H	0.62024277172364	1.24939332198243	8.21372764447351
H	1.61681360879802	2.34825149073447	7.18862559987419
H	-1.57745726752520	1.33913805541821	4.53559880687440

Int-4 (Pathway A)

C	-2.99464225132960	5.9980553596652	3.60188269816502
C	-3.76385873411630	4.86141095542614	3.26520961744609
C	-5.10941174695267	4.71531168999198	3.66232329314187
C	-5.66211545903874	5.7220008629114	4.46466774834818
C	-4.91328203331991	6.83795687886227	4.83781715575732

C	-3.59798865380520	6.98000098418210	4.39899579776793
N	-3.15585737728853	3.85345972593632	2.44670601221799
C	-2.47905963896304	2.76944161389602	2.86095815625020
B	-2.52882558694590	2.02130009545049	4.31396733408425
C	-3.10849735138966	2.77625318160457	5.64892950085840
C	-2.26335207366300	3.90716622827708	6.28626575147110
C	-0.86983060404060	3.49081301327090	6.67375445893808
O	-0.74810077502664	3.27624226145222	7.98982531547534
C	0.46873684005079	2.67363974608385	8.42167427605224
C	-5.95891668772317	3.54124000103138	3.19643412747952
C	-6.78239999505183	2.89779011903056	4.31980440605711
C	-1.57782566449556	6.21262844525877	3.07618246853403
C	-1.56277312281310	7.36965977632614	2.06057558142081
C	-3.06027729610314	4.05887376026767	0.99152738276401
N	-1.86259480354364	2.20850774099886	1.80623045791519
C	-2.25189394256821	2.83903486692914	0.53321826659616
C	-0.90097501429821	1.13958363187494	1.81959170962426
C	-1.26175695983482	-0.12350248597521	1.30822661743683
C	-0.270371171767326	-1.11400377964829	1.24594661774855
C	1.02395248271509	-0.86278341976827	1.68682567804021
C	1.35632356375539	0.39107069029041	2.20020703831443
C	0.41172265180467	1.42113276531809	2.27335746478796
C	-2.66172509076224	-0.44404091405352	0.80252200142912
C	-2.68410890599289	-0.53240532556619	-0.73400052865445
C	0.80380507151458	2.79528412754441	2.80778086792931
C	2.03494579479083	2.7689817612191	3.71816717642922
C	-6.86454787459732	3.98286207333519	2.03237803670357
C	-0.53200552561787	6.44340219104425	4.17771097624766
CI	-3.86714620252080	0.66017395787733	3.86581563851279
C	1.02496238271742	3.80358600608737	1.66638954240217
C	-3.22207438720640	-1.73152300843096	1.42475455753559
C	-3.33241103866969	1.68187003528092	6.66488736743414
O	-2.46396084180658	1.04276277991587	7.21191691884535
O	-4.64696756048980	1.47364681253657	6.90654821064852
C	-4.96031699843249	0.3399538471452	7.70844682192628
O	0.05337136529484	3.37376674203980	5.89595966988227
H	-2.17544198532143	4.7249296234908	5.56376760230571
H	-4.08659806152315	3.21765929146765	5.43263374811057
H	1.84521325883454	3.47417555756064	1.00765604190958
H	1.29342258735023	4.79075787815510	2.07510454292255
H	0.13202831686340	3.93668638127910	1.04027285720734
H	-0.02125442152084	3.15395503759468	3.43833949378201
H	-5.28110293166432	2.76144668394387	2.82523146376369
H	-7.58542571655164	4.74994822996308	2.36059019886505
H	-7.43623273149087	3.12610830969278	1.64051501869585
H	-6.28298472938128	4.41424376676230	1.20163167958128
H	-4.46594163421317	0.39922936406925	6.89000537992976
H	-4.63234116473441	-0.58346900681689	7.20591618348335
H	-6.05150478773083	0.33821684956659	7.82745604287057
H	-3.02677912240306	7.86652369234799	4.68340165413171
H	-5.36307918832421	7.60923980478123	5.46817568300771
H	-6.69616488078462	5.62954246705233	4.80192278428911
H	-6.14440395506606	2.55147092331526	5.14467704116988
H	-7.31454592815756	2.0174536332279	3.92640398643798
H	-7.54157411249615	3.5886952968201	4.72243617308673
H	-1.27004535464438	5.30113857057278	2.54766887434917
H	-0.80845189028699	7.28228492284558	4.83623800026878
H	0.43998425081306	6.69021167335248	3.72128406231590
H	-0.38395136756153	5.54577016049612	4.79287809114824
H	-1.78525181154540	8.33029830243494	2.55264897096915
H	-2.31331036756722	7.22810553629320	1.26654664211314
H	-0.57132330288057	7.45575526801548	1.58735440969478
H	-2.56170738613866	5.0149932130090	0.77349607395916
H	-4.06823270541475	4.09349750278940	0.55348263231730
H	-2.86067251478685	2.14224563882099	-0.05942137616856
H	-1.36115852394416	3.09647496606782	-0.05649144027263
H	1.91124174770787	2.04425318453082	4.53390405829842
H	2.16605686520048	3.75652702913212	4.183114665450396
H	2.95628497931099	2.53295423105762	3.15981575242155
H	2.37246796717555	0.56930870504301	2.55103856466404
H	1.78152339886802	-1.64917523696829	1.63743566031954
H	-0.52475472829206	-2.10037670275075	0.85313026819208
H	-3.32685897795948	0.36818740903062	1.12673755847130

C	-3.30730044702908	0.71318396028061	1.58165572460357	B	-0.16604166587650	0.09283569792929	-1.40457995438620
C	-4.23483367419858	-0.30829341426918	0.91061927954181	C	0.80377655506315	-1.13088519274012	-1.93914862010282
C	-0.29808987611372	4.202847373406939	-0.70800699139709	C	1.64215568767176	-0.48872554484458	-3.05290150885864
C	0.23860383531365	4.99893676115567	0.49369520871751	C	1.00248036259246	0.83952938674345	-3.30377347338627
C	-0.23851032048705	1.79870749724045	2.22517996389746	C	1.43576608912005	1.61494154311528	-4.22777552744071
N	1.36344900571622	0.83348626354524	0.80891871069742	C	0.86969769825712	2.95637815147117	-4.36524365815017
C	1.22916241894510	1.35325517727603	2.17693695474595	C	-2.03411201321312	-0.16624406329411	2.09250188552068
C	2.63074413641568	0.36312938210482	0.32898058085104	C	-2.52199968049549	-0.02193203772388	3.54189236567025
C	3.51478295943758	1.29318372859954	-0.27451849347048	C	-1.96648580581165	3.68145734072296	-1.29755863277846
C	4.73893209025500	0.82390208881011	-0.76887389720408	C	-2.37026164664737	3.67791270583988	-2.77631958835948
C	5.08860006921784	-0.52126935466415	-0.65616792270815	C	-2.16868061486727	-1.61466034397489	1.59603477981238
C	4.23727610323664	-1.40670188991985	0.00043195478392	C	-2.13150494382029	5.08266626716888	-0.68654024649762
C	3.00765196768259	-0.98426737514443	0.52799812142541	O	0.03243170773560	1.14674168752589	-2.56394444590763
C	3.21166535029783	2.78388341316696	-0.32479457944529	C	1.51015747479308	-0.98882845898118	3.05644343883525
C	3.55825543242797	3.43739435829314	-1.66962204401703	C	4.35007735435500	2.27162266061379	-2.52487113308112
C	2.17839267947336	-1.93903389720123	1.36918670310003	C	-0.09719185772185	-2.20821613120740	-2.45919164271137
C	2.83930227430275	-2.11213848154399	2.74856803248819	O	-0.44493495833672	-2.35251170388159	-3.60836706625700
C	-3.81433560438508	1.107638408108125	2.97808580443204	O	-0.53356604754907	-2.99963818417384	-1.45413926046648
C	-0.26310612506547	5.06701919810258	-1.97214235837814	C	-1.50259164845245	-3.98715119242356	-1.80166758457569
C	1.82821652248378	-0.18393472765984	-2.94655233082966	H	-3.15475654328904	5.47252441215073	-0.82598967408868
C	1.34932203634359	1.18311236220949	-3.28459940196077	H	-1.40690128779406	5.76636604061998	-1.15319400785250
O	0.54259401767257	1.73089144634690	-2.51506723255765	H	-1.92192623334547	5.07349529755652	0.39472244466004
O	1.79764427637898	1.70735820207004	-4.36150786799530	H	-0.89087640002960	3.46210288336337	-1.25849526942286
C	1.23403424690518	3.04433111722040	-4.72155482938187	H	0.5958698300149	-1.08867493425816	1.14169749784646
C	1.93885081442628	-3.29811587685302	0.70138453414387	H	2.41152508732362	-1.36025794586811	3.57010572144052
C	3.94742111853903	3.51972187937999	0.81072273252834	H	0.62828347513977	-1.34349594376029	3.61332523720967
O	-0.57416394585641	-0.9259798380641	-4.13833158066631	H	1.52419989372863	0.10888763882069	3.11192543769394
CI	-0.99321580192924	-1.40494756148389	0.55084595226827	H	-1.10423409993394	-4.67705342140658	-2.56083017277375
H	-0.43002584542014	5.84170031614522	0.73283765909977	H	-2.41193135183031	-3.51420563453193	-2.20280183527002
H	1.23894428942888	5.40840816700813	0.27654897107855	H	-1.73245277580445	-4.5286860949479	-0.87560828016834
H	0.32214517794583	4.37424992487162	1.39385055691126	H	1.43372153960337	-1.54897615223633	-1.15152271554016
H	0.38554916926220	3.36764364290416	-0.88932726100997	H	5.77045557094078	0.35331868995675	-1.16078052094591
H	1.8000453066633	-1.49975876711811	1.502193297785146	H	5.80653345688685	-1.91190192494682	-0.14373602381468
H	3.82215727339716	-2.60733944362053	2.66882887368152	H	3.83878191441871	-2.74134358434175	1.10168282901015
H	1.20119554481711	-2.72969029255909	3.40102032396529	H	1.29775790362337	-3.38988866349274	0.52683532755620
H	3.00160288435193	-1.14353639967825	3.24941169354126	H	0.39931354749332	-3.31636858811748	2.054440472061892
H	-2.32061691095672	-3.90564830632603	-2.742601241927676	H	2.157586664368759	-3.52061976724228	2.090857311416995
H	-1.60149330270129	-3.38559678733596	-4.31644813355038	H	2.76684972595388	2.59791612497597	-1.14525635529163
H	-2.74249366283277	-2.30825611178332	-3.46257273639600	H	5.43510721995922	2.07882008540048	-2.56787448807139
H	1.02300210787290	-1.49204454522392	-1.36097466418956	H	4.17158220371573	3.28137429913163	-2.92585183676286
H	5.42974512562050	1.52150544534679	-1.24643940308449	H	3.85453232706701	1.55760902984736	-3.19938745294390
H	6.04049411279023	-0.87451600673844	-1.06100240701020	H	5.66337604232022	3.00133660104535	-0.24874375659238
H	4.53453509667119	-2.45010775851534	0.12234665835336	H	4.27626824345479	3.10311601671342	0.85771390236025
H	1.40915441419969	-3.18296989916007	-0.25423861173259	H	4.36476227126527	4.21790984639089	-0.52226659714699
H	1.28920243690148	-3.91006394849520	1.34531313533112	H	2.08106544431505	3.14284872366866	0.86912365905964
H	2.87434261847201	-3.85839317894587	0.53294955201277	H	1.97414254885642	2.016932621403102	2.28482528991203
H	2.13470248304477	2.91025443823730	-0.16300518879796	H	-0.40399793293863	2.57841077173904	2.42816453144942
H	4.64736282998744	3.52293167203471	-1.81092031044755	H	-0.10194798922555	3.74420739706145	1.07803763713705
H	3.14518357741955	4.45754524666441	-1.71314306906768	H	-2.25202463633413	2.67628344622364	-3.21798642399118
H	3.16349755691759	2.86965272455336	-2.52147032704557	H	-1.72804004232947	4.38091967094135	-3.32949498642968
H	5.03881250108377	3.44839100593248	0.67491600321565	H	-3.41549246607395	3.99577641406443	-3.92798763757933
H	3.71167045613133	3.09456781969469	1.79728219285968	H	-4.65211246942007	3.26235866429886	-1.19270101315028
H	3.67431126456273	4.58737307905121	0.82441898289719	H	-5.91154027639810	1.60793527164050	0.16132710618008
H	1.93758815514559	2.18104582815825	2.33824157094354	H	-4.69922500930533	0.04917448307983	1.660803943242629
H	1.44680563182669	0.56299919272192	2.90890271269126	H	-0.96470045177163	0.08220369767643	2.09288350306515
H	-0.80025466606758	1.08253814589320	2.793644115714549	H	-3.22711853633704	-1.91770057112604	1.55056849386894
H	-0.38306228387794	2.80314136346590	2.645899898667564	H	-1.65235274830378	-2.30740660646491	2.27929415283018
H	-0.69292918453128	4.53349707827019	-2.83200742360340	H	-1.73839941336689	-1.74174866508649	0.59180960684540
H	0.77836369602351	5.33456214583920	-2.21322943874813	H	-2.42382824325740	1.01671110677770	3.89507974641510
H	-0.81357306157235	6.01293786324948	-1.84559414158719	H	-1.93372085076344	-0.66956413026213	4.2123239877392
H	-2.73613201675387	5.20579110552229	-1.40170349823056	H	-3.57992741284254	-0.31106417286460	3.64651038375203
H	-4.98364145269704	4.36712739151036	-0.80196539582448	H	2.68821413371526	-0.31993654722731	-2.75517127680417
H	-5.21563432565354	2.31255051848925	0.56596114154965	H	1.01239827261838	3.51237832869395	-3.41622403023911
H	-2.34658573419424	0.19207888994922	1.67604129210123	H	-0.19532852229587	2.86473540770417	-4.61171365854083
H	-5.25558659358042	0.08223745773782	0.75988059323992	H	1.42821041724577	3.40644990786493	-5.19219354173142
H	-4.30415904800991	-1.21126188893404	1.53719228352296	H	-1.34074013574239	-0.174497152535435	-1.34491200512760
H	-3.81464448317608	-0.61918069667406	-0.05597890286788	H	1.64456380018487	-1.06617764055612	-3.99106502753470
H	-3.13435161433124	1.82106891534161	3.47260094962389	CI	1.334787918411403	4.43754888030849	-1.26694799987884
H	-3.89756529221329	0.21620539926868	3.62100470475208				
H	-4.80924227134995	1.58242839302182	2.93237246727061				
H	2.74619863717493	-0.06973719815362	-2.34942004607951				
H	1.48641814830113	3.79883544269954	-3.96546964496195				
H	0.14193323747668	2.95555636705447	-4.80232061652326				
H	1.67736844958353	3.30142954757292	-5.68979105419333				
H	-1.27665536656790	0.62460223448372	-1.64749141585109				
H	2.07903475808892	-0.74125953260508	-3.85915041358120				

Int-5 (Pathway A)

C	-2.71257337781374	2.64128987160434	-0.48869080124053
C	-2.04251254881048	1.73638305657642	0.35989639540640
C	-2.74076620415193	0.80305929063712	1.15685207461811
C	-4.13777850839175	0.77072238823717	1.06290590662052
C	-4.82069278969004	1.64623343960771	0.22052142859588
C	-4.11214858298777	2.57281950452636	-0.54058395351510
N	-0.60804218653081	1.78952980301247	0.47589442581581
C	0.27396081354673	0.97909998290261	-0.11071238337464
N	1.50021684422176	1.16935499783204	0.39373020769431
C	1.52013757711825	2.3188589444913	1.33011004251526
C	0.03818066065484	2.711443581628259	1.42771563411778
C	2.65675118379063	0.33082021581706	0.21617590586240
C	3.77416309480216	0.82073289963039	-0.49667129853277
C	4.89991662596564	-0.01017510371430	-0.61145183683084
C	4.92168191023129	-2.78739700936447	-0.04169940869257
C	3.81072341586859	-1.74403986512045	0.66261997030708
C	2.66288835826025	-0.95711552243067	0.81232618368637
C	3.79636488773044	2.21144333204783	-1.09565358162593
C	4.57693464523276	3.18822980877623	-0.19738093975288
C	1.47165283389997	-1.48927464608809	1.60265981725211
C	1.33510367616841	-3.0155977408451	1.56030459778418

TS6 (Pathway A)

C	-2.70990470565515	2.67465388302921	-0.55993147493676
C	-2.06931020742100	1.71311492314846	0.24770704567026
C	-2.79344506252685	0.76252993955894	0.99918644491508
C	-4.18865369535377	0.75818795962505	0.88268186507989
C	-4.84328206711070	1.68102296824072	0.06857877578905
C	-4.10927011690367	2.63346058016628	-0.6346350780708
N	-0.63609734671905	1.73835584165022	0.3705272946657
C	0.23683949674162	0.91042555660614	-0.21128950324290
N	1.47530484544622	1.15586942862101	0.24749167480491
C	1.49789621932501	2.3449027643434	1.13830916408376
C	0.00892061627134	2.65455849647730	1.23939015396118
C	2.63810722296513	0.32343739175692	0.09646106296527
C	3.76953287660776	0.83003442617616	-0.57764972834037
C	9.40418727534361	0.00894303590768	-0.67249253585238
C	4.91868272313181	-1.26560049159062	-0.11941069445432
C	3.79627548522457	-1.74327845089401	0.55875268684834
C	2.64169543322874	-0.96469302539311	0.69465261507090
C	3.82173434766107	2.23545002457151	-1.1505486592019
C	4.66653061411201	3.16661370506234	-0.26341428136299
C	1.44914491746310	-1.49364660806926	1.48659442351402
C	1.42639882447581	-0.310881263538712	1.62783071832551
B	-0.24323922020235	0.00570865970903	-1.50454687867454
C	0.72740586679004	-1.18505780829544	-2.13089630876575
C	1.19257080750787	-0.6130733687464	-3.48262635377977
C	0.74071843129405	0.82185285275245	-3.49152622975125
O	1.22076846383697	1.72050951419349	-4.21706242859310
C	1.22032653807456	3.31042578993400	-3.72942425233254
C	-2.11519794363706	-0.23233232656370	1.92738072728440
C	-2.58489828810445	-0.05829943405729	3.37982489410111

C -1.93995189443793 3.76042402313739 -1.28886336290065
C -2.29703431663097 3.83161165137035 -2.77889100130960
C -2.30121568761015 -1.67961191533874 1.44541598289135
C -2.13962526016747 5.12786500291157 -0.61296969891051
O -0.14947676933541 1.08334317393025 -2.59619602723128
C 1.38070553736512 -0.83832692255231 2.87723475620340
C 4.32221519239247 2.47462114617739 -2.60032916858508
C -0.10108241551597 -2.42230947461518 -2.29675000813431
O -0.62500088100594 -2.80561503879197 -3.31622226743327
O -0.25113742150777 -3.07003969488837 -1.11695190754837
C -1.11234541143846 -4.20621816820714 -1.12476677789519
H -3.16339315932464 5.50885460568641 -0.76652010460539
H -1.41342490311315 5.84495405402169 -1.02371541112731
H -1.96846215709950 5.06772855945198 0.47372045129127
H -0.86781554941519 3.53695655604372 -1.22424133473432
H 0.53578532363837 -1.22672341408378 0.93662839115688
H 2.29178612111443 -1.06489788314177 3.45395239543955
H 0.51624776071342 -1.21946266646309 3.44292950206588
H 1.28619053693273 0.25429430932148 2.82070565002786
H -0.76137294678606 -4.95988358435904 -1.84550572933724
H -2.13816108422739 -3.91442211932831 -1.39677137432644
H -1.09117756944799 -4.61162751925977 -0.10537848550528
H 1.57701770462860 -1.41840007578107 -1.48120018304791
H 5.78861728305474 0.38365320934795 -1.19096479837410
H 5.80892197035563 -1.89314672285985 -0.20901019061362
H 3.82524575085578 -2.74181995697854 0.99361677889509
H 1.50941838319329 -3.51342331185739 0.65090916430867
O 4.7372451157166 -3.33045481533191 2.08143117152610
H 2.2386840540662 -3.38300015010494 2.28386879677960
H 2.81032765722204 2.65628718706557 -1.14832484167811
H 5.36664840984835 1.93465687062711 -2.68553909025908
H 4.28336343778871 3.31040432049416 -2.97035140568356
H 3.70551257107272 1.65264153375228 -3.26606815466749
H 5.73852810749861 2.91542845078838 -0.32484431560392
H 4.36877014099072 3.09783493052474 0.79413922733483
H 4.51905154394927 4.20829185027980 -0.5866886358904
H 1.98985366568472 3.18365519305943 0.62505881932354
H 2.03088212718985 2.10747181430096 2.06897179001592
H -0.37085028495714 2.44732449852441 2.34357561455978
H -0.21464419564470 -3.69562178494972 1.06078998313548
H -2.09715776169785 2.87341050480241 -3.28124743668852
H -1.69821044241478 4.61883248114382 -3.26399343098156
H -3.35671408147447 4.08871012078627 -2.93840013028253
H -4.63024576277680 3.36469550072824 -1.25593735916251
H -5.93328746958656 1.66315021082552 -0.01017303296297
H -4.77139767053387 0.02332352964821 1.44282956642386
H -1.03865099508976 -0.02415975688648 1.91443860829398
H -3.36635303382065 -1.96186107662563 1.43512065153034
H -1.77617700722400 -2.37978553382018 2.11518771279503
H -1.90115689908496 -1.81392866390371 0.43142549826816
H -2.43691393534060 0.97667814902706 3.72676178679413
H -2.02320013679631 -0.72883916399990 4.05059672448327
H -3.65469573242441 -0.29693506591819 3.49141250901541
H 2.27665339538069 -0.66226060750713 -3.65806314443263
H 1.38901984405288 2.16606020334003 -2.34214371702624
H 0.21851642363387 3.66375322273233 -3.49318638929509
H 2.05969084459483 3.76167663423810 -3.79834444809731
H -1.39746218280683 -0.32073721653609 -1.34894665827146
H 0.69286444409074 -1.14338549355868 -4.31203848221731
Cl 1.42701318250699 4.98352114878231 -1.37684421284327

Product (Pathway A)

C -2.79430791943466 2.68645698370179 -0.46900468639918
C -2.05714733188590 1.74794908795000 0.29612643863469
C -2.67891771988537 0.70530077508714 1.01144860225756
C -4.07950486080054 0.62780433211623 0.96748812161384
C -4.82572964303763 1.54497119206010 0.23472019048956
C -4.18727705211408 2.55960423742818 -0.48122684311819
N -0.63263317131913 1.90045940325289 0.36735707633001
C 0.25267207314468 1.65865120132370 -0.61147380040610
N 1.44703131895866 2.14205065854634 -0.25573271694570
C 1.41922195176926 2.81970134195678 1.04970138248595
C 0.01431662248727 2.48056244931073 1.56265548954865
C 2.64054040029687 2.16082410548250 -1.05212125485308
C 3.57484476275361 1.11632646235722 -0.91322563221440
C 4.74773125425703 1.19267787886612 -1.67662357788567
C 4.97682776668884 2.26320036626989 -2.53944590828162
C 4.03656896817167 3.28704979685607 -2.65427409531559
C 2.85159647617971 3.26007061357890 -1.90912038396322
C 3.34824308786186 -0.05203489060478 0.03451623674436
C 4.27185997077040 0.05478731954538 1.26006548966854
C 1.81938088879441 4.36843636508574 -2.06648720236167
C 1.10118671960533 4.26340237867493 -3.42097022151059
B 0.1016999471267 0.68532645159783 -1.93374005453917
O 0.42530767275524 -0.65230431100958 -1.3424758632376
C -0.55945788505420 -1.54927592354500 -1.44618003101599
O -0.50329694684941 -2.65043281813427 -0.95246036027034
C -1.88868331839569 -0.29178838708716 1.84869625203167
C -2.33889790413623 -1.74653220431947 1.64968084412505
C -2.10024959541607 3.77990192889332 -1.27894635076306
C -1.71152796511378 4.98115754528904 -0.40040695543781
C -1.97240399929082 0.08388261626033 3.34111755388357
C -2.91037719172601 4.25293588408205 -2.49054972406831
C -1.40166967463968 0.46761037041842 -2.60662722714196
C -1.27909736678816 0.69874623636806 -4.07595451484312
O -1.35814529388009 2.02899054462405 -4.36714808797784
C -1.14014982235141 2.38439119689767 -5.72750263486936
C -1.73065398058576 -0.98234461188091 -2.24285044797964
C 2.42517636253129 5.762788566716251 -1.85282101045618

C 3.50307288279585 -1.40737928333743 -0.66852060691829
O -1.09231194064932 -0.12985661469760 -4.93481619732449
H 5.33209692092127 -0.01525485577881 0.96604612436882
H 4.06631720913939 -0.76051626231514 1.97253217723207
H 4.14221096972021 1.01331935038826 1.78948126497611
H 2.30772809256522 -0.00295450350043 0.38319223041633
H -1.17440989091355 3.34860029850488 -1.68571547181335
H -2.60837608883615 5.45255111213420 0.03334681255071
H -1.18304509663742 5.74035140449026 -0.99907679516455
H -1.05171003255487 4.69619521291094 0.43064077443713
H -1.86514893230629 1.88434939010453 -6.38793037753170
H -0.12657374620426 2.09894131448484 -6.04976307865740
H -1.26142827196473 3.47413576069351 -5.78428425787501
H -2.14760388306781 1.16552479154091 -2.21893375388536
H -4.58834469005568 -0.16980773056482 1.51146925539104
H -5.91540251082488 1.46560208323070 0.20937295634317
H -4.78673036553240 3.25586711147351 -1.06786961193661
H -3.20359557027049 3.40957189332297 -3.13042818806991
H -2.29373703644665 4.93086511408664 -3.10064437025108
H -3.81315673062591 4.81047363345017 -2.19289813655000
H -0.83652967549935 -0.234508242253749 1.52852120416420
H -3.36871506603165 -1.90433569446933 2.00834236923573
H -1.68416760157349 -2.41754856386429 2.22715711236239
H -2.27275073477740 -2.06426512255101 0.60151738212684
H -3.00520601233878 -0.03148664470054 3.70863917752240
H -1.67705666097019 1.12758579871511 3.52932620351622
H -1.32518503421018 -0.57285315433437 3.94447998960483
H 0.04079220082993 1.73312785526481 2.36870512017285
H -0.54891840230566 3.35183622123315 1.92292451519951
H 1.58491599195991 3.90151304700649 0.910808642714044
H 2.21822817879621 2.43175860033972 1.69627221425137
H 2.83153131265721 -1.47124293972779 -1.53470271196344
H 3.22996956608338 -2.22190429327726 0.02054798989385
H 4.54036247390449 -1.579854854213278 -0.99992487007744
H 5.48954646518134 0.39522606700886 -1.59787462440145
H 5.89551002787083 2.29915438070324 -3.13045907879827
H 4.22401719892525 4.11744268129671 -3.33863211800862
H 1.05273723068054 4.22953536317921 -1.29116969110769
H 1.81088025053266 4.39359139481747 -4.25419372210903
H 0.32837156190758 5.04471517162495 -3.50961709648857
H 0.61229085917674 3.28694442959496 -3.53778699556105
H 2.93697730929581 5.83567710080855 -0.87979040619469
H 1.63684281214097 6.53235372935491 -1.88525201209041
H 3.15962945600656 0.61215153752622 -2.63527118920104
H -2.64364760062263 -1.07716122318158 -1.63504794527036
H 0.94950155647451 1.03121206943151 -2.73586690298547
H -1.86446056161430 -1.61087092141451 -3.17322318208579

Reactant (2) (Pathway B)

C 3.65919618667100 1.56269612862183 -0.11460930063547
C 2.98839765472355 0.42387209469622 0.62124941059555
N 3.40239282074930 -0.86782847961032 0.05145791693399
C 4.62528112092092 -1.07507633442166 -0.48056644652601
N 5.49128695967365 -0.02811250919262 -0.46726290043721
C 5.15266681746187 1.33239514981125 -0.02945315280320
C 6.89020650636506 -0.16915411490155 -0.79765363184351
C 7.33656778521501 0.25499968390230 -2.06663786262762
C 8.70998043258884 0.21577534096292 -2.32662699777257
C 9.61130175742107 -0.23234899971939 -1.35983271184321
C 9.14645191864631 -0.65284196096835 -0.11625625628453
C 7.77843534312585 -0.62740970907805 0.19340997299461
C 6.36275539224921 0.67843948067247 -3.15681215063354
C 6.42974483142515 -0.27847579965788 -4.35877768497159
C 7.30825579221973 -1.07931445861207 1.56892975312798
C 7.80633557420498 -0.12518930113701 2.66699858613449
B 5.14898367092711 -2.36462382814997 -1.27206510085543
C 5.31353193709239 -3.95442830345056 -0.9580934940142
C 4.83531183873539 -4.80210881083660 0.14522783762919
O 3.69006716147103 -5.05076928925998 0.45415686545663
C 2.45161508339866 -1.93102171952706 0.27945089613638
C 1.49486320035461 -2.23699249819124 -0.71392932439874
C 0.54976441058714 -3.22375264455717 -0.41141766381585
C 0.53465603617895 -3.85392579124316 0.83360042897621
C 1.46157242576256 -3.50351924500698 1.80768346186162
C 2.43903658490513 -2.53361982898441 1.55217008300230
C 1.45719429492921 -1.50344455561357 -2.05150632061954
C 0.60217582475014 -0.22508748685684 -1.95602802249627
C 3.39083456471923 -2.11231566121361 2.66695320302515
C 4.23311027185957 -3.26493499920176 3.226341214444996
C 0.94978595599457 -2.36714872221253 -3.21247754979756
C 2.61380041932154 -1.40914251970041 3.79434770744052
C 4.29058222451744 -3.53047001608421 -1.98563857652675
C 4.49565597167611 -3.77842912909279 -3.42263014817375
O 5.80231641667817 -3.93280517133934 -3.76343161569344
C 6.06543539418838 -4.13182683022476 -5.14450012685993
O 5.88877660981209 -5.36662776817393 0.80872563712520
C 5.56838027213297 -6.36360371304738 1.76913100884226
C 7.71145746644869 -2.53155230375043 1.86270671795271
C 6.58230132052953 2.13632601200272 -3.58923390587077
O 3.61809651857078 -3.82456248463186 -4.26277803386799
H 8.90612103507246 -0.13779057347340 2.73878949323338
H 7.40389228570569 -0.42072348286512 3.64983203157380
H 7.50048190268583 0.91492848301583 2.46923641465180
H 6.20984082644387 -1.04415777451471 1.58010915974453
H 2.49030198528080 -1.20929551746718 -2.29156713447821
H -0.43996876994006 -0.47714905473731 -1.699744712262045
H 0.59345117294390 0.30331118123104 -2.92317429640593
H 0.96711074043092 0.479537027661525 -1.19558219890562
H 5.73032425046214 -3.26754929245252 -5.73991383758443

H 5.54780279888087 -5.02729281528378 -5.52274331071660
H 7.15281834228561 -4.25346338546316 -5.23642518193156
H 3.26420162801156 -3.71268728145567 -1.67044348336904
H 1.43996353865917 -4.00208804663147 2.77901195941257
H -0.20994604238896 -4.62628870043711 1.04151892481298
H -0.18795363620976 -3.50732469079284 -1.162674558997198
H 1.53365362744702 -3.28907558609007 -3.32700117025491
H 1.05100011592527 -1.80902067148539 -4.15648254653501
H -0.11760885522186 -2.61679788233699 -3.09586733447605
H 4.10355787471616 -1.38704281239356 2.25000771270534
H 3.60162350359857 -4.08810844020301 3.59435359696613
H 4.84589970281127 -2.90783014396680 4.07032827739061
H 4.91008894711476 -3.66882777060839 2.46577002946448
H 1.93017241149733 -2.11144949453711 4.29792155532951
H 2.00267750929433 -0.57680776305329 3.41132374519575
H 3.30448365140446 -1.00988351113543 4.55523247479024
H 3.25068099190560 0.46169586173285 1.69240647871877
H 1.89490628033020 0.47315904836031 0.55893627147446
H 5.70889743547890 2.03239900284414 -0.66818416885221
H 5.51472027864782 1.48637832897935 1.00315747448501
H 7.30096897906935 -3.22284660778068 1.11403188575890
H 7.3203431438703 -2.83935241324920 2.84999394666117
H 8.80722395782687 -2.64845143760135 1.87810573767278
H 9.85786861473227 -1.00791233560330 0.63276780784291
H 10.68122867850774 -0.25947456049148 -1.58106797733685
H 9.08006206816848 0.52649329468391 -3.30651521136615
H 5.34656435819583 0.59861852785267 -2.74316182464519
H 7.40473265162735 -0.20994328275751 -4.86851951171797
H 5.684843475274639 -0.02849883433419 -5.09471287110562
H 6.28340107775931 -1.1883025114753 4.03589648561288
H 6.50900415432725 2.83141467725875 -2.73700979580513
H 5.83290285760974 2.43621753475377 -4.3396606737384
H 7.57824258190866 2.27356183437154 -4.04084336621275
H 6.27595669790751 -4.29756941894665 -1.34061540126152
H 4.95355917830310 -7.15971237078802 1.31784216647248
H 5.00619744416943 -5.94213630547965 2.61728071653134
H 6.52264537331040 -6.77383711631598 2.11994055124597
H 6.08696473803852 -2.02935717331406 -1.93426041104003
H 3.33129172265327 1.58022524458291 -1.16682342221320
H 3.39280633957360 2.52864933055169 0.33953541732488

RC (Pathway B)

C 3.41359862755114 1.37205164293424 -0.73784618286068
C 2.86332612361515 0.45583063954040 0.18266440171923
C 3.53276186138708 0.73167212747765 0.53851199899892
C 4.77542899689768 -0.99471361337328 -0.05462632006294
C 3.54216454423553 -0.10033004884065 -0.95847060286758
C 4.66205534787942 1.06903434431598 -1.29591134089148
N 1.66144748704186 0.80792301810896 0.91242426665565
C 0.40875975683183 0.41174622915523 0.57527101147159
N -0.58750885225690 0.64434906156276 1.45553476067367
C -0.39631798535724 1.4194662982493 2.69737957951627
C 1.96999975745595 1.53783722066585 2.15141079700521
C -1.89495340614966 0.02207134357696 1.40876130086562
C -0.3188993159102 0.84774379839968 1.26058876610011
C -4.29319195749037 0.27741569682246 1.46963888598284
C -4.42941023048639 1.06468242238920 1.80416598893638
C -3.29851167998940 -1.87280094901701 1.90697073662872
C -2.01136005257616 -1.35486292041092 1.71497366546473
C -2.94093150629993 2.31296761158579 0.85769246671233
C -3.71815054813437 2.59188928137402 -0.44182530395642
C -0.80026306199879 -2.26417848285522 1.89162687057229
C -0.35106980765202 -2.31660014083897 3.36165740828714
B 0.23651473841945 -0.17766001605279 -0.90108444812707
C -0.76569681583777 0.71423359737314 -1.85331247826190
C -1.00663842002918 -0.76427536823035 -1.74146833452096
C -2.38716879050871 -1.22851831761923 -1.47809866471406
O -2.4503457386924 2.58576833647246 -1.48513438450513
C -3.75998891702931 -3.14476704597895 -1.39461184039447
C 2.93990712663080 -1.74366195248571 1.50640435315128
C 2.58322767718608 -0.04598111305546 0.77375214523158
C 2.68131506699877 2.6397643438356 -1.14354338621865
C 3.18745648682022 3.8785881384326 -0.38681975510010
C 3.85878419073995 -2.00558935092047 2.70857018388968
C 2.75457614745185 2.88264103666397 -2.65656891588708
O -0.33576212121652 1.38037336980339 -3.06826791521692
O -0.36902194337942 2.60693375174042 -3.24097932893559
O 0.1911133817065 0.57938413176115 -4.03521986307129
C 0.51184870931719 1.19071331079882 -5.26356616971764
C -1.02681325715095 -3.67869073140056 1.34264604698877
C -3.43126200050876 3.26314629039590 1.96375825250639
O -3.7966421144207 -0.54573925087918 -1.35582699026049
Cl -0.47865131045407 4.29827320570642 -0.90676975943455
H 4.80659399461868 -2.47574778620801 2.40083153008587
H 3.3699333447223 2.68378692342768 3.426716337787112
H 4.10736048950493 -1.07038053435239 3.23521604060868
H 2.00382309774487 -1.32724162328061 1.90151465549726
H -1.88720571557280 2.54795569903639 0.65382985648975
H -4.50651072445678 3.12080100840027 2.15969253322781
H -3.28083867393352 4.30916309449520 1.65307377263716
H -2.90458228188812 3.11715534986264 2.92031714303860
H 1.35294727363788 1.88164014396383 -5.10889064189587
H -0.32626381471777 1.75174751123173 -5.70323188089272
H 0.81176203471188 0.36922614728715 -5.92590101193103
H -1.45780928996141 1.332258677883778 -1.28339812324302
H -3.41599981771170 -2.92900474883144 2.15280295643663
H -5.42223572670386 -1.49165244811689 1.96732831858001
H -5.18296541112282 0.89840892859884 1.34936002120872
H -3.50361244677239 1.83357536726652 -1.20537577791944

H -3.44371379523499 3.58499889602541 -0.82828907348162
H -4.80607655803705 2.57805916814924 -0.26399117462346
H 0.02155187936414 -1.83868771097490 1.30335302566727
H -1.78980992515495 -4.22839062851331 1.91684127560691
H -0.09496398256960 -4.25959349994603 1.41049917857674
H -1.33575212291359 -3.64090309432307 0.28924313123976
H -1.14604021081692 -2.73968478677522 3.99723221438066
H -0.10905051830511 -1.31831876354968 3.75521274465635
H 0.54530721711728 -2.94803931307570 3.47272144433586
H -0.24720369592930 0.71960402419281 3.53724653114544
H -1.32604325268568 1.95900577651937 2.89775400484426
H 2.85262715221477 2.15794487233654 1.95490394312886
H 2.25007338452286 0.81859595294576 2.94291801182115
H 1.87787852313913 -2.85516251087559 -0.04869547753114
H 2.12214618957634 -3.76766302066479 1.46584041416368
H 3.48187077490397 -3.51886316273855 0.34618635070154
H 5.30630267522487 -1.91512441389385 0.19919033107093
H 6.31505887919273 -0.31675219379103 -1.40702222253001
H 5.10661034474940 1.75994273131319 1.95490394312886
H 1.62243283197516 2.50961313408037 -0.88735977969649
H 3.76098126139272 3.203902146661383 2.97112048069401
H 2.04170559742741 3.666763768665696 -2.94674222349302
H 2.50176795104787 1.96762781367829 -3.21085869553255
H 3.11015732420486 3.76180646868581 0.70449224459279
H 2.58543675441945 4.75648995025573 -0.66675582091032
H 4.24450924694455 4.08223532275181 -0.62643849207084
H -0.57125059994809 -1.35896448913450 -2.54936552331473
H -4.39409165245971 -2.79472442866349 -2.224017503390060
H -4.24285668753876 -2.86363309549068 -0.44774228440144
H -6.33211227776225 -4.23389420299715 -1.44849742523646
H 1.28854083802676 -0.49731139742184 -1.38438987676608
H -0.49327832988281 3.48192405629940 -2.02344136532349
C 0.77559216294038 2.36442581704096 2.56965630538429
H 0.56466881578456 3.13544399859930 1.81089620989323
H 0.96616359092749 2.86617970109281 3.52995660919083

RC-New_mechanism (Pathway B)

C 3.21305212546552 -0.99340252072580 0.24881472980467
C 2.74806442595991 0.33758457448637 0.25237726008639
C 3.39460158837049 1.36306248088048 -0.46985910179467
C 4.49500639571929 1.00519656208081 -1.25719471508397
C 4.95254556198138 -0.30965588503521 -1.30381700115139
C 4.32449140191852 -1.29632904254287 -0.54835964097644
N 1.61868358912863 0.66720743604473 1.09819610975638
C 0.34287857744318 0.576608033893270 0.67252765697932
N -0.63671345423683 0.88272701711962 1.55425786753803
C -0.41118970968372 1.64044166270654 2.80389072592103
C 1.94440752360529 1.05739878719793 2.47386874420825
C -1.99946596417498 0.42046533811979 1.40147257302351
C -2.28543930871112 -0.94505336728664 1.66777600696007
C -3.62455127711144 -1.34854645865781 1.58957980566930
C -4.64204708288588 -0.44659626995793 1.28693104755451
C -4.34101680088841 0.89140944835108 1.05849648916673
C -3.01979407261696 1.55456404735734 1.1435222522061
C -1.20825046599728 -1.96983550368034 2.03956989939464
C -0.61875614860115 0.42046533811979 3.44397749497470
C -2.76113963679745 2.84249994968457 0.89448188550985
C -3.42413499789273 3.36905330534081 -0.38604804298907
B 0.16175888369801 0.35526611431301 -0.91102975513245
C -1.21685740106253 0.13188595254993 -1.76779538119299
C -0.0913623929721 -0.90741204326679 -1.85485534335918
C -0.54158316233360 -2.27472204662095 -1.54355387301468
O 0.26571044038633 -3.20538478525145 -2.103993293301
C -0.11923319693254 -4.56435849110142 -1.91681940559807
C 2.94595073938706 2.816250490480172 -0.39648040298284
C 3.74042277314714 3.58781725933410 0.67411733206384
C 2.59386667096480 -2.06672865471074 1.13207178573646
C 2.43161205618264 -3.41306420902407 0.41648897906556
C 3.05036525250025 3.53810368266354 -1.74386559827281
C 3.40690419120997 -2.24297889457033 2.42737737556712
O 1.48205787610981 0.9271973343592 2.89330380946682
O -0.68271073254223 1.29956105298797 -3.82354216289229
O -2.70221123066897 1.45583766576874 -2.98911312406906
C -2.98764026636547 2.38947931433734 -4.04589581883065
C -3.25249433205465 3.67515179649953 2.09546607303613
C -1.68121705484905 -3.42669376823513 1.95056540746765
O -1.53015785212912 -2.58528511680542 -0.91009399018064
Cl -0.44461677142541 4.16162426466723 -1.93737744240871
Cl 1.24315630092262 3.90807830584865 -4.95279764364293
Cl 2.05317723639621 0.85940704235829 -4.17799237559930
H 4.41853228210556 -2.61641875724171 2.19939366816063
H 2.91970169921476 -2.97004916394671 3.09804351934160
H 3.52396353889473 -1.29654882861283 2.97593461769273
H 1.58830768020063 -1.72608061145684 1.41336742032637
H -1.67617088331438 2.98639197129469 0.77633626546685
H -4.35021199189554 3.62128386065696 2.17518320595175
H -2.97733349833522 4.73460281083696 1.96853014003808
H -2.84586781321934 3.32772160237728 3.05749884117393
H -2.86742151545426 1.90381163921312 -5.02422709706762
H -2.31128804368115 3.25159763514869 -3.97747555993333
H -4.02840234046847 2.69503213488566 -3.88885679989063
H -2.11179294396696 -0.19960363918762 -1.24127655096283
H -3.88046007421401 -2.39218915002237 1.76318144148208
H -5.67712096477877 -0.79277010646972 1.23074266570211
H -5.14470774560456 1.59304650856764 0.82811594047561
H -3.14480632350399 2.76103844326400 -1.25146958291994
H -3.11076994427087 4.40672253601822 -0.57643134200768
H -4.52262040143080 3.36456355055992 -0.29905909716398
H -0.39595748900620 -1.85712385330306 1.30700668971129

H -2.40086561640118 -3.66686129162745 2.75071322849322
H -0.81536659881291 -4.09469899693223 2.084733918067488
H -2.12949103037941 -3.64607080933397 0.97562819744742
H -1.41367292234833 -1.75362392447902 4.20740551918500
H -0.06816457691160 -0.80623191353350 3.53633082986540
H 0.08735435315053 -2.55733449444458 3.68633930927205
H -0.65181211095586 0.993913542600991 3.66032921573370
H -1.13029924927506 2.46532602151040 2.82440586566804
H 2.99580274856652 1.36505499418940 2.49017800465121
H 1.84615083479875 0.18548730996621 3.14215212520122
H 1.95427420740169 -3.28383068615262 -0.56262472837168
H 1.81447066911659 -4.09473036463813 1.02435747493858
H 3.40333365644679 -3.90856753016291 0.26035711204453
H 4.70068612499153 -2.32049117786520 -0.57876643436451
H 5.80592824341174 -0.56627489206913 -1.93608122771732
H 4.99237950199313 1.76679872256566 -1.85795887395951
H 1.88348948003581 2.82416018781792 -0.10983978936378
H 4.0993400580916 3.73316693512954 -2.01990175664872
H 2.53729985531636 4.50940614088645 -1.69343074306346
H 2.59783942067386 2.94280559156095 -2.54503295058030
H 3.65954292503805 3.13874500639741 1.67531061923638
H 3.38384891381748 4.62862697802705 0.74099483029734
H 4.81091172307052 6.31409522088578 0.41318244072995
H 0.54255461457892 -0.87130922594925 -2.74387294003184
H -1.13409330458065 -4.73983014090308 -2.30487681318367
H -0.10312461984647 -4.83658626203192 -0.85021741202395
H 0.61113480032212 -5.16719651313862 -2.47103136719239
H 0.90969323150001 1.13286878961013 -1.43801916987839
H 0.35771255817315 1.00875306401539 -3.83060368752081
H 1.67421821423781 2.61280415824944 -4.70851395943325
H 0.25190382621627 4.04142753622738 -3.05697859246788
C 1.00602981433925 2.16790635528068 2.90156281235629
H 1.21346091493494 2.49056973155176 3.93268274318955
H 1.14776448908115 3.03845589716788 2.24215188953814

TS1 (Pathway B)

C 3.73646728566789 1.71188257815123 -0.30162453265645
C 2.91622674067183 0.65194404730737 0.14115288424950
C 3.24680427982250 -0.70087877108419 -0.10487042594190
C 4.42865740305366 -0.96614410104490 -0.80824727445362
C 5.25839613802712 0.06389575048201 -1.24693169422501
C 4.91059670987046 1.38761795326661 -0.99606017399977
N 1.76778867752792 0.95593811259494 0.97374925674806
C 0.48343190908793 0.85143851458278 0.57245496826075
N -0.48987102869657 1.064314865977733 1.48516511806905
C -0.26865475701281 1.69288577252696 2.79723768132709
C 2.09815364373590 1.30075586752075 2.36378566629640
C -1.82801757588225 0.53607054277067 1.33263638444544
C -2.87657568692209 1.37466919353983 0.90013176405344
C -4.15978881150936 0.81921288619676 0.81105169011715
C -4.39394359597669 -0.51162785669107 1.14674971943930
C -3.35274211785579 -1.30570331449768 1.61536584413205
C -2.05385440125334 -0.79843393923656 1.73766328019582
C -2.66643989801385 2.84402771841814 0.56694529096760
C -3.20343387882495 3.21324967623448 -0.82283942714364
C -0.98098370776268 -1.65451419802201 2.40259852290630
C -1.26458635615221 -1.76703897879633 3.91315232505203
B 0.21288680009116 0.65156887154977 -1.00239214337097
C -1.09180653525854 0.04741027342048 -1.65541313771003
C -0.64811186924366 -1.39312859891550 -1.63561645223755
C -1.59949754623066 -2.41847897126099 -1.40684866785307
O -1.03684601185239 -3.68650112529229 -1.52332306294286
C -1.92959893365789 -4.76357776595367 -1.33339391653103
C 2.38525021238677 -1.85858482912480 0.38221709852785
C 2.36486545061787 -3.04419833471416 -0.59217189054703
C 3.41066833343988 3.17860987390211 -0.04866606053149
C 4.35004929169479 3.79412265754582 1.00405892150922
C 2.83158245336406 -3.22179626248121 1.779695910621129
C 3.45471302877240 4.00687226575303 -1.34187257943824
C -1.38879028492511 0.46618816857264 -3.04703131711511
O -0.83558343188653 1.4623490706168913 -3.64290700100193
O -2.21521444946912 -0.24453941799705 -3.75613685553702
C -2.44634102019342 0.0881901159368 -5.13072983425730
C -0.83466269195914 -3.04968462260262 1.78613114603309
C -3.29974266886118 3.74437751749096 1.64240091404723
O -2.78648099718454 -2.30107017365628 -1.10422808536115
CI 0.18985175542824 2.96524214138764 -1.42302520319724
H 3.87334207706694 -2.68205380575894 1.75523673691456
H 2.19453434728732 -3.14626204561800 2.13529093820991
H 2.78167053443248 -1.51102617682294 2.52180191029788
H 1.34810830618911 -1.50468809472189 0.44613214971172
H -1.58557702833793 3.03564862099669 0.54261258752897
H -4.39415126059974 3.61583092433225 1.67453681066003
H -3.09066205423175 4.80605650586868 1.43226627485192
H -2.91647594849754 3.51462479253223 2.64964880286799
H -1.51676252232509 -0.01895185512909 -5.70866462445394
H -2.81423591124601 1.12039504783403 -5.222159706849031
H -3.20047394731723 -0.62485814869189 -5.48193427124965
H -2.02725851867262 0.12977782977686 -1.08430377661039
H -3.54915656992780 -2.34464728880480 1.88201485883470
H -5.39543226206936 -0.93482664314703 1.04105129858215
H -4.98747675728078 1.44107788783567 0.46326418461694
H -2.75663722521146 2.58073343858530 -1.60091373424375
H -2.94369132586592 4.25576591929207 -1.06368554765043
H -4.29978930174420 3.11427661412056 -0.87736508975453
H -0.01233488708618 -1.14902226532136 2.283178972352002
H -1.77632317281011 -3.61667434726539 1.84046500941402
H -0.07439908587262 -3.62549677109391 2.33769329337264
H -0.53305230541732 -2.993867877234 0.73439527880102

H -2.19498326165386 -2.32933852254322 4.09312468500417
H -1.384498289316960 -0.7803394072574 4.38780819359870
H -0.44508293724998 -2.29864763303802 4.42433132612174
H -0.39272148585747 0.93299747153429 3.58529702099725
H -1.06631133885724 2.43579817981140 2.93972062755540
H 3.12719751212586 1.67257389319324 2.38064249170793
H 2.06995314512029 0.38896363458466 2.98570897794858
H 2.20284866855489 -2.70863474753058 -1.62593838656072
H 1.53773974909914 -3.72403107960866 -0.34325811920623
H 3.30383343426619 -3.62120997631331 -0.55882293980257
H 4.70354670428002 -2.00115366711149 -0.101543298577674
H 6.17745698092232 -0.16796498838030 -1.79119624012540
H 5.55915539520697 2.19127185831320 -1.35033824750299
H 2.37740109479817 3.23227814905034 0.32046297064403
H 4.47897682017156 4.08180634102129 -1.74192438727042
H 3.09939436352737 5.03088831835356 -1.14429168896791
H 2.80049349966541 3.56998599074565 -2.10711649559796
H 4.32734266532723 3.25148335565626 1.96197268332832
H 4.07218277116933 4.84179284309629 1.20394020481611
H 5.39420043027232 3.78638291464638 0.65107036550101
H 0.28447578051279 -1.65451623476867 -2.13200568694482
H -2.77963708259285 -4.7150437819914 -2.03480091463061
H -2.34704987736503 -4.77613525817083 -0.31218874932251
H -1.35270761696693 -5.68388043580110 -1.50629128231629
H 1.21217340889982 0.47338709786903 -1.63778564276108
H -0.35132686253029 2.05930236068358 -2.95254939134707
C 1.10513146963587 2.32259426544269 2.88088323826086
H 1.15717910714671 3.23484333963731 2.2607545487495
H 1.33164270810471 2.60019460419110 3.92093817707573

TS1-New_mechanism (Pathway B)

C 3.21589977862025 -0.58176124186772 -0.20814976812809
C 2.80304521702821 0.73050000714503 0.12123259565883
C 3.53181774120488 1.86765348311688 -0.29181374656037
C 4.68292704015242 1.66163934828399 -1.06519716351469
C 5.10128671537173 0.38142240145665 -1.41099776906553
C 4.37256177815403 -0.72522449000267 -0.98348894117933
N 1.65287865250297 0.91195954791180 0.99299927853441
C 0.36595556193013 0.81969186387747 0.60691867817219
N -0.58842993487780 1.02990561769201 1.54381181404398
C -0.37187449740702 1.82589469086109 2.77061562109865
C 1.95836686864657 1.17048829842667 2.40588924465757
C -1.92539395940157 0.48313863039438 1.44320323871738
C -2.10620713927491 -0.88651116989339 1.76490970277735
C -3.41090936544048 -1.39254391848070 1.74311984278833
C -4.49849764899153 -0.57916575007756 1.43712628204061
C -4.30133733484125 0.76754463646982 1.15147708339516
C -3.01744712920042 1.33094289217052 1.15297709576993
C -0.94686983408588 -1.80230176394508 2.15720725656285
C -0.53217382644816 -1.61920080488348 3.62880460863948
C -2.87149911207205 2.82062911068654 0.87338636396584
C -3.51453590715383 3.23094969735626 -0.45894297792434
B 0.09112504034720 0.59577847923810 -0.9546881380843
C -1.20642479755293 0.04198257241659 -1.65912871696094
C -0.54459116689817 -1.31080243283071 -1.68883088413580
C -1.30037883622160 -2.48264686134408 -1.37282584521066
O -0.54177936548034 -3.62777309176445 -1.48009928963685
C -1.24850115828435 -4.85482271611077 -1.44517113908483
C 3.14078002329157 3.2915307885322 0.08140690569424
C 3.99679975173025 3.82382432052473 1.24532789288166
C 2.46228854178589 -1.82025585748982 0.25961641445012
C 2.57750377392592 -3.00468369785540 -0.70744916554844
C 3.23056560170924 4.25788592943868 -1.10930993682761
C 2.90648769738848 -2.24917394534507 1.66882302739891
C -1.46691246771513 0.55939467130125 -3.00875505337684
C -0.99429774216359 -0.08130173487259 -0.01391967453621
O -2.14838842227177 1.62818795437102 -3.20735714811210
C -2.25957662999727 2.18497027456759 -4.53837926044257
C -3.45607845613459 3.65601562545713 2.02675954035832
C -1.23343797743689 -3.29015974095999 1.91444525945375
O -2.5418746286840984 -2.5418746286840984 -1.07139681135991
CI -0.10339244748300 3.20230397857186 -1.14530880684099
C 1.20708037490260 2.66626433046959 -3.95449967335111
CI 2.32333002164269 -0.64905990150846 -4.03910533728417
H 3.97017688256809 -2.53861551991902 1.66773910094630
H 2.31834273166368 -3.11670124133477 2.00980428177882
H 2.78431303140382 -1.44737140286225 2.41030348212981
H 1.39621874502868 -1.56222853320608 0.30003465421357
H -1.80248463506611 3.04851530361205 0.77648147787184
H -4.54563567578243 3.51036927226293 2.10834148016654
H -3.27283496591787 4.72921660989046 1.85589167635133
H -3.02053098925851 3.38519503270290 3.00183336327622
H -2.69859910706517 1.44171838057414 -5.21754231364938
H -1.25680266522873 2.48245351539989 -4.87372123815050
H -2.91476117691559 3.05545124840297 4.42909390719516
H -2.11208188929271 0.08440513170294 -1.04425920190427
H -3.58062540522351 -2.44711578288141 1.95394840125208
H -5.05081298066187 -1.00214970093215 1.41785313931732
H -5.15952463340447 1.40112233492270 0.9183468666267
H -3.11276821389252 2.63988495570236 -1.29019154707201
H -3.29166767164319 4.28874958913115 -0.66902269649966
H -4.61062276562001 3.11410519635128 -0.43517663509210
H -0.08869421041552 -1.53528911936896 1.52640204897321
H -1.89063472850808 -3.703717163061409 2.69747334362431
H -0.29229239860010 -3.86086200335862 1.94443612813373
H -1.71592648209062 -3.45239877794525 0.94528321204259
H -1.37760920626604 -1.85174343518443 4.29654392257944
H -0.19753254650949 -0.60090551439499 3.86095889270993
H 0.29450497250195 -2.30399673894362 3.87743971701757

H -0.67748132900388 1.21615727157035 3.63231268049798
H -1.05377468964691 2.68505866597374 2.73286939538304
H 3.02391926739596 1.40613219753188 2.48166769502734
H 1.77618416634352 0.25071712890661 2.98652245841658
H 2.37193096889422 -2.70048953548593 -1.74295023974475
H 1.84059580769472 -3.77427481350633 -0.44014619236034
H 3.57966608761645 -3.46266024949692 -0.67432509755336
H 4.70179838749061 -1.72362397299511 -1.27009840844756
H 5.99471296831880 0.24322035954033 -2.02470295378099
H 5.25341567518842 2.52615180568375 -1.40840936495906
H 2.08628272686137 3.27595074585702 0.38471083958824
H 4.27709854673587 4.48827462946939 -1.36848365960635
H 2.73594889530947 5.20841557202581 -0.85562596555231
H 2.73795794007282 3.84794788568855 -1.99944565988429
H 3.92752636200514 3.20052356107623 2.14946262060023
H 3.68374756894251 4.84522941754934 1.51701203458061
H 5.06027231754074 3.86390424448738 0.95824996308786
H 0.47271296749653 -1.42070353425686 -2.06210391274521
H -2.09776107570290 -4.85012413271174 -2.14719895087256
H -1.64329500213297 -5.07430179863243 -0.43972295301361
H -0.52862188012738 -5.63486225029641 -1.73013414818871
H 1.06811221678638 0.67591244805708 -1.62668856242270
H -0.57564758382748 -0.90444100281745 -3.58724004221803
H 1.98002073300999 0.61426186386240 -3.89704230089263
H 0.61542139936172 2.93900720120293 -2.64054424105851
C 1.06604493931014 2.28972080436501 2.91006390293618
H 1.28361276858185 2.52730044175093 3.96205565664392
H 1.24683767858985 3.19702115998855 2.31638184478141

Int-1 (Pathway B)

C -2.25627969478126 -0.78645099189047 2.22045883350406
C -1.48930834921440 0.39949990173871 2.16800972288141
C -2.07120646588053 1.67582790852053 2.32344477296734
C -3.46468493314116 1.74644650419402 2.44716794405912
C -4.24853471490497 0.59359677766894 2.43969674566357
C -3.64676528068027 -0.65898925114126 2.34401919107300
N -0.05294021295647 0.27250799723080 2.06691515280330
C 0.58676455647544 0.09508364795421 0.89126105996753
N 1.84777019829244 -0.38159234816714 0.92349030618453
C 2.56476167927286 -0.6107135362399 2.18932745176562
C 0.61052931924927 0.21973617626863 3.38055309049728
C 2.60978513010793 -0.75034484662681 -0.25611889950811
C 3.70383302301808 0.05323837089238 -0.64021971620437
C 4.51073187803351 -0.39595944544612 -1.69586007783574
C 4.24093444854602 -1.59283783749923 -2.34954304417915
C 3.14572381797497 -2.36379864601802 -1.96246203200143
C 2.30958719003630 -1.96792386297509 -0.9195335494445
C 4.05335157904383 1.37331018102709 0.03740624376122
C 4.16650493467695 2.52112885426906 -0.97862417893338
C 1.12160037518667 -2.83853470957860 -0.51553433762601
C 1.45968540468657 -7.35137127290848 0.67580246583952
B 0.03194121052516 0.64632629371665 -0.5605675127775
C 0.77872108730606 2.45433417957044 -0.46194567904936
C -1.24162024247312 2.95075379195965 2.38768450375751
C -1.20190688912497 3.4992229125839 3.82577060553192
C -1.62303354270354 -2.17395922982466 2.26991716994415
C -2.26230128918531 -3.19447908153716 1.31936943968261
C -1.74179669759856 4.03044664322692 1.41713942767815
C -1.66231381072920 -2.70849532099352 3.71542968116044
C -1.56697697887412 0.75850969113454 -0.92182904569069
C -1.62933911388332 1.63602447604963 -2.13824860468366
O -2.07305701558619 2.87214113050007 -1.88594014548676
C -1.94888102171620 3.82513280510553 -2.94105873307776
C -2.21837935859727 -0.59292493577983 -1.13764198746558
C -1.95306811875800 -1.47051310126849 -2.12882763909659
O -2.51773198978726 -2.70874398659110 -2.08591862304065
C -2.79852990135648 -3.34526247978973 -3.32126998307460
O -1.28417414194452 1.30925203311568 -3.26643746528462
C 0.58013632887585 -3.68380432506388 -1.67482170495066
C 5.35324468349792 1.2684733473931 0.85549881350417
O -1.14285431961912 -1.29199557940684 -3.17931862598154
H -1.02286557921503 -0.31088431382240 -3.31335355225157
H -2.11657917583291 1.28197843376222 -0.13683495812965
H 2.28998766185437 -4.42925736230919 0.41882080221306
H 0.58843943049601 -4.36821796741372 0.94581416773769
H 1.75851421860907 -3.18699194075925 1.56940972438025
H 0.30422322557058 -2.16659468949806 -0.21531751780638
H -0.21791443990849 2.70005737487853 2.07787996190520
H -2.08377455569133 3.79769955005392 4.16216254606861
H -0.55160420057661 4.38727774191282 3.88147859084093
H -0.82491840754963 2.75670851302663 4.54730170207842
H -2.48407114980757 3.48802003022197 -3.84081303128512
H -0.88706492909379 3.97161546711665 -3.19080618709879
H -2.38232662715064 4.75834720568227 -2.56022366447644
H -4.26605425957623 -1.557677618138722 2.37131925916030
H -5.33526575272531 0.67176921415894 2.52569582096921
H -3.94299145319549 2.72286726350913 2.54539210446360
H -1.7998298230811 3.65120638226622 0.38912514628934
H -1.04591156915450 4.88452324944190 1.42131236310412
H -2.73418329848113 4.41058367862586 1.71161149821845
H -0.56870539443319 -2.07742192445123 1.96793511675767
H -3.32413282176077 -3.36306514196522 1.56076793704490
H -1.75293204428949 -4.16593894127315 1.42256569622236
H -2.19890569797952 -2.8857575205790 0.26940838366008
H -2.70136315683584 -2.89530489403350 4.03182534229119
H -1.22645283322807 -1.99810285783757 4.43476320168685
H -1.11039905292467 -3.65954122276967 3.79172889218730
H 0.37766312100217 -0.73963288428171 3.87045133800098
H 0.17055754440875 1.01250156922702 3.99979226904286

H 3.63626601029216 -0.53015687330203 1.98491860896180
H 2.38153901858040 -1.64012140450527 -2.53982193831563
H 0.40544647460812 -3.06546543858844 -2.56513035695440
H -0.38180412728398 -4.13009653790457 -1.38545070279291
H 1.26674695028460 -4.50601060722867 -1.93586722241387
H 2.93407903338101 -3.29141911702740 -2.49384767469515
H 4.87957643612524 -1.92549155162365 -3.17171160023504
H 5.36118580018276 0.21129486807801 -2.01237924787171
H 3.22546185088316 1.63371996111988 0.71130049265491
H 5.03190474646962 2.38531555023847 -1.64732714427179
H 4.30356538912239 3.47893112570313 -0.45078997516733
H 3.25514268981780 2.59609325955368 -1.58543542152946
H 5.31760317062587 0.46909699509832 1.61229080719898
H 5.55892097843301 2.21747223575240 1.37708736835199
H 6.21328286266222 1.05495641473473 0.20021902046092
H -2.99109934589813 -0.89160599920764 -0.43281128285794
H -3.33310080193489 -4.27283328604327 -3.07304566080437
H -1.87945352599853 -3.58838266049107 -3.87659821143530
H -3.44050958425205 -2.71453524702588 -3.96207498465760
H 0.61419462396723 0.08279233669433 -1.44914714410434
C 2.10579116684188 0.38798761346726 3.23018255882369
H 2.34982855623099 1.41160391651386 2.90377324486080
H 2.60900777652252 0.20771617486644 4.19160453519975

TS2 (Pathway B)

C -2.24397618127464 -0.77301117838771 2.10435251930029
C -1.47243090413085 0.41509601130541 2.09142514978198
C -2.06460484537250 1.68829089085881 2.23627771723240
C -3.46225222475387 1.75694053185165 2.31277995479169
C -4.24422608549980 0.60564003714686 2.25719605099173
C -3.63761933333235 -0.64406502185643 2.16920776226279
N -0.02750622734670 0.29113288902509 2.03045617876370
C 0.65619223711900 0.13820297396548 0.87489644971903
N 1.89461213326778 -0.38479297461955 0.94215806678725
C 2.47477475083984 -0.79829213168737 2.22745272220771
C 0.59636142971484 0.25618703698151 3.36775033673034
C 2.72454335648099 -0.68361660165101 -0.20892762821302
C 3.78390470894512 0.18909829417592 -0.53272459621585
C 4.64069337882875 -0.18331843451311 -1.57781941145938
C 4.45784838181200 -1.37816878651147 -2.2697590942876
C 3.40711518040234 -2.22675006757633 -1.92677415180035
C 2.52192409681944 -1.90286892166403 -0.89084675066394
C 4.04239687576342 1.48537261654620 0.22405670142012
C 4.24121768038690 2.68073974234557 -0.71783482749923
C 1.39996745941657 -2.86598191733364 -0.53165886139248
C 1.92629139895816 -0.40393131270010 0.31202299225513
B 0.17855395442573 0.73532519111929 -0.58239436903313
C 0.77397584213215 2.57113476716987 -0.42607662697880
C -1.25321407145949 2.97204683516665 2.34148397797186
C -1.27718119933438 3.51540813369833 3.78171012954572
C -1.62912857310596 -2.16790117491837 2.18282262749693
C -2.35120165763977 -3.229114142777067 1.339190032303782
C -1.73431453601758 4.04889551065149 1.35716459582131
C -1.59375316493061 -2.64501062917099 3.65023908550236
C -1.43524502356466 0.59572504302789 -0.97572248171721
C -1.52251973369610 1.37042146696433 -2.19856367533083
O -1.81573971160134 2.63400223279228 -2.12979886984668
C -1.69645069477720 3.45618258526663 -3.29926412176823
C -1.67529225516318 -0.86518712063186 -1.15838244646012
C -2.64629586246168 -1.34836899167284 -2.03282371420641
O -2.82701194867927 -2.73032291343280 -1.95962966632852
C -3.72257929281183 -3.27865870548259 -2.90242655156466
O -1.23118173524622 0.90359501253291 -3.36960633247272
C 0.63783133214283 -3.36984343934315 -1.76480832396331
C 5.24514469738948 1.346058200713049 1.17418770222388
O -3.30657425064161 -0.69157921302882 -2.86839218838784
H -1.35928071794213 -0.07345187700764 -3.31001037421966
H -2.05488658168678 1.11563641785124 -0.22835798648228
H 2.64690726405651 -4.64471254597320 -0.26210328292194
H 1.09594435141875 -4.69785551136008 0.61528554730683
H 2.43969285008400 -3.69316462594341 -2.3309380625515
H 0.67599557618010 -2.31882050272154 0.08503236718292
H -0.21456883388784 2.73879569929955 2.07152585743633
H -2.30033591453122 3.79546868926690 4.08109191848057
H -0.64376311249941 4.41346637320501 3.86678060494771
H -0.91704217781024 2.77431749009555 4.51322390465574
H -2.27223227342129 3.02575345865703 -4.12974368969576
H -0.63686160678569 3.54340843798782 -3.57939242895043
H -2.09521492253103 4.43544165546436 -3.01194823335931
H -4.25642952345887 -1.54214613267225 2.15058124593026
H -5.33372022058659 0.68184697361079 2.29653687308959
H -3.94421488857209 2.73187239597187 2.40680718388885
H -1.76451364246669 3.66385577547714 0.32969621119442
H -1.04403865361103 4.90733071359859 1.37347000440101
H -2.73609407808208 4.42279374050522 1.62521399663353
H -0.59248476394428 -2.10362218183943 1.81995182048072
H -3.33482845070678 -3.74659469834558 1.77054596075925
H -1.76194868708114 -4.16095218528810 1.3960618465733
H -2.50407958762735 -2.91867985922749 0.29873551554813
H -2.61956548685996 -2.78462606604305 4.02752098107822
H -1.09836746571740 -1.93126507425893 4.32458236834666
H -1.0713103778446 -3.61239027539617 3.72981567100448
H 0.22662372215836 -0.62668260562948 3.90751360488728
H 0.24060332401671 1.13941175713358 3.91598191506439
H 3.55740943809927 -0.89154377551158 2.09092345791163
H 2.08763444015643 -1.7964176072818 2.0003338153377
H 0.31898312768768 -2.52856533985213 -2.3950202078529
H -0.27730277095592 -3.89919855041584 -1.46102594430243
H 1.24980536332750 -4.06155681229436 -2.36663258554220

H 3.26703598247119 -3.16032533666564 -2.47476678678174
H 5.13724708324222 -1.64966483045605 -3.08172650301754
H 5.46538126195601 0.47705527182879 -1.85317801782418
H 3.14677371878894 1.70435324803714 0.82135350736331
H 5.17002065496102 2.58936045224834 -1.30492809755831
H 4.31087377728843 3.6127054204572 -0.13485315019401
H 3.39248604224965 2.77752090375588 -1.40874541331417
H 5.11698499014066 0.52311303345069 1.894398542221009
H 5.39624310134767 2.27544225217336 1.74734488043738
H 6.17033778876500 1.14487111735928 0.60975172200303
H -1.11856017602369 -1.56096298023873 -0.54324606978060
H -3.75729050771021 -4.36097901153798 -2.70781566201902
H -3.38709489920948 -3.10161461243948 -3.93932681678846
H -4.73432422881312 -2.85066224189124 -2.80737381180227
H 0.83424062440160 0.24512441268472 -1.46257988010623
C 2.10751278479072 0.22375381653354 3.28478452572437
H 2.51177464550473 1.20770309933905 2.999658311550178
H 2.53198225502795 -0.04518386819629 4.26344880741810

Int-2 (Pathway B)

C -2.13280643017252 -1.00565957848006 1.83071283694515
C -1.44779916764349 0.23311172267731 1.86819532763352
C -2.13623322338811 1.46250440068712 1.93022076464828
C -3.53463265957323 1.43279076236802 1.84502730048713
C -4.22475980161383 0.23005825627046 1.71794926444945
C -3.53014316937251 -0.97755663416103 1.7368564017067
N -0.00151945168792 0.20763872960321 1.91720430020602
C 0.75554176986694 0.09509797615332 0.80145267040545
N 2.01574833518719 -0.35793337210952 0.94761921188758
C 2.55424521762784 -0.70329585427258 2.27050501790901
C 0.53686305099282 0.21285329398185 3.28963781361423
C 2.90449268711413 -0.66233807336500 -0.15553341224989
C 3.99724412641647 0.18965468343256 -0.41331906816999
C 4.91169760474143 -0.20054872846930 -1.4024227635310
C 4.74921871801583 -1.38915661256865 -2.10808287760496
C 3.65673258865723 -2.21274820013480 -1.8399956961801
C 2.71548065330640 -1.87003143918867 -0.86279371239548
C 4.22635601768562 1.49113638980399 0.34394759379425
C 4.43672488765592 2.67903875614810 -0.60682610963982
C 1.53935242905442 -2.79665317648827 -0.58858510279677
C 1.95218217765954 -3.95817259105223 0.33099302940330
B 0.33078200269035 0.67522717784071 -0.68990121593138
CI 0.97555695309536 2.49076675802254 -0.47224670485896
C -1.41804493775301 2.79311021971180 2.10424778961787
C -1.60418344530806 3.31485472005605 3.54113301739242
C -1.42314828345086 -2.34531974053158 2.01638131402669
C -1.91887301705981 -3.46721414651729 1.09289246223221
C -1.86805653927902 3.85173625196637 1.08730496029552
C -1.55905405889770 -2.8059289936424 3.48208952864229
C -1.22053926613203 0.66703643368010 -1.19158773458223
C -1.30950300983065 1.49944960854436 -2.44425118425458
O -1.71732120660905 2.75982892166297 -2.18605691302502
C -1.69207668468201 3.66298196150772 -3.28348090010976
C -1.65084284484693 -0.76171612305860 -1.50875288086058
C -3.14553551118730 -0.91835430841981 -1.63228860730894
O -3.50882682479149 -2.22505753181148 -1.57412450823678
C -4.90363520435415 -2.48735357556557 -1.68252116350059
O -1.03037103993405 1.12510042241088 -3.56068936616675
C 0.88545760789301 -3.31925586431582 -1.87448309061514
C 5.40839912579190 1.37371896629850 1.32243305861451
O -3.94709090249613 -0.02803756727025 -1.77167477480166
H -1.20567381123302 -1.06731769952077 -2.46991360190745
H -1.90341408161432 1.11333702398009 -0.46571776332427
H 2.72171955275635 -4.58307629281247 -0.15084227164956
H 1.08723381868947 -4.60124478897252 0.56071075757588
H 2.37091281427838 -3.59563617065112 1.282571959722181
H 0.77274246182502 -2.21588045375094 -0.06046453946833
H -0.34751307087840 2.62179172000606 1.92621100761401
H -2.66494733727721 3.53527084818094 3.74470190373293
H -1.03280560404488 4.24535739304091 3.69005542612904
H -1.27318003022210 2.58602816407414 4.29858354804304
H -2.32498089527966 3.30020470428779 -4.10775906647535
H -0.66433872577448 3.78617397026124 -3.65990638311550
H -2.07162674419648 4.62023217373406 -2.90284556956059
H -4.08187861356896 -1.91730337603199 1.67345309654663
H -5.31252775863633 0.23312779845434 1.61761013780991
H -4.08897066057159 2.37273378574496 1.85539017485535
H -1.77496548322791 3.48813481112194 0.05613016833060
H -1.23759403598228 4.74972653543030 1.18615189959562
H -2.91223181182415 4.16070144600921 1.26098321885375
H -0.35386030677532 -2.19654779685135 1.80708020519423
H -2.95125567970462 -3.76243949449418 1.33857078892727
H -1.28866783862079 -4.36095945132692 1.22338084259541
H -1.90825774003610 -3.18430439551974 0.03363878790601
H -2.61235386498721 -3.03039958820920 3.71520571029492
H -1.22680879775097 -2.03849287400114 4.196520303378778
H -0.97025846722798 -3.72093364523818 3.65917658989371
H 0.0639431457956 -0.69958532031261 3.80824683766339
H 0.08343183975908 1.06408302673012 3.81646668548466
H 3.64658759790664 -0.70888105803140 2.19731391467835
H 2.23798737181936 -1.72683026659133 2.54170255809443
H 0.65750977102434 -2.495077201509274 -2.56503378112147
H -0.05611188712761 -3.83866308549126 -1.63725002210721
H 1.53345364336169 -4.0387336508740 -2.40042570403438
H 3.53051170084867 -3.13835418302033 -2.40444647887907
H 5.47284439922781 -1.67371330871883 -2.87600405866398
H 5.76371940195606 0.44495612658217 -1.62491408635672
H 3.31207757955556 1.70660901214468 0.91399728030604
H 5.37828993198544 2.58663448833839 -1.1722537933693

H 4.48840842671199 3.61703841026630 -0.03064196280319
H 3.60157433686148 2.76236162111002 -1.31461373879561
H 5.27853822286978 0.55217036647408 2.04446384473293
H 5.53174947643934 2.30820565074839 1.89377553545342
H 6.35001170628028 1.18557389937794 0.78113857193794
H -1.28859558245456 -1.47881493787193 -0.76319268931959
H -5.01645466643051 -3.57786140763504 -1.62962166897153
H -5.30408624801507 -2.10699542399689 -2.63468374588635
H -5.45688403576083 -2.00596713222122 -0.86073759803604
H 1.02720515765489 0.15013083344767 -1.52333509818486
C 2.04835078509089 0.29769450776301 3.29013204383858
H 2.38661378318962 1.30808926039931 3.01155926391175
H 2.43893741116306 0.07400568291121 4.29394165013910

TS3 (Pathway B)

B 0.11136246146174 -0.30833898251614 -0.76742848999343
C -1.31601438290342 -1.10302786400393 -0.83088156256180
C -1.45316899387341 -2.05724587071577 0.39458150114513
C -1.55705589402147 -3.52136157202606 0.03298735187509
C 1.25532631545790 3.49863954061924 0.99269909559876
C 2.09246070886495 2.31271945028522 1.42679397233216
N 1.69137368556060 1.12312062453512 0.66106740755178
C 0.40742903983811 0.90664468483906 0.31424820869778
N -0.51481507377144 1.80689551015858 0.72264485790131
C -0.19247982890481 1.34355144479154 1.25266218561093
C -1.92456959166798 1.49371071975919 0.79587224683427
C -2.39795073848020 0.84559659308424 1.96075777155043
C -3.76317162844499 0.53715298179829 2.02967681526599
C -4.63173895176999 0.88966755856908 0.99883753648208
C -4.15428123335311 1.59283175094730 -0.10545722172209
C -2.79732440522861 1.91955056177485 -0.22782931846821
C -1.51098566037840 0.58610494411950 3.17592195863746
C -1.80175082423384 1.63625517475900 4.26624173319291
C -2.32302205711671 2.73168605555239 -1.42428584053574
C -2.79670398746323 2.14522561747137 -2.76195269288644
O -2.55799677736986 -4.05827222859397 -0.37520540003916
C 2.77173264625545 0.18891940915859 0.40844922737566
C 3.70856414269663 0.47913781834703 -0.60446886907013
C 4.80442821388184 -0.38388134339390 -0.74860807081691
C 4.96753087493499 -1.48929652603904 0.08078254871985
C 4.03095927213967 -1.7532555118435 1.07880759993315
C 2.92037697574749 -0.92284874015749 1.26741414503884
C 3.59213964665289 1.69182703723647 -1.51891901815635
C 4.63287992461192 2.76755285348532 -1.15963030953988
C 1.93647544814501 -1.22080086391091 2.39050306431458
C 1.62526229212083 -2.71592513701180 2.53486574999340
C 3.71435365089687 1.30973616715530 -3.00166492610982
C 4.32939398922221 -0.63935322605059 3.72594735162235
CI 0.37522822572582 0.71946763411650 -2.39822246973550
C -2.77307317319483 4.19627570158814 -1.29138240208893
C -1.64621002324476 -0.82277364178109 3.76953997697953
C -1.30944585383288 -1.83470615060575 -2.14880687047328
O -0.65827876865588 -2.8183738568188 -2.41732151977448
O -2.10689072451971 -1.23179842021265 -3.05832620690482
C -2.01890195300149 -1.73031547880603 -4.38851841959443
O -0.39370755479344 -4.17355164326395 0.22596842357786
C -0.32803568494871 -5.49303083245222 -0.30714647368832
H -0.60707300382477 -1.92835267632300 1.07894316532608
H -2.17602004135179 -0.43034043107518 -0.85513710130305
H 3.37416226207470 -1.12390951917383 4.03294433565575
H 1.69031890485834 -0.80514641404670 4.5235953117205
H 2.62723456076143 0.44183213235497 3.6594932878296
H 0.98976858797619 -0.72156302957080 2.1443229582966
H -1.22512574217398 2.69797820292561 -1.43718602848084
H -3.87244728317328 4.27642451048582 -1.31300898658538
H -2.37717011867640 4.79907195304333 -2.12609094328392
H -2.43342407406680 4.65861152798800 -0.34956145248052
H -2.26554672067162 -2.80207332825249 -4.42399317099250
H -1.00039563398246 -1.58972692614668 -4.78283023680203
H -2.73789228235296 -1.15063319662577 -4.98192280125324
H 4.29858354804304 0.02051577957179 2.90876568347474
H -5.69104029019704 0.62963477850059 1.06478660269427
H -4.84628759693182 1.88657074904623 -0.89680876948673
H -5.22280137223798 1.08679557713477 -2.85581589868374
H -2.32526489608687 2.69215576370941 -3.59390713286682
H -3.88894359521147 2.24095705611927 -2.88056295697238
H -0.46341654215670 0.70701464150799 2.86579275358921
H -2.65919346135446 -1.00331155220487 4.16229363354379
H -0.94525438947242 -0.9433264643005 4.61062739200123
H -1.42651314134362 -1.60229458110919 3.03072954295715
H -2.82496444226731 1.51522720834155 4.65689107940714
H -1.72008212056472 2.66463611501942 3.88300598220231
H -1.10179645908461 1.52553382878430 5.11047583871847
H -0.40453255048863 3.16480994446877 2.33349723746307
H -0.87763778350122 3.85838454995912 0.77698606219359
H 3.16195690671811 2.47416086311478 1.25720187465864
H 1.95811839333360 2.11993043608891 2.50581300016228
H 1.31295509236559 3.16101240045155 1.58044726264701
H 0.80599879229457 -2.85985879796702 3.25680343605844
H 2.49325726174043 -3.27696372463128 2.91684476207986
H 4.16408666993866 -2.62392655928564 1.72283689804908
H 5.82698496730642 -2.15131328310515 -0.05124709707084
H 5.53996425697412 -0.18487863649615 -1.53050121243465
H 2.58588214661066 2.11237209796656 -1.38580124220597
H 4.72665246471352 0.94928447002349 -3.24661546535288
H 3.51594048963555 2.19001948550481 -3.63427005152931
H 2.98534518991147 0.53244058804776 -3.26510283389507
H 4.55768132756132 3.09456790895221 -0.11061892381282
H 4.50699051988722 3.65617054914788 -1.79949483245056

H 5.65726681235988 2.38932811496366 -1.30953665954724
H -2.37694588127681 -1.80532655547460 0.92998187851973
H 0.66268695433899 -5.88348385776262 -0.04108360344057
H -0.44187509675281 -5.45312052428495 -1.40086224677472
H -1.11951605600967 -6.13144532070679 0.1139280237760
H 1.00360238172672 -1.11510094996755 -0.70549984154125
H 1.42353567140055 3.69920671352050 -0.07722078142993
H 1.53075820755942 4.40291779561040 1.55523477266891

Int-3 (Pathway B)

C -0.92201547505253 0.15668134934879 1.73599855332428
C -0.49658492727229 1.60114915238522 2.10768384680689
C 0.58516209069104 1.72493780898191 3.16257968778020
O 1.78764860796813 1.32512510543893 2.69969376217598
O 0.41856946378507 2.17062572246300 4.27029410887846
C -3.32436675560187 -0.59989286812129 -0.74342683125708
C -2.35083354268450 0.36873644260533 -1.06708283199206
C -2.59226988997322 1.75229288291702 -0.89335468735209
C -3.78313543673481 2.13781097268151 -0.26521489444381
C -4.72201485861667 1.19007603174168 0.13745300696221
C -4.50297850762203 -0.15946500278726 -0.12524021367399
N -1.09722231208545 -0.03649947495157 -1.66811754079574
C -1.12569786379009 -0.14545956853272 -3.13434480548434
C -0.02639870455435 -1.07819839900482 -3.59763833832394
C 1.28707893765504 -0.53294503445378 -3.07777051849787
N 1.20556945826235 -0.29596538716412 1.62572785522310
C 0.03766367035697 -0.19168403395106 -0.95425632118823
C 2.50122404083611 -0.14352101131936 -0.98842885175855
C 2.93535841819323 1.15643364644369 -0.63339154812295
C 4.23671857911505 1.29878535019789 -0.13852956348902
C 5.08520497341157 0.20040225251431 -0.00468537954869
C 4.63233953242801 -1.06939635786058 -0.34708906610154
C 3.33433013363927 -1.270508444839828 -0.83741041857063
C 2.0336817225045 2.37928992855630 -0.76512160091724
C 2.35895431862360 3.49346550767422 0.236771880415118
C 2.87540844655223 -2.68976390251756 -1.14467741524313
C 3.64750074787316 -3.29845796869899 -2.32772913087347
B 0.10104872131500 -0.53264004854202 0.66223883784126
C 2.81603254661935 1.16351835454863 3.66980738270196
C -1.67027745496417 2.82069946859909 -1.46892572288574
C -2.21936781917646 3.30494640242710 -2.82562304627060
C -3.16547050905477 -2.07438820045343 -1.08075902308906
C -3.53280570303878 -2.98928953041348 0.09625746349286
CI -0.21406077404960 -2.45290148628885 0.53814990446062
C -1.45063085807208 4.02711840272837 -0.54655316007570
C -3.99945544113889 -2.43359350989036 -2.32431249375029
C 2.99421423487762 -3.59054079371434 0.09529683783871
C 2.03526400358442 2.94816305685769 -2.19415222178182
C -0.95255851629179 -0.74055738259832 2.94352964618856
O -0.08322222694086 -0.83215019291752 3.78111377380767
O -2.07218162439509 -1.497774485717617 2.98442571476176
C -2.09038480319786 -2.52137308469859 3.97435356563773
H -0.13861484027788 2.10925792378630 1.20189894302537
H -1.94443758284772 0.19788401795083 1.34937273419993
H 3.05113746535998 3.26375522621874 -2.48195377835459
H 1.37530259387237 8.2793111590707 -2.26167620806071
H 1.69100371147425 2.21697551797924 -2.93760341576046
H 1.01138340909769 2.04631348214685 -0.53783438549393
H -2.10534654449086 -2.25236153824386 -1.30329934395303
H -5.07505467338440 -2.28517562115527 -2.13367620584480
H -3.84822072943714 -3.49084267471960 -2.59657042976623
H -3.73575095946155 -1.81767895056575 -3.19892178999706
H -1.97010757958517 -2.09800816492648 4.98301693466420
H -1.27521350700821 -3.23951230797046 3.79468763066472
H -3.06297347604819 -3.02191483436062 3.88098930396697
H -3.98362978533500 3.19753347177766 -0.09826442359911
H -5.63938247072216 1.50826920768142 0.63883685622643
H -5.25804134230952 -0.89269273670740 0.16255912587072
H -3.01290498793215 -2.67442131799323 1.00979203897075
H -3.23730041625646 -4.02610910735457 -0.12909196184128
H -4.61925986738538 -2.98992864857324 2.85069303808450
H -0.69003621710086 2.36083692748077 -1.65077332550098
H -2.37317996428162 4.61535658722283 -0.42151679262327
H -0.69639677537057 4.70135249675053 -0.98165679391978
H -1.10645807456904 3.72671989799060 0.45110741147452
H -3.17972423104069 3.82743267984097 -2.68710941475859
H -2.39921380065356 2.47196536845475 -3.52100247527129
H -1.51582969331797 4.00723796107345 -3.30205080055838
H -0.99823089657121 0.85223139699340 -3.58729870216356
H -2.12167226229960 -0.50772943858586 -3.41809565310359
H 2.11002499082813 -1.23475849288326 -3.25496027501999
H 1.55256027941066 0.40376982946366 -3.59441224673515
H 2.41896234486966 3.09840311028654 1.25876937374237
H 1.57007506156476 4.26067096296748 0.20737158582909
H 3.30822754873062 3.99794249855673 -0.00546218290941
H 4.59469074877649 2.28651308685218 0.15226556443620
H 6.0930480401855 0.33680340052419 0.37938034034657
H 5.29245262059702 -1.92981384884247 -0.21881261570347
H 1.80645124065623 -2.65273588260856 -1.39691736216372
H 4.04705134168833 -3.74119925008333 0.38472299127697
H 2.55929363571714 -4.58085427045484 -0.11516163439992
H 2.44888027936790 -3.15956595761780 0.945117809424900
H 3.57685267234510 -2.68228374404832 -3.23876314369449
H 3.25975323231597 -4.30207485751889 -2.5662940620734
H 4.71872813840234 -3.40333065492365 -2.09055683678947
H -1.35738588463691 2.16628557535365 2.49205245152262
H 3.71066878321582 0.85484000754255 3.11363419102080
H 2.52389612466192 0.38333509062098 4.38892732611565
H 3.00160975821146 2.1025078229962 4.21362978237317

H 1.23400208455470 -0.41506481339833 1.03028613584183
H -0.20258216179076 -2.0915526210910 -3.20214914984266
H -0.00621547085196 -1.13915999068735 -4.69571176332871

TS4 (Pathway B)

C -0.97781296361641 -0.07342132731760 1.79021052214965
C -0.74425079353023 1.40762014309094 2.10244516079473
C 0.57161259507234 1.93757926344738 2.63813267972090
O 1.50790700002854 1.01358627195560 2.84884165158854
O 0.73821660571469 3.12391817356345 2.83627219881064
C -3.33654869038838 -0.54466238631571 -0.74164036171103
C -2.33679219343026 0.41573678912879 -1.00672676355410
C -2.55818892472281 1.79786234450077 -0.79113443024650
C -3.75624972014917 2.18228264869119 -0.17551895493391
C -4.72148854921770 1.23908480564614 0.17063407247029
C -4.52195855432169 -0.10448215691622 -0.13688518528851
N -1.08181220702684 0.00689963263022 -1.60514502842257
C -1.08557102610227 -0.02941430684467 -3.07548191449077
C -0.04528486865949 -1.02017604423790 -3.55617686654201
C 1.29782087351995 -0.58006101152241 -3.01206266962475
N 1.21059994869538 -0.32275784495272 -1.56251727465521
C 0.03983059039986 -0.22079548723977 -0.8898957219895
C 2.50732507513465 -0.17260604528377 -0.92624330484218
C 2.94518907223121 1.13011338326790 -0.57594455853435
C 4.25438576554208 1.27196089485872 -0.09902842429039
C 5.10687675836541 0.17544447562116 0.0502044906453
C 4.65159015665374 -1.09370227635964 -0.31168031724913
C 3.34801547551917 -1.29637461183217 -0.78708747206201
C 2.05012711276699 2.36240399084221 -0.70193372377134
C 2.50804549711281 3.55540843294868 0.14602361907505
C 2.89709144901748 -2.71873417679033 -1.0960267496968
C 3.68036241466471 -3.33086963179045 -2.26431198900862
B 0.08481831116772 -0.68065767200352 0.70392229935697
C 2.74505220889393 1.39976392420479 3.43557828667218
C -1.61650442207903 2.86881880415118 -1.33303496342545
C -2.16222274021040 3.38523152515122 -2.68010675664647
C -3.19409773332718 -2.00864158108459 -1.12853298077339
C -3.58849376502262 -2.96081619953784 0.00937266914848
CI -0.22467408384775 -2.58121667741722 0.42082705731657
C -1.36851958040591 4.06119710792851 -0.39691711087389
C -4.01328151821943 -2.3090536125203 -2.39704032227319
C 3.01130217550217 -3.60992426544187 0.15675782954393
C 1.90637935578066 2.82567592847192 -2.16295473209339
C -1.02490939365204 -0.90396756132934 3.04633913983488
O -0.38905658364593 -0.73382637880427 4.059767266914848
O -1.93138630251814 -1.90813659084193 2.93375679807046
C -1.95780605744294 -2.84875267156722 3.99833160314122
H -0.92304019860317 1.98230583359981 1.18609521142531
H -1.98765949119053 -0.14377650694353 1.36997412250992
H 2.89679702815408 3.04116327250718 -2.59516827622891
H 1.30736818775980 3.74804819608606 -2.21582125211204
H 1.41707871985115 2.07907268305056 -2.79952729802506
H 1.05234102919070 2.07565702245829 -0.33534063646954
H -2.13408235464619 -2.19502891625040 -1.34317942569453
H -5.08974705732342 -2.15139604467512 -2.21887528492834
H -3.87295574041862 -3.35780077860806 -2.70565116490276
H -3.72484736837513 -1.66554375420724 -3.24362753849758
H -2.17324951811221 -2.35673169623953 4.95945993821038
H -0.98920721989802 -3.3663993943221 0.08292146592065
H -2.74795031810859 -3.57034896548166 3.75219836278429
H -3.940595606154374 3.23948486851749 0.02312441290673
H -5.64540410800631 1.55715571092242 0.66009427007789
H -5.29820774470921 -0.8328858714668 0.10333228115177
H -3.05974263659010 -2.70493113208042 0.93680843190597
H -3.321966164449445 -3.99474439649666 -0.26132417733338
H -4.67495757283527 -2.93935119292428 0.19752791970195
H -0.64704028459303 2.39438134054871 -1.52667989835889
H -2.29690828930912 4.61789535263192 -0.194147413024
H -0.67272895516627 4.76686098483298 -0.87736813266947
H -0.93039857795937 3.77364202340952 0.56868930503064
H -3.10423527640803 3.93638661385086 -2.52752787884331
H -2.37446266618852 2.56595083032541 -3.38260462576326
H -1.44094722706609 4.07027698266607 -3.15483810766845
H -0.87606210915117 0.97576663994868 -3.47876716638224
H -2.09834386690934 -0.30552415696023 -3.39454270594554
H 2.05938402658480 -1.35318449907584 -3.16769798075802
H 1.65577085703941 0.32376670075023 -3.53031614801441
H 2.66164678628742 3.29202126807904 1.19917174518956
H 1.73576723115834 4.33787117207947 0.12441180409257
H 3.43676009937268 3.99772864873231 -0.24967239683661
H 4.61911691300893 2.26015003246467 0.1792737344844
H 6.12613023394521 0.31463008530634 0.39409363990603
H 5.31440103260570 -1.95344492856882 -0.19359730992452
H 1.83002904586723 -2.69003642788243 -1.34873256404704
H 4.06276533188423 -3.75484008401211 0.4543190464332
H 2.57930698921746 -4.60246256487489 -0.04833017487422
H 2.45922693908899 -3.17402439608784 0.99969755166998
H 3.61537990559226 -2.71812449179106 -3.17816852038637
H 3.29555170943370 -4.33591230486943 -2.50146115201777
H 4.75006636243378 -3.4338198117194 -2.01958427916783
H -1.50084534839029 1.78422663194196 2.81219158914015
H 3.51504515433971 1.46201780910482 2.65101431698450
H 3.01643844130417 0.61064478717977 4.14999943582772
H 2.65018434202188 2.369985654077049 3.94195903130448
H 1.21779661310990 -0.59045783259196 1.08104133866123
H -0.29599735288203 -2.02841722142509 -3.1892886616655
H -0.01692024062023 -1.05405146934619 -4.65524657569928

Int-4 (Pathway B)

C 3.56148781409943 1.36423435062050 -0.05464802033472
C 2.69490229684685 0.43985482211754 0.56259513404976
C 3.01930456842743 -0.93429679310677 0.66450562922058
C 4.24968375250251 -1.35411188877424 0.14754504229810
C 5.13387690915641 -0.45165368564055 -0.44149910947777
C 4.78665588452549 0.89079862204228 -0.54508141492514
N 1.49392320581671 0.92080671860196 1.22186114416427
C 1.77196693444779 1.65450560737144 2.46954854038110
C 0.55573531731045 2.44368526337040 2.90415285631989
C -0.61999870579105 1.49048475193232 2.92843558815386
N -0.79069769360236 0.88222837862684 1.60024541119917
C 0.24769093208934 0.67878203489125 0.76106146135120
B 0.11217695193591 0.41011463786243 -0.86694183487441
C -1.10756441007428 -0.47811378541440 -1.50241928598830
C -1.26298722482056 -0.04540714286422 -2.93603040842481
O -2.34305531821018 0.75235160385423 -3.10664653418086
C -2.44957705197531 1.382990813685827 4.37869652263444
C -2.13440985882313 0.42491296453162 1.31766734412171
C -3.08130865105451 1.32073639793247 0.77762727255116
C -4.35938613400927 0.82329403680317 0.48775896617343
C -4.69539745470575 -0.50281459740218 0.74697963256020
C -3.76935227155160 -1.34915473441239 1.35400740740053
C -2.48120080034682 -0.90055413534420 1.67169210661959
C -2.78218295782294 2.79431462232550 0.54725613094735
C -3.40660933610811 3.65046522040547 1.66436377138103
C -1.55187419501918 -1.79748608493357 2.48070833410796
C -1.54797627401515 -3.26722034544916 2.03967353271537
C 2.07260152949328 -1.94852996451207 1.29878917834410
C 2.18153573110417 -1.96298657542512 2.83307718165684
C 3.21393637907228 2.83538648691031 -0.24188620389460
C 3.23302259750836 3.22279591941079 -1.72943454293891
C -3.25168040509334 3.282171789084044 -0.83047390352424
C -1.91993541090210 -1.71414240176416 3.97559233244860
CI -0.04851716992710 -2.27289141342823 -1.42223157098296
C 2.24317870718214 -3.36983863264007 0.74984534558697
C 4.14886391385773 3.75361731298142 0.56398343355683
C -0.82383227700915 -1.99089589813155 -1.38024463564811
C 0.18390510015120 -2.53244737822942 -2.3747876717621
O 1.38630759779080 -2.48245686026916 -2.25826522511638
O -0.42936465645350 -3.11769440506943 -3.41935091508517
C 0.40746020643319 -3.44236927862641 -4.52511812328870
O -0.51901207501836 -0.31975387089865 -3.84994853225062
H 3.20605228265972 -2.22438280021087 3.14378011575405
H 1.49694125559933 -7.1201141021836 3.26284297982003
H 1.93461509196484 -0.99192607846504 3.283077882994485
H 1.05189447882432 -1.63665081977271 1.03655829539375
H -1.69200906150657 2.92065955338664 0.57357907549623
H -4.50547385194661 3.56147144349887 1.66096534640002
H -3.15422044902871 4.71370408841769 1.52068146096334
H -3.05837702074688 3.35257436538165 2.66618109059461
H -3.37054740797517 1.97975717233295 -4.34993825729033
H -2.49941682510029 0.63765457255777 -5.18710192056669
H -1.57971819339979 2.03462975387621 -4.55477038058934
H -2.06272209766032 -0.27607741920754 -1.01072347081584
H -4.05557517346519 -2.37424217332082 1.59565959524827
H -5.69175870947227 -0.874101168600988 0.49459911499163
H -5.10043751615835 1.48868856106594 0.04194087614591
H -2.88254335202757 2.61899411576424 -1.62257151708717
H -2.86473526747566 4.29570445230025 -1.02017080013310
H -4.35168981981652 3.33266535872966 -0.88970159051470
H -0.52912691819292 -1.41584549824660 2.36569289667772
H -2.51121780887213 -3.75735849969887 2.25195143765334
H -0.77494264568411 -3.82330692413291 2.59284228449578
H -1.34408783805459 -3.37665478722524 0.96702773604899
H -2.91852895274938 -2.146722950506788 4.14963938450563
H -1.94710642116959 -0.67671095876949 4.33924136067514
H -1.19451796155548 -2.27561273027898 4.58682834759123
H -0.45794869540222 0.70292258642485 3.68353260424117
H -1.55929407063126 1.99752801575414 3.18127058514733
H 2.62914012255195 2.31137278302768 2.28507385834976
H 2.08040354581788 0.94605510937268 3.25549024126138
H 2.22771111847804 -3.36826143483508 -0.34772959836449
H 1.41871608973907 -4.00545912384312 1.11018799622806
H 3.18115358164803 -3.83200529403631 1.09863416914889
H 4.52005038733574 -2.40866478985945 0.19668061161318
H 6.09013048347504 -0.80348411796352 -0.83658697424408
H 5.47151162254424 1.58911004106315 -1.03095180318944
H 2.18124765607473 2.98631181174642 0.10255854375233
H 4.25145989406158 3.16632535563177 -2.14709109302907
H 2.87569094440877 4.25772434137261 -1.85488588318058
H 2.57335510751012 2.56684884853027 -2.31231811424047
H 4.15500512775505 3.51059456436971 1.63903763909266
H 3.84315570285190 4.80703970307490 0.45621099526269
H 5.18883132973554 3.67082313001509 0.208702515189625
H -0.42261599666273 -2.20268274068758 -0.38025587177262
H 1.23210191373648 -4.10386814684314 -4.21889428026346
H 0.82709648948248 -2.51843712967309 -4.95131554172719
H -0.23397636873897 -3.94416727013638 -5.26106144542402
H 1.16790943588124 0.02205278416169 -1.28579745709128
H 0.72145027362963 2.88258352529182 3.89906031939808
H 0.35830967151794 3.26518694071433 2.19662671545690
H -1.75799636400809 -2.56682959904427 -1.49918723879446

TS5 (Pathway B)

C 3.47461915965557 1.32659227562133 -0.34793276600352
C 2.65436446559490 0.39461726023946 0.32768270509313
C 3.05228834530111 -0.96053197992505 0.46562240069959

C 4.27801987152373 -1.35151589831739 -0.08919140956905
C 5.09743878811174 -0.44349041280725 -0.75569963969599
C 4.69184810004917 0.87885733810316 -0.88200196547505
N 1.45999994863623 0.84018446257210 1.02497448310906
C 1.75230227481887 1.6331253165467 2.23418084650053
C 0.49937528941453 2.31444988058792 2.74506980689102
C -0.60044598048270 1.27345040843451 2.81557386569670
N -0.81722625960129 0.70269981815456 1.47893576006881
C 0.19342435739128 0.63441921271503 0.57827054122129
B 0.00851352120353 0.30412249233461 -1.00130544765252
C -1.37923712630991 0.34772644403018 -1.87057375542038
C -0.95255874982950 0.68750968897053 -3.27455217723000
O -1.11222489104638 1.97929437520973 -3.57380267998458
C -0.55683426551306 2.42442188248371 -4.80629185355826
C -2.14463537351818 0.17891547884785 1.24394133135854
C -3.20398282747180 1.03641933317880 0.86294474610582
C -4.46332295856054 0.46178419777107 0.63395392999701
C -4.69365550714141 -0.89691817009994 0.83440703663857
C -3.66668620722438 -1.70598016094670 1.31560623163347
C -2.38482908929291 -1.18562839565005 1.54159342710195
C -3.06473783745517 2.55006966096961 0.81135573882158
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C -1.34050147811623 -2.06653606821279 2.21081932363292
C -1.24601774581327 -3.47424451464327 1.61113753287734
C 2.20847810589295 -1.99417485060334 1.20448071698171
C 2.39152532479385 -1.92242211248596 2.72923421874968
C 3.09987569552154 2.78460475701989 -0.54902711605602
C 2.92356255889397 3.10766230878101 -2.04080100686395
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C 4.11394485907911 3.73324854029058 0.10814704694831
C -2.01776965824138 -1.04773581658006 -1.89537133239827
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C 0.12209449572828 -1.62365514210759 -1.09838143772240
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C 0.10035122662527 -4.10261075452712 -2.08770106068356
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H 3.44548082197539 -2.09060761875711 3.004371713260165
H 1.78347947140702 -2.69461339231604 3.22880355167185
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H 1.16173402252468 -1.77146970701444 0.97515799939067
H -1.9953568587407 2.79514051094393 0.83785229462891
H -4.85351126296046 3.01185848775949 2.00330737403599
H -3.57970175517586 4.25634851773926 2.06748522892884
H -3.40067748834498 2.73907414415652 2.98427689857092
H -0.74113339035100 3.50485533719497 -4.84947370168350
H -1.02937832196636 1.91584100814730 -5.616127848242386
H 0.52530849701276 2.22417422015596 -4.83482016086833
H -2.06222337371425 1.10631063082587 -1.49029274690736
H -3.86500642444442 -2.75793452139056 1.52896174100892
H -5.68380716245040 -1.31989778225972 0.64659668093587
H -5.28424643950074 1.10424714415652 0.30983794297558
H -3.02558825286254 2.83735613631370 -1.35636600235247
H -3.45964823013057 4.2723859407364 -0.43515560203534
H -4.68680277958906 2.98219599477443 -0.63998291744101
H -0.36529916288305 -1.58386298708366 2.08344607170077
H -2.15811979328816 -4.06126663235626 1.80143680287874
H -0.40740995400390 -4.02401798488766 2.06510762182872
H -1.08653798824813 -3.44565758138250 0.5260276215576
H -2.57566646280237 -2.67537633840094 3.91145128308662
H -1.68993747296502 -1.16197670637557 4.18484089299389
H -0.82179616763808 -2.71932564284005 4.23297200348523
H -0.33413648494785 0.47075317012974 3.52729658182245
H -1.55179921287758 1.70501255948692 3.15069986381436
H 2.51740660599044 2.37391328376926 1.96883378165868
H 2.19413566033140 0.97883869494687 3.00362629514477
H 2.41419957240102 -3.49710145088682 -0.37065140907911
H 1.69847161471552 -4.10345569509110 1.14644171094079
H 3.44020335442106 -3.80878598722444 1.05130951663926
H 4.60470378129352 -2.38697648557387 0.00432949041908
H 0.750516438016450 -0.77245413481156 -1.17872752431379
H 5.32680568939776 1.59034594551923 -1.41412032072419
H 2.11189613242792 2.95815905654127 -0.10615620219305
H 3.87045814765802 3.01188831516626 -2.59920614715731
H 2.55171173023022 4.13734714364235 -2.15482383402536
H 2.17225484603849 2.44343148383366 -2.48942038454425
H 4.24486407476485 3.51732547086215 1.18179830496342
H 3.77211954060984 4.77645074942868 0.01270347568714
H 5.10961423305611 3.66494993466734 -0.36135686717961
H -2.70764162203401 -1.18727430605852 -1.05044915856043
H 0.30039755008505 -4.36863859528863 -1.04115666917198
H 0.98971019157334 -3.62132625134117 -2.51801614950008
H -0.17668162045246 -4.99312401621046 -2.66325482960595
H 1.02407829206060 0.48834773328881 -1.60349499903784
H 0.68422437165812 2.75139184213185 3.73771590347220
H 0.20435441671222 3.10942066133896 2.04324306736717
H -2.56245435395647 -1.28735129863839 -2.81865751063062

Int-5 (Pathway B)

C 2.69628784500125 -1.04178203280220 0.72813428149105
C 2.69002002897516 0.265500567751311 0.17877602283417
C 3.76262867279127 0.73719704513708 -0.61258058001512
C 4.82532553804247 -0.14344266676600 -0.87370674719969
C 4.83755389122598 -1.43633608998881 -0.36238358566097
C 3.78119330162928 -1.87642386407493 0.43511685793544
N 1.61222309843824 1.16421924576303 0.54325182941711
C 0.36088519878627 1.06458495004368 0.0589261791420

N	-0.61666199814801	1.81483751044073	0.59442145899142	C	-4.09335347564420	2.29304265988810	-0.83817867855244
C	-0.35744588453881	2.87815942491687	1.58422823608030	C	-4.78561972359895	1.31374346611319	-0.13099487733325
C	1.98420477874519	2.18127232754718	1.55174554694178	C	-4.10584562941716	0.504449212284960	0.77762064765519
C	-0.26333384807006	1.61850551222611	0.30907772973372	C	-2.72871087997639	0.64839600714809	0.98224909573068
C	-2.68660980568456	2.47055018860580	-0.59870230090431	C	-2.00696307173803	3.60439214031290	-1.40469113396298
C	-4.06474438882987	2.28520641085040	-0.78163533791238	C	-2.34598891469799	4.96699709918892	-0.77538802342990
C	-4.76472180697504	1.30264600925259	-0.08546018875938	C	-2.03601269591216	-0.22780635259917	2.01592150688368
C	-4.09454874839587	0.49092366769939	0.82756812410917	C	-2.16114412006520	-1.72013538426165	1.67663418093878
C	-2.72006221721846	0.63975411825927	1.05177036494714	B	-0.14135521517829	0.07703789302290	-1.31277320899637
C	-1.96220162012134	3.58209040208412	-1.33345607573161	O	-0.09667767349671	1.15712636117138	-2.40673961164867
C	-2.25137842023052	4.95102757161953	-0.69412353436639	C	0.80911413898510	0.94674352868387	-3.29759757724487
C	-2.03667468771908	-0.24684232728807	2.08266596046712	O	1.24482101310565	1.87459563017440	-4.01645787426703
C	-2.12155529766922	-1.73050072793640	1.69594723792325	C	3.88993964807679	2.14959359454595	-1.17399860993963
B	-0.06146506156686	0.20188203939440	-1.28039806996427	C	4.31638391980030	2.24613631865770	-2.64583631000654
O	0.16973323484148	1.28387672303474	-2.40918846306185	C	1.51902072157005	-1.54563473938608	1.53327447741126
C	1.05219646018954	0.92813623594106	-3.22776035445827	C	1.71446472847032	-1.05415022999122	2.97769870343455
O	1.47659298226675	1.70193446403513	-4.16063936793013	C	4.87766544559072	2.94632652783519	-0.30024616104683
C	3.82500669168016	2.15828953623581	-1.14055307819563	C	1.33056503172071	-3.06660794057435	1.51544494306487
C	4.31368452219889	2.26644867138903	-2.59192483981403	C	0.76845858752303	-1.11819069471816	-2.021339903177386
C	1.57360141908248	-1.54665613235391	1.62785512426926	O	-0.18665027040687	-2.22125056980193	-2.36660601903773
C	1.84215496765360	-1.16537542481198	3.09360355868861	O	-0.44390879678045	-3.00403323491393	-1.29068018888738
C	4.7188805765455	3.04697271242927	-0.25380376581625	C	-1.43246390240839	-4.01534376214521	-1.46991772144966
C	1.31278761600248	-3.05256627578288	1.50351820983646	C	1.35299967546713	-0.45706764659569	-3.28192032156995
C	0.80657219497273	-1.06260155028508	-1.90507336539039	C	-2.54663540461118	0.07569740417094	3.43338585319842
C	-0.20507669411869	-2.05094971099358	-2.40178301175672	C	-2.31441558753411	3.61151121086610	-2.90765391921347
O	-0.64128170235266	-2.84890972062414	-1.40146077188740	O	-0.71586319184200	-2.40314695039162	-3.4814501186659
C	-1.71032595449708	-3.73732187438507	-1.72283839043285	C	1.23150245117618	3.44641690951511	-3.01827738209332
C	1.60628891231176	-0.44959362740722	-3.06333078290970	CI	1.40988747230975	5.01228125804409	-1.03111248145450
C	-2.59014200035622	0.003571718666848	3.49418076485812	H	-3.39278039683732	5.25176022236373	-0.97489123268736
C	-2.29161879532298	3.60963872141001	-2.83035098285322	H	-1.67461191989437	5.73793084237526	-1.18272961422142
O	-0.63246949760235	-2.12510662349930	-3.53077778722157	H	-2.20556438232736	4.95417465971281	0.31587035568071
C	1.02172788152360	3.0699577275365	-4.205944907723961	H	-0.92637109267013	3.46507896844836	-1.28856298861769
CI	1.36056764908245	4.44424734220526	-0.97334221291669	H	0.58404636371062	-1.11357705593834	1.15292308845244
H	-3.29063612868314	5.27392989302497	-0.878426731795498	H	2.61995093399941	-1.503754566547714	3.41646539259169
H	-1.55606100917915	5.69815323911694	-1.10556064442201	H	0.85414445853425	-1.33854088639528	3.60502877514253
H	-2.09640979019335	4.92765184254200	0.39490167230709	H	1.82776524532039	0.03629523165990	3.03419214916045
H	-0.87889658240731	3.42518402196324	-1.24094994863321	H	-1.15209652031158	-4.699397722345987	-2.28506708721620
H	0.64801460571932	-1.04352013290425	1.31988666390393	H	-2.40779835992280	-3.56617792132701	-1.71212878443120
H	2.74227793569954	-1.68015334411032	3.46722908885824	H	-1.49069971728753	-4.55791783905624	-0.51773657649987
H	0.99233233128036	-1.45508389171830	3.73305398503200	H	1.55042786182659	-1.52838748607022	-1.37936290105393
H	2.00532026927696	-0.08553305439852	3.21427715988923	H	5.66104793602963	0.15631470282375	-1.53221361595096
H	-1.41979615702530	4.42334634606175	-2.53261726502840	H	5.62542491227224	-2.15643921147279	-0.64724273041271
H	-2.59883089980950	-3.1727789849360	-2.04401606713139	H	3.73017738258479	-2.91779903185163	0.74750596352513
H	-1.92752284578302	4.29799663483330	-0.80511398932037	H	1.20110497557601	-3.44285398495676	0.49178548997785
H	1.45576377182744	-1.55672831147062	-1.18145623580146	H	0.42695488864942	-3.31372551875525	2.08437298321478
H	5.56821821227258	0.20280447221612	-1.48832916997873	H	2.17506603727281	-3.59161353875747	1.98952506801721
H	5.67446384366310	-2.10541709500165	-0.57816689275828	H	2.91883075727039	2.64930205714125	-1.07799604032111
H	3.80122321815470	-2.89039497088394	0.83502574710220	H	5.32575150933566	1.83616384227945	-2.80716447317647
H	1.10066869476537	-3.34183806672871	0.46415511518016	H	4.34840289349176	3.30426311921228	-2.94794022064831
H	0.43638972621591	-3.32710111793671	2.10903069471192	H	3.62216315926380	1.72472291168951	-3.31889722759785
H	2.15957711736343	-3.65129291157050	1.87421962032250	H	5.91257074686574	2.60062850444093	-0.45865341543202
H	2.81610135961971	2.59894616710609	-1.10336123859482	H	4.65578052613089	2.84755006814345	0.77180196546278
H	5.39248155947470	2.05880591615095	-2.68617766259593	H	4.81635969997457	4.01469513362757	-0.55875652381490
H	4.14381704848398	3.2959058385170	-2.94460877081757	H	2.28508054443200	3.12398767417756	0.83302097515983
H	3.78304294422477	1.59009546559960	-3.27566317675876	H	2.84364412581432	1.84887381852307	1.96070588931643
H	5.78596824370022	2.80431258687466	-0.39562776657434	H	-1.2687223210317	3.10270247015383	1.99223646142039
H	4.49301114786878	2.93320481459699	0.81495529558986	H	-0.12504362913692	3.83376795752302	0.81882735391781
H	4.54723008769005	4.10140628035127	-0.51841466325051	H	-2.01521389700585	2.66479975437316	-3.37984554625623
H	2.26604562044680	3.09603572771771	1.00511662499465	H	-1.77460929619114	4.43741939471534	-3.39866080639893
H	2.84750941601066	1.79157124465225	2.10589360117642	H	-3.38560373144553	3.77337699391681	-3.10804781226403
H	-1.27878675227624	3.01891866209754	2.16327347615612	H	-4.63498350372332	2.93870896669185	-1.53201250662713
H	-0.11891235759321	3.79817024823137	1.02218742261249	H	-5.86124285311610	1.18817668967245	-0.27843298747248
H	-2.09959925779124	2.63251625332265	-3.29949300769446	H	-4.65596755388600	-0.25038361125591	1.34420098390426
H	-1.66635391816697	4.36705974056175	-3.32833330556452	H	-0.96649312536204	0.01682998045457	2.00696505008739
H	-3.34359048622397	3.87791883873045	-3.02364202084453	H	-3.21467858156836	-2.04211202475462	1.6663981628556
H	-4.59704958511755	2.92915779490344	-1.48435667554390	H	-1.63627226819893	-2.32989531815471	2.42912618047640
H	-5.83815200254145	1.17479329175389	-0.24728882741004	H	-1.72548498528317	-1.94155241113344	0.69183702921856
H	-4.64913441202884	-0.26944834203836	1.38249981904165	H	-2.42734365281882	1.14249633234854	3.68131941061891
H	-0.97264290122549	0.02117668759057	2.10857209060585	H	-1.99020392622478	-0.51400542668823	4.18046411133908
H	-3.16862170288084	-2.06866450943137	1.63810936557564	H	-3.61515698377040	-0.17220315614569	3.53865425589400
H	-1.61285457370810	-2.35457054782098	2.44776635917522	H	2.45164217466037	-0.41083170776645	-3.29113913428599
H	-1.64964655523509	-1.91621383366380	0.72008367800358	H	1.29708696357815	2.91226898021805	-2.09103616689394
H	-2.50173045314400	1.06532337412239	3.77476128224124	H	0.26796991746945	3.852647115591927	-3.30397479180307
H	-2.03881417670401	-0.59428725213436	4.23840121526474	H	2.12914433376537	3.87071593845286	-3.45519602993821
H	-3.65471590469237	-0.27164246191805	3.56582334227166	H	-1.28022111991123	-0.2710505972516	-1.13097336857967
H	2.68246061464547	-0.37071500529731	-2.85030240731737	H	1.02734752375295	-0.97386644031309	-4.19995927850549
H	1.16209271820382	3.56694764816159	-3.21605747461687	C	0.82323819753145	2.58951305515895	2.30032035399018
H	-0.03575211626535	3.10041162647095	-4.49583819305815	H	0.57048171436577	1.76226623791266	2.98258701571308
H	1.64275567773074	3.55769756850584	-4.97678889793595	H	1.09725327627692	3.46150129544864	2.91228181736001
H	-1.24024466993804	-0.03274322518702	-1.24998551820370				
H	1.48601422531204	-0.99544519487485	-4.01261389411479				
H	0.81521831971272	2.49551775594955	2.46304888012924				
H	0.56202074004526	1.63543176767366	3.10447981723596				
H	1.08052283648876	3.33792120833195	3.11912543860617				

TS6 (Pathway B)

C	2.65260345752270	-1.05445607907951	0.63957771167288
C	2.66974309966556	0.2541352614556	0.09097064514733
C	3.76059920380534	0.71568270092098	-0.67877164579128
C	4.81201928281435	-0.17976099466961	-0.93481445240848
C	4.79753752008817	-1.47564753904072	-0.43428033737990
C	3.72783009891520	-1.90244170593221	0.35213908725411
N	1.59734834185027	1.16999896214537	0.42768412303936
C	0.33288543868627	1.01543565754944	-0.01361022301992
N	-0.62698294764288	1.81665635106493	0.48170881098540
C	-0.35303172646030	2.93176135637700	1.41262094591690
C	1.98235011021103	2.22699960335555	1.39573147222505
C	-2.04164862321280	1.61941333735771	0.22562947877969
C	-2.71217182839956	2.47431276130930	-0.67426629173551

C	-2.77958283552080	4.33094170884522	-2.33782839349305	H	-4.83051705048417	3.11239080854826	-1.06467391532474
C	-1.77092028106523	-0.37486600300186	1.76211876329704	H	-2.61397475838251	3.51928222123273	-3.05916164644556
C	-1.96778280146789	-0.03541035211629	3.25401218143647	H	-2.25336714049448	5.22313433020195	-2.71377758609180
B	0.09261295408024	0.88344921894428	-1.78868071290718	H	-3.85347001031072	4.57593359061490	-2.31170311346250
C	-1.37765597302749	0.63914845993763	-2.53765678695521	H	-0.71106239930936	-0.22589844789657	1.50271998145961
C	-1.70450535363956	-0.81362781599025	-2.18069614844184	H	-3.11847301311512	-2.10249281299970	1.86409345571323
C	-0.47839492030258	-1.41225758349508	-1.50165587750012	H	-1.40845777944901	-2.47785351821977	2.13593018236861
O	-0.33976670197592	-2.56695620555198	-1.17144406277213	H	-1.97136865208130	-2.16895994990960	0.49233967829465
C	3.26737606590654	-0.07829205781558	0.07211764837125	H	-3.00767774750667	-0.24088765031698	3.55643686887276
C	3.32047625865350	-1.51665030330553	-0.45895713918792	H	-1.76731869394677	1.02159088889895	3.48019466440834
C	1.98789614658403	4.36554564514569	-2.15712720624264	H	-1.30619393384149	-0.65366941255545	3.88206443383876
C	2.80735049757963	5.66109156359974	-2.06303282331421	H	-0.00799791089330	1.93272544384477	2.53202582078583
C	4.30832584858407	0.12856285813933	1.18850764149489	H	-1.27328403243822	3.12504255853445	2.18644600265141
C	1.10927643742055	4.34239023456518	-3.41676231223752	H	2.69213140327109	3.78879082291240	0.66950403534925
O	0.44591634660185	-0.47673238525146	-1.27732839398145	H	2.42581051884029	2.38302225644445	1.71050868797045
C	-2.09472271111038	-1.85909664191790	1.53692221917099	H	2.57476303271733	-1.66925347956568	-1.24862133638201
C	-2.45606807045939	5.12908997578680	0.03743264304012	H	3.09023386287712	-2.22371021195450	0.35380366359734
C	-1.13060226739632	0.80687299943264	-4.00196617594119	H	4.32096612902213	-1.77241683098401	-0.84483146479138
O	-0.81495532770394	-0.05369338908877	-4.78876909604685	H	5.17284342764532	-0.01761537244355	-1.87059124733532
O	-1.26053246721101	2.10995079140031	-4.38452465719444	H	5.58770667551058	1.71746049164381	-3.58783124146755
C	-0.92818631859648	2.39750255600637	-5.73828845294834	H	4.14271651730034	3.73039236992797	-3.70443359724897
H	5.32928891580583	-0.03917552424570	0.80793523529165	H	1.30312060647658	4.35332564339449	-1.29667960745346
H	4.13723376488834	-0.58035315878519	2.01510197205263	H	1.72826707259102	4.34352285443541	-4.32889608660846
H	4.27921232913251	1.15021812524629	1.60039693207549	H	0.45814500632464	5.23176142932324	-3.44997073753018
H	2.26563304348715	0.06144058255800	0.50165028649483	H	0.47051390647643	3.44996728499633	-3.44182553987873
H	-1.15808316632743	3.81955151800409	-1.06194377447112	H	3.43205607399692	5.68049755439301	-1.15532790329478
H	-3.53114511507677	5.34021430927561	0.15775725873284	H	2.14017167726218	6.53814055821407	-2.04009196807692
H	-1.96932712412505	6.04696715092944	-0.33075136470619	H	3.47769179915596	5.78064770908665	-2.92909867621327
H	-2.05319211147167	4.90748248424552	1.03720464320341	H	-2.54914651531074	-0.88955055958826	-1.48030912071719
H	-1.55939796772316	1.81993116675326	-6.43084966924857	H	0.91508900869624	1.27255564216515	-2.58919098293889
H	0.12493016619323	2.14987257763598	-5.94310218903009	H	-1.94627292354939	-1.42994303204759	-3.05876754372634
H	-1.09722923286354	3.47374833434628	-5.87487059530389	C	0.73914128662360	3.74063425255635	1.62274384316385
H	-2.16498588096218	1.33446131773554	-2.24134137252489	H	1.01743043167335	4.18176427645338	2.59145503328261
H	-4.42313674889178	-0.53522836452806	1.16599154390162	H	0.37218325010211	4.55402098613109	0.97663541444646
H	-5.83086295768639	1.06463190756896	-0.09321070373581				