

Supporting Information

Ligand-Enabled, Palladium-Catalyzed β -C(sp³)-H Arylation of Weinreb Amides

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1. General Information

Weinreb amides were synthesized from corresponding carboxylic acids which were obtained from commercial sources or prepared following literature procedures. Solvents were obtained from Sigma-Aldrich, Alfa-Aesar, Oakwood, and Acros and used directly without further purification. Analytical thin layer chromatography was performed on 0.25 mm silica gel 60-F254. Visualization was carried out with UV light. ^1H NMR was recorded on Bruker instrument (600 MHz). Chemical shifts were reported in parts per million (ppm) referenced to 0.0 ppm for tetramethylsilane. ^{13}C NMR was recorded on Bruker instrument (150 MHz), and were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to 77.16 ppm for center line of chloroform. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Coupling constants, J , were reported in Hertz unit (Hz). High-resolution mass spectra (HRMS) were recorded on an Agilent Mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

2. Experimental Section

2.1. Preparation of substrates

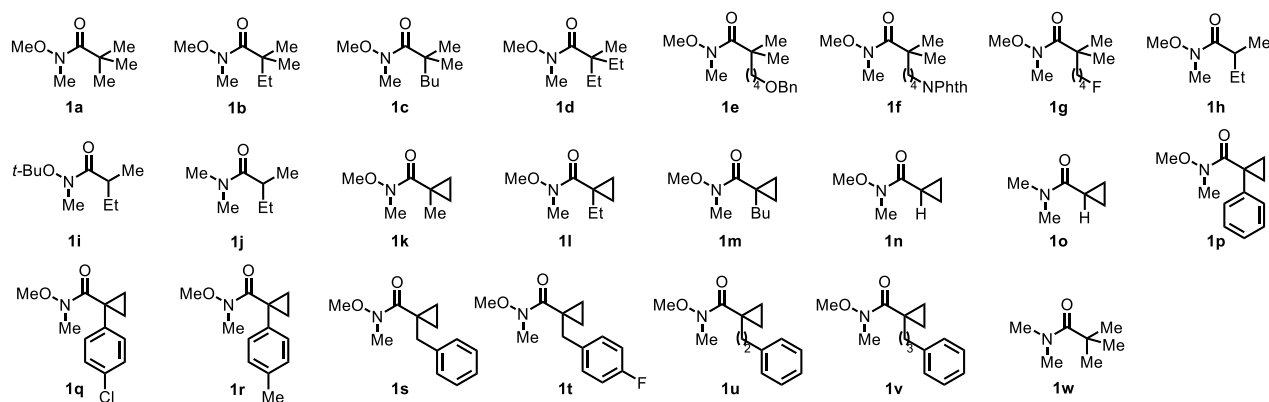


Table S1. List of substrates

- General procedure for the preparation of substrates **1a-w**.

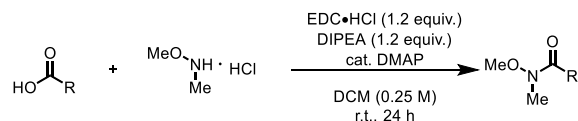


Figure S1. Preparation of substrates **1a-w**

To a stirring solution of corresponding carboxylic acid (5 mmol), *N*-(3-dimethylaminopropyl)-*N'*-ethylcarbodiimide hydrochloride (932 mg, 6 mmol), and *N,O*-dimethylhydroxylamine hydrochloride (585 mg, 6 mmol) in DCM (20 mL) were added *N,N*-diisopropylethylamine (1.05 mL, 6 mmol) and a small amount of 4-(dimethylamino)pyridine. The reaction was allowed to stir for 24 h at room temperature. Upon completion, the organic layer was washed with 0.2 M HCl (aq) and sat. Na_2CO_3 (aq). The combined organic layers were dried over anhydrous MgSO_4 , filtered, and concentrated *in vacuo*. The crude residue was purified by flash chromatography to afford substrate **1**. As a representative example, substrate **1a** was purified using hexanes/ethyl acetate as eluent to give 675 mg (93% yield) of product as a colorless oil.

(For **1i**, *N*-methyl-*O*-*tert*-butylhydroxylamine hydrochloride¹ was used instead. For **1j**, **1o**, and **1w**, dimethylamine hydrochloride was used instead.)

- General procedure for the preparation of corresponding carboxylic acids for substrates **1b-e**, **1g**.

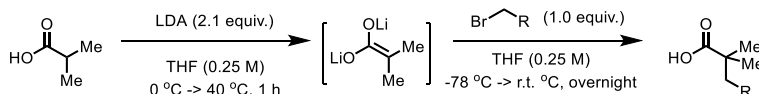


Figure S2. Preparation of Carboxylic acids for 1b-e, 1g

To a stirring solution of diisopropylamine (21 mmol, 3.0 mL) in THF (40 mL) was added 2.5 M *n*-BuLi solution (21 mmol, 8.4 mL) dropwise at -78 °C. The resulting solution was stirred for 30 min at 0 °C. Isobutyric acid (10 mmol, 910 μ L) was added dropwise at the same temperature, and the reaction mixture was stirred for 1 h at 40 °C. After cooling to -78 °C, corresponding alkyl bromide (10 mmol) was added dropwise. The reaction mixture was slowly warmed to room temperature overnight. The reaction mixture was quenched with water, and diluted with EtOAc. The layers were separated, and the organic layer was extracted with water. The aqueous layer was combined, and acidified to pH < 4 with 3 M HCl (aq.). Then, the aqueous layer was extracted with EtOAc. The combined organic layers were dried over anhydrous Na₂SO₄, filtered and concentrated *in vacuo*. The crude carboxylic acid was used without further purification.

(For **1d**, 2-ethylbutyric acid and methyl iodide was used instead.)

- General procedure for the preparation of corresponding carboxylic acids for substrates **1l-m**, **1s-v**.

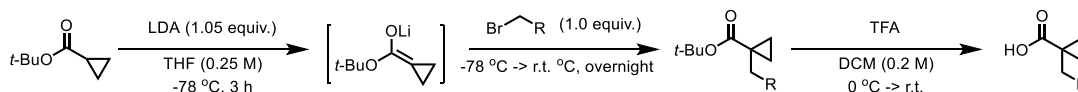


Figure S3. Preparation of Carboxylic acids for 1l-m, 1s-v

To a stirring solution of diisopropylamine (10.5 mmol, 1.5 mL) in THF (40 mL) was added 2.5 M *n*-BuLi solution (10.5 mmol, 4.2 mL) dropwise at -78 °C. The resulting solution was stirred for 30 min at 0 °C. After cooling to -78 °C, *tert*-butyl cyclopropanecarboxylate (10 mmol, 1.42 g) was added dropwise. The resulting solution was stirred for 3 h at same temperature. Corresponding alkyl bromide (10 mmol) was added dropwise, and the reaction mixture was warmed to room temperature overnight. The reaction mixture was quenched with sat. NH₄Cl (aq.). The layers were separated, and the aqueous layer was extracted with Et₂O. The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, filtered and concentrated *in vacuo*. The crude ester was dissolved in DCM (40 mL) and cooled to 0 °C. To the resulting solution was added trifluoroacetic acid (10 mL) dropwise. The reaction mixture was stirred at room temperature until completion was indicated by TLC. The solvent was removed *in vacuo*, and the crude carboxylic acid was used without further purification.

- Procedure for the preparation of **1f**.

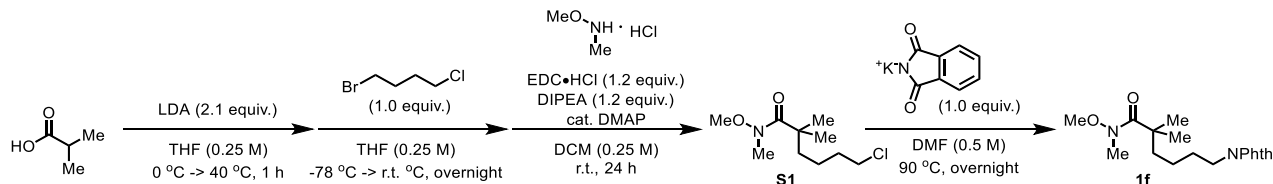
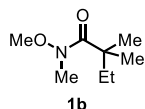


Figure S4. Preparation of 1f

S1 was prepared following the general procedures above using 1-bromo-4-chlorobutane. The suspension of **S1** (2.5 mmol, 555 mg) and potassium phthalimide (2.5 mmol, 465 mg) in DMF (5 mL) was stirred overnight at 90 °C. The

reaction mixture was cooled to room temperature, and diluted with EtOAc. The organic layer was washed with water and brine. The combined organic layers were dried over anhydrous MgSO_4 , filtered, and concentrated *in vacuo*. The crude residue was purified by flash chromatography to afford substrate **1f**.

- Full characterization of new compounds

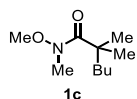


N-Methoxy-N,2,2-trimethylbutanamide (1b) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 3.67 (s, 3H), 3.18 (s, 3H), 1.66 (q, J = 7.5 Hz, 2H), 1.21 (s, 6H), 0.85 (t, J = 7.5 Hz, 3H).

^{13}C NMR (150 MHz, CDCl_3): δ 178.83, 60.58, 43.68, 33.88, 32.41, 25.32, 9.60.

HRMS (ESI-TOF): m/z calculated for $\text{C}_8\text{H}_{18}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 160.1332, found 160.1335.

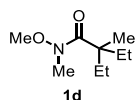


N-Methoxy-N,2,2-trimethylhexanamide (1c) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 3.66 (s, 3H), 3.17 (s, 3H), 1.62 – 1.58 (m, 2H), 1.28 (p, J = 7.0 Hz, 2H), 1.22 (s, 6H), 1.24 – 1.17 (m, 2H), 0.89 (t, J = 7.3 Hz, 3H).

^{13}C NMR (150 MHz, CDCl_3): δ 178.97, 60.60, 43.27, 39.73, 33.90, 27.42, 25.84, 23.44, 14.21.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{10}\text{H}_{22}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 188.1645, found 188.1649.

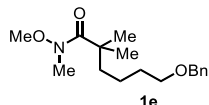


2-Ethyl-N-methoxy-N,2-dimethylbutanamide (1d) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 3.66 (s, 3H), 3.18 (s, 3H), 1.86 (dq, J = 15.0, 7.5 Hz, 2H), 1.44 (dq, J = 13.8, 7.5 Hz, 2H), 1.15 (s, 3H), 0.84 (t, J = 7.5 Hz, 6H).

^{13}C NMR (150 MHz, CDCl_3): δ 178.31, 60.44, 48.10, 33.89, 31.05, 21.83, 9.37.

HRMS (ESI-TOF): m/z calculated for $\text{C}_9\text{H}_{20}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 174.1489, found 174.1494.

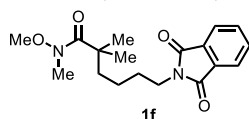


6-(Benzyloxy)-N-methoxy-N,2,2-trimethylhexanamide (1e) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 7.36 – 7.30 (m, 4H), 7.29 – 7.25 (m, 1H), 4.49 (s, 2H), 3.65 (s, 3H), 3.46 (t, J = 6.7 Hz, 2H), 3.16 (s, 3H), 1.64 – 1.57 (m, 4H), 1.35 – 1.28 (m, 2H), 1.22 (s, 6H).

^{13}C NMR (150 MHz, CDCl_3): δ 178.78, 138.78, 128.46, 127.77, 127.60, 73.06, 70.47, 60.60, 43.29, 39.82, 33.89, 30.47, 25.75, 21.87.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{17}\text{H}_{28}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$ 294.2064, found 294.2067.

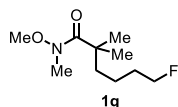


6-(1,3-Dioxoisindolin-2-yl)-N-methoxy-N,2,2-trimethylhexanamide (1f) (Colorless oil)

¹H NMR (600 MHz, CDCl₃): δ 7.84 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.71 (dd, *J* = 5.4, 3.0 Hz, 2H), 3.66 (t, *J* = 7.6 Hz, 2H), 3.66 (s, 3H), 3.15 (s, 3H), 1.69 – 1.63 (m, 4H), 1.33 – 1.26 (m, 2H), 1.22 (s, 6H).

¹³C NMR (150 MHz, CDCl₃): δ 178.60, 168.49, 133.96, 132.30, 123.27, 60.61, 43.17, 39.45, 38.01, 33.85, 29.17, 25.70, 22.48.

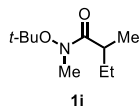
HRMS (ESI-TOF): *m/z* calculated for C₁₈H₂₅N₂O₄⁺ [M+H]⁺ 333.1809, found 333.1807.

**6-Fluoro-N-methoxy-N,2,2-trimethylhexanamide (1g) (Colorless oil)**

¹H NMR (600 MHz, CDCl₃): δ 4.43 (dt, *J* = 47.3, 6.2 Hz, 2H), 3.67 (s, 3H), 3.17 (s, 3H), 1.73 – 1.62 (m, 4H), 1.38 – 1.32 (m, 2H), 1.23 (s, 6H).

¹³C NMR (150 MHz, CDCl₃): δ 178.63, 84.11 (d, *J* = 164.3 Hz), 60.64, 43.23, 39.70, 33.89, 31.07 (d, *J* = 19.5 Hz), 25.70, 20.96 (d, *J* = 5.5 Hz).

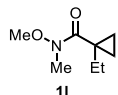
HRMS (ESI-TOF): *m/z* calculated for C₁₀H₂₁FNO₂⁺ [M+H]⁺ 206.1551, found 206.1562.

**N-(tert-Butoxy)-N,2-dimethylbutanamide (1i) (Colorless oil)**

¹H NMR (600 MHz, CDCl₃): δ 3.26 (s, 3H), 2.94 (br s, 1H), 1.67 (dp, *J* = 14.9, 7.4 Hz, 1H), 1.43 – 1.36 (m, 1H), 1.31 (s, 9H), 1.07 (d, *J* = 6.8 Hz, 3H), 0.88 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (150 MHz, CDCl₃): δ 181.74, 82.39, 39.52, 37.32, 27.82, 27.20, 16.77, 12.14.

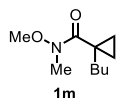
HRMS (ESI-TOF): *m/z* calculated for C₁₀H₂₂NO₂⁺ [M+H]⁺ 188.1645, found 188.1646.

**1-Ethyl-N-methoxy-N-methylcyclopropane-1-carboxamide (1l) (Colorless oil)**

¹H NMR (600 MHz, CDCl₃): δ 3.72 (s, 3H), 3.25 (s, 3H), 1.61 (q, *J* = 7.5 Hz, 2H), 1.00 – 0.94 (m, 5H), 0.58 – 0.54 (m, 2H).

¹³C NMR (150 MHz, CDCl₃): δ 173.45, 60.77, 34.14, 28.80, 26.79, 11.71, 11.54.

HRMS (ESI-TOF): *m/z* calculated for C₈H₁₆NO₂⁺ [M+H]⁺ 158.1176, found 158.1177.

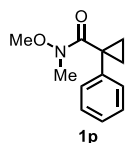
**1-Butyl-N-methoxy-N-methylcyclopropane-1-carboxamide (1m) (Colorless oil)**

¹H NMR (600 MHz, CDCl₃): δ 3.72 (s, 3H), 3.24 (s, 3H), 1.58 – 1.54 (m, 2H), 1.40 – 1.34 (m, 2H), 1.34 – 1.27 (m, 2H), 1.00 – 0.96 (m, 2H), 0.88 (t, *J* = 7.2 Hz, 3H), 0.57 – 0.54 (m, 2H).

¹³C NMR (150 MHz, CDCl₃): δ 173.68, 60.76, 35.65, 34.13, 29.91, 25.73, 22.82, 14.15, 11.81.

HRMS (ESI-TOF): *m/z* calculated for C₁₀H₂₀NO₂⁺ [M+H]⁺ 186.1489, found 186.1495.



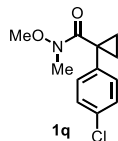


N-Methoxy-N-methyl-1-phenylcyclopropane-1-carboxamide (1p) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 7.32 – 7.25 (m, 4H), 7.20 (tt, J = 6.4, 1.6 Hz, 1H), 3.18 (br s, 3H), 3.12 (s, 3H), 1.45 – 1.41 (m, 2H), 1.15 – 1.11 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3): δ 173.37, 140.99, 128.47, 127.50, 126.54, 60.06, 33.91, 29.97, 13.85.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{12}\text{H}_{16}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 206.1176, found 206.1184.

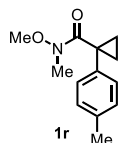


1-(4-Chlorophenyl)-N-methoxy-N-methylcyclopropane-1-carboxamide (1q) (Yellow oil)

^1H NMR (600 MHz, CDCl_3): δ 7.27 (d, J = 8.6 Hz, 2H), 7.21 (d, J = 8.6 Hz, 2H), 3.21 (br s, 3H), 3.12 (s, 3H), 1.46 – 1.42 (m, 2H), 1.11 – 1.07 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3): δ 173.05, 139.70, 132.32, 129.02, 128.61, 60.19, 33.82, 29.53, 13.96.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{12}\text{H}_{15}\text{ClNO}_2^+$ $[\text{M}+\text{H}]^+$ 240.0786, found 240.0792.

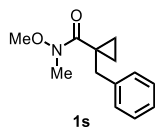


N-Methoxy-N-methyl-1-(p-tolyl)cyclopropane-1-carboxamide (1r) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 7.16 (d, J = 8.1 Hz, 2H), 7.10 (d, J = 7.9 Hz, 2H), 3.23 (br s, 3H), 3.12 (s, 3H), 2.31 (s, 3H), 1.42 – 1.38 (m, 2H), 1.11 – 1.07 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3): δ 173.41, 137.94, 136.16, 129.18, 127.37, 60.17, 33.98, 29.62, 21.17, 13.76.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{13}\text{H}_{18}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 220.1332, found 220.1335.

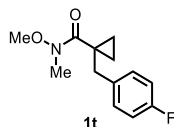


1-Benzyl-N-methoxy-N-methylcyclopropane-1-carboxamide (1s) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 7.29 – 7.25 (m, 2H), 7.23 – 7.17 (m, 3H), 3.70 (s, 3H), 3.12 (s, 3H), 3.00 (s, 2H), 1.10 – 1.07 (m, 2H), 0.73 – 0.69 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3): δ 173.22, 138.96, 129.08, 128.44, 126.56, 60.76, 40.74, 33.99, 26.06, 11.60.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{13}\text{H}_{18}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 220.1332, found 220.1339.



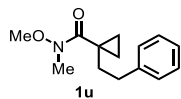
1-(4-Fluorobenzyl)-N-methoxy-N-methylcyclopropane-1-carboxamide (1t) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 7.18 (dd, J = 8.7, 5.4 Hz, 2H), 6.95 (t, J = 8.7 Hz, 2H), 3.71 (s, 3H), 3.13 (s, 3H),

2.96 (s, 2H), 1.12 – 1.08 (m, 2H), 0.72 – 0.68 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3): δ 173.08, 161.77 (d, $J = 244.2$ Hz), 134.72 (d, $J = 3.2$ Hz), 130.38 (d, $J = 9.2$ Hz), 115.23 (d, $J = 21.0$ Hz), 60.81, 40.04, 33.89, 26.21 (d, $J = 1.1$ Hz), 11.62.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{13}\text{H}_{17}\text{FNO}_2^+$ $[\text{M}+\text{H}]^+$ 238.1238, found 238.1246.

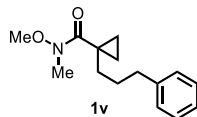


N-Methoxy-N-methyl-1-phenethylcyclopropane-1-carboxamide (1u) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 7.28 – 7.24 (m, 2H), 7.19 – 7.14 (m, 3H), 3.72 (s, 3H), 3.23 (s, 3H), 2.74 – 2.69 (m, 2H), 1.91 – 1.86 (m, 2H), 1.07 – 1.03 (m, 2H), 0.61 – 0.58 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3): δ 173.31, 142.03, 128.50, 128.42, 125.94, 60.86, 38.02, 34.10, 34.03, 25.78, 12.09.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{14}\text{H}_{20}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 234.1489, found 234.1493.



N-Methoxy-N-methyl-1-(3-phenylpropyl)cyclopropane-1-carboxamide (1v) (Colorless oil)

^1H NMR (600 MHz, CDCl_3): δ 7.28 – 7.24 (m, 2H), 7.19 – 7.15 (m, 3H), 3.65 (s, 3H), 3.20 (s, 3H), 2.62 (t, $J = 7.6$ Hz, 2H), 1.77 – 1.70 (m, 2H), 1.61 – 1.56 (m, 2H), 1.01 – 0.97 (m, 2H), 0.56 – 0.52 (m, 2H).

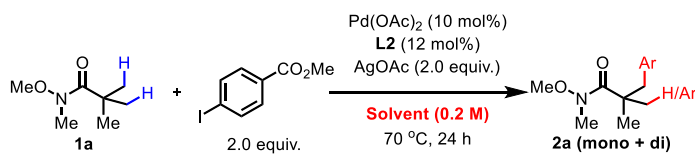
^{13}C NMR (150 MHz, CDCl_3): δ 173.51, 142.32, 128.54, 128.37, 125.83, 60.73, 35.75, 35.34, 34.08, 29.24, 25.60, 11.88.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{15}\text{H}_{22}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 248.1645, found 248.1653.

2.2 Preparation of Ligands

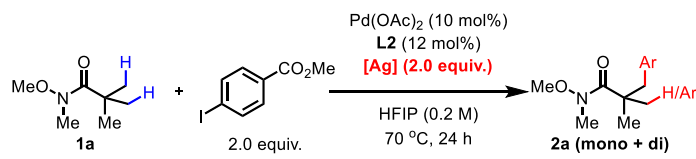
L3² and **L7**³ were synthesized following literature procedures. Other ligands were obtained from commercial sources.

2.3 Optimization of Reaction Conditions



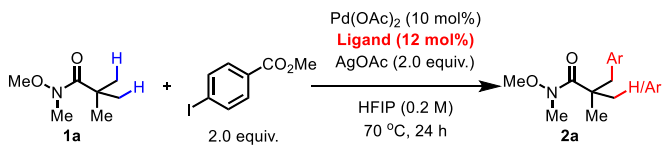
entry 1	HFIP	60% + 9%
entry 2	TFE	31% + 1%
entry 3	DCE	0%
entry 4	Toluene	0%
entry 5	<i>t</i> -AmOH	0%
entry 6	DMF	0%
entry 7	CH_3CN	0%
entry 8	Dioxane	0%

Table S2. Solvent screening



entry 1	AgOAc	60% + 9%
entry 2	AgTFA	10% mono
entry 3	Ag ₂ O	0%
entry 4	Ag ₂ CO ₃	44% + 2%

Table S3. Silver source screening



No Ligand <5%	 L1 , <5%	 L2 , 69% (81% at 80 °C) mono:di = 7:1 (5:1 at 80 °C)	 L3 , 74% mono:di = 10:1
 L4 , <5%	 L5 , <5%	 L6 , <5%	 L7 , <5%
PivOH L8 , <5%	Ac-Gly-OH L9 , 22% mono:di = 10:1	Ac-Val-OH L10 , 21% mono:di = >20:1	 L11 , 9%
 L12 , 0%	 L13 , <5%	 L14 , 8%	 L4 + L14 , 0%

Table S4. Ligand screening

Procedure for Ligand Screening: A sealed tube with magnetic stir bar was charged with $\text{Pd}(\text{OAc})_2$ (10 mol%, 2.2 mg), ligand (12 mol%), AgOAc (0.2 mmol, 33.4 mg), methyl 4-iodobenzoate (0.2 mmol, 52.4 mg), and substrate **1a** (0.1 mmol, 14.5 mg) in air. Then, HFIP (0.5 mL) was added as solvent. The reaction mixture was stirred at 70 °C for 24 hours. Upon completion, the reaction mixture was cooled to room temperature, diluted with EtOAc, filtered through a celite plug, and concentrated *in vacuo*. The yield was determined by ¹H NMR analysis of the crude product using CH₂Br₂ as the internal standard.

2.4 General Procedure for Pd-catalyzed C–H Arylation

Substrate Scope

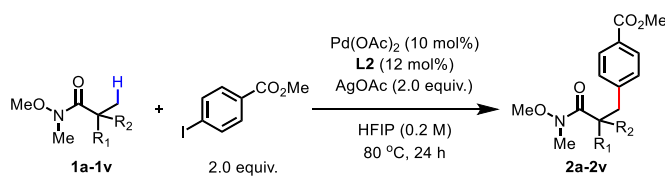
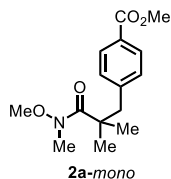


Figure S5. Pd-catalyzed C–H Arylation: Substrate Scope

A sealed tube with magnetic stir bar was charged with Pd(OAc)₂ (10 mol%, 2.2 mg), **L2** (12 mol%, 1.9 mg), AgOAc (0.2 mmol, 33.4 mg), methyl 4-iodobenzoate (0.2 mmol, 52.4 mg), and substrate **1** (0.1 mmol) in air. Then, HFIP (0.5 mL) was added as solvent. The reaction mixture was stirred at 80 °C for 24 hours. Upon completion, the reaction mixture was cooled to room temperature, diluted with EtOAc, filtered through a celite plug, and concentrated *in vacuo*. The crude reaction mixture was purified on silica gel using hexanes/EtOAc as eluent to afford the desired products.



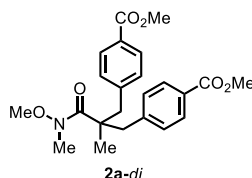
Methyl 4-(3-(methoxy(methyl)amino)-2,2-dimethyl-3-oxopropyl)benzoate (2a-mono)

2a-mono (17.4 mg, 62% yield) was obtained as a colorless oil by following the general procedure.

¹H NMR (600 MHz, CDCl₃): δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 8.3 Hz, 2H), 3.89 (s, 3H), 3.71 (s, 3H), 3.19 (s, 3H), 3.02 (s, 2H), 1.25 (s, 6H).

¹³C NMR (150 MHz, CDCl₃): δ 177.75, 167.25, 144.21, 130.35, 129.37, 128.32, 60.77, 52.09, 45.15, 44.38, 34.10, 25.53.

HRMS (ESI-TOF): *m/z* calculated for C₁₅H₂₂NO₄⁺ [M+H]⁺ 280.1543, found 280.1546.



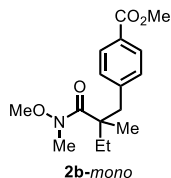
Dimethyl 4,4'-(2-(methoxy(methyl)carbamoyl)-2-methylpropane-1,3-diyl)dibenzoate (2a-di)

2a-di (9.8 mg, 14% yield) was obtained as a colorless oil by following the general procedure.

¹H NMR (600 MHz, CDCl₃): δ 7.93 (d, *J* = 8.4 Hz, 4H), 7.23 (d, *J* = 8.4 Hz, 4H), 3.90 (s, 6H), 3.57 (s, 3H), 3.44 (d, *J* = 13.2 Hz, 2H), 3.16 (s, 3H), 2.77 (d, *J* = 13.2 Hz, 2H), 1.13 (s, 3H).

¹³C NMR (150 MHz, CDCl₃): δ 176.09, 167.21, 143.61, 130.51, 129.49, 128.55, 60.74, 52.16, 49.49, 45.33, 34.37, 22.19.

HRMS (ESI-TOF): *m/z* calculated for C₂₃H₂₈NO₆⁺ [M+H]⁺ 414.1911, found 414.1913.



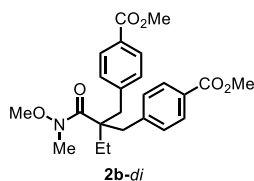
Methyl 4-(2-(methoxy(methyl)carbamoyl)-2-methylbutyl)benzoate (2b-mono)

2b-mono (18.7 mg, 64% yield) was obtained as a colorless oil by following the general procedure.

¹H NMR (600 MHz, CDCl₃): δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 3.89 (s, 3H), 3.70 (s, 3H), 3.29 (d, *J* = 13.2 Hz, 1H), 3.19 (s, 3H), 2.76 (d, *J* = 13.2 Hz, 1H), 1.96 (dq, *J* = 14.9, 7.5 Hz, 1H), 1.49 (dq, *J* = 15.0, 7.5 Hz, 1H), 1.14 (s, 3H), 0.92 (t, *J* = 7.5 Hz, 3H).

¹³C NMR (150 MHz, CDCl₃): δ 177.05, 167.28, 144.26, 130.40, 129.39, 128.29, 60.58, 52.11, 48.88, 44.20, 34.17, 31.40, 22.12, 9.51.

HRMS (ESI-TOF): m/z calculated for $C_{16}H_{24}NO_4^+$ $[M+H]^+$ 294.1700, found 294.1710.



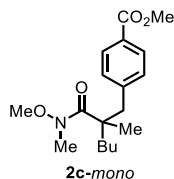
Dimethyl 4,4'-(2-ethyl-2-(methoxy(methyl)carbamoyl)propane-1,3-diyl)dibenzoate (2b-di)

2b-di (2.7 mg, 6% yield) was obtained as a colorless oil by following the general procedure.

1H NMR (600 MHz, $CDCl_3$): δ 7.93 (d, J = 8.2 Hz, 4H), 7.21 (d, J = 8.2 Hz, 4H), 3.90 (s, 6H), 3.66 (s, 3H), 3.21 (s, 3H), 3.16 (d, J = 14.7 Hz, 2H), 3.07 (d, J = 14.7 Hz, 2H), 1.67 (q, J = 7.4 Hz, 2H), 0.97 (t, J = 7.4 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 176.51, 167.19, 143.95, 130.19, 129.60, 128.42, 60.52, 52.23, 52.18, 39.56, 34.46, 25.81, 9.12.

HRMS (ESI-TOF): m/z calculated for $C_{24}H_{30}NO_6^+$ $[M+H]^+$ 428.2068, found 428.2074.



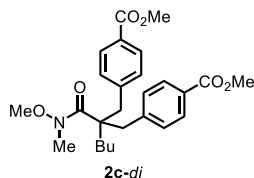
Methyl 4-(2-(methoxy(methyl)carbamoyl)-2-methylhexyl)benzoate (2c-mono)

2c-mono (20.4 mg, 63% yield) was obtained as a colorless oil by following the general procedure.

1H NMR (600 MHz, $CDCl_3$): δ 7.92 (d, J = 8.2 Hz, 2H), 7.19 (d, J = 8.2 Hz, 2H), 3.89 (s, 3H), 3.69 (s, 3H), 3.30 (d, J = 13.2 Hz, 1H), 3.18 (s, 3H), 2.75 (d, J = 13.2 Hz, 1H), 1.92 – 1.83 (m, 1H), 1.44 (td, J = 13.3, 3.8 Hz, 1H), 1.36 – 1.18 (m, 4H), 1.15 (s, 3H), 0.91 (t, J = 7.0 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 177.19, 167.24, 144.24, 130.40, 129.35, 128.26, 60.58, 52.07, 48.38, 44.47, 38.73, 34.16, 27.20, 23.38, 22.67, 14.21.

HRMS (ESI-TOF): m/z calculated for $C_{18}H_{28}NO_4^+$ $[M+H]^+$ 322.2013, found 322.2017.



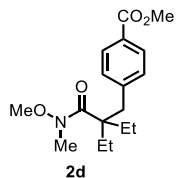
Dimethyl 4,4'-(2-butyl-2-(methoxy(methyl)carbamoyl)propane-1,3-diyl)dibenzoate (2c-di)

2c-di (2.3 mg, 5% yield) was obtained as a colorless oil by following the general procedure.

1H NMR (600 MHz, $CDCl_3$): δ 7.93 (d, J = 8.4 Hz, 4H), 7.19 (d, J = 8.3 Hz, 4H), 3.90 (s, 6H), 3.65 (s, 3H), 3.21 (s, 3H), 3.15 (d, J = 14.7 Hz, 2H), 3.09 (d, J = 14.8 Hz, 2H), 1.61 – 1.57 (m, 2H), 1.40 – 1.33 (m, 2H), 1.31 – 1.24 (m, 2H), 0.89 (t, J = 7.3 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 176.68, 167.20, 144.00, 130.19, 129.59, 128.42, 60.52, 52.18, 51.70, 39.92, 34.47, 33.29, 26.57, 23.11, 14.24.

HRMS (ESI-TOF): m/z calculated for $C_{26}H_{34}NO_6^+$ $[M+H]^+$ 456.2381, found 456.2392.



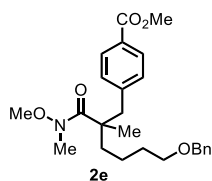
Methyl 4-(2-ethyl-2-(methoxy(methyl)carbamoyl)butyl)benzoate (2d)

2d (19.5 mg, 63% yield) was obtained as a colorless oil by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.92 (d, J = 8.3 Hz, 2H), 7.18 (d, J = 8.3 Hz, 2H), 3.89 (s, 3H), 3.71 (s, 3H), 3.20 (s, 3H), 3.04 (s, 2H), 1.69 – 1.57 (m, 4H), 0.91 (t, J = 7.5 Hz, 6H).

^{13}C NMR (150 MHz, CDCl_3): δ 177.14, 167.25, 144.49, 130.33, 129.39, 128.21, 60.42, 52.37, 52.09, 37.90, 34.23, 25.41, 8.96.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{17}\text{H}_{26}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 308.1856, found 308.1865.



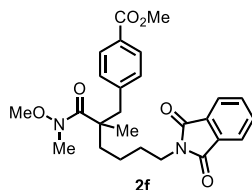
Methyl 4-(6-(benzyloxy)-2-(methoxy(methyl)carbamoyl)-2-methylhexyl)benzoate (2e)

2e (19.8 mg, 46% yield) was obtained as a colorless oil by following the general procedure. Trace amount of *di*-product was observed in crude ^1H NMR.

^1H NMR (600 MHz, CDCl_3): δ 7.91 (d, J = 8.3 Hz, 2H), 7.36 – 7.31 (m, 4H), 7.28 (td, J = 6.0, 2.8 Hz, 1H), 7.18 (d, J = 8.3 Hz, 2H), 4.49 (s, 2H), 3.89 (s, 3H), 3.67 (s, 3H), 3.46 (t, J = 6.6 Hz, 2H), 3.28 (d, J = 13.2 Hz, 1H), 3.17 (s, 3H), 2.76 (d, J = 13.3 Hz, 1H), 1.90 (td, J = 12.9, 4.2 Hz, 1H), 1.63 – 1.58 (m, 2H), 1.50 – 1.38 (m, 2H), 1.39 – 1.28 (m, 1H), 1.16 (s, 3H).

^{13}C NMR (150 MHz, CDCl_3): δ 177.03, 167.26, 144.12, 138.71, 130.41, 129.39, 128.47, 128.31, 127.76, 127.63, 73.07, 70.30, 60.60, 52.10, 48.41, 44.44, 38.78, 34.17, 30.40, 22.63, 21.70.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{25}\text{H}_{34}\text{NO}_5^+$ $[\text{M}+\text{H}]^+$ 428.2431, found 428.2437.



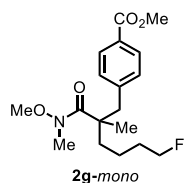
Methyl 4-(6-(1,3-dioxoisindolin-2-yl)-2-(methoxy(methyl)carbamoyl)-2-methylhexyl)benzoate (2f)

2f (25.1 mg, 54% yield) was obtained as a colorless oil by following the general procedure. Trace amount of *di*-product was observed in crude ^1H NMR.

^1H NMR (600 MHz, CDCl_3): δ 7.91 (d, J = 8.1 Hz, 2H), 7.84 (dd, J = 5.3, 3.1 Hz, 2H), 7.71 (dd, J = 5.4, 3.0 Hz, 2H), 7.18 (d, J = 8.2 Hz, 2H), 3.89 (s, 3H), 3.68 (s, 3H), 3.71 – 3.64 (m, 2H), 3.27 (d, J = 13.3 Hz, 1H), 3.16 (s, 3H), 2.75 (d, J = 13.3 Hz, 1H), 1.93 (td, J = 12.9, 4.3 Hz, 1H), 1.77 – 1.61 (m, 2H), 1.49 (td, J = 13.0, 4.6 Hz, 1H), 1.40 (tdt, J = 13.9, 10.4, 5.3 Hz, 1H), 1.32 (dtd, J = 17.6, 8.9, 8.1, 5.0 Hz, 1H), 1.16 (s, 3H).

^{13}C NMR (150 MHz, CDCl_3): δ 176.85, 168.43, 167.18, 143.95, 133.99, 132.22, 130.34, 129.36, 128.30, 123.26, 60.61, 52.05, 48.28, 44.52, 38.59, 37.93, 34.12, 29.11, 22.55, 22.29.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{26}\text{H}_{31}\text{N}_2\text{O}_6^+$ $[\text{M}+\text{H}]^+$ 467.2177, found 467.2177.



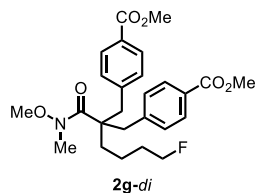
Methyl 4-(6-fluoro-2-(methoxy(methyl)carbamoyl)-2-methylhexyl)benzoate (2g-mono)

2g-mono (22.5 mg, 66% yield) was obtained as a colorless oil by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.92 (d, J = 8.3 Hz, 2H), 7.19 (d, J = 8.3 Hz, 2H), 4.44 (dt, J = 47.3, 6.0 Hz, 2H), 3.89 (s, 3H), 3.69 (s, 3H), 3.26 (d, J = 13.2 Hz, 1H), 3.18 (s, 3H), 2.80 (d, J = 13.3 Hz, 1H), 1.93 (td, J = 13.4, 12.2, 5.6 Hz, 1H), 1.74 – 1.65 (m, 2H), 1.50 – 1.42 (m, 2H), 1.41 – 1.35 (m, 1H), 1.18 (s, 3H).

^{13}C NMR (150 MHz, CDCl_3): δ 176.89, 167.22, 143.95, 130.39, 129.40, 128.37, 83.93 (d, J = 164.5 Hz), 60.62, 52.10, 48.31, 44.48, 38.56, 34.17, 30.98 (d, J = 19.7 Hz), 22.57, 20.82 (d, J = 5.3 Hz).

HRMS (ESI-TOF): m/z calculated for $\text{C}_{18}\text{H}_{27}\text{FNO}_4$ $[\text{M}+\text{H}]^+$ 340.1910, found 340.1921.



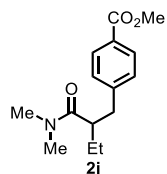
Dimethyl 4,4'-(2-(4-fluorobutyl)-2-(methoxy(methyl)carbamoyl)propane-1,3-diyl)dibenzoate (2g-di)

2g-di (2.6 mg, 5% yield) was obtained as a colorless oil by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.94 (d, J = 8.3 Hz, 4H), 7.20 (d, J = 8.3 Hz, 4H), 4.41 (dt, J = 47.3, 5.8 Hz, 2H), 3.90 (s, 6H), 3.68 (s, 3H), 3.22 (s, 3H), 3.22 (d, J = 14.6 Hz, 2H), 3.07 (d, J = 14.6 Hz, 2H), 1.81 – 1.47 (m, 6H).

^{13}C NMR (150 MHz, CDCl_3): δ 176.34, 167.14, 143.69, 130.12, 129.67, 128.54, 83.69 (d, J = 164.6 Hz), 60.54, 52.19, 51.79, 40.00, 34.48, 32.88, 30.69 (d, J = 19.8 Hz), 20.14 (d, J = 4.8 Hz).

HRMS (ESI-TOF): m/z calculated for $\text{C}_{26}\text{H}_{33}\text{FNO}_6$ $[\text{M}+\text{H}]^+$ 474.2286, found 474.2294.



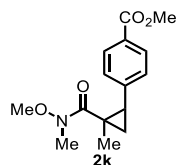
Methyl 4-(2-(dimethylcarbamoyl)butyl)benzoate (2j)

2j (9.0 mg, 34% yield) was obtained as a colorless oil by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.93 (d, J = 8.2 Hz, 2H), 7.24 (d, J = 8.2 Hz, 2H), 3.90 (s, 3H), 2.99 (dd, J = 12.9, 9.6 Hz, 1H), 2.88 (td, J = 9.7, 4.8 Hz, 1H), 2.85 (s, 3H), 2.76 (dd, J = 12.9, 5.0 Hz, 1H), 2.68 (s, 3H), 1.82 – 1.73 (m, 1H), 1.58 – 1.50 (m, 1H), 0.90 (t, J = 7.4 Hz, 3H).

^{13}C NMR (150 MHz, CDCl_3): δ 174.91, 167.22, 146.01, 129.73, 129.10, 128.28, 52.15, 45.31, 39.34, 37.27, 35.70, 26.37, 12.08.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{15}\text{H}_{22}\text{NO}_3$ $[\text{M}+\text{H}]^+$ 264.1594, found 264.1598.



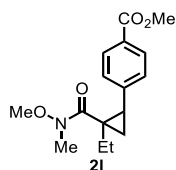
Methyl 4-(2-(methoxy(methyl)carbamoyl)-2-methylcyclopropyl)benzoate (2k)

2k (26.8 mg, 97% yield) was obtained as a colorless oil by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.90 (d, J = 8.4 Hz, 2H), 7.15 (d, J = 8.3 Hz, 2H), 3.89 (s, 3H), 3.33 (s, 3H), 2.89 (s, 3H), 2.19 (dd, J = 8.4, 6.7 Hz, 1H), 1.85 (t, J = 6.1 Hz, 1H), 1.52 (s, 3H), 1.16 (dd, J = 8.4, 5.7 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 167.07, 144.64, 129.44, 128.02, 126.89, 60.55, 52.07, 33.67, 32.38, 31.74, 22.59, 20.19. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{15}\text{H}_{20}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 278.1387, found 278.1392.

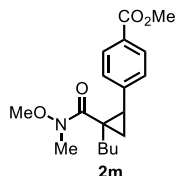
**Methyl 4-(2-ethyl-2-(methoxy(methyl)carbamoyl)cyclopropyl)benzoate (2l)**

2l (28.7 mg, 99% yield) was obtained as a colorless oil by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.90 (d, J = 8.4 Hz, 2H), 7.15 (d, J = 8.4 Hz, 2H), 3.89 (s, 3H), 3.32 (s, 3H), 2.89 (s, 3H), 2.39 (br s, 1H), 2.21 (dd, J = 8.6, 6.5 Hz, 1H), 1.84 – 1.75 (m, 1H), 1.18 – 1.08 (m, 2H), 1.03 (t, J = 7.4 Hz, 3H).

^{13}C NMR (150 MHz, CDCl_3): δ 167.14, 144.68, 129.50, 128.02, 126.94, 60.53, 52.11, 38.72, 33.86, 30.76, 30.09, 18.37, 11.49. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{16}\text{H}_{22}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 292.1543, found 292.1547.

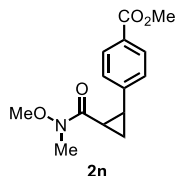
**Methyl 4-(2-butyl-2-(methoxy(methyl)carbamoyl)cyclopropyl)benzoate (2m)**

2m (31.3 mg, 98% yield) was obtained as white solid by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.89 (d, J = 7.6 Hz, 2H), 7.14 (d, J = 7.6 Hz, 2H), 3.88 (s, 3H), 3.32 (s, 3H), 2.88 (s, 3H), 2.37 (br s, 1H), 2.19 (t, J = 7.1 Hz, 1H), 1.82 (t, J = 5.5 Hz, 1H), 1.53 – 1.43 (m, 1H), 1.42 – 1.30 (m, 3H), 1.20 – 1.12 (m, 1H), 1.11 – 1.00 (m, 1H), 0.90 (t, J = 6.0 Hz, 3H).

^{13}C NMR (150 MHz, CDCl_3): δ 167.09, 144.59, 129.43, 127.95, 126.92, 60.46, 52.05, 37.69, 36.87, 33.74, 30.67, 29.53, 22.73, 18.83, 14.07. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{18}\text{H}_{26}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 320.1856, found 320.1866.

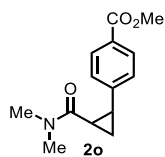
**Methyl 4-(2-(methoxy(methyl)carbamoyl)cyclopropyl)benzoate (2n)**

2n (4.7 mg, 18% yield) was obtained as a colorless oil by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.92 (d, J = 8.4 Hz, 2H), 7.30 (d, J = 8.3 Hz, 2H), 3.88 (s, 3H), 3.68 (s, 3H), 3.02 (s, 3H), 2.62 (br s, 1H), 2.57 (q, J = 8.6 Hz, 1H), 1.87 (q, J = 6.4 Hz, 1H), 1.37 (td, J = 8.2, 5.1 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 170.63, 167.22, 142.80, 129.39, 128.99, 128.38, 61.75, 52.10, 32.80, 25.50, 21.23, 10.69.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{14}\text{H}_{18}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 264.1230, found 264.1234.



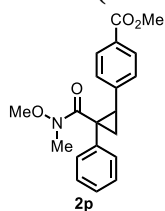
Methyl 4-(2-(dimethylcarbamoyl)cyclopropyl)benzoate (2o)

2o (21.5 mg, 87% yield) was obtained as yellow solid by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.90 (d, J = 8.4 Hz, 2H), 7.22 (d, J = 8.4 Hz, 2H), 3.88 (s, 3H), 2.97 (s, 3H), 2.72 (s, 3H), 2.50 (td, J = 8.9, 7.0 Hz, 1H), 2.27 – 2.21 (m, 1H), 1.89 – 1.85 (m, 1H), 1.36 (td, J = 8.4, 5.4 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 168.46, 167.17, 143.40, 129.41, 128.21, 127.79, 52.07, 36.91, 35.46, 24.62, 24.15, 11.28.

HRMS (ESI-TOF): m/z calculated for $\text{C}_{14}\text{H}_{18}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$ 248.1281, found 248.1289.



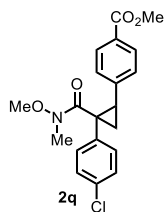
Methyl 4-(2-(methoxy(methyl)carbamoyl)-2-phenylcyclopropyl)benzoate (2p)

2p (20.0 mg, 59% yield) was obtained as white solid by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.96 (d, J = 8.2 Hz, 2H), 7.41 (br s, 2H), 7.37 – 7.32 (m, 4H), 7.28 – 7.24 (m, 1H), 3.90 (s, 3H), 3.16 (t, J = 7.7 Hz, 1H), 2.80 (br s, 3H), 2.70 (s, 3H), 2.37 (t, J = 5.7 Hz, 1H), 1.31 (br s, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 167.11, 142.94, 140.66, 129.41, 128.72, 128.44, 128.20, 127.05, 59.91, 52.13, 40.66, 33.05, 28.64, 20.18. (One aromatic carbon peak cannot be found due to overlap/Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{20}\text{H}_{22}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 340.1543, found 340.1547.



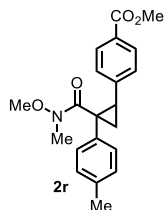
Methyl 4-(2-(4-chlorophenyl)-2-(methoxy(methyl)carbamoyl)cyclopropyl)benzoate (2q)

2q (27.1 mg, 72% yield) was obtained as white solid by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.96 (d, J = 8.1 Hz, 2H), 7.40 – 7.29 (m, 6H), 3.90 (s, 3H), 3.10 (t, J = 7.9 Hz, 1H), 2.87 (br s, 3H), 2.71 (s, 3H), 2.36 (t, J = 6.0 Hz, 1H), 1.27 (br s, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 170.82, 167.05, 142.49, 139.36, 132.84, 129.44, 128.84, 128.58, 128.19, 60.05, 52.15, 40.07, 33.10, 28.93, 20.24. (One aromatic carbon peak cannot be found due to overlap)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{20}\text{H}_{21}\text{ClNO}_4^+$ $[\text{M}+\text{H}]^+$ 374.1154, found 374.1156.



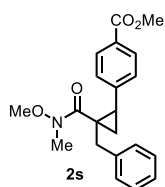
Methyl 4-(2-(methoxy(methyl)carbamoyl)-2-(p-tolyl)cyclopropyl)benzoate (2r)

2r (23.9 mg, 68% yield) was obtained as a colorless oil by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.95 (d, J = 8.3 Hz, 2H), 7.33 (d, J = 8.3 Hz, 2H), 7.29 (br s, 2H), 7.16 (d, J = 7.9 Hz, 2H), 3.90 (s, 3H), 3.11 (t, J = 7.8 Hz, 1H), 2.84 (br s, 3H), 2.70 (s, 3H), 2.34 (s, 3H), 2.34 – 2.30 (m, 1H), 1.28 (br s, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 171.48, 167.12, 143.13, 137.60, 136.73, 129.40, 128.38, 128.08, 59.98, 52.12, 40.38, 33.08, 28.71, 21.15, 20.37. (Two aromatic carbon peaks cannot be found due to overlap)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{21}\text{H}_{24}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 354.1700, found 354.1698.



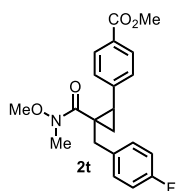
Methyl 4-(2-benzyl-2-(methoxy(methyl)carbamoyl)cyclopropyl)benzoate (2s)

2s was obtained as mixture with **1s** in 10:1 ratio (22.0 mg, 59% yield) as white solid by following the general procedure.

^1H NMR (600 MHz, CDCl_3): δ 7.90 (d, J = 8.4 Hz, 2H), 7.33 – 7.29 (m, 2H), 7.26 – 7.20 (m, 3H), 7.17 (d, J = 8.4 Hz, 2H), 3.88 (s, 3H), 3.65 (br s, 1H), 3.27 (s, 3H), 2.84 (s, 3H), 2.64 (d, J = 14.4 Hz, 1H), 2.27 (dd, J = 8.6, 6.8 Hz, 1H), 1.90 (t, J = 6.1 Hz, 1H), 1.31 (dd, J = 8.7, 5.8 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 167.12, 144.34, 137.91, 129.51, 129.24, 128.60, 128.15, 127.19, 126.90, 60.73, 52.12, 41.72, 37.70, 33.71, 30.05, 18.33. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{21}\text{H}_{24}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 354.1700, found 354.1702.



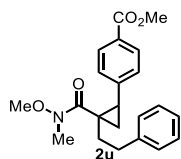
Methyl 4-(2-(4-fluorobenzyl)-2-(methoxy(methyl)carbamoyl)cyclopropyl)benzoate (2t)

2t (23.3 mg, 63% yield) was obtained as white solid by following the general procedure. Structure was confirmed by X-Ray analysis of the crystal obtained using chloroform/hexanes as recrystallization solvents.

^1H NMR (600 MHz, CDCl_3): δ 7.91 (d, J = 7.2 Hz, 2H), 7.24 – 7.18 (m, 2H), 7.17 (d, J = 7.2 Hz, 2H), 6.99 (t, J = 7.9 Hz, 2H), 3.88 (s, 3H), 3.66 (br s, 1H), 3.25 (s, 3H), 2.85 (s, 3H), 2.55 (d, J = 14.4 Hz, 1H), 2.28 (t, J = 7.4 Hz, 1H), 1.92 (t, J = 5.2 Hz, 1H), 1.31 (t, J = 6.8 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 169.84, 167.07, 161.91 (d, J = 244.8 Hz), 144.16, 133.74, 130.53 (d, J = 7.9 Hz), 129.53, 128.20, 127.14, 115.41 (d, J = 21.2 Hz), 60.74, 52.11, 41.09, 37.86, 33.66, 30.15, 18.58.

HRMS (ESI-TOF): m/z calculated for $C_{21}H_{23}FNO_4^+$ $[M+H]^+$ 372.1606, found 372.1610.



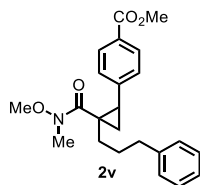
Methyl 4-(2-(methoxy(methyl)carbamoyl)-2-phenethylcyclopropyl)benzoate (2u)

2u was obtained as mixture with **1u** in 96:4 ratio (25.3 mg, 67% yield) as a colorless oil by following the general procedure.

1H NMR (600 MHz, $CDCl_3$): δ 7.90 (d, J = 8.3 Hz, 2H), 7.28 (t, J = 7.6 Hz, 2H), 7.21 – 7.18 (m, 3H), 7.14 (d, J = 8.4 Hz, 2H), 3.89 (s, 3H), 3.32 (s, 3H), 2.90 (s, 3H), 2.85 – 2.67 (m, 3H), 2.23 (dd, J = 8.5, 6.7 Hz, 1H), 1.87 (t, J = 6.1 Hz, 1H), 1.36 (td, J = 13.4, 5.4 Hz, 1H), 1.16 (dd, J = 8.5, 5.9 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 167.13, 144.38, 141.54, 129.51, 128.54, 128.48, 128.13, 127.04, 126.14, 60.66, 52.14, 39.17, 37.62, 33.76, 33.70, 30.89, 18.89. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $C_{22}H_{26}NO_4^+$ $[M+H]^+$ 368.1856, found 368.1859.



Methyl 4-(2-(methoxy(methyl)carbamoyl)-2-(3-phenylpropyl)cyclopropyl)benzoate (2v)

2v (29.1 mg, 76% yield) was obtained as a colorless oil by following the general procedure.

1H NMR (600 MHz, $CDCl_3$): δ 7.88 (d, J = 8.3 Hz, 2H), 7.27 (t, J = 7.6 Hz, 2H), 7.19 – 7.15 (m, 3H), 7.12 (d, J = 8.4 Hz, 2H), 3.87 (s, 3H), 3.22 (s, 3H), 2.82 (s, 3H), 2.70 (dt, J = 14.4, 7.4 Hz, 1H), 2.61 (dt, J = 14.1, 7.5 Hz, 1H), 2.38 (br s, 1H), 2.19 – 2.14 (m, 1H), 1.89 – 1.81 (m, 2H), 1.77 – 1.69 (m, 1H), 1.12 (dd, J = 8.3, 5.8 Hz, 1H), 1.06 (ddd, J = 13.8, 11.3, 5.6 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 167.09, 144.45, 141.93, 129.43, 128.53, 128.40, 127.99, 126.96, 125.93, 60.41, 52.08, 37.50, 36.35, 35.56, 33.65, 30.64, 28.87, 18.77. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $C_{23}H_{28}NO_4^+$ $[M+H]^+$ 382.2013, found 382.2015.

Aryl Iodide Scope

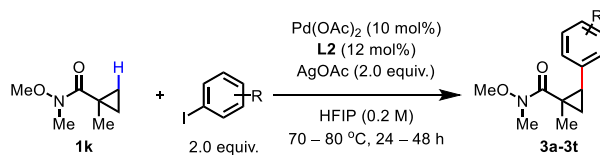
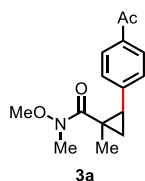


Figure S6. Pd-catalyzed C–H Arylation: Aryl Iodide Scope

A sealed tube with magnetic stir bar was charged with $Pd(OAc)_2$ (10 mol%, 2.2 mg), **L2** (12 mol%, 1.9 mg), $AgOAc$ (0.2 mmol, 33.4 mg), $Ar-I$ (0.2 mmol), and substrate **1k** (0.1 mmol, 14.3 mg) in air. Then, HFIP (0.5 mL) was added as solvent. The reaction mixture was stirred at 70 or 80 °C for 24 or 48 hours. Upon completion, the reaction mixture was cooled to room temperature, diluted with EtOAc, filtered through a celite plug, and concentrated *in vacuo*. The crude reaction mixture was purified on silica gel using hexanes/EtOAc as eluent to afford the desired products.



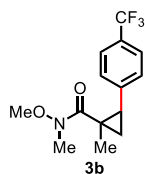
2-(4-Acetylphenyl)-N-methoxy-N,1-dimethylcyclopropane-1-carboxamide (**3a**)

3a (23.1 mg, 88% yield) was obtained as a colorless oil by following the general procedure (70 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 3.36 (s, 3H), 2.90 (s, 3H), 2.56 (s, 3H), 2.20 (dd, *J* = 8.5, 6.6 Hz, 1H), 1.86 (t, *J* = 6.1 Hz, 1H), 1.53 (s, 3H), 1.17 (dd, *J* = 8.5, 5.7 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 197.76, 144.94, 135.19, 128.27, 127.10, 60.63, 33.69, 32.45, 31.74, 26.61, 22.63, 20.29. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₅H₂₀NO₃⁺ [M+H]⁺ 262.1438, found 262.1446.



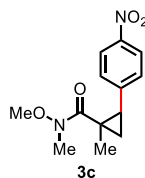
N-Methoxy-N,1-dimethyl-2-(4-(trifluoromethyl)phenyl)cyclopropane-1-carboxamide (**3b**)

3b (24.7 mg, 86% yield) was obtained as a colorless oil by following the general procedure (70 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 7.47 (d, *J* = 8.2 Hz, 2H), 7.19 (d, *J* = 8.2 Hz, 2H), 3.38 (s, 3H), 2.89 (s, 3H), 2.20 (dd, *J* = 8.4, 6.7 Hz, 1H), 1.85 (t, *J* = 6.1 Hz, 1H), 1.53 (s, 3H), 1.15 (dd, *J* = 8.5, 5.7 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 143.18, 128.43 (q, *J* = 31.9 Hz), 127.35, 125.02 (q, *J* = 3.7 Hz), 124.38 (q, *J* = 271.8 Hz), 60.61, 33.68, 32.16, 31.41, 22.58, 19.99. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₄H₁₇F₃NO₂⁺ [M+H]⁺ 288.1206, found 288.1211.



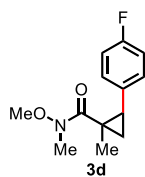
N-Methoxy-N,1-dimethyl-2-(4-nitrophenyl)cyclopropane-1-carboxamide (**3c**)

3c (21.9 mg, 83% yield) was obtained as a colorless oil by following the general procedure (70 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 8.09 (d, *J* = 8.8 Hz, 2H), 7.23 (d, *J* = 8.8 Hz, 2H), 3.43 (s, 3H), 2.90 (s, 3H), 2.25 (dd, *J* = 8.4, 6.6 Hz, 1H), 1.90 (t, *J* = 6.2 Hz, 1H), 1.55 (s, 3H), 1.23 (dd, *J* = 8.4, 5.8 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 147.29, 146.42, 127.80, 123.42, 60.87, 33.51, 33.14, 31.58, 22.67, 20.83. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₃H₁₇N₂O₄⁺ [M+H]⁺ 265.1183, found 265.1186.



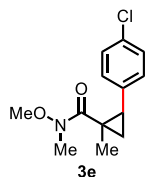
2-(4-Fluorophenyl)-*N*-methoxy-*N*,1-dimethylcyclopropane-1-carboxamide (3d)

3d (18.8 mg, 79% yield) was obtained as a colorless oil by following the general procedure (80 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 7.05 (dd, *J* = 8.1, 5.5 Hz, 2H), 6.92 (t, *J* = 8.5 Hz, 2H), 3.39 (s, 3H), 2.91 (s, 3H), 2.16 – 2.10 (m, 1H), 1.76 (t, *J* = 6.1 Hz, 1H), 1.49 (s, 3H), 1.07 (dd, *J* = 8.4, 5.8 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 161.57 (d, *J* = 244.3 Hz), 134.30, 128.53 (d, *J* = 7.6 Hz), 114.95 (d, *J* = 21.3 Hz), 60.56, 33.81, 31.22, 30.96, 22.50, 19.38. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₃H₁₇FO₂⁺ [M+H]⁺ 238.1238, found 238.1248.



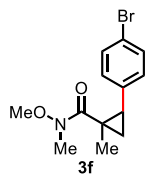
2-(4-Chlorophenyl)-*N*-methoxy-*N*,1-dimethylcyclopropane-1-carboxamide (3e)

3e (19.7 mg, 77% yield) was obtained as a colorless oil by following the general procedure (80 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 7.19 (d, *J* = 8.5 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 3.39 (s, 3H), 2.91 (s, 3H), 2.11 (dd, *J* = 8.6, 6.7 Hz, 1H), 1.78 – 1.74 (m, 1H), 1.49 (s, 3H), 1.09 (dd, *J* = 8.6, 5.7 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 137.34, 131.92, 128.40, 128.25, 60.61, 33.81, 31.58, 31.10, 22.54, 19.62. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₃H₁₇ClNO₂⁺ [M+H]⁺ 254.0942, found 254.0949.



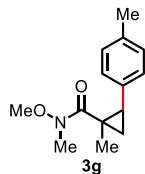
2-(4-Bromophenyl)-*N*-methoxy-*N*,1-dimethylcyclopropane-1-carboxamide (3f)

3f (23.9 mg, 80% yield) was obtained as a colorless oil by following the general procedure (80 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 7.34 (d, *J* = 8.5 Hz, 2H), 6.96 (d, *J* = 8.5 Hz, 2H), 3.39 (s, 3H), 2.92 (s, 3H), 2.10 (dd, *J* = 8.6, 6.6 Hz, 1H), 1.77 – 1.74 (m, 1H), 1.49 (s, 3H), 1.09 (dd, *J* = 8.6, 5.7 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 137.91, 131.19, 128.78, 119.94, 60.63, 33.77, 31.58, 31.17, 22.54, 19.63. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₃H₁₇BrNO₂⁺ [M+H]⁺ 298.0437, found 298.0444.



N-Methoxy-*N*,1-dimethyl-2-(*p*-tolyl)cyclopropane-1-carboxamide (3g)

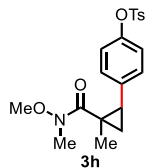
3g (12.9 mg, 55% yield) was obtained as yellow oil by following the general procedure (80 °C, 48 h).

¹H NMR (600 MHz, CDCl₃): δ 7.03 (d, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 8.1 Hz, 2H), 3.34 (s, 3H), 2.92 (s, 3H), 2.28 (s, 3H), 2.09 (dd, *J* = 8.6, 6.7 Hz, 1H), 1.77 – 1.73 (m, 1H), 1.48 (s, 3H), 1.05 (dd, *J* = 8.7, 5.5 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 135.76, 135.56, 128.90, 126.83, 60.46, 34.03, 31.51, 31.13, 22.64, 21.11, 19.35.

(Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $C_{14}H_{20}NO_2^+$ $[M+H]^+$ 234.1489, found 234.1496.



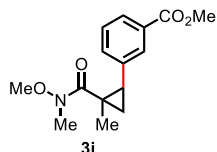
4-(2-(Methoxy(methyl)carbamoyl)-2-methylcyclopropyl)phenyl 4-methylbenzenesulfonate (3h)

3h (33.8 mg, 87% yield) was obtained as a colorless oil by following the general procedure (80 °C, 24 h).

1H NMR (600 MHz, $CDCl_3$): δ 7.66 (d, J = 8.3 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 6.99 (d, J = 8.7 Hz, 2H), 6.83 (d, J = 8.7 Hz, 2H), 3.33 (s, 3H), 2.85 (s, 3H), 2.44 (s, 3H), 2.11 (dd, J = 8.5, 6.7 Hz, 1H), 1.72 (t, J = 6.1 Hz, 1H), 1.48 (s, 3H), 1.07 (dd, J = 8.5, 5.7 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 148.05, 145.44, 137.86, 132.50, 129.81, 128.57, 128.08, 122.02, 60.49, 33.73, 31.68, 30.98, 22.44, 21.82, 19.57. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $C_{20}H_{24}NO_5S^+$ $[M+H]^+$ 390.1370, found 390.1376.



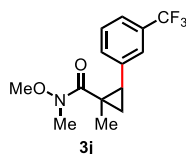
Methoxy 3-(2-(methoxy(methyl)carbamoyl)-2-methylcyclopropyl)benzoate (3i)

3i (23.4 mg, 84% yield) was obtained as a colorless oil by following the general procedure (70 °C, 24 h).

1H NMR (600 MHz, $CDCl_3$): δ 7.86 (t, J = 1.7 Hz, 1H), 7.83 (d, J = 7.7 Hz, 1H), 7.30 (t, J = 7.7 Hz, 1H), 7.21 (d, J = 7.8 Hz, 1H), 3.90 (s, 3H), 3.37 (s, 3H), 2.89 (s, 3H), 2.21 (dd, J = 8.5, 6.7 Hz, 1H), 1.85 (t, J = 6.1 Hz, 1H), 1.52 (s, 3H), 1.13 (dd, J = 8.6, 5.7 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 167.20, 139.21, 130.67, 129.98, 129.25, 128.30, 127.49, 60.52, 52.23, 33.86, 31.51, 31.40, 22.56, 19.51. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $C_{15}H_{20}NO_4^+$ $[M+H]^+$ 278.1387, found 278.1394.



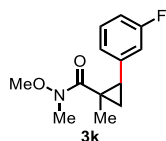
N-Methoxy-N,1-dimethyl-2-(3-(trifluoromethyl)phenyl)cyclopropane-1-carboxamide (3j)

3j (25.2 mg, 88% yield) was obtained as a colorless oil by following the general procedure (70 °C, 24 h).

1H NMR (600 MHz, $CDCl_3$): δ 7.41 (d, J = 7.3 Hz, 1H), 7.41 (s, 1H), 7.34 (t, J = 7.7 Hz, 1H), 7.23 (d, J = 7.9 Hz, 1H), 3.38 (s, 3H), 2.89 (s, 3H), 2.21 (dd, J = 8.5, 6.6 Hz, 1H), 1.86 – 1.83 (m, 1H), 1.52 (s, 3H), 1.14 (dd, J = 8.6, 5.7 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$): δ 139.93, 130.44 (q, J = 32.0 Hz), 129.95, 128.61, 124.60, 124.27 (q, J = 272.3 Hz), 122.97 (q, J = 3.8 Hz), 60.54, 33.66, 31.74, 31.30, 22.51, 19.60. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $C_{14}H_{17}F_3NO_2^+$ $[M+H]^+$ 288.1206, found 288.1209.



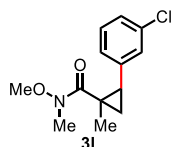
2-(3-Fluorophenyl)-N-methoxy-N,1-dimethylcyclopropane-1-carboxamide (3k)

3k (17.6 mg, 74% yield) was obtained as a colorless oil by following the general procedure (80 °C, 48 h).

¹H NMR (600 MHz, CDCl₃) δ 7.18 (td, *J* = 7.9, 6.2 Hz, 1H), 6.88 – 6.83 (m, 2H), 6.81 (dt, *J* = 10.4, 2.0 Hz, 1H), 3.38 (s, 3H), 2.93 (s, 3H), 2.13 (dd, *J* = 8.5, 6.7 Hz, 1H), 1.77 (t, *J* = 6.1 Hz, 1H), 1.50 (s, 3H), 1.11 (dd, *J* = 8.5, 5.7 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 162.81 (d, *J* = 245.2 Hz), 141.61, 129.58 (d, *J* = 8.5 Hz), 122.61 (d, *J* = 2.2 Hz), 114.10 (d, *J* = 21.6 Hz), 113.10 (d, *J* = 21.1 Hz), 60.52, 33.84, 31.71, 31.40 (d, *J* = 2.1 Hz), 22.56, 19.79. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₃H₁₇FNO₂⁺ [M+H]⁺ 238.1238, found 238.1245.



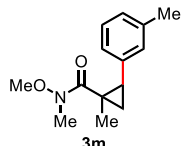
2-(3-Chlorophenyl)-N-methoxy-N,1-dimethylcyclopropane-1-carboxamide (3l)

3l (19.3 mg, 76% yield) was obtained as a colorless oil by following the general procedure (80 °C, 48 h).

¹H NMR (600 MHz, CDCl₃): δ 7.17 – 7.14 (m, 1H), 7.14 – 7.09 (m, 2H), 6.94 (dt, *J* = 7.3, 1.6 Hz, 1H), 3.40 (s, 3H), 2.92 (s, 3H), 2.11 (dd, *J* = 8.6, 6.6 Hz, 1H), 1.79 – 1.75 (m, 1H), 1.50 (s, 3H), 1.10 (dd, *J* = 8.5, 5.7 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 141.03, 134.02, 129.41, 127.48, 126.38, 124.93, 60.54, 33.86, 31.63, 31.26, 22.54, 19.68. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₃H₁₇ClNO₂⁺ [M+H]⁺ 254.0942, found 254.0950.



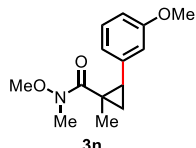
N-Methoxy-N,1-dimethyl-2-(*m*-tolyl)cyclopropane-1-carboxamide (3m)

3m (11.0 mg, 47% yield) was obtained as a colorless oil by following the general procedure (80 °C, 48 h).

¹H NMR (600 MHz, CDCl₃): δ 7.11 (t, *J* = 7.6 Hz, 1H), 6.96 (d, *J* = 7.5 Hz, 1H), 6.89 (s, 1H), 6.88 (d, *J* = 7.9 Hz, 1H), 3.33 (s, 3H), 2.91 (s, 3H), 2.28 (s, 3H), 2.09 (dd, *J* = 8.6, 6.6 Hz, 1H), 1.78 – 1.74 (m, 1H), 1.48 (s, 3H), 1.07 (dd, *J* = 8.7, 5.6 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 138.61, 137.68, 128.12, 127.61, 127.04, 124.00, 60.29, 34.09, 31.75, 31.19, 22.67, 21.54, 19.40. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₄H₂₀NO₂⁺ [M+H]⁺ 234.1489, found 234.1496.



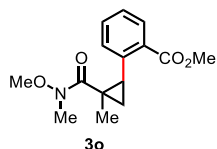
N-Methoxy-2-(3-methoxyphenyl)-N,1-dimethylcyclopropane-1-carboxamide (3n)

3n (13.1 mg, 53% yield) was obtained as a colorless oil by following the general procedure (80 °C, 48 h).

^1H NMR (600 MHz, CDCl_3): δ 7.13 (t, J = 7.9 Hz, 1H), 6.70 (dd, J = 8.2, 2.4 Hz, 1H), 6.68 (d, J = 7.7 Hz, 1H), 6.64 (t, J = 2.0 Hz, 1H), 3.76 (s, 3H), 3.35 (s, 3H), 2.94 (s, 3H), 2.10 (dd, J = 8.5, 6.7 Hz, 1H), 1.79 – 1.75 (m, 1H), 1.49 (s, 3H), 1.08 (dd, J = 8.6, 5.6 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 159.56, 140.50, 129.18, 119.31, 112.54, 111.88, 60.43, 55.28, 33.99, 31.87, 31.38, 22.66, 19.68. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{14}\text{H}_{20}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$ 250.1438, found 250.1444.



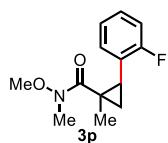
Methyl 2-(2-(methoxy(methyl)carbamoyl)-2-methylcyclopropyl)benzoate (**3o**)

3o (15.0 mg, 54% yield) was obtained as a colorless oil by following the general procedure (80 °C, 48 h).

^1H NMR (600 MHz, CDCl_3): δ 7.85 (dd, J = 7.8, 1.2 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 6.98 (d, J = 7.9 Hz, 1H), 3.92 (s, 3H), 3.37 (s, 3H), 3.11 (t, J = 7.8 Hz, 1H), 2.88 (s, 3H), 1.98 – 1.83 (m, 1H), 1.56 (s, 3H), 1.07 (dd, J = 8.5, 5.6 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 168.52, 139.47, 131.87, 131.29, 130.41, 125.95, 125.85, 60.26, 52.13, 33.95, 31.83, 28.96, 22.52, 18.86. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{15}\text{H}_{20}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 278.1387, found 278.1397.



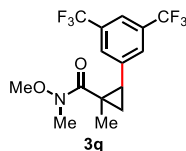
2-(2-Fluorophenyl)-*N*-methoxy-*N*,1-dimethylcyclopropane-1-carboxamide (**3p**)

3p (10.6 mg, 45% yield) was obtained as a colorless oil by following the general procedure (80 °C, 24 h).

^1H NMR (600 MHz, CDCl_3): δ 7.13 (tdd, J = 7.1, 5.3, 1.6 Hz, 1H), 7.02 – 6.98 (m, 2H), 6.87 – 6.82 (m, 1H), 3.35 (s, 3H), 2.92 (s, 3H), 2.47 – 2.42 (m, 1H), 1.89 – 1.85 (m, 1H), 1.53 (s, 3H), 1.09 (dd, J = 8.7, 5.6 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 162.30 (d, J = 244.6 Hz), 127.52 (d, J = 8.1 Hz), 126.19 (d, J = 3.4 Hz), 125.63, 123.91 (d, J = 3.5 Hz), 114.77 (d, J = 22.4 Hz), 60.33, 33.87, 31.25, 23.88 (d, J = 6.2 Hz), 22.37, 18.01. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{13}\text{H}_{17}\text{FNO}_2^+$ $[\text{M}+\text{H}]^+$ 238.1238, found 238.1245.



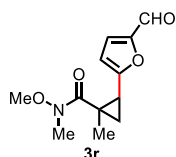
2-(3,5-Bis(trifluoromethyl)phenyl)-*N*-methoxy-*N*,1-dimethylcyclopropane-1-carboxamide (**3q**)

3q (27.7 mg, 78% yield) was obtained as a colorless oil by following the general procedure (70 °C, 24 h).

^1H NMR (600 MHz, CDCl_3): δ 7.67 (s, 1H), 7.55 (s, 2H), 3.49 (s, 3H), 2.87 (s, 3H), 2.28 (dd, J = 8.5, 6.6 Hz, 1H), 1.89 (t, J = 6.2 Hz, 1H), 1.56 (s, 3H), 1.20 (dd, J = 8.5, 5.8 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3): δ 141.85, 131.30 (q, J = 33.1 Hz), 127.70, 123.49 (q, J = 272.6 Hz), 119.99 (hept, J = 3.5 Hz), 60.78, 33.35, 32.11, 30.89, 22.45, 19.99. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): m/z calculated for $\text{C}_{15}\text{H}_{16}\text{F}_6\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 356.1080, found 356.1079.



2-(5-Formylfuran-2-yl)-N-methoxy-N,1-dimethylcyclopropane-1-carboxamide (3r)

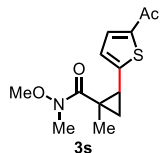
3r (19.0 mg, 80% yield) was obtained as a colorless oil by following the general procedure (80 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 9.47 (s, 1H), 7.14 (d, *J* = 3.6 Hz, 1H), 6.10 (d, *J* = 3.5 Hz, 1H), 3.52 (s, 3H), 3.07 (s, 3H), 2.29 (dd, *J* = 8.7, 6.5 Hz, 1H), 1.83 – 1.80 (m, 1H), 1.51 (s, 3H), 1.23 (dd, *J* = 8.8, 5.5 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 176.60, 161.25, 151.75, 123.65, 107.34, 60.77, 33.85, 31.88, 24.29, 21.67, 19.81.

(Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₂H₁₆NO₄⁺ [M+H]⁺ 238.1074, found 238.1083.



2-(5-Acetylthiophen-2-yl)-N-methoxy-N,1-dimethylcyclopropane-1-carboxamide (3s)

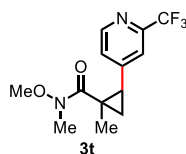
3s (18.4 mg, 69% yield) was obtained as yellow solid by following the general procedure (80 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 7.47 (d, *J* = 3.9 Hz, 1H), 6.67 (d, *J* = 3.9 Hz, 1H), 3.52 (s, 3H), 3.02 (s, 3H), 2.48 (s, 3H), 2.33 (dd, *J* = 8.5, 6.5 Hz, 1H), 1.82 (t, *J* = 6.0 Hz, 1H), 1.51 (s, 3H), 1.25 (dd, *J* = 8.5, 5.6 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 190.29, 152.69, 141.66, 132.90, 124.04, 60.87, 33.78, 33.06, 27.03, 26.55, 22.23,

22.08. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₃H₁₈NO₃S⁺ [M+H]⁺ 268.1002, found 268.1003.



N-Methoxy-N,1-dimethyl-2-(2-(trifluoromethyl)pyridin-4-yl)cyclopropane-1-carboxamide (3t)

3t (12.4 mg, 43% yield) was obtained as a colorless oil by following the general procedure (80 °C, 24 h).

¹H NMR (600 MHz, CDCl₃): δ 8.53 (d, *J* = 5.0 Hz, 1H), 7.43 (s, 1H), 7.14 (d, *J* = 4.8 Hz, 1H), 3.47 (s, 3H), 2.90 (s, 3H), 2.23 – 2.18 (m, 1H), 1.90 (t, *J* = 6.1 Hz, 1H), 1.56 (s, 3H), 1.28 – 1.24 (m, 1H).

¹³C NMR (150 MHz, CDCl₃): δ 150.93, 149.61, 147.99 (q, *J* = 34.3 Hz), 124.33, 121.73 (q, *J* = 274.3 Hz), 119.54, 60.86, 33.37, 33.30, 30.62, 22.52, 20.70. (Carbon peak for amide carbonyl was very broad and showed weak intensity)

HRMS (ESI-TOF): *m/z* calculated for C₁₃H₁₆F₃N₂O₂⁺ [M+H]⁺ 289.1158, found 289.1163.

2.5 Procedure for gram-scale reaction / 1 mol% Pd Loading

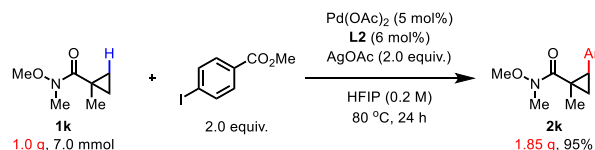


Figure S7. Gram-Scale C–H Arylation

A 150 mL sealed vessel with magnetic stir bar was charged with Pd(OAc)₂ (5 mol%, 79 mg), **L2** (6 mol%, 67 mg), AgOAc (14.0 mmol, 2.34 g), Ar-I (14.0 mmol, 3.67 g), and substrate **1k** (7.0 mmol, 1.00 g) in air. Then, HFIP (35 mL) was added as solvent. The reaction tube was sealed and stirred at 80 °C for 24 hours. Upon completion, the reaction mixture was cooled to room temperature, diluted with EtOAc, filtered through a plug of silica and celite, and concentrated *in vacuo*. The crude reaction mixture was purified on silica gel using hexanes/EtOAc as eluent to afford **2k** (1.85 g, 95% yield).

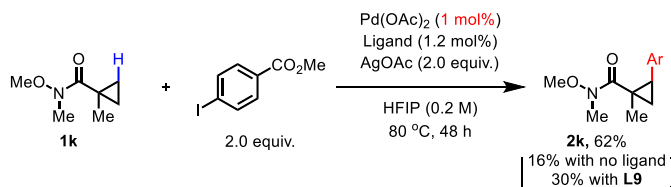


Figure S8. 1 mol% Pd Loading

A sealed tube with magnetic stir bar was charged with Pd(OAc)₂ (1 mol%, 1.1 mg), ligand (1.2 mol%, **L2**: 1.0 mg, **L9**: 0.7 mg), AgOAc (1.0 mmol, 167 mg), Ar-I (1.0 mmol, 262 mg), and substrate **1k** (0.5 mmol, 71.5 mg) in air. Then, HFIP (2.5 mL) was added as solvent. The reaction tube was sealed and stirred at 80 °C for 48 hours. Upon completion, the reaction mixture was cooled to room temperature, diluted with EtOAc, filtered through a celite plug, and concentrated *in vacuo*. The crude reaction mixture was purified on silica gel using hexanes/EtOAc as eluent to afford **2k**.

2.6 Comparison with Ligand-Free Protocols

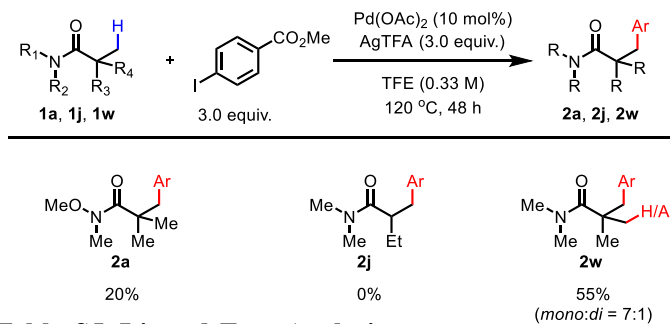
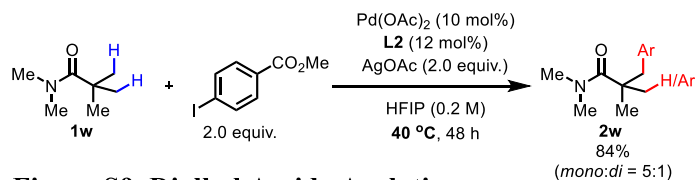
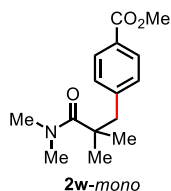


Table S5. Ligand-Free Arylation

Conditions A: A sealed tube with magnetic stir bar was charged with Pd(OAc)₂ (10 mol%, 2.2 mg), AgTFA (0.1 mmol, 22.1 mg), methyl 4-iodobenzoate (0.1 mmol, 26.2 mg), and substrate **1a** (0.1 mmol, 14.5 mg) in air. Then, TFE (0.3 mL) was added as solvent. The reaction mixture was stirred at 120 °C for 16 hours, cooled to room temperature, and second batch of AgTFA (0.1 mmol, 22.1 mg) and methyl 4-iodobenzoate (0.1 mmol, 26.2 mg). The reaction mixture was stirred at 120 °C for 16 hours, cooled to room temperature, and third batch of AgTFA (0.1 mmol, 22.1 mg) and methyl 4-iodobenzoate (0.1 mmol, 26.2 mg). The reaction mixture was stirred at 120 °C for 16 hours. Upon completion, the reaction mixture was cooled to room temperature, diluted with EtOAc, filtered through a celite plug, and concentrated *in vacuo*. The yield was determined by ¹H NMR analysis of the crude product using CH₂Br₂ as the internal standard.



Conditions **B** (**2w**): A sealed tube with magnetic stir bar was charged with Pd(OAc)₂ (10 mol%, 2.2 mg), **L2** (12 mol%, 1.9 mg), AgOAc (0.2 mmol, 33.4 mg), methyl 4-iodobenzoate (0.2 mmol, 52.4 mg), and substrate **1w** (0.1 mmol, 12.9 mg) in air. Then, HFIP (0.5 mL) was added as solvent. The reaction mixture was stirred at 40 °C for 48 hours. Upon completion, the reaction mixture was cooled to room temperature, diluted with EtOAc, filtered through a celite plug, and concentrated *in vacuo*. The crude reaction mixture was purified on silica gel using hexanes/EtOAc as eluent to afford the desired products as an inseparable mixture of **2w-mono** and **2w-di** (24.0 mg, 5:1, 84%).

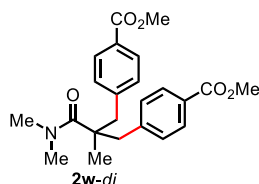


Methyl 4-(3-(dimethylamino)-2,2-dimethyl-3-oxopropyl)benzoate (**2w-mono**)

¹H NMR (600 MHz, CDCl₃): δ 7.93 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 8.3 Hz, 2H), 3.90 (s, 3H), 3.04 (br s, 6H), 3.00 (s, 2H), 1.28 (s, 6H).

¹³C NMR (150 MHz, CDCl₃): δ 176.17, 167.19, 143.96, 130.33, 129.41, 128.43, 52.12, 46.29, 43.72, 38.75, 26.59.

HRMS (ESI-TOF): *m/z* calculated for C₁₅H₂₂NO₃⁺ [M+H]⁺ 264.1594, found 264.1600.



Dimethyl 4,4'-(2-(dimethylcarbamoyl)-2-methylpropane-1,3-diyl)dibenzoate (**2w-di**)

¹H NMR (600 MHz, CDCl₃): δ 7.93 (d, *J* = 8.3 Hz, 4H), 7.23 (d, *J* = 8.3 Hz, 4H), 3.90 (s, 6H), 3.53 (d, *J* = 13.2 Hz, 2H), 2.75 (br s, 6H), 2.67 (d, *J* = 13.2 Hz, 2H), 1.20 (s, 3H).

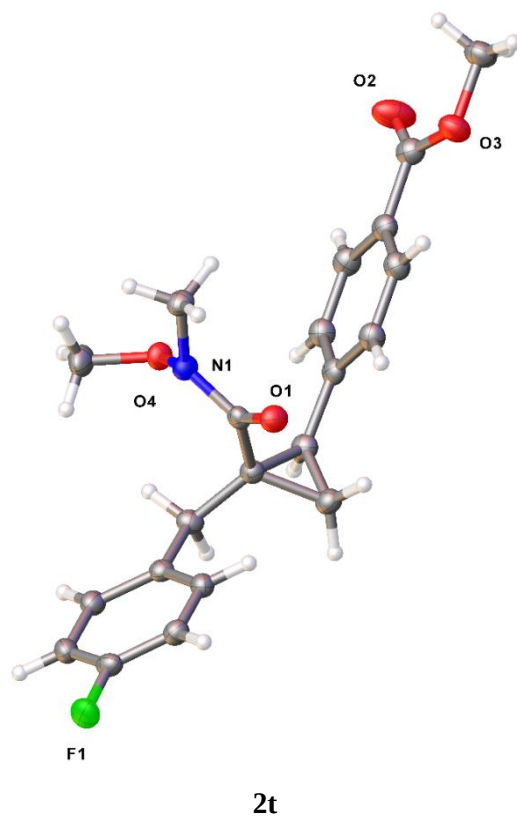
¹³C NMR (150 MHz, CDCl₃): δ 174.72, 167.15, 143.61, 130.39, 129.47, 128.61, 52.16, 49.87, 47.62, 38.85, 23.17.

HRMS (ESI-TOF): *m/z* calculated for C₂₃H₂₈NO₅⁺ [M+H]⁺ 398.1962, found 398.1967.

*Preparation and characterization of **2a** and **2j** is described in 2.5.

*The results using Conditions **B** without ligand were analyzed by ¹H NMR analysis of the crude product using CH₂Br₂ as the internal standard.

2.7 X-Ray Crystallographic Data of 2t



Crystal data and structure refinement for 2t. (CCDC 1841524)

Crystal data and structure refinement for Yu103.

Report date	2018-05-04	
Identification code	CPBNF	
Empirical formula	C ₂₁ H ₂₂ F N O ₄	
Molecular formula	C ₂₁ H ₂₂ F N O ₄	
Formula weight	371.39	
Temperature	100.0 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 2 ₁ /c 1	
Unit cell dimensions	a = 27.4465(18) Å	∠ = 90°.
	b = 6.4873(4) Å	∠ = 112.954(2)°.
	c = 22.0138(15) Å	∠ = 90°.
Volume	3609.3(4) Å ³	
Z	8	
Density (calculated)	1.367 Mg/m ³	
Absorption coefficient	0.840 mm ⁻¹	

F(000)	1568
Crystal size	0.219 x 0.135 x 0.126 mm ³
Crystal color, habit	Colorless Block
Theta range for data collection	1.748 to 68.379°.
Index ranges	-33<=h<=32, -7<=k<=7, -25<=l<=26
Reflections collected	54256
Independent reflections	6618 [R(int) = 0.0625, R(sigma) = 0.0378]
Completeness to theta = 68.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.3129 and 0.2122
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6618 / 0 / 493
Goodness-of-fit on F ²	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0987
R indices (all data)	R1 = 0.0414, wR2 = 0.1021
Extinction coefficient	n/a
Largest diff. peak and hole	0.243 and -0.224 e.Å ⁻³

2.8 Computational study

DFT calculations were performed using *Gaussian09* suite of quantum chemical programs (rev. A.02)⁴. All geometry optimizations and frequency calculations were computed using the dispersion-corrected ω B97X-D hybrid density functional⁵ with SDD basis set⁶ for Pd and 6-31+G(d) basis set⁷ for other atoms. Solvent effects of HFIP were incorporated for all calculations using the SMD continuum solvation model⁸ (Solvent=Generic, parametrization via non-standard input⁹). All located transition states were connected to the nearest minima by the Intrinsic Reaction Coordinate (IRC) calculations¹⁰, performed at the same level of theory with subsequent optimization of the resulting structures. Frequency analysis was carried out for the optimized geometries to verify them as either minima or saddle points by the presence of zero or one imaginary harmonic vibrational frequency, respectively. Single point energy corrections were computed at the SMD(HFIP, Generic)-M06¹¹/SDD,6-311++G(d,p) level of theory. Enthalpies and quasi-harmonic Gibbs free energies were evaluated at the reaction temperature of 343.15 K and adjusted¹² to the standard state concentration of 1 mol·l⁻¹. The quasi-rigid-rotor-harmonic-oscillator approximation was applied¹² to vibrational frequencies, switching to a free rotor description of vibrational entropy below 100 cm⁻¹, as proposed by Grimme¹³, and a damping function was used to interpolate a smooth transition from the RRHO description at the cut-off frequency¹². Relative enthalpies and free energies were calculated with reference to infinitely separated reactants.

Results and Discussion

Breaking the C–H bond is one of the key steps in C(sp³)–H bond activation reactions. Thus, the focus of this study was to model the C–H cleavage step of a weakly binding Weinreb amide substrate, whereupon gaining insight into the enabling effect of the designed ligand. This is achieved by examining ligand influence on the C–H activation step free energy profile, and comparing those effects amongst the selected ligands.

The C–H bond breaking was modelled to proceed via the following four species from separated reactants:

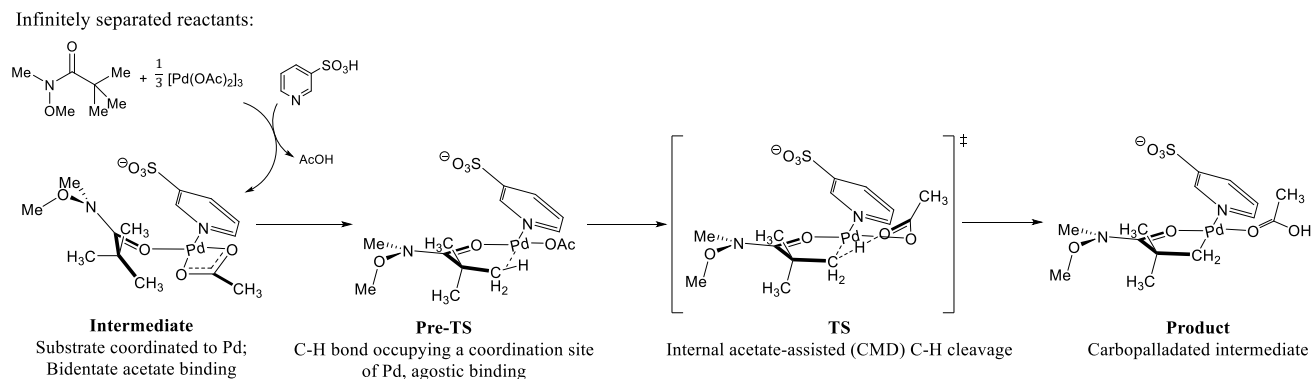


Figure S10. Modelling of C–H activation step

2.8.1. Analysis of conformational space: comparison of structures and energy profiles

N,O-dimethyl Weinreb amide of pivalic acid was chosen as the model substrate. Although structurally simple, this molecule has the following points of structural and conformational variability when bound to Pd (Fig. 11):

1. cis/trans isomerism;
2. conformational flexibility about the Pd–N bond (corresponding to ligand rotation);
3. conformational flexibility about the N–O bond (corresponding to the OMe-group rotation).

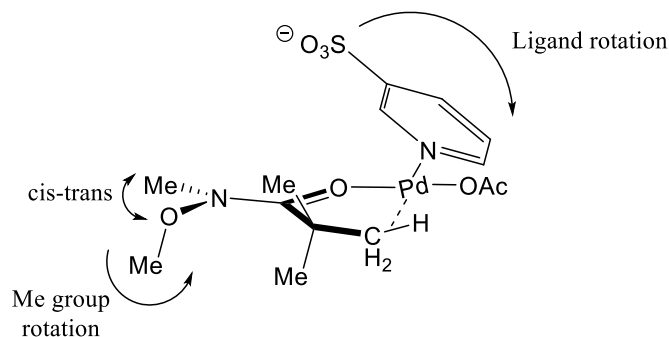


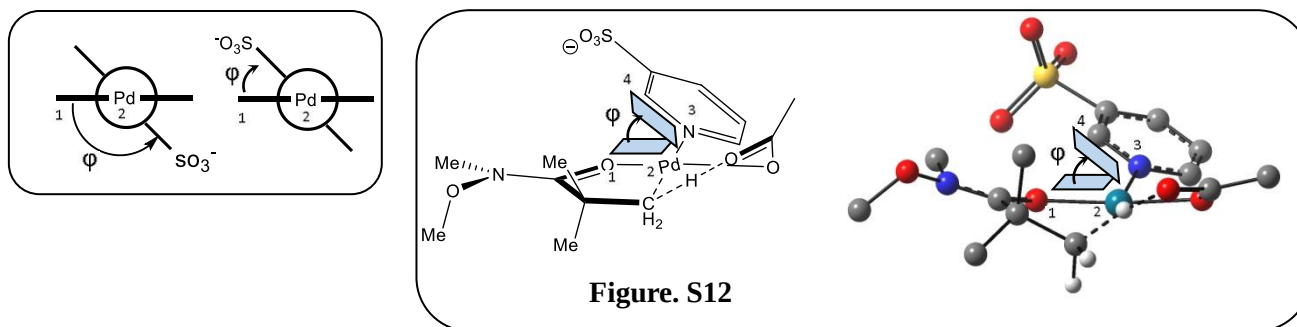
Figure S11. Example: Pre-TS structure

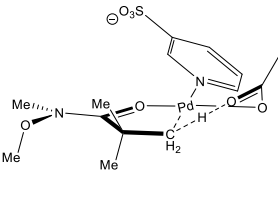
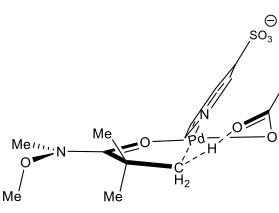
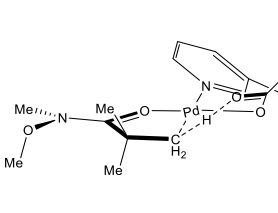
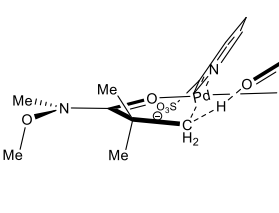
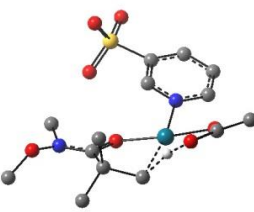
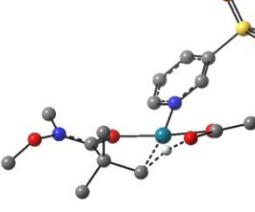
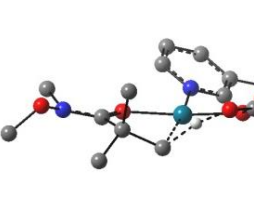
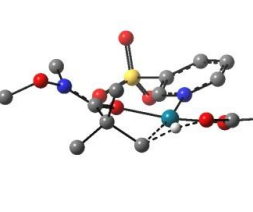
Thus, a description of the C–H cleavage free energy profile with comparison of ligand effects would require analysis of these conformational arrangements. For both cis & trans amides, conformational sampling with optimization showed that the OMe group can take two positions (up and down), whilst the ligand SO_3^- group can point either towards or away from the substrate.

2.8.1.1. Conformational and structural effects on TS energies

Selected conformations of C–H cleavage transition states from the sampling-optimization studies are summarized in separate tables for the cis- and trans-amides. Gibbs free energies are in kcal/mol. Four main roto-conformations were located for the ligand with different orientations of the SO_3^- group in space where the ligand is tilted relative to the O–Pd–O axis (Conf. 1-4). Conformations 5 and 6 correspond to nearly planar ligand orientations and are also given where found.

- ΔG_{HFIP} is the quasi-harmonic Gibbs free energy of the species relative to separated reactants (lowest values in each series of conformations are highlighted in red).
- $\Delta\Delta G_{\text{HFIP}}$ is the free energy barrier between the TS and the pre-TS intermediate.
- $\varphi_{\text{dihedral (Pd-L)}}$ is the dihedral angle 1-2-3-4 along Pd–L bond (Fig. 12) from the optimized TS structures, $-180^\circ < \varphi < 180^\circ$ (positive values are clockwise and negative are anticlockwise from the 1-2 bond):



	Conformation 1	Conformation 2	Conformation 3	Conformation 4
TS				
3D model				
ΔG_{HFIP} kcal* mol^{-1}	26.56	27.44	28.15	26.28
Φ_{dihedral} (Pd-L)	24.3°	152.9°	-153.4°	-25.0°
$\Delta\Delta G_{\text{HFIP}}$ pre-TS-TS barrier kcal* mol^{-1}	8.59	7.71	8.31	8.35

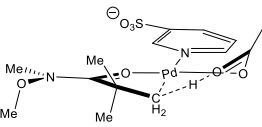
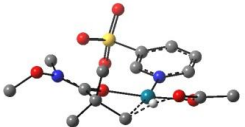
	Conformation 5	Conformation 6
TS		Not found (optimization converges to Conf. 2)
3D model		
ΔG_{HFIP} kcal* mol^{-1}	25.64	
Φ_{dihedral} (Pd-L)	-0.6°	
$\Delta\Delta G_{\text{HFIP}}$ pre-TS-TS barrier kcal* mol^{-1}	8.20	

Table S6. Located TS conformations for Trans-amide (OMe down)

	Conformation 1	Conformation 2	Conformation 3	Conformation 4
TS				
ΔG_{HFIP} kcal* mol^{-1}	26.36	28.93	29.22	28.64
Φ_{dihedral} (Pd-L)	20.7°	150.0°	-151.4°	-19.9°
$\Delta\Delta G_{\text{HFIP}}$ pre-TS-TS barrier kcal* mol^{-1}	7.92	6.88	8.73	8.94

	Conformation 5	Conformation 6
TS		
ΔG_{HFIP} kcal* mol^{-1}	27.83	29.54
Φ_{dihedral} (Pd-L)	1.4°	177.9°
$\Delta\Delta G_{\text{HFIP}}$ pre-TS-TS barrier kcal* mol^{-1}	10.59	6.70

Table S7. Located TS conformations for Trans-amide (OMe up)

	Conformation 1	Conformation 2	Conformation 3	Conformation 4
TS				
ΔG_{HFIP} kcal* mol^{-1}	25.62	27.55	27.90	24.85
Φ_{dihedral} (Pd-L)	13.6°	164.0°	-154.4°	-15.4°
$\Delta\Delta G_{\text{HFIP}}$ pre-TS-TS barrier kcal* mol^{-1}	9.44	6.75	7.54	7.03

	Conformation 5	Conformation 6
TS		
ΔG_{HFIP} kcal* mol^{-1}	26.84	28.00
Φ_{dihedral} (Pd-L)	1.9°	175.9°
$\Delta\Delta G_{\text{HFIP}}$ pre-TS-TS barrier kcal* mol^{-1}	10.06	7.96

Table S8. Located TS conformations for Cis-amide (OMe down)

	Conformation 1	Conformation 2	Conformation 3	Conformation 4
TS				
ΔG_{HFIP} kcal* mol^{-1}	25.53	27.70	28.24	25.52
Φ_{dihedral} (Pd-L)	33.3°	154.2°	-152.0°	-17.0°
$\Delta\Delta G_{\text{HFIP}}$ pre-TS-TS barrier kcal* mol^{-1}	7.18	8.36	7.53	9.17

	Conformation 5	Conformation 6
TS		Not found (optimization converged to Conf. 2)
ΔG_{HFIP} kcal* mol^{-1}	26.49	
Φ_{dihedral} (Pd-L)	-3.1°	
$\Delta\Delta G_{\text{HFIP}}$ pre-TS-T S barrier kcal* mol^{-1}	7.96	

Table S9. Located TS conformations for Cis-amide (OMe up)

2.8.1.2. C–H cleavage energy profiles comparison for 3-pyridinesulfonate ligand

Diagrams below illustrate comparatively the C–H cleavage step free energy profiles corresponding to TS conformations 1-4 located for the 3-pyridinesulfonate ligand. Variation of both free energies and activation barriers is shown depending on the substrate and ligand spacial arrangement. All energy diagrams are drawn to scale.

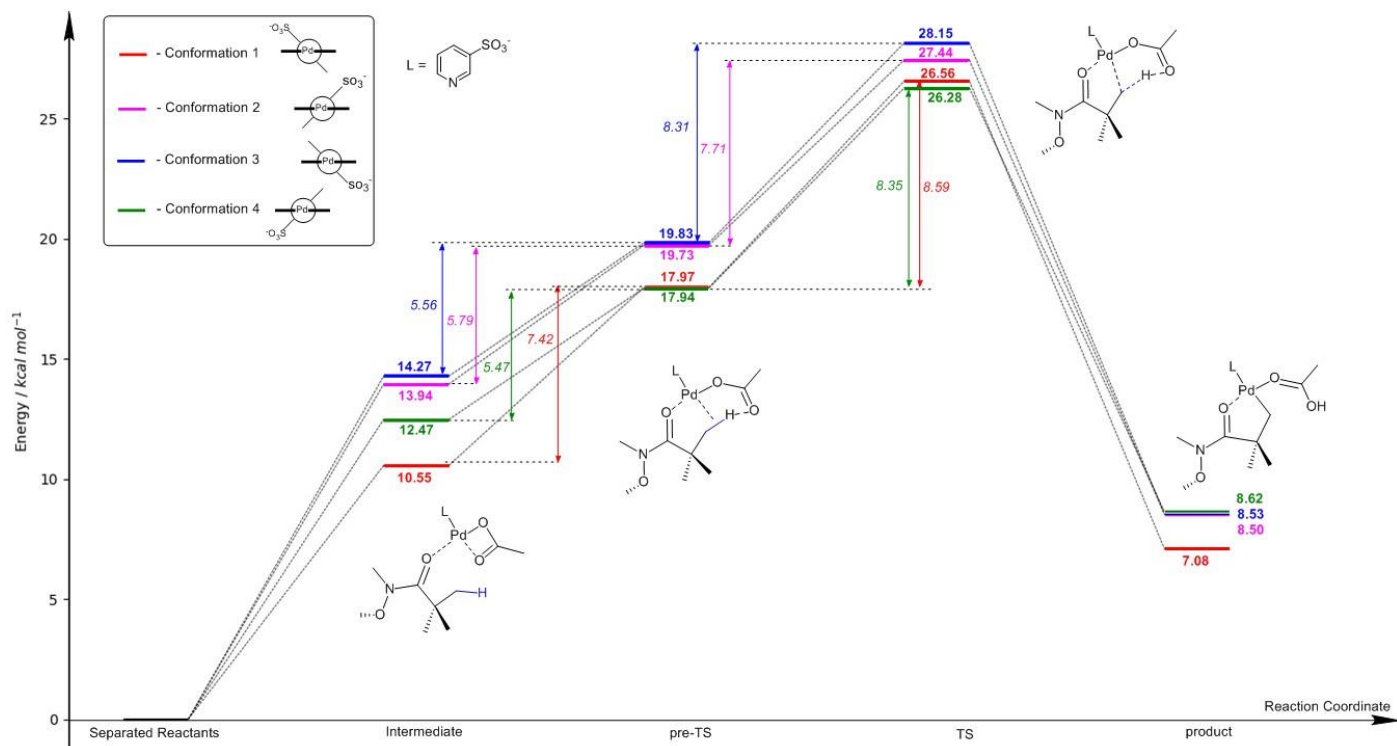


Diagram S1. Comparison of free energy profiles for conformations of Trans-amide (OMe down)

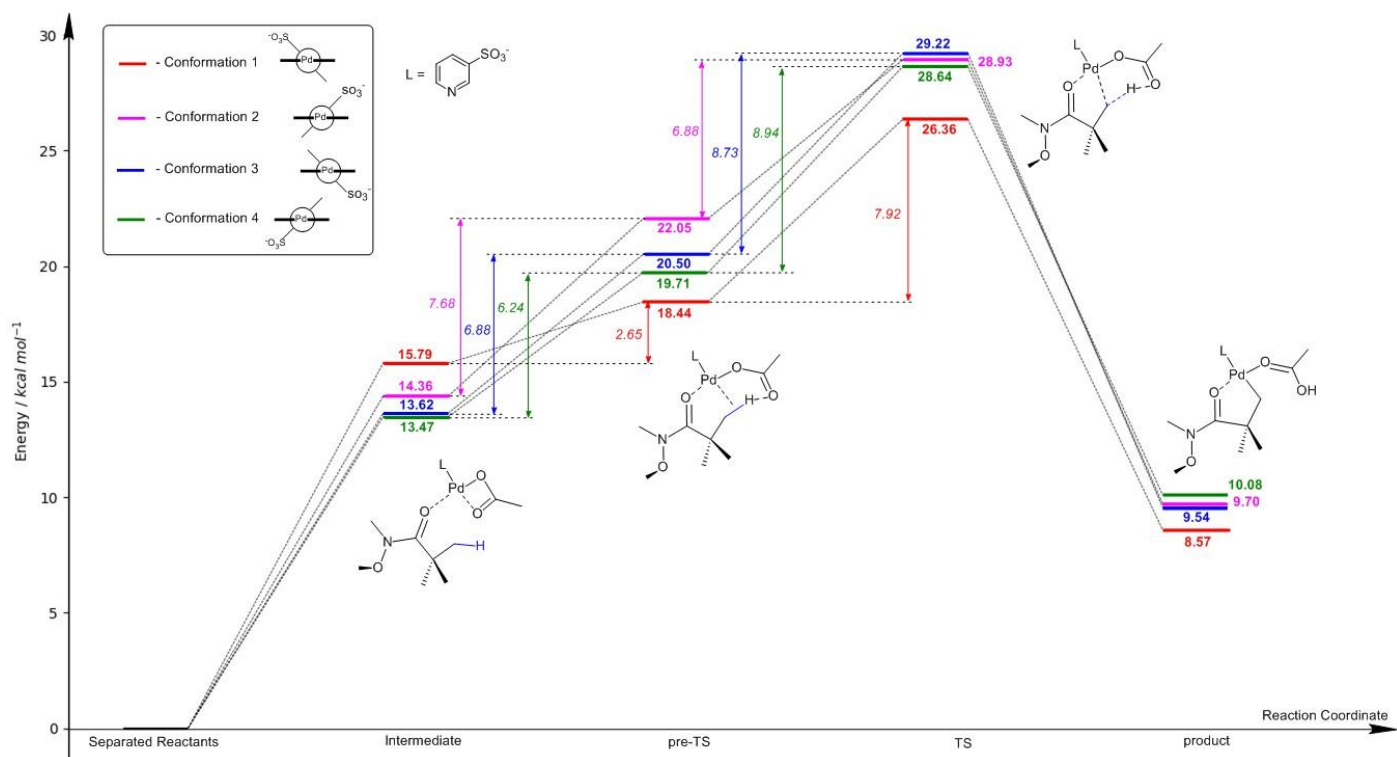


Diagram S2. Comparison of free energy profiles for conformations of Trans-amide (OMe up)

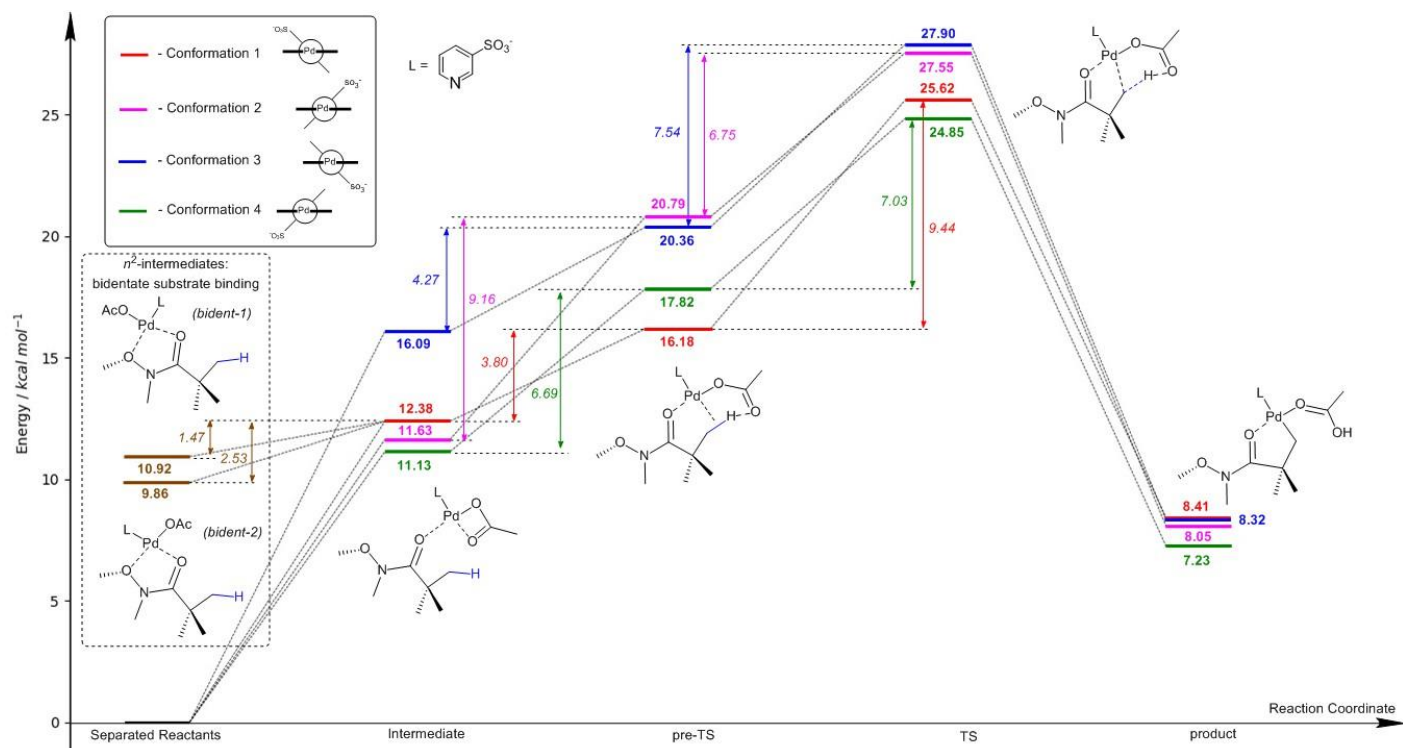


Diagram S3. Comparison of free energy profiles for conformations of Cis-amide (OMe down)

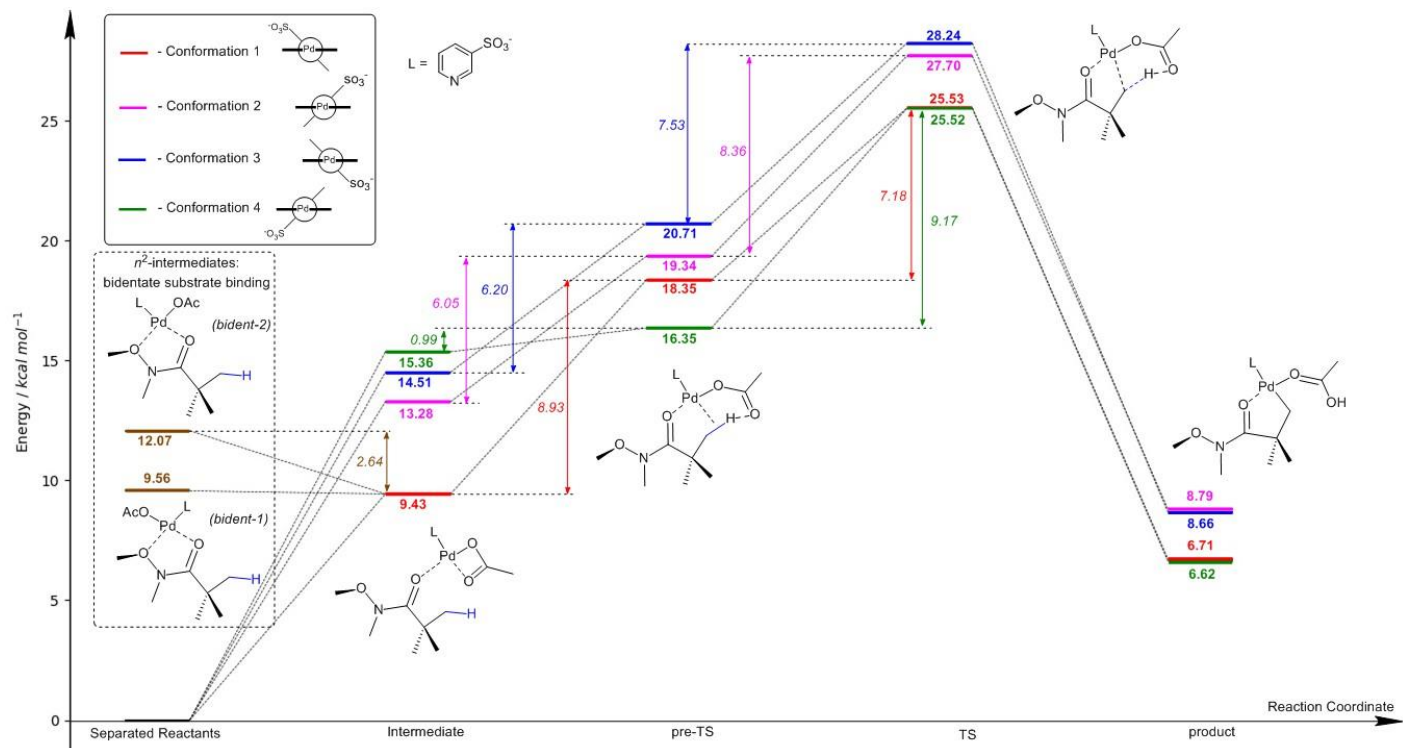


Diagram S4. Comparison of free energy profiles for conformations of Cis-amide (OMe up)

2.8.2. Comparison of ligand effects on the C-H cleavage free energy profile

For the selected ligands, full C-H cleavage step free energy profiles are compared separately for cis/trans amides with OMe pointing up/down. For 3-pyridinesulfonate ligand, conformation 1 was chosen for the purposes of comparison. The difference in ligand enabling and its effect on free energies are demonstrated comparatively. All energy diagrams are drawn to scale.

3-pyridinesulfonate ligand is shown to consistently have the strongest free energy lowering effect on the C-H cleavage profile compared to the ligands presented.

For the intermediate structures for Ac-Gly-OH ligand, calculations on structures with Ac-oxygen coordinated to Pd indicate higher free energies (see Fig. 13 and Table S10) than pre-TS species, presumably owing to the high deformational strain necessary to achieve the Ac-oxygen occupying a vacant coordination site on Pd center (Fig. 13). Thus, intermediates with tridentate mode of binding of Ac-Gly-OH are unlikely to be involved and were omitted for this ligand in the TS diagrams below.

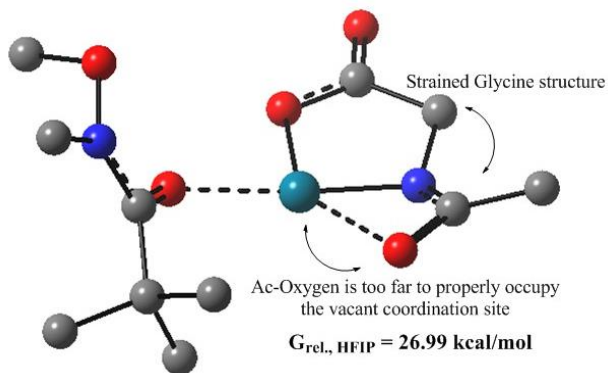


Figure S13. Substrate coordinated intermediate with tridentate binding of Ac-Gly-OH

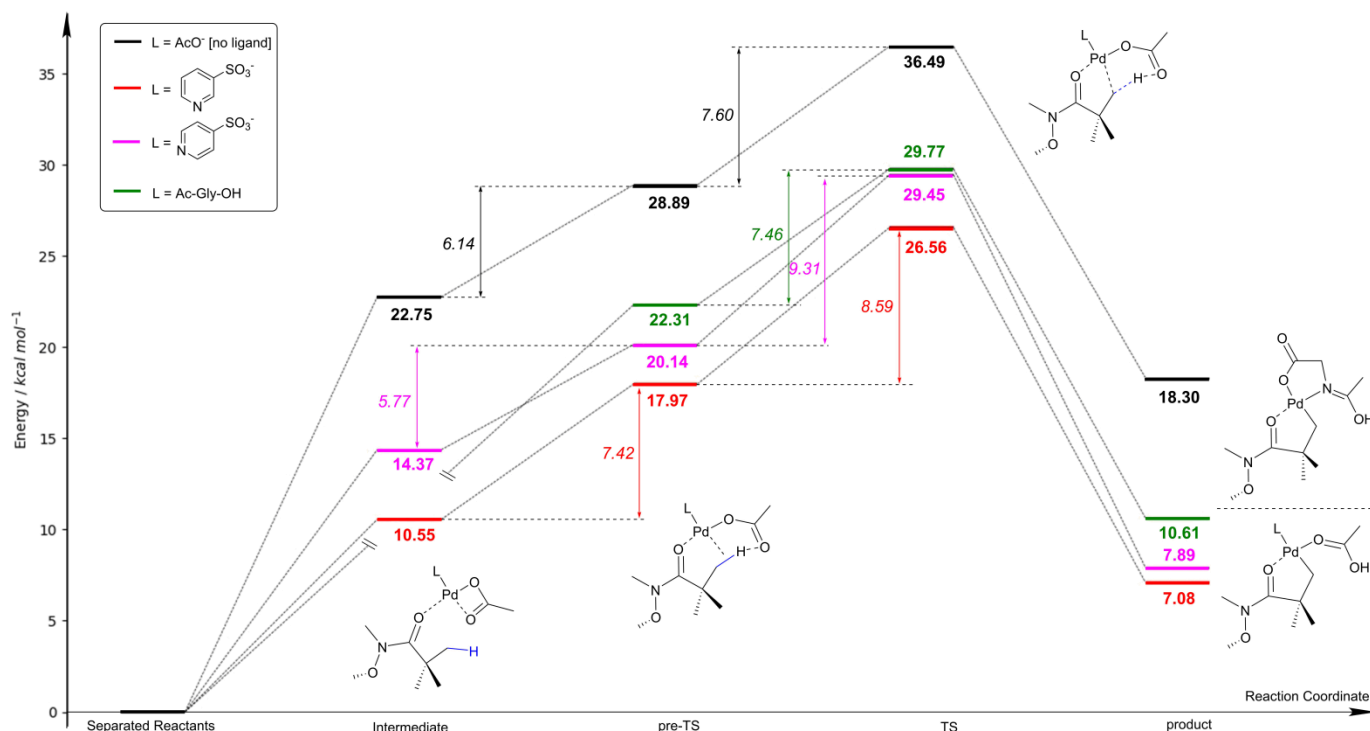


Diagram S5. Comparison of free energy profiles with selected ligands for Trans-amide (OMe down)

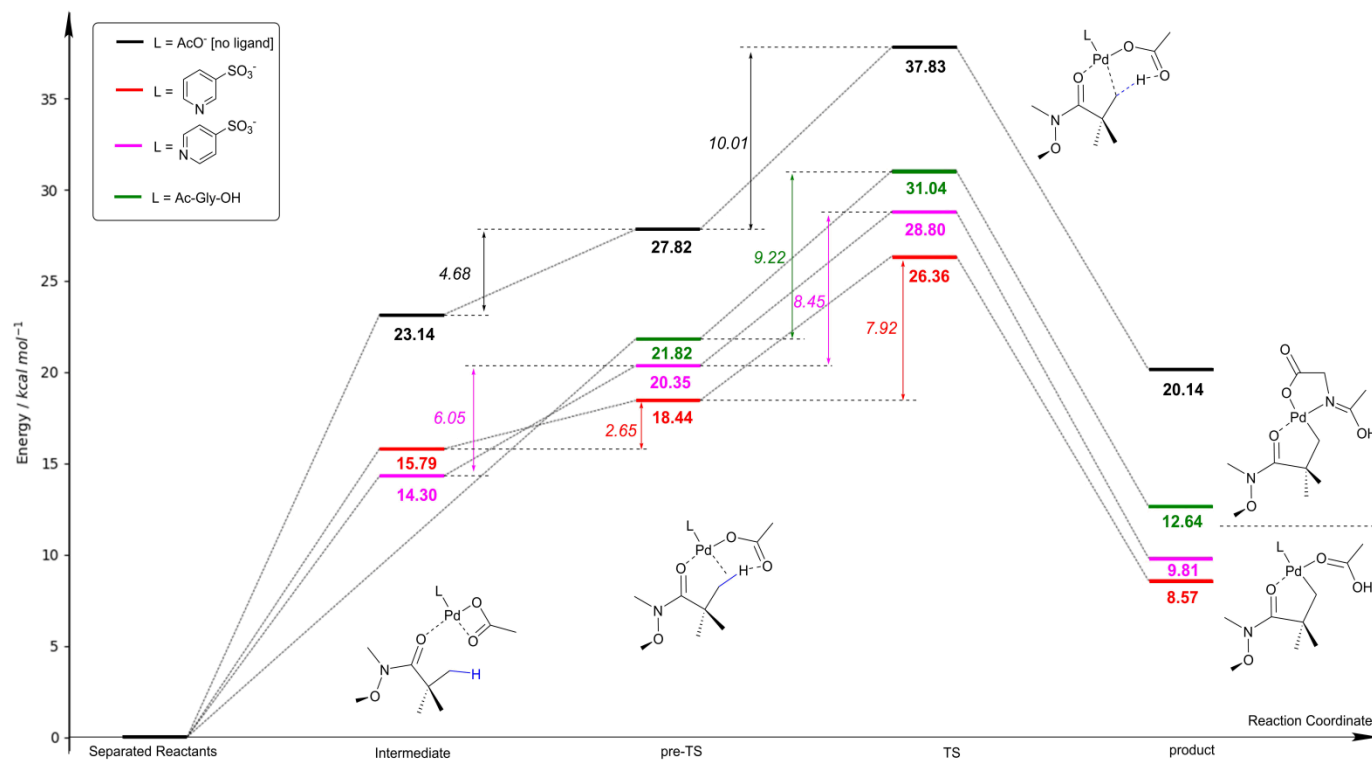


Diagram S6. Comparison of free energy profiles with selected ligands for Trans-amide (OMe up)

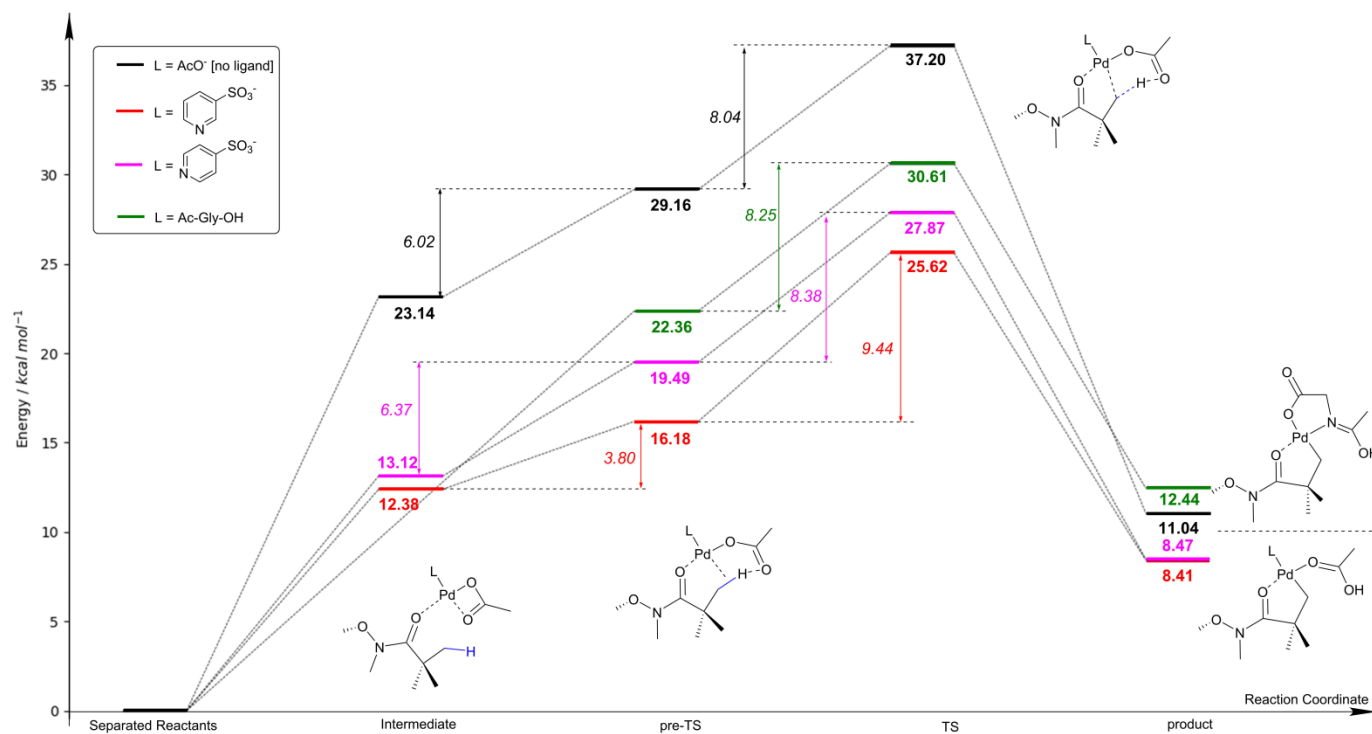


Diagram S7. Comparison of free energy profiles with selected ligands for Cis-amide (OMe down)

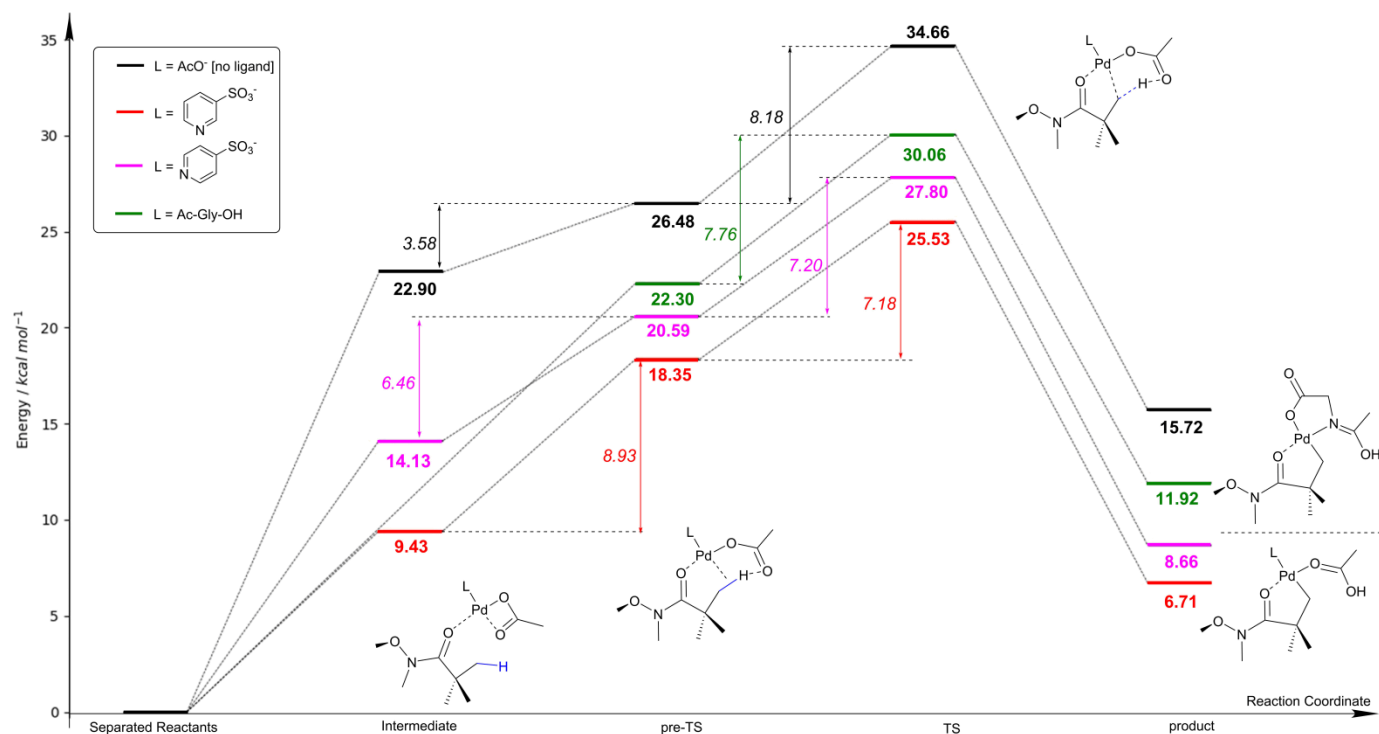


Diagram S8. Comparison of free energy profiles with selected ligands for Cis-amide (OMe up)

Choosing the lowest TS energy pathway for each ligand (cis/trans; OMe up/down, and conformation where appropriate are given in brackets) results in the following overall diagram.

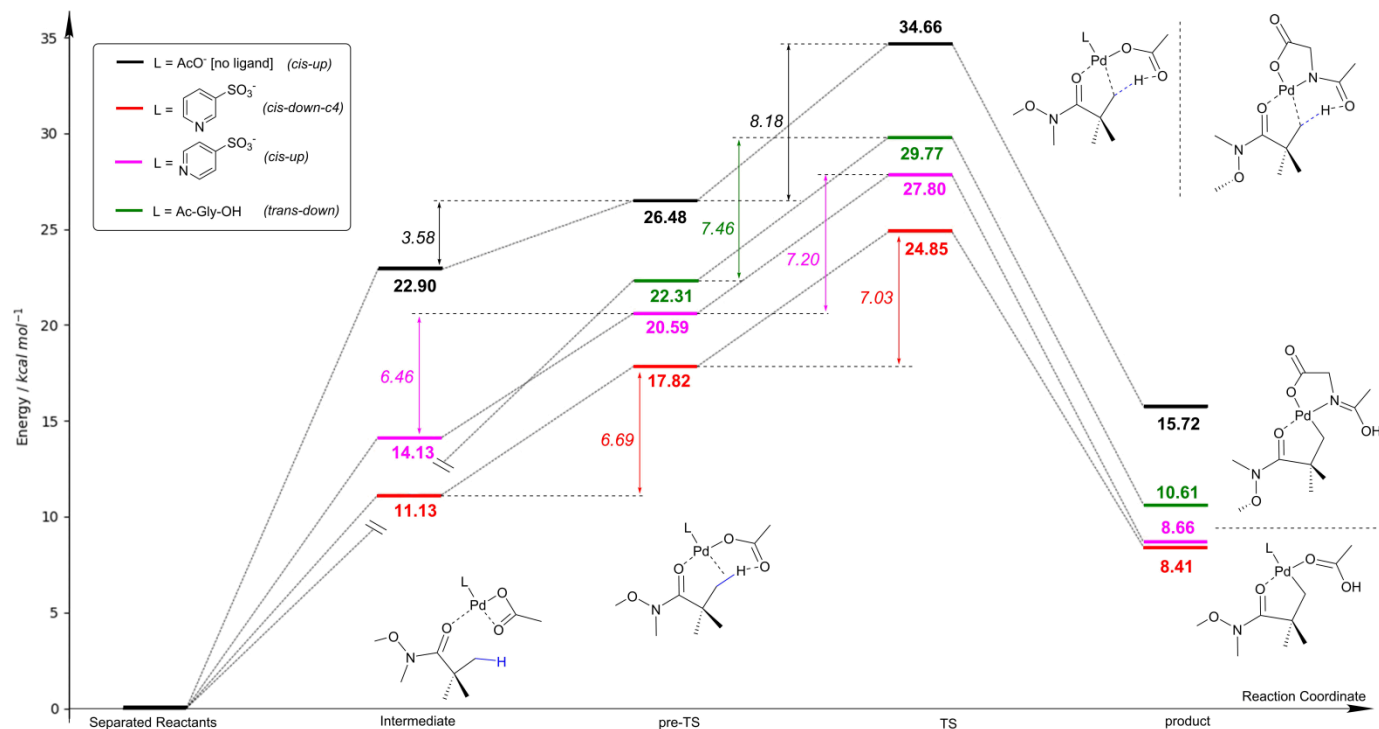


Diagram S9. Comparison of free energy profiles with selected ligands for the lowest TS energy conformations

Overall, DFT data supports the observations of 3-pyridinesulfonate ligand demonstrating superior enabling properties, consistently lowering the free energies of all species in the C–H cleavage step more than the other ligands considered. In contrast, the reaction is much less feasible without a ligand, and although *N*-Ac-glycine is also shown to possess enabling properties, it is significantly less powerful compared to pyridinesulfonates. Notably, the TS barrier values (pre-TS – TS, confirmed by IRC) follow a similar trend, correlating with the observed reactivity.

2.8.3. Combination of the comparative free energy profiles: overall ligand comparison

Free energies of all optimized species are plotted for each ligand, allowing to compare the overall variation of free energies depending on the substrate or ligand arrangement around the Pd center.

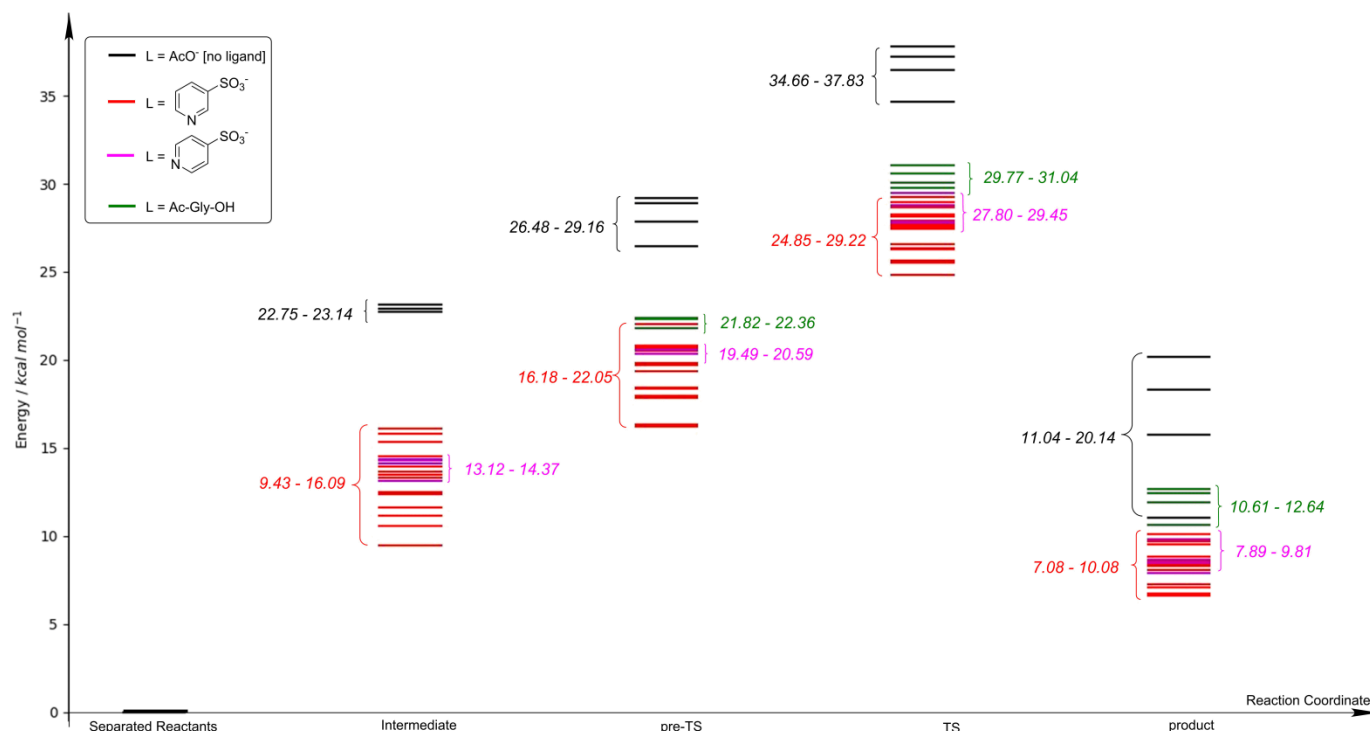


Diagram S10. Overlay of the free energy profiles for each ligand. Ranges of free energies are given in kcal/mol.

It is worth noting that 3-pyridinesulfonate is shown to consistently have the strongest energy-lowering properties in all the conformational and structural arrangements considered. In addition, the corresponding species span the broadest range of free energies with more energy levels available at each stage of C–H cleavage due to greater ligand conformational variation, which may contribute to smaller energy gaps, and thus, easier transitions, between the corresponding species involved.

2.8.4. Comparison of ΔG Values of the Acetate Dissociation Step

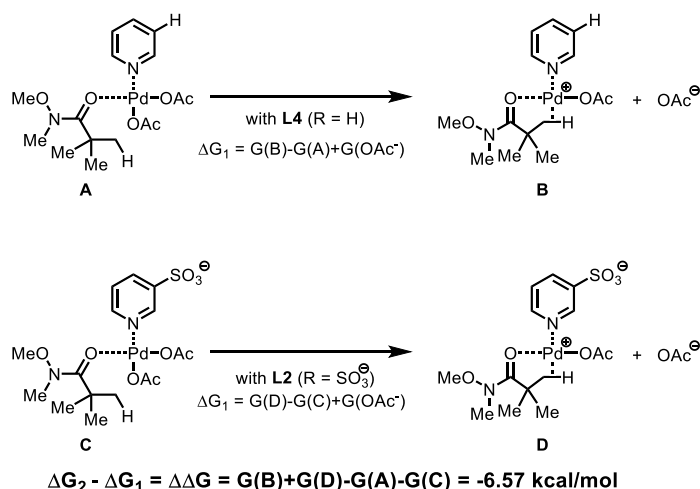


Figure S14. Relative tendency to lose an acetate from diacetate complex

The acetate dissociation step from diacetate complexes **A** and **C** to form pre-transition state complexes **B** and **D** was studied via DFT calculation. Due to the extensive H-bonding that the acetate anion would experience, we concluded that the calculation of the free energy of acetate anion would require more extensive optimization, including explicit solvation effects. Therefore, instead of calculating and comparing the ΔG values for the acetate dissociation from complexes **A** (ΔG_1) and **C** (ΔG_2), we calculated the difference between the ΔG values ($\Delta\Delta G$ value), which is not affected by the free energy of the acetate anion. The $\Delta\Delta G$ value shows the relative tendency of the di-acetate complexes (**A,C**) to lose an acetate and access the active pre-transition state (**B,D**). In accordance with our initial hypothesis, the $\Delta\Delta G (= \Delta G_2 - \Delta G_1)$ value was calculated to be -6.57 kcal/mol, showing that the acetate-dissociation step is favored with the pyridine-3-sulfonic acid ligand more than with the simple pyridine ligand.

2.8.5. Energies for Calculated Structures

Notation

The following notation for structures is used in Table S10 and Section 2.7.5. [Important*: The Ligand numberings are different with the manuscript due to revision of the manuscript.]

Substrate: **III** – N-methoxy-N-methylpivalamide;

Ligands: **L0** – AcO^- as the ligand;

LPy – pyridine;

L2 – 3-pyridinesulfonic acid;

L3 – Ac-Gly-OH;

L4 – 4-pyridinesulfonic acid.

Otherwise structure ID name is constructed as:

SubstrateLigand[**III** followed by a number]–**cis/trans_OME-up/down**[position of the amide OMe group]–**species**[intermediate, pre-TS, TS, or product]–**conformer**[conformation number as introduced in Section 2.7.1].

The bidentate substrate binding intermediates *III2-cis_OME-down/up_int_bident-1* and *III2-cis_OME-down/up_int_bident-2* are given as introduced in diagrams S3 and S4.

Structure	ZPE	E	H	qh-G	Imaginary frequency	Δ qh-G
Pd ₃ (OAc) ₆	0.321088	-1754.378175	-1754.015385	-1754.125896	-	-
[AcOH] ₂	0.126369	-458.052557	-457.913119	-457.963844	-	-
III-cis_OMe-down	0.222419	-480.72466	-480.485863	-480.542141	-	-
III-trans_OMe-down	0.223107	-480.729431	-480.490362	-480.545631	-	-
III-cis_OMe-up	0.223081	-480.724579	-480.485463	-480.540887	-	-
III-trans_OMe-up	0.222229	-480.729525	-480.490908	-480.547191	-	-
LPy	0.090434	-248.158051	-248.061073	-248.096373	-	-
L2	0.107236	-871.917104	-871.798394	-871.845935	-	-
L3	0.119009	-436.95416	-436.823336	-436.871195	-	-
L4	0.107091	-871.917511	-871.798986	-871.846454	-	-
III0-cis_OMe-down_int	0.329748	-1065.487103	-1065.126780	-1065.213898	-	23.14
III0-cis_OMe-down_pre-TS	0.329563	-1065.477708	-1065.117713	-1065.204305	-	29.16
III0-cis_OMe-down_TS	0.324415	-1065.460338	-1065.106087	-1065.191485	-1487.02	37.20
III0-cis_OMe-down_prod	0.327868	-1065.504122	-1065.145587	-1065.233180	-	11.04
III0-trans_OMe-down_int	0.329961	-1065.491782	-1065.131380	-1065.218010	-	22.75
III0-trans_OMe-down_pre-TS	0.330320	-1065.483018	-1065.122728	-1065.208222	-	28.89
III0-trans_OMe-down_TS	0.325465	-1065.467010	-1065.112399	-1065.196108	-1537.68	36.49
III0-trans_OMe-down_prod	0.330029	-1065.498971	-1065.138575	-1065.225105	-	18.30
III2-cis_OMe-down_int_bident-1_conf-1	0.374853	-1708.410649	-1708.000095	-1708.097386	-	10.92
III2-cis_OMe-down_int_bident-2_conf-1	0.373713	-1708.41079	-1708.001044	-1708.099075	-	9.86
III2-cis_OMe-down_int_conf-1	0.375049	-1708.408826	-1707.998223	-1708.095051	-	12.38
III2-cis_OMe-down_int_conf-2	0.372810	-1708.407983	-1707.999897	-1708.096253	-	11.63
III2-cis_OMe-down_int_conf-3	0.373934	-1708.401271	-1707.991457	-1708.089137	-	16.09
III2-cis_OMe-down_int_conf-4	0.373707	-1708.409358	-1707.999923	-1708.097046	-	11.13
III2-cis_OMe-down_pre-TS_conf-1	0.374067	-1708.400502	-1707.991747	-1708.089001	-	16.18
III2-cis_OMe-down_pre-TS_conf-2	0.373633	-1708.393399	-1707.983953	-1708.081648	-	20.79
III2-cis_OMe-down_pre-TS_conf-3	0.373643	-1708.394178	-1707.984734	-1708.082336	-	20.36
III2-cis_OMe-down_pre-TS_conf-4	0.373722	-1708.398424	-1707.989015	-1708.086383	-	17.82
III2-cis_OMe-down_pre-TS_conf-5	0.373178	-1708.393833	-1707.990752	-1708.088041	-	16.78
III2-cis_OMe-down_pre-TS_conf-6	0.373906	-1708.401366	-1707.984647	-1708.082842	-	20.05
III2-cis_OMe-down_TS_conf-1	0.369234	-1708.383167	-1707.979338	-1708.073951	-1515.13	25.62
III2-cis_OMe-down_TS_conf-2	0.368971	-1708.378818	-1707.974945	-1708.070885	-1499.22	27.55
III2-cis_OMe-down_TS_conf-3	0.369342	-1708.378544	-1707.974209	-1708.070323	-1520.52	27.90
III2-cis_OMe-down_TS_conf-4	0.367972	-1708.382069	-1707.978878	-1708.075180	-1528.26	24.85
III2-cis_OMe-down_TS_conf-5	0.370145	-1708.382388	-1707.977877	-1708.072008	-1532.50	26.84
III2-cis_OMe-down_TS_conf-6	0.369136	-1708.378549	-1707.974547	-1708.070158	-1500.35	28.00
III2-cis_OMe-down_prod_conf-1	0.374315	-1708.414117	-1708.004216	-1708.101387	-	8.41
III2-cis_OMe-down_prod_conf-2	0.373328	-1708.412854	-1708.003470	-1708.101962	-	8.05

III2-cis_OMe-down_prod_conf-3	0.373813	-1708.413148	-1708.003388	-1708.101521	-	8.32
III2-cis_OMe-down_prod_conf-4	0.373900	-1708.414948	-1708.005104	-1708.103261	-	7.23
III2-trans_OMe-down_int_conf-1	0.372725	-1708.411772	-1708.002764	-1708.101469	-	10.55
III2-trans_OMe-down_int_conf-2	0.373494	-1708.407404	-1707.997866	-1708.096068	-	13.94
III2-trans_OMe-down_int_conf-3	0.373571	-1708.407492	-1707.998112	-1708.095530	-	14.27
III2-trans_OMe-down_int_conf-4	0.373772	-1708.410583	-1708.001040	-1708.098408	-	12.47
III2-trans_OMe-down_pre-TS_conf-1	0.373982	-1708.401752	-1707.991976	-1708.089638	-	17.97
III2-trans_OMe-down_pre-TS_conf-2	0.373352	-1708.397884	-1707.988642	-1708.086842	-	19.73
III2-trans_OMe-down_pre-TS_conf-3	0.373753	-1708.398203	-1707.988618	-1708.086669	-	19.83
III2-trans_OMe-down_pre-TS_conf-4	0.373609	-1708.401549	-1707.992186	-1708.089694	-	17.94
III2-trans_OMe-down_pre-TS_conf-5	0.373040	-1708.401475	-1707.992478	-1708.090474	-	17.45
III2-trans_OMe-down_TS_conf-1	0.369147	-1708.384645	-1707.980755	-1708.075944	-1526.87	26.56
III2-trans_OMe-down_TS_conf-2	0.368868	-1708.382563	-1707.978771	-1708.074554	-1523.77	27.44
III2-trans_OMe-down_TS_conf-3	0.369238	-1708.382400	-1707.978525	-1708.073420	-1527.52	28.15
III2-trans_OMe-down_TS_conf-4	0.368047	-1708.38298	-1707.979632	-1708.076394	-1519.16	26.28
III2-trans_OMe-down_TS_conf-5	0.368971	-1708.38552	-1707.981518	-1708.077412	-1523.82	25.64
III2-trans_OMe-down_prod_conf-1	0.373528	-1708.418544	-1708.009111	-1708.106990	-	7.08
III2-trans_OMe-down_prod_conf-2	0.373649	-1708.416258	-1708.006675	-1708.104732	-	8.50
III2-trans_OMe-down_prod_conf-3	0.374125	-1708.417278	-1708.007593	-1708.104688	-	8.53
III2-trans_OMe-down_prod_conf-4	0.373978	-1708.416688	-1708.006944	-1708.104532	-	8.62
III3-cis_OMe-down_int	0.321200	-1044.381147	-1044.030725	-1044.115114	-	26.99
III3-cis_OMe-down_pre-TS	0.320780	-1044.387984	-1044.038080	-1044.122498	-	22.36
III3-cis_OMe-down_TS	0.316624	-1044.37205	-1044.027389	-1044.109346	-1479.69	30.61
III3-cis_OMe-down_prod	0.322424	-1044.406727	-1044.055846	-1044.138307	-	12.44
III3-trans_OMe-down_int	0.321507	-1044.388342	-1044.037980	-1044.121323	-	25.28
III3-trans_OMe-down_pre-TS	0.322035	-1044.393885	-1044.043319	-1044.126060	-	22.31
III3-trans_OMe-down_TS	0.316292	-1044.376961	-1044.032688	-1044.114169	-1515.84	29.77
III3-trans_OMe-down_prod	0.321474	-1044.411392	-1044.061006	-1044.144705	-	10.61
III4-cis_OMe-down_int	0.374001	-1708.406695	-1707.996951	-1708.094400	-	13.12
III4-cis_OMe-down_pre-TS	0.372589	-1708.393837	-1707.984964	-1708.084243	-	19.49
III4-cis_OMe-down_TS	0.368875	-1708.378891	-1707.975071	-1708.070896	-1511.54	27.87
III4-cis_OMe-down_prod	0.373449	-1708.412719	-1708.003282	-1708.101810	-	8.47
III4-trans_OMe-down_int	0.373630	-1708.407503	-1707.997978	-1708.095896	-	14.37
III4-trans_OMe-down_pre-TS	0.373663	-1708.398289	-1707.988802	-1708.086699	-	20.14
III4-trans_OMe-down_TS	0.369897	-1708.381815	-1707.977593	-1708.071864	-1549.21	29.45
III4-trans_OMe-down_prod	0.373185	-1708.416822	-1708.007509	-1708.106224	-	7.89
III0-cis_OMe-up_int	0.330216	-1065.487363	-1065.126813	-1065.213024	-	22.90
III0-cis_OMe-up_pre-TS	0.328955	-1065.479595	-1065.119980	-1065.207316	-	26.48
III0-cis_OMe-up_TS	0.324760	-1065.464155	-1065.109949	-1065.194281	-1529.78	34.66
III0-cis_OMe-up_prod	0.329419	-1065.497167	-1065.137058	-1065.224469	-	15.72
III0-trans_OMe-up_int	0.329653	-1065.491971	-1065.131623	-1065.218947	-	23.14
III0-trans_OMe-up_pre-TS	0.329744	-1065.485200	-1065.125122	-1065.211488	-	27.82

III0-trans_OMe-up_TS	0.325355	-1065.46637	-1065.111846	-1065.195535	-1509.56	37.83
III0-trans_OMe-up_prod	0.330080	-1065.497448	-1065.137028	-1065.223730	-	20.14
III2-cis_OMe-up_int_bident-1_conf-1	0.373660	-1708.409926	-1708.000156	-1708.098291	-	9.56
III2-cis_OMe-up_int_bident-2_conf-1	0.373782	-1708.405759	-1707.995922	-1708.094305	-	12.07
III2-cis_OMe-up_int_conf-1	0.372921	-1708.408979	-1707.999722	-1708.098509	-	9.43
III2-cis_OMe-up_int_conf-2	0.374800	-1708.406337	-1707.996156	-1708.092363	-	13.28
III2-cis_OMe-up_int_conf-3	0.374309	-1708.402936	-1707.992868	-1708.090414	-	14.51
III2-cis_OMe-up_int_conf-4	0.374401	-1708.401658	-1707.991455	-1708.089048	-	15.36
III2-cis_OMe-up_pre-TS_conf-1	0.374818	-1708.397925	-1707.987738	-1708.084286	-	18.35
III2-cis_OMe-up_pre-TS_conf-2	0.373851	-1708.39454	-1707.984979	-1708.082715	-	19.34
III2-cis_OMe-up_pre-TS_conf-3	0.374046	-1708.392559	-1707.982744	-1708.080530	-	20.71
III2-cis_OMe-up_pre-TS_conf-4	0.373764	-1708.399732	-1707.990285	-1708.087475	-	16.35
III2-cis_OMe-up_pre-TS_conf-5	0.375187	-1708.398198	-1707.987770	-1708.083989	-	18.54
III2-cis_OMe-up_TS_conf-1	0.369168	-1708.381409	-1707.977401	-1708.072846	-1554.73	25.53
III2-cis_OMe-up_TS_conf-2	0.369891	-1708.379434	-1707.975125	-1708.069395	-1499.56	27.70
III2-cis_OMe-up_TS_conf-3	0.369155	-1708.377162	-1707.973183	-1708.068530	-1499.55	28.24
III2-cis_OMe-up_TS_conf-4	0.369865	-1708.383137	-1707.978941	-1708.072862	-1497.77	25.52
III2-cis_OMe-up_TS_conf-5	0.370960	-1708.382759	-1707.977621	-1708.071311	-1511.22	26.49
III2-cis_OMe-up_prod_conf-1	0.374037	-1708.415392	-1708.005740	-1708.102840	-	6.71
III2-cis_OMe-up_prod_conf-2	0.374304	-1708.411841	-1708.001772	-1708.099520	-	8.79
III2-cis_OMe-up_prod_conf-3	0.374170	-1708.41224	-1708.002391	-1708.099727	-	8.66
III2-cis_OMe-up_prod_conf-4	0.374202	-1708.415855	-1708.006123	-1708.102983	-	6.62
III2-trans_OMe-up_int_conf-1	0.374591	-1708.407952	-1707.997748	-1708.094668	-	15.79
III2-trans_OMe-up_int_conf-2	0.373668	-1708.408428	-1707.998906	-1708.096945	-	14.36
III2-trans_OMe-up_int_conf-3	0.374915	-1708.412412	-1708.002276	-1708.098130	-	13.62
III2-trans_OMe-up_int_conf-4	0.373588	-1708.410327	-1708.000877	-1708.098373	-	13.47
III2-trans_OMe-up_pre-TS_conf-1	0.373464	-1708.401986	-1707.992642	-1708.090449	-	18.44
III2-trans_OMe-up_pre-TS_conf-2	0.373268	-1708.396062	-1707.986988	-1708.084704	-	22.05
III2-trans_OMe-up_pre-TS_conf-3	0.373341	-1708.398132	-1707.988800	-1708.087172	-	20.50
III2-trans_OMe-up_pre-TS_conf-4	0.373435	-1708.399965	-1707.990706	-1708.088433	-	19.71
III2-trans_OMe-up_pre-TS_conf-5	0.372745	-1708.402752	-1707.993827	-1708.092367	-	17.24
III2-trans_OMe-up_pre-TS_conf-6	0.374411	-1708.396191	-1707.986212	-1708.083438	-	22.84
III2-trans_OMe-up_TS_conf-1	0.368517	-1708.38521	-1707.981535	-1708.077834	-1510.04	26.36
III2-trans_OMe-up_TS_conf-2	0.368505	-1708.381386	-1707.977927	-1708.073741	-1498.48	28.93
III2-trans_OMe-up_TS_conf-3	0.369046	-1708.381610	-1707.977766	-1708.073263	-1506.56	29.22
III2-trans_OMe-up_TS_conf-4	0.368713	-1708.381896	-1707.978120	-1708.074189	-1523.98	28.64
III2-trans_OMe-up_TS_conf-5	0.369791	-1708.385044	-1707.980649	-1708.075493	-1535.38	27.83
III2-trans_OMe-up_TS_conf-6	0.369043	-1708.381101	-1707.977178	-1708.072761	-1502.47	29.54
III2-trans_OMe-up_prod_conf-1	0.373723	-1708.417126	-1708.007416	-1708.106176	-	8.57
III2-trans_OMe-up_prod_conf-2	0.373415	-1708.415247	-1708.005724	-1708.104381	-	9.70
III2-trans_OMe-up_prod_conf-3	0.373713	-1708.416429	-1708.006963	-1708.104631	-	9.54
III2-trans_OMe-up_prod_conf-4	0.373406	-1708.414835	-1708.005341	-1708.103769	-	10.08

III3-cis_OMe-up_int	0.321129	-1044.383632	-1044.033489	-1044.117173	-	24.91
III3-cis_OMe-up_pre-TS	0.321396	-1044.387726	-1044.037373	-1044.121333	-	22.30
III3-cis_OMe-up_TS	0.316919	-1044.372844	-1044.028215	-1044.108961	-1481.94	30.06
III3-cis_OMe-up_prod	0.322866	-1044.406861	-1044.055591	-1044.137872	-	11.92
III3-trans_OMe-up_int	0.321130	-1044.388689	-1044.038702	-1044.121771	-	25.98
III3-trans_OMe-up_pre-TS	0.32022	-1044.393381	-1044.043981	-1044.128396	-	21.82
III3-trans_OMe-up_TS	0.316076	-1044.376033	-1044.031839	-1044.113704	-1516.82	31.04
III3-trans_OMe-up_prod	0.321777	-1044.410513	-1044.060079	-1044.143029	-	12.64
III4-cis_OMe-up_int	0.373607	-1708.403127	-1707.993645	-1708.091536	-	14.13
III4-cis_OMe-up_pre-TS	0.373982	-1708.393063	-1707.983278	-1708.081234	-	20.59
III4-cis_OMe-up_TS	0.368860	-1708.377584	-1707.973745	-1708.069756	-1535.69	27.80
III4-cis_OMe-up_prod	0.374090	-1708.412326	-1708.002566	-1708.100250	-	8.66
III4-trans_OMe-up_int	0.373534	-1708.408786	-1707.999261	-1708.097566	-	14.30
III4-trans_OMe-up_pre-TS	0.372942	-1708.398228	-1707.989181	-1708.087925	-	20.35
III4-trans_OMe-up_TS	0.368166	-1708.381325	-1707.978024	-1708.074454	1542.79	28.80
III4-trans_OMe-up_prod	0.373506	-1708.415696	-1708.006197	-1708.104727	-	9.81
III2-cis_OMe-down_c4_diOAc	0.426086	-1937.008490	-1936.540031	-1936.650403	-	-
IIIPy-cis_OMe-up_opt_diOAc	0.422701	-1313.700514	-1313.239952	-1313.341447	-	-
IIIPy-cis_OMe-up_pre-TS	0.370834	-1085.080816	-1084.678852	-1084.766953	-	-

Table S10. Zero-point energy corrections (ZPE), electronic energies (E), enthalpies (H), quasi-harmonic Gibbs free energies (qh-G (T=343.15 K)) for all computed structures are given in Hartree at the SMD_(HFIP, Generic)-M06/SDD,6-311++(d,p)//SMD_(HFIP, Generic)- ω B97X-D/SDD,6-31+G(d) level of theory. Imaginary frequencies are in cm⁻¹, and relative free energies (Δ qh-G) are in kcal/mol.

2.8.6. Cartesian coordinates (Å) of all calculated structures at the SMD_(HFIP, Generic)- ω B97X-D/SDD, 6-31+G(d) level of theory.

Pd ₃ (OAc) ₆				O	1.36840900	-1.86427100	1.60129000
				O	2.63685600	-0.03907200	1.22849400
Pd	0.16392000	-1.78673200	-0.02070700	C	3.28765800	-1.54203600	2.93614200
C	-2.14563300	-1.41473800	1.87865500	H	3.83680600	-2.43124100	2.60671700
O	-1.33252600	-2.18588300	1.29332300	H	3.99340000	-0.74500900	3.17852800
O	-2.33430700	-0.18867800	1.61445100	H	2.70655400	-1.81688200	3.82197800
C	-0.27783100	2.59884500	-1.90157600	[AcOH] ₂			
O	0.81395100	2.54507800	-1.26544500	C	-1.95247300	0.05933000	-0.00624700
O	-1.30739000	1.89882100	-1.66581100	C	-3.44353100	0.08286800	0.05884300
C	-0.38579000	3.59631000	-3.01716700	H	-3.78242800	-0.44388000	0.95699400
H	-1.15967100	3.28746400	-3.72399000	H	-3.80312700	1.11302200	0.06940200
H	-0.67276800	4.56325200	-2.58649600	H	-3.85107100	-0.44470700	-0.81058800
H	0.57527100	3.71611500	-3.52308600	O	-1.25285000	1.06582000	-0.10733700
C	-2.99886400	-2.00992800	2.95875200	O	-1.44035500	-1.16498900	0.04405700
H	-2.47927600	-2.83126100	3.45740300	H	-0.44481400	-1.14132400	-0.02253100
H	-3.28914200	-1.24077100	3.67863100	C	1.95247300	-0.05932000	-0.00649600
H	-3.90923100	-2.40619100	2.49236000	C	3.44352500	-0.08294500	0.05879900
Pd	1.50540300	1.09603800	-0.01520000	H	3.78221000	0.44261200	0.95773700
C	-0.17638000	2.51316700	1.95166200	H	3.80312000	-1.11311000	0.06815300
O	-1.23427000	2.29289800	1.29320200	H	3.85126700	0.44578400	-0.80982700
O	0.97870800	2.07298900	1.67147400	O	1.25282400	-1.06575000	-0.10797800
C	-2.13071900	-1.51067300	-1.87105600	O	1.44038600	1.16499500	0.04421000
O	-1.01873700	-2.07071400	-1.63259400	H	0.44484000	1.14139500	-0.02235700
O	-2.59134600	-0.49251600	-1.27972600	III-cis_OMe-down			
C	-2.98003700	-2.14472200	-2.93189000	C	1.46899500	-0.03447000	0.08489900
H	-3.67737700	-1.42171200	-3.36066700	C	0.01797100	-0.45158600	-0.21570100
H	-2.34392900	-2.57783800	-3.70854100	O	-0.24980400	-1.61091900	-0.54641400
H	-3.55324500	-2.95694600	-2.46899000	N	-1.01343500	0.43663300	-0.04018400
C	-0.30320300	3.34512900	3.19322800	C	1.96676300	0.98997300	-0.95260900
H	-0.56465600	2.67777700	4.02361800	H	1.51576400	1.97882400	-0.83994000
H	0.64289100	3.83844300	3.42704700	H	3.05035200	1.11367200	-0.84106200
H	-1.10413700	4.08033700	3.08266500	H	1.77228500	0.63975800	-1.97370800
Pd	-1.66866800	0.80053600	-0.01344600	C	2.34029500	-1.29366400	-0.03889800
C	2.34153500	-0.97507400	-1.94129900	H	3.38079300	-1.03357300	0.18803700
O	1.71560400	-1.89146900	-1.33339400	H	2.02498800	-2.07531100	0.66030000
O	2.28706700	0.26283500	-1.67883500	H	2.30600600	-1.71011600	-1.05136800
C	3.24266600	-1.39418800	-3.06497000	C	1.60090600	0.49886700	1.52230700
H	2.70283900	-2.06195600	-3.74288800				
H	3.61534500	-0.51951300	-3.60243700				
H	4.09026700	-1.94901900	-2.64698800				
C	2.35966900	-1.11042000	1.83896900				

H	1.24954300	-0.24682400	2.24580600
H	2.65699000	0.70355000	1.73458500
H	1.04713200	1.42493900	1.70102200
C	-1.01642000	1.88749000	-0.13396800
H	-1.91578000	2.24847500	0.37153400
H	-0.15662700	2.32338700	0.36884900
H	-1.03816300	2.21276200	-1.18066200
O	-2.23903300	-0.04700700	-0.49352700
C	-2.95217500	-0.71600400	0.54424000
H	-2.40488400	-1.60225200	0.88516500
H	-3.14373700	-0.03656700	1.38303500
H	-3.89793000	-1.01738300	0.08760400

III-cis_OMe-up

C	-1.46445500	0.00813000	0.06934900
C	-0.03446700	-0.50520500	-0.19082700
O	0.18810600	-1.71869000	-0.28545600
N	0.99508500	0.37230200	-0.37271000
C	-1.54330800	0.82919300	1.36991100
H	-1.10756100	1.82720200	1.27859200
H	-2.59651100	0.96218100	1.64365400
H	-1.04471400	0.31145500	2.19878700
C	-2.36432500	-1.22737800	0.22353900
H	-3.39231000	-0.90009800	0.41748700
H	-2.36964200	-1.83792100	-0.68582900
H	-2.04434800	-1.86405500	1.05601700
C	-1.97442400	0.81790500	-1.13601900
H	-1.88567600	0.23975200	-2.06354000
H	-3.03511700	1.05230200	-0.98712100
H	-1.44935800	1.76680800	-1.27815000
C	1.11682800	1.78183000	-0.03888200
H	1.97508200	2.16533600	-0.59609400
H	0.23997900	2.33929100	-0.36278300
H	1.27972300	1.94265400	1.03203700
O	2.22279500	-0.22706800	-0.60468800
C	2.91011400	-0.55481800	0.60438600
H	3.21363800	0.35150600	1.14142100
H	2.29030200	-1.19147400	1.24565300
H	3.79792500	-1.10292800	0.28125300

III-trans_OMe-down

C	1.30769500	-0.26144600	0.03131400
C	0.21835300	0.80228800	-0.17379500
O	0.51724100	1.97541900	-0.43253200
N	-1.10926100	0.48804200	-0.07496700
C	-2.10835600	1.50959400	0.20083700
H	-2.27583200	1.58435200	1.28213300
H	-1.75045400	2.46550500	-0.18281700
H	-3.04735400	1.26096000	-0.29997900
C	1.36717900	-0.60758200	1.53177100
H	0.43351000	-1.05189100	1.88999800
H	2.17532800	-1.32872700	1.70570500
H	1.57870600	0.28606000	2.13194500
C	2.64583600	0.36368100	-0.38775800
H	3.45360400	-0.35145700	-0.19274800
H	2.65966200	0.60313300	-1.45758600
H	2.86042500	1.28257000	0.16746700
C	1.07872100	-1.52659600	-0.81271100
H	0.83967000	-1.27537800	-1.85347300
H	2.00184900	-2.11876100	-0.82211300
H	0.28521100	-2.16169800	-0.41353100
O	-1.43566500	-0.74403300	0.47444700
C	-2.28042000	-1.50126200	-0.38962900
H	-3.26524700	-1.03259000	-0.49465700
H	-1.82084500	-1.63178900	-1.37489700
H	-2.39006300	-2.46972500	0.10382900

III-trans_OMe-up

C	-1.32584700	-0.22747300	0.02842900
C	-0.18541400	0.79283200	-0.12357400
O	-0.40004600	1.96596300	-0.47848400
N	1.08674500	0.46166600	0.19743700
C	2.18124600	1.41349500	0.18888200
H	2.59778300	1.55296100	-0.81534600
H	1.82678400	2.37703800	0.56243200
H	2.95346000	1.03945700	0.86582300
C	-1.15602300	-1.41077200	-0.94169200
H	-0.34231700	-2.07936100	-0.65162500
H	-2.08011700	-2.00156700	-0.94954400

H	-0.97715500	-1.06263000	-1.96635100
C	-2.63993500	0.49096800	-0.30775900
H	-3.47426000	-0.20730900	-0.17260100
H	-2.80894700	1.35324600	0.34618500
H	-2.65753600	0.84348000	-1.34504700
C	-1.39272200	-0.71801500	1.48637400
H	-1.52104800	0.12485300	2.17694200
H	-2.25654800	-1.38312300	1.60652800
H	-0.49556000	-1.26948200	1.78201200
O	1.41194100	-0.84114300	0.51594500
C	2.22661900	-1.44938700	-0.48828100
H	1.77030100	-1.34385800	-1.47836000
H	3.23496000	-1.02071500	-0.49099800
H	2.28029100	-2.50309600	-0.20607500

Pyridine (LPy)

C	-1.14145800	-0.71862000	0.00000100
C	1.14141700	-0.71869700	0.00000700
C	1.19572000	0.67102100	-0.00000100
C	0.00004700	1.38389200	-0.00000700
C	-1.19567000	0.67110700	0.00000900
H	-2.06148000	-1.29840100	0.00000100
H	2.06139100	-1.29855200	0.00002300
H	2.15615900	1.17778400	0.00001100
H	0.00008200	2.47085100	-0.00002400
H	-2.15607400	1.17793400	0.00001800
N	-0.00005900	-1.42312000	-0.00001100

3-pyridinesulfonic acid (L2)

C	-0.92991600	-1.23156500	-0.02917000
C	-2.32135500	-1.22791500	0.00142800
H	-0.38579200	-2.17198800	-0.05141000
H	-2.88621500	-2.15264400	0.01130000
C	-0.23958500	-0.01991400	-0.03413100
C	-0.94062700	1.16598200	-0.02925800
H	-0.47576800	2.14480200	-0.05276500
S	1.55825300	0.00548300	0.00323000
O	1.89784900	-0.36875500	1.38986600
O	1.95777900	-1.00583500	-0.99213800

O	1.91864000	1.39004500	-0.34940700
C	-2.98895200	-0.01991700	0.02253400
H	-4.06739300	0.07362500	0.05120200
H	-2.79238300	2.01015200	0.00612400
N	-2.28514700	1.12637900	0.00126900

4-pyridinesulfonic acid (L4)

C	-2.31314000	1.18036600	-0.00198100
C	-0.93373900	1.21927500	-0.03190000
C	-0.23764800	0.01484200	-0.03782200
C	-0.91759800	-1.20218200	-0.03391800
C	-2.29469600	-1.18482000	-0.00013900
H	-2.93686200	2.06597100	0.00838900
H	-0.41801700	2.17326200	-0.05355100
H	-0.39290600	-2.15135500	-0.05547600
H	-2.90537300	-2.07928600	0.01455500
H	-3.96228800	-0.01420500	0.05289500
N	-2.94475700	-0.00592700	0.01890800
S	1.56695700	0.00333300	0.00359700
O	1.96939700	1.37527900	-0.34797400
O	1.87636300	-0.37721300	1.39550900
O	1.94653600	-1.01945500	-0.98780300

Ac-Gly-OH (L3)

N	0.50584200	-0.41132400	0.02499800
C	-1.90716300	0.11138300	-0.00238800
C	-0.49799400	0.63248500	0.06679100
C	1.83829400	-0.19641300	-0.00402100
O	-2.87095800	0.85324400	-0.01574700
O	2.63020500	-1.15501000	0.00550100
H	-0.43550200	1.21836600	0.99203400
H	-0.38321400	1.33100000	-0.76867200
C	2.32365400	1.22469700	-0.04375700
H	1.99789500	1.76979400	0.85001300
H	3.41488400	1.22125600	-0.08559800
H	1.93040900	1.75332400	-0.91945900
H	0.20637100	-1.37942000	0.08563500
O	-1.99469900	-1.21949000	-0.03559000
H	-2.92886700	-1.49791200	-0.06200100

III0-cis_OMe-down_int

C	-2.40747800	-2.11240500	-0.62399500
O	-1.14113600	-2.13004000	-0.46306100
Pd	-1.20790700	-0.16258000	0.20467700
C	1.77841600	-0.11885600	0.13995100
C	2.30087200	-1.44715500	0.70667600
C	1.42823700	-1.81219200	1.91929900
H	0.39029100	-2.01552700	1.63602200
H	1.83065000	-2.72182700	2.37891900
N	2.41917200	0.54735600	-0.82552500
O	0.73950800	0.42153200	0.61810600
C	2.17835800	-2.57252500	-0.33777200
H	2.80133200	-2.41147800	-1.22221500
H	2.49985900	-3.51407800	0.12260400
H	1.14092500	-2.69371200	-0.66848000
C	3.75353400	-1.28708200	1.19922200
H	4.48579800	-1.23688100	0.39003100
H	3.86308900	-0.38947000	1.81997200
H	4.01673400	-2.15436000	1.81497200
H	1.43059900	-1.01758200	2.67318700
C	-3.16023200	-3.30085400	-1.09494400
H	-2.52159600	-3.92103000	-1.72951800
H	-3.46404500	-3.89148100	-0.22194900
H	-4.05937400	-2.98787600	-1.63211100
O	-2.99576400	-1.00903100	-0.33298700
O	1.81066400	1.71274000	-1.24248900
C	2.21122000	2.84652900	-0.46492900
H	1.98947900	2.68841100	0.59528900
H	3.27664600	3.05712500	-0.61109400
H	1.60938200	3.66965700	-0.85614900
C	3.67736000	0.30754700	-1.51743200
H	3.56036300	0.71863500	-2.52295000
H	4.50604800	0.81160800	-1.01202200
H	3.88769100	-0.75483900	-1.60883800
O	-1.80481200	1.62371500	0.87128900
C	-1.56039400	2.69928800	0.17812900
C	-2.03725700	3.96333400	0.84931400
O	-0.99706400	2.70693800	-0.92355300
H	-3.11411800	3.89620500	1.04004200

H	-1.82954000	4.83288300	0.22126200
H	-1.53767700	4.08218300	1.81699800

III0-cis_OMe-down_pre-TS

C	3.43724900	-0.81230500	0.36971100
O	2.73763900	-1.64748200	0.96348900
C	-1.74327100	-0.55182600	-0.14773600
C	-1.26919300	-1.99257600	0.08493100
C	-0.11418000	-2.27243500	-0.89856600
H	0.87919200	-1.85765300	-0.56567600
H	0.13396400	-3.33869700	-0.87460100
N	-2.86415700	-0.05450600	0.37197800
O	-1.04255200	0.24371000	-0.84260900
C	-0.74277300	-2.11071200	1.52806700
H	-1.55111900	-2.07432900	2.26465600
H	-0.22142500	-3.06767900	1.64295700
H	-0.02902500	-1.30932100	1.75740200
C	-2.37000900	-3.02782600	-0.20899800
H	-3.15440500	-3.04288700	0.54865000
H	-2.83294800	-2.85325700	-1.18745100
H	-1.92030400	-4.02622000	-0.22315200
H	-0.34688200	-2.00966000	-1.93370300
C	4.92313800	-0.71130900	0.58910100
H	5.32675700	-1.68042500	0.89397100
H	5.43070800	-0.35141500	-0.31007000
H	5.10626600	0.00861500	1.39626400
O	2.95350100	0.05937500	-0.46754200
Pd	0.96802300	0.07081500	-0.67726800
O	1.09306000	2.04774600	-0.41795100
C	0.43641200	2.53600500	0.60012400
C	0.47835300	4.04045300	0.68870400
O	-0.19269500	1.85671300	1.41930200
H	1.37106300	4.44683900	0.20611300
H	0.43692800	4.34594500	1.73807300
H	-0.40613800	4.44111600	0.17869000
O	-3.04346300	1.30112200	0.18362300
C	-3.78274500	1.58555100	-1.00934500
H	-3.26010200	1.19779500	-1.89016800
H	-4.79571400	1.17240100	-0.94518100
H	-3.82765900	2.67557300	-1.04998400

C	-3.94977800	-0.68314600	1.11284700
H	-4.44367100	0.11951400	1.66371600
H	-4.66760900	-1.16039700	0.44099200
H	-3.57098000	-1.40055300	1.83947000

III0-cis_OMe-down_TS

C	3.21796000	-1.30391500	0.02935700
O	2.34960000	-2.15710400	0.39354200
C	-1.86408100	-0.36444900	0.02515600
C	-1.26973200	-1.75543000	0.22402000
C	-0.05476900	-1.82133400	-0.72956800
H	1.20437000	-1.74751100	-0.12034000
H	0.29058300	-2.86421600	-0.76559700
N	-3.12583100	-0.04034600	0.30461300
O	-1.11688700	0.56017000	-0.41119800
C	-0.79271200	-1.84958700	1.68815500
H	-1.63692300	-1.88334100	2.38555500
H	-0.20148800	-2.76470200	1.81435100
H	-0.15782300	-0.99399000	1.95261200
C	-2.21188300	-2.91793400	-0.12546600
H	-2.99592400	-3.07995300	0.61664200
H	-2.67685700	-2.78132800	-1.10856200
H	-1.62127800	-3.84005000	-0.16327200
H	-0.32595400	-1.60832200	-1.77166800
C	4.66326700	-1.56255400	0.30331400
H	4.89231600	-2.61799300	0.13335400
H	5.29698700	-0.92414800	-0.31547600
H	4.85577100	-1.33854900	1.35951100
O	2.88282100	-0.21933200	-0.54395700
Pd	0.86649200	0.13125600	-0.56175600
O	1.31590700	2.13635100	-0.48317300
C	1.05704900	2.70782500	0.65066400
C	1.31995100	4.19430000	0.68205400
O	0.61964700	2.10250500	1.64643900
H	0.69911600	4.69504000	-0.06921700
H	2.36775300	4.39174000	0.42954700
H	1.09691200	4.60725000	1.66859600
O	-3.46143500	1.27769000	0.06478700
C	-3.90386600	1.46738500	-1.28468200
H	-3.10906900	1.20585500	-1.99159800

H	-4.80686500	0.87886400	-1.48098700
H	-4.12822500	2.53340700	-1.35516800
C	-4.20685700	-0.83055800	0.87818100
H	-4.93351400	-0.11488300	1.26748600
H	-4.68834700	-1.46435800	0.13005000
H	-3.84251400	-1.42888900	1.71405500

III0-cis_OMe-down_prod

C	3.43993700	-1.11676200	-0.11230900
O	3.56484700	-0.36879600	0.95295300
C	-2.08656500	-0.19913900	0.09632600
C	-1.57943200	-1.58179300	0.48412800
C	-0.35447200	-1.82616700	-0.43249900
H	2.80243500	0.29154800	1.12510500
H	0.27090500	-2.62729400	-0.01825300
N	-3.34438500	0.21603300	0.25427700
O	-1.24602200	0.63433500	-0.35717000
C	-1.13107300	-1.46422800	1.95561100
H	-1.97868600	-1.24844100	2.61714700
H	-0.68185800	-2.41237400	2.27273200
H	-0.38088100	-0.67106300	2.07757500
C	-2.55819700	-2.75110000	0.30697300
H	-3.31349400	-2.81211200	1.09437900
H	-3.06192400	-2.71400600	-0.66540900
H	-1.98133700	-3.68285300	0.34349000
H	-0.67864900	-2.11656400	-1.44304300
C	4.61070800	-1.99528100	-0.40095100
H	4.86339100	-2.57680300	0.49167600
H	4.38129000	-2.65916400	-1.23621600
H	5.47748900	-1.37214200	-0.64846500
O	2.44339400	-1.12665400	-0.85224200
Pd	0.64217000	-0.11756700	-0.59605100
O	1.45182000	1.93063500	-0.62448500
C	1.75370500	2.36480800	0.53061600
C	1.76434400	3.85701400	0.74888500
O	2.01675400	1.60774400	1.51437900
H	0.80483200	4.14709100	1.19533600
H	1.87994500	4.39495500	-0.19545600
H	2.55744000	4.14010900	1.44697900
O	-3.58201600	1.53308400	-0.08876800

C	-3.97609200	1.65808000	-1.45894000
H	-3.18774500	1.28850300	-2.12388300
H	-4.91681400	1.12513300	-1.63852600
H	-4.12150400	2.72965300	-1.60926300
C	-4.49451800	-0.47184500	0.82505700
H	-5.23241900	0.29896200	1.05284000
H	-4.92827100	-1.18877500	0.12421500
H	-4.22353800	-0.96279100	1.76073900

III0-cis_OMe-up_int

C	2.11252700	-2.28752700	0.70489100
O	0.85100800	-2.10038900	0.63541700
Pd	1.17204500	-0.23885900	-0.21677500
C	-1.81613400	0.17179000	-0.22465100
C	-2.40281600	-1.06898900	-0.91756700
C	-1.42917800	-1.51908400	-2.01880100
H	-0.47268300	-1.86785000	-1.61543100
H	-1.88172100	-2.35746100	-2.55947100
N	-2.50258300	0.85709300	0.70042900
O	-0.67447400	0.61833100	-0.52168600
C	-2.55631800	-2.21791200	0.09575400
H	-3.27214300	-1.99716100	0.89300900
H	-2.91481600	-3.10968800	-0.43137700
H	-1.59415300	-2.46297900	0.55957800
C	-3.74482900	-0.73092600	-1.60121800
H	-4.57842200	-0.62792600	-0.90352000
H	-3.67032400	0.19357200	-2.18623200
H	-4.00107000	-1.54284400	-2.29032900
H	-1.23001100	-0.71715100	-2.73792800
C	2.70406500	-3.53253400	1.25348300
H	1.92208800	-4.16564300	1.67930700
H	3.21688900	-4.07011800	0.44786500
H	3.44644600	-3.27859600	2.01664800
O	2.84741100	-1.33320600	0.26183900
O	-1.87275200	1.99257000	1.17808200
C	-1.16216800	1.71888200	2.39162500
H	-1.85617900	1.42118800	3.18616900
H	-0.40648400	0.94266500	2.23246900
H	-0.67632300	2.66154700	2.64997900
C	-3.89211100	0.79104800	1.12917000

H	-3.93566000	1.14603700	2.16054400
H	-4.51726900	1.43574400	0.50405400
H	-4.26721900	-0.22874600	1.11489800
O	1.93055800	1.40727000	-1.07057600
C	1.82239400	2.53774000	-0.43364600
C	2.31822100	3.73745300	-1.19968300
O	1.33177700	2.65120500	0.69737900
H	3.06167100	3.45523200	-1.94964200
H	2.73596600	4.47461500	-0.50811800
H	1.46528700	4.19752800	-1.71362700

III0-cis_OMe-up_pre-TS

C	3.32113800	-1.07094600	0.47075900
O	2.56110200	-1.71391600	1.21220400
C	-1.89636300	-0.46881600	-0.27307500
C	-1.45860500	-1.89384400	0.08836700
C	-0.18843100	-2.20838700	-0.72990000
H	0.76185200	-1.84686000	-0.23008800
H	0.03361600	-3.27919400	-0.67762100
N	-3.13005600	-0.00914400	-0.06080900
O	-1.06472900	0.34863500	-0.76644600
C	-1.11167400	-1.90926400	1.59040300
H	-2.00532400	-1.79292400	2.21179100
H	-0.63897900	-2.86541800	1.84119000
H	-0.40680700	-1.10491100	1.83883300
C	-2.49070400	-2.97628800	-0.26967400
H	-3.36156100	-2.97920700	0.38659300
H	-2.83039900	-2.87921500	-1.30730200
H	-2.01492100	-3.95699600	-0.16362800
H	-0.27685900	-1.95697400	-1.79127500
C	4.81611900	-1.22720000	0.54584600
H	5.33253500	-0.39163100	0.06669400
H	5.12525800	-1.31660200	1.59119400
H	5.09466200	-2.15410400	0.02961700
O	2.90405600	-0.24493500	-0.44316200
Pd	0.92991100	-0.01793400	-0.61717400
O	1.30393200	1.95103900	-0.65169100
C	0.85583200	2.61085300	0.38028800
C	1.10681100	4.09474300	0.30758300
O	0.25881500	2.08656300	1.32982000

H	0.78762600	4.57727700	1.23433800
H	0.54617400	4.51538400	-0.53483100
H	2.16959800	4.29035300	0.13069100
O	-3.36755900	1.27368400	-0.51556400
C	-3.12364600	2.25151400	0.50596700
H	-3.80129500	2.10110000	1.35391200
H	-2.08044700	2.21664000	0.83592600
H	-3.33630400	3.20896300	0.02661800
C	-4.30907300	-0.65719200	0.50051100
H	-4.98949300	0.13829700	0.80874000
H	-4.81356800	-1.27554900	-0.24559300
H	-4.05423400	-1.23905200	1.38612400

III0-cis_OMe-up_TS

C	3.28107500	-1.11529800	0.32252100
O	2.45381400	-2.01849300	0.66312400
C	-1.84257500	-0.54116900	-0.26201100
C	-1.20377200	-1.87369800	0.11946900
C	0.13058700	-1.94177600	-0.66187900
H	1.32320200	-1.72849000	0.05226900
H	0.53885700	-2.95502000	-0.52893800
N	-3.13630700	-0.25875300	-0.11591100
O	-1.10333000	0.38190600	-0.71414800
C	-0.91224700	-1.83276100	1.63289200
H	-1.83488000	-1.83501000	2.22350300
H	-0.32625000	-2.71666200	1.91076900
H	-0.33103200	-0.93881700	1.89599400
C	-2.04667400	-3.10308900	-0.25676700
H	-2.90059300	-3.25994100	0.40545100
H	-2.40704300	-3.03924400	-1.29014900
H	-1.41670900	-3.99591800	-0.17715500
H	-0.01474200	-1.86157300	-1.74662600
C	4.73116800	-1.27870500	0.64142700
H	5.25517700	-0.32487500	0.55425400
H	4.85011700	-1.69629300	1.64487900
H	5.16235400	-1.98999400	-0.07326400
O	2.90618700	-0.08082700	-0.31416000
Pd	0.89575000	0.09033500	-0.56229900
O	1.23348900	2.11391700	-0.59298200
C	0.72256800	2.78335300	0.39112400

C	0.95469700	4.27321300	0.32401000
O	0.07478000	2.26961700	1.32119100
H	0.61390000	4.75717100	1.24271000
H	0.40182100	4.68723000	-0.52727500
H	2.01726200	4.48310200	0.16207900
O	-3.52110500	0.99186300	-0.56077100
C	-3.38729800	1.98472400	0.46730200
H	-4.02963000	1.74046000	1.32139500
H	-2.34448900	2.08494300	0.78620500
H	-3.72890100	2.91015400	-0.00037600
C	-4.23498000	-1.05915800	0.40935100
H	-5.03878400	-0.36201200	0.65166500
H	-4.60377800	-1.76683500	-0.33727000
H	-3.94218900	-1.57420700	1.32432900

III0-cis_OMe-up_prod

C	3.46401100	-1.05060900	0.31562300
O	2.92484600	-1.34183700	1.48884300
C	-1.92456900	-0.54021100	-0.26454700
C	-1.24620600	-1.84335100	0.13557100
C	0.09842300	-1.83852400	-0.63864400
H	1.99779300	-1.03303300	1.54376800
H	0.78066800	-2.58235100	-0.20679000
N	-3.23002300	-0.29647000	-0.14069700
O	-1.19467500	0.40239500	-0.68826400
C	-0.98433300	-1.75593800	1.65266200
H	-1.91622700	-1.79873400	2.22780700
H	-0.35981800	-2.60210400	1.96167400
H	-0.46673300	-0.82340800	1.91263000
C	-2.02090000	-3.12153400	-0.21704800
H	-2.85013900	-3.32978800	0.46450700
H	-2.40522500	-3.08581800	-1.24295100
H	-1.32870100	-3.96923800	-0.14973400
H	-0.06495900	-2.08950100	-1.69730900
C	4.89353200	-1.43785200	0.19610900
H	5.25739100	-1.20306900	-0.80509000
H	5.47798600	-0.89898100	0.94957000
H	4.99706700	-2.50936500	0.39760900
O	2.83856000	-0.50887200	-0.59891900
Pd	0.81145700	0.02431400	-0.60158500

O	1.37646900	2.11914500	-0.53420300
C	0.80610100	2.83092300	0.36852700
C	1.07808800	4.31857200	0.30128100
O	0.04545000	2.36994200	1.25201700
H	0.76998100	4.81949900	1.22294900
H	0.51172400	4.74459200	-0.53614700
H	2.14013900	4.50607300	0.11127600
O	-3.64854700	0.94919700	-0.57064700
C	-3.49590700	1.94454900	0.45235400
H	-4.05198200	1.65720100	1.35200800
H	-2.43843900	2.10872200	0.68734000
H	-3.92941700	2.84963400	0.02210000
C	-4.30235600	-1.13348000	0.38138300
H	-5.13675100	-0.46579500	0.60409000
H	-4.63254000	-1.86694500	-0.35834300
H	-4.00080200	-1.62577500	1.30661500

III0-trans_OMe-down_int

C	-2.42849200	-2.11007000	-0.66786000
O	-1.16290800	-2.07023400	-0.50657500
Pd	-1.32516300	-0.11377800	0.18473700
C	1.67331900	0.04804300	0.21648400
C	2.18028400	-1.24367600	0.86375600
C	1.18600700	-1.68500900	1.94812300
H	0.21603500	-1.97392600	1.53127400
H	1.59766200	-2.56192600	2.46014200
N	2.33998500	0.67269500	-0.75212000
O	0.58221200	0.60165600	0.55657300
C	2.27558500	-2.34184400	-0.21338200
H	3.02847500	-2.10983400	-0.97216800
H	2.55473400	-3.28755300	0.26613800
H	1.31065200	-2.48868000	-0.71383300
C	3.54772300	-1.01992000	1.53908500
H	4.35426000	-0.87312100	0.81832100
H	3.51992600	-0.16308000	2.22295700
H	3.79408600	-1.90931500	2.13046700
H	1.02302000	-0.90196900	2.69690300
C	-3.12593300	-3.29911900	-1.21732000
H	-2.49315900	-4.18547000	-1.13079800
H	-4.07594500	-3.44943100	-0.69673300

H	-3.34204900	-3.11713800	-2.27704200
O	-3.07108400	-1.04508500	-0.34585000
O	-1.99866400	1.64155800	0.86860800
C	-1.75648100	2.71882200	0.18018000
C	-2.19788500	3.99180600	0.85533100
O	-1.19517800	2.72533700	-0.92331800
H	-3.11664000	3.83170800	1.42714800
H	-2.34264900	4.78088000	0.11237700
H	-1.41410100	4.30922600	1.55377000
O	3.56876400	0.20680400	-1.15300900
C	4.61913300	1.13434900	-0.85549600
H	4.51796600	2.04900100	-1.44844300
H	4.63304500	1.37540600	0.21235600
H	5.53316500	0.60992600	-1.14059500
C	1.78525200	1.79349900	-1.50555500
H	0.74428100	1.58217500	-1.75909700
H	1.83344600	2.72353000	-0.93166600
H	2.36516700	1.88292700	-2.42602900

III0-trans_OMe-down_pre-TS

Pd	1.02194500	-0.07037800	-0.63046700
C	3.21395300	-1.43038700	0.54077400
O	2.35241600	-1.93849900	1.27486800
C	4.68182600	-1.70860300	0.72518900
H	5.08225800	-0.99100600	1.45185500
H	4.82391000	-2.71667000	1.12432200
H	5.23007900	-1.58748300	-0.21285100
C	-1.80537600	-0.08051200	-0.26061700
C	-1.68200500	-1.58681200	-0.02501600
C	-0.43411500	-2.09242700	-0.76856700
H	0.52309700	-1.85892900	-0.21447600
H	-0.38181900	-3.18496000	-0.70930000
N	-2.82954700	0.63829800	0.17970500
C	-2.85385100	2.09506700	0.16347900
H	-1.83713000	2.46974100	0.29848700
H	-3.26219100	2.47900700	-0.77579400
H	-3.46894100	2.41973700	1.00554400
O	-0.89379500	0.57993300	-0.85360800
C	-1.50055500	-1.83033400	1.48497100
H	-2.37160100	-1.49509800	2.05676500

H	-1.36187200	-2.90302500	1.66103700
H	-0.60928300	-1.31042700	1.85920800
C	-2.88891100	-2.36218600	-0.58182700
H	-3.79810900	-2.18776800	-0.00504400
H	-3.07658600	-2.10700600	-1.63121800
H	-2.66694000	-3.43411100	-0.53302000
H	-0.41972400	-1.83338600	-1.83185100
O	2.93641100	-0.60462200	-0.42594100
O	1.71739300	1.80387900	-0.59757500
C	1.28393300	2.60247900	0.33702100
C	1.89464500	3.97998700	0.27639300
O	0.45967300	2.28520800	1.20310300
H	2.97193800	3.90701200	0.46404800
H	1.43592000	4.62754500	1.02748100
H	1.76036800	4.41524100	-0.71931100
O	-3.86504800	0.01051100	0.82650400
C	-5.10482600	0.15447200	0.12359300
H	-5.42024000	1.20260800	0.09584800
H	-5.02419200	-0.24937300	-0.89080800
H	-5.81627800	-0.42811600	0.71148500

III0-trans_OMe-down_TS

C	3.07230500	-1.59533200	0.35758100
O	2.07764700	-2.32944000	0.65685500
C	-1.78291300	-0.05134800	-0.25924500
C	-1.42889700	-1.50034400	0.05183200
C	-0.13946800	-1.80497000	-0.74388900
H	1.05379100	-1.84418700	-0.00592800
H	0.06515500	-2.88244100	-0.65621000
N	-2.91755000	0.54027400	0.08908600
C	-3.10780300	1.98284900	-0.01586400
H	-3.26433300	2.28084700	-1.05632500
H	-3.98120200	2.24627500	0.58315500
H	-2.22887700	2.49396800	0.38940300
O	-0.92626400	0.69970200	-0.82323100
C	-1.14884500	-1.58371300	1.56650400
H	-2.06869800	-1.45747300	2.14753500
H	-0.71486800	-2.56330700	1.80071000
H	-0.43285000	-0.81049500	1.87551400
C	-2.51041900	-2.51032900	-0.36195800

H	-3.40242400	-2.45347000	0.26522000
H	-2.80086100	-2.37703700	-1.41029700
H	-2.09736600	-3.52021200	-0.25587600
H	-0.27048600	-1.65838500	-1.82336100
C	4.44648300	-2.01196600	0.76972200
H	4.70101500	-2.94986200	0.26415700
H	5.17867700	-1.24500100	0.51209100
H	4.46129200	-2.19904000	1.84809000
O	2.92551000	-0.51507000	-0.29718800
Pd	0.99264100	0.04579900	-0.59982600
O	1.70458500	1.96453700	-0.51925100
C	1.23557500	2.73378400	0.41069500
C	1.82003400	4.12592400	0.42410800
O	0.38838700	2.38017300	1.25047700
H	1.88425800	4.53056700	-0.59088200
H	2.83897000	4.07692500	0.82713500
H	1.22129800	4.78746200	1.05534700
O	-3.86622700	-0.17712700	0.77548900
C	-5.06956800	-0.34141500	0.01693200
H	-5.55264600	0.62457800	-0.16383500
H	-4.86739400	-0.84998000	-0.93091800
H	-5.70908900	-0.95946200	0.64996300

III0-trans_OMe-down_prod

C	3.29982300	-1.47624400	0.35860100
O	2.69077600	-1.69660800	1.51418100
C	-1.87129200	-0.04968400	-0.25642900
C	-1.45494200	-1.46891600	0.09852500
C	-0.14525000	-1.71649800	-0.69289400
H	1.80596900	-1.27889100	1.53869800
H	0.39867400	-2.56769100	-0.26351500
N	-3.04178400	0.50031000	0.05138100
C	-3.28441800	1.93323800	-0.06368000
H	-3.51373700	2.21155400	-1.09622000
H	-4.12622800	2.17899600	0.58648500
H	-2.39752800	2.47745400	0.27518300
O	-1.02541000	0.72286100	-0.80251500
C	-1.18355600	-1.46556100	1.61824400
H	-2.11403500	-1.34918300	2.18535100
H	-0.72229900	-2.41698800	1.90727800

H	-0.50619900	-0.64792200	1.89981900
C	-2.47630500	-2.55690700	-0.26264400
H	-3.34690100	-2.55954100	0.39884500
H	-2.81853800	-2.45624500	-1.29898200
H	-1.98400300	-3.53277100	-0.16998800
H	-0.36829600	-1.94273200	-1.74623100
C	4.67982000	-2.02410000	0.28025500
H	4.66035300	-3.09982900	0.48367100
H	5.09697500	-1.83571200	-0.70974300
H	5.29819600	-1.54799300	1.04894200
O	2.77714800	-0.86904000	-0.57895600
Pd	0.88460900	-0.00707800	-0.66697400
O	1.77997800	1.96207700	-0.51195800
C	1.31245100	2.73271700	0.40162200
C	1.90022800	4.12736300	0.44828200
O	0.44043700	2.39169400	1.23585900
H	1.97848500	4.54680000	-0.56019900
H	2.91496800	4.07130400	0.86173500
H	1.29869300	4.78589600	1.08083500
O	-3.96188300	-0.23966300	0.75561900
C	-5.14616400	-0.48624000	-0.00825100
H	-5.64955600	0.45270500	-0.26317300
H	-4.91279400	-1.05167300	-0.91631700
H	-5.78245200	-1.07969000	0.65105300

III0-trans_OMe-up_int

C	-1.22048600	2.70295300	0.52226700
O	-0.11263200	2.10074200	0.30382900
Pd	-1.13228000	0.39161800	-0.24472300
C	1.52619000	-0.73365300	-0.34370000
C	2.47764600	0.04202800	-1.25857800
C	1.67371700	0.54088200	-2.46825800
H	0.93491400	1.29644800	-2.17642400
H	2.36379100	1.00333800	-3.18292300
N	1.90069100	-1.25729800	0.81682600
O	0.33251900	-0.99194300	-0.71098600
C	3.11105200	1.26048800	-0.56210700
H	3.85024300	0.97736000	0.18973300
H	3.62710100	1.85920500	-1.32197200
H	2.35090000	1.89862700	-0.09669500

C	3.56833000	-0.93275800	-1.74623300
H	4.18630900	-1.30205400	-0.92178800
H	3.12546200	-1.79366700	-2.26165300
H	4.22205900	-0.41204500	-2.45527900
H	1.14914800	-0.27385400	-2.97771500
C	-1.27064200	4.10216900	1.01356400
H	-0.39816600	4.65620600	0.65783300
H	-2.19592200	4.58138800	0.68305700
H	-1.25481600	4.09036300	2.11015100
O	-2.28335400	2.01962700	0.30912400
O	-2.48261300	-0.98051000	-0.79686300
C	-2.75906000	-1.93297100	0.04553500
C	-3.80724600	-2.89771000	-0.44672800
O	-2.21788000	-2.05100500	1.15385600
H	-4.71772400	-2.35023100	-0.71400900
H	-4.03342400	-3.64082700	0.32154100
H	-3.44825100	-3.40309200	-1.34993200
O	3.18854400	-1.08033100	1.26262400
C	3.22838400	-0.28414800	2.45448400
H	2.70988100	0.66777800	2.30205100
H	2.79120100	-0.82426700	3.30073200
H	4.29123500	-0.11334800	2.63450400
C	1.03146000	-2.09083400	1.64044900
H	0.36673600	-1.47731800	2.25720600
H	0.43405100	-2.73445300	0.99334100
H	1.67256500	-2.71020000	2.27089400

III0-trans_OMe-up_pre-TS

C	3.26782000	-0.85613000	0.78610000
O	2.44246200	-1.56410700	1.38152600
C	-1.69736100	-0.39671700	-0.57069000
C	-1.40437500	-1.82925700	-0.10566900
C	-0.17676500	-2.33495100	-0.88655300
H	0.80521700	-1.94798900	-0.50102000
H	-0.04081700	-3.40508100	-0.69690400
N	-2.80277400	0.25946500	-0.24955400
C	-3.10623400	1.61197800	-0.69169500
H	-2.65713000	1.77609100	-1.67145100
H	-4.19241200	1.69706600	-0.77298000
H	-2.71744500	2.35181800	0.01545900

O	-0.89379400	0.21149200	-1.35181800
C	-1.10135800	-1.85839700	1.40456500
H	-2.01028100	-1.74447100	2.00062600
H	-0.64906700	-2.82414400	1.65682800
H	-0.38993200	-1.07349000	1.68828200
C	-2.57708700	-2.76245100	-0.45893400
H	-3.48914400	-2.50291000	0.08212200
H	-2.78933000	-2.73722700	-1.53456500
H	-2.30493100	-3.79008800	-0.19216000
H	-0.26699200	-2.19290900	-1.96649200
C	4.72195300	-0.83110900	1.17863900
H	5.20799400	-1.73256800	0.78695200
H	5.23067400	0.04715200	0.77345400
H	4.80916400	-0.84857300	2.26908300
O	2.96840400	-0.10017000	-0.23078000
Pd	1.05984400	-0.01192200	-0.78057200
O	1.23970300	1.96814300	-0.54310000
C	0.45951100	2.50518900	0.35517500
C	0.53017200	4.00976800	0.39701500
O	-0.30647400	1.86921700	1.08870800
H	-0.20315600	4.40727700	-0.31596100
H	1.51960900	4.37207900	0.10500400
H	0.26970300	4.36717300	1.39681700
O	-3.67282800	-0.29545500	0.65791800
C	-3.66023200	0.42035900	1.90301100
H	-2.63352200	0.57955300	2.24876700
H	-4.18291300	1.37716800	1.80268200
H	-4.20473600	-0.22640500	2.59324500

III0-trans_OMe-up_TS

C	3.12665300	-1.26382700	0.56584600
O	2.22445200	-2.15373200	0.67425900
C	-1.73611900	-0.27922200	-0.52018700
C	-1.25876900	-1.68980400	-0.18300300
C	0.09574800	-1.85394100	-0.91325700
H	1.24190800	-1.78280700	-0.10241100
H	0.40138800	-2.90768900	-0.82690900
N	-2.94634100	0.19523500	-0.26178000
C	-3.33853300	1.55492800	-0.60868200
H	-3.06472200	1.75533300	-1.64743900

H	-4.42322800	1.62293100	-0.50840200
H	-2.84495400	2.28152600	0.04658600
O	-0.94986500	0.52453100	-1.11470100
C	-1.04203400	-1.82028000	1.33713300
H	-1.99084200	-1.90159300	1.87482600
H	-0.46371300	-2.73046300	1.53662200
H	-0.47809600	-0.96571700	1.73307300
C	-2.23679200	-2.76075300	-0.69202000
H	-3.18967300	-2.73941200	-0.15768100
H	-2.43287200	-2.63949000	-1.76382000
H	-1.78502900	-3.74827700	-0.54172600
H	0.00891800	-1.69930900	-1.99569000
C	4.46221000	-1.48621600	1.19680600
H	4.91937700	-2.38473000	0.76937000
H	5.11448200	-0.62599500	1.03702200
H	4.32677700	-1.65945600	2.26944800
O	2.91940600	-0.18435700	-0.07289600
Pd	0.99498800	0.11104000	-0.65780600
O	1.42410000	2.10055700	-0.45597800
C	0.74468200	2.75377800	0.43200400
C	1.05952000	4.22848400	0.49317000
O	-0.11953700	2.24498600	1.16941900
H	0.50869300	4.73898200	-0.30666900
H	2.12704500	4.40233900	0.32738700
H	0.75233100	4.65124600	1.45320000
O	-3.83730700	-0.56696600	0.45400100
C	-4.02684000	-0.05294300	1.78062500
H	-3.06378700	0.12004000	2.27050300
H	-4.61295400	0.87187600	1.76164700
H	-4.58446700	-0.83519000	2.29914700

III0-trans_OMe-up_prod

C	3.20775200	-1.33735400	0.55301300
O	2.47292800	-1.44850300	1.64872100
C	-1.85005200	-0.20744300	-0.49531100
C	-1.34025600	-1.60685600	-0.17525600
C	0.02123100	-1.70130000	-0.91225600
H	1.63604700	-0.94543700	1.56975800
H	0.61029500	-2.53738400	-0.51317100
N	-3.11155900	0.19661400	-0.34161500

C	-3.51630300	1.57132200	-0.59348800
H	-3.16320800	1.87272500	-1.58234300
H	-4.60746000	1.60532000	-0.58268000
H	-3.09974300	2.25213700	0.15787900
O	-1.03881500	0.65420400	-0.94837200
C	-1.12532400	-1.70355500	1.34989900
H	-2.06827600	-1.87281300	1.87854500
H	-0.45984600	-2.54733200	1.56914700
H	-0.66335100	-0.79039400	1.74813600
C	-2.26355600	-2.73220100	-0.66570200
H	-3.20412700	-2.78186600	-0.11053900
H	-2.49473200	-2.61699200	-1.73108100
H	-1.74165800	-3.68891000	-0.54037800
H	-0.12955200	-1.86113200	-1.98992700
C	4.53873700	-1.99076600	0.65390200
H	4.39856400	-3.05286000	0.88247400
H	5.08654200	-1.87666000	-0.28201300
H	5.09877600	-1.54072200	1.48014200
O	2.81603200	-0.75038200	-0.46024300
Pd	0.91398100	0.06551200	-0.70543700
O	1.70736600	2.05722100	-0.35936700
C	1.04491100	2.80907700	0.44389600
C	1.47359400	4.26066800	0.49039800
O	0.08055900	2.42070400	1.14511400
H	1.08003300	4.77151400	-0.39731900
H	2.56461000	4.34657800	0.46407100
H	1.08102100	4.75783300	1.38183500
O	-3.97754300	-0.60132200	0.37284600
C	-4.18043300	-0.11173900	1.70612800
H	-3.22549800	0.12789400	2.18384300
H	-4.83332200	0.76764500	1.70462700
H	-4.67335200	-0.93348900	2.22947400

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C	-3.11218500	-0.85919700	0.22205400
C	-3.50189600	-2.04459700	0.83217500
C	-2.52235300	-2.98481400	1.14127400
H	-4.54939500	-2.22969900	1.05397900
H	-2.77544600	-3.92798500	1.61290400
N	-0.84291100	-1.54358800	0.26047800

C	2.97632500	-2.61480100	-0.72279600
O	3.14246200	-1.36574000	-0.53282900
Pd	1.11037900	-1.18237100	-0.07992500
C	1.39271600	1.82007200	0.17357200
C	2.71561200	2.04424900	0.92241600
C	2.86502700	0.94481900	1.98840500
H	3.01410300	-0.04557300	1.54979300
H	3.75077200	1.16856400	2.59286800
N	0.90007300	2.72768700	-0.67566900
O	0.68848000	0.78794100	0.37044100
C	3.90466200	1.94821700	-0.05177900
H	3.88743600	2.71530400	-0.83121800
H	4.83547600	2.07393600	0.51326400
H	3.93767700	0.96823300	-0.54061800
C	2.69448000	3.39870800	1.66226000
H	2.82477500	4.26095200	1.00612400
H	1.76130500	3.52783800	2.22360600
H	3.52059700	3.41639900	2.38110900
H	1.99749200	0.90541100	2.65657700
C	-1.77452600	-0.63749400	-0.06542100
H	-1.42289400	0.25475600	-0.57046300
O	-5.61762600	-0.19670200	-0.00070200
O	-4.01750700	1.49880200	0.82948000
O	-3.97938700	0.84345900	-1.54469200
S	-4.29458000	0.43493600	-0.15932300
C	4.07932600	-3.52078700	-1.12407600
H	5.04472800	-3.03535500	-0.96263800
H	4.01858400	-4.45554600	-0.55904700
H	3.96847400	-3.75753400	-2.18889800
O	1.77767800	-3.05226500	-0.55776100
C	-1.20044200	-2.70233800	0.84556700
H	-0.40206900	-3.40089300	1.07464700
O	-0.29877500	2.39375400	-1.27430000
C	-1.41848800	2.99266400	-0.60369100
H	-1.45872700	2.66149100	0.43915200
H	-1.36793500	4.08535700	-0.66176700
H	-2.29108300	2.63114700	-1.15137500
C	1.38342500	4.04041700	-1.08386800
H	1.02407600	4.19704300	-2.10322600
H	0.99524600	4.82803400	-0.43308200
H	2.46980500	4.07480600	-1.10330000

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C	3.31656300	-0.54225700	-0.11401000
C	3.74625100	-1.74324100	-0.66287500
C	2.78741000	-2.69166900	-1.00698300
H	4.80495800	-1.93376500	-0.81359800
H	3.07028900	-3.64461300	-1.44054900
N	1.05210300	-1.24216500	-0.25946500
C	-2.31210800	-3.29852300	-0.14059100
O	-3.19477800	-2.65266300	-0.72130800
Pd	-0.88672400	-0.81265500	0.06456600
C	-1.61876500	1.90894700	-0.10211000
C	-1.41975800	3.39456400	-0.40378100
C	0.07101800	3.70881600	-0.18892800
H	0.71329800	3.13064700	-0.85885500
H	0.23468300	4.77182300	-0.39426900
N	-2.82122700	1.37263900	0.12581600
O	-0.58863900	1.17341000	-0.09571500
C	-1.76186900	3.63035200	-1.88872700
H	-2.81302400	3.43865600	-2.12428800
H	-1.55040800	4.67678500	-2.13475400
H	-1.14431800	2.99526300	-2.53388700
C	-2.24365200	4.29804700	0.52862100
H	-3.31523300	4.28895700	0.31887200
H	-2.09263700	4.02571900	1.57968700
H	-1.90137600	5.33044300	0.40003900
H	0.37979200	3.50795800	0.84301400
C	1.96323900	-0.31274500	0.07007700
H	1.59045500	0.61107300	0.49966000
O	5.80231800	0.14604800	0.22704700
O	4.19843100	1.86890900	-0.54152700
O	4.09785400	1.05024600	1.78174700
S	4.46359100	0.74478600	0.38183100
C	-2.43093700	-4.78200600	0.09308300
H	-3.48382600	-5.07491800	0.11955500
H	-1.94524900	-5.30652300	-0.73919600
H	-1.92889800	-5.07795900	1.01833600
O	-1.20397800	-2.77785200	0.29928300
C	1.44911700	-2.41546300	-0.78766800
H	0.67063900	-3.13029800	-1.02617300

O	-2.82258200	-0.00467000	0.41832300
C	-3.35759600	-0.28071500	1.74182300
H	-2.78387500	0.26807400	2.49182900
H	-4.41690600	-0.01898000	1.76391800
H	-3.23464200	-1.35676400	1.86547100
C	-4.16874700	1.89410400	-0.06102300
H	-4.77224400	1.07065700	-0.45080600
H	-4.58864200	2.26120600	0.87758600
H	-4.16715100	2.68210900	-0.80962400

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C	-3.61156100	0.16420300	0.05061100
C	-4.17878700	1.38123200	-0.30335600
C	-3.33254800	2.42168700	-0.67713800
H	-5.25687400	1.51250100	-0.28496100
H	-3.72761700	3.39093700	-0.96120000
N	-1.43301900	1.02382400	-0.34857200
C	1.70840800	3.01580900	0.65997200
O	2.25621200	2.26281200	1.47211400
Pd	0.56035400	0.66203200	-0.42966200
C	2.78046600	-1.01444800	-0.14741400
C	4.21256900	-1.30643600	0.28662600
C	5.09511400	-0.19772600	-0.31446700
H	4.82274400	0.78929100	0.07308900
H	6.13805200	-0.39808500	-0.04717000
N	1.79598800	-1.92228300	-0.11241800
O	2.52049300	0.16854000	-0.50227600
C	4.24486400	-1.18090300	1.82429400
H	3.67393400	-1.97121400	2.32329900
H	5.28471300	-1.25522700	2.16200500
H	3.84659100	-0.20987900	2.14531300
C	4.72879100	-2.67049400	-0.19065800
H	4.29208200	-3.51375000	0.34855800
H	4.54866500	-2.81071400	-1.26313000
H	5.81040900	-2.71158500	-0.02383800
H	5.01896100	-0.17258600	-1.40778700
C	-2.23468500	0.01223800	0.01562100
H	-1.75483000	-0.92243700	0.29207200
O	-6.00080200	-0.78971900	0.48351400
O	-4.26354100	-2.29490300	-0.44627800

O	-4.13745700	-1.58286200	1.90873200
S	-4.60052300	-1.24958600	0.54479900
C	1.93008600	4.50618600	0.65208900
H	2.63952800	4.78764600	1.43332000
H	2.31226300	4.82023800	-0.32522800
H	0.97702800	5.02091300	0.81694100
O	0.88596400	2.61574000	-0.27419000
C	-1.96417200	2.21323400	-0.68802000
H	-1.26432300	2.99411600	-0.96587500
O	0.54679300	-1.45947700	-0.57172400
C	0.23048100	-2.00997500	-1.88105100
H	0.98113300	-1.68178700	-2.60328800
H	0.18527100	-3.09786500	-1.80680900
H	-0.75471100	-1.60726200	-2.11768600
C	1.72576000	-3.27936100	0.41808000
H	0.67955700	-3.45839900	0.67525300
H	2.06060100	-4.01599800	-0.31431000
H	2.30811000	-3.35227200	1.33573600

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C	-3.26777800	-0.42589200	-0.50204700
C	-3.30168600	-1.37531900	-1.51433200
C	-2.16902800	-1.54005700	-2.30755300
H	-4.19313600	-1.97463500	-1.67528300
H	-2.14643900	-2.26991800	-3.10948200
N	-1.03685800	0.14918600	-1.06754100
C	1.33002900	3.22489900	0.37358900
O	2.17470500	2.27687200	0.21432100
Pd	0.66999400	1.05189300	-0.50061700
C	2.40255800	-1.20152800	0.05214600
C	3.91280200	-1.27605800	-0.20033300
C	4.17741700	-0.60018100	-1.55553700
H	3.89382700	0.45902600	-1.53840000
H	5.24898600	-0.66296400	-1.77492600
N	1.83331500	-1.63705800	1.17885600
O	1.67006800	-0.70937900	-0.85762300
C	4.66269300	-0.47487500	0.88469500
H	4.72422700	-0.99272400	1.84452700
H	5.68963600	-0.30209200	0.54397100
H	4.19334300	0.50348300	1.04772100

C	4.39159100	-2.73563600	-0.27859600
H	4.23465000	-3.29417300	0.64868600
H	3.87889300	-3.26998500	-1.08689800
H	5.46646300	-2.74747600	-0.49167100
H	3.63065900	-1.08949100	-2.36835600
C	-2.12231000	0.33061000	-0.30459200
H	-2.05365500	1.08347400	0.47572300
O	-5.71736100	-1.06055700	0.11462200
O	-4.10798500	-0.62201100	1.94310500
O	-4.94612900	1.25003200	0.56978400
S	-4.63913200	-0.19461000	0.62983600
C	1.70709200	4.53136200	0.96500200
H	2.76368200	4.73988200	0.77934300
H	1.07690700	5.32608700	0.55777000
H	1.54439600	4.47996600	2.04861400
O	0.12364100	2.96663000	0.01999900
C	-1.04726000	-0.77222600	-2.04932400
H	-0.13125000	-0.88997600	-2.61863300
O	0.48654700	-1.35642700	1.31340500
C	-0.32913800	-2.46806300	0.92079800
H	-0.19342100	-2.68825100	-0.14249700
H	-0.09408000	-3.35204000	1.52363700
H	-1.35333200	-2.14714200	1.12510700
C	2.41346400	-2.07414000	2.44076100
H	2.52378800	-1.22185200	3.11721000
H	1.72679800	-2.79811500	2.88504800
H	3.36967600	-2.56795800	2.29162800

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C	3.49139900	-0.94430900	0.11674400
C	3.30569100	-2.30674300	-0.07841500
C	2.01981200	-2.76914600	-0.34345700
H	4.14559500	-2.99314200	-0.02943400
H	1.82418800	-3.82268700	-0.51080200
N	1.17193600	-0.54708800	-0.20146000
C	-0.43839000	3.17176300	-0.76128900
O	-1.48984500	2.51221100	-0.46541500
Pd	-0.34664900	0.78803400	-0.29102300
C	-2.91763300	-0.69019700	0.25774200
C	-3.61636500	0.09659700	1.37652000

C	-2.53817300	0.65330900	2.32226100
H	-1.93064500	1.43031800	1.84650400
H	-3.03519800	1.11119600	3.18426100
N	-3.60073100	-1.40758400	-0.64144900
O	-1.65568000	-0.74481600	0.18108600
C	-4.41730800	1.28106100	0.80414300
H	-5.28446600	0.97716400	0.21187300
H	-4.78958100	1.88710500	1.63800300
H	-3.78495100	1.91993500	0.17839300
C	-4.51236600	-0.85116800	2.20012600
H	-5.41780700	-1.16229200	1.67486800
H	-3.96084300	-1.74996100	2.50239200
H	-4.83142500	-0.33059900	3.10951300
H	-1.87044300	-0.13349500	2.68924000
C	2.40574200	-0.08365800	0.04838400
H	2.51131500	0.98763900	0.19699200
O	6.02133700	-1.38823600	0.57998300
O	5.39009700	0.58818500	-0.77286000
O	4.94409200	0.56752500	1.65303000
S	5.11287900	-0.23581200	0.42286100
C	-0.46828200	4.62271900	-1.06462600
H	-1.44509400	5.04055400	-0.81162700
H	0.32223900	5.13587700	-0.50850800
H	-0.27532700	4.76502700	-2.13434600
O	0.65566900	2.49427700	-0.79263800
C	0.97597600	-1.86361200	-0.39851900
H	-0.03923600	-2.17424800	-0.61040600
O	-2.82919100	-2.07780300	-1.57105500
C	-2.55527200	-3.42245100	-1.15488900
H	-2.06703000	-3.43078800	-0.17473400
H	-3.47503900	-4.01673800	-1.12876700
H	-1.88232900	-3.81957000	-1.91692700
C	-5.02249000	-1.68675000	-0.79229300
H	-5.19208700	-1.86293700	-1.85675900
H	-5.31879200	-2.57317500	-0.22505500
H	-5.62757500	-0.83428700	-0.49463100

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C	3.21454900	-0.55186700	0.02691900
C	3.65918600	-1.56231800	0.87023900

C	2.72427400	-2.44873000	1.39553400
H	4.71378800	-1.65605700	1.11185500
H	3.02082900	-3.25554000	2.05672000
N	0.97464800	-1.29874200	0.25640300
C	-2.81650200	-2.78527500	-0.13385400
O	-3.02128800	-1.55127300	-0.38896900
Pd	-1.00553500	-1.16572600	-0.12004000
C	-1.59070700	1.69796100	0.01234600
C	-2.86349100	2.17942300	-0.69495800
C	-2.88301700	1.55477500	-2.09995400
H	-2.93524600	0.46150700	-2.06288800
H	-3.77325400	1.91545000	-2.62705700
N	-1.21902100	2.15417900	1.20916100
O	-0.84400300	0.84394800	-0.55850100
C	-4.10746100	1.67631900	0.06499400
H	-4.19993400	2.08574000	1.07517300
H	-5.00245200	1.97768000	-0.49177300
H	-4.10794900	0.58191900	0.13911200
C	-2.86434900	3.71229900	-0.85061500
H	-3.07075900	4.24613200	0.07996200
H	-1.90516300	4.06866900	-1.24566500
H	-3.64604900	3.99274900	-1.56472200
H	-2.00064000	1.84078800	-2.68313400
C	1.86347700	-0.44175800	-0.26599400
H	1.47544100	0.32701400	-0.92592000
O	5.60108600	0.48900200	0.06536200
O	4.50191600	0.14889800	-2.12546600
O	3.69948300	1.92460700	-0.61009300
S	4.36081300	0.60856900	-0.72597900
C	-3.90298500	-3.79347900	-0.14564500
H	-4.70431200	-3.47150500	-0.81553000
H	-3.50979100	-4.76631200	-0.45216100
H	-4.30867800	-3.88723700	0.86905300
O	-1.60321200	-3.10296900	0.14899900
C	1.38996500	-2.28927500	1.06830300
H	0.62561800	-2.95646000	1.45576800
O	-0.05973600	1.60610100	1.71784300
C	1.08850800	2.40503800	1.39285800
H	1.16018300	2.55165900	0.31113900
H	1.04553000	3.36923400	1.91045500
H	1.94160900	1.83111500	1.75756100

C	-1.76597400	3.21041600	2.04999200
H	-1.51488100	2.95685000	3.08183700
H	-1.32981900	4.17938600	1.79354500
H	-2.84863800	3.25776900	1.97082400

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C	-2.87490700	-1.30510200	-0.03754900
C	-3.10616600	-2.60909500	0.38427500
C	-2.00393500	-3.41452300	0.65490600
H	-4.11869800	-2.98858300	0.49476000
H	-2.12580700	-4.44251200	0.97859600
N	-0.52596700	-1.62241500	0.13064900
C	3.29035000	-2.75594900	-0.36071800
O	3.97644700	-1.86440900	-0.87432600
Pd	1.31060100	-0.73653700	0.10808300
C	0.97143000	2.17685500	0.05282100
C	2.49668900	2.30048200	0.12869300
C	3.08588100	0.89815000	0.38250000
H	2.92481400	0.21118400	-0.49271100
H	4.18044300	0.92931600	0.38263200
N	0.15711900	3.22071300	-0.11262800
O	0.39565200	1.05437400	0.15540400
C	3.05274100	2.81484500	-1.21176600
H	2.78192800	3.85254000	-1.42012200
H	4.14639000	2.76038400	-1.18475800
H	2.70162000	2.19485000	-2.04466900
C	2.91975900	3.18286700	1.31721700
H	2.67834100	4.23968800	1.18353500
H	2.45007100	2.83716800	2.24485600
H	4.00593300	3.11094400	1.43931900
H	2.81260400	0.49675500	1.37006200
C	-1.57891800	-0.84642400	-0.17300600
H	-1.37131600	0.15443900	-0.52828100
O	-5.33575500	-0.91643100	-0.81720000
O	-4.43839300	0.46707400	1.02487400
O	-3.64733600	0.84631500	-1.27735400
S	-4.19799300	-0.12466200	-0.30991400
C	3.75063100	-4.18751000	-0.29555800
H	4.84282100	-4.22981600	-0.27708000
H	3.33173900	-4.69897100	0.57534000

H	3.39879900	-4.70255200	-1.19798500
O	2.10339400	-2.55945100	0.14156700
C	-0.72600200	-2.88944600	0.53187300
H	0.15900400	-3.47572100	0.75487300
O	-1.17662500	2.90842300	-0.31207500
C	-1.92409100	2.90606200	0.91241700
H	-1.63825500	2.05674800	1.54124400
H	-1.78231100	3.84969600	1.45014900
H	-2.96523500	2.80939700	0.60190700
C	0.41710200	4.61545700	-0.42573900
H	0.21463100	4.78956000	-1.48658800
H	-0.24867900	5.23378000	0.18189800
H	1.44085800	4.89172400	-0.19565000

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C	-3.03030400	-2.50578900	0.24479700
C	-3.30773300	-1.15031000	0.09909400
H	-3.82574600	-3.22080500	0.43561900
N	-1.00237000	-0.66717200	-0.19684700
C	-0.62485200	3.19258800	0.14460400
O	0.38223600	3.33933800	0.85075400
Pd	0.52234900	0.68146300	-0.40838400
C	3.10345600	-0.55505300	0.10279900
C	3.65161800	0.87501600	0.09675200
C	2.72285900	1.72140200	-0.79372600
H	1.79791400	2.05973800	-0.23545900
H	3.15489500	2.71443900	-0.95567100
N	3.83549300	-1.61654500	0.43819300
O	1.89795400	-0.78945900	-0.21528600
C	3.60192800	1.42744700	1.53410100
H	4.24696200	0.86103600	2.21286300
H	3.94534100	2.46773200	1.52672300
H	2.57820000	1.41150300	1.92851300
C	5.06565400	0.98466500	-0.49933900
H	5.84345000	0.61542800	0.16992400
H	5.14209400	0.46004400	-1.45820600
H	5.28181000	2.04276000	-0.68008800
H	2.54841200	1.28860400	-1.78418200
C	-0.71728000	-1.97634200	-0.07071000
H	0.32677200	-2.26117800	-0.13725100

C	-1.71363300	4.22549600	0.05886300
H	-1.40598900	5.13773700	0.57496100
H	-1.94839800	4.44663400	-0.98714300
H	-2.62286400	3.83247400	0.52783800
O	-0.83837700	2.12740400	-0.57909100
C	-2.27986300	-0.25242700	-0.12462000
H	-2.46111500	0.81093200	-0.24007000
S	-5.00109300	-0.56239300	0.16500500
O	-5.60575600	-1.29559400	1.29629300
O	-4.90422400	0.89619400	0.37305900
O	-5.57862600	-0.93712700	-1.14362500
C	-1.70789100	-2.91886700	0.15164500
H	-1.43454200	-3.96324800	0.25552300
O	3.16924300	-2.82430700	0.38987800
C	3.35876900	-3.47673900	-0.87182800
H	2.95580100	-2.86487800	-1.68564300
H	4.41963400	-3.69276000	-1.04034000
H	2.79920200	-4.40999200	-0.78919200
C	5.21010800	-1.73482900	0.91010900
H	5.26046300	-2.68020300	1.45386800
H	5.92368800	-1.75201900	0.08306600
H	5.45498600	-0.93614300	1.60941100

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C	3.05139400	-2.24048900	-0.86585200
C	3.29929300	-1.05194000	-0.19168300
H	3.86414800	-2.92095500	-1.10291600
N	0.99705900	-0.49068900	-0.25857400
C	0.38210300	3.28240500	-0.54427400
O	-0.74582800	3.35375600	-1.05298800
Pd	-0.51859200	0.74467400	0.25532600
C	-3.01886200	-0.68377100	0.11310700
C	-3.68021600	0.67798900	0.34548200
C	-2.69303500	1.56034000	1.13465300
H	-1.90926700	2.04063000	0.47399700
H	-3.19373700	2.48112700	1.45220500
N	-3.68625900	-1.76502100	-0.28836100
O	-1.77217000	-0.83901800	0.28752800
C	-3.94656000	1.34078400	-1.01899600
H	-4.67396800	0.78505900	-1.61831700
H	-4.34448900	2.34799400	-0.85327400

H	-3.01778100	1.43443200	-1.59501000
C	-4.96021500	0.57228700	1.19148000
H	-5.79148100	0.10632600	0.66066400
H	-4.78009600	0.01469200	2.11771000
H	-5.28190300	1.58313300	1.46334200
H	-2.30417200	1.08625200	2.04070800
C	0.73412100	-1.63716100	-0.91637300
H	-0.30117100	-1.83304900	-1.17524500
C	1.39264300	4.39002700	-0.65875900
H	1.13263300	5.04901300	-1.49068900
H	1.38815900	4.97265000	0.27038200
H	2.39934900	3.98407700	-0.79435700
O	0.78036000	2.25574700	0.15397000
C	2.25406100	-0.18953600	0.10024700
H	2.40682700	0.74990600	0.62315200
S	4.94937100	-0.59675100	0.34412100
O	5.85720200	-1.47968600	-0.41378000
O	5.06977100	0.83529900	0.00216700
O	4.95543200	-0.84703300	1.80173700
C	1.74137900	-2.53133900	-1.23370800
H	1.49526700	-3.44240200	-1.76832500
O	-2.90811000	-2.88124800	-0.52238400
C	-2.68431100	-3.64876700	0.66717000
H	-2.17413600	-3.04816100	1.42713200
H	-3.63091200	-4.04307100	1.05256600
H	-2.03982300	-4.46785900	0.34229000
C	-5.09385000	-1.97812000	-0.60297100
H	-5.12030500	-2.79718200	-1.32418300
H	-5.66417000	-2.25779700	0.28634300
H	-5.53017800	-1.10065000	-1.07774400

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C	3.25087300	-2.34989600	0.57109900
C	2.99705800	-1.04899100	0.14764900
H	4.26038500	-2.66874000	0.81624300
N	0.67509200	-1.51717900	-0.02326400
C	-2.91220800	-2.98950300	0.12322400
O	-3.54963000	-2.16497500	0.79487300
Pd	-1.19935400	-0.80475400	-0.36672400
C	-1.22996300	2.07341000	0.09845900

C	-2.75376000	1.95554100	0.01071100
C	-3.06805100	0.73965200	-0.88280100
H	-3.01178900	-0.23078100	-0.30378400
H	-4.13686800	0.70734100	-1.11772300
N	-0.59819300	3.19387600	0.44318500
O	-0.49128700	1.07662400	-0.16263200
C	-3.31471000	1.69467300	1.42135400
H	-3.11750700	2.52746400	2.10322900
H	-4.39979700	1.55892500	1.35323000
H	-2.88673200	0.78022900	1.85100700
C	-3.41398100	3.17847300	-0.64706800
H	-3.43858800	4.05419000	0.00258700
H	-2.91355400	3.44656000	-1.58455500
H	-4.45453600	2.92931800	-0.88057200
H	-2.53295500	0.74912600	-1.83815200
C	0.90113700	-2.78077500	0.37433400
H	0.03806300	-3.43197300	0.44946700
C	-3.30794400	-4.43879500	0.05517800
H	-2.89680200	-4.92750900	-0.83155600
H	-2.91300900	-4.94324700	0.94571800
H	-4.39767000	-4.52869300	0.07061100
O	-1.83584000	-2.68674000	-0.54645700
C	1.70434000	-0.65965200	-0.14441500
H	1.47666700	0.35020400	-0.46295800
S	4.32733100	0.13875000	-0.05748600
O	5.14963100	-0.00387500	1.16220600
O	5.03073900	-0.29007900	-1.28634900
O	3.65227200	1.44603000	-0.18375300
C	2.17863800	-3.22603000	0.68037900
H	2.31997200	-4.25044300	1.00725500
O	0.78117100	3.10837100	0.45713100
C	1.34259400	3.60237100	-0.76652500
H	1.01695300	2.98799400	-1.61324700
H	1.06541200	4.65057300	-0.92408300
H	2.42165900	3.51806300	-0.62979900
C	-1.10494700	4.49014800	0.87938700
H	-0.29154600	4.95708200	1.43797700
H	-1.37478500	5.12793000	0.03474900
H	-1.94919000	4.37158100	1.55801900

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C	2.91456600	-1.16601000	0.02601700
C	3.20806900	-2.48367600	-0.30248400
C	2.14862900	-3.34008600	-0.58887000
H	4.23620500	-2.83461300	-0.32819100
H	2.32065600	-4.38105600	-0.83990600
N	0.59165500	-1.57025400	-0.25310100
C	-2.98526400	-2.76961500	0.63855600
O	-3.43321600	-1.81505200	1.28930300
Pd	-1.28347300	-0.79521500	-0.37283900
C	-1.09550600	2.08337800	-0.11222300
C	-2.62651000	2.10458200	-0.13678700
C	-3.10168600	0.87505200	-0.93559600
H	-3.07383100	-0.07316300	-0.32264400
H	-4.18351500	0.93053300	-1.09531200
N	-0.34599900	3.10404100	0.30042500
O	-0.46325600	1.04297200	-0.46447300
C	-3.14793100	1.97916100	1.30717700
H	-2.88556000	2.84565500	1.92156700
H	-4.24065400	1.90190500	1.28246200
H	-2.75699100	1.07613800	1.79114000
C	-3.18890300	3.35331200	-0.83685900
H	-3.08466800	4.26046500	-0.23986700
H	-2.70963400	3.51590000	-1.80920600
H	-4.26020400	3.20519500	-1.00926800
H	-2.63566800	0.78333700	-1.92111300
C	1.60014500	-0.73807000	0.05031800
H	1.34182400	0.28026400	0.31310000
O	5.34846600	-0.69050600	0.84117000
O	4.40770200	0.70225500	-0.97618400
O	3.58137300	0.98502200	1.32532900
S	4.18301200	0.06373300	0.33938900
C	-3.53668200	-4.16330300	0.75841900
H	-2.73269600	-4.90439900	0.72480900
H	-4.10517400	-4.26250100	1.68621600
H	-4.20710700	-4.35507000	-0.08793400
O	-2.01774100	-2.64265800	-0.22595700
C	0.85087600	-2.85393900	-0.56076100
H	-0.00293300	-3.48518900	-0.78375900
O	1.00366600	2.82963200	0.42557800
C	1.74024900	3.13986900	-0.76523300

H	1.40939700	2.51061000	-1.59793700
H	1.63368800	4.20139500	-1.01505800
H	2.78020600	2.91903300	-0.51631700
C	-0.70571100	4.47094000	0.66005800
H	0.14768300	4.87724600	1.20445900
H	-0.89514200	5.08041400	-0.22637100
H	-1.56592200	4.48865700	1.32972300

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C	-3.03050000	-2.55459400	0.23370300
C	-3.31291300	-1.20395800	0.09227900
H	-3.82967600	-3.27834300	0.36481000
N	-1.00246100	-0.68850400	-0.10195800
C	-0.70059700	3.18934300	0.16893800
O	0.27112200	3.40031800	0.90850800
Pd	0.51533900	0.67419600	-0.30623400
C	3.13118100	-0.53225300	0.08444800
C	3.67415200	0.89607600	0.00160100
C	2.65072400	1.74972600	-0.76912700
H	1.77783200	2.06070900	-0.11457000
H	3.05197100	2.75386900	-0.94194700
N	3.89520800	-1.57952800	0.39213800
O	1.90640700	-0.78172900	-0.12729000
C	3.80618400	1.45908900	1.42860300
H	4.49908200	0.87983400	2.04629300
H	4.18106800	2.48694000	1.37016800
H	2.83190800	1.48322200	1.93087600
C	5.00023100	0.98201600	-0.77443000
H	5.85616400	0.61441300	-0.20734700
H	4.94275100	0.43331400	-1.72166100
H	5.20085700	2.03327200	-1.00624800
H	2.39745800	1.34519100	-1.75536700
C	-0.70907400	-1.99861600	0.02937200
H	0.33975300	-2.27110500	0.00408100
C	-1.82222600	4.17804000	0.00399600
H	-2.55123800	4.01043500	0.80624600
H	-1.44033100	5.19832700	0.09561600
H	-2.33085100	4.04432700	-0.95409000
O	-0.86102400	2.08927100	-0.51182700
C	-2.28310200	-0.29123400	-0.07920600

H	-2.47156600	0.77072400	-0.20662600
S	-4.99150600	-0.56967400	0.09158600
O	-5.85722300	-1.74190200	0.32472100
O	-5.01783200	0.42904700	1.18109000
O	-5.15211700	0.03506700	-1.24756500
C	-1.69662700	-2.95163300	0.19566200
H	-1.41697100	-3.99467600	0.29690800
O	3.23111000	-2.78708600	0.45784000
C	3.29281500	-3.49728500	-0.78490800
H	2.84831000	-2.90367300	-1.59074500
H	4.32784900	-3.76365000	-1.02568500
H	2.70420300	-4.40021300	-0.61214200
C	5.30899400	-1.67517600	0.73556400
H	5.41503400	-2.57943000	1.33712800
H	5.93391300	-1.75505100	-0.15699600
H	5.62275500	-0.83155700	1.34864400

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C	2.96115700	-1.23203800	0.08223500
C	3.22474300	-2.58570000	-0.07946000
C	2.14615700	-3.43975100	-0.30265600
H	4.24061200	-2.96715900	-0.02866100
H	2.29637100	-4.50594300	-0.43374700
N	0.62730300	-1.60172800	-0.21349700
C	-3.25101500	-2.48508500	0.50314400
O	-3.84883000	-1.37869100	0.67954600
Pd	-1.25566100	-0.73212800	-0.41144300
C	-1.02632000	2.05555500	-0.14763200
C	-2.55085300	1.95295800	-0.11255700
C	-2.90673300	0.62640900	-0.82594200
H	-3.17337600	-0.47847100	0.01052600
H	-4.00276100	0.55338200	-0.87430500
N	-0.30944500	3.09582100	0.26941300
O	-0.36219900	1.06638500	-0.58181100
C	-3.01466300	1.87739700	1.35364500
H	-2.81378800	2.80143200	1.90489900
H	-4.09555900	1.69720500	1.37689400
H	-2.52578200	1.04697100	1.87794400
C	-3.24185700	3.09795200	-0.87315700
H	-3.21910100	4.05293500	-0.34264900

H	-2.79293900	3.24140600	-1.86263800
H	-4.29670800	2.83809800	-1.01436500
H	-2.60292600	0.62977000	-1.88109000
C	1.65655000	-0.77631100	0.02345600
H	1.42226100	0.27008500	0.17345200
O	5.43790500	-0.70768800	0.73727100
O	4.37049300	0.62282900	-1.06292300
O	3.68120400	0.96466600	1.27055800
S	4.23429200	0.01611800	0.28075600
C	-3.90123600	-3.75630600	0.93726700
H	-4.62945800	-4.05194800	0.17310100
H	-3.15925900	-4.55030300	1.04532900
H	-4.43893900	-3.59660000	1.87570100
O	-2.11001000	-2.54202300	-0.05783200
C	0.86383200	-2.91640700	-0.37236300
H	-0.00034600	-3.54663700	-0.56070000
O	1.05204800	2.87030100	0.39739100
C	1.77841600	3.07767000	-0.82250600
H	1.54343800	2.29401300	-1.55066500
H	1.56255800	4.06958400	-1.23350900
H	2.82879900	3.01520700	-0.53034300
C	-0.69849500	4.33838400	0.91094500
H	-0.43595000	4.29372100	1.97171300
H	-0.15932200	5.16072700	0.43341000
H	-1.76411600	4.51926300	0.80847900

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C	-3.18659600	-2.51685800	-0.11501300
C	-3.38732300	-1.15185200	0.03605200
H	-4.02094000	-3.21038100	-0.06724100
N	-1.06220900	-0.72935600	-0.24465300
C	-0.37201500	3.21774700	-0.02586600
O	0.81831600	3.34613600	0.39455100
Pd	0.54922500	0.59102500	-0.41388800
C	3.05905500	-0.61195900	0.16988100
C	3.48686800	0.85157200	0.12682800
C	2.45107900	1.57070400	-0.76321000
H	1.46933900	2.29634300	-0.07858000
H	2.78298600	2.60922000	-0.90861600
N	3.85865500	-1.61483300	0.52361000

O	1.86356100	-0.91722000	-0.12600200
C	3.40921500	1.42039000	1.55697900
H	4.14994200	0.96267200	2.22056400
H	3.60254800	2.49876500	1.52035400
H	2.41330800	1.26901900	1.98994400
C	4.87845600	1.07381900	-0.48742900
H	5.69511100	0.78895100	0.17884400
H	4.98859800	0.53501100	-1.43530800
H	4.99739200	2.14277200	-0.69587300
H	2.42725200	1.16741100	-1.78455600
C	-0.85281300	-2.05344800	-0.37773600
H	0.17306200	-2.37107900	-0.53010300
C	-1.33852300	4.35113700	0.07013400
H	-2.32362200	3.97662500	0.36160600
H	-0.98292200	5.09829600	0.78221300
H	-1.43297200	4.81387900	-0.91931300
O	-0.77277500	2.13179300	-0.55887300
C	-2.30849500	-0.28191700	-0.03632700
H	-2.43204600	0.79071300	0.07274800
S	-5.01266800	-0.44462100	0.31355200
O	-5.92516900	-1.59465400	0.47044600
O	-4.86000800	0.36911500	1.54001500
O	-5.27985300	0.37283600	-0.89001500
C	-1.88714100	-2.97118600	-0.32423500
H	-1.67407400	-4.02791300	-0.44453200
O	3.25678100	-2.85636000	0.55176000
C	3.40341700	-3.54744800	-0.69427200
H	2.95586200	-2.97176200	-1.51136800
H	4.46003000	-3.75171600	-0.89995200
H	2.86330700	-4.48555800	-0.55367100
C	5.25310500	-1.62549200	0.94663900
H	5.39296000	-2.55310200	1.50447800
H	5.93749300	-1.60957300	0.09516800
H	5.46402800	-0.79690700	1.62290800

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C	3.21965700	-2.25817600	-0.84053600
C	3.41671400	-1.03606900	-0.21188500
H	4.05988800	-2.91332100	-1.05167700
N	1.08670400	-0.56983700	-0.28766200

C	0.10881700	3.33592500	-0.30134900
O	-1.15336800	3.39711300	-0.41548200
Pd	-0.53337000	0.63901600	0.20707400
C	-3.00562100	-0.74603500	0.03991500
C	-3.51641500	0.68672700	0.16594100
C	-2.41228500	1.45702200	0.92216700
H	-1.61502400	2.29034800	0.13678700
H	-2.80134500	2.45543200	1.16699200
N	-3.77999000	-1.79762700	-0.21596300
O	-1.76395200	-0.97251800	0.17514100
C	-3.67234300	1.27970700	-1.24813500
H	-4.49415100	0.81405900	-1.80174300
H	-3.87985700	2.35312500	-1.16273400
H	-2.74879500	1.16425100	-1.82762800
C	-4.82075100	0.80799600	0.97022000
H	-5.69989800	0.45629900	0.42710000
H	-4.75329000	0.26609200	1.92069900
H	-4.99015400	1.86614200	1.19839000
H	-2.19603500	1.02007100	1.90583000
C	0.88150800	-1.74944600	-0.90419700
H	-0.14618600	-1.99171500	-1.15663200
C	0.94281400	4.54658700	-0.56162700
H	0.41970200	5.22920100	-1.23485900
H	1.10953200	5.05727900	0.39465900
H	1.91417100	4.26187000	-0.97256400
O	0.69211600	2.26391600	0.06358800
C	2.33277800	-0.21144600	0.05316900
H	2.45102200	0.74866400	0.54749700
S	5.04350300	-0.48314500	0.30016400
O	5.99238700	-1.43273900	-0.31365800
O	5.15198100	0.89688500	-0.21931300
O	5.01468900	-0.53970500	1.77880800
C	1.92170700	-2.61553500	-1.19406100
H	1.71442000	-3.55638600	-1.69256100
O	-3.12409700	-3.00988700	-0.31540800
C	-2.96550000	-3.63810500	0.96360000
H	-2.32892100	-3.03113200	1.61581500
H	-3.94128500	-3.81504300	1.42845100
H	-2.47747600	-4.58963300	0.74461300
C	-5.21240100	-1.89080300	-0.47561300
H	-5.35701500	-2.80528700	-1.05328600

H	-5.78596300	-1.95449300	0.45229800
H	-5.55147400	-1.05259800	-1.08314100

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C	3.31808100	-2.38164400	0.56450100
C	3.07182300	-1.07598000	0.15119800
H	4.32401500	-2.70745200	0.81544400
N	0.74389600	-1.53076200	-0.04502000
C	-3.07555200	-2.78177100	0.01255200
O	-3.75936800	-1.77023700	0.36319200
Pd	-1.16333400	-0.75989400	-0.37253700
C	-1.21224400	2.04477700	0.09642600
C	-2.70961200	1.75334900	0.10520700
C	-2.89267200	0.49541300	-0.77676000
H	-3.11744300	-0.71742300	-0.10305100
H	-3.97077200	0.33891400	-0.92316900
N	-0.65800300	3.21935700	0.38243900
O	-0.41257800	1.09927400	-0.17690400
C	-3.11850800	1.42888800	1.55572600
H	-3.06837000	2.31345200	2.19972900
H	-4.14982900	1.05599700	1.55974500
H	-2.47722400	0.64840500	1.98209100
C	-3.58355100	2.87720600	-0.47256600
H	-3.66502200	3.74274300	0.18819900
H	-3.21855700	3.21163600	-1.45025300
H	-4.59754200	2.48621800	-0.61120200
H	-2.51614900	0.64670200	-1.79711300
C	0.96623900	-2.79559100	0.34839000
H	0.09638800	-3.44076300	0.42391300
C	-3.62679000	-4.15628500	0.20091600
H	-3.23595900	-4.83815000	-0.55757300
H	-3.30640400	-4.51906800	1.18544400
H	-4.71842900	-4.13824300	0.17898600
O	-1.90519500	-2.65482300	-0.47543200
C	1.78147800	-0.68351700	-0.14912400
H	1.56378900	0.33071100	-0.46044300
S	4.39393600	0.12397700	-0.01963500
O	5.21222300	-0.04161500	1.20069500
O	5.11277300	-0.25897900	-1.25573300
O	3.70911900	1.42992100	-0.11717000

C	2.23958800	-3.25354100	0.65851800
H	2.37545300	-4.28111300	0.97832100
O	0.72374800	3.23265100	0.37073700
C	1.23979400	3.59796400	-0.91606100
H	0.91996600	2.87837700	-1.67723100
H	0.92086900	4.61193200	-1.18292700
H	2.32499400	3.56371800	-0.80057600
C	-1.25914500	4.47801300	0.80237900
H	-0.47019000	5.03361200	1.31315200
H	-1.61974200	5.05623300	-0.05139700
H	-2.06407500	4.30168500	1.51595800

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C	3.01171400	-1.21587300	0.10385700
C	3.26853800	-2.58048400	0.08778600
C	2.18212900	-3.44565100	-0.02992000
H	4.28358700	-2.95941800	0.17056400
H	2.32423800	-4.52097600	-0.04318400
N	0.67084300	-1.59965200	-0.12374200
C	-3.23907700	-2.59209300	0.29460100
O	-3.85960300	-1.51272600	0.54419400
Pd	-1.22208100	-0.74194600	-0.35746400
C	-1.06788000	2.06178300	-0.00074200
C	-2.58420800	1.90362700	0.00796400
C	-2.88275000	0.60594400	-0.78223300
H	-3.16685400	-0.54978800	-0.02110200
H	-3.97431500	0.51809900	-0.87999000
N	-0.40545600	3.16867100	0.32303000
O	-0.35499300	1.06609700	-0.32637800
C	-3.06317500	1.72742300	1.46142200
H	-2.88575200	2.62159700	2.06753000
H	-4.14112800	1.52867700	1.45559900
H	-2.56471700	0.87677500	1.94144500
C	-3.30600000	3.07129700	-0.68359500
H	-3.32325700	3.98296700	-0.08164200
H	-2.85035200	3.29908200	-1.65415000
H	-4.34849300	2.78434900	-0.86010300
H	-2.53835400	0.66496500	-1.82316300
C	1.71016300	-0.76169100	-0.00028100
H	1.48813400	0.29750500	0.02420100

O	5.47711300	-0.64797300	0.74217300
O	4.46269400	0.49719000	-1.20682900
O	3.73121400	1.09272400	1.06341900
S	4.29153100	0.03800000	0.19130600
C	-3.88903900	-3.91022200	0.55800000
H	-3.13647100	-4.66021100	0.81265800
H	-4.63343700	-3.82185700	1.35215300
H	-4.39671300	-4.22868300	-0.36078900
O	-2.07061900	-2.58625500	-0.21341900
C	0.90081500	-2.92518500	-0.13632100
H	0.03164400	-3.56834300	-0.23237200
O	0.97126800	3.04025000	0.34716900
C	1.57132900	3.27101000	-0.93443400
H	1.17008200	2.57702500	-1.68084200
H	1.41994500	4.31039500	-1.24587900
H	2.63406000	3.07125900	-0.77592300
C	-0.88279600	4.49453700	0.68994700
H	-0.06406000	4.97349400	1.23017600
H	-1.13340800	5.08937900	-0.19185300
H	-1.73604700	4.43108400	1.36513700

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C	-3.16903200	-2.49300500	0.32332300
C	-3.39019600	-1.13721900	0.12694900
H	-4.0006200	-3.17178800	0.49078900
N	-1.05620600	-0.73833500	-0.11544500
C	-0.38188000	3.19392200	0.04378300
O	0.80863000	3.32449100	0.46522800
Pd	0.55384000	0.57905000	-0.37425100
C	3.09300900	-0.61135300	0.11274300
C	3.49732100	0.85815500	0.11313600
C	2.44018400	1.58480000	-0.74675600
H	1.46567700	2.28832900	-0.03248600
H	2.76027500	2.62868400	-0.87721800
N	3.91698400	-1.62095700	0.38197400
O	1.88793500	-0.91757200	-0.13765600
C	3.41807000	1.36549000	1.56644600
H	4.17011100	0.88866300	2.20378600
H	3.59243100	2.44769600	1.57727100
H	2.42725400	1.17887400	1.99752600

C	4.88057800	1.13491800	-0.49643300
H	5.70656900	0.84549500	0.15599200
H	5.00164300	0.63528900	-1.46417300
H	4.97256900	2.21342200	-0.66570500
H	2.40312100	1.20300200	-1.77567900
C	-0.82913000	-2.05420200	0.06843200
H	0.20546500	-2.37914200	0.04361400
C	-1.36588500	4.30346100	0.20892800
H	-1.84544100	4.18888900	1.18881400
H	-0.85864400	5.27026800	0.18086800
H	-2.13810800	4.24700500	-0.56152600
O	-0.77357600	2.11381500	-0.50739800
C	-2.31781300	-0.28299100	-0.08777000
H	-2.45999500	0.78367200	-0.24107700
S	-5.04122200	-0.43851600	0.10835300
O	-5.95175900	-1.57634500	0.34388700
O	-5.04479600	0.56980500	1.19028700
O	-5.17303600	0.16241800	-1.23624800
C	-1.85619000	-2.95392200	0.29346800
H	-1.62630900	-4.00370300	0.44107200
O	3.33514800	-2.87419500	0.37927100
C	3.29515500	-3.44422200	-0.93558700
H	2.69166600	-2.82418300	-1.60756500
H	4.30861300	-3.57267500	-1.33065100
H	2.82022200	-4.41733400	-0.79661400
C	5.32450000	-1.63022100	0.75863200
H	5.49801100	-2.58478000	1.25826100
H	5.97719900	-1.55716900	-0.11432400
H	5.54470200	-0.83454600	1.47049200

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C	2.92189000	-1.35618500	0.09485200
C	3.16688100	-2.70879200	-0.10635800
C	2.07517200	-3.53934700	-0.35547000
H	4.17703900	-3.10720100	-0.06451400
H	2.21145900	-4.60373800	-0.51587500
N	0.57513600	-1.67947200	-0.21872300
C	-3.25024600	-2.63341400	0.51754000
O	-3.43768800	-1.88364600	1.59109900
Pd	-1.31988400	-0.58933500	-0.47925700

C	-0.94777600	2.16978400	-0.15829900
C	-2.46925000	2.06373100	-0.08152700
C	-2.82347000	0.70783700	-0.75625300
H	-2.87863400	-1.07885600	1.56822300
H	-3.79399500	0.35021000	-0.39094700
N	-0.21461100	3.22576600	0.20203700
O	-0.29952100	1.15435200	-0.54596500
C	-2.86247900	2.02344100	1.40632800
H	-2.63537600	2.96147000	1.92380000
H	-3.94121500	1.84878400	1.48804500
H	-2.34371600	1.21182000	1.93102000
C	-3.21493300	3.18618800	-0.82259700
H	-3.27737900	4.11978200	-0.25601400
H	-2.75390000	3.39446500	-1.79466600
H	-4.24477900	2.85545800	-1.00172700
H	-2.88969300	0.82677500	-1.84756200
C	1.62086600	-0.88618700	0.04856300
H	1.40612700	0.16090200	0.22684200
O	5.39387300	-0.86137700	0.80366800
O	4.38817100	0.47201400	-1.02738100
O	3.64767700	0.83821800	1.28656600
S	4.20806500	-0.12661100	0.31545100
C	-4.03271300	-3.89667700	0.51239600
H	-5.08481100	-3.67969900	0.72126300
H	-3.92869800	-4.39639000	-0.45145000
H	-3.66052600	-4.55052300	1.30909500
O	-2.48558200	-2.31578600	-0.40007300
C	0.80162300	-2.98828700	-0.41784600
H	-0.07128300	-3.59861200	-0.63727200
O	1.14258200	2.98040600	0.35113600
C	1.87617400	3.14011400	-0.86985200
H	1.59432700	2.36960500	-1.59453300
H	1.71513100	4.14091300	-1.28576500
H	2.92305900	3.01779300	-0.58288300
C	-0.59605200	4.48123400	0.81959600
H	-0.37645300	4.44635300	1.89102600
H	-0.02194900	5.28666100	0.35430500
H	-1.65299600	4.68103200	0.66613700

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C	-3.17161300	-2.59387800	0.35903800
C	-3.38794300	-1.23730600	0.14139200
H	-3.99908000	-3.26290100	0.57847400
N	-1.05271000	-0.86230500	-0.17632100
C	-0.86776400	3.09184200	-0.09548900
O	-0.32755800	3.25705100	1.10045200
Pd	0.65305500	0.50992200	-0.41873700
C	3.23480200	-0.49394400	0.15328200
C	3.43110600	1.00897200	0.27406100
C	2.30101900	1.62374900	-0.58625800
H	0.21513900	2.48713600	1.36477600
H	2.14304100	2.67239100	-0.30399200
N	4.19544500	-1.39837800	0.33562600
O	2.06915600	-0.92562500	-0.10017400
C	3.22746700	1.35819800	1.76112700
H	4.01972100	0.93280300	2.38740600
H	3.24748100	2.44731500	1.88309000
H	2.26349300	0.98603000	2.12872200
C	4.77365800	1.55436700	-0.23423000
H	5.59958800	1.40085100	0.46488900
H	5.04395400	1.11997500	-1.20311200
H	4.66791100	2.63629600	-0.37580400
H	2.56633700	1.58785100	-1.65342400
C	-0.83851700	-2.17248700	0.03063100
H	0.19453100	-2.50545300	-0.01354200
C	-1.80989100	4.17041400	-0.49187000
H	-1.41245700	5.14818400	-0.20750900
H	-2.00178200	4.12621900	-1.56470700
H	-2.75181600	4.01706600	0.04853800
O	-0.63697800	2.11228600	-0.81260900
C	-2.31233800	-0.40384800	-0.12526500
H	-2.45771700	0.65759400	-0.29994900
S	-5.04343600	-0.55374400	0.16147300
O	-5.77458200	-1.33138900	1.18405100
O	-4.86518100	0.87174700	0.51108200
O	-5.56695100	-0.75785300	-1.20838300
C	-1.86566500	-3.06652200	0.29913900
H	-1.64074400	-4.11494000	0.46466300
O	3.79514400	-2.71352500	0.21284000
C	3.96619500	-3.19571200	-1.12507600
H	3.36716000	-2.60363100	-1.82527000

H	5.02452500	-3.17944000	-1.40815300
H	3.60157300	-4.22439000	-1.09406800
C	5.58784400	-1.23413000	0.73099700
H	5.90655500	-2.19957000	1.12942600
H	6.22437700	-0.96322600	-0.11468400
H	5.67894500	-0.49770200	1.53046800

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C	3.24521200	-2.41269300	-0.83660200
C	3.42298400	-1.18047500	-0.22207400
H	4.09511800	-3.06066200	-1.03182600
N	1.08294200	-0.73263000	-0.31902000
C	0.76946600	3.18794200	-0.15673100
O	-0.01930300	3.49235600	-1.17364500
Pd	-0.63718100	0.53469000	0.18205900
C	-3.23307900	-0.57503400	-0.01084600
C	-3.52064900	0.91826000	0.02346800
C	-2.28039800	1.54423300	0.70448500
H	-0.65455200	2.77418500	-1.36468500
H	-2.23232900	2.61749300	0.48135300
N	-4.16419800	-1.52487900	-0.08661200
O	-2.02137300	-0.95068900	-0.00701900
C	-3.61954500	1.37962700	-1.44352400
H	-4.49368500	0.94838000	-1.94482600
H	-3.72094200	2.47060700	-1.47155000
H	-2.72412300	1.09851100	-2.01092800
C	-4.76799200	1.34674900	0.80996500
H	-5.70377800	1.18410900	0.26919300
H	-4.82811300	0.84169300	1.78036600
H	-4.69152900	2.42337900	1.00273500
H	-2.34138000	1.42231200	1.79635900
C	0.90357000	-1.92254000	-0.92005500
H	-0.11935500	-2.17766000	-1.18309600
C	1.77109500	4.23621100	0.16818800
H	2.24406100	4.59650900	-0.74987500
H	1.25344500	5.08227100	0.63543700
H	2.51656800	3.84047300	0.85912600
O	0.67472500	2.13494000	0.48110200
C	2.32389000	-0.36859200	0.02689800
H	2.42841400	0.59315000	0.52283500

S	5.03790700	-0.60183800	0.29234800
O	5.99935900	-1.58649500	-0.24332100
O	5.16986400	0.74810100	-0.30045100
O	4.97953400	-0.57435100	1.77214400
C	1.95203600	-2.78725600	-1.19265200
H	1.75792800	-3.73862300	-1.67689400
O	-3.67991400	-2.81551200	-0.16165400
C	-3.51921800	-3.39644400	1.13802600
H	-2.83676800	-2.79581800	1.74887600
H	-4.49055300	-3.50322100	1.63384700
H	-3.08429700	-4.38008600	0.95016500
C	-5.61281000	-1.42324900	-0.19854800
H	-5.95445200	-2.37098200	-0.61897400
H	-6.08752000	-1.26859200	0.77342000
H	-5.89003900	-0.62846300	-0.89114500

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C	3.37863700	-2.50115100	0.23792100
C	3.10218200	-1.14392000	0.09816400
H	4.39672200	-2.85592900	0.37545100
N	0.76425900	-1.58735600	-0.10285600
C	-3.05220100	-2.96134200	0.15930900
O	-3.48502500	-2.34565900	1.24654100
Pd	-1.21448600	-0.65365800	-0.38956400
C	-1.20259400	2.14054800	0.02743400
C	-2.68831400	1.81389500	0.08145500
C	-2.83867900	0.47911900	-0.69546000
H	-3.02074700	-1.49740500	1.39516900
H	-3.78156400	-0.00833500	-0.41593800
N	-0.66638400	3.33663700	0.26486600
O	-0.39620500	1.18970400	-0.19500000
C	-3.03422500	1.59966100	1.56925600
H	-2.94338900	2.52848500	2.14355800
H	-4.06959600	1.25023300	1.65212900
H	-2.37706000	0.84966000	2.02507300
C	-3.61969600	2.86265100	-0.54329700
H	-3.76844100	3.74032700	0.09116700
H	-3.25594300	3.19359700	-1.52271100
H	-4.60294100	2.40110800	-0.69283700
H	-2.85014300	0.66112600	-1.78025700

C	1.02337000	-2.89632100	0.02701900
H	0.16867800	-3.56607600	-0.00363300
C	-3.68191300	-4.28770800	-0.06926700
H	-3.31063000	-4.72586000	-0.99633500
H	-3.44947200	-4.94213300	0.77806400
H	-4.76982000	-4.17074200	-0.11118100
O	-2.19904700	-2.48504000	-0.59585500
C	1.79504100	-0.72652700	-0.06913700
H	1.56228300	0.32661900	-0.17779900
S	4.39852700	0.09065100	0.13335800
O	5.07584700	-0.09384600	1.43585600
O	5.27350600	-0.23179300	-1.01642800
O	3.69752000	1.38614900	0.00118400
C	2.31177900	-3.39147300	0.19698000
H	2.47025000	-4.45981500	0.30010700
O	0.71531300	3.36015400	0.31796100
C	1.29833300	3.64720200	-0.95928300
H	1.03159100	2.87350700	-1.68687400
H	0.98267500	4.63524700	-1.31312800
H	2.37554000	3.63881600	-0.77971200
C	-1.30813000	4.60765300	0.57397400
H	-0.54039200	5.24138500	1.02106900
H	-1.69738600	5.09360600	-0.32388900
H	-2.10222000	4.47441200	1.31020000

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C	3.17917900	-0.69234300	-0.23987100
C	3.66505000	-1.99281400	-0.24725600
C	2.74570600	-3.03917800	-0.28935500
H	4.73290500	-2.18697900	-0.20716500
H	3.07188800	-4.07352200	-0.29500500
N	0.94268500	-1.48160600	-0.30172300
C	-2.90071600	-2.62036200	0.48408900
O	-3.08064300	-1.37733300	0.26619400
Pd	-1.04679400	-1.16519900	-0.12608800
C	-1.39226300	1.80566900	-0.20154400
C	-2.73871600	2.15746800	-0.84844400
C	-2.99000800	1.17444200	-2.00527800
H	-3.06596600	0.13644800	-1.66570800
H	-3.94106100	1.43787100	-2.48133700

N	-0.84853900	2.54514800	0.76869600
O	-0.72426200	0.80793300	-0.60390100
C	-3.87845500	2.00860400	0.17647500
H	-3.77229700	2.66867300	1.04228300
H	-4.82792800	2.25541900	-0.31227000
H	-3.94479400	0.97722600	0.54162800
C	-2.68455900	3.57643500	-1.45127300
H	-2.72179800	4.37435500	-0.70729100
H	-1.77785100	3.70932200	-2.05359700
H	-3.54891400	3.71029600	-2.11074400
H	-2.20355400	1.23466300	-2.76517600
C	1.81305800	-0.46359000	-0.27853700
H	1.39333900	0.53644600	-0.28199700
O	5.57746700	0.22940800	0.22123100
O	4.20199100	1.34139700	-1.51174600
O	3.61889900	1.60538100	0.86946700
S	4.24778100	0.74785800	-0.15805700
C	-4.00951400	-3.54484500	0.82054600
H	-4.95930300	-3.00543600	0.82205500
H	-4.03881200	-4.35517600	0.08444800
H	-3.82865500	-3.99013300	1.80483300
O	-1.68636500	-3.03529900	0.38594800
C	1.39258100	-2.75151300	-0.30539100
H	0.64085000	-3.53531200	-0.31370700
O	0.42507900	2.17744000	1.16127200
C	0.40234100	1.30586800	2.29777300
H	-0.08282700	1.79306300	3.15059600
H	-0.10782100	0.36584100	2.05732900
H	1.45451900	1.12103900	2.52256100
C	-1.21906100	3.83493600	1.32952100
H	-0.95040100	3.82751200	2.38844400
H	-0.66874900	4.63400400	0.82432600
H	-2.28881600	4.00892800	1.25920100

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C	3.09433900	-0.85816600	-0.06849800
C	3.40218800	-2.09386800	-0.62341100
C	2.36289500	-2.99137900	-0.85358900
H	4.42747200	-2.34274300	-0.88264700
H	2.54730900	-3.96541800	-1.29354200

N	0.78806100	-1.42095600	-0.00603500
C	-2.36216500	-3.26886800	0.05078000
O	-2.47179900	-3.02182100	-1.15921000
Pd	-1.08329600	-0.72409000	0.18978300
C	-1.30674000	2.06058100	-0.13532900
C	-0.77057300	3.48491100	-0.26481900
C	0.42817500	3.43203500	-1.23188900
H	0.12581500	3.07602800	-2.22372300
H	0.82910200	4.44521200	-1.34131100
N	-2.55460800	1.76861500	0.24846800
O	-0.49315900	1.12225600	-0.37169800
C	-1.80180300	4.48017600	-0.81689600
H	-2.57496300	4.74971700	-0.09499400
H	-1.27951100	5.40529800	-1.08325900
H	-2.28382600	4.09901400	-1.72451600
C	-0.26955900	3.90816700	1.13066700
H	-1.07591600	3.94926400	1.87058500
H	0.49904200	3.21694800	1.49459400
H	0.17455600	4.90702200	1.05726200
H	1.23406300	2.78864300	-0.86611900
C	1.78028700	-0.55147800	0.23914600
H	1.50487900	0.40137700	0.67722200
O	5.53557600	-0.04933500	-0.48771100
O	3.73295600	1.64384800	-0.29712700
O	4.49753200	0.43160300	1.70787800
S	4.33419600	0.40367200	0.23821500
C	-2.88278800	-4.54624500	0.65311400
H	-3.70210200	-4.93967900	0.04585000
H	-2.07043400	-5.28353100	0.66038100
H	-3.21295200	-4.39491000	1.68442300
O	-1.75917000	-2.47699700	0.88907100
C	1.06463000	-2.62431500	-0.54184800
H	0.22614300	-3.27984400	-0.74819200
O	-2.88948200	0.39967500	0.22110200
C	-3.80031400	0.11151900	-0.87796900
H	-4.70421400	0.71196400	-0.75627500
H	-3.29850500	0.31725000	-1.82619900
H	-4.03019300	-0.94833400	-0.77113500
C	-3.61484800	2.58860500	0.82288900
H	-4.23750400	3.04538700	0.05158900
H	-4.22028200	1.92351100	1.44304500

H	-3.18963200	3.34974300	1.47593700
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C	-3.62090600	0.15377200	-0.11690300
C	-4.17936100	1.42084900	-0.00103300
C	-3.32391700	2.51056500	0.12728400
H	-5.25791100	1.55112800	-0.01911000
H	-3.70961400	3.52012300	0.21873200
N	-1.43148700	1.06631800	0.02371600
C	1.80230000	3.26449400	0.08123200
O	2.37341900	2.88610200	1.10928000
Pd	0.56540100	0.70225600	0.04309200
C	2.73538900	-1.08744800	-0.10339600
C	4.17118600	-1.54534200	-0.34917700
C	4.97620400	-0.30674600	-0.77397300
H	4.96086800	0.47462600	-0.00909900
H	6.01727600	-0.60266200	-0.94121200
N	1.71461000	-1.94203800	0.05664100
O	2.52683000	0.15318500	0.00386800
C	4.70321100	-2.07284400	0.99789300
H	4.16187700	-2.96310900	1.33566900
H	5.75808400	-2.34501900	0.88102500
H	4.63213500	-1.30606600	1.77787400
C	4.29685500	-2.61829800	-1.44427500
H	3.99987300	-3.61289100	-1.10417200
H	3.71791700	-2.35752800	-2.33780900
H	5.35012800	-2.68387700	-1.73677400
H	4.58553100	0.12071600	-1.70473400
C	-2.24425100	0.00495300	-0.10439700
H	-1.77492900	-0.96893800	-0.21595300
O	-5.97345700	-0.83511700	-0.63559000
O	-3.97236500	-2.16069400	-1.25030000
O	-4.59965000	-1.91005400	1.12108100
S	-4.63893400	-1.31907300	-0.23418700
C	2.11519200	4.57625600	-0.58856100
H	2.76162200	5.18372900	0.04938900
H	2.62503500	4.37843100	-1.53880800
H	1.19374600	5.12217400	-0.81437200
O	0.88401900	2.57500000	-0.54133100
C	-1.95495900	2.30093400	0.13881700

H	-1.25222300	3.12063400	0.23409900
O	0.52254000	-1.36199600	0.53478400
C	0.37735500	-1.60085700	1.96758400
H	0.36946200	-2.67715500	2.14877900
H	1.19309300	-1.10659700	2.50015600
H	-0.58983300	-1.16593200	2.22155900
C	1.60560600	-3.38335500	-0.14503400
H	0.57226200	-3.65676400	0.07336500
H	1.79727600	-3.63178600	-1.18887400
H	2.27086700	-3.93482000	0.52184600

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C	3.49008100	-0.94150100	0.11995500
C	3.31373900	-2.30123300	-0.10135900
C	2.03213400	-2.76617700	-0.38170500
H	4.15806900	-2.98286300	-0.06203200
H	1.84390800	-3.81738800	-0.57067400
N	1.16827400	-0.55392400	-0.19363400
C	-0.53775000	3.14326300	-0.69572200
O	-1.56953400	2.44856600	-0.40786800
Pd	-0.36944200	0.76064900	-0.24345400
C	-2.86851700	-0.85157200	0.36978200
C	-3.58768800	-0.09248000	1.49303000
C	-2.52687200	0.55970300	2.39582200
H	-1.97345900	1.35420100	1.88463200
H	-3.03318800	1.01764600	3.25243400
N	-3.52250200	-1.63524600	-0.49700300
O	-1.61385100	-0.80558000	0.23642100
C	-4.47929100	1.01509500	0.90183800
H	-5.29470400	0.62558500	0.28483700
H	-4.93042900	1.58150600	1.72446300
H	-3.89054600	1.71130900	0.29354500
C	-4.40104000	-1.07005600	2.36722700
H	-5.31445000	-1.43018200	1.89061100
H	-3.79703200	-1.93843200	2.65720300
H	-4.70331200	-0.55113700	3.28326700
H	-1.80881300	-0.17462500	2.77710200
C	2.39875800	-0.08733300	0.06680700
H	2.49589600	0.98170300	0.23696600
O	6.01843300	-1.38061900	0.58955300

O	5.38706100	0.59720100	-0.76048900
O	4.93565300	0.57153000	1.66435500
S	5.10839600	-0.22942900	0.43326700
C	-0.60291300	4.59737300	-0.97853000
H	-1.58463000	4.99432100	-0.71174900
H	0.18297100	5.11755000	-0.42230300
H	-0.42113600	4.75727000	-2.04779300
O	0.57571200	2.49918700	-0.73842700
C	0.98147000	-1.86741900	-0.42274100
H	-0.03104800	-2.18530100	-0.64416400
O	-2.71950200	-2.34966000	-1.36741500
C	-2.51492700	-1.64298100	-2.59509000
H	-3.46903000	-1.47171300	-3.10600300
H	-2.00138600	-0.69201700	-2.41709400
H	-1.88469800	-2.30132000	-3.19601200
C	-4.89589000	-2.11431000	-0.53964200
H	-5.13940000	-2.29953100	-1.58811900
H	-4.98998900	-3.04907400	0.02057700
H	-5.59351600	-1.36950500	-0.16569000

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C	3.23057100	-0.50806200	0.50054700
C	3.22575400	-1.51383500	1.45838800
C	2.07309800	-1.70396400	2.21633800
H	4.10370500	-2.13504900	1.60916900
H	2.02395800	-2.47337800	2.97910400
N	0.99579800	0.06750300	1.04992200
C	-1.01938800	3.29260200	-0.42403700
O	-1.99352200	2.47659700	-0.29800100
Pd	-0.65582500	1.06332700	0.48317400
C	-2.49068400	-1.23589000	0.06820800
C	-3.98123100	-0.87323800	0.03309800
C	-4.25515100	0.07634500	1.21199100
H	-3.65338000	0.98985400	1.16468400
H	-5.31096900	0.36806800	1.18547300
N	-1.95197000	-2.15605800	-0.73577400
O	-1.73289200	-0.64468500	0.89189200
C	-4.27093300	-0.11998300	-1.28035600
H	-4.10495000	-0.73332200	-2.17137700
H	-5.32070400	0.19513300	-1.28459600

H	-3.64844900	0.77914800	-1.36144600
C	-4.89436600	-2.10388700	0.19409500
H	-4.96740600	-2.71620200	-0.70712900
H	-4.56391600	-2.74251800	1.02181000
H	-5.90752000	-1.75753700	0.42600300
H	-4.06139500	-0.41055600	2.17453600
C	2.10220400	0.27708800	0.32411400
H	2.06098700	1.07750400	-0.41061500
O	5.69862600	-1.10741700	-0.09639900
O	4.10329900	-0.64670300	-1.93178200
O	4.91206700	1.20536900	-0.51632000
S	4.61792300	-0.24065700	-0.60484100
C	-1.17630700	4.64566300	-1.00938700
H	-2.02882900	5.15303000	-0.54751800
H	-0.26061400	5.22418700	-0.86811300
H	-1.38185900	4.54364300	-2.08138600
O	0.12629100	2.86455300	-0.02664900
C	0.96826100	-0.90562200	1.97834700
H	0.03970900	-1.03086600	2.52394400
O	-0.60578500	-2.39561000	-0.53372700
C	0.19780400	-1.79410400	-1.55749400
H	0.00987600	-2.25875800	-2.53146700
H	0.00860800	-0.71667400	-1.61066700
H	1.23017600	-1.99082000	-1.25917700
C	-2.57799400	-3.14097900	-1.60991900
H	-1.84057800	-3.43790300	-2.35685100
H	-2.87874600	-4.02406300	-1.03941800
H	-3.42783900	-2.71520600	-2.13823300

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C	-3.28454500	0.40335000	0.06629000
C	-3.82725200	1.50732600	0.71030600
C	-2.96388900	2.50545800	1.15407400
H	-4.89998100	1.58682300	0.86072200
H	-3.33723600	3.38775500	1.66215800
N	-1.09696500	1.28595800	0.31390200
C	2.57294200	2.95477700	-0.30030000
O	2.90373800	1.72519300	-0.32837300
Pd	0.89620000	1.21162600	-0.00368700
C	1.58652400	-1.74563200	0.06803500

C	2.42741300	-1.98311000	-1.19436100
C	1.89285800	-1.07085100	-2.31073800
H	2.05912800	-0.01018700	-2.10087500
H	2.42700400	-1.30611700	-3.23756500
N	1.68614900	-2.52260800	1.15340700
O	0.72268300	-0.82821100	0.12790800
C	3.90083300	-1.62469500	-0.92686100
H	4.36914300	-2.27005100	-0.17708700
H	4.46562900	-1.73802900	-1.85930800
H	4.00083700	-0.58460400	-0.59501400
C	2.27118800	-3.43862900	-1.68170400
H	2.81127900	-4.16678900	-1.07423800
H	1.21476500	-3.73108400	-1.71490200
H	2.67224600	-3.51320900	-2.69817900
H	0.82292000	-1.22797700	-2.48513400
C	-1.91363500	0.31390100	-0.11633800
H	-1.45202100	-0.53633700	-0.60634400
O	-5.65379100	-0.68181900	-0.03671100
O	-4.24809500	-0.70876400	-2.07015400
O	-3.66689200	-2.15953900	-0.16110000
S	-4.31100100	-0.90593600	-0.60531000
C	3.54349600	4.06176600	-0.47307100
H	4.50223600	3.67391300	-0.82479400
H	3.14133600	4.79351700	-1.18094500
H	3.68403100	4.56407600	0.49116600
O	1.32330600	3.19366000	-0.10225300
C	-1.60502400	2.36884400	0.93334100
H	-0.89630600	3.12710900	1.25169900
O	0.74187300	-2.28652000	2.13312400
C	1.20436900	-1.35332700	3.11301200
H	2.13724300	-1.70069900	3.57069300
H	1.33910900	-0.36111600	2.66875700
H	0.40994100	-1.32922500	3.86155200
C	2.42038200	-3.75065700	1.41603700
H	2.63993200	-3.77146400	2.48584600
H	1.81235200	-4.62278600	1.15859200
H	3.36638900	-3.76991300	0.88074700

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C	-3.60932200	1.67338700	-0.90609700
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C	-3.14827500	0.55639200	-0.21917800
H	-4.67308500	1.81498300	-1.07776200
N	-0.90496800	1.28389400	-0.47020700
C	2.10542300	3.48166200	0.65556500
O	2.70147100	2.86333200	1.54740400
Pd	1.06872700	0.94282900	-0.17004800
C	1.67755100	-1.91659900	-0.19809400
C	3.13794000	-1.51351400	0.03163100
C	3.26475600	0.00706700	-0.17373600
H	2.77278600	0.58602200	0.66082700
H	4.29797700	0.32979000	-0.01168400
N	1.29465800	-3.19021400	-0.30861500
O	0.75187600	-1.05204000	-0.25830500
C	3.52047900	-1.83896000	1.48671300
H	3.52562500	-2.91402700	1.68708700
H	4.52810600	-1.45643100	1.68201300
H	2.82903000	-1.36095500	2.19013700
C	4.09699600	-2.17183300	-0.97636000
H	4.29423400	-3.22234800	-0.75897000
H	3.71332200	-2.08806700	-1.99963500
H	5.05857700	-1.64966500	-0.93366300
H	3.02799000	0.31497600	-1.20290900
C	-1.33082700	2.37876100	-1.12604800
H	-0.56922900	3.07892100	-1.45246600
C	2.27111500	4.96587400	0.46922300
H	1.42707400	5.39880300	-0.07371500
H	2.38668000	5.44891800	1.44366100
H	3.18636800	5.14113200	-0.10927900
O	1.31711400	2.91855200	-0.21482300
C	-1.78967700	0.37808700	-0.02547800
H	-1.39579500	-0.49183400	0.48745000
S	-4.28511600	-0.63233700	0.49701300
O	-5.51581100	-0.51160500	-0.30821600
O	-3.60184500	-1.93588500	0.37720600
O	-4.45200000	-0.19185600	1.90014900
C	-2.67702200	2.59544400	-1.36964800
H	-2.98364700	3.48156800	-1.91473500
O	-0.02772900	-3.37688800	-0.65856000
C	-0.86292400	-3.62834400	0.47869200
H	-0.54175000	-4.53669200	1.00087600
H	-0.85866000	-2.77482300	1.16351000

H	-1.85889300	-3.76998800	0.05651900
C	2.07363400	-4.41963800	-0.37120900
H	1.40270400	-5.23756900	-0.10337200
H	2.45492600	-4.58881700	-1.38150600
H	2.88457000	-4.40799000	0.35470000

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C	-3.00240800	-2.38528800	-0.59711900
C	-3.19909000	-1.08707800	-0.14725600
H	-3.80609700	-3.11492300	-0.55602400
N	-0.95603400	-0.51793600	-0.67360700
C	-0.53119400	3.20336000	0.29111700
O	0.39104800	3.18586300	1.11894200
Pd	0.60824700	0.77705600	-0.59747300
C	3.03129800	-0.69003400	-0.03774400
C	3.70140500	0.67586400	0.12812400
C	2.90167100	1.69605700	-0.70374500
H	1.96014200	2.03072100	-0.17329300
H	3.41849400	2.66120800	-0.71017800
N	3.59084700	-1.83133600	0.35954100
O	1.88003300	-0.79315100	-0.55878400
C	3.63507800	1.09450900	1.60803300
H	4.23434300	0.44489800	2.25269600
H	4.02210300	2.11455600	1.70793800
H	2.59972200	1.08680800	1.97002200
C	5.14226600	0.68469900	-0.41316100
H	5.84359300	0.14355100	0.22362200
H	5.19054100	0.26395800	-1.42392900
H	5.49069200	1.72163300	-0.46343500
H	2.76761000	1.40226800	-1.74989100
C	-0.74733800	-1.77231000	-1.12238700
H	0.24140400	-2.00015800	-1.50266000
C	-1.58396800	4.27665300	0.28597100
H	-2.01874800	4.40704200	-0.70837000
H	-2.38495900	3.97513600	0.97220200
H	-1.16102700	5.21819200	0.64561800
O	-0.69411800	2.28350400	-0.61985100
C	-2.16157900	-0.16839800	-0.20332100
H	-2.28241200	0.85645200	0.12969100
S	-4.77400700	-0.52242200	0.50342400

O	-5.60631300	-1.73530900	0.62542700
O	-4.44044800	0.10971200	1.79797800
O	-5.26580100	0.44509200	-0.50004400
C	-1.74984600	-2.72471200	-1.10200100
H	-1.54403600	-3.72150200	-1.47671800
O	2.87876300	-2.97202100	0.04782200
C	1.92791500	-3.30675500	1.06689000
H	2.43437400	-3.49120800	2.02080900
H	1.18040300	-2.51425800	1.17749900
H	1.45741300	-4.22340700	0.70664900
C	4.89309500	-2.12005600	0.94337300
H	4.78199500	-3.03922300	1.52157800
H	5.64365900	-2.27907500	0.16443700
H	5.20270300	-1.33218800	1.62659400

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C	3.11681200	-2.28511600	-0.72897300
C	3.33553100	-1.07633400	-0.08115700
H	3.94286500	-2.95835600	-0.93892300
N	1.02697100	-0.54780200	-0.20337100
C	0.44774500	3.19647200	-0.78557300
O	-0.63747700	3.23801200	-1.38409900
Pd	-0.50954800	0.71714300	0.17050300
C	-3.06363100	-0.66435100	0.32887800
C	-3.67265700	0.73340700	0.47941300
C	-2.57026400	1.69996400	0.95182600
H	-1.88527600	2.00469200	0.09954300
H	-2.99631900	2.68972000	1.14539500
N	-3.80554900	-1.76494400	0.19211000
O	-1.80732700	-0.83339600	0.27972300
C	-4.15796000	1.19575800	-0.90785600
H	-4.95899600	0.56287500	-1.30121600
H	-4.54376200	2.21800200	-0.82650900
H	-3.33076900	1.20056900	-1.62822900
C	-4.79741500	0.79483000	1.52741400
H	-5.73138200	0.35350300	1.17864000
H	-4.50284300	0.30618600	2.46270000
H	-5.00661800	1.84655600	1.74924900
H	-2.08584700	1.39178800	1.88590000
C	0.79370400	-1.71756900	-0.82751600

H	-0.23367500	-1.92801100	-1.09939400
C	1.45587100	4.30820500	-0.88674900
H	1.31932800	4.84511000	-1.82895600
H	1.28924300	5.00851700	-0.05919900
H	2.47765400	3.92732500	-0.80871700
O	0.79661000	2.21559800	-0.00165600
C	2.27322600	-0.22208700	0.17006300
H	2.40888900	0.73619100	0.66112800
S	4.96762700	-0.58422400	0.47764400
O	5.90582700	-1.45418700	-0.25840600
O	5.06589700	0.84764100	0.12710500
O	4.95529200	-0.82473300	1.93700400
C	1.81691000	-2.60567100	-1.10739000
H	1.59273000	-3.53452200	-1.62049200
O	-3.08604000	-2.94104900	0.10782900
C	-2.85381600	-3.31569200	-1.25569700
H	-3.79112400	-3.60362100	-1.74503300
H	-2.37752900	-2.49786900	-1.80601900
H	-2.18368300	-4.17533700	-1.19674400
C	-5.24438800	-1.98192000	0.28132100
H	-5.45277000	-2.92629700	-0.22367600
H	-5.56543800	-2.06070900	1.32293000
H	-5.79772200	-1.20055000	-0.23701500

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C	3.22246400	-2.26770200	0.58503100
C	2.96659100	-1.02782400	0.00700900
H	4.23310100	-2.55466000	0.86387300
N	0.64365800	-1.50758800	-0.08609000
C	-2.95530500	-2.87517100	0.33338200
O	-3.48841800	-1.97077800	0.99275500
Pd	-1.23128300	-0.80300500	-0.42179200
C	-1.17289200	2.09768200	-0.11077100
C	-2.70040100	2.04657200	-0.19600600
C	-3.07224400	0.80791400	-1.03398900
H	-3.03682500	-0.14072200	-0.42280000
H	-4.14359300	0.81238100	-1.25916300
N	-0.48531700	3.18231700	0.24151100
O	-0.47961000	1.06739800	-0.36084200
C	-3.26785700	1.87620400	1.22570500

H	-3.06508600	2.74929200	1.85384700
H	-4.35396300	1.74690100	1.16243200
H	-2.85017400	0.98695900	1.71352000
C	-3.30656900	3.27013000	-0.90287700
H	-3.27867000	4.17505300	-0.29440800
H	-2.80665100	3.47095100	-1.85719000
H	-4.36124500	3.06216800	-1.11263000
H	-2.54135800	0.75403400	-1.98970800
C	0.86982600	-2.71377700	0.46118400
H	0.00469100	-3.34670700	0.62235200
C	-3.44288800	-4.29797600	0.35170400
H	-4.40895800	-4.36421800	0.85684000
H	-3.52422400	-4.68812400	-0.66762900
H	-2.71562900	-4.91858400	0.88836600
O	-1.91068100	-2.67839400	-0.42355200
C	1.67419300	-0.67805200	-0.32892800
H	1.45487300	0.27672500	-0.79073000
S	4.28243500	0.15858100	-0.27323900
O	4.89980400	0.33953000	1.05828600
O	5.18597000	-0.48219100	-1.25262500
O	3.60221600	1.36696600	-0.77842800
C	2.15050100	-3.12403100	0.80276800
H	2.29318300	-4.10252900	1.24828800
O	0.89098800	3.05521300	0.18408600
C	1.42632600	2.56365700	1.42231100
H	1.13637700	3.21993800	2.25038500
H	1.09139400	1.53820600	1.60918200
H	2.50914800	2.58639900	1.28633900
C	-0.92529200	4.52635900	0.59488800
H	-0.09915700	4.99260200	1.13407800
H	-1.13995000	5.11992300	-0.29720100
H	-1.78649100	4.49595900	1.26236600

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C	3.12743900	-0.84974300	-0.02107600
C	3.49040100	-2.17742800	0.15983900
C	2.48194000	-3.13446900	0.19383100
H	4.53584900	-2.45189600	0.27179800
H	2.70586800	-4.18643700	0.33373000
N	0.82895000	-1.44143200	-0.11386300

C	-2.64223500	-3.11772800	0.41752500
O	-3.23415900	-2.30239700	1.13993900
Pd	-1.12294000	-0.86740400	-0.31073200
C	-1.44314400	2.01945700	-0.13088500
C	-2.94611600	1.73643400	-0.21935200
C	-3.13159900	0.35436400	-0.87441400
H	-2.97006000	-0.48401100	-0.12900300
H	-4.19333900	0.16373400	-1.06335900
N	-0.94065000	3.23350100	0.08928200
O	-0.59379100	1.08149600	-0.23048400
C	-3.50714100	1.67581600	1.21474800
H	-3.40922900	2.63261200	1.73712400
H	-4.57154800	1.42023500	1.17093300
H	-2.99482500	0.90245800	1.80044900
C	-3.71129000	2.74515100	-1.09466000
H	-3.84833200	3.71736200	-0.62040100
H	-3.21879100	2.89043800	-2.06258600
H	-4.71243100	2.34397400	-1.28442700
H	-2.62945400	0.25655800	-1.84335600
C	1.79257200	-0.50709500	-0.16283100
H	1.48075400	0.51984500	-0.32200700
O	5.59778500	-0.16090700	0.39983600
O	4.40562100	0.85949900	-1.51520000
O	3.81486400	1.51664600	0.78692500
S	4.35245000	0.45823300	-0.09267400
C	-2.99509100	-4.57929700	0.40767300
H	-4.07136500	-4.70260900	0.55648400
H	-2.67836000	-5.06070200	-0.52089800
H	-2.47880300	-5.06536700	1.24477700
O	-1.65540600	-2.79094400	-0.36904000
C	1.16373000	-2.73514100	0.05892200
H	0.34939200	-3.44975800	0.08253600
O	0.43609500	3.32430500	0.03200600
C	1.04598900	3.12064500	1.31454600
H	0.65505600	3.83824300	2.04467500
H	0.88761600	2.09373600	1.66005700
H	2.10703900	3.30263300	1.13970800
C	-1.58331600	4.53363100	0.22904400
H	-0.91076600	5.15975400	0.81860600
H	-1.73504200	4.99957900	-0.74840300
H	-2.52220400	4.45480300	0.77275500

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C	3.68972100	-1.72697800	-0.81986200
C	3.20815500	-0.59827100	-0.16565500
H	4.75900900	-1.88664600	-0.93092800
N	0.96579900	-1.28485400	-0.55237400
C	-2.30770500	-3.17232800	0.69701900
O	-3.08155300	-2.26811900	1.14329900
Pd	-1.06263700	-0.89865300	-0.38445400
C	-1.66871300	1.87928900	-0.27432300
C	-3.03224800	1.30831000	0.10432300
C	-3.08185300	-0.12372600	-0.47051600
H	-2.83928200	-1.19439800	0.41317200
H	-4.08903400	-0.52270200	-0.28407400
N	-1.38408700	3.17955200	-0.29390900
O	-0.71899400	1.08624700	-0.55966300
C	-3.11354500	1.24812600	1.64132000
H	-3.13618300	2.24759500	2.08754800
H	-4.03129300	0.72362600	1.93151600
H	-2.26328900	0.69836100	2.06098200
C	-4.21933200	2.08496500	-0.49026800
H	-4.42183800	3.02814300	0.02044600
H	-4.06831200	2.28639200	-1.55692200
H	-5.12121200	1.47121800	-0.39088600
H	-3.00726400	-0.13046500	-1.56648900
C	1.41696300	-2.38666500	-1.17617400
H	0.66788700	-3.06972100	-1.56285300
C	-2.51078700	-4.58996600	1.11829700
H	-1.87486800	-5.26244700	0.54000100
H	-2.26928400	-4.68023800	2.18317100
H	-3.56422300	-4.85732500	0.99164500
O	-1.35846400	-2.89563500	-0.10478100
C	1.84182200	-0.40070200	-0.05254100
H	1.42864500	0.47175400	0.44279700
S	4.33418900	0.57363200	0.59395200
O	5.57708300	0.46532900	-0.19545800
O	3.66216800	1.88496700	0.48968200
O	4.48449200	0.10839700	1.99190600
C	2.77100800	-2.63585900	-1.33329700
H	3.09488800	-3.53006400	-1.85489200

O	-0.13361900	3.49277600	-0.78582100
C	0.83760200	3.62945100	0.25979400
H	0.60013800	4.48744300	0.89914900
H	0.89266300	2.71455000	0.85702300
H	1.78025200	3.80125600	-0.26228200
C	-2.21723600	4.34296200	-0.02242800
H	-1.54368300	5.17302200	0.19701300
H	-2.82355000	4.60579000	-0.89299100
H	-2.83991900	4.17851200	0.85605000

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C	-3.18895000	-2.34257100	-0.53430200
C	-3.32363700	-1.02775000	-0.10802300
H	-4.03114400	-3.02738100	-0.49331400
N	-1.04411100	-0.58156200	-0.61715800
C	-0.15711400	3.25592500	0.18415200
O	1.04055500	3.25621900	0.60586000
Pd	0.61987600	0.66953700	-0.59646500
C	2.99375400	-0.76573800	-0.04229200
C	3.52629500	0.65668500	0.11368300
C	2.59954700	1.54857100	-0.74223200
H	1.63698700	2.25251100	-0.01075800
H	3.01113900	2.56801900	-0.74819000
N	3.65826100	-1.85721500	0.32820500
O	1.83327600	-0.94628800	-0.52292100
C	3.40621300	1.07395800	1.59250200
H	4.09318100	0.51857800	2.23867700
H	3.64206800	2.14067300	1.68341000
H	2.38529100	0.92595900	1.96383400
C	4.96508400	0.82453300	-0.40367300
H	5.71783000	0.39769200	0.26277100
H	5.08536000	0.38092800	-1.39883000
H	5.18110600	1.89559700	-0.48433000
H	2.60719500	1.26276000	-1.80250200
C	-0.90165300	-1.85322400	-1.03784700
H	0.07961900	-2.14082900	-1.40083100
C	-1.05834900	4.40035200	0.51149400
H	-1.86129600	4.48552500	-0.22342000
H	-1.50665900	4.21320300	1.49485100
H	-0.48233400	5.32716800	0.56869900

O	-0.62056700	2.28648900	-0.50073000
C	-2.23544300	-0.16829900	-0.16372400
H	-2.30065900	0.86423900	0.16483400
S	-4.88624400	-0.37790600	0.48840900
O	-5.76905100	-1.55240800	0.63540000
O	-4.56271500	0.28995200	1.76782300
O	-5.32223800	0.57040100	-0.55950100
C	-1.94855900	-2.75753900	-1.01077400
H	-1.78997200	-3.77184300	-1.36094000
O	3.02683000	-3.05474900	0.05507000
C	2.16481700	-3.45031500	1.13042700
H	2.73556200	-3.55986400	2.05926100
H	1.35285600	-2.72753100	1.26347300
H	1.76320600	-4.41660800	0.82003800
C	4.99932800	-2.02656100	0.86835000
H	5.00679700	-2.97305900	1.41183900
H	5.74281300	-2.06746600	0.06795600
H	5.24088300	-1.23413200	1.57451600

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C	3.26779100	-2.25921600	-0.72706100
C	3.43537100	-1.01528400	-0.13099100
H	4.12007200	-2.90764800	-0.90791900
N	1.09864500	-0.58916600	-0.26743600
C	0.09330600	3.25717900	-0.61323300
O	-1.17059000	3.28087400	-0.74343000
Pd	-0.52409800	0.63398000	0.16889800
C	-3.01466500	-0.74241000	0.32350300
C	-3.51369300	0.69789300	0.37500500
C	-2.34004100	1.53859800	0.91890200
H	-1.61390800	2.24539500	-0.04672700
H	-2.69321500	2.56928700	1.06660300
N	-3.81311000	-1.80655000	0.28733100
O	-1.76593000	-0.96371300	0.26601400
C	-3.82516100	1.13164900	-1.07128000
H	-4.69226300	0.59910200	-1.47602400
H	-4.04416400	2.20564500	-1.08367300
H	-2.96674500	0.95472200	-1.73038700
C	-4.72512400	0.92008800	1.29386100
H	-5.66263100	0.56268500	0.86381900

H	-4.57788800	0.44645300	2.27110700
H	-4.84266600	1.99664800	1.45833400
H	-2.03528900	1.22937600	1.92770500
C	0.92256400	-1.79330000	-0.83986900
H	-0.09598900	-2.06066100	-1.10009900
C	0.90237700	4.44742500	-1.01139000
H	0.47136800	4.91462800	-1.90033400
H	0.86583500	5.17718600	-0.19350900
H	1.94363400	4.17293700	-1.19037500
O	0.68993600	2.24458300	-0.12087300
C	2.33338500	-0.20112600	0.08393400
H	2.42694600	0.77838200	0.54217900
S	5.03955400	-0.44421700	0.43419800
O	6.02784700	-1.26109600	-0.29850700
O	5.07348300	0.99335900	0.09280000
O	5.03487100	-0.69162800	1.89324700
C	1.98220500	-2.64912700	-1.08953700
H	1.79855300	-3.60869900	-1.56079800
O	-3.16509800	-3.02493900	0.28463000
C	-2.94614700	-3.49871600	-1.04973600
H	-3.89979800	-3.67429100	-1.55993600
H	-2.33855700	-2.78810300	-1.61912300
H	-2.41054100	-4.44136500	-0.92403100
C	-5.26815500	-1.90231900	0.28636400
H	-5.51684300	-2.91349700	-0.03898700
H	-5.67596900	-1.75273200	1.28850700
H	-5.70322900	-1.19856300	-0.42394200

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C	3.28587600	-2.30376600	0.63071000
C	3.05020300	-1.06024500	0.05153600
H	4.28846900	-2.59713900	0.93161900
N	0.72345000	-1.52735700	-0.10966200
C	-3.11372200	-2.69007000	0.23770600
O	-3.74992600	-1.62954700	0.52470600
Pd	-1.18469500	-0.76566800	-0.45091600
C	-1.18492200	2.05714900	-0.12851800
C	-2.68552500	1.78822900	-0.06300300
C	-2.90836300	0.48936400	-0.87284600
H	-3.11808100	-0.65398200	-0.09115100

H	-3.99062400	0.32958700	-0.98388000
N	-0.61451000	3.23570900	0.10035400
O	-0.40397100	1.09234500	-0.38789800
C	-3.05469700	1.54471500	1.41433200
H	-2.95314100	2.45762100	2.01060900
H	-4.09637700	1.20823400	1.47365500
H	-2.42317200	0.76397800	1.85567600
C	-3.55913000	2.89588300	-0.67071500
H	-3.61801900	3.78970000	-0.04621100
H	-3.20978000	3.18433800	-1.66840900
H	-4.57964000	2.51084900	-0.77358200
H	-2.55802900	0.57742600	-1.90956600
C	0.93429900	-2.72864600	0.45255000
H	0.05953000	-3.35202300	0.60698800
C	-3.72660500	-4.02368900	0.51084400
H	-4.47852000	-3.94601300	1.29890600
H	-4.21737600	-4.36591700	-0.40856200
H	-2.95613800	-4.75126100	0.77758500
O	-1.96655300	-2.64745700	-0.31669800
C	1.76737300	-0.70655600	-0.31984600
H	1.56463400	0.25152800	-0.78601200
S	4.38169200	0.11259200	-0.19695600
O	5.01476800	0.24482100	1.13313000
O	5.27174600	-0.51350300	-1.19906300
O	3.72039400	1.34659100	-0.66661500
C	2.20297300	-3.15236900	0.82450400
H	2.32993300	-4.13114500	1.27458900
O	0.75769300	3.27514100	-0.06513100
C	1.44601600	2.97101400	1.15688700
H	1.11952900	3.64375100	1.95817800
H	1.28292400	1.92670500	1.44218700
H	2.50005300	3.14130400	0.93298200
C	-1.20322800	4.51621400	0.46942100
H	-0.40058900	5.12057700	0.89487300
H	-1.60441000	5.03385000	-0.40512600
H	-1.97134100	4.38836300	1.23240900

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C	3.18202900	-0.90813300	-0.01667300
C	3.52722500	-2.24740400	0.10440100

C	2.50624400	-3.19262900	0.07782400
H	4.56646400	-2.54226000	0.21985300
H	2.71833600	-4.25264800	0.16766400
N	0.87294700	-1.46515900	-0.17188000
C	-2.86114000	-2.89319400	0.42175200
O	-3.59163200	-1.88903600	0.68436600
Pd	-1.11207100	-0.82938500	-0.35729500
C	-1.39742700	1.99655500	-0.16180100
C	-2.87350900	1.61243300	-0.19825000
C	-2.94503100	0.21317500	-0.84580100
H	-3.04038400	-0.87644800	0.04490400
H	-4.00503400	-0.06526600	-0.92900300
N	-0.94732100	3.22507200	0.08069200
O	-0.51657800	1.09981000	-0.33506800
C	-3.39648100	1.52362600	1.24800200
H	-3.42724100	2.50252900	1.73718100
H	-4.41411100	1.11642700	1.23322300
H	-2.77261600	0.85377300	1.85163200
C	-3.72828500	2.56223000	-1.05597000
H	-3.92827900	3.52245300	-0.57681000
H	-3.25971500	2.74668500	-2.02945600
H	-4.69912100	2.08752400	-1.23584500
H	-2.60581400	0.22219500	-1.89047000
C	1.85212700	-0.54753800	-0.16340400
H	1.55568900	0.48945500	-0.28748000
O	5.64217900	-0.23661600	0.50496400
O	4.52051800	0.82228100	-1.43033100
O	3.85046800	1.44153200	0.85963200
S	4.41370600	0.39359600	-0.01766400
C	-3.29613300	-4.26839500	0.80526400
H	-4.37091400	-4.29316100	0.99557200
H	-3.02529300	-4.97801400	0.01894500
H	-2.76388900	-4.55539300	1.72005000
O	-1.73353000	-2.76106200	-0.15720200
C	1.19460700	-2.76782900	-0.05760300
H	0.37206200	-3.47482800	-0.07894500
O	0.42247600	3.38297900	-0.01191200
C	1.06621700	3.15729200	1.25084900
H	0.67136900	3.84410300	2.00814800
H	0.93841000	2.11774800	1.57051600
H	2.12057100	3.36742400	1.06444400

C	-1.64866000	4.48863100	0.24586100
H	-1.01278500	5.13156900	0.85800300
H	-1.81383700	4.96752500	-0.72343700
H	-2.58917200	4.35138200	0.77549800

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C	3.67364500	-1.92583900	-0.66190400
C	3.22260900	-0.72420100	-0.12444400
H	4.73653600	-2.13486000	-0.74466400
N	0.95248400	-1.37106000	-0.47365100
C	-2.36200300	-3.37831100	0.51819600
O	-2.60112000	-2.85398800	1.70738600
Pd	-1.15487100	-0.77359600	-0.36936500
C	-1.61198100	2.01250600	-0.25511100
C	-2.94183500	1.45117500	0.22442200
C	-2.99655300	0.00353300	-0.32999300
H	-2.24756900	-1.94510500	1.78038700
H	-3.71053300	-0.59258400	0.25353700
N	-1.33828900	3.30767600	-0.40476400
O	-0.66692500	1.19281900	-0.46939500
C	-2.86079600	1.43686200	1.76394700
H	-2.80254900	2.45260700	2.17218200
H	-3.75878100	0.95719000	2.16957900
H	-1.98327800	0.87827800	2.11068600
C	-4.20128700	2.19373700	-0.24315200
H	-4.38277400	3.12876700	0.29293000
H	-4.16989900	2.40048400	-1.31879100
H	-5.06404900	1.54338100	-0.05696000
H	-3.32701000	0.00849500	-1.37919500
C	1.38041200	-2.53370200	-0.98928300
H	0.61233200	-3.22322600	-1.32902900
C	-2.83273300	-4.77987100	0.37333900
H	-2.59197900	-5.15589100	-0.62164500
H	-2.35996800	-5.39850600	1.14363000
H	-3.91525100	-4.81307700	0.53733900
O	-1.80699800	-2.75830200	-0.39349500
C	1.86079600	-0.48097500	-0.04868200
H	1.47737300	0.44876200	0.35920200
S	4.36561100	0.49634500	0.52365500
O	5.58586800	0.36259800	-0.29965700

O	3.67900900	1.79749400	0.37719700
O	4.57270500	0.10753800	1.93779900
C	2.72824200	-2.84650400	-1.10154300
H	3.02924100	-3.79484900	-1.53425500
O	-0.08397400	3.58801600	-0.90568900
C	0.88824300	3.76439100	0.13363100
H	0.68657100	4.68321200	0.69646800
H	0.90000200	2.90229700	0.80674800
H	1.84110100	3.84740000	-0.39241100
C	-2.17168300	4.47929800	-0.17279700
H	-1.50205600	5.34016700	-0.13416700
H	-2.88363400	4.62797200	-0.98837700
H	-2.68787800	4.40469000	0.78509400

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C	-3.17126700	-2.52252800	-0.35520900
C	-3.35077900	-1.17165600	-0.09028900
H	-4.00717400	-3.21344500	-0.28800400
N	-1.04714000	-0.72176000	-0.50842600
C	-0.67569000	3.19713700	0.16970100
O	0.07372400	3.32112100	1.25304200
Pd	0.70428000	0.61183900	-0.57266200
C	3.18912400	-0.62361200	-0.09358400
C	3.51717000	0.85085500	0.10175800
C	2.43283900	1.61317900	-0.69873300
H	0.71406800	2.58620900	1.34122000
H	2.38140800	2.65481900	-0.35915200
N	4.01771500	-1.62733200	0.19362100
O	2.02573600	-0.93677200	-0.49025800
C	3.36801600	1.15883100	1.60467900
H	4.11759600	0.63759700	2.20942100
H	3.50094900	2.23490400	1.76422500
H	2.37452800	0.87424000	1.97256400
C	4.90157600	1.27789800	-0.41194500
H	5.71931500	1.00885100	0.26218300
H	5.10772500	0.85674100	-1.40229400
H	4.90803900	2.36991200	-0.50906500
H	2.67041700	1.61236700	-1.77307400
C	-0.86497400	-2.03149700	-0.76012200
H	0.14399600	-2.33540400	-1.02297400

C	-1.70110300	4.25979700	0.00888000
H	-2.29265000	4.06662100	-0.88707500
H	-2.34500200	4.27617300	0.89484200
H	-1.20657100	5.23427000	-0.06514700
O	-0.55045500	2.27330900	-0.63950300
C	-2.27472700	-0.29855900	-0.18443100
H	-2.39302900	0.76522600	0.00483300
S	-4.94107200	-0.51225600	0.39593400
O	-5.82582200	-1.68685200	0.53315600
O	-4.68452400	0.19060700	1.67334000
O	-5.33152600	0.41044200	-0.69296000
C	-1.89495800	-2.95685700	-0.70420500
H	-1.69648300	-4.00085000	-0.92307100
O	3.50944000	-2.89527200	-0.02163800
C	2.71630700	-3.33544100	1.08934800
H	3.32917600	-3.39830800	1.99565300
H	1.86255500	-2.66739400	1.24769900
H	2.36701700	-4.32937900	0.80302200
C	5.40939700	-1.62019700	0.62299800
H	5.61059000	-2.60492000	1.04792700
H	6.08361600	-1.45202400	-0.22069600
H	5.57797800	-0.87784500	1.40360300

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C	-3.24141000	-2.40332200	0.73319500
C	-3.42542400	-1.15999100	0.14082300
H	-4.08740600	-3.05450700	0.93400900
N	-1.08347000	-0.71438600	0.22756700
C	-0.70917600	3.18155500	0.49973600
O	0.04409700	3.26857600	1.58233200
Pd	0.63049800	0.58416200	-0.20818400
C	3.20190800	-0.59211600	-0.29254800
C	3.53018300	0.88916700	-0.19560100
C	2.26297000	1.62241700	-0.69540500
H	0.65056000	2.50446700	1.66429300
H	2.25352500	2.65290500	-0.31851300
N	4.11153500	-1.56162000	-0.37612700
O	1.98425600	-0.94171300	-0.21324900
C	3.75750000	1.16645100	1.30364400
H	4.64289400	0.64111500	1.67954500

H	3.91276300	2.24103900	1.45335900
H	2.89090400	0.85547000	1.89990900
C	4.72719500	1.37974700	-1.02234000
H	5.69477000	1.13858400	-0.57523700
H	4.69920300	0.98705800	-2.04492200
H	4.66567800	2.47255000	-1.08692700
H	2.24836200	1.65667900	-1.79510100
C	-0.89808400	-1.91956600	0.79298000
H	0.12735500	-2.18547200	1.03315700
C	-1.64198600	4.32185200	0.29993000
H	-1.79293000	4.86802300	1.23307300
H	-1.20340800	4.99875200	-0.44304000
H	-2.59221900	3.95251700	-0.09356700
O	-0.63127800	2.24648800	-0.30340800
C	-2.32868900	-0.34236600	-0.09680700
H	-2.44101600	0.63470000	-0.55952700
S	-5.03952000	-0.59511200	-0.39100700
O	-6.01546700	-1.41814600	0.35265400
O	-5.07551600	0.84166100	-0.04088100
O	-5.06071800	-0.83301900	-1.85205300
C	-1.94526900	-2.78662700	1.06516600
H	-1.74727200	-3.74661100	1.53043200
O	3.59981800	-2.84125400	-0.45898200
C	3.43879400	-3.42897800	0.83739100
H	4.41236100	-3.56985000	1.32087300
H	2.78850200	-2.81136000	1.46552200
H	2.97187900	-4.39743800	0.64778000
C	5.56642700	-1.48600200	-0.42290100
H	5.93898100	-2.50043700	-0.27274400
H	5.91675800	-1.13340400	-1.39546100
H	5.95155700	-0.85645100	0.38068900

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C	3.56759400	-2.20867600	0.02773800
C	3.20205700	-0.86674600	-0.03865900
H	4.60743300	-2.49744300	0.15768900
N	0.90479500	-1.45272700	-0.29351300
C	-2.57551900	-3.24301100	0.36553400
O	-2.84500000	-2.69707500	1.53952200
Pd	-1.16223500	-0.72598400	-0.42525900

C	-1.50707000	2.07142600	-0.18277900
C	-2.91062900	1.54861200	0.08531800
C	-2.95374800	0.14496700	-0.57255900
H	-2.43647200	-1.81228800	1.63044300
H	-3.76847200	-0.44498500	-0.13475500
N	-1.15688200	3.35635500	-0.16532100
O	-0.58457600	1.22233100	-0.37811600
C	-3.03947300	1.42310100	1.61611900
H	-3.01410700	2.40274800	2.10647400
H	-3.99403000	0.94401500	1.86168000
H	-2.22855200	0.81228300	2.03126500
C	-4.05784100	2.38687100	-0.49615200
H	-4.28353100	3.28541300	0.08362000
H	-3.85504900	2.67563200	-1.53362200
H	-4.96438100	1.76972300	-0.49651500
H	-3.13460800	0.23406200	-1.65405200
C	1.24816100	-2.74691900	-0.21938200
H	0.43839500	-3.46833600	-0.28662500
C	-3.15671300	-4.59905500	0.18611300
H	-2.90175800	-5.22701300	1.04554100
H	-4.24851000	-4.50721600	0.15048600
H	-2.79529500	-5.04634900	-0.74040100
O	-1.91387700	-2.67442100	-0.50920500
C	1.87251700	-0.52471300	-0.21084600
H	1.56685400	0.51399500	-0.28745900
S	4.43262200	0.41897300	0.14672100
O	4.93983500	0.25826600	1.52918100
O	5.45794700	0.12791000	-0.87891500
O	3.70599000	1.68732400	-0.06743300
C	2.56495000	-3.16517100	-0.06793600
H	2.79231600	-4.22508500	-0.02128100
O	0.15945400	3.62025300	-0.49292800
C	1.01396300	3.59967000	0.65895300
H	0.71439800	4.37706000	1.37133900
H	0.99616200	2.61660400	1.13817200
H	2.01073300	3.80945100	0.26629400
C	-1.95889100	4.54798600	0.07655900
H	-1.26309100	5.35025200	0.32768700
H	-2.51735500	4.83769500	-0.81733300
H	-2.62995200	4.39936000	0.92261400

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C	-3.29720300	-0.59639500	0.10136400
C	-3.84746500	-1.81075400	-0.28329800
C	-2.99294200	-2.89913900	-0.44365000
H	-4.91587900	-1.90347500	-0.45650800
H	-3.37081600	-3.87295200	-0.73533000
N	-1.11720100	-1.53273900	0.11115200
C	2.72551400	-2.88402400	-0.34963800
O	2.94572500	-1.65808600	-0.07547400
Pd	0.90534100	-1.33670600	0.12094100
C	1.46317000	1.57994300	0.15803100
C	2.79186800	1.86906400	0.86017600
C	2.91329800	0.93240300	2.07147800
H	2.92171600	-0.12405000	1.78480100
H	3.85906700	1.14334500	2.58324500
N	1.04020300	2.26540200	-0.89795100
O	0.67573300	0.66439800	0.56763800
C	3.96064700	1.60486200	-0.10762600
H	3.93019600	2.26414800	-0.98022800
H	4.90433300	1.78641200	0.42036400
H	3.96414400	0.56433900	-0.45180600
C	2.83218200	3.32318100	1.37206300
H	2.97004900	4.04769300	0.56714600
H	1.92264900	3.57972100	1.92795600
H	3.68156900	3.42721200	2.05674300
H	2.09962600	1.09128400	2.78797800
C	-1.93152400	-0.48773700	0.30794300
H	-1.46731700	0.43882300	0.62735500
O	-5.64960700	0.50047300	-0.10380000
O	-4.15534200	1.25533900	1.71873800
O	-3.64448300	1.86933000	-0.61472400
S	-4.28267100	0.88915400	0.29211400
C	3.81272900	-3.84160800	-0.66231700
H	4.72399200	-3.56768000	-0.12455200
H	3.50324800	-4.85848400	-0.40713500
H	4.01729500	-3.79882200	-1.73899500
O	1.49029200	-3.23856600	-0.36023800
C	-1.63419000	-2.72424100	-0.25076100
H	-0.93137000	-3.53945600	-0.39320300
O	1.80687100	3.29079400	-1.39584800

C	1.13890300	4.55811700	-1.30790100
H	0.28705100	4.60135000	-1.99393300
H	0.81403700	4.75423800	-0.28150000
H	1.89377700	5.28408500	-1.61401400
C	-0.20572300	1.98069800	-1.60301100
H	-0.10958900	2.37176400	-2.61747300
H	-0.35359500	0.90123700	-1.65885800
H	-1.05724100	2.44697100	-1.09902200

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C	3.49894000	-0.83263800	0.39809400
C	3.39484100	-1.84311300	1.34512900
C	2.17625200	-2.02150900	1.99478500
H	4.24897900	-2.47451000	1.57246000
H	2.04808300	-2.79380200	2.74545700
N	1.23758000	-0.21554400	0.76267500
C	-0.49823400	3.27325700	-0.47774600
O	-1.53546300	2.54061700	-0.35657900
Pd	-0.31879700	0.96120200	0.26422800
C	-2.66881400	-0.84562500	0.06829200
C	-3.88789400	-0.16665100	0.69019400
C	-3.41773300	0.63623400	1.91169400
H	-2.72282800	1.43780500	1.63849800
H	-4.29002600	1.09900200	2.38634700
N	-2.73906400	-1.62802500	-1.00142400
O	-1.49984000	-0.70119500	0.55140600
C	-4.52401300	0.78773800	-0.33830700
H	-4.91343100	0.25143800	-1.20861700
H	-5.35889400	1.31556000	0.13750200
H	-3.80323500	1.53784500	-0.68302500
C	-4.91350500	-1.21485100	1.16445000
H	-5.43754300	-1.69121400	0.33318300
H	-4.43925000	-1.99038900	1.77774800
H	-5.66598300	-0.71237300	1.78274600
H	-2.92823400	-0.00717800	2.65175600
C	2.40497100	-0.02319000	0.13220600
H	2.43979100	0.78318200	-0.59603000
O	6.01868000	-1.42804000	0.07692400
O	4.65441300	-0.90349200	-1.92145800
O	5.28236800	0.89897500	-0.36485200

S	5.00637100	-0.54306600	-0.53112600
C	-0.54665200	4.67249400	-0.96661700
H	-1.57046800	5.05198800	-0.94294200
H	0.10943100	5.30074300	-0.35671500
H	-0.17441700	4.69519500	-1.99771000
O	0.61945600	2.71517000	-0.17129300
C	1.11371500	-1.19347500	1.67915200
H	0.14344900	-1.29865200	2.15318400
O	-3.95496900	-1.90232100	-1.57641000
C	-4.29446000	-3.29220400	-1.47275100
H	-3.60532100	-3.91007700	-2.05798300
H	-4.30112800	-3.61316200	-0.42655300
H	-5.29729700	-3.35832100	-1.89838300
C	-1.55412000	-2.14014900	-1.68085900
H	-1.85733600	-2.46482100	-2.67740300
H	-0.81569400	-1.34092900	-1.77853200
H	-1.11247700	-2.97418900	-1.12841800

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C	3.60243400	-1.04441900	0.00712300
C	3.39524500	-2.40971900	-0.13770400
C	2.09242600	-2.86633400	-0.31809200
H	4.23074100	-3.10290300	-0.10836600
H	1.87899400	-3.92279300	-0.43909000
N	1.27236100	-0.63172300	-0.20327000
C	-0.35629100	3.14418400	-0.48658700
O	-1.40164800	2.42911400	-0.32544700
Pd	-0.23454700	0.72769700	-0.23120400
C	-2.83221400	-0.68652100	0.15241500
C	-3.40091700	-0.15384600	1.46949400
C	-2.23432500	0.09103800	2.43718000
H	-1.56684600	0.88670500	2.08848200
H	-2.63882700	0.40127800	3.40662700
N	-3.59190000	-1.05794300	-0.87211100
O	-1.58106300	-0.81781300	-0.04268400
C	-4.14440000	1.17151700	1.21568600
H	-5.00907200	1.03557600	0.55931200
H	-4.50479900	1.56288200	2.17438500
H	-3.48128000	1.92239100	0.77120200
C	-4.34705600	-1.18602100	2.11592500

H	-5.29515400	-1.27963800	1.58330300
H	-3.87811900	-2.17435600	2.18659900
H	-4.57456000	-0.85504000	3.13554800
H	-1.63541100	-0.81455500	2.58692800
C	2.52299200	-0.17531000	-0.03798300
H	2.64546300	0.90042100	0.06067400
O	6.14201600	-1.49437700	0.41483800
O	5.48939000	0.46702700	-0.95206400
O	5.09432900	0.47893300	1.48324500
S	5.23489800	-0.34056300	0.26012800
C	-0.42463900	4.61067200	-0.69257500
H	-1.42132600	4.98139900	-0.44346300
H	0.33438900	5.10945300	-0.08261500
H	-0.20903600	4.82678300	-1.74577300
O	0.76014600	2.50808000	-0.48333300
C	1.05368200	-1.95311600	-0.34133400
H	0.02363400	-2.26423900	-0.47570500
O	-4.95975900	-1.00537700	-0.77046300
C	-5.56191300	-2.30332900	-0.85782600
H	-5.43604900	-2.72916100	-1.85866200
H	-5.14856600	-2.97771500	-0.10102100
H	-6.62081600	-2.12082200	-0.66681900
C	-3.04066000	-1.47391500	-2.15620800
H	-3.79965400	-1.29324800	-2.91935200
H	-2.15765400	-0.87211600	-2.37964200
H	-2.76196400	-2.53167900	-2.14137800

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C	-3.16688200	-0.72053400	-0.03936100
C	-3.59399900	-1.67777700	-0.95021600
C	-2.65302500	-2.55843300	-1.47582200
H	-4.63696600	-1.73135000	-1.24792900
H	-2.93557300	-3.32429100	-2.18943600
N	-0.93355900	-1.49961100	-0.20925200
C	2.89839300	-2.88043600	0.02559800
O	3.10800400	-1.64616000	0.26539100
Pd	1.05189000	-1.29222000	0.10831200
C	1.31070600	1.71448700	0.06952800
C	2.64876300	2.15683200	0.66117600
C	2.92459800	1.30754600	1.91114200

H	3.04848400	0.24585000	1.68219800
H	3.85561700	1.65637500	2.37150800
N	0.72399600	2.33331600	-0.94904200
O	0.69350100	0.69700900	0.51686000
C	3.73581500	1.89275000	-0.39986500
H	3.60511400	2.53160200	-1.27977700
H	4.72004300	2.10423400	0.03399800
H	3.72717200	0.84384700	-0.72361400
C	2.65362500	3.63778800	1.08406400
H	2.66094100	4.32225000	0.23386200
H	1.79651700	3.87501600	1.72518900
H	3.56362800	3.82649400	1.66478600
H	2.12182100	1.40817700	2.65062700
C	-1.83091200	-0.65936600	0.32397300
H	-1.45815100	0.07032600	1.03465900
O	-5.53716700	0.36153900	-0.10015000
O	-4.44337400	0.04022300	2.09818600
O	-3.60286900	1.76686000	0.54809400
S	-4.29575600	0.46849100	0.69023200
C	3.98962600	-3.88266700	-0.01131700
H	4.72432200	-3.65439400	0.76587800
H	3.58396700	-4.88879400	0.11843900
H	4.49002100	-3.82022700	-0.98510200
O	1.67356300	-3.20688300	-0.19318900
C	-1.32980500	-2.43704600	-1.09110800
H	-0.55922800	-3.09068100	-1.48948800
O	1.29022700	3.46259900	-1.48736900
C	0.47529800	4.62157900	-1.25724000
H	-0.47822800	4.54123000	-1.78926200
H	0.30123600	4.76527800	-0.18649400
H	1.05602400	5.45056500	-1.66497500
C	-0.48103100	1.82916800	-1.59963000
H	-0.57564300	2.33726200	-2.56034600
H	-0.37277600	0.75771400	-1.78242500
H	-1.36833000	2.01897900	-0.98840000

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C	3.17054700	-0.42507900	-0.04547700
C	3.79587900	-1.50770000	-0.64997700
C	3.00283000	-2.55916200	-1.10337100

H	4.87585800	-1.52860600	-0.76611200
H	3.44255200	-3.43055900	-1.57601000
N	1.04215700	-1.41581200	-0.39162300
C	-1.90476300	-3.54506500	0.74769200
O	-2.49855200	-2.77475500	1.51541600
Pd	-0.96290300	-1.15822300	-0.39958400
C	-1.50795100	1.69515400	-0.24249700
C	-2.96584800	1.30719800	-0.00781500
C	-3.20174400	-0.08134200	-0.63325400
H	-2.82452400	-0.92176300	0.02182600
H	-4.26769200	-0.33035000	-0.60465400
N	-1.01956500	2.92397200	-0.08442200
C	0.42194800	3.17058800	-0.04583500
H	0.88831900	2.74159300	-0.93385000
H	0.58895500	4.24768500	-0.04319000
H	0.85754600	2.73809500	0.86115400
O	-0.63936500	0.82841400	-0.56818500
C	-3.18052500	1.21372000	1.51555100
H	-3.04846500	2.18446200	2.00290700
H	-4.20186100	0.86603400	1.70741400
H	-2.48775100	0.49163000	1.96610300
C	-3.96754100	2.28078900	-0.64997600
H	-4.00671000	3.23675400	-0.12638300
H	-3.73651500	2.45720300	-1.70654700
H	-4.96757200	1.83727500	-0.59460600
H	-2.89629600	-0.14524800	-1.68350700
C	1.79373100	-0.41413200	0.08701100
H	1.27424800	0.40187000	0.57351600
O	5.48308900	0.66874100	0.45595400
O	3.68185800	2.07066600	-0.51524100
O	3.52963700	1.34694500	1.82980300
S	4.05677700	1.04353200	0.48265600
C	-1.95832100	-5.03910000	0.90650500
H	-1.11093100	-5.35048900	1.52979000
H	-2.88361200	-5.32806300	1.41152300
H	-1.87422000	-5.54497900	-0.05917800
O	-1.16619100	-3.13276200	-0.24411400
C	1.62644900	-2.48032600	-0.97071700
H	0.96855700	-3.26397700	-1.33039400
O	-1.82234200	3.87863300	0.49398200
C	-2.04885100	5.00273200	-0.36427900

H	-1.12369900	5.56198800	-0.53588300
H	-2.48413700	4.68427400	-1.31604700
H	-2.75520000	5.62311100	0.19052200

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C	-3.09138800	-2.45662200	-0.64333200
C	-3.30074800	-1.18973500	-0.10593700
H	-3.88427500	-3.19979000	-0.64604600
N	-1.07779300	-0.55844900	-0.63738200
C	-0.75885700	3.19099600	0.20604600
O	0.11265400	3.18740500	1.08654600
Pd	0.45439100	0.76422300	-0.56038800
C	2.91825200	-0.62647800	0.03470600
C	3.57436800	0.74843100	0.13072400
C	2.71165800	1.75037700	-0.65352300
H	1.77962000	2.04679800	-0.08617000
H	3.19640400	2.73195700	-0.67202400
N	3.48104100	-1.73688500	0.49184000
C	2.77904100	-3.01340700	0.56564900
H	2.81881300	-3.54360500	-0.38991300
H	3.25670500	-3.60620500	1.34726600
H	1.73687800	-2.83276100	0.83926100
O	1.75104000	-0.78374800	-0.44846700
C	3.60282800	1.15656000	1.61510900
H	4.20935800	0.46703200	2.21116900
H	4.03480600	2.15961700	1.70398300
H	2.58712000	1.18793700	2.03041900
C	4.98266200	0.78056400	-0.48896300
H	5.71542700	0.24469700	0.11544700
H	4.98284400	0.36708500	-1.50367100
H	5.30814800	1.82449600	-0.55422900
H	2.55444900	1.46398900	-1.69958300
C	-0.85696700	-1.77663800	-1.16273300
H	0.12927700	-1.96462300	-1.57285600
C	-1.74883800	4.31123100	0.04925400
H	-1.36636500	5.01269500	-0.70251600
H	-2.71546600	3.93467200	-0.29684500
H	-1.86385800	4.84368100	0.99665200
O	-0.87605900	2.24443900	-0.68490800
C	-2.28167400	-0.25462000	-0.12048100

H	-2.41485000	0.74100000	0.28672900
S	-4.89659300	-0.75154900	0.58620100
O	-5.10240900	-1.68976100	1.71027900
O	-4.76108700	0.65732300	1.00446400
O	-5.84826300	-0.96051100	-0.52479500
C	-1.84513500	-2.74821500	-1.18165700
H	-1.63292800	-3.71661100	-1.62128900
O	4.72491100	-1.67316100	1.06820000
C	5.69963200	-2.42073200	0.32864500
H	5.46046600	-3.48912400	0.33284000
H	5.77793800	-2.04916600	-0.69780000
H	6.63495900	-2.25204200	0.86502800

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C	3.21005000	-2.25517000	-0.98000500
C	3.37850200	-1.15765400	-0.14016700
H	4.03842400	-2.92758900	-1.18790400
N	1.11809800	-0.52325300	-0.45393400
C	0.76383500	3.31115900	-0.36759600
O	-0.16883500	3.57688400	-1.13623100
Pd	-0.42846100	0.72979700	-0.09311000
C	-2.99455800	-0.64606700	0.00402600
C	-3.62955300	0.71875700	0.26291000
C	-2.51443000	1.75403600	0.49152700
H	-1.92020400	1.94910400	-0.44571200
H	-2.93619900	2.75212500	0.64599700
N	-3.68836400	-1.78043200	-0.02877500
C	-3.09083400	-3.02729300	-0.49804400
H	-2.26501400	-3.31613500	0.15651500
H	-3.85796500	-3.80114600	-0.48038400
H	-2.72576700	-2.90770400	-1.52291000
O	-1.76036900	-0.78653400	-0.27108100
C	-4.42252700	1.10484700	-1.00115400
H	-5.23547800	0.39954100	-1.19599300
H	-4.85854800	2.09986400	-0.85833700
H	-3.77116400	1.14160300	-1.88224000
C	-4.53330500	0.74113700	1.50756600
H	-5.48191700	0.22898700	1.34021100
H	-4.03131000	0.29828800	2.37495700
H	-4.76107500	1.78512700	1.74919600

H	-1.93683700	1.54927600	1.40822700
C	0.93299700	-1.57992000	-1.26331800
H	-0.05489700	-1.70432600	-1.69234200
C	1.80967500	4.31981300	0.02447300
H	1.51721500	4.77327000	0.97921000
H	2.78254700	3.83934200	0.16186900
H	1.87708300	5.10800600	-0.72921100
O	0.92061700	2.15064400	0.20245600
C	2.32058200	-0.30227200	0.10606100
H	2.42316800	0.57063500	0.74378400
S	4.97316400	-0.85002900	0.61593900
O	5.90048100	-0.69594600	-0.52404600
O	4.79409000	0.37913600	1.41409100
O	5.24182600	-2.05726000	1.42548100
C	1.96139800	-2.46450500	-1.54915600
H	1.77499500	-3.29980400	-2.21520700
O	-5.05955700	-1.72938900	0.04557400
C	-5.56603200	-2.41150300	1.19985700
H	-5.37965600	-3.48815500	1.13379000
H	-5.12735800	-2.00654400	2.11644700
H	-6.64044200	-2.22061400	1.17522200

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C	3.64901600	-1.70613200	0.77946000
C	3.20996100	-0.55818300	0.12688900
H	4.68292000	-1.80653600	1.09834200
N	1.00131000	-1.42531300	0.01247100
C	-2.31459700	-3.42575700	0.20661700
O	-3.03314000	-2.66346100	0.87064800
Pd	-0.95047100	-1.05008200	-0.38410600
C	-1.45450600	1.76952000	0.01842600
C	-2.93266800	1.44957000	-0.18977900
C	-3.02881500	0.14341900	-0.99911800
H	-2.83602100	-0.77102700	-0.35995600
H	-4.07292300	-0.06765900	-1.25363900
N	-1.00206000	2.90099500	0.53899000
C	0.40402800	3.10191300	0.88041600
H	0.99352500	3.34588100	-0.00736900
H	0.44973100	3.91850800	1.60315200
H	0.79389500	2.19160500	1.34298700

O	-0.54521800	0.91986600	-0.24394000
C	-3.57306700	1.23417300	1.19439400
H	-3.50093800	2.13213500	1.81661400
H	-4.63363200	0.99273100	1.06133500
H	-3.09801600	0.39524200	1.71939600
C	-3.67217900	2.54266700	-0.98035500
H	-3.82104800	3.44759900	-0.38914500
H	-3.14026000	2.80151200	-1.90272400
H	-4.66053700	2.16170500	-1.25949300
H	-2.47659000	0.17809300	-1.94460800
C	1.40909900	-2.54957700	0.62514500
H	0.65947800	-3.31326400	0.79807200
C	-2.59517800	-4.90059600	0.11356400
H	-1.78779500	-5.43590000	-0.39154200
H	-2.74390800	-5.30800800	1.11857800
H	-3.52696100	-5.04392000	-0.44562600
O	-1.27988100	-3.01568700	-0.47089400
C	1.88607100	-0.44725400	-0.24954500
H	1.51655400	0.43209000	-0.76173400
S	4.32882700	0.78583900	-0.27749400
O	5.06205500	0.31802900	-1.47334800
O	3.44772700	1.94380800	-0.53626000
O	5.18874300	0.93944000	0.91409300
C	2.72811100	-2.71900800	1.01929900
H	3.01856000	-3.63539700	1.52145100
O	-1.88465900	3.89404300	0.87956700
C	-1.70661500	5.06547000	0.07178900
H	-0.71878400	5.50857500	0.23442500
H	-1.84924300	4.83185100	-0.98775600
H	-2.47931300	5.75508300	0.41564900

III2-trans_OMe-down_pre-TS_conf-5

C	-3.92574200	1.50579100	-0.05507400
C	-3.27857000	0.27380400	-0.03997300
H	-5.00400400	1.57169800	0.06253000
N	-1.16880200	1.33374800	-0.30368900
C	1.83437400	3.59046100	0.57704800
O	2.47761700	2.86576800	1.34793800
Pd	0.85813800	1.13885400	-0.40321100
C	1.67705100	-1.63240800	-0.14123100

C	3.11320000	-1.11424700	-0.10477800
C	3.14156000	0.27603400	-0.76116500
H	2.74258600	1.07127300	-0.06261100
H	4.17083300	0.64179300	-0.83720600
N	1.33144300	-2.86170100	0.21957300
C	-0.06398800	-3.26255400	0.39484300
H	-0.56276600	-3.36798100	-0.57118400
H	-0.07024400	-4.21786900	0.92092400
H	-0.58072600	-2.52320100	1.01110000
O	0.69967300	-0.88731300	-0.47867900
C	3.53578200	-0.98182500	1.36988400
H	3.54296000	-1.95130500	1.87652500
H	4.54631600	-0.56076200	1.41663700
H	2.86234300	-0.30365100	1.90930100
C	4.08213000	-2.01328600	-0.89108900
H	4.28241600	-2.95490400	-0.37876500
H	3.69910200	-2.22418700	-1.89611800
H	5.03723800	-1.48739200	-0.99789200
H	2.73572600	0.28488500	-1.77894600
C	-1.77592300	2.53284300	-0.31868600
H	-1.13460300	3.40132100	-0.41749100
C	1.91577100	5.09077300	0.61713800
H	1.00568900	5.48543400	1.08439200
H	2.78238200	5.40121000	1.20600800
H	1.97792000	5.49953700	-0.39602500
O	1.02306500	3.12352600	-0.33109800
C	-1.90608100	0.21634400	-0.17673300
H	-1.37800100	-0.72761400	-0.17845000
S	-4.20636400	-1.24754100	0.17198300
O	-4.89424000	-1.46353100	-1.11830900
O	-3.20038700	-2.28325600	0.48840200
O	-5.13342200	-0.94632800	1.28187100
C	-3.15305600	2.65034800	-0.20587200
H	-3.60440300	3.63615700	-0.22395800
O	2.29810100	-3.71875900	0.68368400
C	2.45742200	-4.87138800	-0.15331000
H	1.55974300	-5.49802900	-0.13777200
H	2.69987700	-4.58022100	-1.17990800
H	3.29175300	-5.41213200	0.29719000

III2-trans_OMe-down_TS_conf-1

C	3.24233400	-0.66425800	-0.01780400
C	3.79845800	-1.86681400	-0.42997000
C	2.93260100	-2.88930500	-0.81419400
H	4.87629700	-2.00216800	-0.45255200
H	3.31411900	-3.84989700	-1.14342900
N	1.04246900	-1.49340800	-0.39490800
C	-2.46982800	-3.18590900	0.61010800
O	-3.23999300	-2.22425900	0.92086300
Pd	-0.98646400	-1.04064500	-0.43443400
C	-1.33724800	1.76077100	-0.24638300
C	-2.76553800	1.31723600	0.03102000
C	-2.92376000	-0.06762700	-0.63716300
H	-2.84948400	-1.19084600	0.21016000
H	-3.97705700	-0.36939900	-0.54317600
N	-0.85856700	2.99017100	-0.08685100
C	0.57799300	3.26439600	-0.13008300
H	1.00077100	2.85822500	-1.05076400
H	0.72316800	4.34481200	-0.11759300
H	1.07939600	2.82541200	0.73974200
O	-0.48257500	0.90223900	-0.62927900
C	-2.93468800	1.18175800	1.55710300
H	-2.84134700	2.15067900	2.05884400
H	-3.93119700	0.77463300	1.76560900
H	-2.19639000	0.49016200	1.98080300
C	-3.82725800	2.26484400	-0.54814500
H	-3.89603300	3.20311900	0.00646900
H	-3.63232700	2.48349300	-1.60414700
H	-4.80356700	1.77147300	-0.48269100
H	-2.76791400	-0.02302400	-1.72319800
C	1.86659900	-0.51463100	0.00047000
H	1.40562900	0.40761900	0.33275200
O	5.61781900	0.34328300	0.39407400
O	3.84206400	1.79812400	-0.55287200
O	3.73467700	1.12397100	1.80726300
S	4.20711400	0.77256400	0.45036700
C	-2.77321200	-4.56519200	1.09477900
H	-2.56474000	-4.60847300	2.16999100
H	-3.83431600	-4.78590900	0.94920000
H	-2.15496400	-5.30235700	0.57919800
O	-1.42749800	-2.99954700	-0.09710100

C	1.56446700	-2.66834500	-0.79234900
H	0.86131900	-3.43296000	-1.10457900
O	-1.65139800	3.92606500	0.53406700
C	-1.95768900	5.03123900	-0.32542400
H	-1.05538500	5.59954900	-0.57378500
H	-2.45074400	4.68552100	-1.23861600
H	-2.63317000	5.65364800	0.26424400

III2-trans_OMe-down_TS_conf-2

C	-3.28161400	-2.44040500	-0.48624900
C	-3.42941800	-1.11450500	-0.08914800
H	-4.11514700	-3.13555400	-0.42614100
N	-1.15774500	-0.65720200	-0.61639900
C	-0.37221000	3.19832900	0.10932500
O	0.81552100	3.24407900	0.55690900
Pd	0.48575100	0.61774100	-0.60829200
C	2.89173000	-0.72060700	0.02301200
C	3.38822800	0.71566000	0.11719100
C	2.43471000	1.56039600	-0.75159200
H	1.44977900	2.25098600	-0.03558000
H	2.81281800	2.59246700	-0.78051500
N	3.54621200	-1.77084700	0.49739700
C	2.96680800	-3.10637400	0.55900000
H	3.09291400	-3.63593800	-0.38965400
H	3.46565000	-3.64770500	1.36515300
H	1.90137800	-3.01958700	0.78899100
O	1.74489800	-0.96987800	-0.47195000
C	3.28042900	1.15264800	1.59183300
H	3.97444300	0.59362300	2.22762600
H	3.51720100	2.22037100	1.66960100
H	2.26254600	1.00926700	1.97410900
C	4.82058500	0.90556800	-0.40936800
H	5.57248200	0.49373600	0.26632100
H	4.94485800	0.45453400	-1.40063300
H	5.01424700	1.98012700	-0.50449700
H	2.45401300	1.25599200	-1.80692800
C	-1.00530200	-1.93103000	-1.01512700
H	-0.02377600	-2.21171300	-1.38350900
C	-1.30972200	4.33714700	0.34031500
H	-1.13473800	5.09010400	-0.43770300

H	-2.34573200	3.99848600	0.27195900
H	-1.11920000	4.79894700	1.31176700
O	-0.78868600	2.20332900	-0.56850900
C	-2.35467000	-0.24606500	-0.16525200
H	-2.43997000	0.79139000	0.13892000
S	-4.99634500	-0.54071700	0.56384700
O	-5.15393300	-1.26846600	1.84153200
O	-4.84403100	0.91863300	0.72797000
O	-5.99902400	-0.93186700	-0.45032300
C	-2.04399200	-2.84897400	-0.96681700
H	-1.87569600	-3.86718600	-1.30052600
O	4.76039400	-1.58148800	1.10885800
C	5.82666900	-2.22474500	0.40087600
H	5.70684200	-3.31274600	0.41891000
H	5.88191700	-1.86098400	-0.62995900
H	6.72638600	-1.94386300	0.95129200

III2-trans_OMe-down_TS_conf-3

C	-3.34112500	-2.33025900	0.72675100
C	-3.51691400	-1.10371400	0.09229100
H	-4.18776100	-2.98463900	0.91658700
N	-1.18699800	-0.65291500	0.22646900
C	-0.27951500	3.22719200	0.44904700
O	0.97712600	3.30495100	0.61387700
Pd	0.43126500	0.58207100	-0.19680100
C	2.94082300	-0.75641800	-0.15713800
C	3.42512900	0.68281900	-0.22585900
C	2.28154000	1.49544800	-0.86627600
H	1.48175500	2.24506700	0.00587900
H	2.64585900	2.51987100	-1.02689900
N	3.73467700	-1.81566500	0.00321700
C	3.19897600	-3.12003400	0.37928400
H	2.42551000	-3.41685500	-0.33018400
H	4.00765200	-3.85040500	0.34587200
H	2.78799400	-3.08119400	1.39357000
O	1.69717600	-1.00826500	-0.20930800
C	3.65480900	1.15344700	1.22567100
H	4.47912800	0.60769500	1.69774400
H	3.90240200	2.22138000	1.21661400
H	2.75031700	1.02405000	1.83179000

C	4.69462800	0.88508900	-1.06871800
H	5.59114200	0.51115900	-0.57028300
H	4.60155900	0.40522900	-2.04954600
H	4.83302300	1.95923500	-1.23535100
H	2.04524700	1.15057700	-1.88204500
C	-1.00393700	-1.83271400	0.84155200
H	0.01461700	-2.08029600	1.12224300
C	-1.14443800	4.40254000	0.76358700
H	-1.03585200	5.13931000	-0.04111800
H	-2.19243600	4.10493500	0.83340000
H	-0.81097100	4.86937100	1.69434000
O	-0.82599700	2.17029300	-0.00337400
C	-2.42541900	-0.28687900	-0.14644700
H	-2.53016400	0.66978400	-0.64777200
S	-5.16053100	-0.56119800	-0.37126800
O	-5.82295100	-0.24141700	0.91230900
O	-4.95647800	0.61544400	-1.24073400
O	-5.76255800	-1.72104100	-1.06132400
C	-2.05643000	-2.69660700	1.10632500
H	-1.86418100	-3.64100200	1.60402400
O	5.03620400	-1.57845900	0.38718900
C	5.98629200	-2.12900200	-0.53085500
H	5.91101600	-3.22026300	-0.57110700
H	5.85843800	-1.70182900	-1.52967300
H	6.95554400	-1.84472400	-0.11713800

III2-trans_OMe-down_TS_conf-4

C	3.85076100	-1.54198900	0.74678500
C	3.37293200	-0.39404000	0.11949500
H	4.90290600	-1.63667300	1.00306800
N	1.17059000	-1.28561800	0.07604700
C	-2.28540400	-3.37111500	0.13557600
O	-3.22403400	-2.52570100	0.27219800
Pd	-0.83943700	-1.00825800	-0.38053300
C	-1.60045300	1.67681700	0.00547800
C	-2.98123600	1.08596500	-0.24238300
C	-2.76357100	-0.22970800	-1.01855900
H	-2.77999900	-1.40690800	-0.24945600
H	-3.75293300	-0.65047000	-1.24969400
N	-1.37819000	2.87060900	0.53552600

C	-0.04926900	3.33178800	0.92310100
H	0.48886800	3.74457300	0.06555000
H	-0.17097400	4.09544500	1.69311400
H	0.51372300	2.49208300	1.33788100
O	-0.55751600	0.99056300	-0.24800900
C	-3.64179300	0.78347800	1.11634700
H	-3.84360800	1.70082200	1.67804400
H	-4.59427700	0.26950600	0.94265600
H	-3.01218000	0.12625100	1.72859200
C	-3.87361300	2.00740900	-1.09117500
H	-4.20939700	2.88826800	-0.53954900
H	-3.35691400	2.33172300	-2.00161200
H	-4.76459500	1.44528100	-1.39432900
H	-2.32058000	-0.05921000	-2.00907800
C	1.61849700	-2.39873800	0.67784700
H	0.88349200	-3.17131900	0.87776300
C	-2.54070200	-4.81373600	0.42718600
H	-1.61976100	-5.39499600	0.35938900
H	-2.97799700	-4.91186900	1.42568100
H	-3.27064800	-5.19663700	-0.29465500
O	-1.12636000	-3.02042800	-0.25728300
C	2.03293500	-0.29130000	-0.20534600
H	1.63487000	0.58673400	-0.70549800
S	4.50180500	0.93905700	-0.27692800
O	5.48379500	0.33479000	-1.20254300
O	3.66937300	1.98998100	-0.89642900
O	5.09426400	1.33307000	1.02006100
C	2.95157800	-2.56116300	1.02764900
H	3.27056100	-3.47627200	1.51480200
O	-2.44892600	3.64656500	0.90296700
C	-2.50476500	4.87443300	0.16744300
H	-1.64649700	5.51210200	0.40390100
H	-2.55212800	4.68043300	-0.90884500
H	-3.42366000	5.35183400	0.51227500

III2-trans_OMe-down_TS_conf-5

C	3.80776000	-1.89834600	0.20248400
C	3.30929000	-0.61144100	0.02683000
H	4.86497200	-2.07079100	0.38441900
N	1.09216800	-1.45125900	-0.21568500

C	-2.48953300	-3.24730100	0.34180300	H	-2.39594500	4.67228600	-1.19150800
O	-3.31114000	-2.32660700	0.63338100	H	-2.79734200	5.66430400	0.24974600
Pd	-0.94844000	-1.00788200	-0.40779100	III2-trans_OMe-down_prod_conf-1			
C	-1.43445100	1.77049300	-0.09848100	C	3.32104800	-0.53197000	-0.08202300
C	-2.86776100	1.26896300	-0.02816200	C	3.89291200	-1.62639000	-0.71810900
C	-2.88955100	-0.08721800	-0.76512800	C	3.05152600	-2.65641400	-1.13339900
H	-2.86637600	-1.24518300	0.03273300	H	4.96397800	-1.67136300	-0.89331300
H	-3.93338600	-0.43075800	-0.80340200	H	3.44733800	-3.53422500	-1.63336700
N	-1.02534200	2.98053000	0.25291500	N	1.13999900	-1.47496500	-0.30830700
C	0.39005100	3.31231900	0.40782500	C	-2.22016700	-3.57126500	0.49756200
H	0.87389400	3.44178800	-0.56365900	O	-2.50701000	-3.03385300	1.67040900
H	0.44943300	4.23976100	0.97941900	Pd	-1.00055500	-0.96868500	-0.34365400
H	0.88576200	2.51594900	0.96896800	C	-1.45537200	1.81287800	-0.19576500
O	-0.50670300	0.96808700	-0.43895500	C	-2.82682300	1.25154100	0.12510200
C	-3.20427800	1.06676300	1.46255600	C	-2.83810300	-0.18443100	-0.46199000
H	-3.21342700	2.01941300	2.00245200	H	-2.17878500	-2.11453800	1.73715500
H	-4.19702400	0.61054800	1.54904900	H	-3.60495600	-0.78918900	0.03902500
H	-2.48119600	0.39743100	1.94347900	N	-1.11848700	3.10510000	-0.23251600
C	-3.89299800	2.19892600	-0.69528700	C	0.28503300	3.51190500	-0.18191300
H	-4.03949800	3.12788200	-0.14085700	H	0.84404400	2.99244300	-0.96235500
H	-3.60666900	2.43735700	-1.72582800	H	0.33863400	4.58633400	-0.36239100
H	-4.85663200	1.67782400	-0.73083600	H	0.71269400	3.28404800	0.79991900
H	-2.61657800	0.01135100	-1.82410000	O	-0.50295400	0.99776500	-0.38098400
C	1.56009900	-2.69963500	-0.04529800	C	-2.89313800	1.20373700	1.66692800
H	0.82946800	-3.50148400	-0.06608500	H	-2.86149300	2.20989900	2.10006900
C	-2.81785300	-4.67183500	0.64469700	H	-3.83092900	0.72565000	1.97221600
H	-1.91321000	-5.21070200	0.93860600	H	-2.06002100	0.62362500	2.08194200
H	-3.57629200	-4.72743800	1.42827700	C	-4.02075300	2.03085300	-0.44028600
H	-3.21442900	-5.13806200	-0.26493800	H	-4.20234600	2.97133100	0.08636900
O	-1.38066600	-2.99090300	-0.22937800	H	-3.88878900	2.24049500	-1.50755800
C	1.95691000	-0.42306300	-0.18933500	H	-4.91714300	1.40832300	-0.33249000
H	1.54630500	0.56660800	-0.34330000	H	-3.06683300	-0.15683000	-1.53767800
S	4.38012500	0.82766100	0.07187900	C	1.94938300	-0.49688300	0.11747000
O	4.99761300	0.90901900	-1.26966700	H	1.47647700	0.34541100	0.61316400
O	3.48024100	1.96215800	0.36900400	O	5.62793900	0.68666400	-0.08332000
O	5.35221500	0.52985700	1.14423600	O	3.55753000	2.05651200	-0.03272800
C	2.90808400	-2.95735600	0.15911100	O	4.24549100	0.78781500	1.96490100
H	3.24051500	-3.98119200	0.29354000	S	4.27851200	0.87164200	0.48655300
O	-1.94368000	3.90065700	0.69562100	C	-2.65472600	-4.98533700	0.36240100
C	-2.05384900	5.00931100	-0.20764100				
H	-1.09843200	5.53655500	-0.29821900				

H	-2.14887100	-5.58844900	1.12427600
H	-3.73205500	-5.05187500	0.54705000
H	-2.41756500	-5.35684300	-0.63515000
O	-1.64600400	-2.95570600	-0.40582500
C	1.68580400	-2.53994300	-0.91935800
H	0.99480600	-3.30941900	-1.25237500
O	-2.01359100	4.00445400	0.31030300
C	-2.42773800	4.99505300	-0.63331800
H	-1.57486700	5.57830800	-0.99561700
H	-2.95787200	4.53826000	-1.47439400
H	-3.10121100	5.64168200	-0.06733600

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C	-3.33181600	-2.59010800	-0.14837100
C	-3.50470300	-1.21472000	-0.01726000
H	-4.17768300	-3.26848900	-0.07190300
N	-1.17074800	-0.84156000	-0.33022300
C	-0.81068700	3.11880700	0.06386200
O	-0.16494700	3.24466500	1.21168300
Pd	0.57428800	0.48713500	-0.46145200
C	3.11385100	-0.64149500	0.03232500
C	3.41160800	0.84486200	0.10266300
C	2.26413800	1.53437800	-0.67253700
H	0.40507300	2.47075900	1.39527700
H	2.17764100	2.58287500	-0.36073600
N	3.97498800	-1.61163600	0.32059700
C	3.56110800	-3.00253400	0.46204100
H	3.42618400	-3.47282300	-0.51614400
H	4.33855700	-3.52750400	1.01892900
H	2.62301800	-3.04950300	1.02311700
O	1.92991500	-1.02312300	-0.23600800
C	3.35322400	1.21979700	1.59746000
H	4.15791200	0.73546900	2.16185300
H	3.46850500	2.30446700	1.70248000
H	2.39460100	0.92906300	2.04363300
C	4.75333200	1.27922700	-0.50588500
H	5.60818100	1.03290300	0.12916900
H	4.90496700	0.83253100	-1.49512400
H	4.73340100	2.36823100	-0.63378300
H	2.46049900	1.51379400	-1.75509000

C	-0.99945700	-2.16614200	-0.46236800
H	0.01734400	-2.50617800	-0.63915000
C	-1.71997700	4.25025500	-0.25322400
H	-1.11443000	5.12282200	-0.52624300
H	-2.36887400	3.98087900	-1.08779000
H	-2.31084000	4.51431100	0.62861600
O	-0.67394200	2.14867800	-0.68832700
C	-2.41027900	-0.37126400	-0.11708700
H	-2.52338100	0.70515200	-0.02857100
S	-5.13420000	-0.54869700	0.30238300
O	-5.51787800	-1.11074200	1.61640800
O	-4.96853100	0.91994900	0.31016300
O	-5.97858100	-1.04948700	-0.80438800
C	-2.05027500	-3.07105500	-0.38263300
H	-1.86049800	-4.13267000	-0.50102000
O	5.22692500	-1.27534700	0.77615600
C	6.25829100	-1.69870600	-0.12233800
H	6.28622500	-2.79090300	-0.19974500
H	6.11835700	-1.24947700	-1.11068300
H	7.18169400	-1.33693800	0.33356500

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C	-3.35956600	-2.42907300	0.71544200
C	-3.52314200	-1.19457700	0.09246500
H	-4.21293400	-3.07560400	0.90255100
N	-1.18221600	-0.76334300	0.22339800
C	-0.80211800	3.14997700	0.33949500
O	-0.10782300	3.28281300	1.45915500
Pd	0.55440600	0.51075900	-0.19697300
C	3.11951400	-0.67487200	-0.12211600
C	3.45570200	0.80128200	-0.07058500
C	2.21454400	1.53229300	-0.63517500
H	0.45989300	2.50212200	1.62317200
H	2.19175300	2.56938500	-0.27715300
N	4.00774700	-1.67370200	-0.10518900
C	3.58513500	-3.02807500	0.24140400
H	2.85801900	-3.38715900	-0.48913400
H	4.46075300	-3.67790600	0.22052300
H	3.14073300	-3.04007500	1.24283100
O	1.90077100	-1.02499900	-0.10390400

C	3.64056500	1.11429000	1.43001100
H	4.49687100	0.57127900	1.84714300
H	3.82061700	2.18826300	1.55437000
H	2.74574000	0.84480400	2.00465500
C	4.69282400	1.24161900	-0.86446500
H	5.63150000	0.96021800	-0.38056200
H	4.68035700	0.83429300	-1.88169100
H	4.67231200	2.33510900	-0.94661200
H	2.24652900	1.54920300	-1.73494500
C	-1.01813200	-1.95341800	0.82104500
H	-0.00054300	-2.21955400	1.09353600
C	-1.73067700	4.27378600	0.05259200
H	-1.17780200	5.21851000	0.06382600
H	-2.20631600	4.12423600	-0.91738400
H	-2.49302000	4.31968900	0.83779000
O	-0.69132100	2.17500800	-0.40901800
C	-2.41937500	-0.38954900	-0.14036200
H	-2.51571100	0.56942200	-0.64113100
S	-5.16077600	-0.63504400	-0.36527600
O	-5.82217100	-0.31401100	0.91985500
O	-4.95109300	0.54558300	-1.22965500
O	-5.77893200	-1.78368300	-1.06147700
C	-2.07659900	-2.81343900	1.08330700
H	-1.89282900	-3.76689900	1.56741200
O	5.30528700	-1.35196900	0.23723900
C	6.23603800	-1.71797200	-0.78422600
H	6.24202500	-2.80166200	-0.94219500
H	6.01184100	-1.20032800	-1.72166100
H	7.20520400	-1.39580300	-0.39819000

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C	-4.09785800	1.40357100	0.14935200
C	-3.47434000	0.16783400	-0.00016700
H	-5.17364100	1.47319200	0.28646100
N	-1.33948300	1.21333500	-0.19334600
C	1.70961800	3.78381100	0.19852200
O	2.15566700	3.41174400	1.38626100
Pd	0.84372100	0.96104700	-0.37025600
C	1.83817100	-1.66081600	-0.02156400
C	3.09938300	-0.82972700	0.11428500

C	2.78282400	0.52467000	-0.56480700
H	1.98167200	2.46531400	1.56424800
H	3.44669500	1.30663600	-0.17450700
N	1.76327800	-2.98272900	0.10343600
C	0.47999700	-3.66778100	0.23158100
H	-0.07982300	-3.60295700	-0.70444600
H	0.67986600	-4.71336500	0.46802300
H	-0.10332000	-3.22025100	1.04230800
O	0.72640500	-1.06443600	-0.17995200
C	3.30048300	-0.64595700	1.63306900
H	3.51487700	-1.60317200	2.12278800
H	4.14717400	0.02806600	1.80674800
H	2.41112200	-0.20793600	2.10258800
C	4.36756300	-1.41398000	-0.52297700
H	4.77800500	-2.25504200	0.04055500
H	4.18495400	-1.73064500	-1.55585700
H	5.12861600	-0.62478400	-0.54792300
H	2.93897800	0.45490200	-1.65178900
C	-1.93637300	2.40699000	-0.05611600
H	-1.28813800	3.27823100	-0.08294600
C	1.93519000	5.22034500	-0.10842300
H	1.38468600	5.50005900	-1.00785300
H	1.62827700	5.83618600	0.74223900
H	3.00801300	5.37948200	-0.26893800
O	1.16270200	3.01187400	-0.59540100
C	-2.10098400	0.10649200	-0.17194700
H	-1.59331200	-0.84648000	-0.29806800
S	-4.43359300	-1.34128200	0.07848800
O	-5.56420100	-1.13777100	-0.85225100
O	-3.50577700	-2.41549900	-0.33136400
O	-4.86394700	-1.44221300	1.49147900
C	-3.30779100	2.54508500	0.11488600
H	-3.74320200	3.53304300	0.22223400
O	2.88218400	-3.67101400	0.51102200
C	3.33315100	-4.58838400	-0.49124300
H	2.57910600	-5.35778300	-0.68818300
H	3.58608500	-4.05874600	-1.41480900
H	4.22459500	-5.05022500	-0.06258400

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C	3.42886100	0.21385700	0.23171800
C	4.07270000	1.38810700	0.60071300
C	3.29829100	2.52372000	0.82485900
H	5.15352300	1.41529400	0.70921800
H	3.75124800	3.46525900	1.11525500
N	1.32097600	1.29523900	0.31980200
C	-2.21050900	3.00940500	-0.81455200
O	-2.60886100	1.82150700	-0.57383700
Pd	-0.66465200	1.29988000	-0.03440800
C	-1.70569400	-1.44476800	0.36616600
C	-2.90862800	-1.34423500	1.30708100
C	-2.71938900	-0.14265000	2.24522100
H	-2.80393300	0.81435100	1.71758000
H	-3.50794000	-0.17086300	3.00520300
N	-1.58622400	-2.39325300	-0.55607100
O	-0.68439600	-0.69243100	0.47729300
C	-4.23389700	-1.17484200	0.54396800
H	-4.54085800	-2.08968700	0.03158600
H	-5.01933000	-0.92278200	1.26582500
H	-4.17836000	-0.35919900	-0.18627400
C	-2.93273000	-2.62595100	2.16805900
H	-3.10223300	-3.52618300	1.57121100
H	-1.99142900	-2.74376100	2.71843400
H	-3.74350600	-2.54554100	2.90139200
H	-1.75333400	-0.17443400	2.75971800
C	2.04962100	0.18979700	0.11563600
H	1.50900800	-0.71177700	-0.14620000
O	5.66757800	-1.10509300	0.40165600
O	3.53434300	-2.38120800	0.37685800
O	4.34599900	-1.28637700	-1.67791400
S	4.33046300	-1.27572800	-0.19712500
C	-3.10999400	4.07373800	-1.31976400
H	-4.15442400	3.77721000	-1.19910700
H	-2.91209200	5.00930400	-0.78799800
H	-2.90082100	4.23722700	-2.38356200
O	-0.96078400	3.23422100	-0.60828100
C	1.92594500	2.44840600	0.66072900
H	1.28307200	3.31226300	0.80204200
O	-2.56624200	-3.34521800	-0.69499800
C	-3.21007100	-3.25678100	-1.97253100
H	-3.64229300	-2.26239900	-2.12180100

H	-2.51058600	-3.49038800	-2.78173200
H	-3.99375900	-4.01548100	-1.93322800
C	-0.33465500	-2.62312600	-1.27581400
H	-0.44527200	-3.54489600	-1.84749600
H	-0.11950100	-1.79168500	-1.95196600
H	0.48592300	-2.74983000	-0.56261700

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C	-3.42567700	-0.59063400	-0.40936700
C	-3.47289400	-1.57000700	-1.39313100
C	-2.34803100	-1.76867700	-2.18981900
H	-4.37316100	-2.15945500	-1.53915800
H	-2.33999500	-2.51830300	-2.97358700
N	-1.19693100	-0.04944800	-1.01456600
C	0.96055500	3.12246200	0.44297500
O	1.88753000	2.28571100	0.17480600
Pd	0.47800600	0.94911400	-0.53289100
C	2.48939100	-1.07074800	-0.23361900
C	3.95779000	-0.70881800	-0.45448000
C	4.03357400	0.25905700	-1.64617400
H	3.54453100	1.21561600	-1.42659200
H	5.08832200	0.46316600	-1.86226000
N	2.06842000	-1.84583500	0.75725900
O	1.60336300	-0.68868000	-1.07075200
C	4.56322900	-0.01123500	0.77890300
H	4.74393200	-0.70182000	1.60520600
H	5.52939000	0.41956900	0.49201400
H	3.92469800	0.80890800	1.12860400
C	4.73510900	-1.99462100	-0.79645800
H	4.72090000	-2.71751700	0.02440200
H	4.32310300	-2.47621200	-1.69141200
H	5.78026200	-1.73720800	-1.00393100
H	3.57535300	-0.16124800	-2.54719200
C	-2.27332500	0.16343200	-0.24514700
H	-2.19464000	0.95068500	0.50164000
O	-5.90727200	-1.12319200	0.18965000
O	-4.31906000	-0.65983600	2.02879500
O	-5.06462300	1.17839000	0.56352900
S	-4.80961300	-0.27218100	0.68839000
C	1.24457400	4.43024900	1.07847300

H	2.22857500	4.78945000	0.76514600
H	0.46581000	5.15365200	0.82528800
H	1.25544500	4.29281100	2.16663900
O	-0.23292400	2.74940100	0.14875700
C	-1.22156400	-0.99579900	-1.97083400
H	-0.31571100	-1.12104700	-2.55423500
O	2.97673700	-2.35262900	1.65370500
C	2.76181000	-1.85347100	2.98047300
H	2.75390700	-0.75890700	2.98567300
H	1.83043300	-2.24467100	3.40198200
H	3.61150900	-2.23245100	3.55073200
C	0.68388200	-2.27930700	0.90961300
H	0.68591100	-3.19692200	1.50073300
H	0.08043400	-1.51391100	1.40847900
H	0.26554200	-2.49613700	-0.07462700

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C	3.68740500	-0.73404800	-0.21615300
C	3.67349600	-2.03454900	-0.70217600
C	2.45089600	-2.58951400	-1.07064100
H	4.59610200	-2.60106300	-0.78647300
H	2.38716900	-3.59898400	-1.46202100
N	1.32799100	-0.58426900	-0.44470900
C	-0.77743800	2.86661100	0.36349900
O	-1.72199900	2.02054300	0.20202500
Pd	-0.33952200	0.53272300	-0.16905900
C	-2.72675900	-1.05444700	-0.16911600
C	-3.25785700	-1.73491100	1.08985100
C	-2.09825800	-2.52222800	1.71847100
H	-1.26210300	-1.87129700	1.99585100
H	-2.46085400	-3.01730700	2.62605800
N	-3.49633600	-0.37725800	-1.01134700
O	-1.48930000	-1.15948700	-0.46577500
C	-3.73124300	-0.66198400	2.09076300
H	-4.66422800	-0.18774300	1.77712500
H	-3.90999300	-1.14022400	3.06057900
H	-2.96858800	0.11442200	2.23399400
C	-4.39510700	-2.71103100	0.74246700
H	-5.27945000	-2.19875900	0.35492800
H	-4.06402100	-3.44647700	-0.00071400

H	-4.68685200	-3.25489700	1.64828700
H	-1.71635300	-3.29273000	1.03990300
C	2.49947100	-0.02964100	-0.09990200
H	2.46990100	0.98873700	0.27904300
O	6.24184100	-0.96891800	0.23069400
O	5.39558800	1.18353400	-0.65636700
O	4.91283100	0.54847500	1.67283200
S	5.20197900	0.07490400	0.30197000
C	-1.03826000	4.30069000	0.63279200
H	-2.04975300	4.43176300	1.02526600
H	-0.29728700	4.69442500	1.33395200
H	-0.94616900	4.85311300	-0.31018400
O	0.41299000	2.40207300	0.24953500
C	1.29544100	-1.84108900	-0.92753100
H	0.32173500	-2.23706000	-1.19481800
O	-4.81287300	-0.15270000	-0.69038600
C	-5.07751200	1.24396000	-0.48064900
H	-4.37306100	1.66773600	0.24275300
H	-5.03209600	1.79355200	-1.42629600
H	-6.09543100	1.26960700	-0.08810000
C	-3.03020600	0.18917400	-2.26937400
H	-3.87274800	0.18905900	-2.96472500
H	-2.65069900	1.20729600	-2.13363400
H	-2.23749600	-0.44635200	-2.66746000

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C	-3.36616800	0.42668700	0.04244900
C	-3.90901500	1.52625300	0.69244100
C	-3.05446300	2.56377500	1.05799900
H	-4.97172100	1.57013600	0.91244400
H	-3.42648100	3.44763400	1.56442700
N	-1.19523900	1.37705400	0.15265200
C	2.59647100	2.92432100	0.02887700
O	2.84192200	1.69540400	-0.20827000
Pd	0.80981000	1.27471500	-0.10024100
C	1.48615500	-1.59249400	-0.20196500
C	2.74599400	-1.83830100	-1.03495400
C	2.70159600	-0.91010200	-2.25940300
H	2.79283900	0.14652700	-1.98742100
H	3.54461800	-1.15839600	-2.91415000

N	1.16618700	-2.31188200	0.86649500
O	0.61475800	-0.73165600	-0.55491000
C	4.02026000	-1.54356600	-0.22248600
H	4.19664000	-2.28574600	0.56050200
H	4.87958700	-1.57262200	-0.90264900
H	3.98633600	-0.54483900	0.22836800
C	2.73992300	-3.29552000	-1.53724500
H	2.84105800	-4.01902700	-0.72435200
H	1.81456700	-3.51484400	-2.08400900
H	3.58028300	-3.43729600	-2.22629500
H	1.77631700	-1.04521400	-2.82993600
C	-2.00773300	0.38287800	-0.22779900
H	-1.54884000	-0.45209600	-0.74460700
O	-5.68873200	-0.75288300	0.13093300
O	-4.34668600	-0.94897400	-1.93899700
O	-3.63985900	-2.15091100	0.09586300
S	-4.35649800	-0.98175100	-0.45983700
C	3.66703700	3.94710500	0.08991400
H	4.42257900	3.73221000	-0.67108500
H	3.24689900	4.94611200	-0.04847300
H	4.14726200	3.89308400	1.07431400
O	1.35982900	3.21836700	0.21968800
C	-1.70379700	2.45598400	0.77992400
H	-1.00007300	3.23319800	1.06162200
O	2.02484800	-3.28230300	1.32291200
C	2.57325500	-2.93463800	2.60116700
H	3.07551600	-1.96328200	2.55587800
H	1.79610500	-2.92601200	3.37248000
H	3.29404100	-3.72642500	2.81231300
C	-0.12101600	-2.19888600	1.54697500
H	-0.22087300	-3.06271900	2.20577600
H	-0.17925500	-1.27679700	2.13229100
H	-0.93096800	-2.22601300	0.81389700

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C	3.20874200	-0.42577400	-0.09407400
C	3.81178000	-1.61430200	-0.49165700
C	2.99475300	-2.68844400	-0.82829200
H	4.89394100	-1.69656900	-0.54806100
H	3.41433700	-3.63564800	-1.14896100

N	1.05696000	-1.38060800	-0.38958900
C	-1.98068400	-3.35682100	0.93487800
O	-2.67004400	-2.49929600	1.50628800
Pd	-0.94536000	-1.12227800	-0.41120300
C	-1.56161800	1.69394300	-0.43972900
C	-3.03591200	1.29421900	-0.35080800
C	-3.17506400	-0.14028000	-0.89236600
H	-2.84617500	-0.90884900	-0.13269100
H	-4.23308300	-0.41598600	-0.95441400
N	-1.12523900	2.93063700	-0.24152200
C	0.26145700	3.34536500	-0.42987500
H	0.70563600	2.75696000	-1.23394000
H	0.24859400	4.39868700	-0.71886400
H	0.83968600	3.21413900	0.48864300
O	-0.66248500	0.85223000	-0.76160800
C	-3.50793300	1.31067600	1.11332700
H	-3.55361500	2.32370600	1.52018900
H	-4.51687700	0.88581300	1.16160100
H	-2.85680500	0.69514300	1.74719500
C	-3.90429300	2.20336800	-1.23880500
H	-3.91334400	3.23811100	-0.89058100
H	-3.55142000	2.18760200	-2.27685900
H	-4.93354000	1.82787200	-1.22443300
H	-2.75828100	-0.26977200	-1.89731100
C	1.82994500	-0.33797800	-0.04724700
H	1.32582800	0.56897900	0.26173200
O	5.39455000	0.94042600	-0.43055300
O	3.29553100	2.16383200	0.07758100
O	4.41739600	0.84543700	1.83649100
S	4.16863200	1.01292300	0.38816700
C	-2.07869900	-4.81482800	1.28574000
H	-1.80557200	-4.94613800	2.33849300
H	-3.11861900	-5.13891100	1.17098400
H	-1.42855700	-5.42903400	0.65837000
O	-1.12841200	-3.06939600	-0.00747300
C	1.61813400	-2.54131700	-0.77014700
H	0.94334900	-3.34770500	-1.03528700
O	-2.01518000	3.89980700	0.15391000
C	-1.73963200	4.36056800	1.48446300
H	-1.67187800	3.51808600	2.18021400
H	-0.82031500	4.95421300	1.51178500

H	-2.59360900	4.99244400	1.73512200
III2-trans_OMe-up_pre-TS_conf-2			
C	-3.15300100	-2.32124700	-0.79127900
C	-3.29664200	-1.08613700	-0.16711800
H	-3.96871300	-3.03919700	-0.80214300
N	-1.08487100	-0.48207800	-0.76728400
C	-0.59993600	3.16789000	0.36393700
O	0.33571100	3.10396300	1.17456100
Pd	0.49719000	0.77238700	-0.64932200
C	2.90806500	-0.71203600	-0.16335500
C	3.62432800	0.63543700	-0.07176300
C	2.75773400	1.69508100	-0.77213500
H	1.86906800	1.99997000	-0.14162000
H	3.27832300	2.65850800	-0.77957900
N	3.45439500	-1.85586000	0.22396000
C	2.80268200	-3.14529600	0.03018200
H	2.41016300	-3.20566200	-0.98724800
H	3.55776600	-3.92235700	0.15925200
H	1.98706600	-3.28399900	0.74601700
O	1.74923000	-0.82671200	-0.68047100
C	3.82295700	1.06085200	1.39187100
H	4.52570000	0.41249300	1.91947400
H	4.23252100	2.07699100	1.40726900
H	2.86763000	1.07920600	1.93066300
C	4.96262100	0.56388300	-0.82928300
H	5.67233000	-0.11148600	-0.34685500
H	4.80869800	0.22798700	-1.86160400
H	5.40720900	1.56455900	-0.86051000
H	2.53884500	1.46185900	-1.82027200
C	-0.92900300	-1.66756700	-1.38312600
H	0.02582500	-1.84950300	-1.86275700
C	-1.64408000	4.24880500	0.42069000
H	-2.11893200	4.39361700	-0.55313500
H	-2.41565200	3.94170800	1.13732400
H	-1.20156900	5.18365200	0.77423500
O	-0.78591200	2.29391000	-0.58651200
C	-2.25145300	-0.18009600	-0.17223100
H	-2.33510000	0.78896000	0.30551900
S	-4.81889800	-0.67713400	0.68696100

O	-4.78437400	-1.49284900	1.91964800
O	-4.74736100	0.77594800	0.93672700
O	-5.89265800	-1.07866900	-0.24519000
C	-1.94381100	-2.61041300	-1.41070300
H	-1.78197700	-3.55282700	-1.92243900
O	4.68906200	-1.85310200	0.82281100
C	4.60036200	-2.23993900	2.20191600
H	3.85166300	-1.63613000	2.72451400
H	4.36213000	-3.30472400	2.29411100
H	5.59744400	-2.04893400	2.60230300

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C	3.16176300	-2.38858500	-0.73983600
C	3.39889000	-1.18272900	-0.08780100
H	3.97437400	-3.08215300	-0.93912800
N	1.10318100	-0.61126500	-0.22287700
C	0.68104000	3.22398700	-0.63351500
O	-0.38137200	3.41477600	-1.24027100
Pd	-0.41572500	0.69025800	0.10285500
C	-2.99431900	-0.65584700	0.30522400
C	-3.61366800	0.72869900	0.50098400
C	-2.48122500	1.74963400	0.71064300
H	-1.89234600	1.91848200	-0.23628800
H	-2.88810700	2.75678600	0.84614000
N	-3.72573100	-1.76304800	0.24045000
C	-3.16220100	-3.10170600	0.14615700
H	-2.26454100	-3.16079900	0.76371600
H	-3.90662700	-3.79882700	0.53709700
H	-2.91297500	-3.35337300	-0.88919700
O	-1.73753900	-0.84246700	0.23333000
C	-4.42209700	1.13480700	-0.74442200
H	-5.35307600	0.56959000	-0.82535800
H	-4.68197200	2.19591600	-0.66310900
H	-3.84054700	0.99973900	-1.66362100
C	-4.49431000	0.75343900	1.76405200
H	-5.39138500	0.14138900	1.65073800
H	-3.93721400	0.40305500	2.64071900
H	-4.80720600	1.78649100	1.95208800
H	-1.90310400	1.55382200	1.62725100
C	0.85247900	-1.77093100	-0.85551000

H	-0.17546900	-1.95629900	-1.14718300
C	1.76994700	4.26062500	-0.56599500
H	2.74883800	3.79740700	-0.41662600
H	1.77000700	4.86542300	-1.47668600
H	1.56654600	4.92126200	0.28562500
O	0.94911900	2.13383300	0.02549200
C	2.35459500	-0.31136200	0.16337900
H	2.51109400	0.63688500	0.66669000
S	5.06602900	-0.72032700	0.37881600
O	5.73394900	-0.40701000	-0.90238000
O	4.90585800	0.44809900	1.26654600
O	5.61998400	-1.91463900	1.04790700
C	1.86067800	-2.68241300	-1.12765200
H	1.61994700	-3.60640700	-1.64198000
O	-5.09634200	-1.66724800	0.22316600
C	-5.63972300	-2.08589100	-1.03689200
H	-5.19295700	-1.52011400	-1.86077700
H	-5.49268600	-3.15990600	-1.18905800
H	-6.70620300	-1.86792100	-0.95966000

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C	3.57516000	-1.91156300	0.58691600
C	3.16978500	-0.68939400	0.05693500
H	4.61044000	-2.08245900	0.86972900
N	0.92951800	-1.46213100	-0.12043900
C	-2.48421900	-3.21938600	0.49670400
O	-3.18575000	-2.35197200	1.03637700
Pd	-1.02875400	-1.00732800	-0.49441500
C	-1.36423700	1.83749200	-0.30809400
C	-2.87337800	1.60910500	-0.36621400
C	-3.12142800	0.25164800	-1.04804900
H	-2.93253000	-0.61509000	-0.34985800
H	-4.19482100	0.10190500	-1.20737800
N	-0.80360800	2.97139200	0.08287200
C	0.63441900	3.21102000	-0.01649600
H	0.98325100	2.91495200	-1.00818500
H	0.80014600	4.28187300	0.11149600
H	1.17668600	2.65451100	0.75350800
O	-0.53878600	0.94812700	-0.69725500
C	-3.47446900	1.56657200	1.04824400

H	-3.45052100	2.54482600	1.53440900
H	-4.52220700	1.25432500	0.97533400
H	-2.94978700	0.83657800	1.67739500
C	-3.53630400	2.69749200	-1.23039000
H	-3.43518000	3.69115300	-0.78715900
H	-3.10110300	2.71878800	-2.23638800
H	-4.60408100	2.47194500	-1.32772900
H	-2.65036800	0.16551500	-2.03263300
C	1.30251200	-2.64813200	0.38914300
H	0.52629400	-3.39453300	0.51063400
C	-2.71887200	-4.68951500	0.70878400
H	-2.16549000	-4.99984100	1.60391500
H	-3.78116700	-4.87937500	0.88248300
H	-2.35901500	-5.27828100	-0.13877500
O	-1.46665800	-2.94047400	-0.26982300
C	1.85032000	-0.49715400	-0.30122500
H	1.51416300	0.43422200	-0.73667800
S	4.33430000	0.66524000	-0.10775700
O	5.43380300	0.12659900	-0.93383600
O	3.57458600	1.75771300	-0.74758300
O	4.74831000	0.96524200	1.28023300
C	2.61974100	-2.90684300	0.74006800
H	2.87831800	-3.87920400	1.14484400
O	-1.59807800	3.99722000	0.52997400
C	-1.39484500	4.25102000	1.92796600
H	-1.52025300	3.33170300	2.50852800
H	-0.40590900	4.68528500	2.10654100
H	-2.16888400	4.97579400	2.18567000

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C	-3.87905500	1.50469400	-0.45168100
C	-3.24732900	0.32624200	-0.06531100
H	-4.95991200	1.55361600	-0.55136700
N	-1.12016100	1.36511900	-0.24928900
C	1.87383500	3.66787600	0.70026700
O	2.59684100	3.02678300	1.47238500
Pd	0.90157600	1.14009300	-0.23062200
C	1.62642500	-1.68765300	-0.27478300
C	3.09074100	-1.25415100	-0.30726100
C	3.14864600	0.28390000	-0.33343900

H	2.75683400	0.72709400	0.61176600
H	4.18371700	0.63880600	-0.33523700
N	1.24655500	-2.95658500	-0.19849100
C	-0.14730000	-3.37979200	-0.29747700
H	-0.64678800	-2.80287000	-1.07831600
H	-0.14998500	-4.43374100	-0.58085400
H	-0.66777500	-3.24505400	0.65479500
O	0.66576900	-0.85980100	-0.38737500
C	3.86878900	-1.73180500	0.93107900
H	4.08040000	-2.80184500	0.89725800
H	4.82908100	-1.20558700	0.96173500
H	3.33115900	-1.49818900	1.85694200
C	3.72394500	-1.79251800	-1.60395800
H	3.74269200	-2.88627300	-1.62111100
H	3.17647400	-1.43765700	-2.48491900
H	4.75486100	-1.42763600	-1.67516200
H	2.73950100	0.70390500	-1.27419500
C	-1.71109000	2.51407900	-0.61651000
H	-1.05666100	3.35132600	-0.83230700
C	1.84335000	5.17307600	0.67007500
H	2.05272700	5.53225900	-0.34308300
H	0.84017800	5.51986200	0.94329700
H	2.57508900	5.58120800	1.37116500
O	1.05984100	3.12024500	-0.15775200
C	-1.87003400	0.28643800	0.03606100
H	-1.35024800	-0.61151100	0.34529400
S	-4.18090700	-1.16274000	0.30368700
O	-5.20125300	-1.23369500	-0.76134200
O	-3.18109000	-2.24918000	0.26243100
O	-4.75619300	-0.94203400	1.64825600
C	-3.08984200	2.61643800	-0.72012300
H	-3.53050700	3.55906000	-1.02563500
O	2.19975900	-3.94124300	-0.11055800
C	2.15069800	-4.61184800	1.15632000
H	2.27232700	-3.89896300	1.97759500
H	1.21433900	-5.16705900	1.26974700
H	2.98968300	-5.30941100	1.12875000

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C	-3.21679300	-2.50135400	-0.04584500
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C	-3.44670800	-1.12909000	-0.03012200
H	-4.04330600	-3.20527500	0.00791400
N	-1.12191900	-0.68963300	-0.21186100
C	-0.56449900	3.03706000	0.57533200
O	0.45516400	2.98760400	1.27704100
Pd	0.43794300	0.61740200	-0.41922600
C	3.02895100	-0.65793200	-0.24728100
C	3.63058300	0.73391200	-0.44160500
C	2.54727900	1.65203800	-1.03147200
H	1.79933400	1.95779100	-0.23950600
H	2.96398100	2.64203300	-1.24460300
N	3.75341000	-1.71435700	0.09798100
C	3.20811300	-3.06374900	0.17822500
H	2.57283300	-3.24884000	-0.69045100
H	4.04635000	-3.76238600	0.15508700
H	2.63128100	-3.20013800	1.09746700
O	1.79581000	-0.90265100	-0.45673100
C	4.07621700	1.32457000	0.90700700
H	4.93640200	0.79729800	1.32498900
H	4.36942800	2.36843500	0.75064000
H	3.25391400	1.31205100	1.63383200
C	4.79348200	0.67745700	-1.44969700
H	5.65318800	0.13081600	-1.05673800
H	4.47734800	0.20662400	-2.38797400
H	5.11262600	1.70102300	-1.67508500
H	2.13460400	1.28978500	-1.98077600
C	-0.88070500	-2.01248300	-0.20957600
H	0.15519700	-2.32149800	-0.27737200
C	-1.56521100	4.15425300	0.67103500
H	-2.56686500	3.74589500	0.84141700
H	-1.29221300	4.83066600	1.48429200
H	-1.59068300	4.70715800	-0.27464600
O	-0.85410900	2.13052500	-0.31828000
C	-2.38818800	-0.24451300	-0.12151400
H	-2.53814300	0.82931600	-0.13177600
S	-5.11588500	-0.50433600	0.15012300
O	-5.49263800	-0.84706200	1.53818300
O	-5.02357900	0.94719200	-0.10265900
O	-5.90021600	-1.24370300	-0.85962300
C	-1.90415800	-2.94419700	-0.13689700
H	-1.66296000	-4.00155200	-0.14873200

O	5.08561400	-1.55479600	0.39398800
C	5.35187200	-1.82181600	1.77864000
H	4.71939400	-1.20190700	2.42213100
H	5.20366200	-2.88217700	2.00760700
H	6.40317600	-1.56014300	1.90912900

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C	3.26369200	-0.60410100	-0.04160600
C	3.80469400	-1.87246100	-0.22669400
C	2.93357500	-2.92577400	-0.48375200
H	4.87720100	-2.03853900	-0.17728800
H	3.30404800	-3.93367700	-0.63726000
N	1.06272000	-1.44943900	-0.36874500
C	-2.38546300	-3.11935200	0.74542500
O	-3.17083500	-2.15536000	1.00215700
Pd	-0.97277600	-1.02319300	-0.47652200
C	-1.44918300	1.75999700	-0.46782200
C	-2.87301700	1.27421800	-0.21587200
C	-2.94441000	-0.16617300	-0.77041500
H	-2.82649700	-1.18582400	0.18580200
H	-3.98199600	-0.51755000	-0.66933500
N	-1.05393200	3.02081900	-0.35313800
C	0.31269000	3.47169300	-0.58745400
H	0.74151500	2.90419800	-1.41424300
H	0.26506700	4.52699300	-0.86530700
H	0.92732800	3.34526100	0.30842800
O	-0.55323500	0.93120500	-0.83041700
C	-3.15002100	1.24852600	1.29927300
H	-3.27287600	2.25439800	1.70939100
H	-4.08149300	0.69840600	1.47800500
H	-2.34720800	0.73861900	1.84520500
C	-3.92326800	2.12584200	-0.94964400
H	-4.02145300	3.12643000	-0.52277900
H	-3.68205900	2.22163600	-2.01474200
H	-4.89509100	1.62557100	-0.86745700
H	-2.76895900	-0.20685000	-1.85337300
C	1.89496400	-0.42698800	-0.11707300
H	1.44310600	0.54650900	0.02965600
O	5.48765700	0.68904100	-0.48456400
O	3.44030700	1.98751300	0.04486400

O	4.56829000	0.67557500	1.80673800
S	4.28288300	0.81544500	0.36149400
C	-2.66439800	-4.47007900	1.31732200
H	-2.50393600	-4.42928300	2.40082800
H	-3.71218500	-4.73174200	1.14375100
H	-2.00510300	-5.22299300	0.88190600
O	-1.35612300	-2.95882600	0.01435700
C	1.56881400	-2.68150800	-0.54387000
H	0.85783800	-3.47904000	-0.73589500
O	-1.94676300	3.95182000	0.11818700
C	-1.60259700	4.41612500	1.43102400
H	-1.38416200	3.57614900	2.09796300
H	-0.75162400	5.10384700	1.39203900
H	-2.49224300	4.95002100	1.77034700

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C	-3.36045100	-2.28388500	-0.70578400
C	-3.42911600	-1.02177600	-0.12321200
H	-4.22395800	-2.94400200	-0.70967800
N	-1.16656500	-0.58397600	-0.70539300
C	-0.21723500	3.20791500	0.18708000
O	0.99425900	3.19978800	0.56699900
Pd	0.51905000	0.63248500	-0.67590700
C	2.88651900	-0.80732000	-0.16270500
C	3.44906700	0.60525600	-0.05341600
C	2.49357200	1.50865700	-0.85888500
H	1.56273000	2.20513900	-0.08000400
H	2.91132500	2.52572300	-0.86884500
N	3.54982600	-1.89692400	0.19832800
C	3.03665100	-3.24663400	0.01812000
H	2.56048100	-3.32509600	-0.96111000
H	3.88559900	-3.93216100	0.04966200
H	2.31265600	-3.50277000	0.79729800
O	1.73054700	-1.00246000	-0.66173700
C	3.46256800	1.06212800	1.41748800
H	4.24591500	0.56089000	1.99264400
H	3.65674800	2.14113200	1.44996600
H	2.49428600	0.88747700	1.90223600
C	4.85150900	0.71157900	-0.67854200
H	5.60594500	0.15639400	-0.11643800

H	4.84917000	0.34655200	-1.71234100
H	5.14561500	1.76752400	-0.69497900
H	2.45911000	1.23610500	-1.92238200
C	-1.08479300	-1.80345000	-1.26444600
H	-0.13274000	-2.07497700	-1.70664200
C	-1.10832100	4.34717000	0.55858300
H	-1.92984700	4.44337400	-0.15417000
H	-1.53132500	4.14383500	1.54980600
H	-0.53175900	5.27361800	0.61485500
O	-0.70585500	2.25019000	-0.49641500
C	-2.32341600	-0.18902900	-0.14848300
H	-2.35449200	0.80821400	0.27745400
S	-4.92798900	-0.49029400	0.70348800
O	-4.95493200	-1.26354200	1.96438700
O	-4.76832300	0.96326300	0.90747500
O	-6.02338400	-0.85607700	-0.21911600
C	-2.16265300	-2.67496500	-1.29058300
H	-2.05514800	-3.64429100	-1.76528700
O	4.76044500	-1.76272500	0.83362600
C	4.67984500	-2.15685800	2.21008400
H	3.85477400	-1.64224600	2.71298900
H	4.56237700	-3.24198000	2.29956600
H	5.63670400	-1.85195100	2.63724400

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C	-3.31403300	-2.30002100	0.74462500
C	-3.50177600	-1.06300400	0.13428900
H	-4.15801900	-2.95529300	0.94304100
N	-1.16873900	-0.62072000	0.22402400
C	-0.15960700	3.22846700	0.55087000
O	1.10671600	3.26019500	0.65858500
Pd	0.44342000	0.60200900	-0.23554000
C	2.91541900	-0.78859200	-0.35733100
C	3.43589200	0.64078000	-0.44023800
C	2.26872700	1.49301200	-0.98312200
H	1.54578600	2.22017500	-0.02332600
H	2.63776900	2.51751100	-1.13584300
N	3.68387100	-1.87037800	-0.30313000
C	3.15139100	-3.22330000	-0.23613300
H	2.29357900	-3.30227700	-0.90625200

H	3.93262000	-3.90600300	-0.57606900
H	2.84387600	-3.47834000	0.78287600
O	1.66217300	-1.00953400	-0.35697800
C	3.79936100	1.11833200	0.97895800
H	4.70794900	0.63219400	1.34625400
H	3.97786200	2.19972300	0.95443300
H	2.98292500	0.92923400	1.68641000
C	4.63089000	0.79773500	-1.39489600
H	5.54516800	0.35117400	-0.99849700
H	4.41818000	0.34693200	-2.37136700
H	4.81387900	1.86702700	-1.55118200
H	1.96048700	1.18413200	-1.99119300
C	-0.97242000	-1.81439500	0.80712700
H	0.05404500	-2.07100700	1.05001700
C	-0.97234600	4.40377300	0.98201600
H	-2.03024500	4.23981200	0.76986900
H	-0.82833800	4.56132300	2.05638400
H	-0.61473100	5.29930400	0.46411700
O	-0.75991600	2.21015300	0.07865400
C	-2.41410300	-0.24270900	-0.11072100
H	-2.52651900	0.72447000	-0.58999000
S	-5.15239300	-0.51974300	-0.30438200
O	-5.80118100	-0.20961900	0.98823000
O	-4.95975400	0.66220500	-1.16922600
O	-5.75998900	-1.67602400	-0.99596400
C	-2.02157600	-2.67817400	1.08497500
H	-1.82135500	-3.63251300	1.56001500
O	5.03878000	-1.72183600	-0.13103800
C	5.44878000	-2.10745300	1.18828800
H	4.83070500	-1.61278900	1.94463100
H	5.40321800	-3.19472800	1.31057300
H	6.48396300	-1.76993800	1.26343000

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C	3.84258800	-1.61994400	0.72472900
C	3.38621400	-0.44804900	0.12840000
H	4.89429800	-1.74812200	0.96649500
N	1.15963000	-1.28771600	0.08135200
C	-2.33181700	-3.28667400	0.24742800
O	-3.24369400	-2.41433800	0.38487900

Pd	-0.84957200	-0.98097400	-0.40332400
C	-1.59572600	1.73836800	-0.24114400
C	-2.98213800	1.13013100	-0.41013800
C	-2.76524300	-0.23706800	-1.09254200
H	-2.79468800	-1.33955800	-0.22340400
H	-3.75034300	-0.67176300	-1.31288500
N	-1.36627300	3.00464200	0.07609100
C	-0.02795700	3.57800500	0.14633000
H	0.53909900	3.28335400	-0.73926400
H	-0.13365500	4.66391700	0.14979000
H	0.49709800	3.24511500	1.04659300
O	-0.55783800	1.03011900	-0.44676000
C	-3.64392600	0.91867300	0.96373700
H	-3.94586800	1.86508000	1.42085400
H	-4.54552800	0.31028600	0.82732300
H	-2.97798600	0.38480800	1.65210800
C	-3.87515000	1.99166700	-1.32013800
H	-4.14167800	2.94539300	-0.85819400
H	-3.38110100	2.19353900	-2.27786500
H	-4.79983900	1.44049400	-1.52697900
H	-2.30785900	-0.13643900	-2.08618600
C	1.58858500	-2.42343600	0.65742600
H	0.84015700	-3.18478500	0.84939000
C	-2.58643400	-4.70574300	0.63445600
H	-2.23882000	-4.84649100	1.66510800
H	-3.65488600	-4.92729000	0.59345700
H	-2.02253800	-5.38319900	-0.01116900
O	-1.17886100	-2.97935100	-0.19903500
C	2.04472800	-0.30902500	-0.17906300
H	1.66224100	0.59276200	-0.64550600
S	4.52298400	0.89761100	-0.20208900
O	5.73966100	0.23902500	-0.72093400
O	3.83809600	1.76126000	-1.18585200
O	4.73072900	1.55163800	1.10885700
C	2.91997000	-2.62265000	0.99200200
H	3.22208000	-3.55576800	1.45513200
O	-2.42581800	3.81006000	0.41673100
C	-2.42166200	4.12593500	1.81675900
H	-2.33809500	3.21592900	2.41908500
H	-1.60891800	4.81843700	2.05900400
H	-3.38452600	4.61035400	1.98880600

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C	3.79280500	-1.95987700	0.19818500
C	3.30255700	-0.66207500	0.08414100
H	4.85825300	-2.14985900	0.29920600
N	1.06566900	-1.46543400	-0.06989200
C	-2.57504700	-3.16558100	0.40924000
O	-3.38369300	-2.21325100	0.63820100
Pd	-0.95481400	-0.99212600	-0.35699600
C	-1.40998300	1.80970200	-0.29791700
C	-2.85566000	1.33274900	-0.25464300
C	-2.85474300	-0.07851900	-0.88430400
H	-2.89418900	-1.16872200	0.00627900
H	-3.89929600	-0.41315100	-0.95822000
N	-1.01349500	3.06761400	-0.16666700
C	0.37686500	3.48870300	-0.30517400
H	0.83438200	2.95537300	-1.14075900
H	0.37009600	4.55772100	-0.52813600
H	0.94526800	3.29860500	0.61030500
O	-0.47752100	0.96779200	-0.49997700
C	-3.32181200	1.24013500	1.20912400
H	-3.43575200	2.22974200	1.66189000
H	-4.29670800	0.73944400	1.23775300
H	-2.62532600	0.64854900	1.81531700
C	-3.80036700	2.22584300	-1.07691600
H	-3.98801400	3.18820700	-0.59691900
H	-3.39553600	2.40836200	-2.07944500
H	-4.76035800	1.70916000	-1.18954600
H	-2.52065700	-0.06478800	-1.93027700
C	1.52280200	-2.72307800	0.04518200
H	0.78137200	-3.51504100	0.02431800
C	-2.96082400	-4.56464000	0.75707000
H	-3.89191900	-4.81971400	0.24064700
H	-2.17259000	-5.26608900	0.47846500
H	-3.15007500	-4.62579800	1.83404800
O	-1.43589500	-2.95400900	-0.11726600
C	1.94421000	-0.44869800	-0.04046300
H	1.54071600	0.55245900	-0.12152900
S	4.39997500	0.75475500	0.06760300
O	5.20930200	0.59253200	-1.16032900

O	3.50785700	1.93262800	0.03982400
O	5.19856400	0.63521800	1.30699600
C	2.87552100	-3.00389700	0.18509100
H	3.19837500	-4.03548300	0.27699700
O	-1.93946500	4.03611800	0.13122700
C	-1.78244900	4.53214300	1.46718800
H	-1.77648000	3.70938500	2.18935300
H	-0.86651100	5.12528500	1.55889000
H	-2.65489300	5.16912800	1.62321300

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C	-3.30468100	-2.49457600	-0.02954900
C	-3.48993900	-1.11613000	0.01264700
H	-4.14974700	-3.17422500	0.04103700
N	-1.15172400	-0.74491000	-0.22654800
C	-0.33163400	3.15121000	0.29588500
O	0.90918700	3.25552000	0.53561100
Pd	0.47705300	0.55853300	-0.45152200
C	2.99787700	-0.72347600	-0.23432000
C	3.46086600	0.72735900	-0.19740400
C	2.35805500	1.54099600	-0.90788200
H	1.47301400	2.23117900	-0.08035100
H	2.71205000	2.57853500	-0.99425600
N	3.78900900	-1.77091200	-0.04437800
C	3.34597700	-3.14863600	-0.20295100
H	2.71123900	-3.21806400	-1.08946100
H	4.23652000	-3.76142700	-0.35445300
H	2.79538300	-3.49510800	0.67686400
O	1.78276800	-0.99786700	-0.49798800
C	3.58570400	1.19526800	1.26499900
H	4.45452500	0.74953700	1.75897700
H	3.71159800	2.28463000	1.27783800
H	2.68506500	0.95539400	1.84258800
C	4.78117600	0.94874800	-0.95590400
H	5.63840100	0.50524200	-0.44596800
H	4.72743300	0.53748500	-1.97074400
H	4.95626600	2.02744200	-1.04094800
H	2.22065300	1.23188600	-1.95288100
C	-0.96048900	-2.07486600	-0.25857800
H	0.06338300	-2.41790300	-0.35982600

C	-1.25807200	4.27058200	0.63331400
H	-2.28505100	3.90656500	0.70744500
H	-0.94146500	4.74527000	1.56567500
H	-1.20230500	5.01872400	-0.16669000
O	-0.81492300	2.11124400	-0.25650000
C	-2.40201300	-0.26728600	-0.08819400
H	-2.52082300	0.81107500	-0.06213300
S	-5.13272100	-0.43902600	0.23684800
O	-5.49685800	-0.78749700	1.62764400
O	-4.99647800	1.01267800	0.00229000
O	-5.96689300	-1.13352400	-0.76664600
C	-2.01034700	-2.97709100	-0.16770600
H	-1.80656100	-4.04183300	-0.20446400
O	5.08143900	-1.56845000	0.36935400
C	5.26765700	-1.95657600	1.73711700
H	4.50623900	-1.49801500	2.37591200
H	5.24673000	-3.04653200	1.84129100
H	6.25882000	-1.57717200	1.99249400

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C	3.28250200	-0.60693300	-0.03971000
C	3.83982300	-1.85925000	-0.27933600
C	2.97744200	-2.91894600	-0.54320600
H	4.91631500	-2.00666400	-0.27024800
H	3.36048200	-3.91483300	-0.74015800
N	1.07897500	-1.47769100	-0.32975500
C	-2.24091100	-3.40762900	0.70504500
O	-2.59418900	-2.71769400	1.77663300
Pd	-1.04300700	-0.93338200	-0.50228700
C	-1.47136200	1.84432000	-0.44168600
C	-2.86515100	1.30552900	-0.15157000
C	-2.86794900	-0.14331500	-0.71121700
H	-2.31496000	-1.78211000	1.71512300
H	-3.66369700	-0.72949500	-0.23473300
N	-1.10842900	3.12322200	-0.41559900
C	0.26751200	3.56493800	-0.61552100
H	0.71925200	2.98905700	-1.42450000
H	0.23780300	4.61835000	-0.90193800
H	0.85917700	3.43700500	0.29643700
O	-0.54818400	1.02025100	-0.73067600

C	-3.05913600	1.28311700	1.37628600
H	-3.16645700	2.29210400	1.78621000
H	-3.97704300	0.73203500	1.61102300
H	-2.22218900	0.78925300	1.88526200
C	-3.99724600	2.09899300	-0.81997000
H	-4.18086000	3.06133900	-0.33530700
H	-3.78319200	2.27853300	-1.87999900
H	-4.91806300	1.50582200	-0.76084200
H	-3.04813300	-0.13410600	-1.79645500
C	1.90765900	-0.45498700	-0.07227600
H	1.44895400	0.51161700	0.10742900
O	5.49118300	0.72006900	-0.46803000
O	3.41887300	1.98548400	0.05034200
O	4.55962700	0.69450800	1.81802900
S	4.27795000	0.82474800	0.36986800
C	-2.60242900	-4.84751500	0.76382800
H	-2.22724700	-5.28139500	1.69609400
H	-3.69431700	-4.94101300	0.76732400
H	-2.18792100	-5.36985800	-0.09919300
O	-1.66828300	-2.90584500	-0.26710000
C	1.60702400	-2.68925200	-0.55916000
H	0.90234400	-3.48980000	-0.76941300
O	-2.01952400	4.06451800	0.00261500
C	-1.69690400	4.59165600	1.29697600
H	-1.45695000	3.78604000	1.99787000
H	-0.86521600	5.30119900	1.23508500
H	-2.60201600	5.11315100	1.61432100

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C	-3.28739500	-2.56783200	-0.35567600
C	-3.42422300	-1.22262600	-0.02351100
H	-4.13068900	-3.24957600	-0.27833000
N	-1.13679700	-0.80647400	-0.55403400
C	-0.84559100	3.13039000	-0.03843100
O	-0.31345400	3.17607100	1.17148700
Pd	0.59834400	0.53636100	-0.61032200
C	3.13105200	-0.61355100	-0.13836100
C	3.37453200	0.85194800	0.17727800
C	2.28432000	1.60660300	-0.62578700
H	0.20088500	2.36797300	1.37014900

H	2.15959600	2.62091700	-0.22622400
N	4.05245300	-1.57216500	-0.11035100
C	3.76472900	-2.94931900	-0.47766400
H	3.17967800	-2.95568100	-1.40049200
H	4.71935800	-3.44811500	-0.65714000
H	3.20674100	-3.46620900	0.31037900
O	1.96312500	-0.97862600	-0.48434400
C	3.15360200	1.04777100	1.68972800
H	3.95466600	0.58325800	2.27401800
H	3.15313300	2.12063100	1.91425900
H	2.19524600	0.62672200	2.01674600
C	4.75358800	1.38774700	-0.23575500
H	5.55245400	1.07031100	0.43905900
H	5.01499600	1.07707300	-1.25405400
H	4.71211600	2.48383000	-0.22238600
H	2.56781500	1.68214500	-1.68609300
C	-0.99516500	-2.10496300	-0.86085800
H	-0.00566700	-2.42064100	-1.18133300
C	-1.72727400	4.28116000	-0.36182200
H	-1.92917300	4.30516900	-1.43370200
H	-2.67060400	4.15929100	0.18340100
H	-1.26182400	5.21381800	-0.03051800
O	-0.64832400	2.20097300	-0.82772100
C	-2.33687600	-0.37247000	-0.13797400
H	-2.42430500	0.67999000	0.11156200
S	-4.98750600	-0.60565700	0.59184500
O	-5.19239500	-1.30740400	1.87877800
O	-4.80674100	0.85361300	0.73852100
O	-5.98181100	-0.98813300	-0.43422300
C	-2.04331900	-3.01382700	-0.78324000
H	-1.87877400	-4.05300800	-1.04791800
O	5.26900600	-1.31572200	0.47496200
C	5.36533500	-1.91315000	1.77569000
H	4.48012800	-1.67813900	2.37530200
H	5.49536900	-2.99767200	1.69656200
H	6.25639600	-1.46715700	2.22137500

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C	-3.34073800	-2.43034300	0.75555800
C	-3.51085300	-1.18995600	0.14615600

H	-4.19324000	-3.07520700	0.95218600
N	-1.16632900	-0.76974100	0.23868400
C	-0.81260300	3.12236000	0.33980700
O	-0.08884100	3.25915500	1.43891300
Pd	0.55751700	0.50227800	-0.22479100
C	3.13532500	-0.65950700	-0.24541500
C	3.45277000	0.82210500	-0.14534400
C	2.19872600	1.53056200	-0.71180900
H	0.50116600	2.49030200	1.57913600
H	2.17144100	2.57334400	-0.37083300
N	4.02178900	-1.63422000	-0.41060500
C	3.66405000	-3.04048900	-0.52158600
H	2.75189700	-3.13341200	-1.11486000
H	4.48278200	-3.54772300	-1.03670900
H	3.50214000	-3.48721600	0.46463900
O	1.91802100	-1.02214000	-0.14757700
C	3.60463800	1.13156000	1.35717100
H	4.49051700	0.64529400	1.77918500
H	3.71885800	2.21354600	1.49003900
H	2.72567000	0.80552500	1.92594300
C	4.68816100	1.31033800	-0.91507800
H	5.62559000	1.08573800	-0.39968200
H	4.73616000	0.87756600	-1.92070700
H	4.61279400	2.39962800	-1.02117600
H	2.21796300	1.52642200	-1.81205200
C	-0.99525300	-1.96638700	0.82054500
H	0.02682700	-2.23876100	1.06953900
C	-1.74988300	4.24336800	0.07454700
H	-2.41659400	3.97884600	-0.74748500
H	-2.32044000	4.47374300	0.97932900
H	-1.16757600	5.13333600	-0.19187500
O	-0.70928100	2.15295800	-0.41733100
C	-2.40850000	-0.38583700	-0.09589600
H	-2.50960700	0.57981400	-0.58251900
S	-5.15265900	-0.62616900	-0.29246500
O	-5.80315200	-0.31152800	0.99963100
O	-4.94971600	0.55842900	-1.15311900
O	-5.77755800	-1.77048900	-0.99009700
C	-2.05270700	-2.82368800	1.09590900
H	-1.86469400	-3.78224800	1.56811900
O	5.35930600	-1.33142200	-0.44174500

C	6.03575600	-1.75166900	0.74770900
H	5.53862500	-1.35516400	1.63846800
H	6.09574000	-2.84423100	0.79919000
H	7.03896000	-1.33167100	0.65237600

III2-trans_OMe-up_prod_conf-4

C	-3.99936000	1.32663600	0.78937000
C	-3.48809500	0.18758000	0.17343400
H	-5.05431800	1.39747800	1.04023700
N	-1.30208000	1.14056900	0.12248000
C	1.75391300	3.71333100	0.12371000
O	2.46014300	3.29006200	1.15982200
Pd	0.81294700	0.90295200	-0.41279400
C	1.88854500	-1.69734900	-0.20530100
C	3.13629900	-0.82946900	-0.22528000
C	2.69322500	0.47466900	-0.93469000
H	2.33927700	2.33087300	1.31259300
H	3.40725300	1.27974500	-0.72187300
N	1.87047800	-3.02373600	-0.11836100
C	0.63944600	-3.80055600	-0.11083200
H	-0.03578400	-3.41092900	-0.87605900
H	0.89747700	-4.83288900	-0.35580300
H	0.14239900	-3.75272300	0.86320100
O	0.75037200	-1.13428500	-0.27734700
C	3.51944500	-0.53465500	1.23855800
H	3.92314800	-1.42333500	1.73447200
H	4.29669300	0.23779200	1.25378400
H	2.65925900	-0.17499300	1.81603500
C	4.33414200	-1.42135600	-0.98318200
H	4.84694000	-2.20751500	-0.42349400
H	4.03122200	-1.82891600	-1.95437300
H	5.05267300	-0.61408900	-1.17171900
H	2.65220400	0.32527100	-2.02400400
C	-1.79131500	2.24211200	0.71138700
H	-1.08199300	3.04102000	0.90702700
C	1.86559900	5.17272800	-0.13541200
H	1.59709800	5.72693400	0.76986600
H	2.90561000	5.41434100	-0.38111300
H	1.21138800	5.45303500	-0.96193300
O	1.05894700	2.96632200	-0.57139900

C	-2.13997600	0.12474800	-0.14091900
H	-1.71293900	-0.74852500	-0.62568300
S	-4.56078800	-1.20282900	-0.18093200
O	-5.80703100	-0.59684400	-0.69701700
O	-3.83745500	-2.02123100	-1.17662200
O	-4.74593000	-1.88742300	1.11872600
C	-3.12842500	2.37437800	1.06085700
H	-3.47653900	3.28596900	1.53507300
O	3.04175800	-3.69403700	0.14021500
C	3.09138900	-4.17831400	1.48853500
H	2.85074100	-3.37961400	2.19711700
H	2.40869400	-5.02397900	1.62464900
H	4.12232200	-4.51068000	1.62417300

III3-cis_OMe-down_int

C	-2.11467800	0.11524700	-0.09583600
C	-2.56827600	-1.27077000	-0.57446100
C	-1.72507100	-1.64483600	-1.80581700
H	-0.66888100	-1.80592800	-1.56119600
H	-2.10719900	-2.58291200	-2.22302200
N	-2.80032200	0.81403700	0.82082800
O	-1.07801400	0.65497500	-0.56280800
C	-2.30975700	-2.30525900	0.53750500
H	-2.94079700	-2.15082400	1.41813000
H	-2.52120800	-3.30801600	0.14854400
H	-1.26135700	-2.28180300	0.86050500
C	-4.04597300	-1.26259400	-1.01133600
H	-4.75100200	-1.20330100	-0.17982100
H	-4.25123000	-0.43376900	-1.69982500
H	-4.25956500	-2.19742100	-1.54130500
H	-1.77816600	-0.87449300	-2.58296800
O	-2.23999100	2.02623200	1.17216600
C	-2.69023900	3.09006000	0.32718000
H	-2.44879800	2.88238100	-0.72036900
H	-3.76677800	3.25322000	0.45150500
H	-2.14052400	3.96807800	0.67166800
C	-4.05109800	0.55442000	1.51874900
H	-3.98994300	1.09501500	2.46611900
H	-4.91252000	0.91523200	0.94996200
H	-4.16744400	-0.50341600	1.74484700

Pd	0.89730900	-0.06543800	-0.35608100
N	2.71831100	-0.61695400	-0.07239000
O	1.74502900	1.75737800	-0.64031600
C	3.00971400	1.77649100	-0.31173200
C	3.63404200	0.47843300	0.20471300
C	2.47946700	-1.71198700	0.64365500
O	3.69562100	2.79985500	-0.38889200
O	1.29201200	-2.16461700	0.48376100
H	3.81801800	0.60520900	1.27923700
H	4.59862200	0.32829200	-0.28960300
C	3.45689100	-2.34668200	1.56671500
H	3.32879800	-1.91111700	2.56620300
H	3.26389200	-3.42100800	1.63123600
H	4.48656700	-2.16858400	1.24353700

III3-cis_OMe-down_pre-TS

Pd	0.72265400	0.09563100	0.03376800
N	2.65604500	-0.28826300	-0.02330600
O	1.34669400	1.97083400	0.15811800
C	2.64172400	2.13836000	0.19713700
C	3.49770100	0.89204100	0.12930700
C	3.15348300	-1.51013100	-0.22472300
O	3.14916800	3.25848000	0.29045300
O	2.40427700	-2.50549100	-0.39289300
H	4.09309300	0.85919900	1.05149200
H	4.19716100	1.01519900	-0.70638600
C	4.65310500	-1.68711300	-0.24976100
H	5.12281600	-1.28865800	0.65672900
H	4.87619300	-2.75369400	-0.33293400
H	5.09377800	-1.16615000	-1.10846400
C	-2.22721600	-0.04530000	0.13775100
C	-2.06846600	-1.56929000	0.09749900
C	-0.60602100	-1.90211700	-0.24993400
H	0.08773400	-1.65093200	0.60075900
H	-0.45580600	-2.98489300	-0.29224400
N	-3.42617000	0.54504500	0.20140000
C	-4.77770900	0.00639100	0.23655800
H	-5.37912800	0.71397500	0.81112800
H	-5.19578500	-0.09380600	-0.76884600
H	-4.81083100	-0.95037900	0.75306000

O	-1.22691000	0.72452500	0.12558800
C	-2.36945700	-2.14390100	1.49458000
H	-3.40705200	-1.99112200	1.80316300
H	-2.17899600	-3.22278300	1.48493300
H	-1.71848500	-1.68914400	2.25006700
C	-2.94087400	-2.21172500	-0.99532500
H	-4.00534000	-2.21500000	-0.75388900
H	-2.80398000	-1.70243400	-1.95647300
H	-2.63638800	-3.25626700	-1.12104800
H	-0.30178500	-1.53436200	-1.24169800
O	-3.40218100	1.92604200	0.23232600
C	-3.37275300	2.49174600	-1.08326500
H	-3.36288500	3.57022400	-0.91459300
H	-2.46582100	2.18664900	-1.61641300
H	-4.26917900	2.20900700	-1.64600100

III3-cis_OMe-down_TS

Pd	0.65515900	0.24021400	-0.18442100
N	2.56012700	-0.29601200	-0.17357800
O	1.47655400	2.05130700	0.29016200
C	2.77069400	2.09704100	0.23064300
C	3.51201400	0.79337000	-0.02943100
C	2.85796600	-1.56516500	-0.02491600
O	3.41934400	3.14087700	0.37790300
O	1.90859300	-2.43049200	-0.05014500
H	4.20139900	0.63002300	0.80709900
H	4.11462300	0.92721100	-0.93626600
C	4.26380600	-2.03537900	0.18422700
H	4.57097700	-1.82029400	1.21519700
H	4.31483400	-3.11443900	0.02335100
H	4.96274800	-1.52960000	-0.48888700
C	-2.17397900	-0.01422300	0.10533300
C	-1.76046800	-1.48027500	-0.02142800
C	-0.47081600	-1.49001600	-0.87395700
H	0.76704200	-1.72297100	-0.31409500
H	-0.26875600	-2.53990900	-1.13084900
N	-3.42372800	0.38994400	0.34310300
C	-4.63301100	-0.36671500	0.64389900
H	-5.29455900	0.31724600	1.17805200
H	-5.13157400	-0.71497600	-0.26380100

H	-4.41075400	-1.20353200	1.30682500
O	-1.28941300	0.88351900	-0.00519800
C	-1.45620500	-2.00693400	1.39458200
H	-2.37167900	-2.13117900	1.98310500
H	-0.95934500	-2.98127700	1.31544600
H	-0.78482300	-1.32902800	1.93419000
C	-2.78950000	-2.37815600	-0.72762900
H	-3.66963300	-2.59273200	-0.11924400
H	-3.11428700	-1.94384300	-1.68005700
H	-2.31464100	-3.34098600	-0.94508800
H	-0.61712200	-1.01248200	-1.85191700
O	-3.59790300	1.75738800	0.44163200
C	-3.77812000	2.37032300	-0.84031600
H	-3.96727200	3.42228000	-0.61760400
H	-2.86947600	2.27338900	-1.44412600
H	-4.64151400	1.93573100	-1.35551700

III3-cis_OMe-down_prod

Pd	-0.57755400	0.22481600	0.08034700
N	-2.54869400	-0.32069500	0.18169000
O	-1.52945100	2.05726300	-0.52098800
C	-2.75333900	2.11838900	-0.15325500
C	-3.38916500	0.85337900	0.42643900
C	-3.09001100	-1.46172500	-0.05358700
O	-3.46628700	3.13940100	-0.22274700
O	-2.33945600	-2.50644800	-0.43133800
H	-4.38460500	0.74877100	-0.01278500
H	-3.51273300	1.00576900	1.50576300
C	-4.54190200	-1.78909300	0.03160500
H	-5.05822400	-1.40660800	-0.85698300
H	-4.66878000	-2.87348600	0.06331100
H	-5.00136400	-1.34487300	0.91800500
C	2.23573500	-0.04096100	-0.10481800
C	1.78668400	-1.47697100	0.13857300
C	0.42097300	-1.34065000	0.85678100
H	-1.42479800	-2.21410600	-0.61165300
H	-0.07012100	-2.32015000	0.88953700
N	3.50046000	0.32811000	-0.31550400
C	4.71731600	-0.45854000	-0.44577400
H	5.39527800	0.13504500	-1.06343000

H	5.18425600	-0.65105400	0.52372900
H	4.52202000	-1.39439000	-0.96952000
O	1.35487500	0.86879600	-0.12355900
C	1.60638400	-2.14906000	-1.23625200
H	2.56253600	-2.26751200	-1.75893200
H	1.17389400	-3.14654700	-1.09525400
H	0.93349000	-1.56891200	-1.87823400
C	2.72519700	-2.30852500	1.02738200
H	3.62587800	-2.65147100	0.51167600
H	3.02338700	-1.75735000	1.92651300
H	2.18183900	-3.20328500	1.35319200
H	0.58147100	-1.03551500	1.90285900
O	3.70118300	1.68149500	-0.51183500
C	3.84952700	2.37530800	0.73182600
H	4.05245300	3.41052300	0.45019400
H	2.92354200	2.31947500	1.31495200
H	4.69440900	1.96886400	1.29801800

III3-cis_OMe-up_int

C	-2.14201500	0.22986200	-0.28429900
C	-2.73874100	-1.18511600	-0.21569800
C	-2.06509600	-2.03829000	-1.30531100
H	-0.99649700	-2.19272700	-1.11869000
H	-2.53982200	-3.02552300	-1.31684200
N	-2.65915600	1.25957100	0.40293600
O	-1.13692200	0.46960000	-1.00358000
C	-2.42580900	-1.81291100	1.15547100
H	-2.90146600	-1.28709300	1.98942000
H	-2.79225200	-2.84605200	1.16527100
H	-1.34402400	-1.83947200	1.33857400
C	-4.25271500	-1.17571000	-0.50504500
H	-4.85546900	-0.77475200	0.31198900
H	-4.47935900	-0.60337200	-1.41273300
H	-4.58465000	-2.20661100	-0.67033000
H	-2.18368300	-1.59167800	-2.29869900
O	-2.06749000	2.48378600	0.15531400
C	-0.99556900	2.75536600	1.06537600
H	-1.38136800	2.90312600	2.08084200
H	-0.25503600	1.95076000	1.05115800
H	-0.54774900	3.67921400	0.69462700

C	-3.84182600	1.37615200	1.24128900
H	-3.64812800	2.16701100	1.96918100
H	-4.71749900	1.65063500	0.64563300
H	-4.02529500	0.45745600	1.79402900
Pd	0.82196200	-0.19241000	-0.54025400
N	2.60679400	-0.72987900	-0.07910900
O	1.67776200	1.64754200	-0.71954000
C	2.88601500	1.67708100	-0.22956400
C	3.50061300	0.36308200	0.26357600
C	2.29630600	-1.82099900	0.61238800
O	3.53668200	2.72171300	-0.13109600
O	1.11417100	-2.24826500	0.35568100
H	3.65524000	0.45191500	1.34572900
H	4.48001000	0.23569400	-0.20873400
C	3.18974400	-2.47916600	1.59978800
H	2.98830100	-2.05946400	2.59370600
H	2.98326400	-3.55256700	1.62975200
H	4.24271300	-2.30460700	1.35893000

III3-cis_OMe-up_pre-TS

Pd	0.71266500	0.06399500	-0.07941200
N	2.64556600	-0.29169800	0.09692100
O	1.32289100	1.93743600	-0.26566400
C	2.60491900	2.13613700	-0.11032100
C	3.46023900	0.91616700	0.15149000
C	3.17778600	-1.51465400	0.11785400
O	3.09882400	3.26480100	-0.16341400
O	2.46442700	-2.54720300	0.03326800
H	3.92557300	1.05420100	1.13694200
H	4.26443400	0.90991900	-0.59364600
C	4.67850700	-1.65333100	0.22413800
H	5.10196200	-1.02504300	1.01483700
H	4.91628100	-2.70044400	0.42731000
H	5.15190400	-1.36246500	-0.72194800
C	-2.24459000	-0.06469400	-0.13625600
C	-2.11813800	-1.58531400	0.01107300
C	-0.64015200	-1.97133100	-0.17870300
H	-0.00950100	-1.59011800	0.67221200
H	-0.49744500	-3.04921400	-0.05627600
N	-3.42669600	0.56107400	-0.10432200

C	-4.79277000	0.06702600	-0.07161500
H	-5.38201800	0.77224300	0.51901500
H	-5.20467400	0.00963900	-1.08356800
H	-4.85535300	-0.90323800	0.41297000
O	-1.23304400	0.67652700	-0.27108400
C	-2.54249700	-2.01956100	1.42448500
H	-3.60326700	-1.85007700	1.62638200
H	-2.35180700	-3.09203200	1.53992400
H	-1.96245300	-1.48611700	2.18642400
C	-2.91672200	-2.30848000	-1.08905100
H	-3.99695800	-2.26703100	-0.93441300
H	-2.69219500	-1.88568900	-2.07521500
H	-2.63070300	-3.36580800	-1.09886600
H	-0.26817500	-1.73865400	-1.18648700
O	-3.38822400	1.91966600	-0.36293000
C	-3.06225500	2.67757700	0.80966600
H	-3.17586900	3.71935600	0.50368700
H	-3.76049400	2.44728200	1.62161700
H	-2.02888700	2.48679600	1.11590600

III3-cis_OMe-up_TS

Pd	0.65071800	0.18273700	-0.41457500
N	2.52560100	-0.34879300	-0.05330900
O	1.44523900	2.04635200	-0.15387200
C	2.72745100	2.08049600	0.03329900
C	3.46517600	0.75106600	0.10248300
C	2.75763500	-1.57649200	0.34914900
O	3.36580300	3.13411600	0.15880100
O	1.80323900	-2.43533900	0.30683500
H	3.98776300	0.71178300	1.06510600
H	4.22642900	0.75022500	-0.68733600
C	4.09247200	-2.00488400	0.87400100
H	4.22338400	-1.61799300	1.89222000
H	4.13818400	-3.09558400	0.90671200
H	4.91164400	-1.61874600	0.25983300
C	-2.17289600	-0.01066000	-0.19719100
C	-1.78107600	-1.48816600	-0.11107900
C	-0.45892300	-1.62964800	-0.89889000
H	0.72903200	-1.78211900	-0.21671000
H	-0.25913200	-2.70621200	-0.99912300

N	-3.39505300	0.44973900	0.07737600
C	-4.61254200	-0.23355000	0.49197000
H	-5.21901400	0.49732100	1.03080700
H	-5.17530000	-0.59490900	-0.37304200
H	-4.38904200	-1.05045200	1.17660200
O	-1.29709600	0.84191700	-0.52279600
C	-1.52554100	-1.85460600	1.36377400
H	-2.44973800	-1.86872700	1.95132200
H	-1.07316100	-2.85254400	1.41047900
H	-0.82577100	-1.14954600	1.82740600
C	-2.81517300	-2.43140900	-0.74903800
H	-3.72096800	-2.55350800	-0.15210600
H	-3.10044100	-2.09215600	-1.75164200
H	-2.36414500	-3.42476100	-0.84982700
H	-0.54953100	-1.29147600	-1.93919600
O	-3.58603100	1.79961800	-0.15380300
C	-3.23099300	2.58651000	0.99029500
H	-3.48766400	3.61121600	0.71483300
H	-3.81327300	2.27895800	1.86646000
H	-2.15887400	2.51147100	1.19522400

III3-cis_OMe-up_prod

Pd	0.57756800	0.21433600	-0.19576200
N	2.53547600	-0.36690600	-0.06298400
O	1.53811900	2.10483800	0.18010300
C	2.78595700	2.08768700	-0.10261100
C	3.42858400	0.73619500	-0.42339400
C	3.01631100	-1.46769200	0.39210600
O	3.51730200	3.09607600	-0.15539500
O	2.20049000	-2.40489700	0.89241100
H	4.38415200	0.68527200	0.10557000
H	3.63877100	0.71565700	-1.49990600
C	4.45288100	-1.86016600	0.43902100
H	4.94880000	-1.36454600	1.28227000
H	4.52333900	-2.94034900	0.58739100
H	4.97055800	-1.57981100	-0.48203500
C	-2.24288600	-0.01640900	-0.19795900
C	-1.80130500	-1.47639300	-0.22720600
C	-0.37371100	-1.44318300	-0.82516900
H	1.29268800	-2.05034500	0.96476800

H	0.11038800	-2.41462000	-0.66639100
N	-3.50914200	0.38060400	-0.05388200
C	-4.74463600	-0.37683500	0.05567900
H	-5.43775800	0.22242800	0.65001200
H	-5.18435300	-0.55741200	-0.92956700
H	-4.58576600	-1.31575800	0.58195400
O	-1.35650100	0.88582800	-0.27321800
C	-1.75141300	-1.99318300	1.22266200
H	-2.74749400	-2.05183500	1.67535000
H	-1.32336700	-3.00233900	1.22745500
H	-1.12471400	-1.35014700	1.85199400
C	-2.67706600	-2.38592300	-1.10637800
H	-3.60364100	-2.70418300	-0.62126700
H	-2.92705200	-1.90259700	-2.05788100
H	-2.10790100	-3.29432400	-1.33658800
H	-0.42909600	-1.28998000	-1.91424700
O	-3.72334700	1.74309900	-0.14428600
C	-3.57787500	2.38609600	1.12740800
H	-3.78131500	3.43997900	0.92784400
H	-4.30713800	1.99340900	1.84538000
H	-2.55910600	2.26544300	1.50913100

III3-trans_OMe-down_int

C	-1.96215500	0.20479800	-0.33904900
C	-2.51040200	-1.22436600	-0.40055200
C	-1.78305000	-1.97584800	-1.52623300
H	-0.70521600	-2.06126200	-1.35292200
H	-2.18484100	-2.99368600	-1.58536000
N	-2.46104600	1.13084900	0.47890700
O	-0.96922200	0.56816000	-1.03634900
C	-2.21952100	-1.90904700	0.94973100
H	-2.73730200	-1.41319200	1.77830200
H	-2.56713000	-2.94807200	0.90506600
H	-1.14309000	-1.92464000	1.16630100
C	-4.01932100	-1.25821600	-0.71048700
H	-4.63249100	-0.94293800	0.13554600
H	-4.26520400	-0.63585500	-1.57910700
H	-4.30016700	-2.28954900	-0.95302800
H	-1.93914700	-1.49344400	-2.49774500
Pd	0.98601200	-0.07167300	-0.52292200

N	2.76234400	-0.57998500	0.00190800
O	1.81710800	1.77894200	-0.68390100
C	3.00353800	1.83167400	-0.13943300
C	3.62695000	0.52782900	0.36914300
C	2.45043700	-1.67696900	0.68320400
O	3.62602000	2.88972200	-0.01287900
O	1.28827300	-2.13048000	0.38664000
H	3.75372300	0.61757200	1.45466200
H	4.61980400	0.41817000	-0.07919500
C	3.32200200	-2.31682300	1.70210600
H	3.08203800	-1.89617500	2.68693000
H	3.12921900	-3.39292700	1.72950900
H	4.37961600	-2.12888100	1.49405500
O	-3.54148200	0.83282700	1.27388900
C	-4.69564500	1.60280300	0.91697600
H	-5.49527800	1.20718500	1.54576200
H	-4.54250500	2.66397000	1.13978900
H	-4.93785000	1.46708700	-0.14186400
C	-1.83375300	2.43067600	0.68832900
H	-0.74623000	2.32090700	0.65767100
H	-2.14156100	3.15080800	-0.07512200
H	-2.13208600	2.78338900	1.67785300

III3-trans_OMe-down_pre-TS

Pd	0.82299900	0.18004600	0.02845000
N	2.71642700	-0.37663000	0.01428700
O	1.62044300	2.00142100	-0.12311400
C	2.92327700	2.05105200	-0.05374100
C	3.65587300	0.73491700	0.07603200
C	3.12055900	-1.64513400	-0.09976900
O	3.53796200	3.11942200	-0.08918100
O	2.30423000	-2.59607900	-0.18452400
H	4.20348200	0.75814200	1.02769400
H	4.40239700	0.69605400	-0.72597600
C	4.60512700	-1.92640600	-0.12379700
H	5.11864400	-1.47445600	0.73216600
H	4.75853900	-3.00780500	-0.10260200
H	5.06210200	-1.52388500	-1.03602300
C	-2.13579700	0.21058500	0.07880300
C	-2.07532700	-1.31540500	0.13271900

C	-0.61946400	-1.75971000	-0.07857800
H	0.04281500	-1.43214000	0.77316700
H	-0.51740600	-2.84488700	0.01629100
N	-3.28155200	0.88473600	0.14652400
O	-1.09611800	0.93386300	0.02454200
C	-2.54166600	-1.77260600	1.52681900
H	-3.59428800	-1.53246800	1.70164300
H	-2.41939600	-2.85857900	1.60640800
H	-1.94053200	-1.30493700	2.31560600
C	-2.91560700	-1.96919700	-0.97898000
H	-3.98678300	-1.90006100	-0.78139800
H	-2.70151000	-1.51815700	-1.95466400
H	-2.65724900	-3.03244400	-1.03653100
H	-0.25075800	-1.52684300	-1.08833100
O	-4.46645000	0.20185600	0.28210300
C	-5.33191000	0.39135400	-0.84334900
H	-6.18919500	-0.25193200	-0.63657200
H	-5.66015300	1.43382500	-0.91433400
H	-4.83933100	0.08492400	-1.77138900
C	-3.33218800	2.33687500	0.24791200
H	-3.17470300	2.80496100	-0.72826100
H	-4.31288000	2.60884800	0.64167900
H	-2.56364300	2.68118300	0.94398700

III3-trans_OMe-down_TS

Pd	-0.76908000	-0.27436200	-0.34362200
N	-2.58556000	0.46166900	-0.08592200
O	-1.75993900	-2.03878000	-0.02494700
C	-3.04771500	-1.92760400	0.08185900
C	-3.64705300	-0.53050500	-0.01680600
C	-2.70580900	1.71305300	0.28890600
O	-3.79960700	-2.89762000	0.24779500
O	-1.65660400	2.45783000	0.31145700
H	-4.29704700	-0.37898200	0.85109600
H	-4.27487800	-0.50282800	-0.91658600
C	-4.01531700	2.30941900	0.70221300
H	-4.19853000	2.08288300	1.75993300
H	-3.96794400	3.39459000	0.58658100
H	-4.85063600	1.91419100	0.11798000
C	2.05399800	-0.31465500	-0.07493200

C	1.82812400	1.19123000	-0.16704400
C	0.49550600	1.39958600	-0.91564100
H	-0.64733700	1.69097500	-0.18902300
H	0.38052600	2.47977900	-1.08478500
N	3.18642300	-0.87270800	0.34488700
O	1.11011200	-1.11763200	-0.35022400
C	1.70709900	1.74468400	1.26589900
H	2.65088100	1.65282600	1.81329700
H	1.43609600	2.80600000	1.21724400
H	0.92120000	1.22315700	1.82542700
C	2.93531100	1.92330600	-0.94512400
H	3.87339200	1.97741700	-0.38974500
H	3.12036600	1.44829000	-1.91547900
H	2.60476000	2.95102300	-1.13429100
H	0.52571700	0.99047700	-1.93466900
O	4.22696300	-0.06792400	0.74495500
C	5.38442200	-0.24231800	-0.08024800
H	6.10195000	0.48946600	0.29573600
H	5.79703700	-1.25090200	0.03029400
H	5.15030300	-0.03822500	-1.12978300
C	3.31755400	-2.29575500	0.63016600
H	3.62676600	-2.85373200	-0.25847200
H	4.05907400	-2.40726000	1.42408600
H	2.35582700	-2.68084900	0.97724500

III3-trans_OMe-down_prod

Pd	0.67930400	-0.31649400	0.15542600
N	2.56829700	0.47885300	0.14887300
O	1.85998000	-2.07513300	-0.29959300
C	3.08617200	-1.93562100	0.03323100
C	3.55739300	-0.54916700	0.47501000
C	2.95965400	1.63843900	-0.24453800
O	3.93416300	-2.85007500	0.04189600
O	2.07880400	2.53615100	-0.70599800
H	4.52349500	-0.36096900	0.00044200
H	3.71903700	-0.58185900	1.55951400
C	4.36371400	2.14122100	-0.26640200
H	4.90128200	1.69723400	-1.11292200
H	4.35579900	3.22570900	-0.39622700
H	4.89497800	1.88596600	0.65431400

C	-2.15347200	-0.30854900	-0.01703900
C	-1.83798000	1.16608100	0.17523800
C	-0.44924600	1.19509000	0.85060700
H	1.20163800	2.12037700	-0.81301700
H	-0.04124100	2.21129600	0.80370500
N	-3.35591300	-0.79295700	-0.31633900
O	-1.20378700	-1.15127500	0.02747600
C	-1.77275300	1.78881000	-1.23326300
H	-2.75617400	1.78899900	-1.71618600
H	-1.43267300	2.82799300	-1.15219500
H	-1.07113600	1.24511500	-1.87728300
C	-2.82612400	1.94634000	1.05618000
H	-3.77465100	2.15412700	0.55509800
H	-3.02866500	1.42000100	1.99573000
H	-2.36468400	2.90832400	1.31057500
H	-0.54911300	0.94380700	1.91840600
O	-4.40128300	0.08193900	-0.49555300
C	-5.41356600	-0.09042400	0.50277700
H	-6.13796400	0.70128000	0.30339800
H	-5.89917100	-1.06675600	0.40051000
H	-4.99095500	0.02404800	1.50591000
C	-3.59205600	-2.18298000	-0.68255000
H	-3.76310400	-2.80170000	0.20329900
H	-4.46947600	-2.21229600	-1.33211200
H	-2.72533400	-2.56156400	-1.22961600

III3-trans_OMe-up_int

C	-1.96089800	0.30480300	-0.52160500
C	-2.93173700	-0.86822100	-0.36409400
C	-2.58861200	-1.90602800	-1.44222900
H	-1.58138100	-2.31754700	-1.30722900
H	-3.30387200	-2.73352500	-1.37410000
N	-2.04181500	1.40674900	0.22423700
O	-1.05430300	0.26841200	-1.40781800
C	-2.74573200	-1.52472400	1.01768100
H	-3.13520800	-0.90669500	1.83030300
H	-3.29344500	-2.47439600	1.03215900
H	-1.68789100	-1.74693600	1.21100800
C	-4.38226000	-0.39776900	-0.57037400
H	-4.70895400	0.30187900	0.20352300

H	-4.49851000	0.08840300	-1.54683800
H	-5.04918600	-1.26771900	-0.54756200
H	-2.65473700	-1.48159200	-2.44973700
Pd	0.88485000	-0.23327200	-0.68534600
N	2.56698700	-0.80356200	0.05083200
O	1.83925700	1.56669800	-0.83466100
C	2.98084700	1.57390900	-0.20560800
C	3.43987400	0.28056400	0.47202100
C	2.10656700	-1.83160100	0.75820900
O	3.68092600	2.58644100	-0.11428000
O	0.95098100	-2.22805100	0.36712300
H	3.40462600	0.44421700	1.55608600
H	4.48057000	0.08780700	0.19301200
C	2.81936700	-2.46908100	1.89498700
H	2.42041700	-2.06609300	2.83433300
H	2.63856600	-3.54795900	1.88028500
H	3.89389600	-2.26825600	1.85583900
O	-2.98310300	1.47767800	1.22553200
C	-2.38453200	1.54940700	2.52400500
H	-3.22042700	1.42969700	3.21591700
H	-1.65699800	0.74332800	2.66530300
H	-1.91196700	2.52386700	2.68535700
C	-1.18994800	2.57444900	0.05996900
H	-0.31283500	2.52429300	0.71294900
H	-0.86289800	2.63468900	-0.97860200
H	-1.78676400	3.45705700	0.30347600

III3-trans_OMe-up_pre-TS

Pd	0.81263200	0.18469300	-0.03557400
N	2.69924400	-0.36913000	0.11829200
O	1.61295300	2.00983000	-0.05420600
C	2.91326200	2.05762700	0.05084000
C	3.64267700	0.73911200	0.17059300
C	3.09535900	-1.64541300	0.11571900
O	3.52817700	3.12661300	0.05597900
O	2.27194800	-2.59235500	0.06135400
H	4.20169700	0.76033200	1.11514700
H	4.37967600	0.70047900	-0.64150200
C	4.57717800	-1.93591500	0.16993100
H	5.05191200	-1.46297300	1.03705300

H	4.72413400	-3.01663200	0.22920800
H	5.07892700	-1.55885800	-0.72936300
C	-2.13793100	0.20127800	-0.19444000
C	-2.06675100	-1.32649200	-0.17121500
C	-0.59322400	-1.75020700	-0.28844300
H	-0.01081900	-1.47211200	0.63263500
H	-0.48941900	-2.83866600	-0.25757200
N	-3.29287500	0.86334100	-0.22982000
O	-1.10249000	0.93121000	-0.22919800
C	-2.62498600	-1.87586300	1.15338400
H	-3.70929600	-1.76629100	1.21997100
H	-2.39598000	-2.94550300	1.21644700
H	-2.16134400	-1.38076600	2.01479900
C	-2.81820700	-1.91393400	-1.37937800
H	-3.89408000	-1.73305300	-1.32120600
H	-2.44240900	-1.49113800	-2.31848200
H	-2.65286800	-2.99696000	-1.40630600
H	-0.14184900	-1.45841200	-1.25070600
O	-4.47888700	0.17526900	-0.12584000
C	-5.15402700	0.46300400	1.10632500
H	-5.98697400	-0.24167200	1.13385200
H	-4.49006100	0.29934100	1.96103000
H	-5.53839600	1.48802300	1.11347700
C	-3.37012000	2.31085500	-0.36163700
H	-2.61008600	2.64775600	-1.06944400
H	-4.35744900	2.55545700	-0.75773700
H	-3.21397000	2.80744600	0.60102000

III3-trans_OMe-up_TS

Pd	-0.75144600	-0.27499200	-0.36321700
N	-2.56553500	0.43366100	-0.00428700
O	-1.69017100	-2.04584800	0.03411400
C	-2.96858600	-1.95903400	0.23181800
C	-3.59806600	-0.57355000	0.18914100
C	-2.69640000	1.69855800	0.31846200
O	-3.68832700	-2.94328900	0.44493000
O	-1.66646900	2.46622700	0.25557100
H	-4.14108600	-0.42663600	1.12940800
H	-4.33311500	-0.56576500	-0.62527600
C	-4.00032000	2.28490300	0.76233200

H	-4.13868100	2.09915800	1.83459600
H	-3.98192000	3.36492400	0.59911500
H	-4.84926200	1.84807700	0.22940600
C	2.08505100	-0.29418800	-0.30517600
C	1.83263700	1.21198200	-0.33718100
C	0.45873700	1.41174000	-1.01423500
H	-0.66052500	1.70195100	-0.25219600
H	0.33376300	2.49279900	-1.17075100
N	3.27971100	-0.84359200	-0.09862300
O	1.13150800	-1.10322800	-0.51937000
C	1.77542000	1.76190600	1.10019600
H	2.76349200	1.77647600	1.56981600
H	1.40054100	2.79169700	1.06936000
H	1.09302900	1.17561500	1.72687900
C	2.88841200	1.96485400	-1.16755300
H	3.86285000	1.99563300	-0.67639500
H	3.01056900	1.51092600	-2.15822200
H	2.54861900	2.99694400	-1.31141100
H	0.43545600	1.01023400	-2.03597700
O	4.33142100	-0.04557500	0.28572500
C	4.67778600	-0.24961400	1.66234400
H	5.37407600	0.55857800	1.89363500
H	3.79059500	-0.18220600	2.30006600
H	5.17376700	-1.21602600	1.80150300
C	3.51312900	-2.27955500	-0.12067500
H	2.94166500	-2.72190400	-0.93879700
H	4.57815600	-2.43815700	-0.30378200
H	3.21478600	-2.74748100	0.82278900

III3-trans_OMe-up_prod

Pd	0.66876300	-0.30846900	0.12017400
N	2.56666100	0.46098100	0.08425000
O	1.81657000	-2.06266300	-0.44252000
C	3.04637600	-1.95316100	-0.11057000
C	3.54282200	-0.58873500	0.37040600
C	2.96732200	1.63479700	-0.25183600
O	3.88031500	-2.88024800	-0.13072400
O	2.09333400	2.55662800	-0.67657800
H	4.50796800	-0.40019800	-0.10652500
H	3.71048400	-0.65793300	1.45235300

C	4.37504900	2.12672100	-0.24851700
H	4.90396200	1.73224300	-1.12456900
H	4.37536600	3.21748600	-0.30858000
H	4.90748600	1.80697900	0.65106500
C	-2.17493300	-0.30729500	0.20343700
C	-1.84358700	1.16990700	0.34699900
C	-0.40681400	1.18976400	0.92045200
H	1.21442300	2.15065700	-0.80523200
H	-0.00416700	2.20682900	0.85148300
N	-3.40157400	-0.82595500	0.18942100
O	-1.21780500	-1.13430100	0.09203300
C	-1.85922500	1.78877900	-1.06413900
H	-2.87632500	1.86335300	-1.46307600
H	-1.44688700	2.80338700	-1.01092800
H	-1.24971100	1.20618400	-1.76502200
C	-2.76114600	1.96840100	1.28546400
H	-3.73696900	2.18264500	0.84354200
H	-2.91637800	1.44758900	2.23729500
H	-2.27291000	2.92551700	1.50627100
H	-0.42691200	0.92734500	1.98998700
O	-4.48859500	0.01522700	0.15335100
C	-5.09756900	0.04565000	-1.14306000
H	-5.81170500	0.87013500	-1.09551800
H	-4.35084200	0.23240200	-1.92110300
H	-5.63113500	-0.88926300	-1.34558100
C	-3.66684200	-2.24688900	0.02615900
H	-2.94245000	-2.81832900	0.60913500
H	-4.67004200	-2.43973400	0.41267900
H	-3.60121600	-2.54764500	-1.02464800

III4-cis_OMe-down_int

C	-3.78466300	-0.20021800	-0.10590100
C	-3.40974100	1.13760700	-0.10395000
H	-4.14211600	1.93659600	-0.05634600
N	-1.11911700	0.48472500	-0.24551900
C	2.04834600	3.16985700	-0.16115700
O	2.63347600	2.03394400	-0.23839200
Pd	0.82400300	1.06735100	-0.28839200
C	2.49790400	-1.34518100	-0.01953600
C	3.37525900	-2.24366700	-0.89452500

C	2.53681700	-2.65424600	-2.11753300
H	2.21425300	-1.78662200	-2.70063400
H	3.14925800	-3.29325200	-2.76282800
N	2.79990200	-1.04858300	1.24663900
O	1.46242000	-0.85839300	-0.55990400
C	4.55804200	-1.37809900	-1.37761200
H	5.26111700	-1.13412000	-0.57494000
H	5.11151300	-1.92391200	-2.15021300
H	4.19805100	-0.43670300	-1.81149200
C	3.84693100	-3.52149400	-0.18274900
H	4.62806400	-3.34827900	0.56003500
H	3.00840700	-4.03386800	0.30456400
H	4.26395700	-4.20542200	-0.93008700
H	1.64605900	-3.22084000	-1.82247300
C	-1.48252700	-0.80965700	-0.23791400
H	-0.68966400	-1.54529000	-0.30686300
C	2.80629800	4.44035400	-0.05590500
H	3.86626000	4.26151000	-0.25137700
H	2.40570800	5.17106100	-0.76544600
H	2.68465500	4.84713300	0.95461800
O	0.76692300	3.14161600	-0.16536600
C	-2.06092500	1.44174600	-0.17580800
H	-1.71638900	2.47166100	-0.18296200
O	1.91882000	-0.20640900	1.89388800
C	0.92529500	-0.93195900	2.63023200
H	0.38568500	-1.62476700	1.97702000
H	1.38369900	-1.46920400	3.46748800
H	0.24678600	-0.16227600	3.00329000
C	3.95234400	-1.40423800	2.06581000
H	4.04013400	-0.62328300	2.82383300
H	3.81336100	-2.37129400	2.55477500
H	4.86905800	-1.40211000	1.47876100
S	-5.51906600	-0.66310500	0.02171000
O	-5.73630900	-0.87692700	1.46873700
O	-6.27140100	0.48169700	-0.52821100
O	-5.63725700	-1.89849600	-0.77705100
C	-2.81176900	-1.19074200	-0.17312500
H	-3.07148200	-2.24481000	-0.18945300

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C	-3.64247800	-0.36788900	0.01539900
C	-3.32336800	0.85730700	-0.55128500
H	-4.08918300	1.53422200	-0.91477500
N	-1.00756400	0.40814400	-0.20944300
C	0.81175300	3.73970000	0.29397400
O	1.64769600	3.48153900	1.17076500
Pd	0.95099400	0.96469800	-0.31882300
C	2.70232400	-1.33040600	0.07361300
C	3.85032200	-0.32056700	0.11081400
C	3.35544500	0.99464200	-0.52067500
H	2.68239400	1.57115800	0.18583600
H	4.17271700	1.72057900	-0.58036300
N	2.87424600	-2.63393300	0.29460700
O	1.51024800	-0.96591500	-0.15673700
C	4.21893500	-0.04667600	1.58048700
H	4.65619100	-0.91961500	2.07260500
H	4.95649800	0.76211100	1.61643200
H	3.33695000	0.26620000	2.15128600
C	5.06334500	-0.78580600	-0.71256100
H	5.61514200	-1.59853200	-0.23767300
H	4.76049100	-1.10714300	-1.71596700
H	5.75835700	0.05375000	-0.81950500
H	2.99135200	0.87090800	-1.54910700
C	-1.31604100	-0.78775400	0.33042800
H	-0.49129100	-1.40833100	0.66359000
C	0.22083800	5.11325000	0.12706600
H	-0.00385500	5.32153900	-0.92263200
H	-0.71853300	5.15533300	0.69234800
H	0.90278200	5.86659000	0.52908800
O	0.34683600	2.85299200	-0.54063900
C	-1.98748900	1.21642700	-0.64362200
H	-1.68915600	2.16974100	-1.06351400
O	1.72043800	-3.38969600	0.25019600
C	1.45625500	-3.88059500	-1.07057800
H	1.34283200	-3.05119400	-1.77672300
H	2.25217300	-4.55977700	-1.39467100
H	0.51497600	-4.42516600	-0.97749100
C	4.05825800	-3.42300500	0.61423900
H	3.69226400	-4.30726900	1.14020000
H	4.59085300	-3.73228800	-0.28838900
H	4.72474700	-2.88286700	1.28463600

S	-5.35590600	-0.88883200	0.19194100
O	-5.52558900	-1.11611700	1.64222700
O	-6.16448100	0.22523900	-0.33887800
O	-5.44665700	-2.12806700	-0.60727600
C	-2.62647900	-1.20842100	0.45927200
H	-2.83435700	-2.17527400	0.90677400

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C	-3.77046600	-0.21036500	0.02531400
C	-3.37816200	1.04405800	-0.41908900
H	-4.10339700	1.80131100	-0.69698300
N	-1.08593300	0.41240800	-0.18111700
C	1.36263400	3.56680300	0.22952400
O	2.48900900	3.09590600	0.58038900
Pd	0.94584600	0.85063100	-0.36529100
C	2.60771200	-1.41585300	0.05854000
C	3.66653300	-0.31918400	0.08154000
C	3.08216100	0.84666100	-0.74386800
H	2.56323000	1.90712300	0.01321900
H	3.86277400	1.61266900	-0.85359200
N	2.84797300	-2.69315700	0.34223400
O	1.40844700	-1.11173200	-0.22205300
C	3.85256700	0.13333700	1.54384000
H	4.31809200	-0.64483500	2.15698800
H	4.49795400	1.01946300	1.56636700
H	2.89283100	0.40707900	1.99751200
C	5.00507600	-0.72691100	-0.55476900
H	5.60224000	-1.39131400	0.07326300
H	4.85717900	-1.20268600	-1.53088700
H	5.59966900	0.17935000	-0.71338400
H	2.86266000	0.55621400	-1.78014700
C	-1.47141800	-0.80401900	0.24944100
H	-0.68597400	-1.50880100	0.50217900
C	1.04376700	5.00201500	0.48812800
H	0.15446300	5.30656600	-0.06713000
H	0.85991800	5.12991200	1.56134500
H	1.90202600	5.62427900	0.21819700
O	0.48500200	2.83623900	-0.33335400
C	-2.02095900	1.31840200	-0.50848100
H	-1.66824700	2.28445700	-0.85331100

O	1.74088800	-3.51830000	0.33295900
C	1.50590400	-4.09724700	-0.95692100
H	1.26932700	-3.32028400	-1.69160100
H	2.37109100	-4.68774200	-1.27765700
H	0.64215300	-4.74775700	-0.80847800
C	4.07481800	-3.36937000	0.74309500
H	3.76545300	-4.26072800	1.29186100
H	4.67187300	-3.66653400	-0.12263800
H	4.66335600	-2.74715000	1.41656400
S	-5.51098800	-0.63982400	0.18006600
O	-5.70464900	-0.88306100	1.62541100
O	-6.25610700	0.52604800	-0.33342800
O	-5.66637300	-1.85989400	-0.63975600
C	-2.80471900	-1.15351800	0.36390800
H	-3.06850500	-2.14768600	0.71026200

III4-cis_OMe-down_pro

C	-3.81935300	-0.43632500	0.04135700
C	-3.46651000	0.80050100	-0.48008700
H	-4.21715200	1.51432100	-0.80310700
N	-1.14974000	0.25897800	-0.20232900
C	0.73945800	3.72884700	0.06538400
O	1.30704100	3.60923400	1.25411300
Pd	0.98040800	0.75930600	-0.35861600
C	2.85532200	-1.30418200	0.11452000
C	3.69364700	-0.04888000	0.29776200
C	2.95184700	1.03883200	-0.51436800
H	1.47648300	2.67238900	1.48197900
H	3.28131200	2.03541400	-0.19355400
N	3.32793300	-2.54551300	0.21495600
O	1.61591200	-1.16646000	-0.12207400
C	3.66097300	0.28079800	1.80349400
H	4.17933500	-0.48410300	2.39357500
H	4.16266600	1.24021800	1.97425200
H	2.63166500	0.35781600	2.17414300
C	5.14228500	-0.12389200	-0.20700300
H	5.81442300	-0.65668400	0.47022500
H	5.20205100	-0.58369100	-1.19962000
H	5.52282600	0.90053100	-0.29593900
H	3.16746200	0.93218300	-1.58785100

C	-1.50396500	-0.94157900	0.28896600
H	-0.69423300	-1.60789800	0.57437300
C	0.37402300	5.12057500	-0.30356300
H	0.13550700	5.17027100	-1.36704500
H	-0.50304200	5.41943900	0.28281900
H	1.19321800	5.80198900	-0.05715000
O	0.51687000	2.76793600	-0.67683800
C	-2.11588700	1.10767300	-0.58158100
H	-1.79490700	2.06671300	-0.97967600
O	2.39741300	-3.55162400	0.04760200
C	2.26243300	-3.92250100	-1.32949000
H	1.89663700	-3.07720500	-1.92244800
H	3.21687100	-4.29090500	-1.72155700
H	1.52164900	-4.72425000	-1.32770800
C	4.64226800	-3.02117300	0.62599400
H	4.50031000	-4.04881300	0.96618500
H	5.35847000	-3.00836000	-0.19884300
H	5.01676400	-2.43766100	1.46774400
S	-5.54563000	-0.90441000	0.22272800
O	-5.72066600	-1.14311700	1.67201800
O	-6.32540500	0.24012900	-0.28956400
O	-5.68699800	-2.13332900	-0.58717600
C	-2.82586100	-1.33100300	0.42852400
H	-3.06172700	-2.31181400	0.82938100

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C	-3.84604800	-0.17550500	-0.08042100
C	-3.43697900	1.13566100	-0.28268900
H	-4.14788000	1.92806600	-0.49175000
N	-1.16908100	0.46054200	0.01265300
C	1.95690900	3.10876600	0.32026400
O	2.57957000	1.99958400	0.19719500
Pd	0.77790200	1.00175900	0.05068700
C	2.47710400	-1.41940500	-0.20900200
C	3.41568200	-1.20325300	-1.40492800
C	2.67278300	-0.36557800	-2.45889700
H	2.48694000	0.65759600	-2.11321300
H	3.29685300	-0.30173200	-3.35703300
N	2.83825400	-2.12251000	0.86804800
O	1.29586600	-0.96304700	-0.21068400

C	4.67901400	-0.43004500	-0.98001800
H	5.33207200	-0.99398700	-0.30872300
H	5.26206000	-0.19242200	-1.87716100
H	4.41508400	0.51319700	-0.48782400
C	3.76029000	-2.56094800	-2.04917300
H	4.37999300	-3.20352000	-1.41977300
H	2.84858100	-3.11221900	-2.30868300
H	4.31758700	-2.37964600	-2.97489500
H	1.71740400	-0.81919700	-2.74156200
C	-1.56552900	-0.80830800	0.22129500
H	-0.79019000	-1.53823100	0.42521300
C	2.66243900	4.40041000	0.49426500
H	3.59296400	4.40176800	-0.07970300
H	2.01790200	5.22795500	0.18786700
H	2.90998800	4.52355100	1.55564700
O	0.67523800	3.03368300	0.29878400
C	-2.08136100	1.41784800	-0.22292600
H	-1.70675500	2.42601500	-0.37319000
O	1.85930400	-2.27016000	1.83098500
C	1.92368200	-1.22656600	2.81171800
H	2.87447700	-1.26560800	3.35458600
H	1.78947800	-0.24328000	2.34468200
H	1.09474200	-1.43918900	3.48942600
C	3.97184200	-2.99228200	1.13932000
H	4.23966300	-2.87322500	2.19156400
H	3.69198100	-4.03271900	0.94922800
H	4.83613800	-2.72495400	0.53946300
S	-5.58692100	-0.62647900	-0.16755500
O	-5.92392100	-1.11328500	1.18717700
O	-6.29224400	0.61108600	-0.54993400
O	-5.62900400	-1.68428500	-1.19800700
C	-2.90151900	-1.16290400	0.18232800
H	-3.18435400	-2.19764000	0.34924200

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C	-3.67820200	-0.37183600	-0.10104000
C	-3.34607400	0.93451400	-0.42930800
H	-4.10489700	1.67452400	-0.66028100
N	-1.03448600	0.40834600	-0.17362300
C	0.82779900	3.73128200	0.47828600

O	1.63291900	3.45457800	1.37607200
Pd	0.93344700	0.95555200	-0.18410900
C	2.74319200	-1.33643000	-0.12147400
C	3.88722900	-0.31949000	-0.18160400
C	3.29410300	1.07750800	-0.44011000
H	2.69556400	1.44207700	0.44329800
H	4.08206100	1.83727200	-0.43648700
N	2.95923300	-2.65193700	-0.06759700
O	1.52766400	-0.97503000	-0.08426000
C	4.60351300	-0.28369100	1.18164900
H	5.09516400	-1.22839200	1.42878300
H	5.37217600	0.49607100	1.15654600
H	3.89867300	-0.04384700	1.98571600
C	4.85832800	-0.61302100	-1.33988200
H	5.52202200	-1.45566800	-1.14136200
H	4.31593500	-0.80608300	-2.27236900
H	5.49272200	0.26605100	-1.49479900
H	2.82799000	1.16514800	-1.43338100
C	-1.35730000	-0.86227400	0.13722100
H	-0.54112700	-1.54366200	0.34565800
C	0.30447800	5.12408300	0.25173400
H	0.45391800	5.41241500	-0.79399300
H	-0.77268400	5.14682000	0.45218600
H	0.81111100	5.83177900	0.91154200
O	0.35050800	2.85232300	-0.35971000
C	-2.00643900	1.29108900	-0.45561600
H	-1.69568900	2.29987800	-0.70176800
O	1.82248700	-3.43394400	-0.13080200
C	1.33787900	-3.77388600	1.17433700
H	2.06230900	-4.39950500	1.70705200
H	1.11603800	-2.87117800	1.75212700
H	0.42244300	-4.33864900	0.98870900
C	4.17979500	-3.43797700	-0.18455600
H	4.00526000	-4.38196900	0.33571800
H	4.40311200	-3.64502100	-1.23472200
H	5.02065100	-2.94741400	0.29979100
S	-5.39814000	-0.88789700	0.00118500
O	-5.61942100	-1.10833200	1.44561700
O	-6.17841300	0.23115100	-0.56035500
O	-5.47272300	-2.12899400	-0.79597600
C	-2.67164100	-1.28795500	0.18605200

H	-2.88845800	-2.32006600	0.44180900
III4-cis_OMe-up_TS			
C	-3.78005200	-0.20331200	-0.06428400
C	-3.37512100	1.09119700	-0.35735400
H	-4.09349200	1.88239000	-0.54474600
N	-1.09015700	0.40970400	-0.19258300
C	1.38219200	3.50408900	0.48233200
O	2.51486500	3.00758100	0.76632600
Pd	0.94522100	0.84956600	-0.34186400
C	2.64100400	-1.43379800	-0.20839100
C	3.69637300	-0.33427900	-0.14410400
C	3.06038500	0.91002700	-0.79679700
H	2.56663600	1.86813300	0.09794100
H	3.82614600	1.69737000	-0.84589300
N	2.90261300	-2.72630800	-0.02721900
O	1.42567200	-1.11984600	-0.40165600
C	3.98441600	-0.03756700	1.34049100
H	4.46526800	-0.88408600	1.84207900
H	4.65611000	0.82616500	1.40764200
H	3.06135400	0.20846300	1.87906600
C	4.99037000	-0.66096500	-0.90947300
H	5.64264800	-1.35665600	-0.37834900
H	4.77798400	-1.06433100	-1.90589100
H	5.55543200	0.26828500	-1.03974400
H	2.79960900	0.74191400	-1.85031200
C	-1.49027400	-0.84530400	0.08300400
H	-0.71404500	-1.58540500	0.24197400
C	1.08540100	4.93035600	0.81004900
H	1.38654400	5.54640800	-0.04618800
H	0.01622400	5.07459200	0.98029900
H	1.66237400	5.24627800	1.68232900
O	0.48946700	2.81959300	-0.11664000
C	-2.01490600	1.35969800	-0.40939500
H	-1.65024500	2.35735000	-0.63062100
O	1.81497800	-3.56691400	-0.16007500
C	1.18428600	-3.80305900	1.10471500
H	1.86636600	-4.32440800	1.78547600
H	0.85005400	-2.86055800	1.55108200
H	0.32737400	-4.43859800	0.87443400

C	4.16768700	-3.42996700	0.14102200
H	3.93802900	-4.39779600	0.58977500
H	4.65279200	-3.59368400	-0.82467100
H	4.82503100	-2.89316000	0.82301500
S	-5.52275600	-0.62310500	0.05767100
O	-5.74005200	-0.85951700	1.50080100
O	-6.25064100	0.54666300	-0.47067400
O	-5.67186800	-1.84437900	-0.76005900
C	-2.82744700	-1.19080400	0.16224200
H	-3.10670000	-2.21614300	0.38440500

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C	-3.82474400	-0.37777300	-0.02469500
C	-3.45561700	0.91787900	-0.35924100
H	-4.19655800	1.68133600	-0.57279200
N	-1.14609000	0.30900000	-0.16871600
C	0.85324200	3.71950600	0.30022600
O	1.46880400	3.49395800	1.44930900
Pd	0.99203600	0.78619400	-0.34650300
C	2.85237400	-1.34149300	-0.15677600
C	3.73291500	-0.12119800	0.06521000
C	2.95737200	1.05406500	-0.57617900
H	1.60756000	2.53837200	1.60647700
H	3.31796600	2.00745100	-0.16767900
N	3.29536500	-2.59768800	-0.17830300
O	1.60097900	-1.16232700	-0.27392900
C	3.83078900	0.06366300	1.59192200
H	4.38226900	-0.75927100	2.06069900
H	4.36160000	0.99733000	1.81019400
H	2.83573100	0.11748600	2.05000800
C	5.13250200	-0.17029200	-0.56525700
H	5.84744700	-0.76796300	0.00584600
H	5.09744400	-0.54347300	-1.59488100
H	5.52457300	0.85305000	-0.59839500
H	3.11040800	1.06281300	-1.66578000
C	-1.51753600	-0.94051500	0.16003500
H	-0.71829100	-1.64947500	0.35688200
C	0.55129400	5.15257000	0.04687400
H	1.48082700	5.73008100	0.08602900
H	0.07500600	5.27000400	-0.92689100

H	-0.10755300	5.52642500	0.83813600
O	0.55354500	2.82370700	-0.49456000
C	-2.10056900	1.21693700	-0.42041900
H	-1.76434900	2.21540400	-0.68740300
O	2.34254300	-3.55587400	-0.46368300
C	1.73528600	-4.07763300	0.72223700
H	2.47939800	-4.57935600	1.35117000
H	1.23634400	-3.28167500	1.28435600
H	1.00274000	-4.80198400	0.36127900
C	4.64368200	-3.12657200	-0.01916900
H	4.54092100	-4.19430600	0.18174700
H	5.23052400	-2.99647600	-0.93134900
H	5.14348900	-2.66778200	0.83491900
S	-5.55653300	-0.84167300	0.09105300
O	-5.78169200	-1.07024300	1.53506600
O	-6.31227800	0.30323400	-0.45484300
O	-5.67761100	-2.07431000	-0.71570600
C	-2.84460500	-1.32749600	0.24613000
H	-3.09415100	-2.35035300	0.51019500

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C	3.91826400	-0.31608800	0.08442900
C	3.56828300	0.98828300	-0.23874400
H	4.31624600	1.73736900	-0.47504700
N	1.26923500	0.43114400	0.05768800
C	-1.65743000	3.25573800	-0.40791200
O	-2.36724600	2.22579700	-0.15039600
Pd	-0.64261600	1.08824000	0.03323400
C	-2.51689200	-1.16511500	0.20894100
C	-3.63698600	-0.97079400	1.23089500
C	-3.03689900	-0.28073100	2.46398900
H	-2.66613000	0.72367000	2.23075800
H	-3.81782600	-0.17904500	3.22590700
N	-2.70596700	-1.70692100	-0.98629100
O	-1.31870700	-0.81381900	0.47064100
C	-4.74385600	-0.07287900	0.64456700
H	-5.24305400	-0.53440400	-0.21189000
H	-5.49757900	0.10577100	1.42065100
H	-4.34351000	0.89935100	0.33421300
C	-4.21075100	-2.33405300	1.66095700

H	-4.79132100	-2.81233600	0.86872600
H	-3.41597700	-3.01885600	1.98006400
H	-4.88214300	-2.17832800	2.51291400
H	-2.21331100	-0.86010700	2.89501200
C	1.60611000	-0.83633100	0.35678300
H	0.79641800	-1.51867600	0.58807700
C	-2.24852400	4.57782900	-0.72418500
H	-3.30782300	4.59315600	-0.45846800
H	-1.70679800	5.36664600	-0.19371700
H	-2.14258200	4.75894800	-1.80043400
O	-0.38520200	3.07230400	-0.40187200
C	2.22573200	1.32723400	-0.23937100
H	1.89916700	2.33543300	-0.47736700
O	-3.95180800	-2.15548500	-1.34600700
C	-3.96737200	-3.57489600	-1.55046900
H	-3.39633500	-3.84989000	-2.44355000
H	-3.57545700	-4.09520700	-0.67104800
H	-5.02161800	-3.81400200	-1.70001300
C	-1.66529600	-1.76652100	-2.00607100
H	-2.15708800	-1.89603900	-2.97146300
H	-1.10990800	-0.82509000	-2.01587500
H	-0.97594500	-2.59466700	-1.82004300
C	2.92822600	-1.24619900	0.38306300
H	3.16556900	-2.27232500	0.64552600
S	5.64683900	-0.81667000	0.09330100
O	5.81296000	-1.59585800	-1.15274600
O	6.41093000	0.44472700	0.11683300
O	5.79649700	-1.63342600	1.31535300

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C	-3.78582100	-0.56286800	-0.06048500
C	-3.51328600	0.75045900	-0.41164600
H	-4.30377900	1.44623500	-0.67184500
N	-1.18276000	0.34743300	-0.10749100
C	0.66237200	3.82482900	0.25430000
O	1.65407000	3.67023300	0.97665700
Pd	0.75808900	0.99303800	-0.11698900
C	2.67626900	-1.19429600	0.08129600
C	3.77253300	-0.13886900	-0.05438500
C	3.12115400	1.21669000	-0.37380900

H	2.49201100	1.59235200	0.48516100
H	3.86764500	2.01751800	-0.38638800
N	2.93719600	-2.48135500	0.27676000
C	1.90796300	-3.46640100	0.58375000
H	1.38749800	-3.78845300	-0.32261900
H	2.39959300	-4.31734100	1.05838000
H	1.19157300	-3.03970700	1.28960900
O	1.43651600	-0.90304400	0.08289300
C	4.50015400	-0.03019000	1.29920700
H	5.00307700	-0.96467000	1.56411600
H	5.25499800	0.76134400	1.23656100
H	3.79964800	0.22940900	2.10143400
C	4.75919900	-0.45404500	-1.19250300
H	5.44423400	-1.26214900	-0.93297800
H	4.23319300	-0.71060100	-2.11882600
H	5.36158200	0.44025200	-1.38656400
H	2.66203700	1.24299700	-1.37380300
C	-1.44803100	-0.92986900	0.23037000
H	-0.60309300	-1.56120700	0.47801900
C	0.06116400	5.17892300	-0.00981000
H	0.40318000	5.89288400	0.74330100
H	0.38439000	5.52621800	-0.99856200
H	-1.03159500	5.12768400	-0.01302500
O	0.06234600	2.84536300	-0.36511500
C	-2.19265300	1.17283400	-0.42559500
H	-1.93034000	2.19055200	-0.68917600
O	4.24236100	-2.90183500	0.34111300
C	4.57642900	-3.78476100	-0.73826200
H	4.01027300	-4.71947500	-0.66968900
H	4.40115400	-3.30189300	-1.70487700
H	5.64011000	-3.98599000	-0.59965600
S	-5.47890700	-1.16458800	0.02523900
O	-5.70965900	-1.38039600	1.46871200
O	-6.30913000	-0.09335600	-0.55854400
O	-5.47538200	-2.41642300	-0.75936700
C	-2.73983200	-1.42113600	0.26351800
H	-2.91267900	-2.45699400	0.53777800

III4-trans_OMe-down_TS

C	-3.87773800	-0.46327100	-0.03619800
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C	-3.55879500	0.84519900	-0.36934600
H	-4.32659300	1.58489000	-0.57013300
N	-1.23309500	0.31897600	-0.20499400
C	0.99767500	3.59834300	0.37546200
O	2.14414500	3.18614500	0.73517500
Pd	0.77319000	0.89259100	-0.35579100
C	2.62187600	-1.24949200	-0.04425400
C	3.60577300	-0.09126200	-0.06311700
C	2.89098300	1.08518900	-0.75737000
H	2.31058400	2.03775900	0.09960300
H	3.59767500	1.92419600	-0.83230900
N	2.93797200	-2.50520400	0.24545800
C	1.92431800	-3.52262900	0.50196700
H	1.41133900	-3.79961900	-0.42266000
H	2.42618900	-4.39592400	0.91952900
H	1.19961200	-3.14948000	1.23128600
O	1.38126700	-1.03893700	-0.23698600
C	3.90332000	0.26146100	1.40825300
H	4.44310600	-0.54835100	1.91059100
H	4.52318600	1.16484300	1.44285000
H	2.97837900	0.46158900	1.96176300
C	4.90978800	-0.37927200	-0.82402600
H	5.56970200	-1.05656800	-0.27811700
H	4.71045400	-0.79529800	-1.81791900
H	5.44441300	0.56772400	-0.95973700
H	2.65789300	0.86206400	-1.80793700
C	-1.54968000	-0.94874800	0.11919100
H	-0.72464100	-1.62968200	0.29637600
C	0.58260400	5.00179200	0.67234100
H	0.79748300	5.23612200	1.71890700
H	1.17337900	5.68036200	0.04647700
H	-0.47956300	5.14260000	0.46324100
O	0.19101800	2.84418900	-0.25838000
C	-2.21949400	1.19831800	-0.44263000
H	-1.92438300	2.20954100	-0.69983400
O	4.22716000	-2.79998300	0.61606500
C	4.86459300	-3.69224600	-0.30625000
H	4.32672800	-4.64412500	-0.36619900
H	4.94273100	-3.23590500	-1.29779300
H	5.85735800	-3.85395100	0.11742000
S	-5.59174600	-0.98590100	0.10108600

O	-5.78767800	-1.20884100	1.54906800
O	-6.38877000	0.12892600	-0.44649700
O	-5.67721300	-2.22738900	-0.69526400
C	-2.86130200	-1.37795400	0.21944200
H	-3.07089400	-2.40945300	0.48413200

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C	-3.91334500	-0.59215400	-0.01022800
C	-3.60779200	0.70197800	-0.40982100
H	-4.38299700	1.41350200	-0.67451900
N	-1.27246200	0.22369900	-0.17459000
C	0.55821900	3.72605300	0.25197600
O	1.16826200	3.53768500	1.41039400
Pd	0.83702300	0.80025400	-0.37795200
C	2.78768200	-1.22354400	-0.07474100
C	3.59945500	0.04267500	0.11627500
C	2.79161600	1.15422800	-0.59452900
H	1.36395200	2.59253700	1.57061900
H	3.09982100	2.13982500	-0.22268600
N	3.26446800	-2.47092300	-0.01986400
C	2.35898300	-3.61112500	0.07986100
H	1.63698400	-3.57790500	-0.73752100
H	2.94256500	-4.52900900	0.00109700
H	1.82664500	-3.59555700	1.03732400
O	1.53544200	-1.11822800	-0.24838800
C	3.63480600	0.28883700	1.63964900
H	4.18154700	-0.50437900	2.16129100
H	4.13944900	1.24155000	1.83711300
H	2.62251500	0.34194200	2.05861100
C	5.02301500	0.02430200	-0.45438700
H	5.71513000	-0.56542900	0.15112000
H	5.03611300	-0.35317700	-1.48280600
H	5.39468000	1.05592200	-0.47612900
H	2.96713000	1.12366200	-1.68029600
C	-1.58165900	-1.02375100	0.21953500
H	-0.74780800	-1.67914300	0.45839500
C	0.19040900	5.14118100	-0.01136200
H	-0.44719000	5.50749100	0.80006100
H	1.10093800	5.75041800	-0.01986100
H	-0.32739400	5.22447600	-0.96724500

O	0.31914900	2.81369800	-0.54479400
C	-2.26990700	1.06632100	-0.48011900
H	-1.98461200	2.06533100	-0.79934700
O	4.50902600	-2.64459700	0.55303700
C	5.43601400	-3.28214800	-0.32912100
H	5.12184300	-4.30416100	-0.56501200
H	5.56388700	-2.70309400	-1.24840700
H	6.37092300	-3.30842200	0.23434800
S	-5.62112000	-1.13444000	0.12205900
O	-5.89375200	-1.13484200	1.57634200
O	-6.41312600	-0.14023600	-0.62951900
O	-5.64121400	-2.48822100	-0.46970800
C	-2.88822900	-1.47507800	0.31558600
H	-3.08922200	-2.49517100	0.62751600

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C	-3.94388600	-0.26066900	-0.06976700
C	-3.55036000	1.06166000	0.11676000
H	-4.26985600	1.85020800	0.31446200
N	-1.27850100	0.41286200	-0.19936000
C	1.82876200	3.07992400	0.18701800
O	2.46161900	1.98506400	-0.00368000
Pd	0.66450200	0.97289700	-0.16729300
C	2.42918100	-1.31948000	-0.21433300
C	3.56939500	-1.38439500	-1.22852700
C	3.08060800	-0.71385400	-2.52122100
H	2.88238600	0.35419000	-2.36405000
H	3.86331500	-0.80211600	-3.28285600
N	2.55106600	-1.69457100	1.05126700
O	1.26484800	-0.95338400	-0.58871500
C	4.82674700	-0.63603700	-0.74795400
H	5.36744100	-1.17574100	0.03182000
H	5.50625200	-0.52444600	-1.60067700
H	4.58215600	0.36918600	-0.38419800
C	3.88591000	-2.86752400	-1.49688000
H	4.25767400	-3.37188200	-0.59875500
H	2.99693100	-3.40073700	-1.85478800
H	4.65853100	-2.93565000	-2.27110200
H	2.17031700	-1.17904100	-2.91112500
C	-1.66106900	-0.85681900	-0.40679200

H	-0.88100900	-1.57456100	-0.63229700
C	2.52692500	4.37001300	0.39857800
H	3.45088400	4.39601700	-0.18539500
H	1.87457200	5.20393500	0.12832900
H	2.78533800	4.45721600	1.46098900
O	0.54839700	2.99031800	0.19862400
C	-2.20288700	1.36179200	0.04742800
H	-1.83917600	2.37511800	0.19288300
O	3.75324800	-2.18116900	1.50095600
C	4.33931400	-1.33376600	2.49943700
H	4.45050300	-0.31212900	2.12301600
H	3.74667700	-1.34257800	3.42019200
H	5.31753400	-1.77870100	2.68897000
C	1.44523200	-1.71312500	2.00100700
H	1.66212500	-2.48363300	2.74308700
H	1.32887700	-0.74077100	2.48981300
H	0.52327300	-1.97112000	1.47745300
C	-2.99412700	-1.23298700	-0.34669100
H	-3.27110300	-2.26828400	-0.51465000
S	-5.68882200	-0.67809300	0.05896200
O	-6.04633400	-0.32248200	1.44836200
O	-6.34497000	0.17855500	-0.95033100
O	-5.77381000	-2.12248900	-0.22905900

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C	-3.72814000	-0.50367100	0.00590500
C	-3.44053100	0.69386300	-0.63208300
H	-4.21509300	1.28580400	-1.10840500
N	-1.13965000	0.41399200	-0.09095400
C	0.69876200	3.82470200	0.47794900
O	1.69901500	3.62416800	1.17793100
Pd	0.78481500	1.02671800	-0.18767200
C	2.60967800	-1.24160800	-0.24124700
C	3.74824100	-0.22260400	-0.26271600
C	3.15165700	1.18017100	-0.47389200
H	2.56507400	1.52248200	0.42414100
H	3.93907100	1.94019100	-0.47264000
N	2.81978400	-2.55307900	-0.22024100
C	1.75000100	-3.53974500	-0.30030000
H	1.00569500	-3.20464500	-1.02511400

H	2.19244700	-4.47456800	-0.64917000
H	1.27393700	-3.68884600	0.67340100
O	1.38354600	-0.90223900	-0.28675600
C	4.50287700	-0.23071500	1.07863200
H	5.09284600	-1.13942700	1.21082500
H	5.19403400	0.61903800	1.09668800
H	3.81351800	-0.12512800	1.92423500
C	4.69773300	-0.50893800	-1.44056500
H	5.23479800	-1.45146500	-1.31375400
H	4.14614400	-0.54548400	-2.38739600
H	5.43382800	0.30011400	-1.50464800
H	2.66293000	1.29094800	-1.45464700
C	-1.41682300	-0.74848900	0.53029100
H	-0.58456500	-1.28209100	0.97547500
C	0.06115400	5.18314000	0.34921800
H	0.72885900	5.95150800	0.74581600
H	-0.18123100	5.39786000	-0.69601100
H	-0.87556100	5.19467600	0.91889800
O	0.09042600	2.89447100	-0.20452900
C	-2.12366800	1.12914500	-0.65638300
H	-1.84223300	2.06009300	-1.13517200
O	4.10163800	-3.02797900	-0.08720900
C	4.30358700	-3.67565300	1.17710600
H	3.98157900	-3.02942400	1.99975300
H	3.77328600	-4.63265900	1.21415400
H	5.38044000	-3.84721600	1.22439400
S	-5.40507800	-1.15165000	0.06370700
O	-5.65272700	-1.39040600	1.49973200
O	-6.25965800	-0.10476300	-0.52781900
O	-5.34254000	-2.39547800	-0.73272300
C	-2.70746000	-1.23648800	0.60487300
H	-2.90099100	-2.17161700	1.12140000

III4-trans_OMe-up_TS

C	-3.84846600	-0.37478300	0.00771000
C	-3.51657900	0.92502800	-0.34640100
H	-4.27684600	1.67007300	-0.55553500
N	-1.19797600	0.37171900	-0.18905000
C	1.15449400	3.51937000	0.54507500
O	2.30531200	3.04919100	0.80147000

Pd	0.80606900	0.89791500	-0.40617200
C	2.57004500	-1.31958000	-0.32306600
C	3.59878700	-0.19613900	-0.26868900
C	2.91130900	1.04629500	-0.87476600
H	2.40368900	1.95843600	0.06464600
H	3.65350900	1.85627200	-0.91914800
N	2.85850300	-2.60670400	-0.17576900
C	1.86949000	-3.67091600	-0.28170100
H	1.16685100	-3.42343400	-1.07970200
H	2.39939700	-4.58856900	-0.54524500
H	1.32704900	-3.80350300	0.65933600
O	1.34651500	-1.05335500	-0.55408600
C	3.97150100	0.09670500	1.19665400
H	4.57922100	-0.70242400	1.62996400
H	4.55691300	1.02307700	1.23279000
H	3.07808300	0.24089200	1.81562900
C	4.85179300	-0.50775700	-1.10530400
H	5.47711200	-1.27904200	-0.65180100
H	4.58098400	-0.82740000	-2.11853100
H	5.44880700	0.40735400	-1.19083500
H	2.63857700	0.89796300	-1.92852200
C	-1.52572800	-0.88345700	0.16986900
H	-0.70516200	-1.56510300	0.36690900
C	0.79258900	4.90472600	0.96797400
H	1.35607500	5.19107300	1.85898100
H	1.05479300	5.59141800	0.15407200
H	-0.28239900	4.97687400	1.14965900
O	0.28976700	2.84184400	-0.10023500
C	-2.17359100	1.26028900	-0.43460300
H	-1.86765000	2.26316000	-0.71183500
O	4.12945400	-2.96746400	0.19923000
C	4.17640700	-3.43710000	1.55379700
H	3.65378500	-2.74550700	2.22219100
H	3.74940500	-4.44201600	1.63457000
H	5.24101700	-3.46570800	1.79367800
S	-5.56823900	-0.88040300	0.14241700
O	-5.77162100	-1.10242500	1.58952800
O	-6.35308600	0.24170900	-0.40773600
O	-5.66173800	-2.12065700	-0.65496100
C	-2.84179500	-1.29573800	0.28092600
H	-3.06261800	-2.31905600	0.56717500

III4-trans_OMe-up_prod

C	-3.90471900	-0.56518600	0.02595400
C	-3.59150300	0.73995900	-0.32718100
H	-4.36371600	1.47017700	-0.54554700
N	-1.25894000	0.22883300	-0.14045800
C	0.60553900	3.72891100	0.27679200
O	1.23148300	3.53650600	1.42610000
Pd	0.84944300	0.79925900	-0.35971300
C	2.80447600	-1.23687200	-0.21729000
C	3.62726300	0.01643500	0.02181800
C	2.79754300	1.15246000	-0.62474900
H	1.41119300	2.58837400	1.58709900
H	3.12178400	2.12475000	-0.23180100
N	3.28617600	-2.46696500	-0.35403600
C	2.44305100	-3.62140900	-0.62678300
H	1.69944200	-3.34521100	-1.37753800
H	3.08154500	-4.41033200	-1.02897200
H	1.93514100	-3.96649700	0.27936900
O	1.53876100	-1.12439400	-0.30016200
C	3.70892000	0.21386700	1.54820000
H	4.33314800	-0.55401900	2.01740400
H	4.16203200	1.18961500	1.75813800
H	2.71575900	0.18577300	2.01224500
C	5.03436600	0.02427400	-0.59235100
H	5.75173100	-0.56417700	-0.01536800
H	5.02482300	-0.35233800	-1.62158400
H	5.38941400	1.06188600	-0.61864200
H	2.93717000	1.15371900	-1.71628700
C	-1.57548800	-1.02980600	0.21130200
H	-0.74474200	-1.70087200	0.41598200
C	0.25426300	5.14754600	0.01004000
H	-0.37928100	5.52269900	0.82068900
H	1.17108000	5.74701900	-0.00081800
H	-0.26363700	5.23336400	-0.94560400
O	0.33917800	2.81538800	-0.50948000
C	-2.25059700	1.09259500	-0.40168300
H	-1.95750600	2.09987400	-0.68679400
O	4.62147500	-2.69791500	-0.13455300
C	4.85063000	-3.36401200	1.11266000

H	4.33984100	-2.84680100	1.93082400
H	4.52512300	-4.40882100	1.06223300
H	5.93226400	-3.32229300	1.25427000
S	-5.61591100	-1.09621200	0.15241200
O	-5.82699600	-1.31752400	1.59936000
O	-6.41769700	0.01189100	-0.40424700
O	-5.69210300	-2.34109500	-0.64089900
C	-2.88559300	-1.47042900	0.30735100
H	-3.09477300	-2.49834300	0.58694900

III2-cis_OMe-down_c4_diOAc

C	2.76415100	-3.06173300	0.58053900
H	2.96488400	-4.06085100	0.95216700
N	1.14562600	-1.43765400	-0.08964500
C	-2.38767000	-3.22789000	0.31496500
O	-3.02739100	-2.66170400	1.21325000
Pd	-0.80039800	-0.78401300	-0.14807900
C	-0.74798600	2.16838600	0.18045300
C	-1.28141800	3.26192700	-0.75319600
C	-1.10121500	2.74933700	-2.19193000
H	-1.64431600	1.81035000	-2.35528400
H	-1.49158000	3.50043200	-2.88784900
N	-0.83154100	2.24616100	1.51305200
O	-0.15626800	1.18148100	-0.33475200
C	-2.78541800	3.50922200	-0.52456700
H	-3.00374800	4.08076900	0.38022400
H	-3.17715200	4.08312000	-1.37169700
H	-3.33744600	2.56419100	-0.47442300
C	-0.45707700	4.54899900	-0.57685900
H	-0.56164700	4.99528600	0.41716200
H	0.60770000	4.35500900	-0.75187200
H	-0.79209400	5.29223000	-1.30957200
H	-0.04780400	2.57702700	-2.43340700
C	2.13333600	-0.56848800	-0.35030500
H	1.83962900	0.40539900	-0.72801000
C	-2.75186100	-4.62189100	-0.13728300
H	-3.26222800	-5.15562800	0.66938800
H	-3.43789400	-4.54111900	-0.98965100
H	-1.86857400	-5.17776200	-0.46488200
O	-1.39101200	-2.70724600	-0.33032400

C	1.45431800	-2.66592700	0.36776300
H	0.62108800	-3.33072400	0.56500100
O	-0.38215100	1.12738300	2.18813400
C	0.99197200	1.26190400	2.57058500
H	1.62499500	1.48260700	1.70459900
H	1.10459000	2.04528500	3.32908500
H	1.25559400	0.29085400	2.99443200
C	-1.60057100	3.12491700	2.37940600
H	-2.60129200	2.71360300	2.54310200
H	-1.07309800	3.19000900	3.33333400
H	-1.66505100	4.12905200	1.96708500
C	3.46238000	-0.89919200	-0.13890200
C	3.79629600	-2.16239200	0.33086700
H	4.83373400	-2.43082800	0.50830200
C	-3.58900500	-0.32071700	-0.81512000
O	-3.36342300	-0.81995400	-1.93078000
C	-4.99574300	-0.05982900	-0.33825700
H	-5.68976800	-0.00279700	-1.18082600
H	-5.28742300	-0.90030900	0.30626500
H	-5.05003200	0.85279500	0.26302700
O	-2.67170600	-0.02966700	0.04610700
S	4.70108200	0.35316000	-0.46576000
O	5.95433800	-0.18188900	0.10347600
O	4.72834600	0.49966300	-1.93774200
O	4.19856600	1.56276800	0.22329400

IIIPy-cis_OMe-up_opt_diOAc

C	-4.21840600	-1.94105900	-1.03880600
H	-5.16730200	-1.69934400	-1.50610800
N	-2.02464900	-1.23177700	-0.42546100
C	-2.32968200	2.25309300	0.83380400
O	-1.73314300	2.05948200	1.90487200
Pd	-0.61786400	0.23616100	-0.26788600
C	2.04761700	-1.05499400	0.04569900
C	3.26787800	-0.90099700	-0.87438100
C	2.73282300	-0.56566800	-2.27797800
H	2.16004800	0.36957300	-2.28816900
H	3.58288600	-0.45292100	-2.96022600
N	2.15497100	-1.15519200	1.37338400
O	0.90971700	-1.13858700	-0.49328600

C	4.18163300	0.25400600	-0.42463300
H	4.77538900	0.02486900	0.46343500
H	4.88703000	0.47958600	-1.23225800
H	3.60111700	1.16220600	-0.22410300
C	4.02547400	-2.23908100	-0.95243300
H	4.48386900	-2.53396400	-0.00340400
H	3.35204400	-3.04512000	-1.26723300
H	4.82665200	-2.15696400	-1.69586000
H	2.08602800	-1.35886800	-2.66610400
C	-1.78207700	-2.44713700	0.09920400
H	-0.80398200	-2.60224700	0.54185300
C	-3.44867400	3.26005800	0.72583500
H	-3.37395300	4.00081200	1.52591000
H	-3.43937600	3.75400500	-0.24999200
H	-4.40628100	2.73444200	0.82724500
O	-2.08425000	1.61276100	-0.26595300
C	-3.21988600	-0.98068100	-0.98834800
H	-3.36534600	0.01352000	-1.39844700
O	0.95958400	-1.31487800	2.04379800
C	0.62969500	-0.18514600	2.86886800
H	1.18742500	-0.22309100	3.81117800
H	0.82542800	0.75163100	2.34159300
H	-0.43945600	-0.29054800	3.06442600
C	3.31488600	-1.15466500	2.25213900
H	3.51142900	-0.15333200	2.64540100
H	3.08675200	-1.83651700	3.07540900
H	4.19690600	-1.53138000	1.74183500
C	-2.73778900	-3.45070100	0.08686500
H	-2.50429000	-4.41383700	0.52861000
C	-3.97846700	-3.19689600	-0.48986100
H	-4.74531800	-3.96579500	-0.51147600
C	0.98342400	2.56946700	-0.82382000
O	0.41990500	2.58274800	-1.93335600
C	1.95381400	3.65995900	-0.44335200
H	2.68877400	3.79682200	-1.24329500
H	1.40023800	4.60084500	-0.33982500
H	2.46407700	3.44542300	0.49864400
O	0.79132900	1.66074800	0.07085900

IIIPy-cis_OMe-up_pre-TS

C	3.60090100	2.46617700	0.54082000
H	4.57036400	2.44864100	1.02677300
N	1.68106200	1.25426600	-0.17995700
C	2.39674700	-2.56311300	0.37688800
O	1.40695800	-2.99204500	0.98847600
Pd	0.64575400	-0.47836400	-0.34772900
C	-2.19589900	0.08295800	-0.13585900
C	-2.39082700	-1.43613200	-0.14408000
C	-1.18069400	-2.06594700	-0.86388100
H	-0.26665700	-2.13855300	-0.19964700
H	-1.34531900	-3.14038200	-0.99683500
N	-3.16968400	0.95718800	0.11799000
O	-1.05524100	0.59150400	-0.34956000
C	-2.41892600	-1.94224800	1.31053100
H	-3.23710600	-1.50002800	1.88683300
H	-2.55838200	-3.02897600	1.30377200
H	-1.47312500	-1.72524100	1.82185700
C	-3.64792800	-1.86930300	-0.91806000
H	-4.57444800	-1.67766000	-0.37528100
H	-3.70701500	-1.38158500	-1.89739300
H	-3.59821700	-2.95036100	-1.08490100
H	-1.00213000	-1.65104500	-1.86097400
C	1.13916900	2.39011800	-0.66028800
H	0.16662700	2.31280300	-1.13368200
C	3.71328900	-3.28848600	0.41095900
H	4.04864600	-3.36106600	1.45140800
H	3.56833600	-4.30814100	0.03796700
H	4.47562500	-2.78361200	-0.18657500
O	2.38109900	-1.46582100	-0.32275300
C	2.88878800	1.28493500	0.41054200
H	3.27752500	0.34272100	0.77759000
C	1.80080800	3.60234700	-0.56007800
H	1.33413300	4.49420500	-0.96449400
C	3.05054100	3.64610800	0.05075200
H	3.58673500	4.58601700	0.14183200
O	-2.80959000	2.28565000	-0.00739800
C	-2.27046800	2.81517500	1.21145700
H	-2.06136000	3.86250100	0.98579500
H	-3.00957000	2.74711200	2.01739800
H	-1.34664100	2.29699500	1.48812000
C	-4.59482100	0.78313200	0.36757000

H	-4.78428000	-0.09294200	0.98586300		H	-5.15078400	0.72192400	-0.57164800
H	-4.92716200	1.66264100	0.92178200					

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4. ^1H and ^{13}C NMR Spectra

