Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Synergistic Catalysis: Enantioselective Synthesis of Alkylbenzoxazoles by Pd(II) and Secondary Amine Catalysis. Scope, Limitations and Mechanistic Insight

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Supporting information

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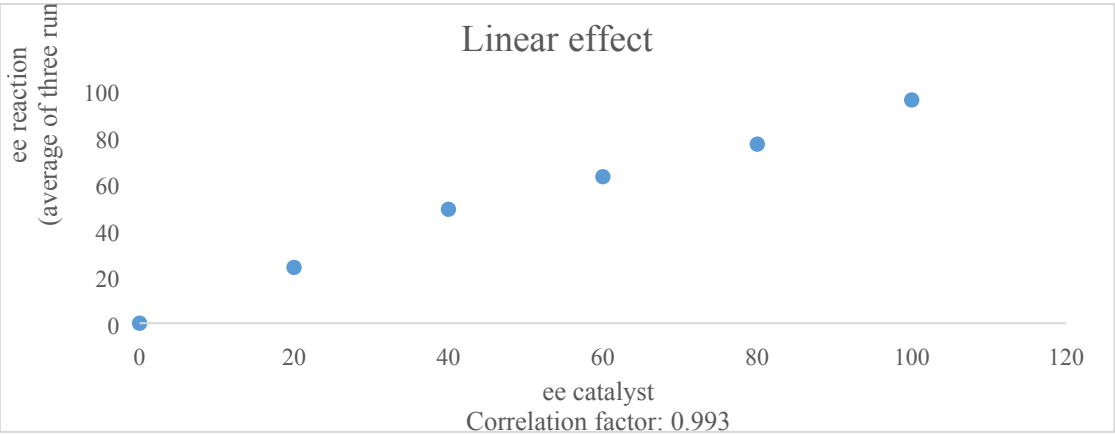
1. General information

Thin layer chromatography (TLC) was performed on Merck TLC Silicagel 60 F254. The products' spots were visualized by UV-light at 254 nm. Column chromatography was performed using silica gel (Geduran Si60, 40-63 µm). ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR, 2D-NMR were recorded with a Bruker DPX400 NMR. Chemical shifts (δ) are reported in ppm relative to residual solvent signals ($CHCl_3$, 7.26 ppm for ^{1}H NMR; $CDCl_3$, 77.16 ppm for ^{13}C NMR). ^{19}F NMR spectra were acquired in proton-decoupled mode. HRMS were recorded using a MaXis (Bruker Daltonics, Bremen, Germany) mass spectrometer equipped with a Time of Flight (TOF) analyzer. Optical rotations were performed on an Optical Activity PolAAr 2001 machine. The HPLC analysis were performed on a Perkin Elmer Flexar HPLC and an Agilent 1220 Infinity LC system HPLC.

2. Linear effect



Graph of the linear effect of the ee of the catalyst and the ee of the product of the cyclopropanation

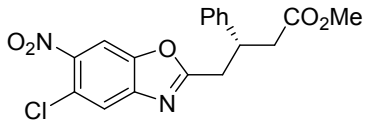
3. Opening of cyclopropanes 8 to give products 10

3.1. General procedure

To a suspension of the 3-benzyl-4,5-dimethylthiazol-3-ium chloride salt catalyst **9** (20 mol%) in CH_2Cl_2 (0.5 mL/0.2 mmol) at rt were added in this sequence: cyclopropane **8** (1 equiv), MeOH (3 equiv) and DIPEA (40 mol%). The resulting solution was stirred for 16 h and the reaction completion was checked by ^{1}H NMR. The product was purified by flash column chromatography on silica gel, to afford the final ester **10**.

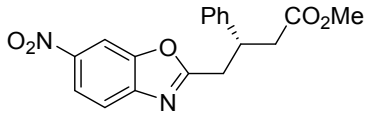
3.2. Characterization data for new compounds

methyl (*S*)-4-(5-chloro-6-nitrobenzo[d]oxazol-2-yl)-3-phenylbutanoate, 10a



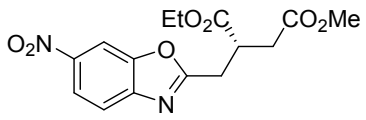
Following the general procedure, the product was isolated in 84% yield as a yellow oil by FC on silica gel using hexane/EtOAc 3:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.03 (s, 1H), 7.78 (s, 1H), 7.32 – 7.19 (m, 5H), 3.88 (dddd, *J* = 7.4 Hz, 1H), 3.60 (s, 3H), 3.42 (dd, *J* = 15.3, 7.1 Hz, 1H), 3.33 (dd, *J* = 15.3, 8.1 Hz, 1H), 2.83 (qd, *J* = 15.9, 7.4 Hz, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 171.9, 170.5, 148.3, 145.1, 144.7, 141.6, 129.0 (2C), 127.6, 127.2 (2C), 123.6, 122.4, 108.6, 51.9, 40.3, 39.9, 35.4. **HRMS (ESI+) *m/z*** calculated for $C_{18}H_{16}ClN_2O_5$ $[M+H]^+$: 375.0742; found: 375.0744. **HPLC**: ODH, hexane/*i*PrOH 85:15, 0.7 mL/min, λ = 210 nm; t_R = 54.05 min; t_S = 56.73 min; >99% ee. $[\alpha]_D^{21}$ **(S catalyst)** = − 57.9 (*c* 0.9, $CHCl_3$).

methyl (*S*)-4-(6-nitrobenzo[d]oxazol-2-yl)-3-phenylbutanoate, 10b



Following the general procedure, the product was isolated in 79% yield as a yellow oil by FC on silica gel using hexane/EtOAc 5:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.37 (d, *J* = 2.1 Hz, 1H), 8.26 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.32 – 7.21 (m, 5H), 3.91 (dddd, *J* = 7.5 Hz, 1H), 3.59 (s, 3H), 3.43 (dd, *J* = 15.3, 7.3 Hz, 1H), 3.35 (dd, *J* = 15.2, 7.8 Hz, 1H), 2.89 (dd, *J* = 15.9, 7.3 Hz, 1H), 2.81 (dd, *J* = 15.9, 7.5 Hz, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 171.9, 169.9, 150.0, 146.6, 145.2, 141.8, 129.0 (2C), 127.5, 127.2 (2C), 120.5, 119.8, 107.2, 51.9, 40.4, 40.0, 35.5. **HRMS** (ESI+) *m/z* calcd. for $C_{18}H_{17}N_2O_5$ $[M+H]^+$: 341.1132; found: 341.1135. $[\alpha]_D^{21}$ **(S catalyst)** = – 53.2 (*c* 0.9, $CHCl_3$).

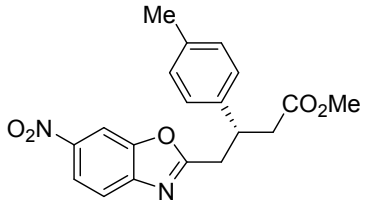
1-ethyl 4-methyl (*S*)-2-((6-nitrobenzo[d]oxazol-2-yl)methyl)succinate, 10c



Following the general procedure, the product was isolated in 54% yield as a yellow oil by FC on silica gel using hexane/EtOAc 4:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.41 (d, *J* = 2.1 Hz, 1H), 8.29 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.76 (d, *J* = 8.7 Hz, 1H), 4.18 (q, *J* = 7.1 Hz, 2H), 3.70 (s, 3H), 3.59 – 3.44 (m, 2H), 3.30 (dd, *J* = 15.9, 6.7 Hz, 1H), 2.91 (dd, *J* = 16.9, 6.7 Hz, 1H), 2.77 (dd, *J* = 16.9, 6.2 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 172.5, 171.7, 169.4, 150.1,

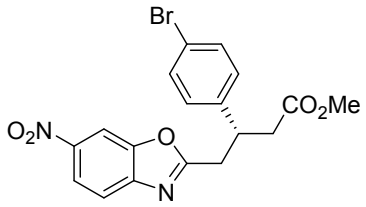
150.0, 146.6, 120.7, 119.9, 107.3, 61.6, 52.2, 39.0, 35.1, 30.2, 14.2. **HRMS** (ESI+) *m/z* calcd. for $C_{15}H_{17}N_2O_7$ $[M+H]^+$: 337.1030; found: 337.1027. $[\alpha]_D^{21}$ **(S catalyst)** = + 2.2 (*c* 0.8, $CHCl_3$).

methyl (*S*)-4-(6-nitrobenzo[d]oxazol-2-yl)-3-(p-tolyl)butanoate, 10d



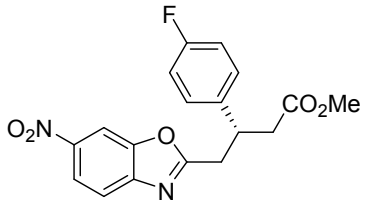
Following the general procedure, the product was isolated in 74% yield as a yellow oil by FC on silica gel using hexane/EtOAc 5:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.36 (d, *J* = 1.9 Hz, 1H), 8.25 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.13 – 7.07 (m, 4H), 3.86 (dddd, *J* = 7.3 Hz, 1H), 3.58 (s, 3H), 3.38 (d, *J* = 7.3 Hz, 1H), 3.31 (dd, *J* = 15.2, 7.9 Hz, 1H), 2.85 (dd, *J* = 15.9, 7.3 Hz, 1H), 2.77 (dd, *J* = 15.8, 7.5 Hz, 1H), 2.28 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 172.0, 170.0, 150.0, 146.7, 145.2, 138.8, 137.1, 129.7 (2C), 127.0 (2C), 120.5, 119.8, 107.2, 51.9, 40.5, 39.6, 35.6, 21.2. **HRMS** (ESI+) *m/z* calcd. for $C_{19}H_{19}N_2O_5$ $[M+H]^+$: 355.1288; found: 355.1291. $[\alpha]_D^{21}$ **(S catalyst)** = − 15.7 (*c* 0.9, $CHCl_3$).

methyl (*S*)-3-(4-bromophenyl)-4-(6-nitrobenzo[d]oxazol-2-yl)butanoate, 10e



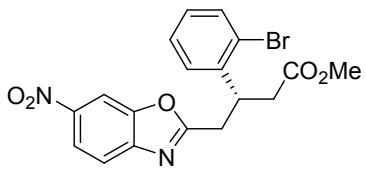
Following the general procedure, the product was isolated in 72% yield as a yellow oil by FC on silica gel using hexane/EtOAc 3:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.38 (d, *J* = 2.1 Hz, 1H), 8.28 (dd, *J* = 8.8, 2.1 Hz, 1H), 8.17 (d, *J* = 8.8 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.46 (d, *J* = 8.7 Hz, 2H), 4.05 (dddd, *J* = 7.5 Hz, 1H), 3.62 (s, 3H), 3.48 (dd, *J* = 15.6, 6.9 Hz, 1H), 3.38 (dd, *J* = 15.6, 8.1 Hz, 1H), 2.95 (dd, *J* = 16.2, 6.7 Hz, 1H), 2.84 (dd, *J* = 16.2, 8.0 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.2, 168.8, 150.0, 149.2, 147.4, 146.3, 145.4, 128.4 (2C), 124.3 (2C), 120.7, 120.0, 107.3, 52.1, 39.9, 39.6, 34.9. **HRMS** (ESI+) *m/z* calcd. for $C_{18}H_{16}BrN_2O_5$ $[M+H]^+$: 419.0237; found: 419.0234. $[\alpha]_D^{21}$ **(S catalyst)** = − 25.2 (*c* 0.9, $CHCl_3$).

methyl (*S*)-3-(4-fluorophenyl)-4-(6-nitrobenzo[d]oxazol-2-yl)butanoate, 10f



Following the general procedure, the product was isolated in 77% yield as a yellow oil by FC on silica gel using hexane/EtOAc 5:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.37 (d, *J* = 1.9 Hz, 1H), 8.26 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.24 – 7.17 (m, 2H), 7.02 – 6.92 (m, 2H), 3.89 (dddd, *J* = 7.4 Hz, 1H), 3.59 (s, 3H), 3.40 (dd, *J* = 15.3, 7.1 Hz, 1H), 3.30 (dd, *J* = 15.3, 8.0 Hz, 1H), 2.86 (dd, *J* = 15.9, 7.0 Hz, 1H), 2.76 (dd, *J* = 15.9, 7.8 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** 171.7, 169.6, 162.0 (d, *J* = 245.9 Hz), 150.0, 146.5, 145.2, 137.4, 128.8 (d, *J* = 8.0 Hz, 2C), 120.6, 119.8, 115.8 (d, *J* = 21.4 Hz, 2C), 107.1, 51.9, 40.4, 39.3, 35.5. **^{19}F NMR (376 MHz, $CDCl_3$)** δ -115.0. **HRMS** (ESI+) *m/z* calcd. for $C_{18}H_{16}FN_2O_5$ $[M+H]^+$: 359.1038; found: 359.1040. $[\alpha]_D^{21}$ **(S catalyst)** = − 70.9 (*c* 1.0, $CHCl_3$).

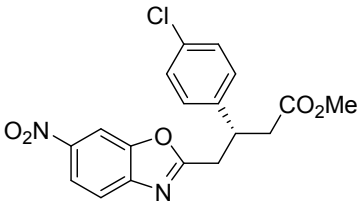
methyl (*S*)-3-(2-bromophenyl)-4-(6-nitrobenzo[d]oxazol-2-yl)butanoate, 10g



Following the general procedure, the product was isolated in 59% yield as a yellow oil by FC on silica gel using hexane/EtOAc

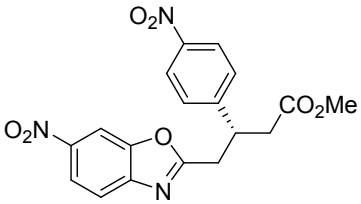
5:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.38 (d, *J* = 2.0 Hz, 1H), 8.26 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.74 (d, *J* = 8.7 Hz, 1H), 7.56 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.27 (dd, *J* = 5.0, 1.8 Hz, 2H), 7.10 (ddd, *J* = 8.1, 6.0, 3.1 Hz, 1H), 4.41 (dddd, *J* = 7.2 Hz, 1H), 3.60 (s, 3H), 3.42 (dd, *J* = 7.3, 2.6 Hz, 2H), 2.90 (dd, *J* = 7.2, 5.5 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.6, 169.5, 150.1, 146.6, 145.2, 140.6, 133.6, 128.9, 128.1, 127.6, 124.6, 120.5, 119.8, 107.2, 52.0, 38.7, 38.6, 34.0. **HRMS** (ESI+) *m*/*z* calcd. for $C_{18}H_{16}BrN_2O_5$ $[M+H]^+$: 419.0237; found: 419.0232. $[\alpha]_D^{21}$ **(S catalyst)** = − 9.0 (*c* 0.9, $CHCl_3$).

methyl (*S*)-3-(4-chlorophenyl)-4-(6-nitrobenzo[d]oxazol-2-yl)butanoate, 10h



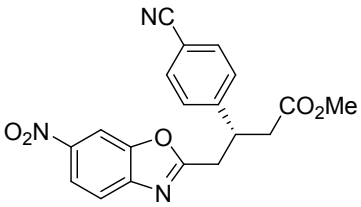
Following the general procedure, the product was isolated in 65% yield as a yellow oil by FC on silica gel using hexane/EtOAc 5:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.29 (d, *J* = 2.1 Hz, 1H), 8.19 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.20 – 7.16 (m, 2H), 7.14 – 7.09 (m, 2H), 3.82 (dddd, *J* = 7.5 Hz, 1H), 3.52 (s, 3H), 3.33 (dd, *J* = 15.4, 7.1 Hz, 1H), 3.23 (dd, *J* = 15.4, 8.1 Hz, 1H), 2.79 (dd, *J* = 16.0, 7.0 Hz, 1H), 2.69 (dd, *J* = 16.0, 7.8 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.6, 169.5, 150.0, 146.5, 145.3, 140.2, 133.3, 129.2 (2C), 128.6 (2C), 120.6, 119.8, 107.2, 52.0, 40.2, 39.3, 35.3. **HRMS** (ESI+) *m*/*z* calcd. for $C_{18}H_{16}ClN_2O_5$ $[M+H]^+$: 375.0742; found: 375.0742. $[\alpha]_D^{21}$ **(S catalyst)** = − 63.0 (*c* 0.9, $CHCl_3$).

methyl (*S*)-4-(6-nitrobenzo[d]oxazol-2-yl)-3-(4-nitrophenyl)butanoate, 10i



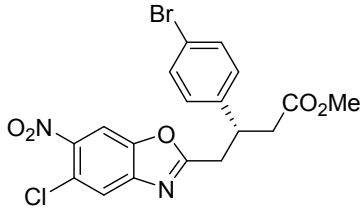
Following the general procedure, the product was isolated in 73% yield as a yellow oil by FC on silica gel using hexane/EtOAc 3:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.36 (d, *J* = 2.1 Hz, 1H), 8.26 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 3.88 (dddd, *J* = 7.4 Hz, 1H), 3.59 (s, 3H), 3.40 (dd, *J* = 15.4, 7.1 Hz, 1H), 3.30 (dd, *J* = 15.4, 8.1 Hz, 1H), 2.86 (dd, *J* = 16.0, 7.0 Hz, 1H), 2.76 (dd, *J* = 16.0, 7.8 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.6, 169.4, 150.0, 146.5, 145.3, 140.7, 132.1 (2C), 129.0 (2C), 121.4, 120.6, 119.9, 107.2, 52.0, 40.2, 39.4, 35.2. **HRMS** (ESI+) *m*/*z* calcd. for $C_{18}H_{16}N_3O_7$ $[M+H]^+$: 386.0983; found: 386.0988. $[\alpha]_D^{21}$ **(S catalyst)** = − 59.9 (*c* 1.0, $CHCl_3$).

methyl (*S*)-3-(4-cyanophenyl)-4-(6-nitrobenzo[d]oxazol-2-yl)butanoate, 10j



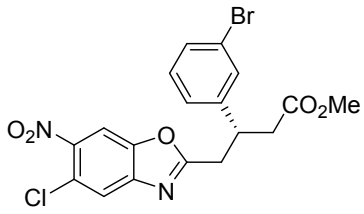
Following the general procedure, the product was isolated in 86% yield as a yellow oil by FC on silica gel using hexane/EtOAc 6:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.37 (d, *J* = 2.1 Hz, 1H), 8.27 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 2H), 3.98 (dddd, *J* = 7.5 Hz, 1H), 3.60 (s, 3H), 3.44 (dd, *J* = 15.6, 7.0 Hz, 1H), 3.34 (dd, *J* = 15.6, 8.1 Hz, 1H), 2.91 (dd, *J* = 16.2, 6.8 Hz, 1H), 2.80 (dd, *J* = 16.2, 7.9 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.3, 168.9, 150.0, 147.2, 146.3, 145.4, 132.8 (2C), 128.3 (2C), 120.7, 119.9, 118.6, 111.7, 107.2, 52.1, 39.8, 39.8, 34.8. **HRMS** (ESI+) *m*/*z* calcd. for $C_{19}H_{16}N_3O_5$ $[M+H]^+$: 366.1084; found: 366.1085. $[\alpha]_D^{21}$ **(S catalyst)** = − 55.2 (*c* 0.9, $CHCl_3$).

methyl (*S*)-3-(4-bromophenyl)-4-(5-chloro-6-nitrobenzo[d]oxazol-2-yl)butanoate, 10k



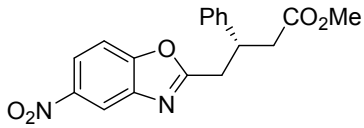
Following the general procedure, the product was isolated in 74% yield as a yellow oil by FC on silica gel using hexane/EtOAc 4:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.02 (s, 1H), 7.77 (s, 1H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 8.5 Hz, 2H), 3.85 (dddd, *J* = 7.4 Hz, 1H), 3.60 (s, 3H), 3.39 (dd, *J* = 15.4, 6.8 Hz, 1H), 3.29 (dd, *J* = 15.4, 8.3 Hz, 1H), 2.84 (dd, *J* = 16.0, 7.1 Hz, 1H), 2.75 (dd, *J* = 16.0, 7.6 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.6, 170.0, 148.3, 145.0, 144.8, 140.6, 132.2 (2C), 129.0 (2C), 123.7, 122.4, 121.5, 108.6, 52.0, 40.2, 39.4, 35.1. **HRMS** (ESI+) *m*/*z* calcd. for $C_{18}H_{15}BrClN_2O_5$ $[M+H]^+$: 452.9847; found: 452.9848. $[\alpha]_D^{21}$ **(S catalyst)** = − 25.9 (*c* 0.3, $CHCl_3$).

methyl (*S*)-3-(3-bromophenyl)-4-(5-chloro-6-nitrobenzo[d]oxazol-2-yl)butanoate, 10l



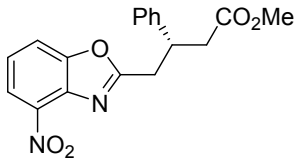
Following the general procedure, the product was isolated in 96% yield as a yellow oil by FC on silica gel using hexane/EtOAc 4:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.03 (s, 1H), 7.78 (s, 1H), 7.39 (d, *J* = 1.6 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.18 – 7.13 (m, 2H), 3.85 (dddd, *J* = 7.4 Hz, 1H), 3.60 (s, 3H), 3.40 (dd, *J* = 15.5, 7.1 Hz, 1H), 3.30 (dd, *J* = 15.5, 8.0 Hz, 1H), 2.85 (dd, *J* = 16.1, 7.2 Hz, 1H), 2.76 (dd, *J* = 16.1, 7.4 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.5, 170.0, 148.3, 145.0, 144.8, 144.0, 130.8, 130.6, 130.4, 126.0, 123.7, 123.0, 122.4, 108.6, 52.0, 40.1, 39.5, 35.0. **HRMS** (ESI+) *m*/*z* calcd. for $C_{18}H_{15}BrClN_2O_5$ $[M+H]^+$: 452.9847; found: 452.9850. $[\alpha]_D^{21}$ **(R catalyst)** = + 38.0 (*c* 0.2, $CHCl_3$).

methyl (*S*)-4-(5-nitrobenzo[d]oxazol-2-yl)-3-phenylbutanoate, 10m



Following the general procedure, the product was isolated in 65% yield as a yellow oil by FC on silica gel using hexane/EtOAc 4:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.52 (d, *J* = 2.2 Hz, 1H), 8.26 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.55 (d, *J* = 8.9 Hz, 1H), 7.32 – 7.17 (m, 5H), 3.89 (dddd, *J* = 7.4 Hz, 1H), 3.58 (s, 3H), 3.40 (dd, *J* = 15.3, 7.4 Hz, 1H), 3.32 (dd, *J* = 15.4, 7.8 Hz, 1H), 2.88 (dd, *J* = 15.9, 7.3 Hz, 1H), 2.80 (dd, *J* = 15.9, 7.5 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 172.0, 168.2, 154.4, 145.3, 141.9, 141.8, 129.0 (2C), 127.5 (2C), 127.2, 121.0, 116.3, 110.7, 51.9, 40.3, 39.9, 35.3. **HRMS** (ESI+) *m*/*z* calcd. for $C_{18}H_{17}N_2O_5$ $[M+H]^+$: 341.1132; found: 341.1135. $[\alpha]_D^{21}$ **(S catalyst)** = − 61.2 (*c* 0.9, $CHCl_3$).

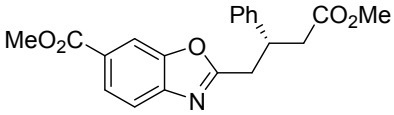
methyl (*S*)-4-(4-nitrobenzo[d]oxazol-2-yl)-3-phenylbutanoate, 10n



Following the general procedure, the product was isolated in 94% yield as a yellow oil by FC on silica gel using hexane/EtOAc 2:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.13 (d, *J* = 8.2 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.42 (t, *J* = 8.2 Hz, 1H), 7.30 – 7.23 (m, 4H), 7.22 – 7.16

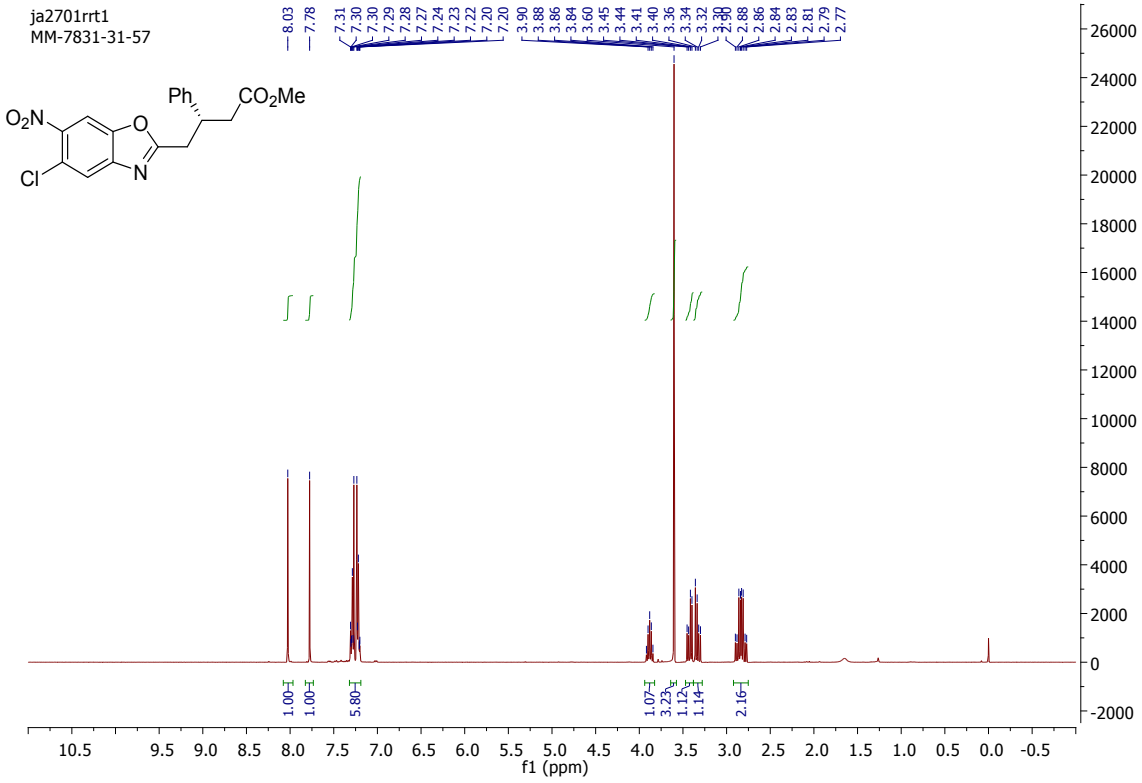
(m, 1H), 3.91 (dddd, *J* = 7.6 Hz, 1H), 3.54 (s, 3H), 3.46 (t, *J* = 7.5 Hz, 1H), 3.39 (dd, *J* = 15.1, 7.6 Hz, 1H), 2.85 (dd, *J* = 15.1, 6.3 Hz, 1H), 2.79 (dd, *J* = 15.1, 6.9 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 172.4, 169.3, 153.0, 142.3, 139.5, 136.4, 129.4 (2C), 127.9, 127.7 (2C), 124.8, 121.3, 117.1, 52.3, 40.8, 40.5, 35.9. **HRMS** (ESI+) *m*/*z* calcd. for $C_{18}H_{17}N_2O_5$ $[M+H]^+$: 341.1132; found: 341.1129. $[\alpha]_D^{21}$ **(R catalyst)** = + 39.9 (*c* 0.8, $CHCl_3$).

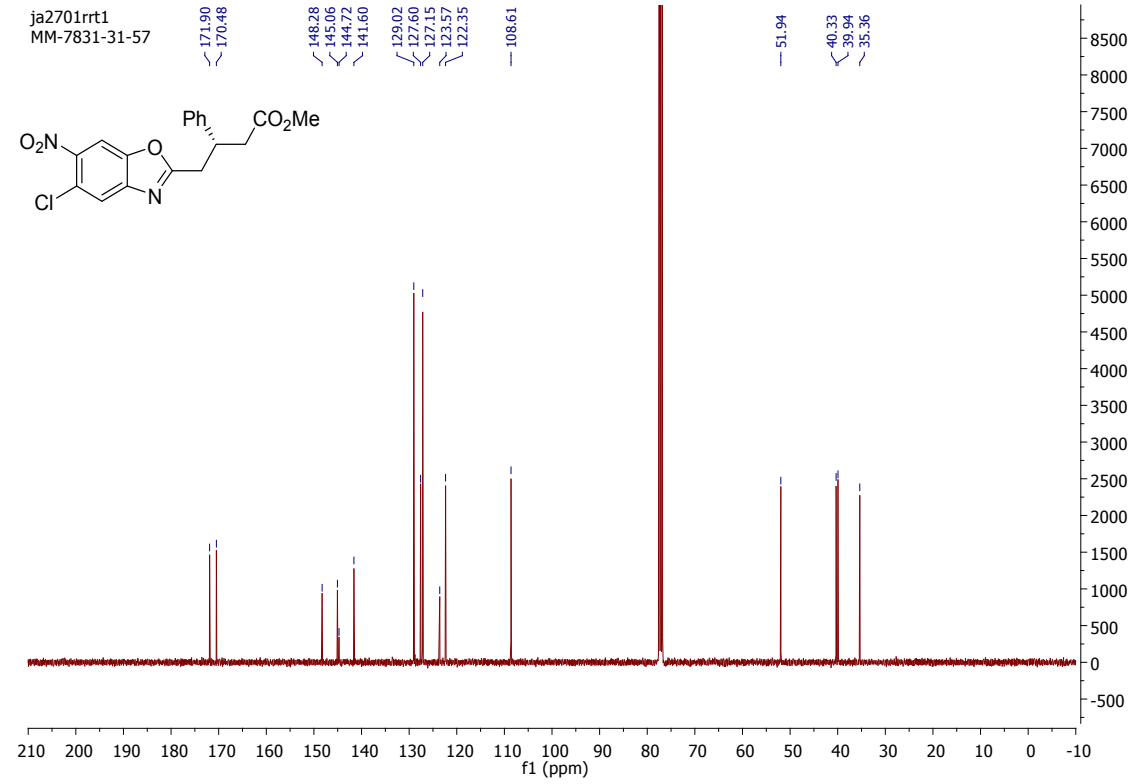
methyl (*S*)-2-(4-methoxy-4-oxo-2-phenylbutyl)benzo[d]oxazole-6-carboxylate, 10o

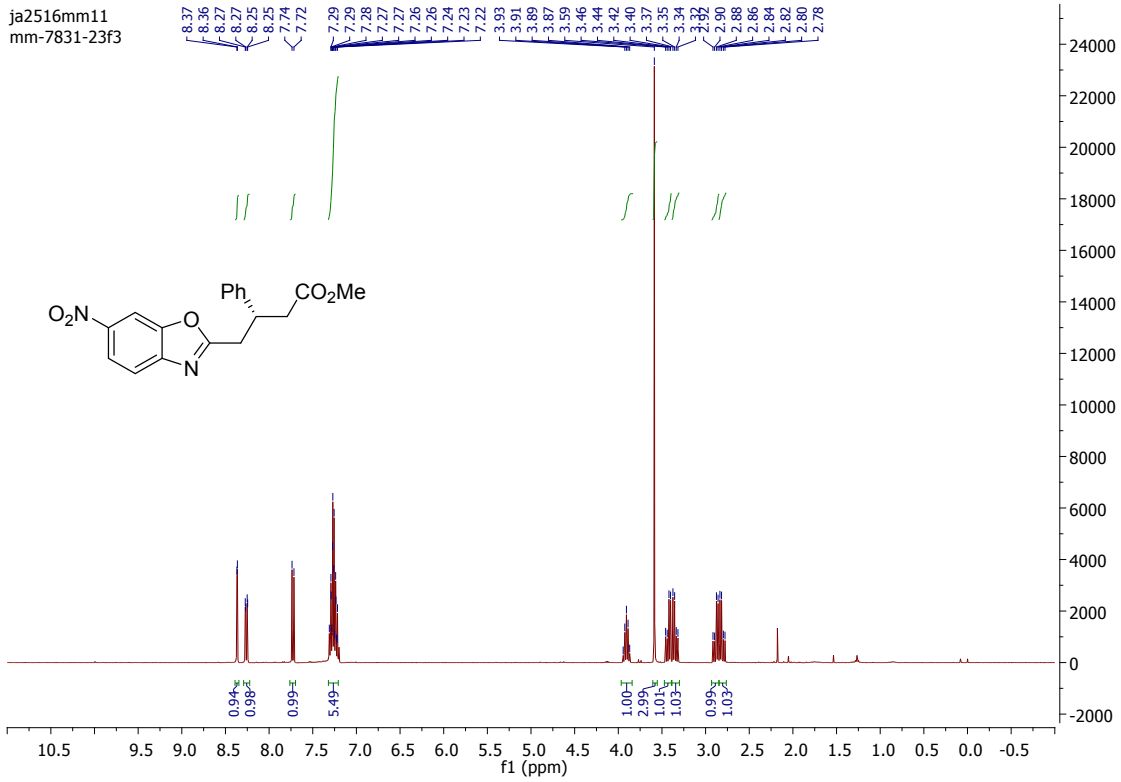


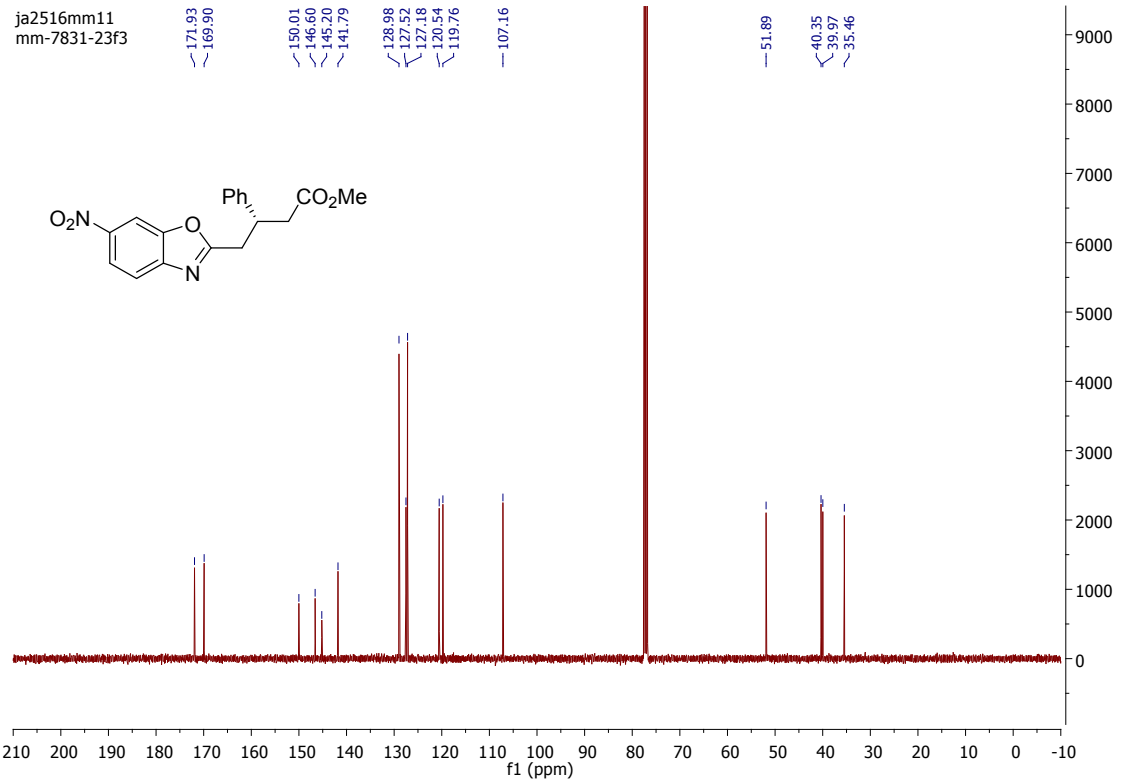
Following the general procedure, the product was isolated in 65% yield as a yellow oil by FC on silica gel using hexane/EtOAc 3:1 as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.08 (d, *J* = 0.8 Hz, 1H), 7.96 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.59 (d, *J* = 8.3 Hz, 1H), 7.25 – 7.12 (m, 5H), 3.88 (s, 3H), 3.83 (dddd, *J* = 7.4 Hz, 1H), 3.49 (s, 3H), 3.30 (dd, *J* = 15.2, 7.7 Hz, 1H), 3.24 (dd, *J* = 15.2, 7.5 Hz, 1H), 2.81 (dd, *J* = 15.8, 7.0 Hz, 1H), 2.72 (dd, *J* = 15.8, 7.8 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 172.0, 167.8, 166.8, 150.6, 145.3, 142.1, 128.9 (2C), 127.4, 127.2 (2C), 127.0, 126.2, 119.5, 112.2, 52.5, 51.8, 40.4, 40.1, 35.5. **HRMS** (ESI+) *m*/*z* calcd. for $C_{20}H_{20}NO_5$ $[M+H]^+$: 354.1336; found: 354.1335. $[\alpha]_D^{21}$ **(S catalyst)** = − 45.0 (*c* 0.9, $CHCl_3$).

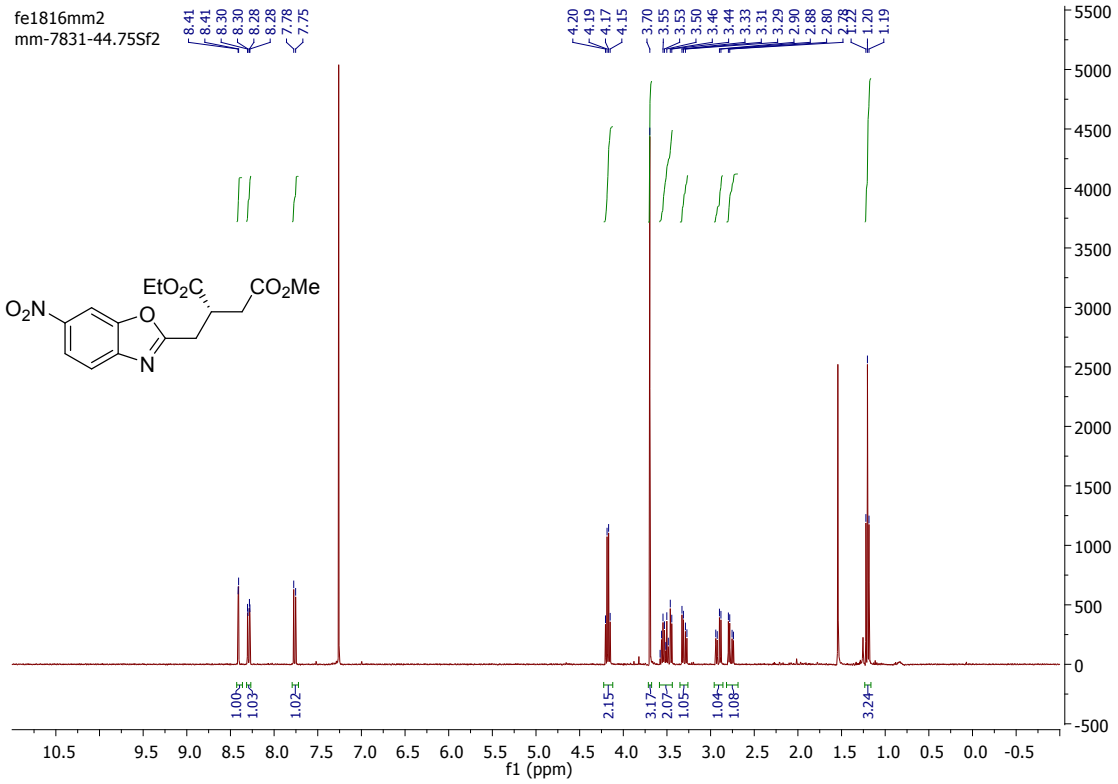
4. NMR spectra

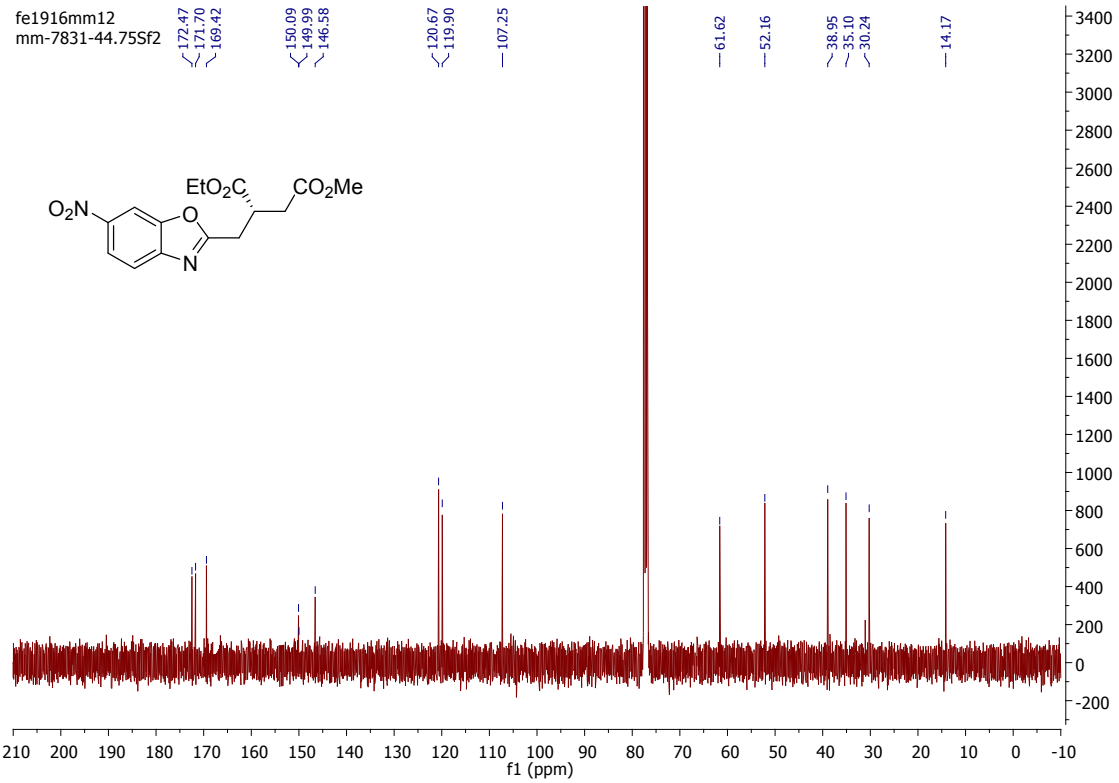


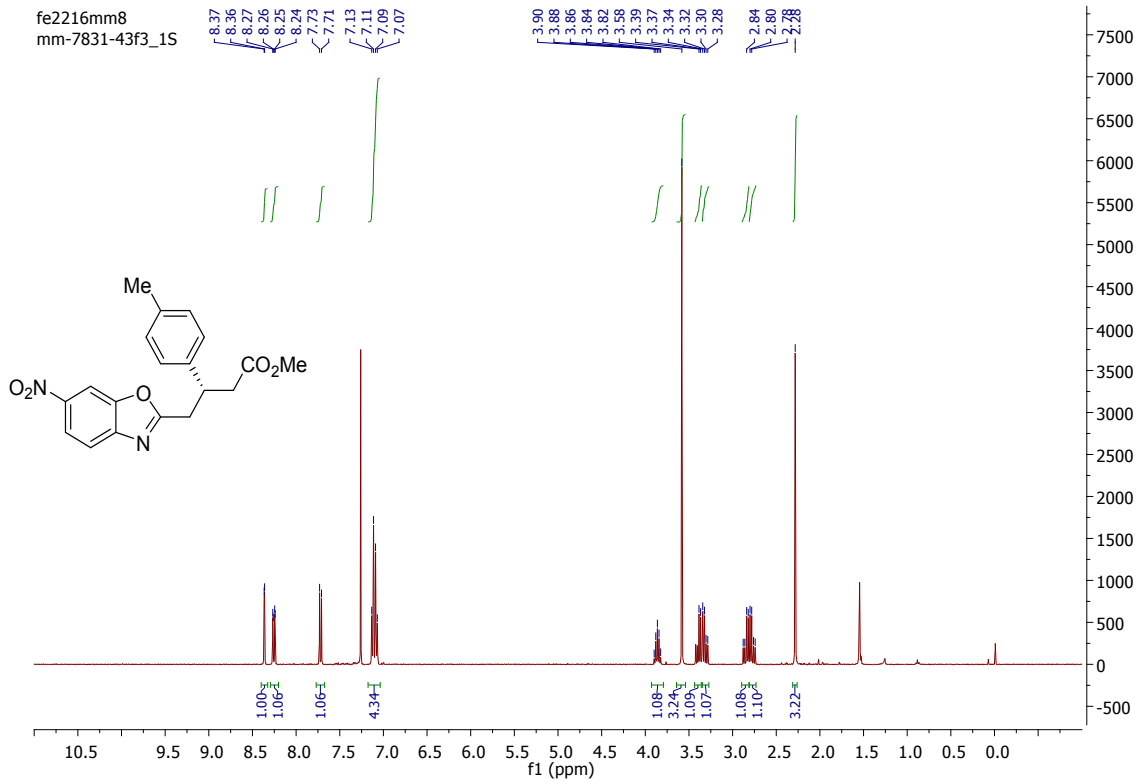


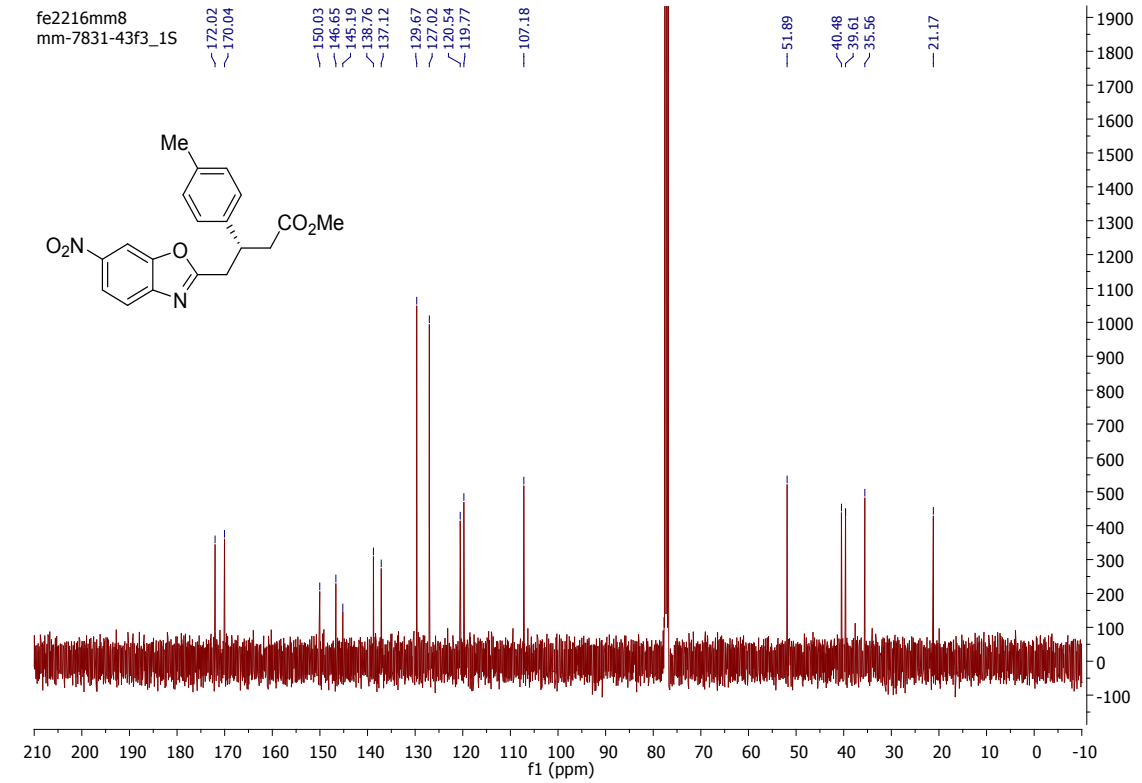

ja2516mm11
mm-7831-23f3
8.37
8.36
8.27
8.27
8.25
8.25
7.74
7.72
7.29
7.29
7.28
7.27
7.27
7.26
7.26
7.24
7.23
7.22
3.93
3.91
3.89
3.87
3.59
3.46
3.44
3.42
3.40
3.37
3.35
3.34
2.92
2.90
2.88
2.86
2.84
2.82
2.80
2.78
Ph
CO2Me
O2N
O
N
0.94
0.98
0.99
5.49
1.00
2.99
1.01
1.03
0.99
1.03
f1 (ppm)

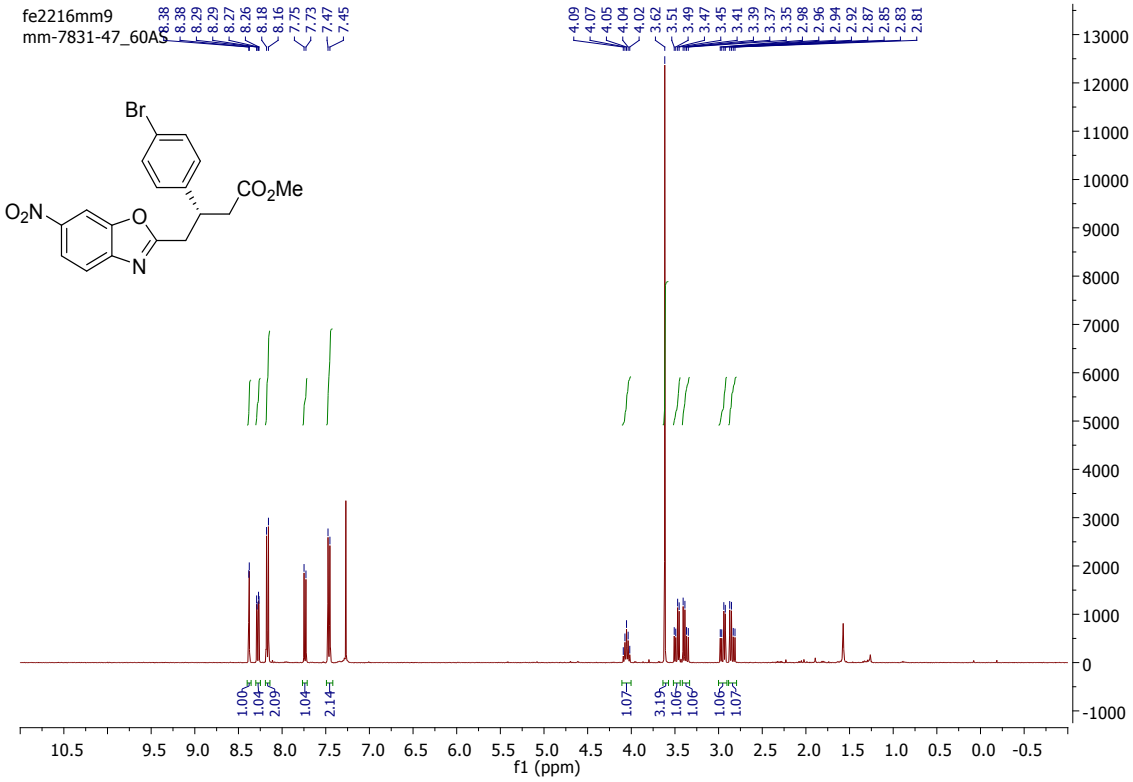

ja2516mm11
mm-7831-23f3
171.93
169.90
150.01
146.60
145.20
141.79
128.98
127.52
127.18
120.54
119.76
107.16
51.89
40.35
39.97
35.46
Ph
CO2Me
O2N
O
N
f1 (ppm)


fe1816mm2
mm-7831-44.75Sf2
8.41
8.41
8.30
8.30
8.28
8.28
7.78
7.75
4.20
4.19
4.17
4.15
3.70
3.55
3.53
3.50
3.46
3.44
3.33
3.31
3.29
2.90
2.88
2.80
1.22
1.20
1.19
EtO2C
CO2Me
O2N
O
N
1.00
1.03
1.02
2.15
3.17
2.07
1.05
1.04
1.08
3.24
f1 (ppm)


fe1916mm12
mm-7831-44.75Sf2
172.47
171.70
169.42
150.09
149.99
146.58
120.67
119.90
107.25
61.62
52.16
38.95
35.10
30.24
14.17
EtO2C
CO2Me
O2N
O
N
f1 (ppm)


fe2216mm8
mm-7831-43f3_1S
Me
CO2Me
O2N
O
N
f1 (ppm)


fe2216mm8
mm-7831-43f3_1S
Me
CO2Me
O2N
O
N
f1 (ppm)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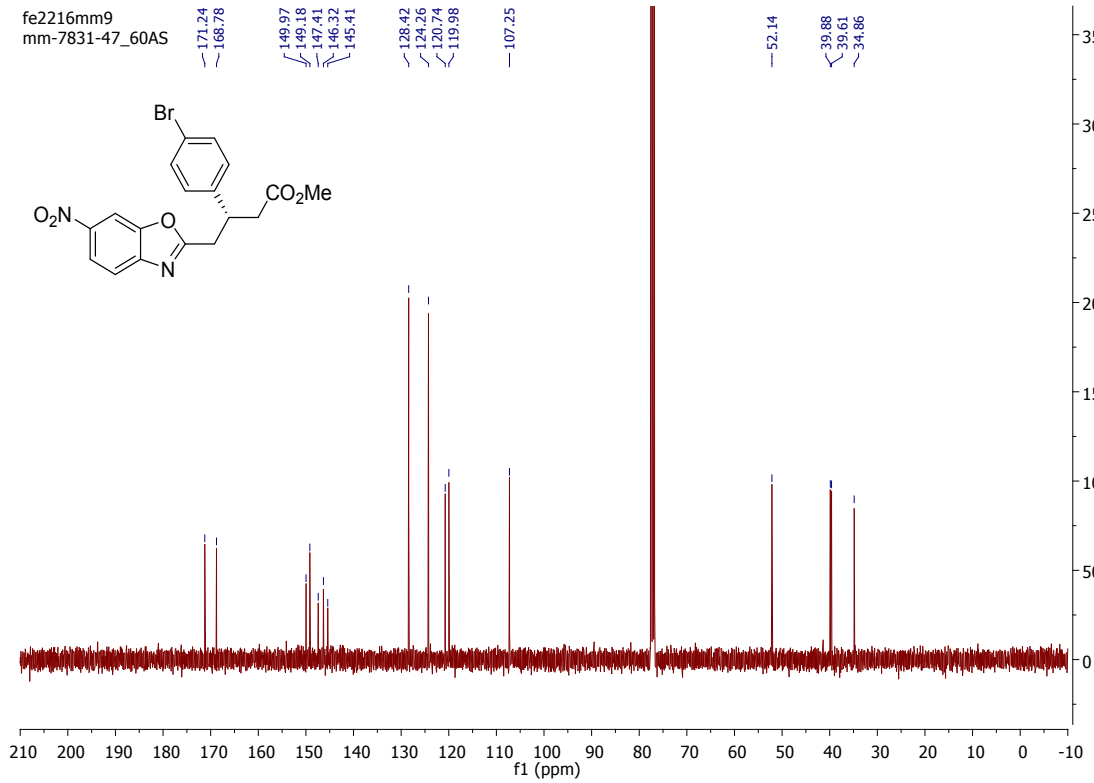
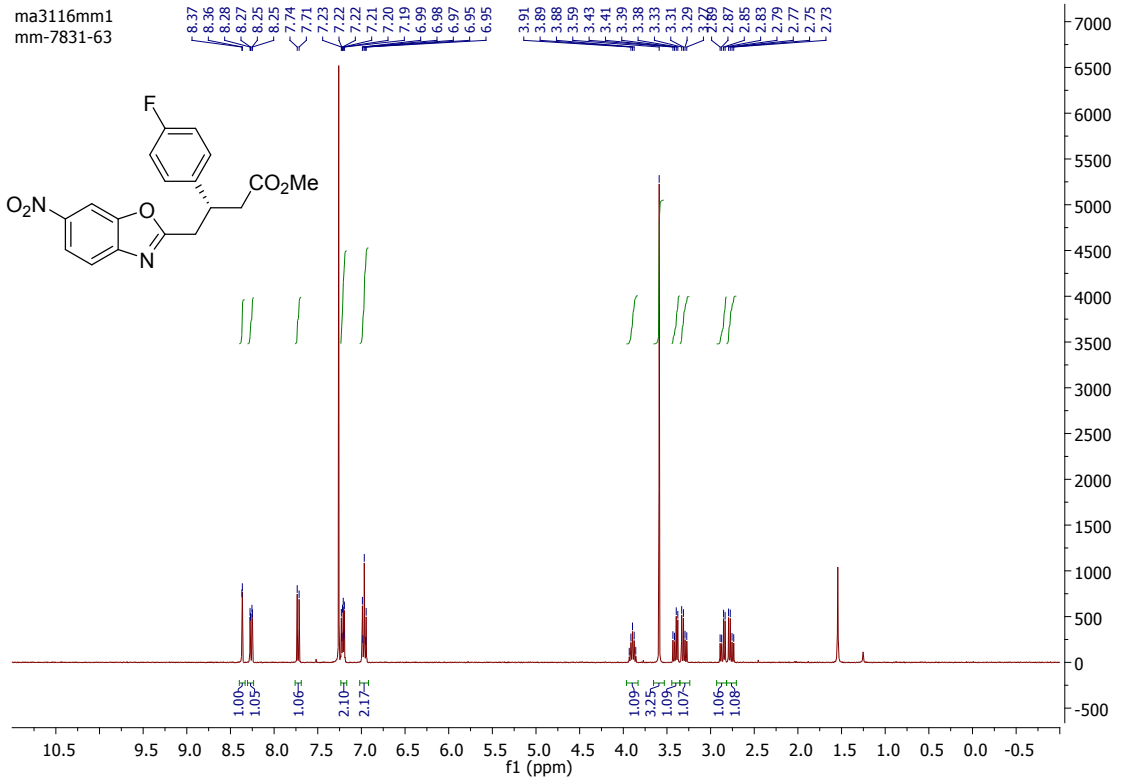
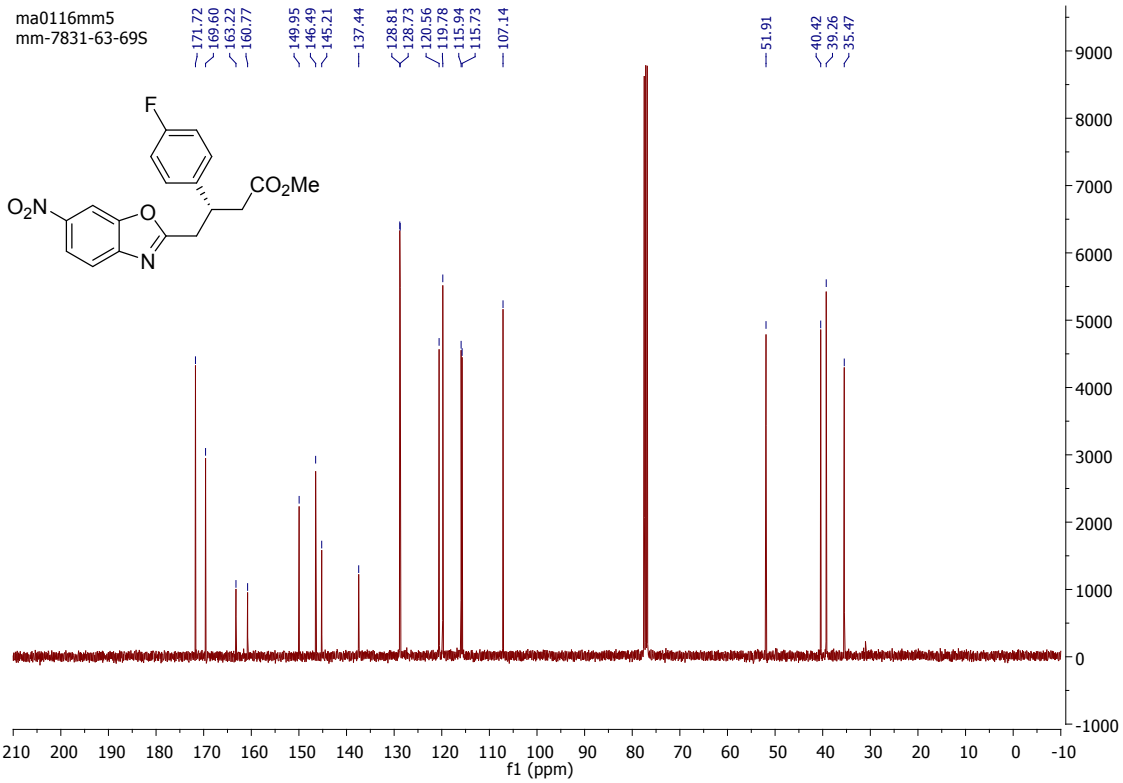
mm-7831-47_60AS
Br
CO2Me
O2N
O
N
f1 (ppm)


fe2216mm9
mm-7831-47_60AS
Br
CO2Me
O2N
O
N
f1 (ppm)


ma3116mm1
mm-7831-63
F
CO2Me
O2N
O
N
f1 (ppm)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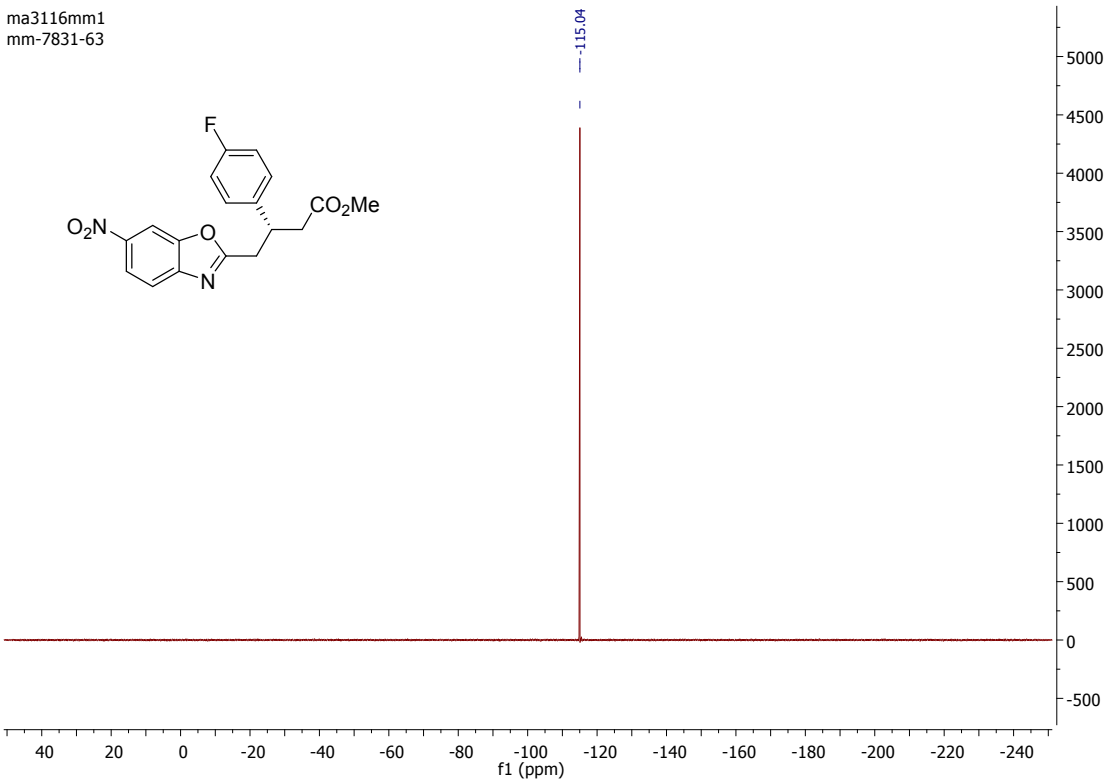
F
CO2Me
O2N
O
N
f1 (ppm)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mm-7831-63
-115.04
F
CO_2Me
O_2N
O
N
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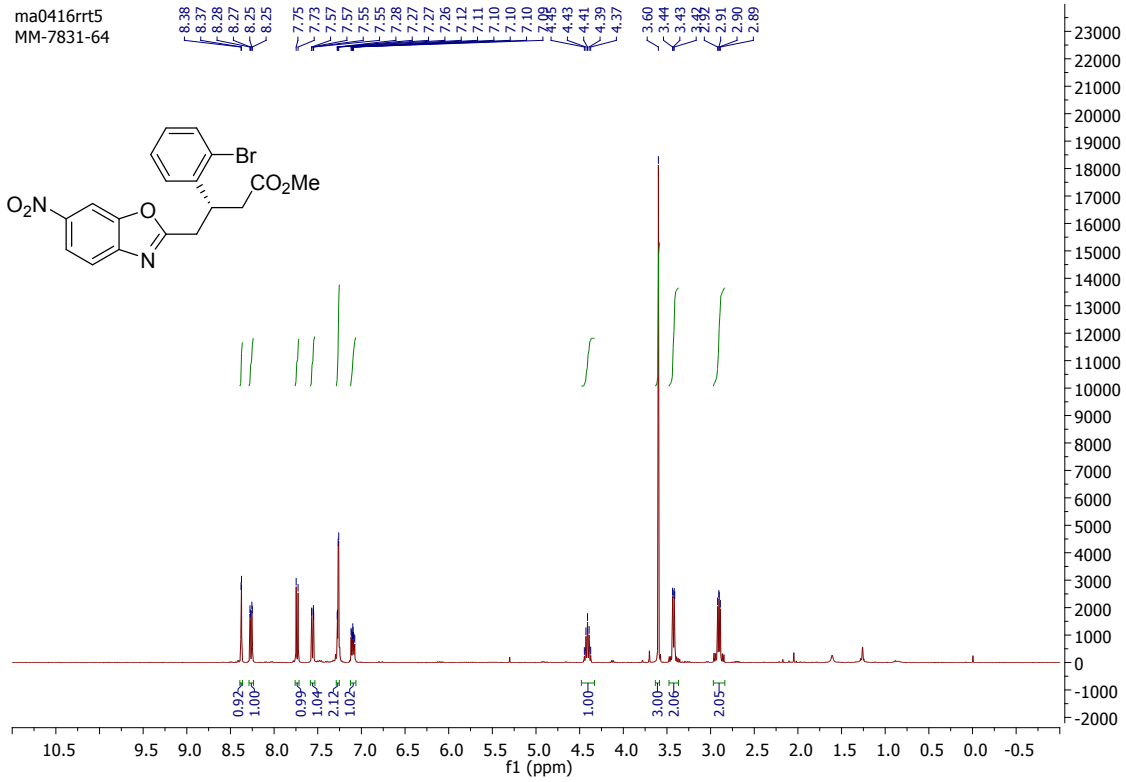
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
f1 (ppm)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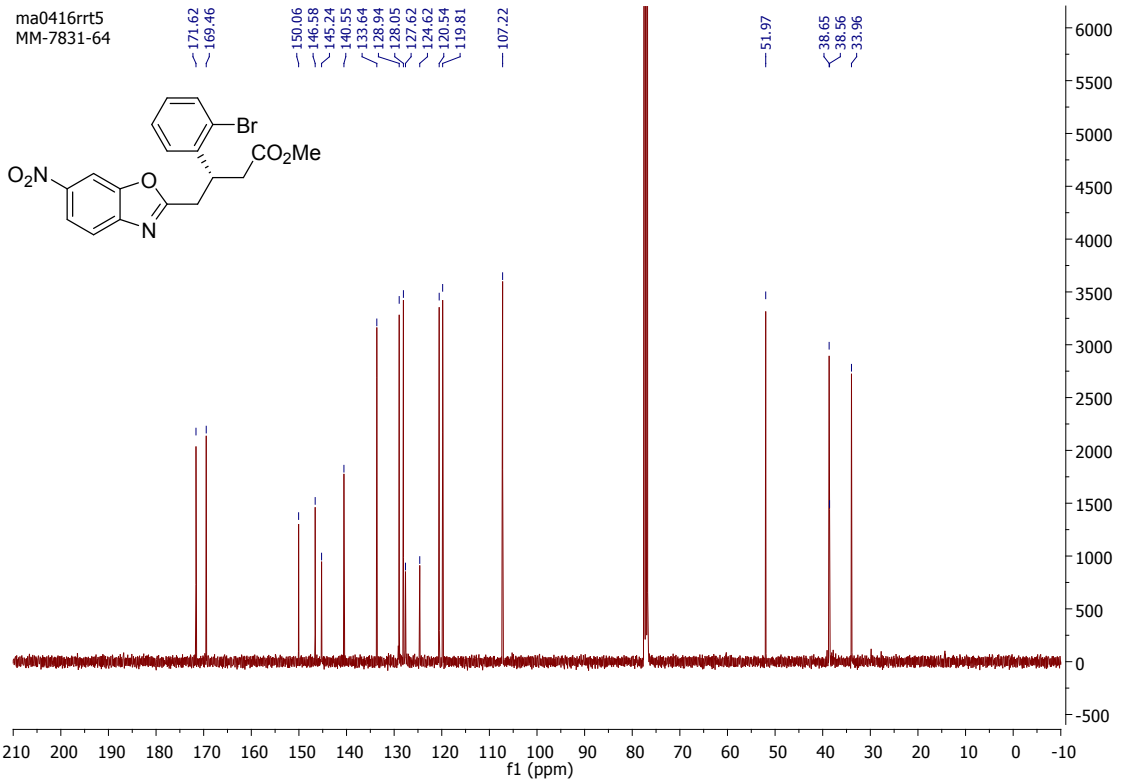
Br
CO2Me
O2N
O
N
f1 (ppm)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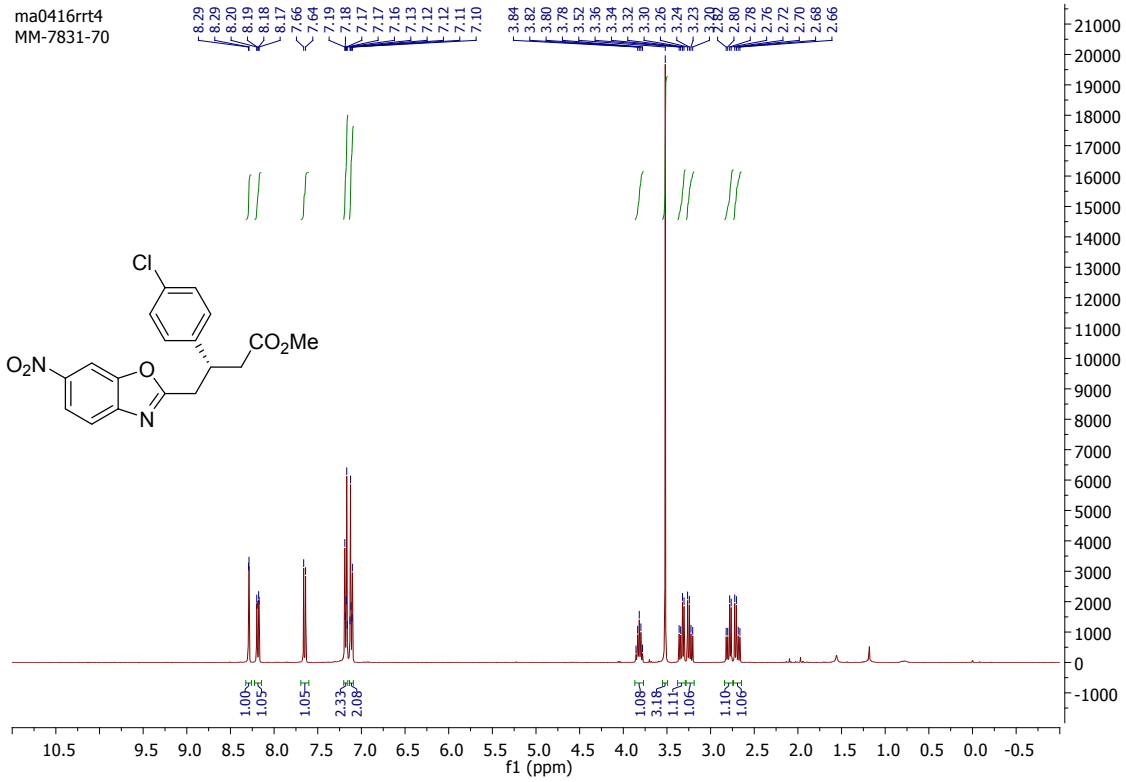
Br
CO2Me
O2N
O
N
f1 (ppm)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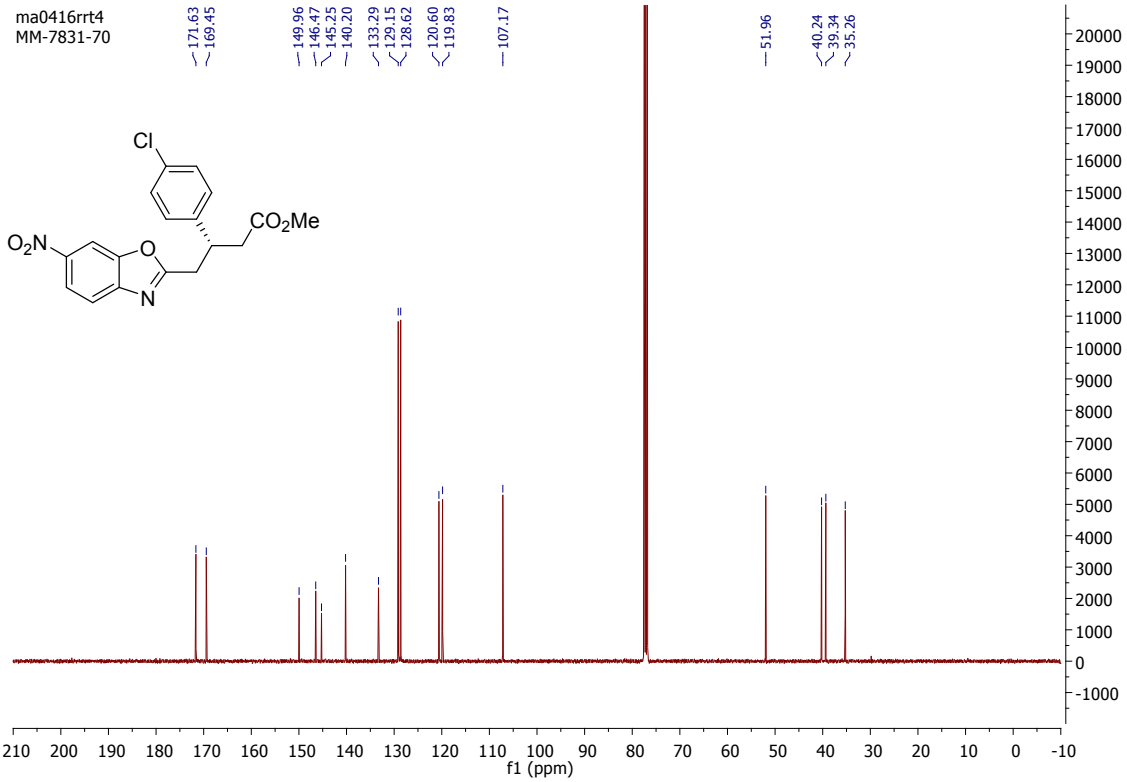
Cl
CO2Me
O2N
O
N
f1 (ppm)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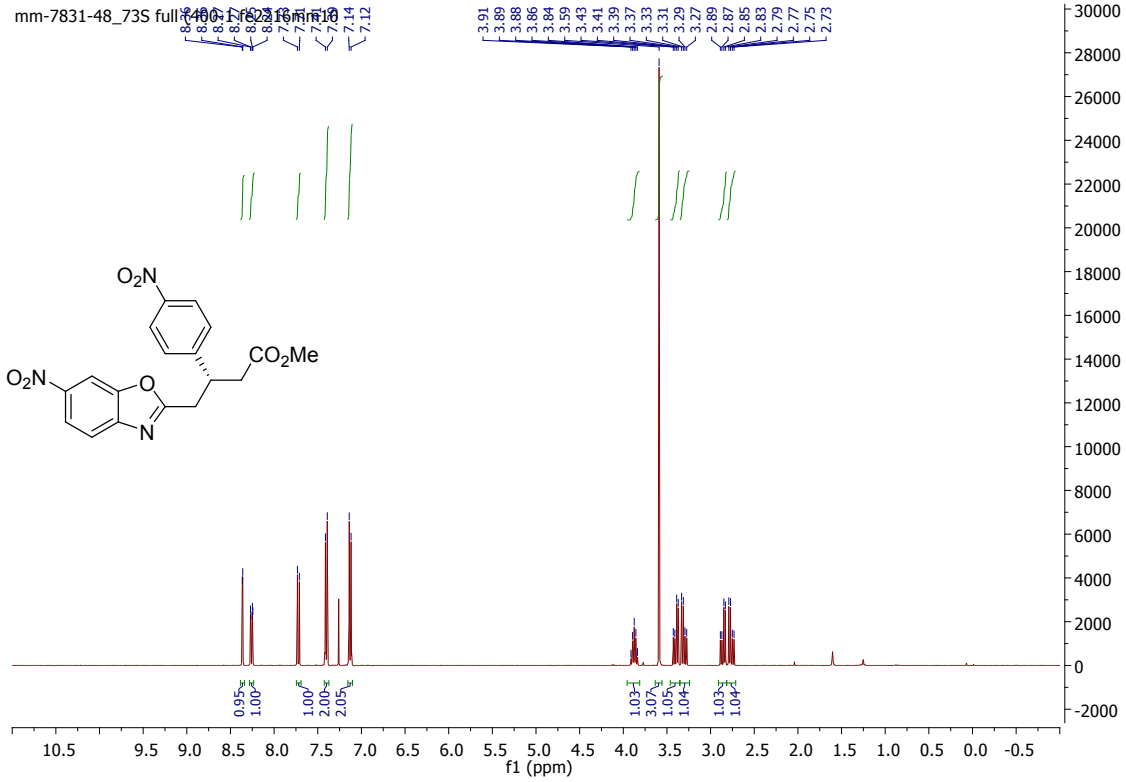
Cl
CO2Me
O2N
O
N
f1 (ppm)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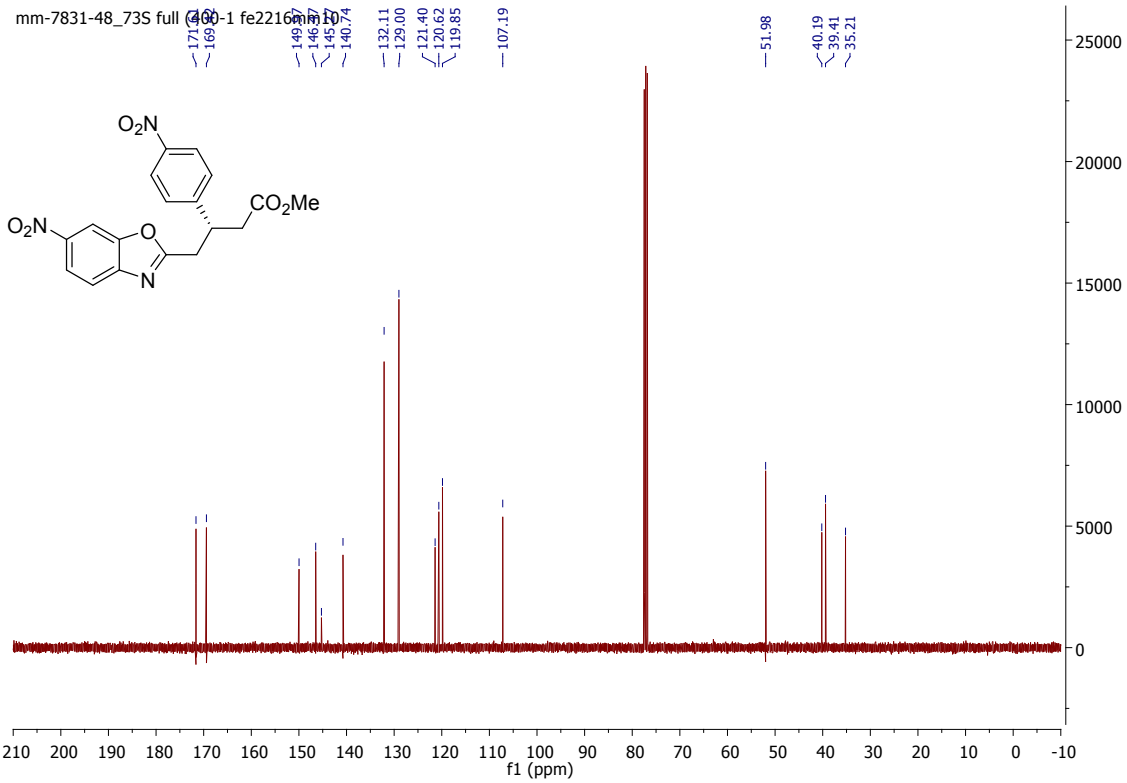
O2N
CO2Me
O2N
O
N
f1 (ppm)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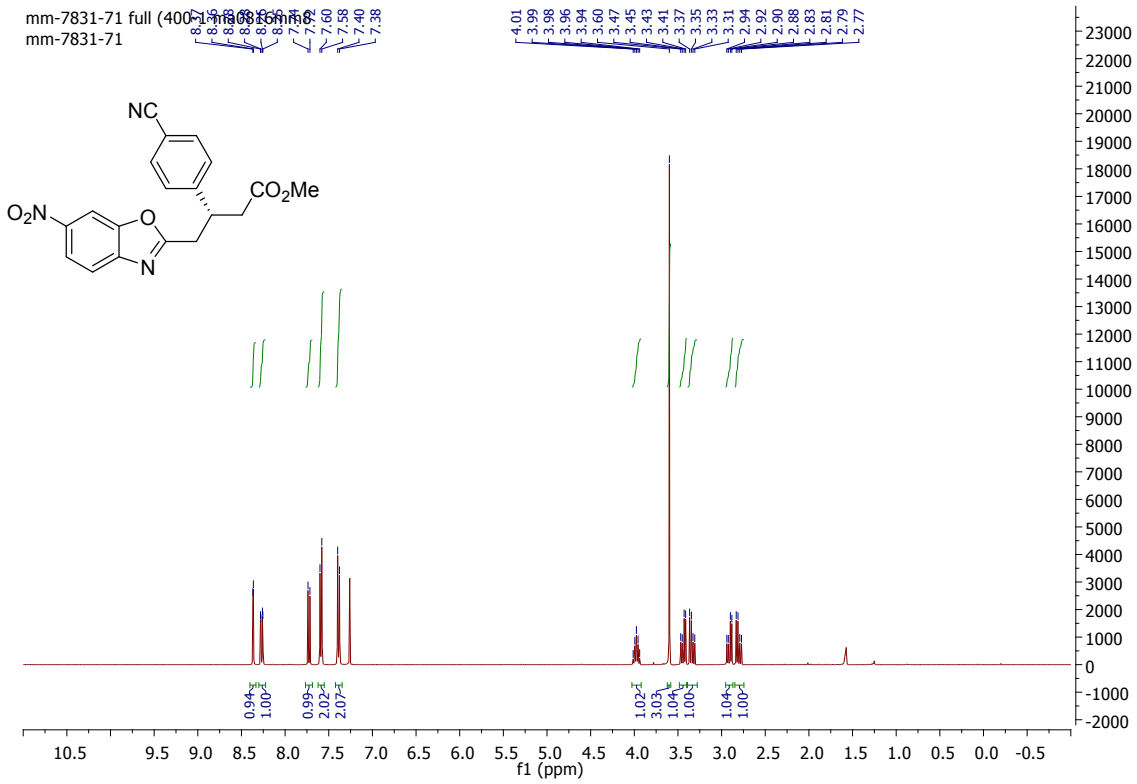
CO2Me
O2N
O
N
f1 (ppm)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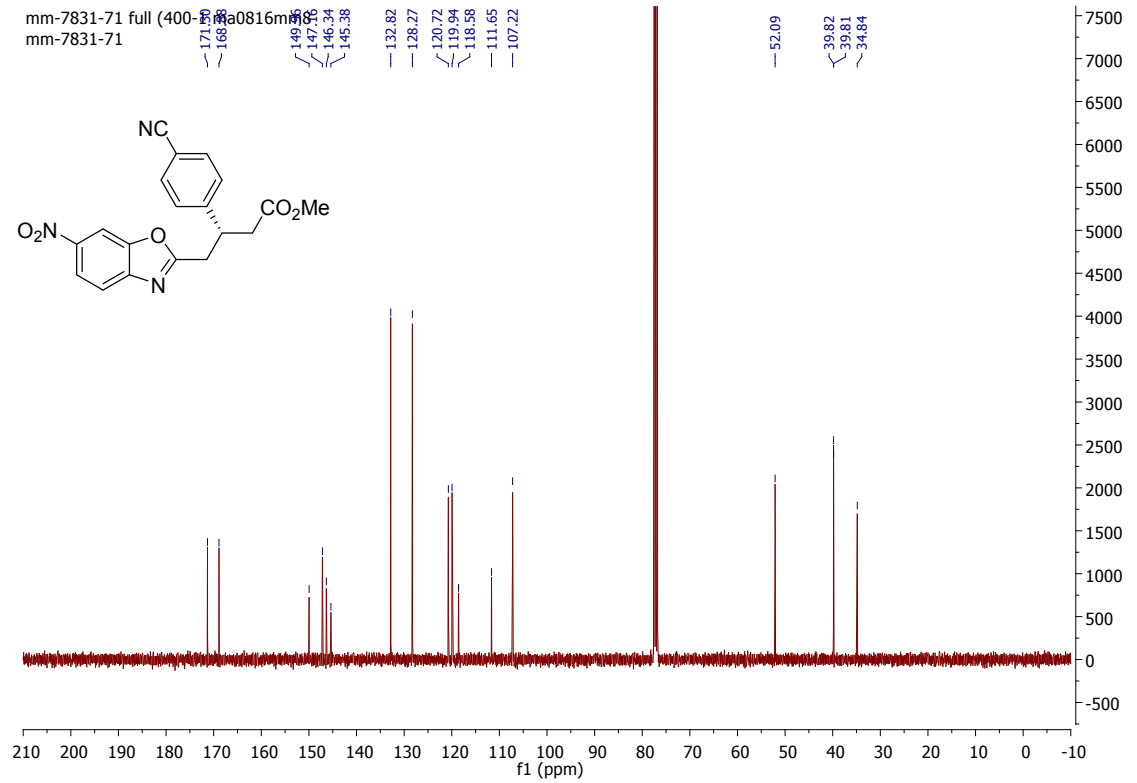
NC
CO2Me
O2N
O
N
f1 (ppm)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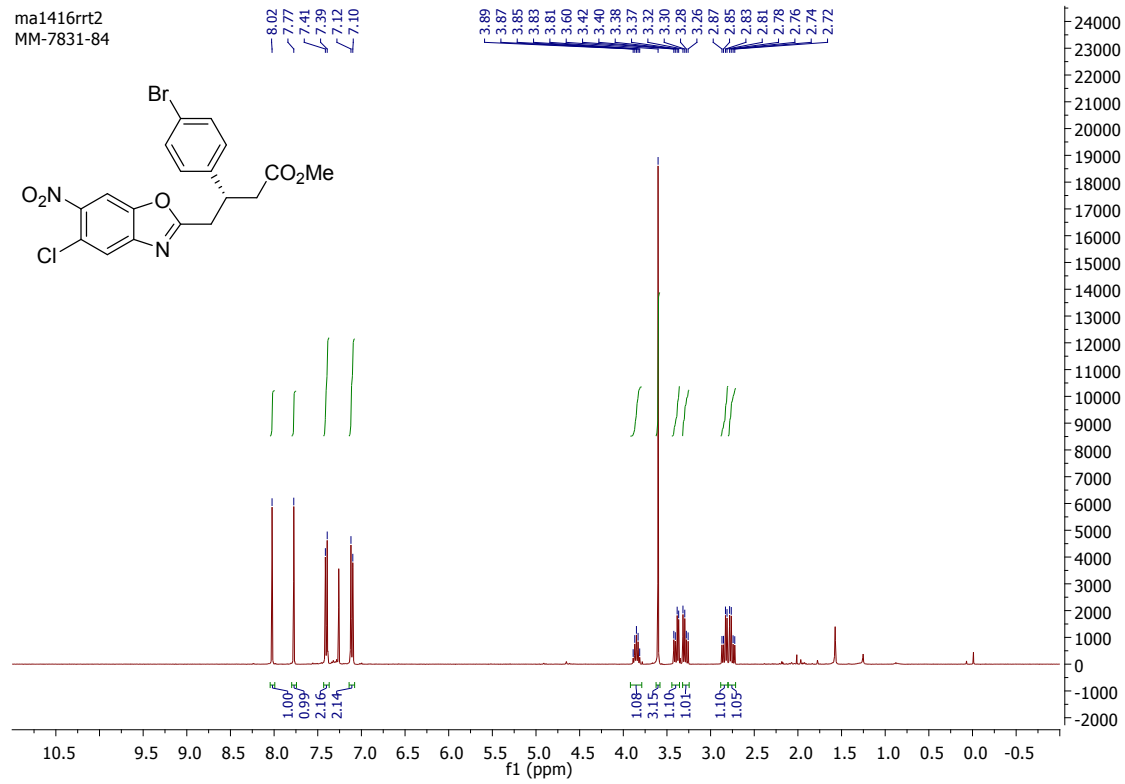
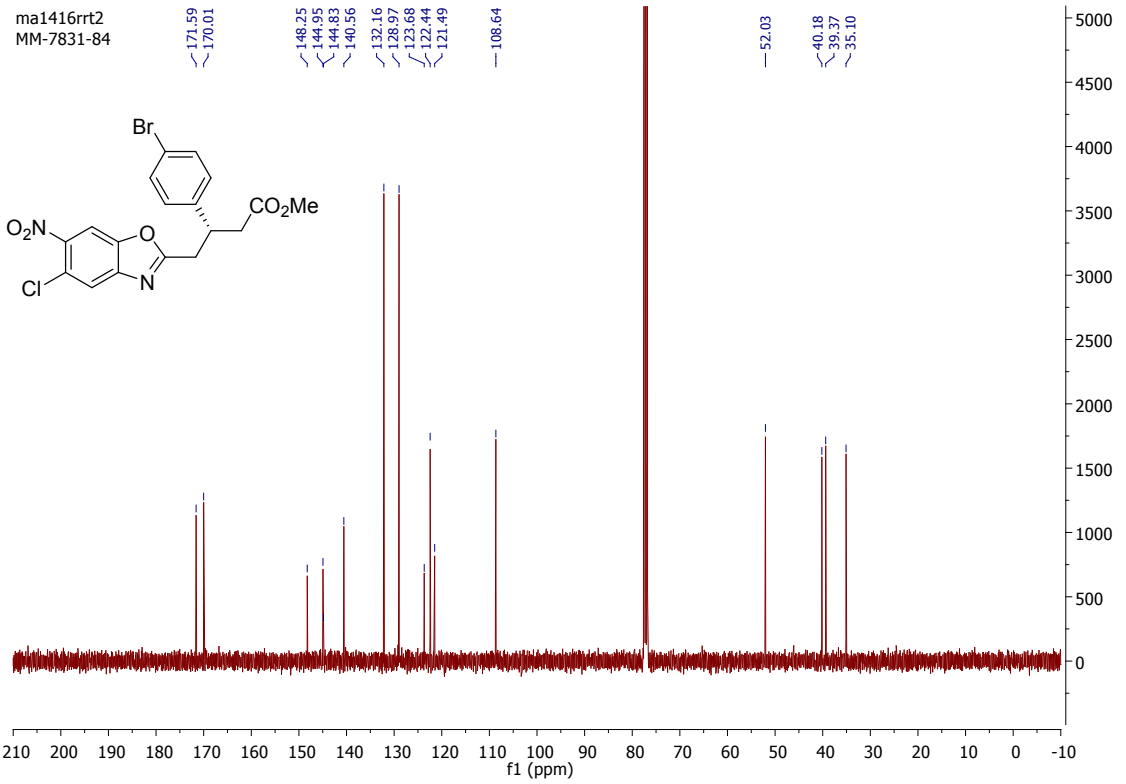
NC
CO2Me
O2N
O
N
f1 (ppm)


ma1416rrt2
MM-7831-84
Br
CO2Me
O2N
Cl
O
N
f1 (ppm)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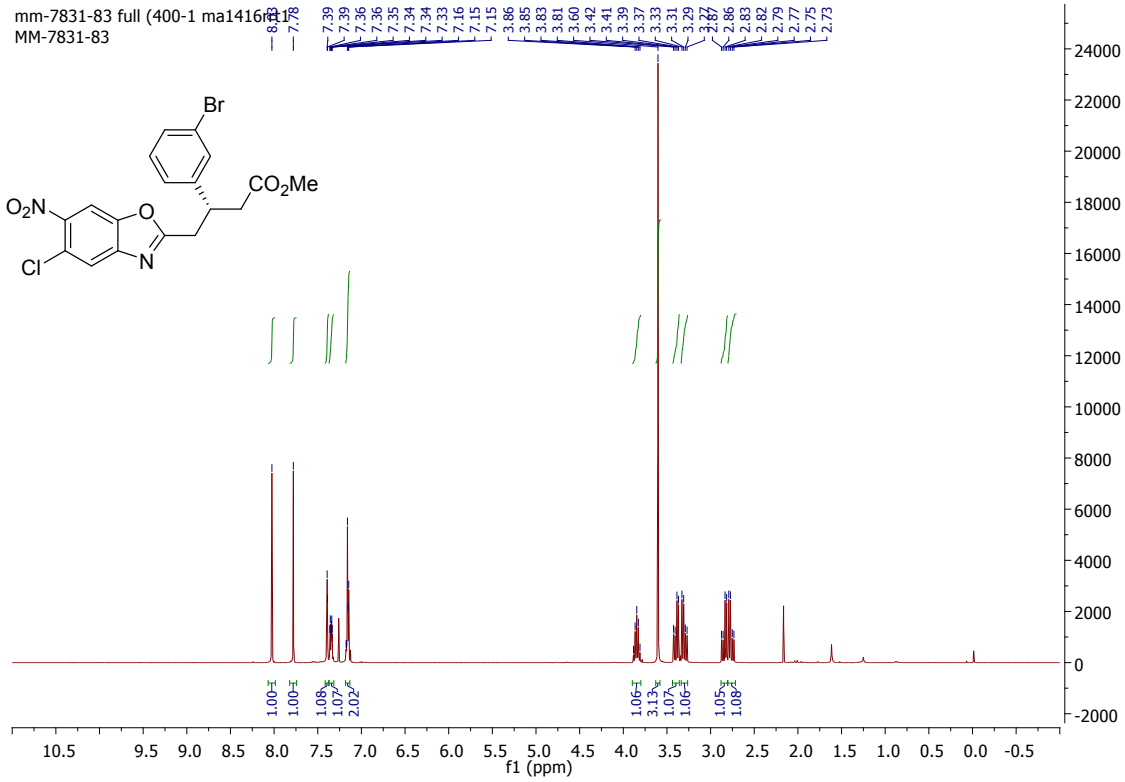
Br
CO2Me
O2N
Cl
O
N
f1 (ppm)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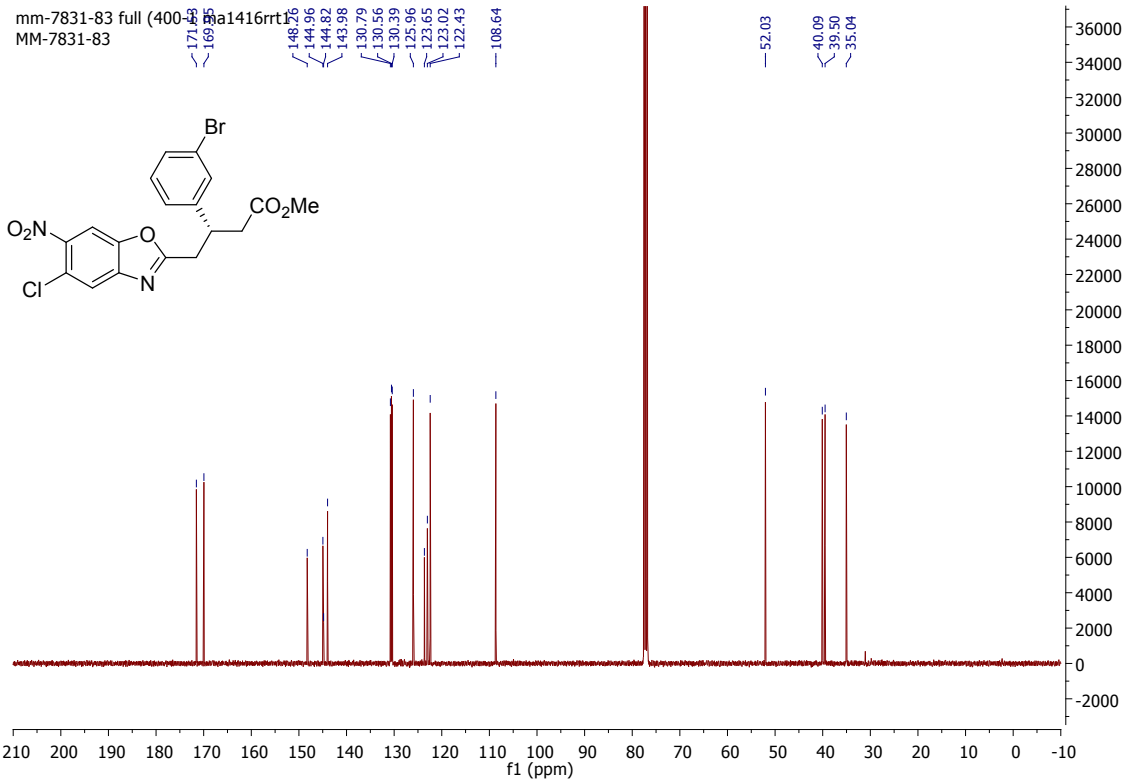
MM-7831-83
Br
CO2Me
O2N
Cl
O
N
f1 (ppm)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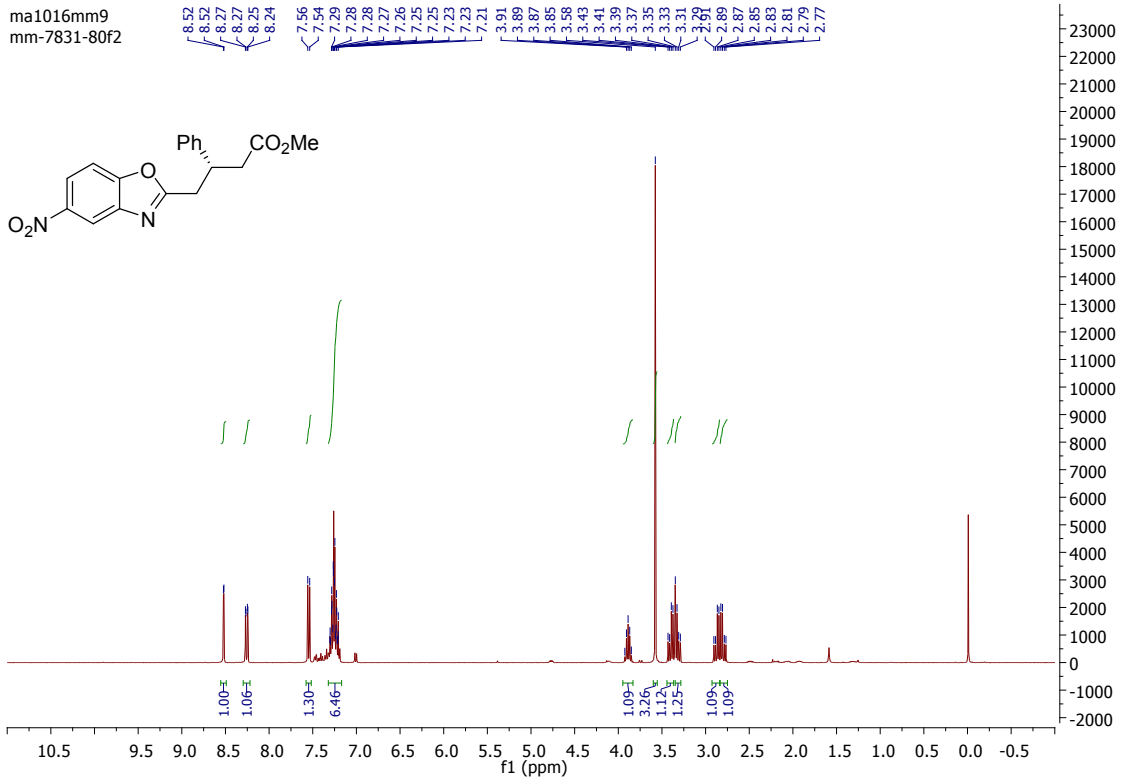
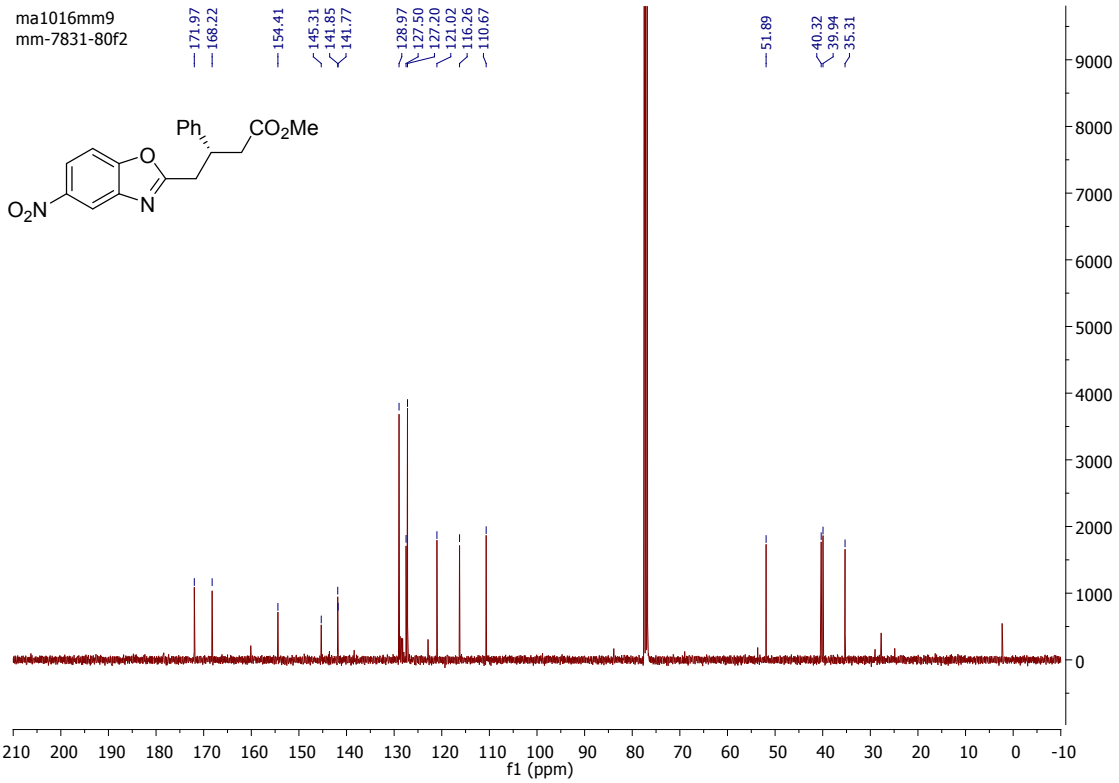
Br
CO2Me
O2N
Cl
O
N
f1 (ppm)


ma1016mm9
mm-7831-80f2
Ph
CO2Me
O2N
O
N
f1 (ppm)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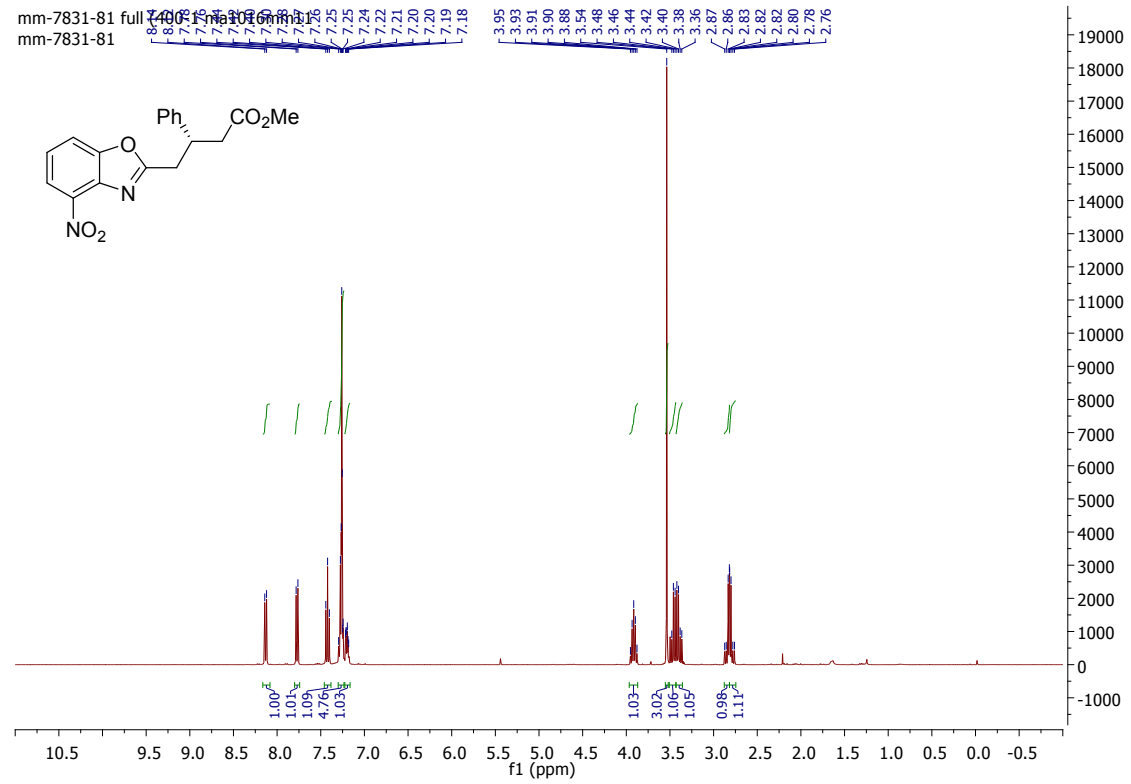
Ph
CO2Me
O2N
O
N
f1 (ppm)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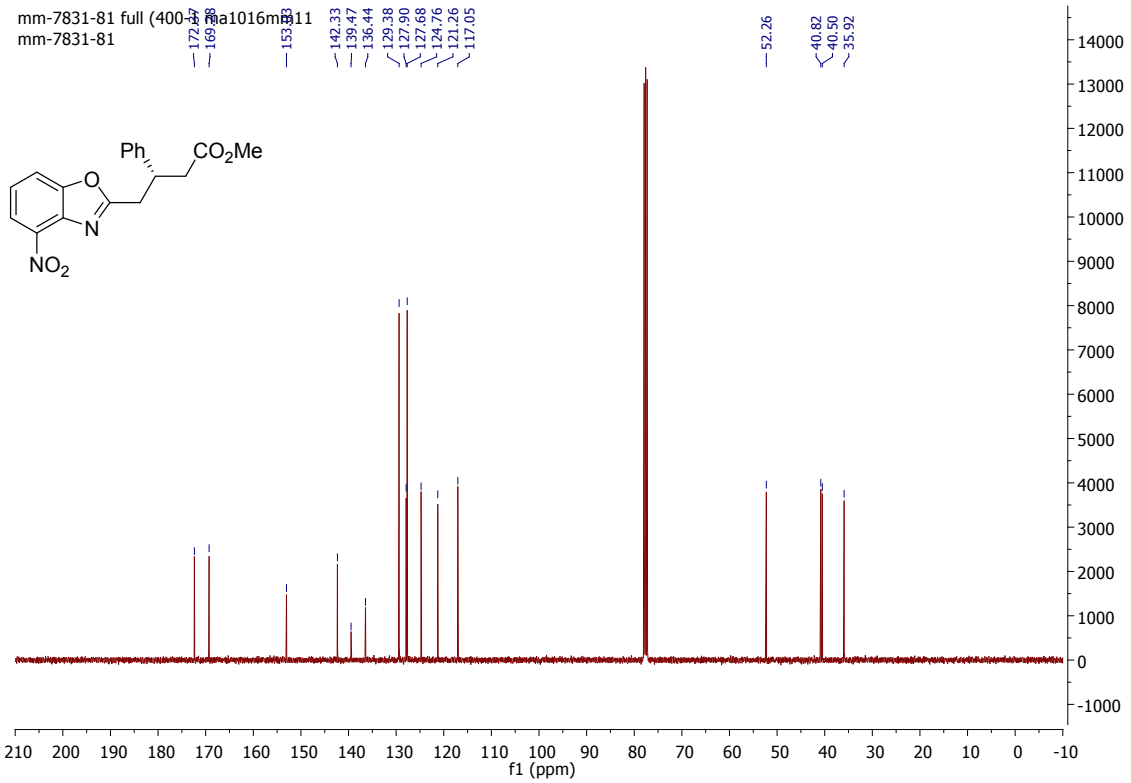
mm-7831-81
Ph
CO2Me
O
N
NO2
f1 (ppm)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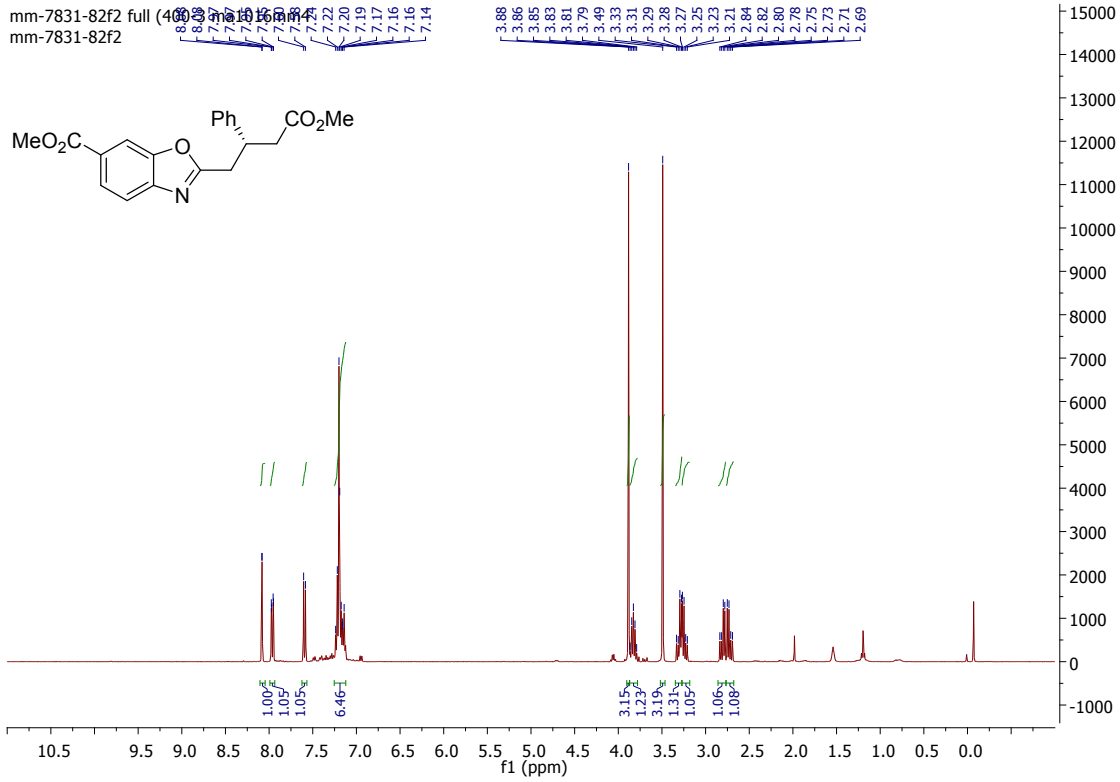
mm-7831-81
Ph
CO2Me
O
N
NO2
f1 (ppm)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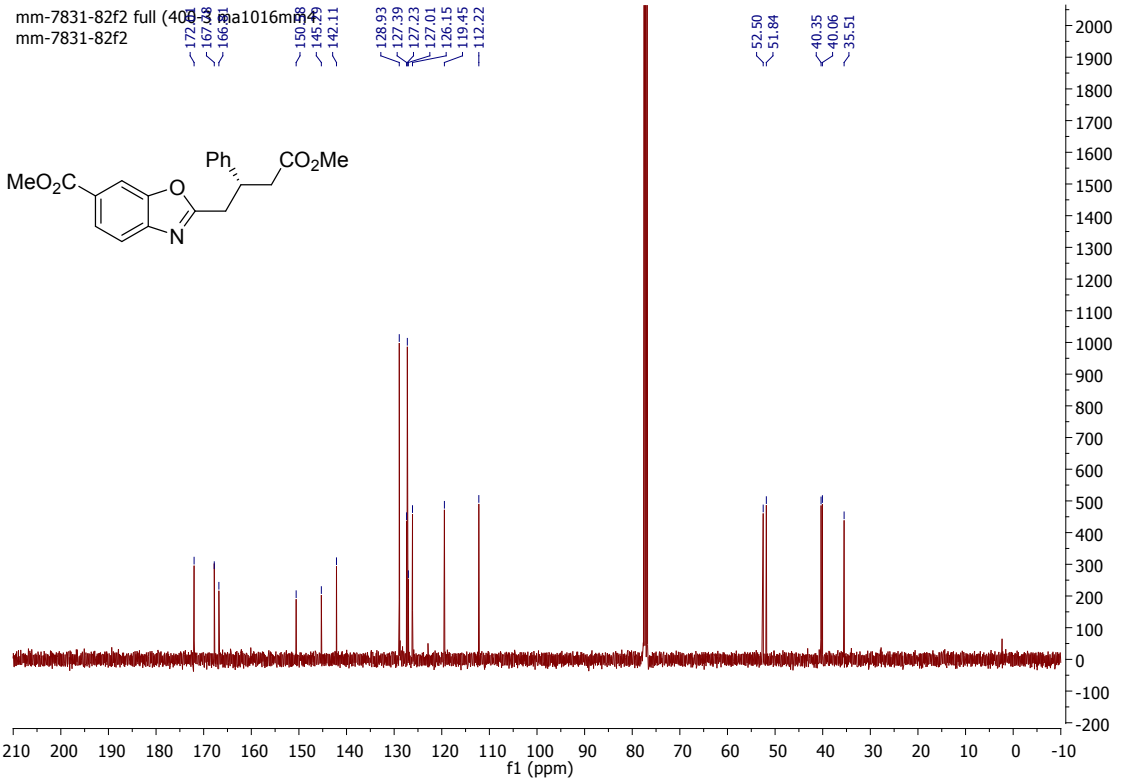
mm-7831-82f2
MeO2C
Ph
CO2Me
O
N
f1 (ppm)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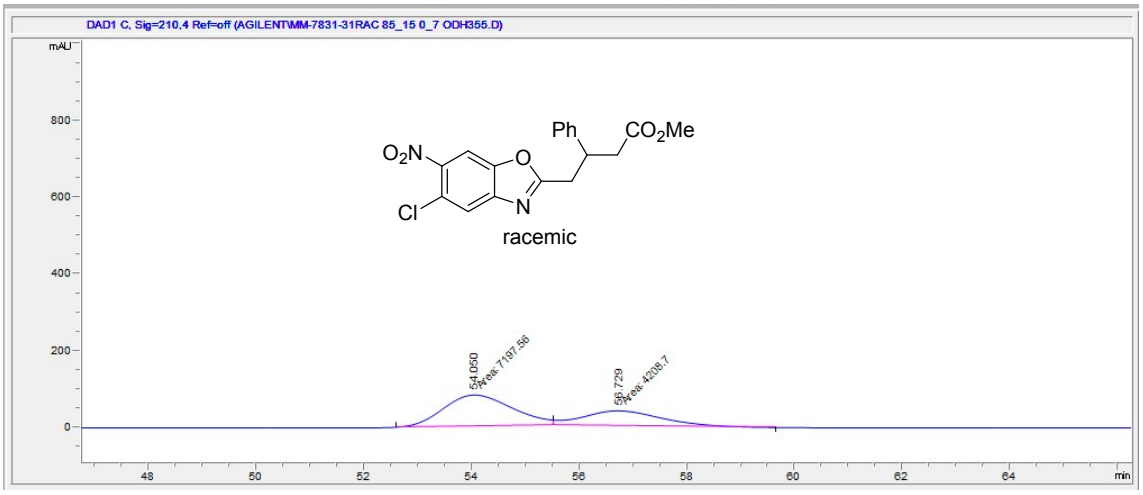
mm-7831-82f2
MeO2C
Ph
CO2Me
O
N
f1 (ppm)

5. HPLC traces



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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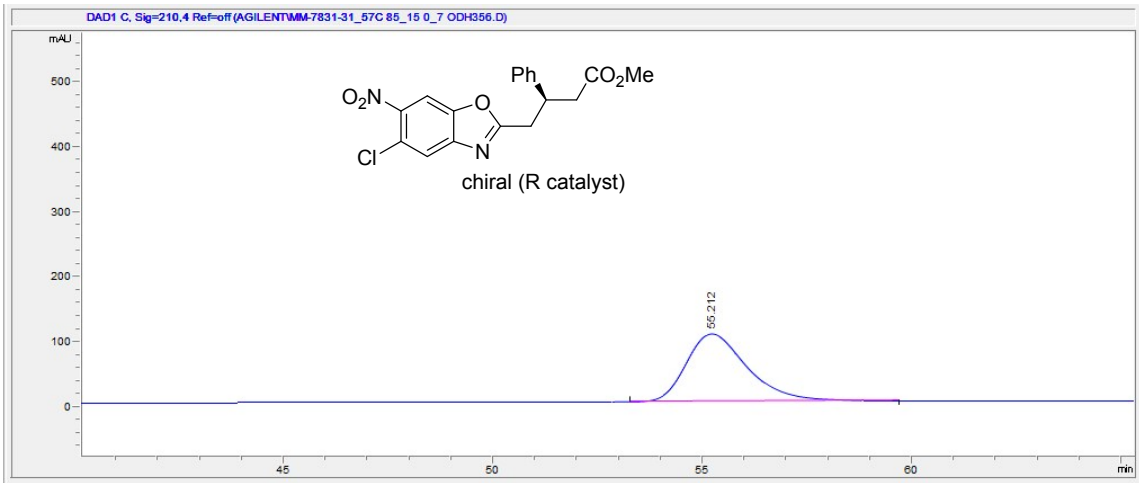
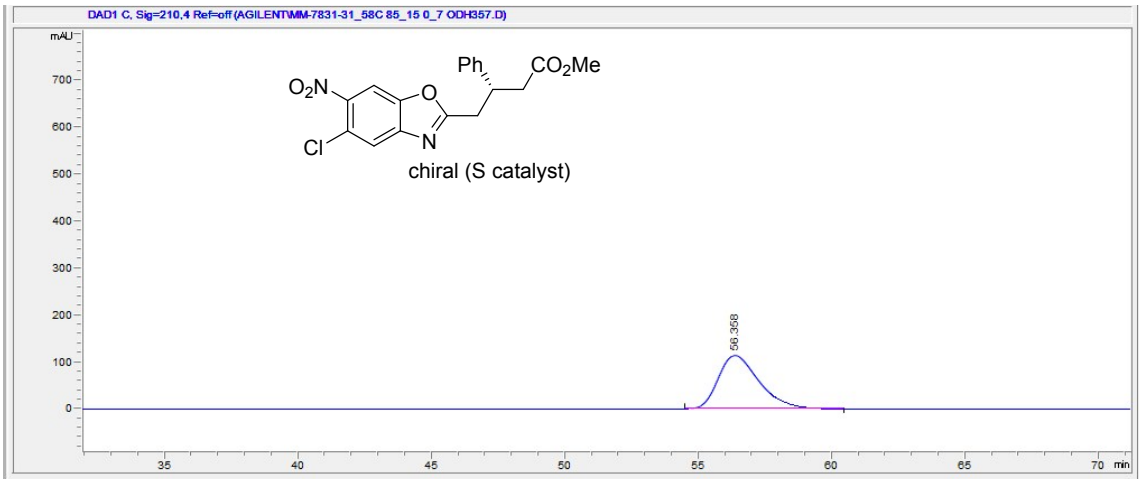


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	55.212	BB	1.3920	1.06790e4	104.34842	100.0000



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	56.358	BB	1.5524	1.19922e4	112.97652	100.0000

6. Computational methods

u All of the calculations were performed using the Gaussian09 program.[1] Computations were done using B3LYP functional[2] in conjunction with Grimme's dispersion correction.[3] Standard basis sets def2SVP and def2TZVP were employed.[4] Geometry full optimizations were made at B3LYP-D3BJ/def2SVP level and then single point calculations at B3LYP-D3BJ/def2TZVP level were carried out in order to obtain more accurate values of the energies. Solvent effects (MeCN) were considered using the PCM model.[5] The nature of stationary points was defined on the basis of calculations of normal vibrational frequencies (force constant Hessian matrix). The optimizations were carried out using the Berny analytical gradient optimization method.[6] Minimum energy pathways for the reactions studied were found by gradient descent of transition states in the forward and backward direction of the transition vector (IRC analysis),[7] using using the Hratchian-Schlegel algorithm.[8] Analytical second derivatives of the energy were calculated to classify the nature of every stationary point, to determine the harmonic vibrational frequencies, and to provide zero-point vibrational energy corrections. The thermal and entropic contributions to the free energies were also obtained from the vibrational frequency calculations, using the unscaled frequencies. Correction to free energy was made by subtracting S_{trans} contribution and considering a 1M concentration. Structural representations were generated using CYLView.[9] For the purpose of comparison between different catalytic cycles (see below) we have calculated the unsubstituted substrate **8t** (Scheme 1, R = H) even though it does not give reaction. This fact does not affect to the comparison between relative energies amongst the different cycles. Once the catalytic cycle was determined we also calculated the real model by adding the nitro group (**8a**; Scheme 1, R = NO_2).

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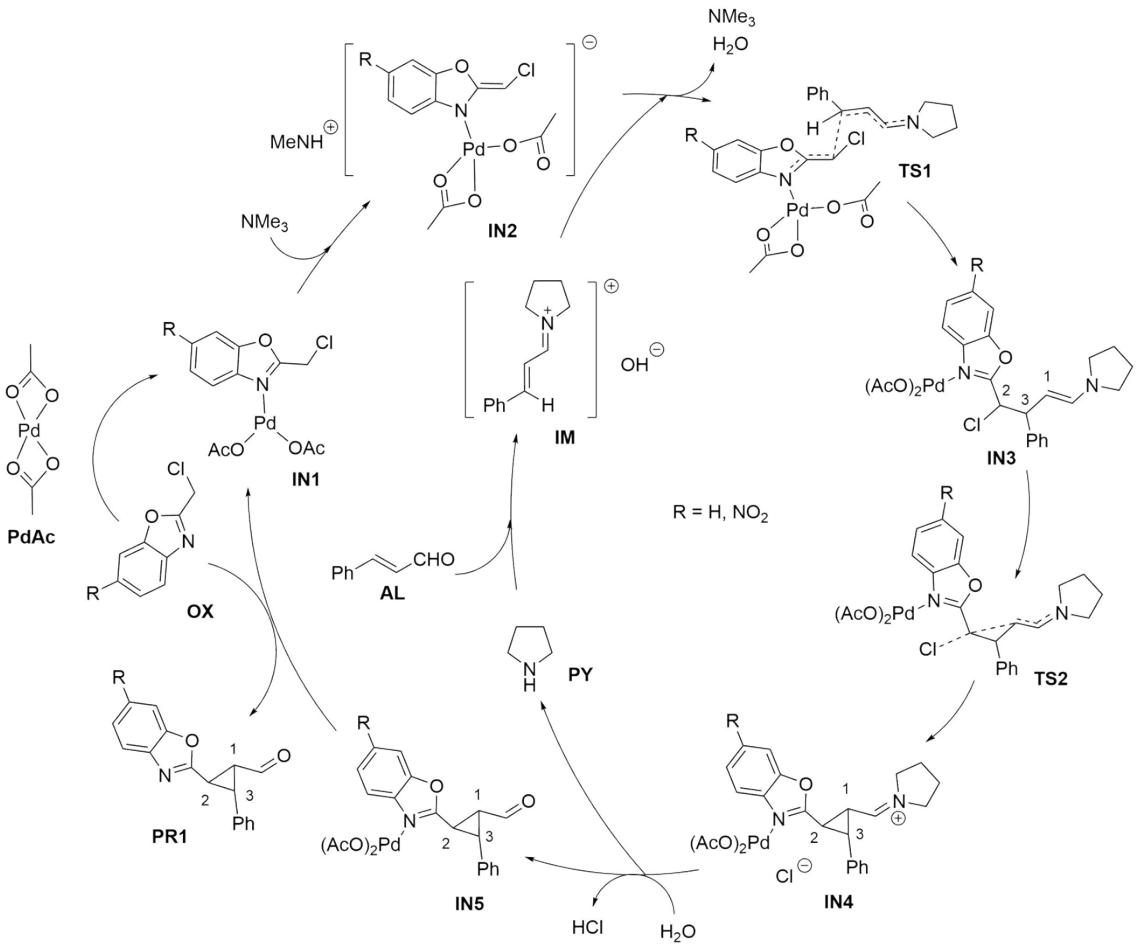
6.1 Catalytic Cycle I



Scheme 1. Catalytic Cycle for the formation of **8a**/**8t**

Energies for the catalytic cycles corresponding to the formation of **8a** are given in Table 1. The optimized geometries for **TS2a** and **TS2b** corresponding to the formation of **8a** are given in Figure 1. In both cases one of the acetates interacts with the iminium but in this case the interaction takes place with an endocyclic hydrogen atom in α-position of the iminium nitrogen. From the spatial distribution of groups in **TS2a** and **TS2b** results evident the small energetic difference found between them. Since a three-membered ring is being formed, once the central atom bearing the phenyl group is placed in the same orientation both structures can be considered pseudoenantiomeric (with opposite relative orientations between the benzoxazole ring and the pyrrolidinyl moiety) and thus, a very similar geometry is found for both transition structures.

Table 1. Calculated (B3LYP-D3BJ/def2TZVP/PCM=MeCN//B3LYP-D3BJ/def2SVP) absolute energies (hartrees) for the catalytic cycle illustrated in Scheme 1 corresponding to **8a**. Both diastereomeric series are considered

	E_0	G	im. freq
AL	-422.084346	-422.082519	
OX	-1103.468921	-1103.350818	
PdAc	-583.924311	-583.922356	
PY	-212.076845	-212.075852	
IM	-558.269925	-558.267182	
IN1	-1688.685522	-1688.482486	
IN2	-1688.213561	-1687.967592	
IN3a	-2248.118785	-2247.674031	
IN3b	-2248.113432	-2247.669734	
IN4a	-2248.116295	-2247.669574	
IN4b	-2248.118187	-2247.675278	
IN5a	-1651.026490	-1650.693144	
IN5b	-1651.021757	-1650.689855	
PR1a	-1065.805119	-1065.540871	
PR1b	-1065.804260	-1065.540435	

TS1a	-	-	
	2248.098338	2247.654853	-222.4
TS1b	-	-	
	2248.093316	2247.650001	-229.2
TS2a	-	-	
	2248.102105	2247.659668	-324.3
TS2b	-	-	
	2248.101711	2247.658226	-352.9

a and **b** series refers to (1*R*,2*R*,3*S*) and (1*S*,2*S*,3*S*), isomers respectively

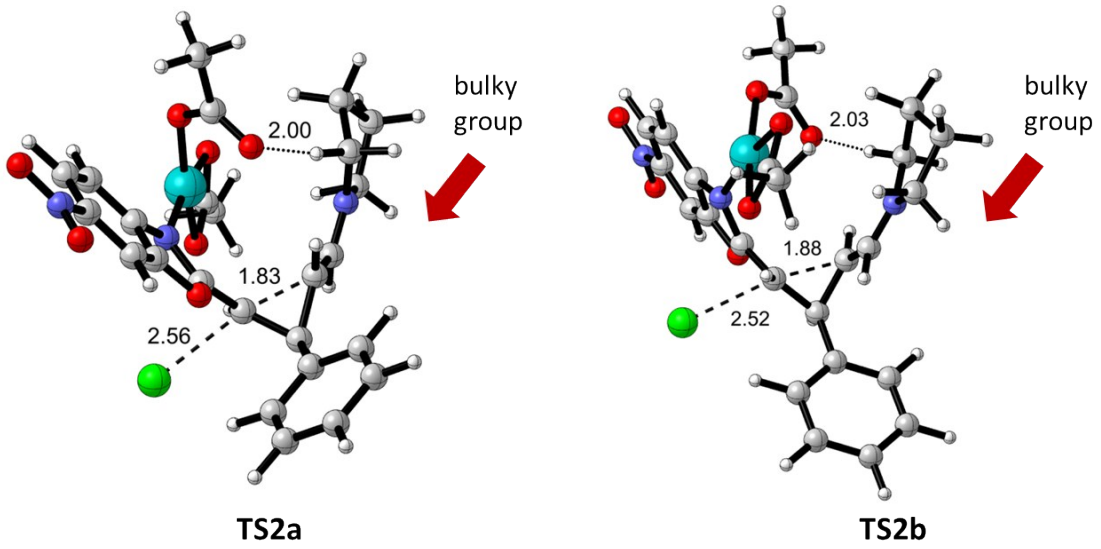


Figure 1. Optimized geometries (B3LYP-D3BJ/Def2SVP) for **TS2a** and **TS2b** (red arrow indicates the position of the bulky group at the original enantiopure catalyst).

Energies for the catalytic cycles corresponding to the formation of **8t** are given in Table 2 and the corresponding energy profiles in Figure 2. Figure 3 collects transition structures **TS1** and **TS2** corresponding to the formation of **8t**. As expected, the presence of the nitro group does not affect the geometry of the transition structures.

Table 2. Calculated (B3LYP-D3BJ/def2TZVP/PCM=MeCN//B3LYP-D3BJ/def2SVP) absolute energies (hartrees) for the catalytic cycle illustrated in Scheme 1 corresponding to **8t**. Both diastereomeric series are considered

	E_0	G	im. freq
AL	-422.084346	-422.082519	
OX	-897.446521	-897.444913	
PdAc	-583.924311	-583.922356	
PY	-212.076845	-212.075852	
IM	-558.269925	-558.267182	
IN1	-1481.41563	-1481.4115	
IN2	-1480.82136	-1480.81681	
IN3a	-2039.41987	-2039.41087	
IN3b	-2039.41272	-2039.40388	
IN4a	-2039.41612	-2039.40738	
IN4b	-2039.41861	-2039.41039	
IN5a	-1443.03617	-1443.02889	
IN5b	-1443.03019	-1443.02345	
PR1a	-859.045714	-859.042386	
PR1b	-859.045494	-859.042311	
TS1a	-2039.38484	-2039.3756	-126.4
TS1b	-2039.37473	-2039.3654	-169.3
TS2a	-2039.35017	-2039.3414	-241.2
TS2b	-2039.35947	-2039.34368	-321.2

a and **b** series refers to (1*R*,2*R*,3*S*) and (1*S*,2*S*,3*S*), isomers respectively

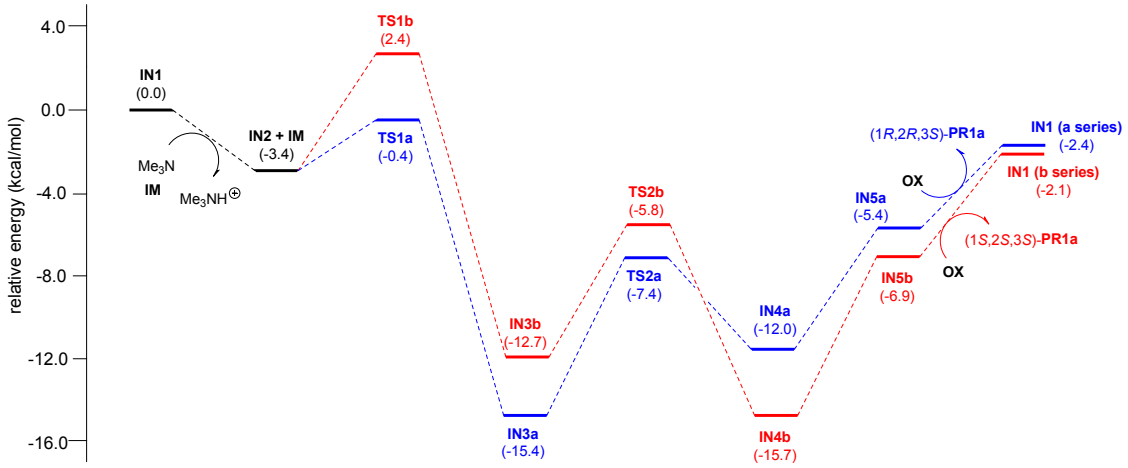


Figure 2. Energy profile for the catalytic cycle corresponding to the formation of (1R,2R,3S)-**8t** (blue trace) and (1S,2S,3S)-**8t** (red trace). Relative energies are given in kcal/mol.

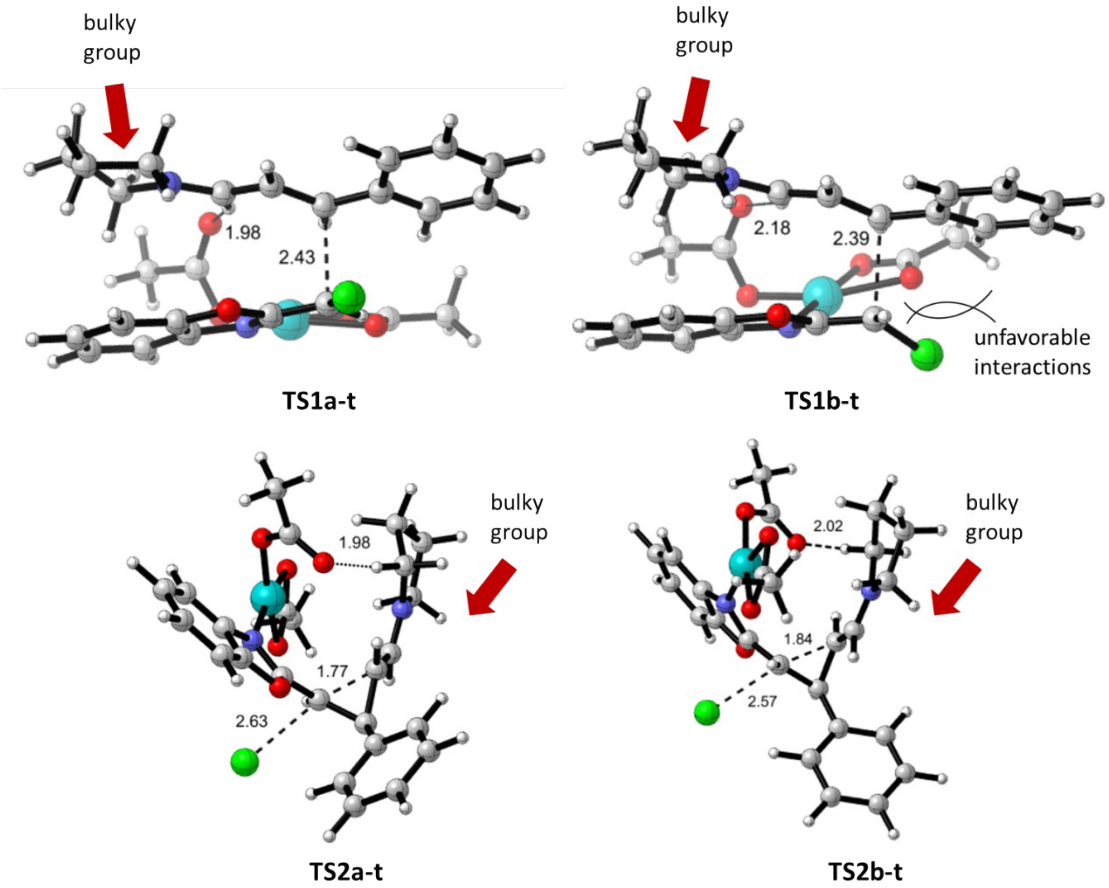
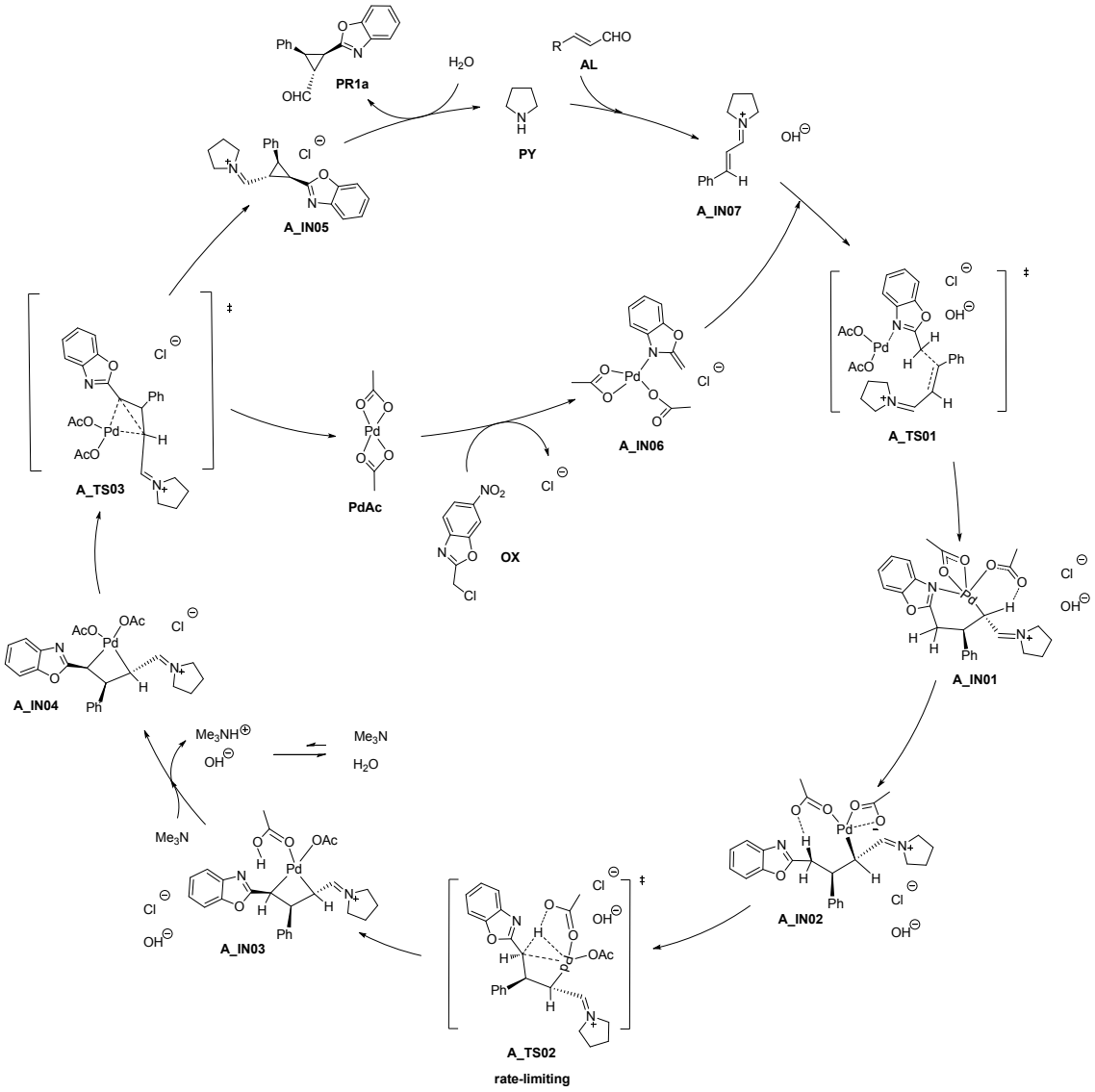


Figure 3. Optimized geometries (B3LYP-D3BJ/Def2SVP) for **TS2a-t** and **TS2b-t** (red arrow indicates the position of the bulky group at the original enantiopure catalyst).

7. Alternative (ruled out) catalytic cycles

7.1. Catalytic Cycle A



Scheme 2. Alternative Catalytic Cycle A

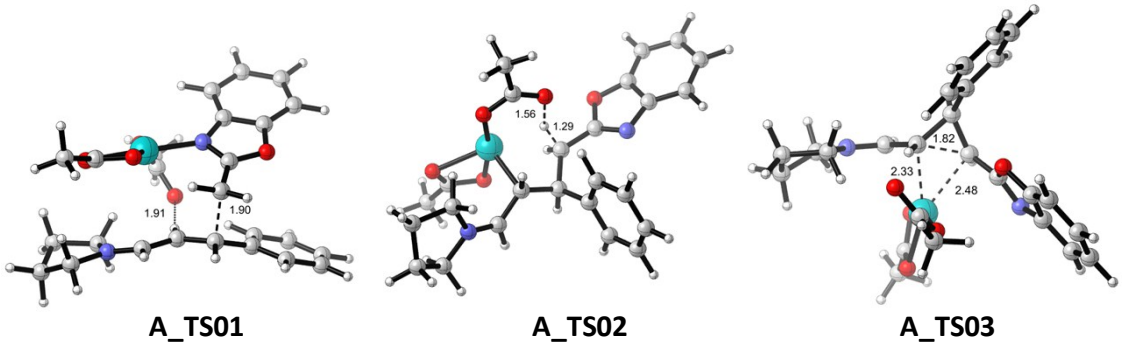


Figure 4. Optimized (B3LYP-D3BJ/def2SVP) geometries of transition structures given in Scheme 3

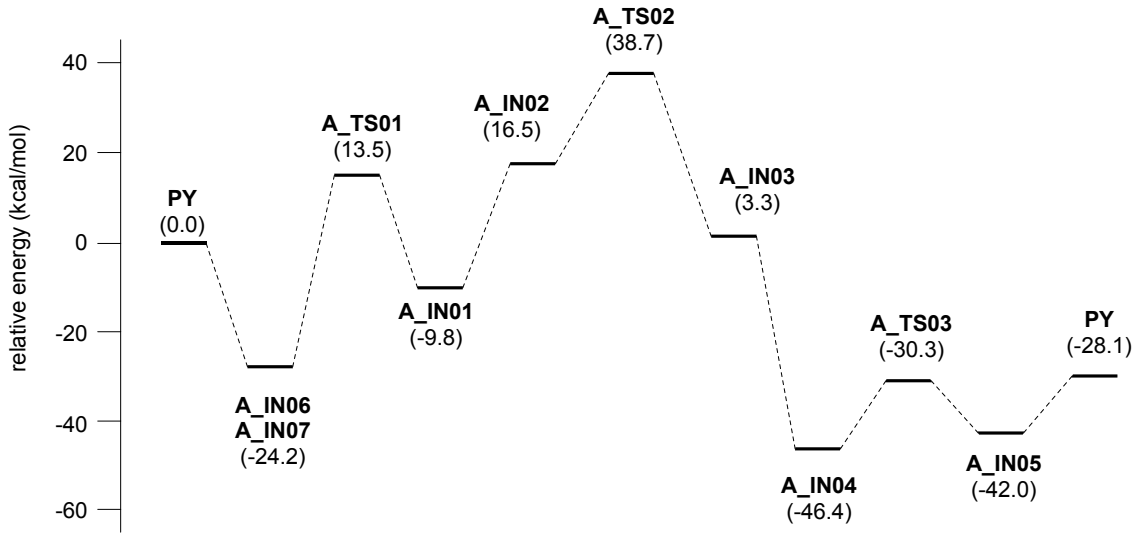
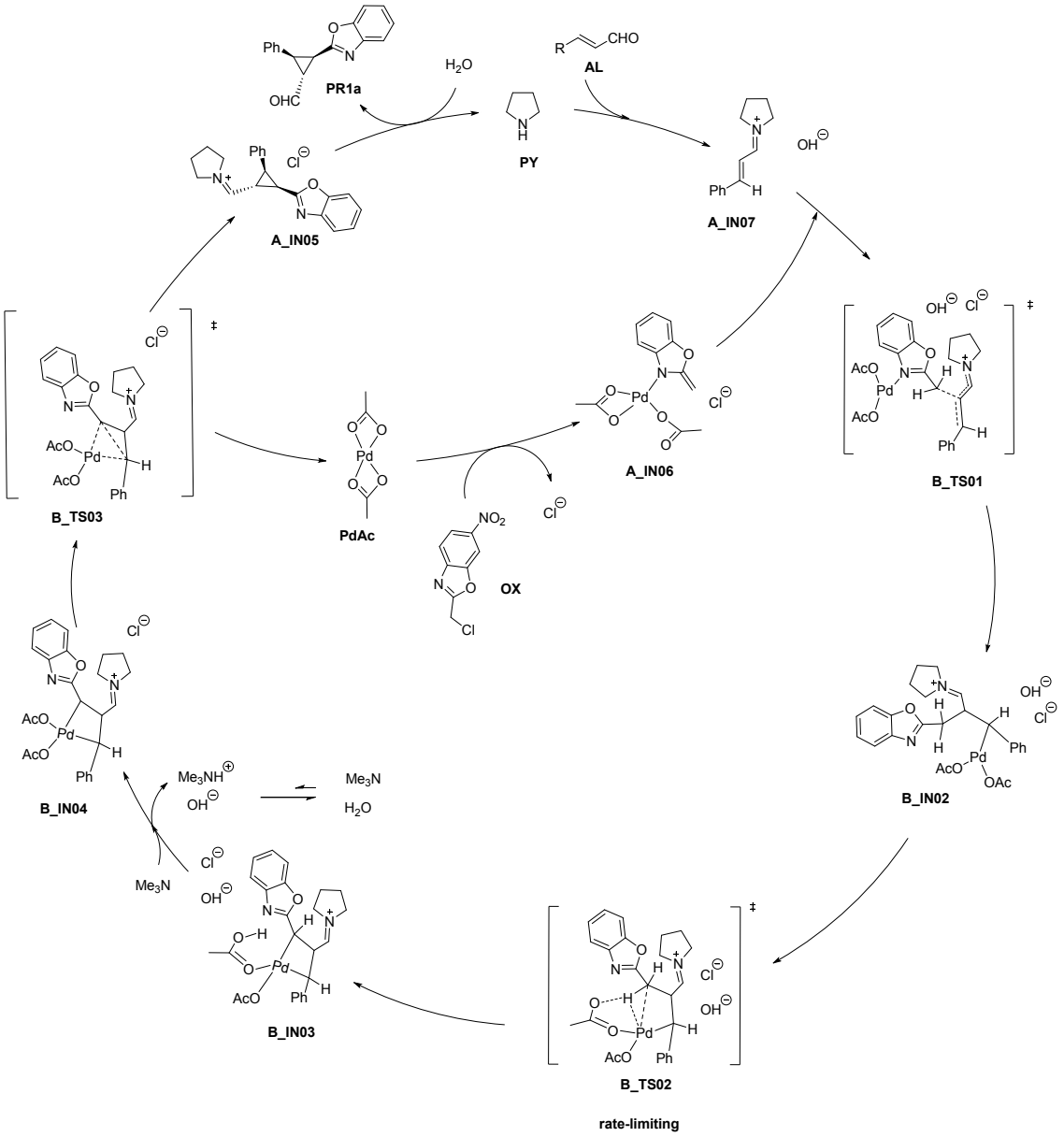


Figure 5. Calculated (B3LYP-D3BJ/def2SVP) energy profile for catalytic cycle illustrated in Scheme 2.

This catalytic cycle was ruled out on the basis of the high activation energy (61.3 kcal/mol) found for the rate-limiting step **A_TS02**.

7.2. Catalytic Cycle B



Scheme 3. Alternative Catalytic Cycle B (no **B_IN01** is defined to keep paralelism with cycle A).

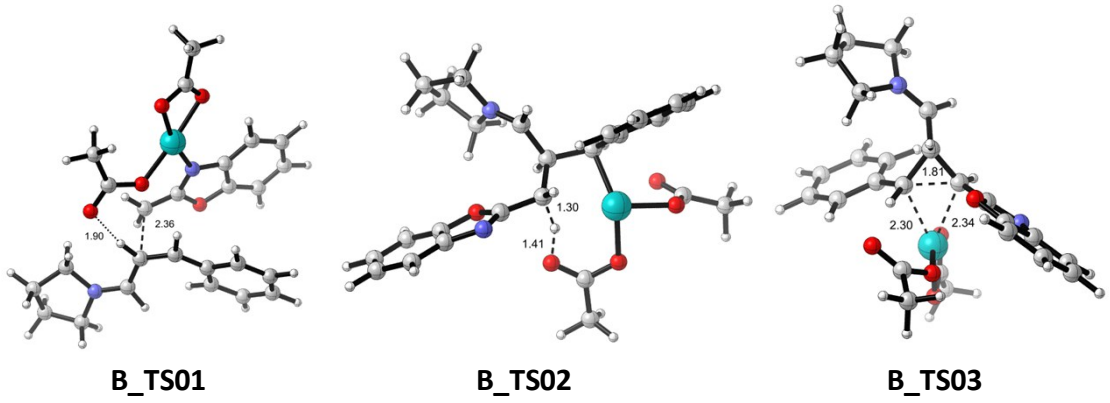


Figure 4. Optimized (B3LYP-D3BJ/def2SVP) geometries of transition structures given in Scheme 3.

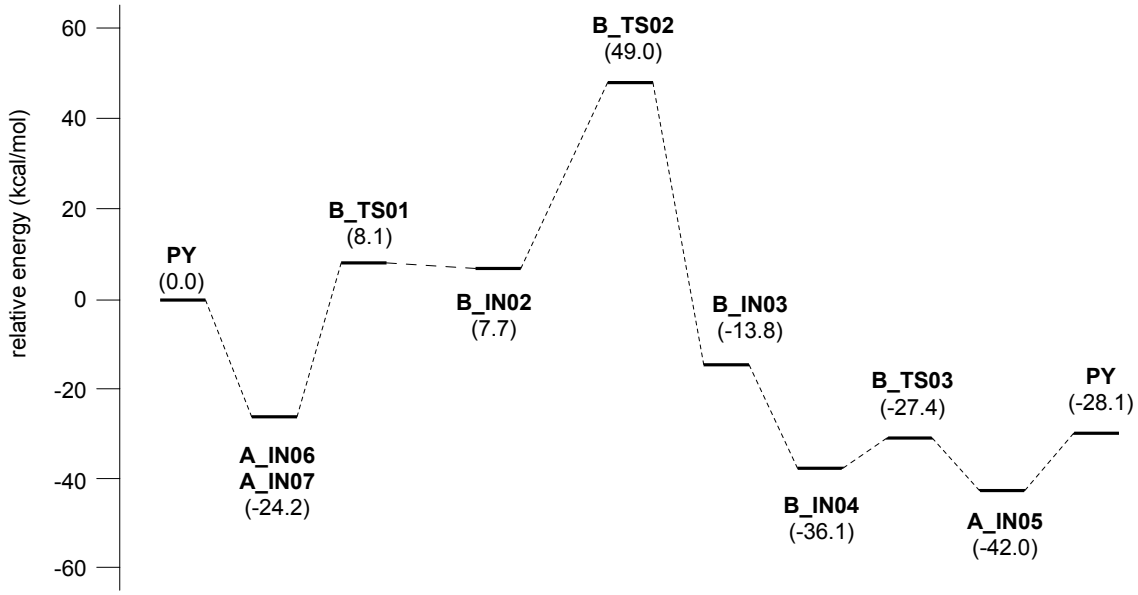


Figure 5. Calculated (B3LYP-D3BJ/def2SVP) energy profile for catalytic cycle illustrated in Scheme 4

This catalytic cycle was also ruled out on the basis of the high activation energy (71.4 kcal/mol) found for the rate-limiting step **B_TS02**.

8. Cartesian Coordinates

8.1. Catalytic Cycle

AL

0 1

C	-0.9333100000	-0.5971950000	0.0002820000
H	-1.1455650000	-1.6740100000	0.0006540000
C	-1.9952450000	0.2371680000	-0.0001390000
H	-1.8976270000	1.3263720000	-0.0007490000
C	-3.3657340000	-0.2861830000	0.0001020000
C	0.4857670000	-0.2466270000	0.0001350000
C	0.9405450000	1.0881640000	0.0002470000
C	1.4440300000	-1.2786820000	-0.0000370000
C	2.3027270000	1.3740850000	0.0000770000
H	0.2190850000	1.9070940000	0.0005580000
C	2.8091540000	-0.9921480000	-0.0002080000
H	1.1059750000	-2.3182510000	-0.0000780000
C	3.2428580000	0.3358310000	-0.0001700000
H	2.6379800000	2.4138310000	0.0001680000
H	3.5366640000	-1.8070370000	-0.0003720000
H	4.3111350000	0.5645260000	-0.0002980000
H	-3.4313190000	-1.4081360000	0.0007010000
O	-4.3651340000	0.3986410000	-0.0002900000

IM

1 1

C	-0.9894990000	-0.8525100000	-0.0331390000
H	-0.9231750000	-1.9467050000	-0.0544440000

C	0.1947430000	-0.1554600000	-0.0344150000
H	0.2026080000	0.9349640000	-0.0123520000
C	1.4217250000	-0.8590910000	-0.0606010000
N	2.6145070000	-0.3219000000	-0.0639200000
C	3.8744130000	-1.1045980000	-0.0771790000
C	2.8902370000	1.1330710000	-0.0277480000
H	3.7742870000	-1.9894900000	0.5662200000
H	4.0681360000	-1.4398710000	-1.1099270000
C	4.9213400000	-0.0938710000	0.3883310000
C	4.4093310000	1.2253680000	-0.2056770000
H	2.3199890000	1.6443280000	-0.8166880000
H	2.5602300000	1.5256550000	0.9482760000
H	4.9370910000	-0.0442380000	1.4888080000
H	5.9310960000	-0.3599240000	0.0487470000
H	4.8258290000	2.1145900000	0.2856480000
H	4.6606660000	1.2865590000	-1.2761780000
C	-2.3264640000	-0.3219870000	-0.0074380000
C	-2.6027970000	1.0673160000	0.0206810000
C	-3.4102620000	-1.2327270000	-0.0102460000
C	-3.9140960000	1.5203610000	0.0451930000
H	-1.7866550000	1.7917400000	0.0231610000
C	-4.7229520000	-0.7738930000	0.0143710000
H	-3.2073050000	-2.3062340000	-0.0319820000
C	-4.9758280000	0.6019720000	0.0421050000
H	-4.1211720000	2.5919550000	0.0667770000
H	-5.5517140000	-1.4842020000	0.0119990000
H	-6.0058180000	0.9651440000	0.0613850000

H	1.3950240000	-1.9546880000	-0.0774370000

IN1

0 1

Pd	-1.2233030000	0.0635570000	-0.0217550000
O	0.0029010000	-0.8692970000	-2.6147190000
C	-0.6354340000	-1.7740760000	-2.1048970000
O	-1.2248150000	-1.7150000000	-0.9296690000
O	-1.7173830000	1.8832570000	0.8714890000
C	-2.9481770000	1.6847160000	0.5924710000
C	-4.0011670000	2.6633300000	1.0085080000
H	-3.6042290000	3.6867010000	0.9640510000
H	-4.2857380000	2.4528930000	2.0522720000
H	-4.8908970000	2.5584350000	0.3742350000
O	-3.2422960000	0.6142980000	-0.0241590000
C	-0.8235190000	-3.1272230000	-2.7738000000
H	-1.8969170000	-3.3303780000	-2.9063820000
H	-0.4208850000	-3.9280270000	-2.1338570000
H	-0.3155790000	-3.1344800000	-3.7461960000
C	1.0632900000	-2.3781870000	1.0255930000
H	0.1068340000	-2.6262810000	0.5502090000
C	1.5192800000	-1.0592780000	0.5348660000
C	2.9518150000	0.5079530000	0.0602430000
C	1.6559920000	0.9978830000	-0.1432640000
C	4.0969480000	1.2619690000	-0.1623370000
C	1.4403030000	2.3054570000	-0.5844340000
C	3.8778610000	2.5691100000	-0.6052440000

H	5.0960830000	0.8568540000	-0.0006090000
C	2.5780910000	3.0789970000	-0.8100900000
H	0.4294120000	2.6855660000	-0.7309470000
H	4.7376170000	3.2141720000	-0.7978980000
H	2.4632970000	4.1081670000	-1.1560280000
N	0.7823350000	-0.0418080000	0.1742810000
O	2.8405970000	-0.7923830000	0.4904060000
Cl	0.8017770000	-2.3166230000	2.8184640000
H	1.8226530000	-3.1428910000	0.8255500000

IN2

-1 1

Pd	-1.2382160000	-0.0928940000	0.0778860000
O	-3.3835670000	-0.1651580000	0.3056780000
C	-3.4772700000	0.8243280000	-0.4750680000
O	-2.4202800000	1.3521630000	-0.9465580000
O	-0.4803420000	-1.4815620000	1.3057180000
C	-0.5295160000	-2.7152030000	0.8994940000
C	0.2635090000	-3.6596280000	1.7960350000
H	0.2633930000	-3.3260520000	2.8433110000
H	1.3048310000	-3.6524720000	1.4326000000
H	-0.1311330000	-4.6817430000	1.7090610000
O	-1.0760210000	-3.1209580000	-0.1198700000
C	-4.8275230000	1.3596240000	-0.8806500000
H	-5.0941140000	0.9416700000	-1.8650910000
H	-4.7868650000	2.4538180000	-0.9781940000
H	-5.5926370000	1.0601640000	-0.1519620000

C	1.7629570000	-1.6476960000	-1.0102940000
H	0.8600150000	-2.2145730000	-1.2175180000
C	1.7286650000	-0.3633170000	-0.5856280000
C	2.5209950000	1.6099960000	0.0400010000
C	1.1128160000	1.6896170000	-0.0095950000
C	3.3288920000	2.6728720000	0.3935210000
C	0.4790330000	2.8953350000	0.3091520000
C	2.6843890000	3.8880880000	0.7129630000
H	4.4150060000	2.5664310000	0.4259550000
C	1.2892830000	3.9859020000	0.6701860000
H	-0.6083850000	2.9702960000	0.2695190000
H	3.2845290000	4.7564280000	0.9965440000
H	0.8124360000	4.9374340000	0.9228260000
N	0.6316370000	0.4590860000	-0.4032850000
O	2.8961940000	0.3415500000	-0.3090180000
Cl	3.2649510000	-2.5529220000	-1.0703020000

IN3a

0 1

Pd	1.0015910000	-1.3588480000	0.6779960000
O	0.6767970000	-2.6031370000	-0.8491810000
C	0.1509600000	-2.1476990000	-1.9544290000
O	-0.1826950000	-0.9874630000	-2.1570040000
O	1.8712180000	-0.2429050000	2.2208610000
C	3.0318860000	-0.5989520000	1.8245150000
C	4.2621770000	-0.0659840000	2.4867180000
H	4.2241040000	1.0332240000	2.4906170000

H	5.1624210000	-0.4138910000	1.9655600000
H	4.2851320000	-0.4002310000	3.5354380000
O	3.0919660000	-1.4203350000	0.8574740000
C	-0.0700480000	-3.2337700000	-2.9936240000
H	0.6922300000	-4.0211930000	-2.9239820000
H	-0.0830120000	-2.7876520000	-3.9966490000
H	-1.0550760000	-3.6922720000	-2.8059600000
C	-0.4253030000	2.3204300000	0.2488800000
C	-0.7907040000	1.4320190000	1.4944800000
H	0.1416860000	1.1598840000	1.9994110000
H	-0.0964930000	3.2671600000	0.7050180000
C	-1.5137450000	0.1783340000	1.1413160000
C	-3.2184060000	-1.0784350000	0.6546020000
C	-2.0511130000	-1.8400610000	0.5248840000
C	-4.4933720000	-1.5771770000	0.4232670000
C	-2.1187470000	-3.1894890000	0.1656660000
C	-4.5551760000	-2.9221330000	0.0499190000
H	-5.3803050000	-0.9519230000	0.5270710000
C	-3.3919570000	-3.7100150000	-0.0703380000
H	-1.2127470000	-3.7839740000	0.0628450000
H	-5.5286680000	-3.3745620000	-0.1501430000
H	-3.4914440000	-4.7589660000	-0.3574230000
N	-0.9860310000	-0.9871500000	0.8446290000
O	-2.8528580000	0.1818530000	1.0488390000
C	0.7347050000	1.7059500000	-0.4859460000
H	0.5287510000	0.8988380000	-1.1895240000
C	2.0088630000	2.0806650000	-0.2264680000

N	3.1385940000	1.5269240000	-0.7586090000
C	4.4673850000	2.1139150000	-0.6127530000
C	3.0916330000	0.4917120000	-1.7827360000
H	4.4358210000	3.2145900000	-0.6870750000
H	4.9095900000	1.8663890000	0.3718460000
C	5.2750460000	1.4771480000	-1.7535210000
C	4.5642260000	0.1360550000	-1.9849500000
H	2.4886440000	-0.3640810000	-1.4478510000
H	2.6188630000	0.8757790000	-2.7088490000
H	5.1986310000	2.1026290000	-2.6580840000
H	6.3424630000	1.3740400000	-1.5084650000
H	4.7661290000	-0.2977250000	-2.9749190000
H	4.8652580000	-0.5993320000	-1.2218600000
C	-1.6467000000	2.5946330000	-0.6111030000
C	-2.0503990000	1.6913700000	-1.6081270000
C	-2.4258020000	3.7366400000	-0.3802870000
C	-3.2131780000	1.9280480000	-2.3452710000
H	-1.4625530000	0.7959450000	-1.8197300000
C	-3.5852950000	3.9755300000	-1.1220170000
H	-2.1241660000	4.4427000000	0.3967220000
C	-3.9850750000	3.0685830000	-2.1064270000
H	-3.5120630000	1.2146030000	-3.1173860000
H	-4.1777580000	4.8734960000	-0.9292290000
H	-4.8915960000	3.2528290000	-2.6885230000
H	2.2044810000	2.8866910000	0.4917020000
Cl	-1.7727090000	2.3580930000	2.7072960000

IN3b

0 1

Pd	-0.9109390000	0.9306090000	1.1452120000
O	-2.3887830000	1.8977050000	0.2196040000
C	-2.6079790000	1.7042980000	-1.0568380000
O	-1.9904020000	0.9327120000	-1.7770550000
O	0.8042560000	0.4348370000	2.2481060000
C	1.1487080000	1.6650200000	2.2671430000
C	2.4833390000	2.0728310000	2.8035760000
H	3.2501130000	1.7996760000	2.0605610000
H	2.5170900000	3.1558910000	2.9755430000
H	2.7024440000	1.5226400000	3.7294770000
O	0.3369870000	2.5075370000	1.7754990000
C	-3.7795110000	2.5207920000	-1.5758100000
H	-3.8604890000	3.4856500000	-1.0575190000
H	-3.6764340000	2.6643280000	-2.6593080000
H	-4.7048070000	1.9519510000	-1.3874600000
C	1.3379110000	-1.5984520000	-0.9393250000
C	0.4537440000	-2.0351940000	0.2640990000
H	0.7529890000	-1.4693470000	1.1508790000
H	0.9848320000	-2.1820700000	-1.8069040000
C	-1.0111620000	-1.8216310000	0.0915680000
C	-3.0501980000	-2.2866800000	-0.5016390000
C	-3.0611450000	-1.1117640000	0.2573470000
C	-4.1943900000	-2.8761630000	-1.0217850000
C	-4.2630380000	-0.4636420000	0.5513650000
C	-5.3939490000	-2.2189660000	-0.7349650000

H	-4.1523010000	-3.7920120000	-1.6116650000
C	-5.4256420000	-1.0408090000	0.0388780000
H	-4.2732380000	0.4560870000	1.1338510000
H	-6.3303510000	-2.6317390000	-1.1158950000
H	-6.3886020000	-0.5675360000	0.2420440000
N	-1.7298210000	-0.8477290000	0.5982180000
O	-1.7472700000	-2.7101680000	-0.5962870000
C	1.1380400000	-0.1201940000	-1.2101130000
H	0.1454330000	0.1827310000	-1.5543440000
C	2.1108330000	0.8089680000	-1.0326340000
N	2.0001860000	2.1551690000	-1.2020330000
C	3.1026990000	3.0814780000	-0.9826630000
C	0.7608590000	2.8274800000	-1.5653520000
H	4.0307100000	2.7235320000	-1.4594360000
H	3.3156970000	3.2112300000	0.0983180000
C	2.5889700000	4.3910300000	-1.5895570000
C	1.0765030000	4.3092570000	-1.3390600000
H	-0.0687760000	2.4783720000	-0.9367360000
H	0.4834010000	2.6036260000	-2.6131380000
H	2.7948310000	4.4058880000	-2.6727450000
H	3.0617380000	5.2787950000	-1.1441820000
H	0.4898830000	4.9741000000	-1.9894400000
H	0.8518110000	4.5709470000	-0.2926980000
C	2.7860570000	-1.9724870000	-0.6860940000
C	3.4142530000	-1.6807740000	0.5351330000
C	3.5388350000	-2.5775000000	-1.6986430000
C	4.7614520000	-1.9885470000	0.7341500000

H	2.8474810000	-1.2035500000	1.3377790000
C	4.8878270000	-2.8856850000	-1.5036790000
H	3.0594820000	-2.8087460000	-2.6533890000
C	5.5043120000	-2.5919050000	-0.2851460000
H	5.2334940000	-1.7591210000	1.6928530000
H	5.4576970000	-3.3606040000	-2.3061220000
H	6.5577680000	-2.8357490000	-0.1279880000
H	3.1096850000	0.4931560000	-0.7197900000
Cl	0.6974590000	-3.7925760000	0.6679840000

IN4a

0 1

Pd	-1.6152170000	-1.2302870000	-0.5711390000
O	-1.5286610000	-2.2700690000	1.1279240000
C	-0.6728000000	-1.9337810000	2.0554570000
O	0.1074270000	-0.9891230000	1.9996290000
O	-2.1932240000	-0.1292900000	-2.2537170000
C	-3.3958280000	-0.0965280000	-1.8258040000
C	-4.4760580000	0.5816650000	-2.6107160000
H	-4.9742270000	-0.1678440000	-3.2469270000
H	-4.0482810000	1.3578390000	-3.2587360000
H	-5.2287910000	1.0072070000	-1.9337140000
O	-3.6451730000	-0.6805950000	-0.7268660000
C	-0.6911320000	-2.8840660000	3.2403530000
H	-0.2587430000	-2.3888470000	4.1193070000
H	-0.0697720000	-3.7590940000	2.9881670000
H	-1.7081000000	-3.2412980000	3.4517140000

C	1.6708750000	2.0977320000	-1.0180360000
C	0.8217040000	0.8565650000	-1.2212900000
H	0.0702980000	0.8915620000	-2.0144160000
H	1.4429170000	2.8716830000	-1.7607010000
C	1.2073600000	-0.5165500000	-0.9080520000
C	2.4536530000	-2.2176580000	-0.3646100000
C	1.1233930000	-2.6446830000	-0.4499980000
C	3.5079460000	-3.0527310000	-0.0246070000
C	0.7809650000	-3.9710290000	-0.1808350000
C	3.1622070000	-4.3816980000	0.2413020000
H	4.5333740000	-2.6873660000	0.0360600000
C	1.8274430000	-4.8285530000	0.1653740000
H	-0.2568580000	-4.2999890000	-0.2206030000
H	3.9461970000	-5.0896240000	0.5179370000
H	1.6069490000	-5.8749060000	0.3869840000
N	0.3704060000	-1.5232140000	-0.8001820000
O	2.4801290000	-0.8759820000	-0.6669140000
C	0.5651350000	1.8193830000	-0.0593830000
H	0.8558680000	1.4360670000	0.9204670000
C	-0.7031640000	2.6108450000	-0.0963740000
N	-1.7919240000	2.0504130000	0.5323520000
C	-3.1022040000	2.6618600000	0.3125550000
C	-1.7211160000	1.6517190000	1.9401900000
H	-3.0520790000	3.7416830000	0.5502530000
H	-3.3867010000	2.5689960000	-0.7476360000
C	-4.0504380000	1.9183080000	1.2764520000
C	-3.1201920000	1.0916720000	2.1991010000

H	-0.9303730000	0.9103750000	2.1023870000
H	-1.5161350000	2.5450920000	2.5629600000
H	-4.6573040000	2.6383470000	1.8445580000
H	-4.7368220000	1.2560220000	0.7325870000
H	-3.4000560000	1.1618690000	3.2599420000
H	-3.1491810000	0.0314170000	1.9107110000
C	3.1016910000	2.0944390000	-0.5763580000
C	3.4521450000	2.6368010000	0.6670190000
C	4.1127620000	1.6099000000	-1.4182850000
C	4.7897970000	2.6755980000	1.0701510000
H	2.6689170000	3.0446010000	1.3098240000
C	5.4483160000	1.6480550000	-1.0169980000
H	3.8458590000	1.1863060000	-2.3897060000
C	5.7901620000	2.1781870000	0.2318000000
H	5.0501630000	3.0997860000	2.0428520000
H	6.2267970000	1.2613780000	-1.6794450000
H	6.8358560000	2.2065800000	0.5476810000
H	-0.9589050000	2.9228080000	-1.1158150000
Cl	-0.2094100000	4.3646990000	0.6835080000

IN4b

0 1

Pd	1.4181770000	-0.9547980000	1.0417800000
O	3.0282590000	-1.2766290000	-0.0868280000
C	3.0648030000	-0.8283850000	-1.3139490000
O	2.1720090000	-0.2017850000	-1.8727390000
O	-0.2447400000	-1.1074560000	2.3004730000

C	-0.1335710000	-2.3796000000	2.3047680000
C	-1.0958710000	-3.2377900000	3.0658850000
H	-0.6061120000	-3.5932940000	3.9865300000
H	-1.9919070000	-2.6639980000	3.3345390000
H	-1.3642610000	-4.1206650000	2.4690830000
O	0.8312630000	-2.8861750000	1.6538000000
C	4.3891360000	-1.1156150000	-2.0008450000
H	4.2560760000	-1.0796760000	-3.0898300000
H	5.1053310000	-0.3300390000	-1.7086780000
H	4.8020350000	-2.0840320000	-1.6877340000
C	-1.9335410000	2.0036870000	-0.5504700000
C	-0.8204650000	1.2431360000	0.1199410000
H	-1.0719820000	0.6346710000	0.9911080000
H	-1.6212710000	2.9079280000	-1.0832740000
C	0.5637530000	1.6891700000	0.1462070000
C	2.3024960000	2.9449520000	-0.2375640000
C	2.7195440000	1.7891240000	0.4334220000
C	3.1674300000	3.9532140000	-0.6362970000
C	4.0665640000	1.5857890000	0.7362870000
C	4.5170200000	3.7476180000	-0.3297370000
H	2.8142960000	4.8429600000	-1.1582400000
C	4.9548910000	2.5884770000	0.3409450000
H	4.3951860000	0.6749890000	1.2355800000
H	5.2486330000	4.5044690000	-0.6198610000
H	6.0193850000	2.4714130000	0.5546660000
N	1.5739990000	1.0229300000	0.6539350000
O	0.9362100000	2.8621510000	-0.4014660000

C	-1.4355860000	0.7338640000	-1.1848830000
H	-0.8265310000	0.8410170000	-2.0839930000
C	-2.1955130000	-0.5523590000	-1.0637460000
N	-1.4295470000	-1.6993990000	-1.0391640000
C	-2.0885660000	-2.9562100000	-0.6861760000
C	-0.4823110000	-1.9794640000	-2.1209150000
H	-2.9723000000	-3.1099890000	-1.3347010000
H	-2.4450720000	-2.9126030000	0.3557480000
C	-1.0195710000	-4.0416840000	-0.9307650000
C	0.1120850000	-3.3285720000	-1.7134320000
H	0.2782050000	-1.1932220000	-2.1972950000
H	-1.0321000000	-2.0491940000	-3.0804420000
H	-1.4493740000	-4.8790810000	-1.4994380000
H	-0.6319940000	-4.4463960000	0.0139030000
H	0.4536620000	-3.9036480000	-2.5858410000
H	0.9793070000	-3.1671050000	-1.0580470000
C	-3.2751390000	2.0991710000	0.1106760000
C	-3.4078150000	2.1150630000	1.5058900000
C	-4.4300610000	2.1941150000	-0.6821260000
C	-4.6686180000	2.2226110000	2.1002220000
H	-2.5174060000	2.0462520000	2.1348110000
C	-5.6883070000	2.3018090000	-0.0891600000
H	-4.3366780000	2.1532630000	-1.7683270000
C	-5.8119600000	2.3163840000	1.3039700000
H	-4.7552710000	2.2340340000	3.1894140000
H	-6.5790120000	2.3666720000	-0.7186480000
H	-6.7984050000	2.3979610000	1.7667650000

H	-2.9005670000	-0.5298680000	-0.2252790000
Cl	-3.4534200000	-0.5369830000	-2.5807410000

IN5a

0 1

Pd	1.8981130000	0.6238800000	-0.0038180000
O	1.3755690000	1.8839600000	1.4560040000
C	0.4528010000	1.4581840000	2.2722510000
O	-0.0989810000	0.3641510000	2.2035520000
O	2.8338720000	-0.7246350000	-1.2856820000
C	3.8545810000	-0.7473970000	-0.5112740000
C	4.9593530000	-1.7273200000	-0.7253830000
H	5.1092680000	-1.9084890000	-1.7984580000
H	4.6466810000	-2.6722870000	-0.2508890000
H	5.8841800000	-1.3759710000	-0.2501430000
O	3.8486390000	0.0518990000	0.4748450000
C	0.0649590000	2.4853850000	3.3211810000
H	-0.4285160000	1.9873350000	4.1655360000
H	-0.6436560000	3.1974070000	2.8665550000
H	0.9409810000	3.0540190000	3.6617550000
C	-1.1206050000	-2.6457550000	-0.6152630000
C	-0.2996370000	-1.5848020000	-1.3080160000
H	0.1946610000	-1.8719130000	-2.2439150000
H	-1.1227720000	-3.5990380000	-1.1528090000
C	-0.6750650000	-0.1651760000	-1.2520810000
C	-1.9472410000	1.5842240000	-1.4975840000
C	-0.7381510000	1.9827580000	-0.9119800000

C	-2.9884020000	2.4603550000	-1.7750870000
C	-0.5137410000	3.3180610000	-0.5657180000
C	-2.7598100000	3.7952210000	-1.4296540000
H	-3.9208330000	2.1212470000	-2.2268800000
C	-1.5492700000	4.2128760000	-0.8380430000
H	0.4177170000	3.6178510000	-0.0871830000
H	-3.5415050000	4.5336710000	-1.6196380000
H	-1.4224790000	5.2669820000	-0.5826730000
N	0.0406240000	0.8292140000	-0.7900190000
O	-1.8800210000	0.2296110000	-1.7116160000
C	0.2255910000	-2.2328030000	-0.0401560000
H	0.2293480000	-1.6196450000	0.8664490000
C	1.3874200000	-3.1416970000	-0.2017600000
C	-2.4106310000	-2.3434970000	0.0741650000
C	-2.5249580000	-1.3590940000	1.0690570000
C	-3.5585880000	-3.0475980000	-0.3198900000
C	-3.7690530000	-1.0840530000	1.6408260000
H	-1.6549480000	-0.8007210000	1.4212540000
C	-4.7996550000	-2.7730020000	0.2578790000
H	-3.4788270000	-3.8189980000	-1.0906930000
C	-4.9097350000	-1.7851390000	1.2396970000
H	-3.8385530000	-0.3165460000	2.4153620000
H	-5.6821470000	-3.3336470000	-0.0598880000
H	-5.8790820000	-1.5678610000	1.6947820000
H	1.3764800000	-3.7368430000	-1.1559600000
O	2.2878520000	-3.2572280000	0.5921720000

IN5b

0 1

Pd	1.6075230000	1.2420910000	-0.0385260000
O	2.4259160000	0.4820030000	1.6201160000
C	1.6539130000	-0.2059050000	2.4156390000
O	0.4653000000	-0.4468770000	2.2244890000
O	0.8264380000	2.4000150000	-1.5692500000
C	1.0774780000	3.4627270000	-0.9024030000
C	0.5786080000	4.7917320000	-1.3620280000
H	0.6349500000	4.8614720000	-2.4571210000
H	-0.4810330000	4.8572750000	-1.0661130000
H	1.1428330000	5.6029930000	-0.8846110000
O	1.7151480000	3.3218720000	0.1885710000
C	2.3908160000	-0.7224830000	3.6404050000
H	1.6872960000	-1.2216580000	4.3183100000
H	3.1714090000	-1.4323250000	3.3247320000
H	2.8951170000	0.1076940000	4.1566400000
C	-2.2090880000	-0.5365660000	0.4764300000
C	-1.3245110000	-0.4667150000	-0.7377190000
H	-1.8516910000	-0.5054460000	-1.6984490000
H	-1.7267930000	-0.9558460000	1.3665630000
C	-0.0208350000	-1.1399280000	-0.7730680000
C	1.3060840000	-2.8633190000	-0.9513230000
C	2.0718610000	-1.7244950000	-0.6744310000
C	1.8516420000	-4.1302740000	-1.1097240000
C	3.4569990000	-1.8089410000	-0.5207850000
C	3.2401710000	-4.2106610000	-0.9639990000

H	1.2337320000	-5.0021590000	-1.3259480000
C	4.0240180000	-3.0751260000	-0.6733070000
H	4.0466850000	-0.9253240000	-0.2777850000
H	3.7292940000	-5.1808900000	-1.0727270000
H	5.1036980000	-3.1928680000	-0.5607060000
N	1.1795200000	-0.6541510000	-0.5937220000
O	-0.0102550000	-2.4713590000	-1.0129130000
C	-1.5564460000	0.7811700000	0.0938530000
H	-0.7520330000	1.0899500000	0.7637190000
C	-2.3152500000	1.8855770000	-0.5429120000
C	-3.6767240000	-0.7910250000	0.3320720000
C	-4.1587500000	-1.7703310000	-0.5467610000
C	-4.5930400000	-0.0679480000	1.1109030000
C	-5.5300730000	-2.0190640000	-0.6518740000
H	-3.4508770000	-2.3468950000	-1.1475630000
C	-5.9628840000	-0.3144570000	1.0063560000
H	-4.2247420000	0.6983090000	1.7979990000
C	-6.4355110000	-1.2905840000	0.1231910000
H	-5.8916110000	-2.7852730000	-1.3419330000
H	-6.6656280000	0.2601910000	1.6144200000
H	-7.5079090000	-1.4817100000	0.0395330000
H	-3.1257190000	1.5649340000	-1.2477420000
O	-2.0951140000	3.0556170000	-0.3390240000

OX

0 1

C	2.4738490000	0.3917330000	0.7249410000

H	2.7864480000	1.4334970000	0.8517000000
C	1.0142120000	0.3557530000	0.4738360000
C	-0.9084930000	-0.6050340000	0.2167960000
C	-1.0232090000	0.7859870000	0.0364960000
C	-1.9784430000	-1.4857550000	0.1140540000
C	-2.2676460000	1.3524090000	-0.2637340000
C	-3.2143720000	-0.9053480000	-0.1875050000
H	-1.8581730000	-2.5600420000	0.2586780000
C	-3.3556040000	0.4853650000	-0.3725380000
H	-2.3698200000	2.4292120000	-0.4062740000
H	-4.0934500000	-1.5466420000	-0.2826030000
H	-4.3427480000	0.8896080000	-0.6072370000
N	0.2364610000	1.3545900000	0.2091390000
O	0.4016910000	-0.8705660000	0.5007850000
Cl	3.4016430000	-0.3067020000	-0.6675930000
H	2.7392910000	-0.1999620000	1.6104820000

PdAc

0 1

Pd	0.0000030000	-0.0000320000	0.0000410000
O	1.7626700000	-1.0821260000	0.0178780000
C	2.4343360000	0.0000160000	0.0181690000
O	1.7625950000	1.0821230000	0.0178950000
O	-1.7626040000	1.0821200000	-0.0178790000
C	-2.4343390000	0.0000100000	-0.0182030000
O	-1.7626680000	-1.0821310000	-0.0178610000
C	3.9276600000	0.0000740000	-0.0132570000

H	4.3163200000	0.9053720000	0.4717040000
H	4.3163900000	-0.9051500000	0.4717860000
H	4.2584590000	0.0000370000	-1.0646270000
C	-3.9276670000	0.0000710000	0.0130610000
H	-4.2585920000	0.0004580000	1.0643890000
H	-4.3162670000	0.9051830000	-0.4723020000
H	-4.3163430000	-0.9053320000	-0.4716940000

PR1a

0 1

C	2.1622540000	0.3618060000	-0.8080670000
C	1.1397530000	1.4731590000	-0.8494800000
H	2.9427360000	0.4588350000	-1.5735040000
H	1.2568830000	2.2218220000	-1.6360250000
C	-0.2706910000	1.2068060000	-0.5391820000
C	-1.9180010000	0.3972900000	0.6187340000
C	-2.3869940000	0.9558750000	-0.5845340000
C	-2.7387860000	-0.2032650000	1.5634890000
C	-3.7543440000	0.9249700000	-0.8796780000
C	-4.1032200000	-0.2283340000	1.2536190000
H	-2.3414830000	-0.6294390000	2.4854440000
C	-4.5994550000	0.3250780000	0.0566210000
H	-4.1338320000	1.3542920000	-1.8081600000
H	-4.8001630000	-0.6888360000	1.9573490000
H	-5.6729130000	0.2815670000	-0.1407440000
N	-1.2949670000	1.4599920000	-1.2898560000
O	-0.5607500000	0.5710710000	0.6421330000

C	1.7729530000	-1.0474120000	-0.4843770000
C	0.8462550000	-1.7181860000	-1.2959990000
C	2.3278120000	-1.7176620000	0.6129550000
C	0.4786340000	-3.0346100000	-1.0122370000
H	0.3986530000	-1.1959640000	-2.1452000000
C	1.9643990000	-3.0368270000	0.8950510000
H	3.0453010000	-1.1990990000	1.2535860000
C	1.0376450000	-3.6975730000	0.0843810000
H	-0.2514870000	-3.5429610000	-1.6464420000
H	2.4031700000	-3.5485630000	1.7549880000
H	0.7483130000	-4.7269840000	0.3086600000
C	2.1832660000	1.4298190000	0.2632050000
H	1.8237130000	1.1534410000	1.2568000000
C	3.2651660000	2.4461790000	0.2429480000
H	3.6088290000	2.7305160000	-0.7905790000
O	3.7603960000	2.9400240000	1.2238830000

PR1b

0 1

C	-1.2457510000	0.1817060000	0.5446430000
C	-0.3030500000	0.3237130000	-0.6133750000
H	-0.7590070000	-0.0262910000	1.5039270000
H	-0.6732760000	0.0436960000	-1.6019580000
C	1.1337450000	0.0766110000	-0.4663250000
C	3.0275540000	0.0482940000	0.5982500000
C	3.1854380000	-0.4479180000	-0.7087170000
C	4.0641010000	0.1519670000	1.5155120000

C	4.4453530000	-0.8714030000	-1.1446790000
C	5.3186270000	-0.2755510000	1.0650860000
H	3.9087820000	0.5422930000	2.5221090000
C	5.5039380000	-0.7766110000	-0.2381820000
H	4.5837830000	-1.2580600000	-2.1554500000
H	6.1742880000	-0.2183290000	1.7414940000
H	6.5020630000	-1.0976940000	-0.5443290000
N	1.9466590000	-0.4087420000	-1.3480680000
O	1.7064980000	0.3826650000	0.7466810000
C	-2.5964930000	-0.4458070000	0.3736890000
C	-3.7077220000	0.0952240000	1.0382970000
C	-2.7695570000	-1.5904150000	-0.4154950000
C	-4.9664890000	-0.4942620000	0.9126840000
H	-3.5825110000	0.9920770000	1.6507260000
C	-4.0296000000	-2.1822380000	-0.5418940000
H	-1.9097900000	-2.0229440000	-0.9328900000
C	-5.1308360000	-1.6353700000	0.1208490000
H	-5.8241370000	-0.0590000000	1.4310850000
H	-4.1501950000	-3.0737340000	-1.1619560000
H	-6.1165630000	-2.0953770000	0.0195610000
C	-0.9331080000	1.5710520000	0.0182880000
H	-0.2882450000	2.2059780000	0.6299260000
C	-1.9426070000	2.3064570000	-0.7877520000
H	-2.5491940000	1.6657060000	-1.4790660000
O	-2.1144810000	3.4986090000	-0.7231780000

PY

0 1

N	-0.0000300000	-1.1650520000	-0.3500870000
C	-1.1578030000	-0.4491920000	0.1705580000
C	1.1578470000	-0.4492040000	0.1703720000
H	-2.0802370000	-0.7429180000	-0.3556980000
H	-1.3242780000	-0.6264210000	1.2578410000
C	-0.7771920000	1.0270960000	-0.0569540000
C	0.7771550000	1.0271620000	-0.0566860000
H	1.3246820000	-0.6266860000	1.2575470000
H	2.0801230000	-0.7427840000	-0.3562470000
H	-1.1605890000	1.3757290000	-1.0270600000
H	-1.2032980000	1.6798940000	0.7191410000
H	1.1609310000	1.3762730000	-1.0264660000
H	1.2028470000	1.6796820000	0.7198700000
H	-0.0000180000	-2.1525750000	-0.1020600000

TS1a

0 1

Pd	-0.2692710000	2.2023550000	0.2872250000
O	1.4985230000	2.8838530000	-0.3455750000
C	1.9974300000	2.4403880000	-1.4599180000
O	1.5288470000	1.5355300000	-2.1460540000
O	-2.3387390000	2.0679820000	0.6893750000
C	-2.5357450000	3.1200520000	-0.0090100000
C	-3.9203730000	3.6396610000	-0.2408710000
H	-4.3385350000	3.1391530000	-1.1298950000
H	-3.8943040000	4.7200100000	-0.4345010000

H	-4.5627300000	3.4085560000	0.6193760000
O	-1.5213430000	3.6762580000	-0.5254310000
C	3.3044310000	3.1174640000	-1.8382420000
H	3.4463760000	3.0696620000	-2.9259020000
H	4.1287100000	2.5656580000	-1.3557480000
H	3.3372680000	4.1567340000	-1.4856710000
C	-1.5392980000	-1.1486590000	-0.8875750000
C	-1.5029650000	-0.7456250000	1.5099420000
H	-2.1963210000	0.0872560000	1.4570950000
H	-1.4223020000	-0.0700310000	-1.0236330000
C	-0.1385390000	-0.5175560000	1.5661880000
C	1.9810350000	-1.0521230000	1.8199210000
C	1.9107150000	0.2923300000	1.4154550000
C	3.1635530000	-1.7169410000	2.0952290000
C	3.0883500000	1.0447020000	1.3350440000
C	4.3430000000	-0.9657220000	1.9738150000
H	3.1660170000	-2.7627970000	2.4053590000
C	4.2952510000	0.3904100000	1.6123480000
H	3.0522740000	2.0962790000	1.0636980000
H	5.3047840000	-1.4375310000	2.1851890000
H	5.2270400000	0.9576530000	1.5527880000
N	0.5644590000	0.5867080000	1.2051550000
O	0.7065260000	-1.5461810000	1.8884320000
C	-0.4008170000	-1.9292820000	-1.1010240000
H	-0.4461670000	-3.0112320000	-0.9688240000
C	0.8167510000	-1.2999220000	-1.3489260000
N	2.0040130000	-1.8959860000	-1.3748730000

C	3.2589850000	-1.2012470000	-1.7091780000
C	2.2201330000	-3.3181400000	-1.1005660000
H	3.0784850000	-0.4558540000	-2.4946070000
H	3.6355970000	-0.6714390000	-0.8196190000
C	4.1926010000	-2.3486180000	-2.0919210000
C	3.7452130000	-3.4762620000	-1.1491150000
H	1.7810190000	-3.5877400000	-0.1264610000
H	1.7170480000	-3.9266910000	-1.8737140000
H	4.0307740000	-2.6395000000	-3.1431980000
H	5.2526460000	-2.0828000000	-1.9731240000
H	4.0511130000	-4.4771040000	-1.4850920000
H	4.1672590000	-3.3093530000	-0.1463230000
C	-2.9151880000	-1.6283280000	-0.8698430000
C	-3.2441690000	-2.9967890000	-0.9099940000
C	-3.9642300000	-0.6891610000	-0.7872970000
C	-4.5755910000	-3.4092330000	-0.8815550000
H	-2.4526910000	-3.7447000000	-0.9681600000
C	-5.2925700000	-1.1018850000	-0.7583180000
H	-3.7135530000	0.3709670000	-0.7148250000
C	-5.6044170000	-2.4660950000	-0.8069780000
H	-4.8131480000	-4.4751480000	-0.9147560000
H	-6.0920720000	-0.3601220000	-0.6919720000
H	-6.6469170000	-2.7921560000	-0.7828930000
H	0.8410370000	-0.2219740000	-1.5493340000
Cl	-2.1366670000	-2.2252470000	2.1734580000

TS1b

0 1

Pd	0.0622480000	-2.0648940000	0.2511540000
O	-1.8177630000	-2.6950530000	-0.0055660000
C	-2.3677880000	-2.2905670000	-1.1126260000
O	-1.8754740000	-1.4789860000	-1.8938310000
O	2.1995540000	-1.9902960000	-0.1629300000
C	2.0441480000	-3.0104840000	-0.9014380000
C	3.1890820000	-3.5962870000	-1.6693990000
H	3.4829460000	-2.8904990000	-2.4625860000
H	2.9016080000	-4.5541840000	-2.1206610000
H	4.0538680000	-3.7275050000	-1.0028170000
O	0.8752550000	-3.5056030000	-0.9819910000
C	-3.7512220000	-2.8720260000	-1.3441630000
H	-3.9629840000	-2.9086960000	-2.4209220000
H	-4.4874560000	-2.2026650000	-0.8683380000
H	-3.8511650000	-3.8681050000	-0.8934500000
C	1.7373280000	1.1880980000	-0.6674670000
C	1.5784860000	0.8285820000	1.7319830000
H	1.6477720000	0.1061050000	-0.7738940000
C	0.2078630000	0.6159200000	1.6932840000
C	-1.8670930000	1.3444550000	1.7904050000
C	-1.8873220000	-0.0448430000	1.5820720000
C	-3.0001540000	2.1263080000	1.9426990000
C	-3.1169340000	-0.7134050000	1.5990310000
C	-4.2293980000	1.4518760000	1.9091810000
H	-2.9284810000	3.2029640000	2.1026150000
C	-4.2761210000	0.0573110000	1.7531130000

H	-3.1590490000	-1.7929040000	1.4906980000
H	-5.1562180000	2.0157740000	2.0338250000
H	-5.2451620000	-0.4470090000	1.7648580000
N	-0.5569040000	-0.4685390000	1.4386150000
O	-0.5630900000	1.7499730000	1.8333460000
C	0.6169590000	1.9599440000	-0.9898560000
H	0.6750360000	3.0478860000	-0.9334390000
C	-0.6078910000	1.3555830000	-1.2722080000
N	-1.7603710000	2.0037990000	-1.4107910000
C	-3.0456710000	1.3575290000	-1.7318300000
C	-1.9043440000	3.4538690000	-1.2579740000
H	-2.8901300000	0.5262200000	-2.4294520000
H	-3.4841710000	0.9405220000	-0.8102670000
C	-3.8888950000	2.5178570000	-2.2558820000
C	-3.4124610000	3.6977370000	-1.3959270000
H	-1.4960750000	3.7759120000	-0.2863560000
H	-1.3283280000	3.9684230000	-2.0479850000
H	-3.6663070000	2.7024270000	-3.3200610000
H	-4.9672750000	2.3252530000	-2.1641310000
H	-3.6373040000	4.6807820000	-1.8332660000
H	-3.8887330000	3.6493580000	-0.4048150000
C	3.1099420000	1.6796860000	-0.5791680000
C	3.4334840000	3.0522400000	-0.5674330000
C	4.1594310000	0.7398160000	-0.5015050000
C	4.7592900000	3.4688330000	-0.4811020000
H	2.6407230000	3.8005420000	-0.6234170000
C	5.4856350000	1.1618320000	-0.4200820000

H	3.9079870000	-0.3217310000	-0.4919310000
C	5.7918930000	2.5254780000	-0.4079410000
H	4.9932180000	4.5362070000	-0.4726580000
H	6.2867130000	0.4211980000	-0.3596650000
H	6.8313190000	2.8555930000	-0.3411850000
H	-0.6817060000	0.2673480000	-1.3888900000
Cl	2.6927140000	-0.3931840000	2.2557210000
H	1.8934080000	1.8408930000	1.9762290000

TS2a

0 1

Pd	-1.6503030000	0.9248730000	0.6252520000
O	-1.7170000000	2.1817780000	-0.9218780000
C	-0.9862070000	1.9557940000	-1.9755130000
O	-0.3017370000	0.9520770000	-2.1671450000
O	-2.0870480000	-0.4274340000	2.1735040000
C	-3.3220540000	-0.3969840000	1.8627060000
C	-4.3390680000	-1.1135200000	2.6981690000
H	-4.5698690000	-0.4908200000	3.5776000000
H	-3.9285240000	-2.0646850000	3.0647790000
H	-5.2643630000	-1.2736490000	2.1295990000
O	-3.6600880000	0.2794160000	0.8408630000
C	-1.0082970000	3.0990660000	-2.9725360000
H	-0.7767170000	2.7224440000	-3.9774610000
H	-0.2224610000	3.8136920000	-2.6780860000
H	-1.9712040000	3.6269350000	-2.9610340000
C	1.5072360000	-2.3535490000	0.4456830000

C	0.8547790000	-1.1590630000	0.9871210000
H	0.0983080000	-1.2709610000	1.7561250000
H	1.3029680000	-3.2320510000	1.0715620000
C	1.1956340000	0.2277480000	0.7026990000
C	2.3278520000	1.9357580000	-0.0110530000
C	1.0401100000	2.3677440000	0.3335540000
C	3.3227720000	2.7841090000	-0.4708450000
C	0.6920290000	3.7151020000	0.2270810000
C	2.9698960000	4.1345340000	-0.5772090000
H	4.3155490000	2.4132700000	-0.7267080000
C	1.6815930000	4.5878370000	-0.2339760000
H	-0.3112440000	4.0553870000	0.4801510000
H	3.7132090000	4.8530290000	-0.9289390000
H	1.4514180000	5.6514280000	-0.3273740000
N	0.3346580000	1.2328850000	0.7277310000
O	2.3834840000	0.5797610000	0.1817830000
C	0.3561060000	-2.0088820000	-0.4821880000
H	0.5691560000	-1.4104680000	-1.3682600000
C	-0.9212340000	-2.5550660000	-0.2869700000
N	-1.9874030000	-2.3843630000	-1.0402740000
C	-3.3204710000	-2.9053360000	-0.6732740000
C	-2.0388140000	-1.5843800000	-2.2757450000
H	-3.2872750000	-4.0000240000	-0.5617810000
H	-3.6229330000	-2.4694610000	0.2895460000
C	-4.2323750000	-2.4360550000	-1.8138060000
C	-3.5130130000	-1.1956650000	-2.3633230000
H	-1.3571270000	-0.7253130000	-2.2098020000

H	-1.7321970000	-2.2220220000	-3.1248240000
H	-4.2991830000	-3.2154610000	-2.5899020000
H	-5.2509170000	-2.2258340000	-1.4595390000
H	-3.8161510000	-0.9377540000	-3.3873700000
H	-3.7010610000	-0.3266120000	-1.7144510000
C	2.9083160000	-2.3573910000	-0.1012100000
C	3.1686470000	-2.7965200000	-1.4042620000
C	3.9718550000	-1.9729890000	0.7289970000
C	4.4812420000	-2.8516910000	-1.8817310000
H	2.3414500000	-3.0954640000	-2.0529250000
C	5.2802660000	-2.0294850000	0.2476920000
H	3.7509150000	-1.5951130000	1.7318170000
C	5.5398200000	-2.4684080000	-1.0552760000
H	4.6750650000	-3.1924220000	-2.9017600000
H	6.1047160000	-1.7203760000	0.8949730000
H	6.5667210000	-2.5079130000	-1.4272590000
H	-1.0880560000	-3.1551200000	0.6155590000
Cl	2.0677850000	-0.2793820000	3.1427220000

TS2b

0 1

Pd	-1.1937640000	1.0112220000	0.9998460000
O	-2.8345610000	1.3730980000	-0.0754470000
C	-2.8790240000	1.0113140000	-1.3254660000
O	-1.9453550000	0.5236340000	-1.9601840000
O	0.5278450000	1.1357860000	2.1928910000
C	0.3937710000	2.4004500000	2.2700800000

C	1.3097000000	3.2167770000	3.1298870000
H	0.9516910000	3.1635640000	4.1708200000
H	2.3259650000	2.7996430000	3.1058650000
H	1.3040690000	4.2674790000	2.8118390000
O	-0.5562800000	2.9354480000	1.6164790000
C	-4.2471030000	1.2027690000	-1.9530580000
H	-4.1456970000	1.3178760000	-3.0401780000
H	-4.8375950000	0.2939840000	-1.7521550000
H	-4.7771370000	2.0583350000	-1.5137200000
C	1.9146190000	-1.6318150000	-0.9961510000
C	0.9855620000	-1.2800150000	0.0761470000
H	1.3129350000	-0.7103780000	0.9391380000
H	1.5392100000	-2.4350530000	-1.6419370000
C	-0.4190800000	-1.6444410000	0.0556460000
C	-2.2121270000	-2.7082580000	-0.5494310000
C	-2.5830300000	-1.6318390000	0.2679870000
C	-3.1177930000	-3.6149920000	-1.0770950000
C	-3.9222360000	-1.4197370000	0.5976610000
C	-4.4605720000	-3.3983860000	-0.7452710000
H	-2.7964240000	-4.4456010000	-1.7059690000
C	-4.8516970000	-2.3235840000	0.0755730000
H	-4.2174060000	-0.5764860000	1.2206080000
H	-5.2202150000	-4.0834010000	-1.1274770000
H	-5.9099580000	-2.1956170000	0.3133600000
N	-1.4102150000	-0.9472870000	0.5814290000
O	-0.8490110000	-2.6662850000	-0.7092370000
C	1.3548820000	-0.2818470000	-1.4281170000

H	0.4984520000	-0.2569520000	-2.1014830000
C	1.9507830000	0.9039600000	-0.9919890000
N	1.5810390000	2.1389450000	-1.2777380000
C	2.2300950000	3.3237990000	-0.6851700000
C	0.4439990000	2.5106570000	-2.1342120000
H	3.3091540000	3.3224870000	-0.9035440000
H	2.1038600000	3.2978410000	0.4077740000
C	1.4834040000	4.5082570000	-1.3108740000
C	0.1065800000	3.9218750000	-1.6564610000
H	-0.3771710000	1.7899990000	-2.0208710000
H	0.7728020000	2.5039230000	-3.1897640000
H	1.9998230000	4.8386620000	-2.2266820000
H	1.4317120000	5.3666170000	-0.6266870000
H	-0.4326700000	4.5030000000	-2.4172660000
H	-0.5191370000	3.8631110000	-0.7528090000
C	3.3892280000	-1.7412670000	-0.7066880000
C	3.8499070000	-2.2365790000	0.5198720000
C	4.3152970000	-1.3684580000	-1.6933430000
C	5.2253050000	-2.3460070000	0.7533900000
H	3.1219290000	-2.5512500000	1.2736550000
C	5.6854820000	-1.4819520000	-1.4571440000
H	3.9563780000	-0.9798040000	-2.6504580000
C	6.1443120000	-1.9699890000	-0.2282590000
H	5.5767940000	-2.7334820000	1.7127650000
H	6.3981820000	-1.1897040000	-2.2324290000
H	7.2172800000	-2.0577960000	-0.0403940000
H	2.8074880000	0.8243050000	-0.3138850000

Cl	0.7670820000	-3.1053360000	1.8718820000

AL

0 1

C	-0.9333100000	-0.5971950000	0.0002820000
H	-1.1455650000	-1.6740100000	0.0006540000
C	-1.9952450000	0.2371680000	-0.0001390000
H	-1.8976270000	1.3263720000	-0.0007490000
C	-3.3657340000	-0.2861830000	0.0001020000
C	0.4857670000	-0.2466270000	0.0001350000
C	0.9405450000	1.0881640000	0.0002470000
C	1.4440300000	-1.2786820000	-0.0000370000
C	2.3027270000	1.3740850000	0.0000770000
H	0.2190850000	1.9070940000	0.0005580000
C	2.8091540000	-0.9921480000	-0.0002080000
H	1.1059750000	-2.3182510000	-0.0000780000
C	3.2428580000	0.3358310000	-0.0001700000
H	2.6379800000	2.4138310000	0.0001680000
H	3.5366640000	-1.8070370000	-0.0003720000
H	4.3111350000	0.5645260000	-0.0002980000
H	-3.4313190000	-1.4081360000	0.0007010000
O	-4.3651340000	0.3986410000	-0.0002900000

IM

1 1

C	-0.9894990000	-0.8525100000	-0.0331390000
H	-0.9231750000	-1.9467050000	-0.0544440000

C	0.1947430000	-0.1554600000	-0.0344150000
H	0.2026080000	0.9349640000	-0.0123520000
C	1.4217250000	-0.8590910000	-0.0606010000
N	2.6145070000	-0.3219000000	-0.0639200000
C	3.8744130000	-1.1045980000	-0.0771790000
C	2.8902370000	1.1330710000	-0.0277480000
H	3.7742870000	-1.9894900000	0.5662200000
H	4.0681360000	-1.4398710000	-1.1099270000
C	4.9213400000	-0.0938710000	0.3883310000
C	4.4093310000	1.2253680000	-0.2056770000
H	2.3199890000	1.6443280000	-0.8166880000
H	2.5602300000	1.5256550000	0.9482760000
H	4.9370910000	-0.0442380000	1.4888080000
H	5.9310960000	-0.3599240000	0.0487470000
H	4.8258290000	2.1145900000	0.2856480000
H	4.6606660000	1.2865590000	-1.2761780000
C	-2.3264640000	-0.3219870000	-0.0074380000
C	-2.6027970000	1.0673160000	0.0206810000
C	-3.4102620000	-1.2327270000	-0.0102460000
C	-3.9140960000	1.5203610000	0.0451930000
H	-1.7866550000	1.7917400000	0.0231610000
C	-4.7229520000	-0.7738930000	0.0143710000
H	-3.2073050000	-2.3062340000	-0.0319820000
C	-4.9758280000	0.6019720000	0.0421050000
H	-4.1211720000	2.5919550000	0.0667770000
H	-5.5517140000	-1.4842020000	0.0119990000
H	-6.0058180000	0.9651440000	0.0613850000

H	1.3950240000	-1.9546880000	-0.0774370000

IN1

0 1

Pd	-1.2233030000	0.0635570000	-0.0217550000
O	0.0029010000	-0.8692970000	-2.6147190000
C	-0.6354340000	-1.7740760000	-2.1048970000
O	-1.2248150000	-1.7150000000	-0.9296690000
O	-1.7173830000	1.8832570000	0.8714890000
C	-2.9481770000	1.6847160000	0.5924710000
C	-4.0011670000	2.6633300000	1.0085080000
H	-3.6042290000	3.6867010000	0.9640510000
H	-4.2857380000	2.4528930000	2.0522720000
H	-4.8908970000	2.5584350000	0.3742350000
O	-3.2422960000	0.6142980000	-0.0241590000
C	-0.8235190000	-3.1272230000	-2.7738000000
H	-1.8969170000	-3.3303780000	-2.9063820000
H	-0.4208850000	-3.9280270000	-2.1338570000
H	-0.3155790000	-3.1344800000	-3.7461960000
C	1.0632900000	-2.3781870000	1.0255930000
H	0.1068340000	-2.6262810000	0.5502090000
C	1.5192800000	-1.0592780000	0.5348660000
C	2.9518150000	0.5079530000	0.0602430000
C	1.6559920000	0.9978830000	-0.1432640000
C	4.0969480000	1.2619690000	-0.1623370000
C	1.4403030000	2.3054570000	-0.5844340000
C	3.8778610000	2.5691100000	-0.6052440000

H	5.0960830000	0.8568540000	-0.0006090000
C	2.5780910000	3.0789970000	-0.8100900000
H	0.4294120000	2.6855660000	-0.7309470000
H	4.7376170000	3.2141720000	-0.7978980000
H	2.4632970000	4.1081670000	-1.1560280000
N	0.7823350000	-0.0418080000	0.1742810000
O	2.8405970000	-0.7923830000	0.4904060000
Cl	0.8017770000	-2.3166230000	2.8184640000
H	1.8226530000	-3.1428910000	0.8255500000

IN2

-1 1

Pd	-1.2382160000	-0.0928940000	0.0778860000
O	-3.3835670000	-0.1651580000	0.3056780000
C	-3.4772700000	0.8243280000	-0.4750680000
O	-2.4202800000	1.3521630000	-0.9465580000
O	-0.4803420000	-1.4815620000	1.3057180000
C	-0.5295160000	-2.7152030000	0.8994940000
C	0.2635090000	-3.6596280000	1.7960350000
H	0.2633930000	-3.3260520000	2.8433110000
H	1.3048310000	-3.6524720000	1.4326000000
H	-0.1311330000	-4.6817430000	1.7090610000
O	-1.0760210000	-3.1209580000	-0.1198700000
C	-4.8275230000	1.3596240000	-0.8806500000
H	-5.0941140000	0.9416700000	-1.8650910000
H	-4.7868650000	2.4538180000	-0.9781940000
H	-5.5926370000	1.0601640000	-0.1519620000

C	1.7629570000	-1.6476960000	-1.0102940000
H	0.8600150000	-2.2145730000	-1.2175180000
C	1.7286650000	-0.3633170000	-0.5856280000
C	2.5209950000	1.6099960000	0.0400010000
C	1.1128160000	1.6896170000	-0.0095950000
C	3.3288920000	2.6728720000	0.3935210000
C	0.4790330000	2.8953350000	0.3091520000
C	2.6843890000	3.8880880000	0.7129630000
H	4.4150060000	2.5664310000	0.4259550000
C	1.2892830000	3.9859020000	0.6701860000
H	-0.6083850000	2.9702960000	0.2695190000
H	3.2845290000	4.7564280000	0.9965440000
H	0.8124360000	4.9374340000	0.9228260000
N	0.6316370000	0.4590860000	-0.4032850000
O	2.8961940000	0.3415500000	-0.3090180000
Cl	3.2649510000	-2.5529220000	-1.0703020000

IN3a

0 1

Pd	1.0015910000	-1.3588480000	0.6779960000
O	0.6767970000	-2.6031370000	-0.8491810000
C	0.1509600000	-2.1476990000	-1.9544290000
O	-0.1826950000	-0.9874630000	-2.1570040000
O	1.8712180000	-0.2429050000	2.2208610000
C	3.0318860000	-0.5989520000	1.8245150000
C	4.2621770000	-0.0659840000	2.4867180000
H	4.2241040000	1.0332240000	2.4906170000

H	5.1624210000	-0.4138910000	1.9655600000
H	4.2851320000	-0.4002310000	3.5354380000
O	3.0919660000	-1.4203350000	0.8574740000
C	-0.0700480000	-3.2337700000	-2.9936240000
H	0.6922300000	-4.0211930000	-2.9239820000
H	-0.0830120000	-2.7876520000	-3.9966490000
H	-1.0550760000	-3.6922720000	-2.8059600000
C	-0.4253030000	2.3204300000	0.2488800000
C	-0.7907040000	1.4320190000	1.4944800000
H	0.1416860000	1.1598840000	1.9994110000
H	-0.0964930000	3.2671600000	0.7050180000
C	-1.5137450000	0.1783340000	1.1413160000
C	-3.2184060000	-1.0784350000	0.6546020000
C	-2.0511130000	-1.8400610000	0.5248840000
C	-4.4933720000	-1.5771770000	0.4232670000
C	-2.1187470000	-3.1894890000	0.1656660000
C	-4.5551760000	-2.9221330000	0.0499190000
H	-5.3803050000	-0.9519230000	0.5270710000
C	-3.3919570000	-3.7100150000	-0.0703380000
H	-1.2127470000	-3.7839740000	0.0628450000
H	-5.5286680000	-3.3745620000	-0.1501430000
H	-3.4914440000	-4.7589660000	-0.3574230000
N	-0.9860310000	-0.9871500000	0.8446290000
O	-2.8528580000	0.1818530000	1.0488390000
C	0.7347050000	1.7059500000	-0.4859460000
H	0.5287510000	0.8988380000	-1.1895240000
C	2.0088630000	2.0806650000	-0.2264680000

N	3.1385940000	1.5269240000	-0.7586090000
C	4.4673850000	2.1139150000	-0.6127530000
C	3.0916330000	0.4917120000	-1.7827360000
H	4.4358210000	3.2145900000	-0.6870750000
H	4.9095900000	1.8663890000	0.3718460000
C	5.2750460000	1.4771480000	-1.7535210000
C	4.5642260000	0.1360550000	-1.9849500000
H	2.4886440000	-0.3640810000	-1.4478510000
H	2.6188630000	0.8757790000	-2.7088490000
H	5.1986310000	2.1026290000	-2.6580840000
H	6.3424630000	1.3740400000	-1.5084650000
H	4.7661290000	-0.2977250000	-2.9749190000
H	4.8652580000	-0.5993320000	-1.2218600000
C	-1.6467000000	2.5946330000	-0.6111030000
C	-2.0503990000	1.6913700000	-1.6081270000
C	-2.4258020000	3.7366400000	-0.3802870000
C	-3.2131780000	1.9280480000	-2.3452710000
H	-1.4625530000	0.7959450000	-1.8197300000
C	-3.5852950000	3.9755300000	-1.1220170000
H	-2.1241660000	4.4427000000	0.3967220000
C	-3.9850750000	3.0685830000	-2.1064270000
H	-3.5120630000	1.2146030000	-3.1173860000
H	-4.1777580000	4.8734960000	-0.9292290000
H	-4.8915960000	3.2528290000	-2.6885230000
H	2.2044810000	2.8866910000	0.4917020000
Cl	-1.7727090000	2.3580930000	2.7072960000

IN3b

0 1

Pd	-0.9109390000	0.9306090000	1.1452120000
O	-2.3887830000	1.8977050000	0.2196040000
C	-2.6079790000	1.7042980000	-1.0568380000
O	-1.9904020000	0.9327120000	-1.7770550000
O	0.8042560000	0.4348370000	2.2481060000
C	1.1487080000	1.6650200000	2.2671430000
C	2.4833390000	2.0728310000	2.8035760000
H	3.2501130000	1.7996760000	2.0605610000
H	2.5170900000	3.1558910000	2.9755430000
H	2.7024440000	1.5226400000	3.7294770000
O	0.3369870000	2.5075370000	1.7754990000
C	-3.7795110000	2.5207920000	-1.5758100000
H	-3.8604890000	3.4856500000	-1.0575190000
H	-3.6764340000	2.6643280000	-2.6593080000
H	-4.7048070000	1.9519510000	-1.3874600000
C	1.3379110000	-1.5984520000	-0.9393250000
C	0.4537440000	-2.0351940000	0.2640990000
H	0.7529890000	-1.4693470000	1.1508790000
H	0.9848320000	-2.1820700000	-1.8069040000
C	-1.0111620000	-1.8216310000	0.0915680000
C	-3.0501980000	-2.2866800000	-0.5016390000
C	-3.0611450000	-1.1117640000	0.2573470000
C	-4.1943900000	-2.8761630000	-1.0217850000
C	-4.2630380000	-0.4636420000	0.5513650000
C	-5.3939490000	-2.2189660000	-0.7349650000

H	-4.1523010000	-3.7920120000	-1.6116650000
C	-5.4256420000	-1.0408090000	0.0388780000
H	-4.2732380000	0.4560870000	1.1338510000
H	-6.3303510000	-2.6317390000	-1.1158950000
H	-6.3886020000	-0.5675360000	0.2420440000
N	-1.7298210000	-0.8477290000	0.5982180000
O	-1.7472700000	-2.7101680000	-0.5962870000
C	1.1380400000	-0.1201940000	-1.2101130000
H	0.1454330000	0.1827310000	-1.5543440000
C	2.1108330000	0.8089680000	-1.0326340000
N	2.0001860000	2.1551690000	-1.2020330000
C	3.1026990000	3.0814780000	-0.9826630000
C	0.7608590000	2.8274800000	-1.5653520000
H	4.0307100000	2.7235320000	-1.4594360000
H	3.3156970000	3.2112300000	0.0983180000
C	2.5889700000	4.3910300000	-1.5895570000
C	1.0765030000	4.3092570000	-1.3390600000
H	-0.0687760000	2.4783720000	-0.9367360000
H	0.4834010000	2.6036260000	-2.6131380000
H	2.7948310000	4.4058880000	-2.6727450000
H	3.0617380000	5.2787950000	-1.1441820000
H	0.4898830000	4.9741000000	-1.9894400000
H	0.8518110000	4.5709470000	-0.2926980000
C	2.7860570000	-1.9724870000	-0.6860940000
C	3.4142530000	-1.6807740000	0.5351330000
C	3.5388350000	-2.5775000000	-1.6986430000
C	4.7614520000	-1.9885470000	0.7341500000

H	2.8474810000	-1.2035500000	1.3377790000
C	4.8878270000	-2.8856850000	-1.5036790000
H	3.0594820000	-2.8087460000	-2.6533890000
C	5.5043120000	-2.5919050000	-0.2851460000
H	5.2334940000	-1.7591210000	1.6928530000
H	5.4576970000	-3.3606040000	-2.3061220000
H	6.5577680000	-2.8357490000	-0.1279880000
H	3.1096850000	0.4931560000	-0.7197900000
Cl	0.6974590000	-3.7925760000	0.6679840000

IN4a

0 1

Pd	-1.6152170000	-1.2302870000	-0.5711390000
O	-1.5286610000	-2.2700690000	1.1279240000
C	-0.6728000000	-1.9337810000	2.0554570000
O	0.1074270000	-0.9891230000	1.9996290000
O	-2.1932240000	-0.1292900000	-2.2537170000
C	-3.3958280000	-0.0965280000	-1.8258040000
C	-4.4760580000	0.5816650000	-2.6107160000
H	-4.9742270000	-0.1678440000	-3.2469270000
H	-4.0482810000	1.3578390000	-3.2587360000
H	-5.2287910000	1.0072070000	-1.9337140000
O	-3.6451730000	-0.6805950000	-0.7268660000
C	-0.6911320000	-2.8840660000	3.2403530000
H	-0.2587430000	-2.3888470000	4.1193070000
H	-0.0697720000	-3.7590940000	2.9881670000
H	-1.7081000000	-3.2412980000	3.4517140000

C	1.6708750000	2.0977320000	-1.0180360000
C	0.8217040000	0.8565650000	-1.2212900000
H	0.0702980000	0.8915620000	-2.0144160000
H	1.4429170000	2.8716830000	-1.7607010000
C	1.2073600000	-0.5165500000	-0.9080520000
C	2.4536530000	-2.2176580000	-0.3646100000
C	1.1233930000	-2.6446830000	-0.4499980000
C	3.5079460000	-3.0527310000	-0.0246070000
C	0.7809650000	-3.9710290000	-0.1808350000
C	3.1622070000	-4.3816980000	0.2413020000
H	4.5333740000	-2.6873660000	0.0360600000
C	1.8274430000	-4.8285530000	0.1653740000
H	-0.2568580000	-4.2999890000	-0.2206030000
H	3.9461970000	-5.0896240000	0.5179370000
H	1.6069490000	-5.8749060000	0.3869840000
N	0.3704060000	-1.5232140000	-0.8001820000
O	2.4801290000	-0.8759820000	-0.6669140000
C	0.5651350000	1.8193830000	-0.0593830000
H	0.8558680000	1.4360670000	0.9204670000
C	-0.7031640000	2.6108450000	-0.0963740000
N	-1.7919240000	2.0504130000	0.5323520000
C	-3.1022040000	2.6618600000	0.3125550000
C	-1.7211160000	1.6517190000	1.9401900000
H	-3.0520790000	3.7416830000	0.5502530000
H	-3.3867010000	2.5689960000	-0.7476360000
C	-4.0504380000	1.9183080000	1.2764520000
C	-3.1201920000	1.0916720000	2.1991010000

H	-0.9303730000	0.9103750000	2.1023870000
H	-1.5161350000	2.5450920000	2.5629600000
H	-4.6573040000	2.6383470000	1.8445580000
H	-4.7368220000	1.2560220000	0.7325870000
H	-3.4000560000	1.1618690000	3.2599420000
H	-3.1491810000	0.0314170000	1.9107110000
C	3.1016910000	2.0944390000	-0.5763580000
C	3.4521450000	2.6368010000	0.6670190000
C	4.1127620000	1.6099000000	-1.4182850000
C	4.7897970000	2.6755980000	1.0701510000
H	2.6689170000	3.0446010000	1.3098240000
C	5.4483160000	1.6480550000	-1.0169980000
H	3.8458590000	1.1863060000	-2.3897060000
C	5.7901620000	2.1781870000	0.2318000000
H	5.0501630000	3.0997860000	2.0428520000
H	6.2267970000	1.2613780000	-1.6794450000
H	6.8358560000	2.2065800000	0.5476810000
H	-0.9589050000	2.9228080000	-1.1158150000
Cl	-0.2094100000	4.3646990000	0.6835080000

IN4b

0 1

Pd	1.4181770000	-0.9547980000	1.0417800000
O	3.0282590000	-1.2766290000	-0.0868280000
C	3.0648030000	-0.8283850000	-1.3139490000
O	2.1720090000	-0.2017850000	-1.8727390000
O	-0.2447400000	-1.1074560000	2.3004730000

C	-0.1335710000	-2.3796000000	2.3047680000
C	-1.0958710000	-3.2377900000	3.0658850000
H	-0.6061120000	-3.5932940000	3.9865300000
H	-1.9919070000	-2.6639980000	3.3345390000
H	-1.3642610000	-4.1206650000	2.4690830000
O	0.8312630000	-2.8861750000	1.6538000000
C	4.3891360000	-1.1156150000	-2.0008450000
H	4.2560760000	-1.0796760000	-3.0898300000
H	5.1053310000	-0.3300390000	-1.7086780000
H	4.8020350000	-2.0840320000	-1.6877340000
C	-1.9335410000	2.0036870000	-0.5504700000
C	-0.8204650000	1.2431360000	0.1199410000
H	-1.0719820000	0.6346710000	0.9911080000
H	-1.6212710000	2.9079280000	-1.0832740000
C	0.5637530000	1.6891700000	0.1462070000
C	2.3024960000	2.9449520000	-0.2375640000
C	2.7195440000	1.7891240000	0.4334220000
C	3.1674300000	3.9532140000	-0.6362970000
C	4.0665640000	1.5857890000	0.7362870000
C	4.5170200000	3.7476180000	-0.3297370000
H	2.8142960000	4.8429600000	-1.1582400000
C	4.9548910000	2.5884770000	0.3409450000
H	4.3951860000	0.6749890000	1.2355800000
H	5.2486330000	4.5044690000	-0.6198610000
H	6.0193850000	2.4714130000	0.5546660000
N	1.5739990000	1.0229300000	0.6539350000
O	0.9362100000	2.8621510000	-0.4014660000

C	-1.4355860000	0.7338640000	-1.1848830000
H	-0.8265310000	0.8410170000	-2.0839930000
C	-2.1955130000	-0.5523590000	-1.0637460000
N	-1.4295470000	-1.6993990000	-1.0391640000
C	-2.0885660000	-2.9562100000	-0.6861760000
C	-0.4823110000	-1.9794640000	-2.1209150000
H	-2.9723000000	-3.1099890000	-1.3347010000
H	-2.4450720000	-2.9126030000	0.3557480000
C	-1.0195710000	-4.0416840000	-0.9307650000
C	0.1120850000	-3.3285720000	-1.7134320000
H	0.2782050000	-1.1932220000	-2.1972950000
H	-1.0321000000	-2.0491940000	-3.0804420000
H	-1.4493740000	-4.8790810000	-1.4994380000
H	-0.6319940000	-4.4463960000	0.0139030000
H	0.4536620000	-3.9036480000	-2.5858410000
H	0.9793070000	-3.1671050000	-1.0580470000
C	-3.2751390000	2.0991710000	0.1106760000
C	-3.4078150000	2.1150630000	1.5058900000
C	-4.4300610000	2.1941150000	-0.6821260000
C	-4.6686180000	2.2226110000	2.1002220000
H	-2.5174060000	2.0462520000	2.1348110000
C	-5.6883070000	2.3018090000	-0.0891600000
H	-4.3366780000	2.1532630000	-1.7683270000
C	-5.8119600000	2.3163840000	1.3039700000
H	-4.7552710000	2.2340340000	3.1894140000
H	-6.5790120000	2.3666720000	-0.7186480000
H	-6.7984050000	2.3979610000	1.7667650000

H	-2.9005670000	-0.5298680000	-0.2252790000
Cl	-3.4534200000	-0.5369830000	-2.5807410000

IN5a

0 1

Pd	1.8981130000	0.6238800000	-0.0038180000
O	1.3755690000	1.8839600000	1.4560040000
C	0.4528010000	1.4581840000	2.2722510000
O	-0.0989810000	0.3641510000	2.2035520000
O	2.8338720000	-0.7246350000	-1.2856820000
C	3.8545810000	-0.7473970000	-0.5112740000
C	4.9593530000	-1.7273200000	-0.7253830000
H	5.1092680000	-1.9084890000	-1.7984580000
H	4.6466810000	-2.6722870000	-0.2508890000
H	5.8841800000	-1.3759710000	-0.2501430000
O	3.8486390000	0.0518990000	0.4748450000
C	0.0649590000	2.4853850000	3.3211810000
H	-0.4285160000	1.9873350000	4.1655360000
H	-0.6436560000	3.1974070000	2.8665550000
H	0.9409810000	3.0540190000	3.6617550000
C	-1.1206050000	-2.6457550000	-0.6152630000
C	-0.2996370000	-1.5848020000	-1.3080160000
H	0.1946610000	-1.8719130000	-2.2439150000
H	-1.1227720000	-3.5990380000	-1.1528090000
C	-0.6750650000	-0.1651760000	-1.2520810000
C	-1.9472410000	1.5842240000	-1.4975840000
C	-0.7381510000	1.9827580000	-0.9119800000

C	-2.9884020000	2.4603550000	-1.7750870000
C	-0.5137410000	3.3180610000	-0.5657180000
C	-2.7598100000	3.7952210000	-1.4296540000
H	-3.9208330000	2.1212470000	-2.2268800000
C	-1.5492700000	4.2128760000	-0.8380430000
H	0.4177170000	3.6178510000	-0.0871830000
H	-3.5415050000	4.5336710000	-1.6196380000
H	-1.4224790000	5.2669820000	-0.5826730000
N	0.0406240000	0.8292140000	-0.7900190000
O	-1.8800210000	0.2296110000	-1.7116160000
C	0.2255910000	-2.2328030000	-0.0401560000
H	0.2293480000	-1.6196450000	0.8664490000
C	1.3874200000	-3.1416970000	-0.2017600000
C	-2.4106310000	-2.3434970000	0.0741650000
C	-2.5249580000	-1.3590940000	1.0690570000
C	-3.5585880000	-3.0475980000	-0.3198900000
C	-3.7690530000	-1.0840530000	1.6408260000
H	-1.6549480000	-0.8007210000	1.4212540000
C	-4.7996550000	-2.7730020000	0.2578790000
H	-3.4788270000	-3.8189980000	-1.0906930000
C	-4.9097350000	-1.7851390000	1.2396970000
H	-3.8385530000	-0.3165460000	2.4153620000
H	-5.6821470000	-3.3336470000	-0.0598880000
H	-5.8790820000	-1.5678610000	1.6947820000
H	1.3764800000	-3.7368430000	-1.1559600000
O	2.2878520000	-3.2572280000	0.5921720000

IN5b

0 1

Pd	1.6075230000	1.2420910000	-0.0385260000
O	2.4259160000	0.4820030000	1.6201160000
C	1.6539130000	-0.2059050000	2.4156390000
O	0.4653000000	-0.4468770000	2.2244890000
O	0.8264380000	2.4000150000	-1.5692500000
C	1.0774780000	3.4627270000	-0.9024030000
C	0.5786080000	4.7917320000	-1.3620280000
H	0.6349500000	4.8614720000	-2.4571210000
H	-0.4810330000	4.8572750000	-1.0661130000
H	1.1428330000	5.6029930000	-0.8846110000
O	1.7151480000	3.3218720000	0.1885710000
C	2.3908160000	-0.7224830000	3.6404050000
H	1.6872960000	-1.2216580000	4.3183100000
H	3.1714090000	-1.4323250000	3.3247320000
H	2.8951170000	0.1076940000	4.1566400000
C	-2.2090880000	-0.5365660000	0.4764300000
C	-1.3245110000	-0.4667150000	-0.7377190000
H	-1.8516910000	-0.5054460000	-1.6984490000
H	-1.7267930000	-0.9558460000	1.3665630000
C	-0.0208350000	-1.1399280000	-0.7730680000
C	1.3060840000	-2.8633190000	-0.9513230000
C	2.0718610000	-1.7244950000	-0.6744310000
C	1.8516420000	-4.1302740000	-1.1097240000
C	3.4569990000	-1.8089410000	-0.5207850000
C	3.2401710000	-4.2106610000	-0.9639990000

H	1.2337320000	-5.0021590000	-1.3259480000
C	4.0240180000	-3.0751260000	-0.6733070000
H	4.0466850000	-0.9253240000	-0.2777850000
H	3.7292940000	-5.1808900000	-1.0727270000
H	5.1036980000	-3.1928680000	-0.5607060000
N	1.1795200000	-0.6541510000	-0.5937220000
O	-0.0102550000	-2.4713590000	-1.0129130000
C	-1.5564460000	0.7811700000	0.0938530000
H	-0.7520330000	1.0899500000	0.7637190000
C	-2.3152500000	1.8855770000	-0.5429120000
C	-3.6767240000	-0.7910250000	0.3320720000
C	-4.1587500000	-1.7703310000	-0.5467610000
C	-4.5930400000	-0.0679480000	1.1109030000
C	-5.5300730000	-2.0190640000	-0.6518740000
H	-3.4508770000	-2.3468950000	-1.1475630000
C	-5.9628840000	-0.3144570000	1.0063560000
H	-4.2247420000	0.6983090000	1.7979990000
C	-6.4355110000	-1.2905840000	0.1231910000
H	-5.8916110000	-2.7852730000	-1.3419330000
H	-6.6656280000	0.2601910000	1.6144200000
H	-7.5079090000	-1.4817100000	0.0395330000
H	-3.1257190000	1.5649340000	-1.2477420000
O	-2.0951140000	3.0556170000	-0.3390240000

OX

0 1

C	2.4738490000	0.3917330000	0.7249410000

H	2.7864480000	1.4334970000	0.8517000000
C	1.0142120000	0.3557530000	0.4738360000
C	-0.9084930000	-0.6050340000	0.2167960000
C	-1.0232090000	0.7859870000	0.0364960000
C	-1.9784430000	-1.4857550000	0.1140540000
C	-2.2676460000	1.3524090000	-0.2637340000
C	-3.2143720000	-0.9053480000	-0.1875050000
H	-1.8581730000	-2.5600420000	0.2586780000
C	-3.3556040000	0.4853650000	-0.3725380000
H	-2.3698200000	2.4292120000	-0.4062740000
H	-4.0934500000	-1.5466420000	-0.2826030000
H	-4.3427480000	0.8896080000	-0.6072370000
N	0.2364610000	1.3545900000	0.2091390000
O	0.4016910000	-0.8705660000	0.5007850000
Cl	3.4016430000	-0.3067020000	-0.6675930000
H	2.7392910000	-0.1999620000	1.6104820000

PdAc

0 1

Pd	0.0000030000	-0.0000320000	0.0000410000
O	1.7626700000	-1.0821260000	0.0178780000
C	2.4343360000	0.0000160000	0.0181690000
O	1.7625950000	1.0821230000	0.0178950000
O	-1.7626040000	1.0821200000	-0.0178790000
C	-2.4343390000	0.0000100000	-0.0182030000
O	-1.7626680000	-1.0821310000	-0.0178610000
C	3.9276600000	0.0000740000	-0.0132570000

H	4.3163200000	0.9053720000	0.4717040000
H	4.3163900000	-0.9051500000	0.4717860000
H	4.2584590000	0.0000370000	-1.0646270000
C	-3.9276670000	0.0000710000	0.0130610000
H	-4.2585920000	0.0004580000	1.0643890000
H	-4.3162670000	0.9051830000	-0.4723020000
H	-4.3163430000	-0.9053320000	-0.4716940000

PR1a

0 1

C	2.1622540000	0.3618060000	-0.8080670000
C	1.1397530000	1.4731590000	-0.8494800000
H	2.9427360000	0.4588350000	-1.5735040000
H	1.2568830000	2.2218220000	-1.6360250000
C	-0.2706910000	1.2068060000	-0.5391820000
C	-1.9180010000	0.3972900000	0.6187340000
C	-2.3869940000	0.9558750000	-0.5845340000
C	-2.7387860000	-0.2032650000	1.5634890000
C	-3.7543440000	0.9249700000	-0.8796780000
C	-4.1032200000	-0.2283340000	1.2536190000
H	-2.3414830000	-0.6294390000	2.4854440000
C	-4.5994550000	0.3250780000	0.0566210000
H	-4.1338320000	1.3542920000	-1.8081600000
H	-4.8001630000	-0.6888360000	1.9573490000
H	-5.6729130000	0.2815670000	-0.1407440000
N	-1.2949670000	1.4599920000	-1.2898560000
O	-0.5607500000	0.5710710000	0.6421330000

C	1.7729530000	-1.0474120000	-0.4843770000
C	0.8462550000	-1.7181860000	-1.2959990000
C	2.3278120000	-1.7176620000	0.6129550000
C	0.4786340000	-3.0346100000	-1.0122370000
H	0.3986530000	-1.1959640000	-2.1452000000
C	1.9643990000	-3.0368270000	0.8950510000
H	3.0453010000	-1.1990990000	1.2535860000
C	1.0376450000	-3.6975730000	0.0843810000
H	-0.2514870000	-3.5429610000	-1.6464420000
H	2.4031700000	-3.5485630000	1.7549880000
H	0.7483130000	-4.7269840000	0.3086600000
C	2.1832660000	1.4298190000	0.2632050000
H	1.8237130000	1.1534410000	1.2568000000
C	3.2651660000	2.4461790000	0.2429480000
H	3.6088290000	2.7305160000	-0.7905790000
O	3.7603960000	2.9400240000	1.2238830000

PR1b

0 1

C	-1.2457510000	0.1817060000	0.5446430000
C	-0.3030500000	0.3237130000	-0.6133750000
H	-0.7590070000	-0.0262910000	1.5039270000
H	-0.6732760000	0.0436960000	-1.6019580000
C	1.1337450000	0.0766110000	-0.4663250000
C	3.0275540000	0.0482940000	0.5982500000
C	3.1854380000	-0.4479180000	-0.7087170000
C	4.0641010000	0.1519670000	1.5155120000

C	4.4453530000	-0.8714030000	-1.1446790000
C	5.3186270000	-0.2755510000	1.0650860000
H	3.9087820000	0.5422930000	2.5221090000
C	5.5039380000	-0.7766110000	-0.2381820000
H	4.5837830000	-1.2580600000	-2.1554500000
H	6.1742880000	-0.2183290000	1.7414940000
H	6.5020630000	-1.0976940000	-0.5443290000
N	1.9466590000	-0.4087420000	-1.3480680000
O	1.7064980000	0.3826650000	0.7466810000
C	-2.5964930000	-0.4458070000	0.3736890000
C	-3.7077220000	0.0952240000	1.0382970000
C	-2.7695570000	-1.5904150000	-0.4154950000
C	-4.9664890000	-0.4942620000	0.9126840000
H	-3.5825110000	0.9920770000	1.6507260000
C	-4.0296000000	-2.1822380000	-0.5418940000
H	-1.9097900000	-2.0229440000	-0.9328900000
C	-5.1308360000	-1.6353700000	0.1208490000
H	-5.8241370000	-0.0590000000	1.4310850000
H	-4.1501950000	-3.0737340000	-1.1619560000
H	-6.1165630000	-2.0953770000	0.0195610000
C	-0.9331080000	1.5710520000	0.0182880000
H	-0.2882450000	2.2059780000	0.6299260000
C	-1.9426070000	2.3064570000	-0.7877520000
H	-2.5491940000	1.6657060000	-1.4790660000
O	-2.1144810000	3.4986090000	-0.7231780000

PY

0 1

N	-0.0000300000	-1.1650520000	-0.3500870000
C	-1.1578030000	-0.4491920000	0.1705580000
C	1.1578470000	-0.4492040000	0.1703720000
H	-2.0802370000	-0.7429180000	-0.3556980000
H	-1.3242780000	-0.6264210000	1.2578410000
C	-0.7771920000	1.0270960000	-0.0569540000
C	0.7771550000	1.0271620000	-0.0566860000
H	1.3246820000	-0.6266860000	1.2575470000
H	2.0801230000	-0.7427840000	-0.3562470000
H	-1.1605890000	1.3757290000	-1.0270600000
H	-1.2032980000	1.6798940000	0.7191410000
H	1.1609310000	1.3762730000	-1.0264660000
H	1.2028470000	1.6796820000	0.7198700000
H	-0.0000180000	-2.1525750000	-0.1020600000

TS1a

0 1

Pd	-0.2692710000	2.2023550000	0.2872250000
O	1.4985230000	2.8838530000	-0.3455750000
C	1.9974300000	2.4403880000	-1.4599180000
O	1.5288470000	1.5355300000	-2.1460540000
O	-2.3387390000	2.0679820000	0.6893750000
C	-2.5357450000	3.1200520000	-0.0090100000
C	-3.9203730000	3.6396610000	-0.2408710000
H	-4.3385350000	3.1391530000	-1.1298950000
H	-3.8943040000	4.7200100000	-0.4345010000

H	-4.5627300000	3.4085560000	0.6193760000
O	-1.5213430000	3.6762580000	-0.5254310000
C	3.3044310000	3.1174640000	-1.8382420000
H	3.4463760000	3.0696620000	-2.9259020000
H	4.1287100000	2.5656580000	-1.3557480000
H	3.3372680000	4.1567340000	-1.4856710000
C	-1.5392980000	-1.1486590000	-0.8875750000
C	-1.5029650000	-0.7456250000	1.5099420000
H	-2.1963210000	0.0872560000	1.4570950000
H	-1.4223020000	-0.0700310000	-1.0236330000
C	-0.1385390000	-0.5175560000	1.5661880000
C	1.9810350000	-1.0521230000	1.8199210000
C	1.9107150000	0.2923300000	1.4154550000
C	3.1635530000	-1.7169410000	2.0952290000
C	3.0883500000	1.0447020000	1.3350440000
C	4.3430000000	-0.9657220000	1.9738150000
H	3.1660170000	-2.7627970000	2.4053590000
C	4.2952510000	0.3904100000	1.6123480000
H	3.0522740000	2.0962790000	1.0636980000
H	5.3047840000	-1.4375310000	2.1851890000
H	5.2270400000	0.9576530000	1.5527880000
N	0.5644590000	0.5867080000	1.2051550000
O	0.7065260000	-1.5461810000	1.8884320000
C	-0.4008170000	-1.9292820000	-1.1010240000
H	-0.4461670000	-3.0112320000	-0.9688240000
C	0.8167510000	-1.2999220000	-1.3489260000
N	2.0040130000	-1.8959860000	-1.3748730000

C	3.2589850000	-1.2012470000	-1.7091780000
C	2.2201330000	-3.3181400000	-1.1005660000
H	3.0784850000	-0.4558540000	-2.4946070000
H	3.6355970000	-0.6714390000	-0.8196190000
C	4.1926010000	-2.3486180000	-2.0919210000
C	3.7452130000	-3.4762620000	-1.1491150000
H	1.7810190000	-3.5877400000	-0.1264610000
H	1.7170480000	-3.9266910000	-1.8737140000
H	4.0307740000	-2.6395000000	-3.1431980000
H	5.2526460000	-2.0828000000	-1.9731240000
H	4.0511130000	-4.4771040000	-1.4850920000
H	4.1672590000	-3.3093530000	-0.1463230000
C	-2.9151880000	-1.6283280000	-0.8698430000
C	-3.2441690000	-2.9967890000	-0.9099940000
C	-3.9642300000	-0.6891610000	-0.7872970000
C	-4.5755910000	-3.4092330000	-0.8815550000
H	-2.4526910000	-3.7447000000	-0.9681600000
C	-5.2925700000	-1.1018850000	-0.7583180000
H	-3.7135530000	0.3709670000	-0.7148250000
C	-5.6044170000	-2.4660950000	-0.8069780000
H	-4.8131480000	-4.4751480000	-0.9147560000
H	-6.0920720000	-0.3601220000	-0.6919720000
H	-6.6469170000	-2.7921560000	-0.7828930000
H	0.8410370000	-0.2219740000	-1.5493340000
Cl	-2.1366670000	-2.2252470000	2.1734580000

TS1b

0 1

Pd	0.0622480000	-2.0648940000	0.2511540000
O	-1.8177630000	-2.6950530000	-0.0055660000
C	-2.3677880000	-2.2905670000	-1.1126260000
O	-1.8754740000	-1.4789860000	-1.8938310000
O	2.1995540000	-1.9902960000	-0.1629300000
C	2.0441480000	-3.0104840000	-0.9014380000
C	3.1890820000	-3.5962870000	-1.6693990000
H	3.4829460000	-2.8904990000	-2.4625860000
H	2.9016080000	-4.5541840000	-2.1206610000
H	4.0538680000	-3.7275050000	-1.0028170000
O	0.8752550000	-3.5056030000	-0.9819910000
C	-3.7512220000	-2.8720260000	-1.3441630000
H	-3.9629840000	-2.9086960000	-2.4209220000
H	-4.4874560000	-2.2026650000	-0.8683380000
H	-3.8511650000	-3.8681050000	-0.8934500000
C	1.7373280000	1.1880980000	-0.6674670000
C	1.5784860000	0.8285820000	1.7319830000
H	1.6477720000	0.1061050000	-0.7738940000
C	0.2078630000	0.6159200000	1.6932840000
C	-1.8670930000	1.3444550000	1.7904050000
C	-1.8873220000	-0.0448430000	1.5820720000
C	-3.0001540000	2.1263080000	1.9426990000
C	-3.1169340000	-0.7134050000	1.5990310000
C	-4.2293980000	1.4518760000	1.9091810000
H	-2.9284810000	3.2029640000	2.1026150000
C	-4.2761210000	0.0573110000	1.7531130000

H	-3.1590490000	-1.7929040000	1.4906980000
H	-5.1562180000	2.0157740000	2.0338250000
H	-5.2451620000	-0.4470090000	1.7648580000
N	-0.5569040000	-0.4685390000	1.4386150000
O	-0.5630900000	1.7499730000	1.8333460000
C	0.6169590000	1.9599440000	-0.9898560000
H	0.6750360000	3.0478860000	-0.9334390000
C	-0.6078910000	1.3555830000	-1.2722080000
N	-1.7603710000	2.0037990000	-1.4107910000
C	-3.0456710000	1.3575290000	-1.7318300000
C	-1.9043440000	3.4538690000	-1.2579740000
H	-2.8901300000	0.5262200000	-2.4294520000
H	-3.4841710000	0.9405220000	-0.8102670000
C	-3.8888950000	2.5178570000	-2.2558820000
C	-3.4124610000	3.6977370000	-1.3959270000
H	-1.4960750000	3.7759120000	-0.2863560000
H	-1.3283280000	3.9684230000	-2.0479850000
H	-3.6663070000	2.7024270000	-3.3200610000
H	-4.9672750000	2.3252530000	-2.1641310000
H	-3.6373040000	4.6807820000	-1.8332660000
H	-3.8887330000	3.6493580000	-0.4048150000
C	3.1099420000	1.6796860000	-0.5791680000
C	3.4334840000	3.0522400000	-0.5674330000
C	4.1594310000	0.7398160000	-0.5015050000
C	4.7592900000	3.4688330000	-0.4811020000
H	2.6407230000	3.8005420000	-0.6234170000
C	5.4856350000	1.1618320000	-0.4200820000

H	3.9079870000	-0.3217310000	-0.4919310000
C	5.7918930000	2.5254780000	-0.4079410000
H	4.9932180000	4.5362070000	-0.4726580000
H	6.2867130000	0.4211980000	-0.3596650000
H	6.8313190000	2.8555930000	-0.3411850000
H	-0.6817060000	0.2673480000	-1.3888900000
Cl	2.6927140000	-0.3931840000	2.2557210000
H	1.8934080000	1.8408930000	1.9762290000

TS2a

0 1

Pd	-1.6503030000	0.9248730000	0.6252520000
O	-1.7170000000	2.1817780000	-0.9218780000
C	-0.9862070000	1.9557940000	-1.9755130000
O	-0.3017370000	0.9520770000	-2.1671450000
O	-2.0870480000	-0.4274340000	2.1735040000
C	-3.3220540000	-0.3969840000	1.8627060000
C	-4.3390680000	-1.1135200000	2.6981690000
H	-4.5698690000	-0.4908200000	3.5776000000
H	-3.9285240000	-2.0646850000	3.0647790000
H	-5.2643630000	-1.2736490000	2.1295990000
O	-3.6600880000	0.2794160000	0.8408630000
C	-1.0082970000	3.0990660000	-2.9725360000
H	-0.7767170000	2.7224440000	-3.9774610000
H	-0.2224610000	3.8136920000	-2.6780860000
H	-1.9712040000	3.6269350000	-2.9610340000
C	1.5072360000	-2.3535490000	0.4456830000

C	0.8547790000	-1.1590630000	0.9871210000
H	0.0983080000	-1.2709610000	1.7561250000
H	1.3029680000	-3.2320510000	1.0715620000
C	1.1956340000	0.2277480000	0.7026990000
C	2.3278520000	1.9357580000	-0.0110530000
C	1.0401100000	2.3677440000	0.3335540000
C	3.3227720000	2.7841090000	-0.4708450000
C	0.6920290000	3.7151020000	0.2270810000
C	2.9698960000	4.1345340000	-0.5772090000
H	4.3155490000	2.4132700000	-0.7267080000
C	1.6815930000	4.5878370000	-0.2339760000
H	-0.3112440000	4.0553870000	0.4801510000
H	3.7132090000	4.8530290000	-0.9289390000
H	1.4514180000	5.6514280000	-0.3273740000
N	0.3346580000	1.2328850000	0.7277310000
O	2.3834840000	0.5797610000	0.1817830000
C	0.3561060000	-2.0088820000	-0.4821880000
H	0.5691560000	-1.4104680000	-1.3682600000
C	-0.9212340000	-2.5550660000	-0.2869700000
N	-1.9874030000	-2.3843630000	-1.0402740000
C	-3.3204710000	-2.9053360000	-0.6732740000
C	-2.0388140000	-1.5843800000	-2.2757450000
H	-3.2872750000	-4.0000240000	-0.5617810000
H	-3.6229330000	-2.4694610000	0.2895460000
C	-4.2323750000	-2.4360550000	-1.8138060000
C	-3.5130130000	-1.1956650000	-2.3633230000
H	-1.3571270000	-0.7253130000	-2.2098020000

H	-1.7321970000	-2.2220220000	-3.1248240000
H	-4.2991830000	-3.2154610000	-2.5899020000
H	-5.2509170000	-2.2258340000	-1.4595390000
H	-3.8161510000	-0.9377540000	-3.3873700000
H	-3.7010610000	-0.3266120000	-1.7144510000
C	2.9083160000	-2.3573910000	-0.1012100000
C	3.1686470000	-2.7965200000	-1.4042620000
C	3.9718550000	-1.9729890000	0.7289970000
C	4.4812420000	-2.8516910000	-1.8817310000
H	2.3414500000	-3.0954640000	-2.0529250000
C	5.2802660000	-2.0294850000	0.2476920000
H	3.7509150000	-1.5951130000	1.7318170000
C	5.5398200000	-2.4684080000	-1.0552760000
H	4.6750650000	-3.1924220000	-2.9017600000
H	6.1047160000	-1.7203760000	0.8949730000
H	6.5667210000	-2.5079130000	-1.4272590000
H	-1.0880560000	-3.1551200000	0.6155590000
Cl	2.0677850000	-0.2793820000	3.1427220000

TS2b

0 1

Pd	-1.1937640000	1.0112220000	0.9998460000
O	-2.8345610000	1.3730980000	-0.0754470000
C	-2.8790240000	1.0113140000	-1.3254660000
O	-1.9453550000	0.5236340000	-1.9601840000
O	0.5278450000	1.1357860000	2.1928910000
C	0.3937710000	2.4004500000	2.2700800000

C	1.3097000000	3.2167770000	3.1298870000
H	0.9516910000	3.1635640000	4.1708200000
H	2.3259650000	2.7996430000	3.1058650000
H	1.3040690000	4.2674790000	2.8118390000
O	-0.5562800000	2.9354480000	1.6164790000
C	-4.2471030000	1.2027690000	-1.9530580000
H	-4.1456970000	1.3178760000	-3.0401780000
H	-4.8375950000	0.2939840000	-1.7521550000
H	-4.7771370000	2.0583350000	-1.5137200000
C	1.9146190000	-1.6318150000	-0.9961510000
C	0.9855620000	-1.2800150000	0.0761470000
H	1.3129350000	-0.7103780000	0.9391380000
H	1.5392100000	-2.4350530000	-1.6419370000
C	-0.4190800000	-1.6444410000	0.0556460000
C	-2.2121270000	-2.7082580000	-0.5494310000
C	-2.5830300000	-1.6318390000	0.2679870000
C	-3.1177930000	-3.6149920000	-1.0770950000
C	-3.9222360000	-1.4197370000	0.5976610000
C	-4.4605720000	-3.3983860000	-0.7452710000
H	-2.7964240000	-4.4456010000	-1.7059690000
C	-4.8516970000	-2.3235840000	0.0755730000
H	-4.2174060000	-0.5764860000	1.2206080000
H	-5.2202150000	-4.0834010000	-1.1274770000
H	-5.9099580000	-2.1956170000	0.3133600000
N	-1.4102150000	-0.9472870000	0.5814290000
O	-0.8490110000	-2.6662850000	-0.7092370000
C	1.3548820000	-0.2818470000	-1.4281170000

H	0.4984520000	-0.2569520000	-2.1014830000
C	1.9507830000	0.9039600000	-0.9919890000
N	1.5810390000	2.1389450000	-1.2777380000
C	2.2300950000	3.3237990000	-0.6851700000
C	0.4439990000	2.5106570000	-2.1342120000
H	3.3091540000	3.3224870000	-0.9035440000
H	2.1038600000	3.2978410000	0.4077740000
C	1.4834040000	4.5082570000	-1.3108740000
C	0.1065800000	3.9218750000	-1.6564610000
H	-0.3771710000	1.7899990000	-2.0208710000
H	0.7728020000	2.5039230000	-3.1897640000
H	1.9998230000	4.8386620000	-2.2266820000
H	1.4317120000	5.3666170000	-0.6266870000
H	-0.4326700000	4.5030000000	-2.4172660000
H	-0.5191370000	3.8631110000	-0.7528090000
C	3.3892280000	-1.7412670000	-0.7066880000
C	3.8499070000	-2.2365790000	0.5198720000
C	4.3152970000	-1.3684580000	-1.6933430000
C	5.2253050000	-2.3460070000	0.7533900000
H	3.1219290000	-2.5512500000	1.2736550000
C	5.6854820000	-1.4819520000	-1.4571440000
H	3.9563780000	-0.9798040000	-2.6504580000
C	6.1443120000	-1.9699890000	-0.2282590000
H	5.5767940000	-2.7334820000	1.7127650000
H	6.3981820000	-1.1897040000	-2.2324290000
H	7.2172800000	-2.0577960000	-0.0403940000
H	2.8074880000	0.8243050000	-0.3138850000

Cl	0.7670820000	-3.1053360000	1.8718820000

8.2. Alternative Catalytic Cycles

AIN01

2 1

Pd	-2.1421340860	-1.6968340158	-0.7476845778
O	-3.4443297641	-1.8941283563	0.8378009304
C	-2.7426517925	-2.8522206435	1.3263428990
O	-1.6428181329	-3.0607997342	0.7066593840
O	-0.9011656791	-1.6236649906	-2.3795441825
C	-1.7015972490	-0.8383068854	-2.9991560462
C	-1.5144843392	-0.4633087263	-4.4196848864
H	-0.4469581737	-0.4555887304	-4.6790998205
H	-1.9885754328	0.5042361992	-4.6323597612
H	-2.0082923615	-1.2299306293	-5.0420091129
O	-2.6937466843	-0.4356784634	-2.2938078898
C	-3.1867152240	-3.6702286772	2.4777046716
H	-3.8437527468	-3.0874858139	3.1373648256
H	-2.3216710131	-4.0715899150	3.0227776272
H	-3.7675986908	-4.5230766199	2.0850963853
C	0.6260694826	-0.1731398174	0.0866174678
C	1.1839758110	-1.5891739174	0.2673560558
H	0.8465717650	-2.2105107758	-0.5794759142
H	0.8116148442	-2.0872969124	1.1735740545
H	0.8137050326	0.1572120270	-0.9426639918
C	2.6694657330	-1.5558173874	0.2852062357
C	4.6607760489	-2.2817007764	0.7165321844

C	4.7233709976	-1.0549327704	0.0119923592
C	5.7722425624	-2.9978345737	1.1173892362
C	5.9725002902	-0.4909171666	-0.3159197933
C	7.0088779005	-2.4180957901	0.7834841374
H	5.7006957929	-3.9471208622	1.6489014793
C	7.1043102613	-1.1917464715	0.0820468300
H	6.0359858193	0.4514862977	-0.8610824175
H	7.9270390912	-2.9339694977	1.0722615997
H	8.0945699583	-0.7963686714	-0.1510316327
N	3.4329049061	-0.6342804613	-0.2407148351
O	3.3273422047	-2.5786960064	0.8825096132
C	-0.7938617502	0.0665888308	0.4751512375
H	-1.1185752082	-0.3056467635	1.4488667121
C	-1.5211621256	1.1524237811	-0.1170731077
N	-2.6264119122	1.6698685737	0.3367813374
C	-3.3804054440	2.7260401485	-0.3877316990
C	-3.3243113494	1.2874518988	1.5891320995
H	-2.6805606496	3.4629637282	-0.8063917044
H	-3.9094375152	2.2294485957	-1.2197560719
C	-4.3476063558	3.2640301571	0.6634468712
C	-4.6669676340	2.0186977207	1.5007881222
H	-3.4163929543	0.1946210537	1.6431262475
H	-2.7066442481	1.6427104843	2.4319217575
H	-3.8542684610	4.0346116528	1.2766688012
H	-5.2362292153	3.7177170438	0.2054581731
H	-5.0675069224	2.2547121579	2.4952773132
H	-5.4036534990	1.3833832320	0.9848728370

C	1.2111335260	0.8586789755	1.0411609604
C	1.4166980878	0.5472633491	2.4084170660
C	1.5654929697	2.1425925106	0.5580960858
C	2.0184305667	1.4748976991	3.2503084080
H	1.1356999219	-0.4327949166	2.7987468716
C	2.1670492737	3.0625702960	1.4047173522
H	1.4223524370	2.3812710726	-0.4979988478
C	2.3930524434	2.7325394130	2.7522670234
H	2.2042308210	1.2243611253	4.2964953219
H	2.4802760348	4.0359035927	1.0219687098
H	2.8655510651	3.4599013458	3.4163467259
H	-1.1376518748	1.5807297063	-1.0476699379

AIN02

2 1

Pd	-0.5357335930	-1.0377649974	-0.3782175309
O	-0.4374381349	-1.7847109261	1.4387566148
C	0.5034177221	-1.4785038413	2.3299935319
O	1.2229538108	-0.4972986258	2.2392187937
O	-1.1862485116	-0.5194954322	-2.2864801168
C	-2.4094585220	-0.5902172694	-1.9159018653
C	-3.5367371916	-0.5256049364	-2.8770068253
H	-3.2764157823	0.1094856852	-3.7349846363
H	-4.4544731607	-0.1812832272	-2.3822443346
H	-3.7174718125	-1.5457361594	-3.2584384848
O	-2.5852135189	-0.7535937676	-0.6537163038
C	0.5734338120	-2.4816439253	3.4522600539

H	1.1803840278	-3.3348698933	3.1069219720
H	-0.4208989696	-2.8671148590	3.7136667536
H	1.0637981154	-2.0243880808	4.3207211088
C	1.0131706898	1.5462861187	-0.7879264507
C	2.3799941514	0.8995422330	-0.5403078084
H	2.7234231034	1.1082103824	0.4868335156
H	3.1288322896	1.3399485123	-1.2150355685
C	2.4111768557	-0.5745214638	-0.6917504793
C	3.3296620667	-2.5512333741	-0.8216127390
C	1.9485204048	-2.7240582217	-0.6729658029
C	4.2273001623	-3.6022896924	-0.9348715580
C	1.3834454745	-4.0000128831	-0.6163151029
C	3.6595511505	-4.8785720439	-0.8803360420
H	5.2988593736	-3.4403801979	-1.0558729905
C	2.2711557356	-5.0721503592	-0.7224257130
H	0.3116454190	-4.1583292681	-0.4886352251
H	4.3104720976	-5.7510967177	-0.9615418322
H	1.8810932179	-6.0908348632	-0.6831112678
N	1.4127126062	-1.4251896316	-0.6110535911
O	3.5798811144	-1.1884157743	-0.8319526085
C	-0.0832766505	1.0397564628	0.1176833690
H	0.2622816994	0.8001549868	1.1328515207
C	-1.3830719451	1.7112915802	0.0104382041
N	-2.2410932654	1.7636845240	0.9707060300
C	-3.5708969947	2.4208748829	0.8544178375
C	-2.0715947717	1.1624706137	2.3220223623
H	-3.4837663995	3.3280722448	0.2414099720

H	-4.2358418885	1.7019630999	0.3465362553
C	-3.9845508363	2.6368950334	2.3071767743
C	-3.4236839633	1.3906846999	3.0052992843
H	-1.7959403352	0.1047313048	2.2102586574
H	-1.2442089539	1.6938554020	2.8195635511
H	-3.5217776826	3.5550690898	2.7021634462
H	-5.0729021430	2.7380652890	2.4098364248
H	-3.3126527830	1.5153863116	4.0902442813
H	-4.0801445586	0.5240309677	2.8334912304
H	-1.6584151317	2.1934440655	-0.9321940570
C	0.9810726593	3.0263876883	-0.4134076232
C	0.5156557899	3.9806368750	-1.3416911551
C	1.3571047819	3.4449994576	0.8844887202
C	0.4705367660	5.3280534123	-0.9944294330
H	0.2321118249	3.6667683199	-2.3496680954
C	1.3015274728	4.7947132271	1.2272831845
H	1.7187685915	2.7210045552	1.6186384946
C	0.8605225299	5.7371960248	0.2907069514
H	0.1470769417	6.0690859455	-1.7284085144
H	1.6135206690	5.1166909856	2.2228108678
H	0.8274040449	6.7959627616	0.5569006854
H	0.7251333280	1.4419146887	-1.8443106930

AIN03

2 1

Pd	0.2968426463	-0.8305902592	0.7887649171
O	-0.7715867395	-2.2173012103	-0.3388398788

C	-1.3361334266	-2.5456015964	-1.3983100249
O	-1.8457034652	-1.6862478440	-2.2391312397
O	1.5168835171	0.1255675607	2.0480528078
C	2.4325748671	-0.7876983896	2.3341835882
C	3.3698636767	-0.4445604428	3.4488882703
H	3.7099002419	0.5984371255	3.3753792492
H	4.2178231829	-1.1409651492	3.4535625454
H	2.8280917857	-0.5413634298	4.4042186187
O	2.4495447950	-1.8390252311	1.6900828340
C	-1.4910674056	-3.9777788670	-1.7790942262
H	-0.7454096688	-4.5986464004	-1.2693665805
H	-1.4405975261	-4.0924266963	-2.8707106636
H	-2.4967589225	-4.3055042414	-1.4622312433
C	0.0881677651	1.4914674801	-0.5905339722
C	-0.8113043689	1.0258776908	0.5676417661
H	-0.5639370247	1.4270191963	1.5553947709
H	-1.9304872974	-0.7796101583	-1.8604681221
H	0.6831080191	2.3220902827	-0.1795236881
C	-2.1935173758	0.7010848241	0.4770941974
C	-4.0891290378	0.0975893845	-0.4325520054
C	-4.2385065544	0.2951552542	0.9668732775
C	-5.1200078501	-0.2804711360	-1.2751659847
C	-5.4974330288	0.1120339875	1.5774322042
C	-6.3582591340	-0.4587044076	-0.6455502526
H	-4.9873063400	-0.4199326758	-2.3483543398
C	-6.5428591440	-0.2669413303	0.7486338749
H	-5.6263688065	0.2670980761	2.6492698967

H	-7.2184332874	-0.7509674399	-1.2520709162
H	-7.5379910601	-0.4202478425	1.1700759945
N	-3.0295032541	0.6542338633	1.4900311252
O	-2.7747486669	0.3548015906	-0.7320435631
C	1.0154434429	0.2880493012	-0.7828420065
H	0.7742104330	-0.3700528223	-1.6226353128
C	2.4489404388	0.4809147661	-0.5662956795
N	3.3546689437	-0.3968751309	-0.8384174765
C	4.8060744282	-0.2002807685	-0.5465413827
C	3.1131149832	-1.7545797474	-1.3934944259
H	5.1173844807	0.7997429175	-0.8780634428
H	4.9233802132	-0.2691655005	0.5471531345
C	5.4806679394	-1.3694728910	-1.2593198031
C	4.4340718383	-2.4858767298	-1.1519614790
H	2.2534725499	-2.2070480098	-0.8835897008
H	2.8896885048	-1.6374795284	-2.4674301637
H	5.6784413135	-1.1134079438	-2.3120400518
H	6.4398170759	-1.6286887887	-0.7922324204
H	4.5887559882	-3.2978531813	-1.8743165729
H	4.4268117016	-2.9193344875	-0.1404990904
C	-0.6391586273	1.9934675518	-1.8258668735
C	-0.5802945154	1.3570745315	-3.0716210135
C	-1.4273837758	3.1470164284	-1.6845006400
C	-1.3120361749	1.8559876336	-4.1558486108
H	0.0436409949	0.4760113739	-3.2346805980
C	-2.1586948059	3.6414095172	-2.7631527691
H	-1.4702900468	3.6651940911	-0.7221296424

C	-2.1063366073	2.9929126155	-4.0026156886
H	-1.2505590971	1.3568771643	-5.1250967051
H	-2.7652254903	4.5411210391	-2.6406169886
H	-2.6735300677	3.3834787214	-4.8498833674
H	2.7913872465	1.4211334293	-0.1203316754

AIN04

1 1

Pd	0.2226544726	-0.4807565534	0.9527817859
C	0.8270105135	0.3123211365	-0.8904464261
C	-0.7977915359	1.3185798634	0.4622947432
H	0.2566780392	-0.2047359923	-1.6648909623
H	-0.8363548669	1.8420857610	1.4198645351
O	1.3364643803	0.6766969259	2.2348101551
C	0.7757929239	0.1829059950	3.2980452819
O	-0.1383235357	-0.6586885144	3.1218525168
O	-0.9025465904	-1.8844768530	-0.0019754501
C	-0.1521728619	-2.9241132208	0.2032412559
O	0.9800743022	-2.7699504444	0.7003530555
C	1.2485571109	0.6100109219	4.6465465076
H	1.4279024215	1.6944091484	4.6597922554
H	0.5148417820	0.3256138114	5.4111629800
H	2.2055374906	0.1077606938	4.8621707470
C	-0.7211404878	-4.2642293311	-0.1582773066
H	-1.3265041410	-4.1993979266	-1.0728589744
H	0.0831076514	-5.0029153249	-0.2661355719
H	-1.3865079016	-4.5864194471	0.6591029044

C	-2.0963269499	0.9029557795	0.0045212369
C	-3.5493667985	0.1170344080	-1.3957811176
C	-4.1473681322	0.3441179326	-0.1330647077
C	-4.2388161339	-0.3782440683	-2.4949952156
C	-5.5112558056	0.0638514387	0.0618522647
C	-5.5916574590	-0.6518517843	-2.2802032897
H	-3.7571635773	-0.5383117434	-3.4598663616
C	-6.2150096782	-0.4360536648	-1.0274814553
H	-5.9823559177	0.2352274865	1.0304007870
H	-6.1900250348	-1.0430520538	-3.1058043548
H	-7.2763740937	-0.6687713451	-0.9220744131
N	-3.1875209164	0.8360990532	0.7215858984
O	-2.2406062794	0.4774588626	-1.2938657421
C	0.2981036803	1.7027530202	-0.5288102682
H	1.0728496871	2.2246252440	0.0544273524
C	2.2142100089	-0.0163235489	-0.7506842245
N	2.8115197274	-1.0150868096	-1.3376355526
C	4.1536459037	-1.5131740589	-0.9566158875
C	2.1673746558	-1.9241577605	-2.3143161019
C	4.0550082701	-3.0035056855	-1.2766511567
H	4.9110703900	-1.0124678748	-1.5829053279
H	4.3486473207	-1.2814578912	0.0983070885
C	3.2202448835	-3.0104217198	-2.5647394785
H	1.2569219823	-2.3301129699	-1.8551364865
H	1.8804249845	-1.3590159245	-3.2132670145
H	3.5133024566	-3.5155741012	-0.4663082156
H	5.0421403765	-3.4701092974	-1.3934454129

H	2.7567229356	-3.9834613198	-2.7747556526
H	3.8455599805	-2.7445262404	-3.4313105000
H	2.8169649536	0.5609349132	-0.0400485346
C	-0.1139022977	2.5773752667	-1.6989031083
C	-1.0418183878	3.6104246566	-1.5088706911
C	0.4510132111	2.3947178350	-2.9658105596
C	-1.4014109648	4.4418591339	-2.5705360238
H	-1.4916761903	3.7703288596	-0.5255896651
C	0.0956783176	3.2293990881	-4.0289104925
H	1.1802384386	1.5978959778	-3.1338198497
C	-0.8340633114	4.2529990912	-3.8343354715
H	-2.1275839592	5.2416485671	-2.4100057920
H	0.5452963529	3.0773632161	-5.0126420570
H	-1.1161511669	4.9031931322	-4.6650346480

AIN05

1 1

Pd	2.6693279884	0.1602880146	0.5157210215
C	-0.9692389573	-0.7674666539	0.7223422809
C	-0.8852280698	-0.1156436432	-0.6005634003
H	-0.4762066862	-0.2279453517	1.5378082254
H	-0.8981145431	-0.7466266190	-1.4896972305
O	2.1485440586	-1.0304033477	-1.0969426965
C	2.8731800190	-0.3104330015	-1.8698075532
O	3.5282924397	0.6185012126	-1.3010683669
O	3.1449323136	1.3954520105	2.0997672900
C	2.3769479650	0.7360574008	2.8689693445

O	1.7398801028	-0.2329196805	2.3281054980
C	2.8880829577	-0.5075511990	-3.3437277514
H	2.7953064914	-1.5739529396	-3.5903291014
H	2.0114676105	0.0255308801	-3.7475113929
H	3.8005025225	-0.0814967710	-3.7800975034
C	2.2513914718	1.0492084836	4.3211595459
H	1.2383605302	0.8165473753	4.6762211731
H	2.9613933732	0.4156585969	4.8776878947
H	2.5050283603	2.1007233203	4.5084916257
C	-0.1727512334	1.1466155257	-0.8113865067
C	0.7287392167	3.0266970798	-0.2031486497
C	1.0008191416	2.7631216300	-1.5575151468
C	1.2100310554	4.1323002903	0.4824938547
C	1.7964811965	3.6455711947	-2.2961666153
C	2.0033405282	5.0050068777	-0.2686488354
H	0.9972238704	4.3016774741	1.5381455403
C	2.2889469152	4.7666412326	-1.6290555923
H	2.0259850010	3.4518215367	-3.3445810230
H	2.4198276057	5.8914363461	0.2139121937
H	2.9190467687	5.4770402373	-2.1677034840
N	0.3937417141	1.5542038895	-1.9008700336
O	-0.0429974874	1.9862340577	0.2645267850
C	-0.9713921061	-2.2598674758	0.8511188458
C	-1.8113338852	-2.8739366427	1.7937560659
C	-0.1208960823	-3.0497863256	0.0672845427
C	-1.8110227788	-4.2610145160	1.9424255995
H	-2.4647287448	-2.2588109033	2.4197299173

C	-0.1207319799	-4.4406864828	0.2212642901
H	0.5625476655	-2.5744264130	-0.6384722659
C	-0.9648719597	-5.0481421293	1.1525780975
H	-2.4655797992	-4.7307898945	2.6800976071
H	0.5500660239	-5.0500317601	-0.3883466843
H	-0.9612608097	-6.1339632361	1.2701818492
C	-2.2295021707	-0.0353782320	0.2210614127
H	-2.4418890348	0.9390372413	0.6607479611
C	-3.3179073319	-0.8068524890	-0.2999871706
H	-3.1040015202	-1.8214889616	-0.6549121380
C	-5.0606165108	0.9113295648	0.0524715158
C	-5.6550183857	-1.2586303675	-0.9156508924
C	-6.5213244989	0.9145977139	-0.4083345286
H	-4.9692749169	0.9698607899	1.1490148034
H	-4.4496616618	1.7101569083	-0.3901940089
C	-6.9101153511	-0.5699991765	-0.3835961127
H	-5.6133859022	-1.2290408350	-2.0167029183
H	-5.5209744928	-2.2966944463	-0.5835567741
H	-6.5932925522	1.3126740546	-1.4326564739
H	-7.1516857024	1.5403625155	0.2371181484
H	-7.7941673828	-0.7973458063	-0.9938601184
H	-7.1169553644	-0.9008507525	0.6467375593
N	-4.5516140051	-0.4139424021	-0.3854385200

AIN06

1 1

Pd	0.7762368853	0.7588960698	1.0127198528

O	1.8216580841	1.8193025356	-0.3095229290
C	2.0090382931	1.3122644239	-1.4949964979
O	1.7466416108	0.1402013223	-1.7790262237
O	-0.5662688787	0.1128768673	2.4250433999
C	-1.0260330415	1.3075060149	2.5550157030
C	-2.0986631788	1.6368087900	3.5288851072
H	-2.7750637069	0.7805595450	3.6543346854
H	-2.6459619790	2.5310477917	3.2031042001
H	-1.6305873965	1.8505981316	4.5042407854
O	-0.4793374688	2.1850946846	1.8132491499
C	2.5797179381	2.2744701544	-2.5071174277
H	3.3941973238	2.8603435631	-2.0584141842
H	1.7857409762	2.9810471379	-2.7966782228
H	2.9256607544	1.7328362821	-3.3956725770
C	-0.0641991816	-2.3785105444	0.0295690045
H	-0.3787723988	-3.3491945843	-0.3581009622
H	-0.7966401847	-1.6816121354	0.4405324638
C	1.2427182464	-2.0402607270	0.0238962026
C	3.3985600673	-2.2951896047	-0.1657862516
C	3.1403631139	-1.0167518129	0.4290280356
C	4.6837554216	-2.7585525265	-0.4159015085
C	4.1989041676	-0.1448890561	0.7883677297
C	5.7084673170	-1.8872385108	-0.0509410460
H	4.8711231211	-3.7321316376	-0.8688329522
C	5.4736370493	-0.6044018850	0.5395684431
H	3.9927152632	0.8317486829	1.2262972003
H	6.7428938334	-2.1950047842	-0.2215289210

H	6.3344430372	0.0159169567	0.7950105886
N	1.8071468472	-0.8666276377	0.4900350311
O	2.2274030643	-2.8952965073	-0.4123758793

AIN07

1 1

C	-1.4389426261	-1.3693761182	-2.1937881718
H	-2.3035697225	-1.8439081150	-1.7148775193
C	-1.3349312228	-0.0037760032	-2.0814216375
H	-0.5011045894	0.5334264347	-2.5349843953
C	-2.3233128601	0.7180235711	-1.3719330102
N	-2.3457380618	2.0134139887	-1.1908918106
C	-3.4143678068	2.7269130909	-0.4498757178
C	-1.3348222116	2.9612323004	-1.7143094255
H	-4.3922460940	2.2810431734	-0.6778567940
H	-3.2222111051	2.6211605417	0.6310490677
C	-3.2526935031	4.1756202445	-0.9075139898
C	-1.7353872080	4.3056529870	-1.0979457558
H	-0.3252288999	2.6284017242	-1.4333487667
H	-1.4031122833	2.9702751193	-2.8147204315
H	-3.7789761073	4.3322607964	-1.8626320867
H	-3.6611250736	4.8868210873	-0.1773862311
H	-1.4477797166	5.1509438080	-1.7369690603
H	-1.2370899978	4.4378116132	-0.1247448146
C	-0.5441880204	-2.2705427094	-2.8697362233
C	0.6242572198	-1.8347222470	-3.5421269724
C	-0.8495042675	-3.6528427738	-2.8597656290

C	1.4498595492	-2.7512475012	-4.1775166963
H	0.8840043793	-0.7750656273	-3.5654282563
C	-0.0189389311	-4.5677609591	-3.4980257853
H	-1.7484378256	-3.9987719645	-2.3436918646
C	1.1305630702	-4.1181231299	-4.1569580364
H	2.3489092645	-2.4098376576	-4.6940528773
H	-0.2630896747	-5.6315288478	-3.4846423132
H	1.7847278396	-4.8344827167	-4.6589958379
H	-3.1568396835	0.1625272699	-0.9269786471

ATS01a

2 1

Pd	-0.9820609839	-1.2208878333	-0.4569141652
O	-0.6121969137	-2.0249052899	1.3226666679
C	-0.0016845202	-1.3330971388	2.2454819120
O	0.3070132765	-0.1462140277	2.1170296987
O	-1.8569313173	-0.5430238498	-2.2185001914
C	-3.0196460121	-0.8714928835	-1.7790543723
C	-4.2227129087	-0.8459095616	-2.6517375849
H	-4.1915632939	0.0167043716	-3.3322387952
H	-5.1432511109	-0.8560229124	-2.0538582398
H	-4.2104764776	-1.7556350433	-3.2762354383
O	-3.0628066354	-1.2490178749	-0.5618422941
C	0.3286721515	-2.1228895050	3.4881420158
H	1.3412168379	-2.5421478231	3.3663454761
H	-0.3715957980	-2.9542534968	3.6371192574
H	0.3403427326	-1.4546979060	4.3587596162

C	0.4982789990	2.4709415592	-0.6509961962
C	0.8047134343	1.1508141848	-1.9876083677
H	1.4080550632	1.7561860041	-2.6680249952
H	-0.2002136473	0.9153739001	-2.3446750440
C	1.5128214262	0.0368699050	-1.4381516958
C	3.2269467077	-1.1751635540	-0.8766924345
C	2.0430184315	-1.8213206189	-0.4294645546
C	4.4982635471	-1.6967884512	-0.6966604032
C	2.1030334224	-3.0639804129	0.2320940613
C	4.5429261696	-2.9259812922	-0.0342231472
H	5.3943959227	-1.1858343116	-1.0494690719
C	3.3694623050	-3.5955245597	0.4159926389
H	1.1974706641	-3.5665383669	0.5692839020
H	5.5132182987	-3.3957191129	0.1414990031
H	3.4791384527	-4.5605550428	0.9144572618
N	0.9968437842	-1.0063356339	-0.7916719253
O	2.8565830735	-0.0126338981	-1.4871459607
C	-0.5467307032	1.8877797385	0.1231842577
H	-0.3044864746	1.2947215199	1.0163321456
C	-1.9076317998	2.0954283940	-0.2360494619
N	-2.9254555476	1.7471088094	0.5058184964
C	-4.3370307949	2.0094399389	0.1256829800
C	-2.8547829861	1.0533989163	1.8129080077
H	-4.4325731988	3.0316974967	-0.2675437150
H	-4.5950669265	1.3001675824	-0.6785933936
C	-5.1235488926	1.7196842893	1.4031563368
C	-4.2949462946	0.6158925775	2.0734772394

H	-2.1213533275	0.2397361824	1.7605897226
H	-2.4949869422	1.7861607645	2.5558727209
H	-5.1653163246	2.6205992314	2.0350673928
H	-6.1557868816	1.4170788706	1.1838087565
H	-4.4996462297	0.5130115523	3.1469633870
H	-4.4751267335	-0.3569329117	1.5921669728
H	-2.1486662653	2.6181375907	-1.1689602305
C	1.8491639228	2.7433584803	-0.1157991883
C	2.6635977371	3.6546452233	-0.8246022770
C	2.3490902860	2.1163332874	1.0440986928
C	3.9406216237	3.9638026742	-0.3661851491
H	2.2850989852	4.1358748562	-1.7311607753
C	3.6304128844	2.4252591184	1.4912110223
H	1.7449971128	1.4013062593	1.6055746010
C	4.4284770296	3.3464521356	0.7914800676
H	4.5565261819	4.6843815643	-0.9073957995
H	4.0124926095	1.9570401130	2.4006166397
H	5.4315628618	3.5828293436	1.1533561203
H	0.1514920069	3.2270348776	-1.3697972032

ATS02a

2 1

Pd	1.2077805535	-1.4059219906	0.0782046782
O	1.0312461155	-1.3321763551	2.0636533470
C	-0.1424137526	-1.1219691177	2.5788791533
O	-1.1365085393	-0.8435433053	1.8878255933
O	1.7458372529	-1.6550122216	-1.8908477741

C	2.9392518769	-2.0872549029	-1.6358540474
C	3.7998243306	-2.6167349261	-2.7278690157
H	3.6465450224	-2.0460686965	-3.6546236596
H	4.8550798724	-2.6157855296	-2.4254535872
H	3.4986781698	-3.6595874029	-2.9257099784
O	3.2994847822	-2.0546595596	-0.4262402364
C	-0.2309158637	-1.2608456180	4.0739265062
H	0.6827649688	-0.8914430254	4.5570246709
H	-1.1213788692	-0.7423642311	4.4489173604
H	-0.3214127291	-2.3348041351	4.3070695408
C	-0.1534172314	0.8596817679	-1.0347084074
C	-1.0004967493	-0.4164620532	-0.8392279750
H	-0.7265952447	-1.1983065742	-1.5578943783
H	-0.7832716979	-0.8243049259	0.3640902019
H	0.1235816663	0.8819037225	-2.0986690623
C	-2.4336330918	-0.3903648628	-0.6836798449
C	-4.3710628257	-1.3501794161	-0.5152499697
C	-4.4711619712	0.0547695551	-0.2421666462
C	-5.4534586991	-2.2102947608	-0.5088030538
C	-5.7291467376	0.6373823384	0.0539464921
C	-6.6812754085	-1.6096862032	-0.2013537427
H	-5.3634487137	-3.2744422138	-0.7278853459
C	-6.8159929648	-0.2139125256	0.0752366910
H	-5.8143677085	1.7052849814	0.2570440178
H	-7.5782621493	-2.2329692514	-0.1746355874
H	-7.8093537518	0.1761150087	0.3043213971
N	-3.2368210684	0.6035675294	-0.3455956828

O	-3.0679788736	-1.6049296989	-0.7926409271
C	1.1028981508	0.6966272623	-0.1894640345
H	0.9709590671	0.9553740404	0.8653477940
C	2.3820458284	1.0945249015	-0.7593399684
N	3.4831974018	1.1910648909	-0.0888508544
C	4.8034110112	1.5013914894	-0.7085427832
C	3.6352140818	0.9487638103	1.3708859786
H	4.6896600264	2.3186943500	-1.4339094714
H	5.1281561433	0.5916733528	-1.2405035110
C	5.7026905295	1.8008857456	0.4881009904
C	5.1489763208	0.8667589123	1.5716424872
H	3.0854202636	0.0436282175	1.6611067284
H	3.1910944102	1.8139916398	1.8920709673
H	5.6009472073	2.8557987965	0.7877769304
H	6.7601621714	1.6187100653	0.2560068249
H	5.4402619865	1.1590078297	2.5888544524
H	5.4879952945	-0.1675561365	1.4057638821
C	-0.7123094962	2.2183667880	-0.6675587871
C	-1.1221582359	2.4976221345	0.6561883931
C	-0.7772851988	3.2313939560	-1.6386327106
C	-1.6062715073	3.7587943165	0.9877131838
H	-1.1036415436	1.7099938424	1.4126231537
C	-1.2630514710	4.4935618549	-1.3032195326
H	-0.4672328252	3.0235461593	-2.6659306562
C	-1.6752816596	4.7603106866	0.0111078152
H	-1.9369891451	3.9656957219	2.0073636713
H	-1.3276524459	5.2732404379	-2.0648267915

H	-2.0513392324	5.7520196730	0.2716905592
H	2.4431008961	1.2798448610	-1.8378474385

ATS03a

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Pd	-1.1527011842	-1.0697561457	-0.1607851140
C	-0.7333619489	1.1978794399	-0.5044329793
C	0.3919688551	0.2454260414	-1.5799420608
H	-0.4370996105	1.2938429220	0.5485371379
H	-0.1135558209	-0.2630139618	-2.4035178318
O	-2.5880756382	-1.4746782572	-1.6059153645
C	-2.9000036534	-2.5760809148	-1.0149133798
O	-2.3049034683	-2.8132300221	0.0792380088
O	0.1176438888	-1.2599889833	1.3552339181
C	0.3234359651	-0.3901223304	2.3039980785
O	-0.1786219476	0.7330666697	2.3487259100
C	-3.8756805372	-3.5288029914	-1.6117061719
H	-4.3663512937	-4.1155402730	-0.8237991331
H	-4.6125266588	-2.9926392540	-2.2246875989
H	-3.3242749595	-4.2243968349	-2.2659668890
C	1.2632611653	-0.9040088863	3.3726158299
H	0.7914815171	-1.7505311979	3.8944608248
H	2.1884184606	-1.2798340670	2.9127452694
H	1.4850340131	-0.1021940220	4.0871432296
C	1.5141763410	-0.5176443608	-1.0535763142
C	3.2585803347	-0.9413221454	0.1441848171
C	2.8946696010	-2.0744001636	-0.6125536136

C	4.3362889719	-0.9068011467	1.0188871044
C	3.6383167650	-3.2591593249	-0.5037555393
C	5.0624974209	-2.0968358516	1.1183186379
H	4.5962388279	-0.0119842022	1.5849409383
C	4.7194534859	-3.2482817232	0.3734010097
H	3.3699362973	-4.1440446590	-1.0819418032
H	5.9228512406	-2.1382836482	1.7895138514
H	5.3232996710	-4.1500093096	0.4920564389
N	1.7717987191	-1.7571689328	-1.3573686166
O	2.3656511486	0.0507202655	-0.1565148210
C	0.2598277953	1.7197366928	-1.5310452610
H	-0.2346189191	2.0990911647	-2.4331132999
C	-2.1435364380	1.2791655288	-0.8221917946
N	-3.0697077743	1.6492929189	0.0081277811
C	-4.5179512014	1.5977105340	-0.3136518702
C	-2.8489075178	2.0304977420	1.4282634203
C	-5.1666413065	1.4755381477	1.0640878539
H	-4.8005984888	2.5396143832	-0.8119384627
H	-4.7106212659	0.7578658606	-0.9940217788
C	-4.2556169911	2.3392269063	1.9475027220
H	-2.3603196649	1.1898735787	1.9436916176
H	-2.1510145115	2.8781949679	1.4728120811
H	-5.1451722953	0.4250255420	1.3962136944
H	-6.2130857045	1.8085657654	1.0578889049
H	-4.3503316173	2.1125695812	3.0175554795
H	-4.4909972828	3.4063400519	1.8102589843
H	-2.4719072994	1.0396011878	-1.8393018470

C	1.3702559965	2.6325536109	-1.0827156270
C	2.2025434360	3.1639731432	-2.0784151497
C	1.6013643311	2.9666872993	0.2576263158
C	3.2580614136	4.0117940882	-1.7405082315
H	2.0253105421	2.9123957629	-3.1277003418
C	2.6556271108	3.8195551652	0.5922002903
H	0.9874725918	2.5510446377	1.0580039551
C	3.4862686735	4.3423944459	-0.4019611184
H	3.9001346385	4.4182003576	-2.5248003810
H	2.8279416328	4.0748788689	1.6400356640
H	4.3086621474	5.0095243374	-0.1349423746

BIN02

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Pd	-0.1424572746	-2.6710918222	-0.3346942659
O	1.7776206548	-3.3647210436	-0.4916000757
C	2.2500348117	-2.1900016242	-0.4640799599
O	1.3682688507	-1.2514385314	-0.3527351078
O	-1.6222469742	-4.0955251887	-0.2812502368
C	-2.5275157487	-3.2215626096	-0.1757811920
C	-3.9721474400	-3.5717467163	-0.1273758686
H	-4.1038793913	-4.5655320478	0.3214310177
H	-4.3592830729	-3.6150858255	-1.1593146127
H	-4.5372324859	-2.8144997188	0.4325280785
O	-2.1107111788	-1.9957900028	-0.1415680042
C	3.7036180540	-1.9054576516	-0.5707657528
H	3.9820552860	-1.0836498525	0.1034650620

H	3.9257263420	-1.5830506305	-1.6005770437
H	4.2838544673	-2.8106585854	-0.3507788484
C	-0.8092264285	1.1313781388	-0.2286183540
C	-0.0572288845	1.7476747984	-1.4521105307
H	-0.4162484136	2.7702410849	-1.6554306621
H	-0.2457993032	1.1509484161	-2.3556865182
H	-0.4156239959	0.1158944253	-0.1193170596
C	1.3904886931	1.7404083189	-1.1225176710
C	3.5170951816	1.5266214350	-1.4220357472
C	3.2478984246	1.7842480287	-0.0623764363
C	4.7909832189	1.3362550866	-1.9376112401
C	4.2991770705	1.8457910108	0.8614819508
C	5.8293404059	1.3985168082	-1.0031053994
H	4.9692873452	1.1500651536	-2.9972728332
C	5.5875571272	1.6452779197	0.3672218499
H	4.1176520962	2.0498994938	1.9176376787
H	6.8573256068	1.2555739026	-1.3419621523
H	6.4369228641	1.6881488637	1.0516574634
N	1.8662894210	1.9177200878	0.0720293296
O	2.3057943990	1.4945061024	-2.0789593822
C	-2.2763800203	1.0025220572	-0.5126566516
H	-2.6021713173	-0.0379572914	-0.6456011867
C	-3.2303365940	1.9975630350	-0.6700170676
C	-4.5657616860	1.5774906781	-1.0161770509
C	-2.9671788245	3.4072237731	-0.5349229495
C	-5.5675781400	2.5067819390	-1.2162612319
H	-4.7690573234	0.5094113513	-1.1214457395

C	-3.9753537463	4.3232469385	-0.7407222857
H	-1.9684883140	3.7588871112	-0.2778885553
C	-5.2729340572	3.8756918957	-1.0804293399
H	-6.5776810139	2.1885923612	-1.4805711162
H	-3.7807456082	5.3931535240	-0.6460972169
H	-6.0644734058	4.6128999044	-1.2419979408
C	-0.4764285392	1.8706348606	1.0449459779
H	-0.3599194326	2.9570298685	1.0399822653
N	-0.3927002372	1.2821475613	2.1834741490
C	-0.4366148507	-0.1930542159	2.4047205321
H	-1.3459143707	-0.6209468964	1.9616140840
H	0.4365310767	-0.6134837901	1.8797906531
C	-0.3281732509	-0.3380909423	3.9221087514
H	-1.3258958838	-0.2857871439	4.3855860194
H	0.1196582273	-1.3000629663	4.2042556836
C	0.5228814771	0.8709007735	4.3312962927
H	0.4414998824	1.1210653168	5.3972116083
H	1.5858561514	0.6909115404	4.1063215418
C	-0.0184204992	1.9896592909	3.4426978851
H	0.7003566602	2.7860524665	3.2073490442
H	-0.9334250887	2.4380127749	3.8619553689

BIN03

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Pd	-0.7375743143	-0.6128857293	-0.3024581824
O	-0.1392019716	-2.1681911146	0.9418493944
C	-0.1598270601	-3.3593133322	0.5516771535

O	-0.6285765087	-3.7440135647	-0.5972116254
O	-1.4575987337	0.5598645726	-1.8602030797
C	-1.9042613154	-0.4481345486	-2.5440709282
C	-2.6346889314	-0.2165821089	-3.8206044070
H	-2.3429714253	0.7372235826	-4.2782488573
H	-3.7148378278	-0.1810447725	-3.5986004381
H	-2.4622933291	-1.0551670661	-4.5088250662
O	-1.7223529642	-1.6032909412	-2.0676984810
C	0.3657574452	-4.4488277173	1.4227140602
H	0.9298387729	-4.0308980350	2.2632964047
H	0.9875605149	-5.1326405836	0.8276597698
H	-0.4881505339	-5.0332270342	1.8043946707
C	1.0457386074	1.3372301115	0.0919898078
C	1.2239041595	0.1223342632	-0.8131718073
H	1.0869448572	0.2313529974	-1.8923023764
H	-1.0116462130	-3.0314662284	-1.1659313373
H	1.9585782288	1.5364554710	0.6781769996
C	2.1357476599	-0.9091530190	-0.4472543958
C	3.3182451938	-2.1119737355	0.9147196745
C	3.1886723681	-2.7593231431	-0.3465217376
C	4.0150179139	-2.6517890920	1.9869734719
C	3.7826001489	-4.0211455664	-0.5622073035
C	4.5877859753	-3.9044514914	1.7516383625
H	4.1114789961	-2.1384240225	2.9439601927
C	4.4737376102	-4.5757693636	0.5039500325
H	3.6968237344	-4.5215768259	-1.5275740995
H	5.1489043532	-4.3863570992	2.5553735380

H	4.9534824845	-5.5495904778	0.3890821787
N	2.4380995136	-1.9650628258	-1.1677040071
O	2.6454712717	-0.9297166363	0.8303775596
C	-0.0616333788	0.7892898885	1.0440997959
H	0.4182859870	0.1934401447	1.8279772453
C	-1.2088972758	1.5676748207	1.5304440200
C	-1.5510885328	1.4435503849	2.8969390720
C	-2.0059465500	2.3982572186	0.7068065594
C	-2.6183870760	2.1621805015	3.4314791729
H	-0.9615259821	0.7870429400	3.5412463573
C	-3.0789461973	3.1037387895	1.2445785818
H	-1.8314824611	2.4410726692	-0.3690221787
C	-3.3813249573	2.9977478571	2.6090307101
H	-2.8608581807	2.0664003062	4.4916928592
H	-3.6987764724	3.7273955934	0.5969203170
H	-4.2228802537	3.5549418883	3.0261328168
C	0.6636055420	2.5663217629	-0.6612603117
H	0.2472732845	2.4688651857	-1.6709149938
N	0.7660539418	3.7496601910	-0.1788778334
C	1.2634243348	4.0923840878	1.1854702243
H	0.7962861206	3.4256660266	1.9212607739
H	2.3538683013	3.9290119261	1.1884594519
C	0.8989986979	5.5695691255	1.3478612068
H	-0.1199679728	5.6602654819	1.7550897209
H	1.5831062665	6.0818258700	2.0368439594
C	0.9591563001	6.1132548548	-0.0855540600
H	0.4125516563	7.0566453016	-0.2144286741

H	2.0011573056	6.2835916102	-0.3989232279
C	0.3362308550	4.9849077466	-0.9027644200
H	0.6536297327	4.9268761894	-1.9522011156
H	-0.7649297261	5.0091627241	-0.8581471812

BIN04

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Pd	0.1615344062	-1.2850111759	0.2859535189
C	-1.2627743370	0.1202285736	0.7513067116
C	0.4771804945	0.4112276181	-0.8451566319
H	-1.2207570384	0.2016979517	1.8405750800
H	0.0993671992	0.1281104571	-1.8318123758
O	-0.6140904130	-2.1490813379	-1.4057672021
C	0.4007685233	-2.9365560937	-1.6112472328
O	1.3744343124	-2.8492647992	-0.8353853071
O	1.0810348033	-0.7131236429	2.0289005021
C	0.7453109288	-1.7715032567	2.7042183572
O	-0.0167185226	-2.6013959991	2.1665944124
C	0.3297328984	-3.9179884068	-2.7381510858
H	-0.1318540722	-3.4544077794	-3.6210477820
H	1.3332389491	-4.2936534833	-2.9736309229
H	-0.3066519816	-4.7628731959	-2.4293115770
C	1.3228532174	-1.9549145138	4.0737373604
H	1.4193988353	-0.9895549361	4.5890451916
H	0.7053519511	-2.6521909182	4.6540656787
H	2.3325409939	-2.3839572038	3.9682055310
C	1.8863486085	0.7535717289	-0.8822037963

C	3.7384921666	1.5909415090	-0.1204456271
C	3.9629025228	0.9079063183	-1.3351634416
C	4.7385503776	2.2282319436	0.6023228697
C	5.2558471114	0.8457880563	-1.8760463712
C	6.0201086010	2.1543611602	0.0493709173
H	4.5384872499	2.7453684833	1.5412357930
C	6.2728065513	1.4771890326	-1.1644749901
H	5.4440697357	0.3181347870	-2.8118159452
H	6.8514545620	2.6315388970	0.5725063047
H	7.2944224608	1.4489623725	-1.5485628495
N	2.7562799143	0.3951447611	-1.7801289008
O	2.4022487599	1.4928592750	0.1577204720
C	-2.5723599071	-0.3213619018	0.2423340723
C	-3.4621649775	-0.9494191428	1.1380367835
C	-2.9678789587	-0.1740601122	-1.1016361172
C	-4.7155485038	-1.3831147691	0.7110469883
H	-3.1523076245	-1.1046813119	2.1743084254
C	-4.2232380321	-0.6048920668	-1.5275412930
H	-2.2750816061	0.2374418989	-1.8390637276
C	-5.1034838217	-1.2051498186	-0.6213636954
H	-5.3918540782	-1.8677381336	1.4182550698
H	-4.5099443944	-0.4913125472	-2.5751708903
H	-6.0845922716	-1.5475053682	-0.9570275656
C	-0.4659108035	1.2335626830	0.0281634758
H	0.1385983868	1.7521748885	0.7934540674
C	-1.2520874648	2.2663755401	-0.7008640922
H	-1.0270020807	2.4562249905	-1.7579493737

C	-2.6582250579	2.8910597712	1.2244618510
C	-3.0026568262	3.9698304908	-0.9469436324
C	-3.6147046815	4.0754847871	1.3657078572
H	-3.1743816301	1.9258878264	1.3393601432
H	-1.7912029516	2.9078644956	1.8990416323
C	-4.2092089135	4.2111616536	-0.0423973907
H	-2.3922853171	4.8790672741	-1.0660367019
H	-3.2401903159	3.5639803072	-1.9388586790
H	-3.0611029771	4.9864754734	1.6428278324
H	-4.3712656817	3.8942926932	2.1403989589
H	-4.6704095619	5.1899530436	-0.2287023170
H	-4.9722148038	3.4361061727	-0.2163409003
N	-2.1932759137	2.9746560003	-0.1852654430

BTS01b

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Pd	-1.7640216925	-1.9133283586	-0.0031776407
O	0.1536826418	-1.8635980428	0.5558266492
C	1.0410278771	-2.8411768387	0.5635411761
O	2.2325825007	-2.5363237421	0.5469968041
O	-2.4814252172	-3.7452767083	0.5455802794
C	-3.6492265486	-3.4501356575	0.1156264752
C	-4.7793284851	-4.4093280075	0.1594736553
H	-4.6886432016	-5.0628872962	1.0378349771
H	-4.7351831341	-5.0426356197	-0.7427409673
H	-5.7377264765	-3.8736427765	0.1610472942
O	-3.7576107125	-2.2730038142	-0.3818539988

C	0.5728377059	-4.2691713113	0.5898412149
H	-0.1116834066	-4.4323107507	1.4345250369
H	1.4369544172	-4.9390351503	0.6646026357
H	0.0044364964	-4.5017282032	-0.3239086450
C	2.2365493116	0.4575590346	0.6875797493
C	0.9167872982	0.1779234765	-1.2468930116
H	1.1097516150	-0.8848368977	-1.1354568856
H	1.6064285000	0.8209132195	-1.7929851086
H	2.3360740879	-0.6419705729	0.6759303387
C	-0.3932607289	0.6407226792	-1.1214984903
C	-1.9800119395	2.1313385741	-1.2826874792
C	-2.5328841045	0.9113944187	-0.7979591906
C	-2.7304398807	3.2789646675	-1.5057970517
C	-3.9146211108	0.8085000166	-0.5211128270
C	-4.0897864325	3.1587200749	-1.2232958263
H	-2.2869690330	4.1996634262	-1.8850397684
C	-4.6678468560	1.9477077134	-0.7411933836
H	-4.3509378511	-0.1290211354	-0.1787756106
H	-4.7413835915	4.0207373141	-1.3832846916
H	-5.7424755893	1.9241114410	-0.5507004963
N	-1.5054710297	0.0114505426	-0.6943532413
O	-0.6552490408	1.9384592157	-1.4639559092
C	1.1325973025	0.9320445330	1.4042655900
H	0.5182962929	0.1167487333	1.8031948537
C	0.6326728777	2.2464026429	1.6364598497
C	-0.3932795742	2.3805231599	2.6145901188
C	1.0621085969	3.4092759411	0.9366666757

C	-0.9224653339	3.6266605290	2.9217537664
H	-0.7419384498	1.4899984535	3.1428731024
C	0.5163427246	4.6473094007	1.2354957187
H	1.7827033866	3.3312872059	0.1224848852
C	-0.4654013459	4.7607045588	2.2365537130
H	-1.6905775871	3.7236133318	3.6912292776
H	0.8407688776	5.5357569838	0.6902797755
H	-0.8841837770	5.7420677082	2.4721441108
C	3.4195347022	1.2146036752	0.3766424648
H	3.5099802901	2.2641170333	0.6744182713
N	4.4739103829	0.6934046338	-0.1758186956
C	4.6098535983	-0.7091050972	-0.6630836319
H	4.1396704826	-1.4146166198	0.0349489300
H	4.0648865854	-0.7746621214	-1.6199591954
C	6.1154309577	-0.8759221339	-0.8624587888
H	6.5895161644	-1.1811040675	0.0836756448
H	6.3420298284	-1.6461737705	-1.6111956064
C	6.5766348224	0.5277691963	-1.2746178195
H	7.6543049422	0.6895775307	-1.1413038222
H	6.3365013432	0.7233884480	-2.3317613698
C	5.7530970215	1.4385410914	-0.3658931474
H	5.5440614583	2.4388259498	-0.7699750368
H	6.2181860409	1.5499131387	0.6274723027

BTS02b

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Pd	-1.8681170141	-0.7836253639	-0.2843794488

O	-1.7497571759	-2.6907289064	0.3411701174
C	-0.6038091608	-3.1726102564	0.6921795464
O	0.4499201019	-2.5124756964	0.6428648305
O	-3.8199983005	-0.9991148894	0.0532896632
C	-4.1451079478	-0.8418815099	1.3258873294
C	-5.5300058820	-1.3485424154	1.6418526890
H	-6.2177173095	-1.2091076795	0.7973566596
H	-5.9007454759	-0.8475490412	2.5453045657
H	-5.4558737076	-2.4306739228	1.8375039979
O	-3.3888034402	-0.3347587791	2.1418938186
C	-0.6288289991	-4.5900862835	1.1972556211
H	-1.0131665165	-4.5760708679	2.2300663814
H	0.3862871410	-5.0038116750	1.1889029861
H	-1.3142012863	-5.1986065532	0.5926753830
C	0.1893721626	0.9589679686	0.4140028447
C	0.4939364021	-0.1700631149	-0.6082908375
H	0.1414682399	0.0198429941	-1.6255751155
H	0.2126272019	-1.3050440197	-0.0473039588
H	0.5365051758	0.6047707141	1.3919666871
C	1.9215463753	-0.5156376169	-0.7551085600
C	3.9298274456	-0.9813280827	-0.0670789088
C	3.8118301063	-1.2024469209	-1.4569190297
C	5.0969579542	-1.1848425214	0.6521227797
C	4.9155798752	-1.6581184858	-2.1940711977
C	6.1868286427	-1.6438456116	-0.0984947478
H	5.1637832986	-1.0245773004	1.7288633924
C	6.0973144938	-1.8741816568	-1.4904360148

H	4.8384755806	-1.8367732937	-3.2671912124
H	7.1335711992	-1.8387428604	0.4095357346
H	6.9801542171	-2.2357419443	-2.0208901554
N	2.5146467583	-0.8916388513	-1.8419733928
O	2.7013123538	-0.5342142535	0.3752696379
C	-1.3225782752	1.1098704161	0.5102914733
H	-1.7426711175	1.1269542131	1.5205578707
C	-2.2000676528	1.5724770741	-0.5285832757
C	-3.5373069938	1.9388780202	-0.1303940646
C	-1.8507585728	1.7066115969	-1.9203770860
C	-4.4510442916	2.3942028999	-1.0563952286
H	-3.8066449055	1.8411586912	0.9223718730
C	-2.7896083551	2.1417115447	-2.8396075138
H	-0.8482410876	1.4738251763	-2.2744338635
C	-4.0858309384	2.4822771484	-2.4135330354
H	-5.4574589739	2.6772479282	-0.7425954781
H	-2.5230872608	2.2244402893	-3.8947685342
H	-4.8196254008	2.8237970331	-3.1484390681
C	0.9189053874	2.2198249444	0.0548156091
H	0.6814812134	2.7120971657	-0.8957815259
N	1.8583922492	2.7444110759	0.7524259766
C	2.3709628587	2.2464115267	2.0715837968
H	1.5347129684	2.1748976323	2.7805559659
H	2.7761975382	1.2400494988	1.8935284171
C	3.4466554917	3.2632856535	2.4632865897
H	3.0077917678	4.0726140356	3.0666780671
H	4.2388608921	2.7954992249	3.0622902204

C	3.9450672039	3.8034828140	1.1170178407
H	4.4676589397	4.7654314600	1.2015004682
H	4.6276980198	3.0882526196	0.6311857991
C	2.6562187981	3.9328077812	0.3114247081
H	2.7709406732	3.9140794543	-0.7800472896
H	2.0857313146	4.8300947791	0.6022742021

BTS03b

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Pd	-0.5883430303	-1.3072492715	0.2785207582
C	0.8849631378	0.3507818714	-0.3462227556
C	-0.1940278248	0.8785570206	1.0040661087
H	0.4084203702	0.3486989662	-1.3400890428
H	0.0609010943	0.4992699302	1.9965463794
O	0.4082510669	-2.2618678545	1.8274291770
C	-0.2528678798	-3.3385394522	1.6092617694
O	-1.0867439843	-3.3057957733	0.6499802255
O	-1.9417764081	-0.8410106425	-1.1102581350
C	-1.6906488271	-0.4595398485	-2.3315670962
O	-0.5782418872	-0.1783708148	-2.7761416882
C	-0.0744909222	-4.5508208530	2.4572186425
H	0.9465625234	-4.5866762512	2.8598659451
H	-0.7805249898	-4.4949727480	3.3020361602
H	-0.3021472987	-5.4556070057	1.8781670260
C	-2.9438044020	-0.3744433234	-3.1786960620
H	-3.3927970698	-1.3749940264	-3.2692183658
H	-3.6849189789	0.2709374386	-2.6841137942

H	-2.6955809499	0.0170671720	-4.1726833581
C	-1.5999563736	1.2600474029	0.8350485991
C	-3.2719265388	2.1531324083	-0.2096170554
C	-3.7122898476	1.4612386854	0.9345854020
C	-4.1178564935	2.8083448702	-1.0928596812
C	-5.0782676339	1.4107546163	1.2380180982
C	-5.4796933276	2.7441382036	-0.7786821069
H	-3.7472198638	3.3327503935	-1.9741884572
C	-5.9483166299	2.0601909651	0.3625849415
H	-5.4361829366	0.8763289044	2.1187776337
H	-6.1994687782	3.2362286405	-1.4360113806
H	-7.0218485291	2.0388476003	0.5602131645
N	-2.6044612795	0.9078147771	1.5690860445
O	-1.9032432162	2.0324432903	-0.2532705018
C	2.0805201767	-0.5225681621	-0.2305940149
C	2.4626745046	-1.2203339949	-1.3931478090
C	2.8539915612	-0.6609366162	0.9341415600
C	3.6158128264	-2.0063410182	-1.3925021284
H	1.8369037054	-1.1423851478	-2.2854355447
C	4.0026678591	-1.4523725642	0.9315876456
H	2.5302022098	-0.2058189296	1.8733735275
C	4.3924369393	-2.1191073808	-0.2350144326
H	3.9045872322	-2.5402947535	-2.3002883721
H	4.5848959232	-1.5666194079	1.8485337850
H	5.2907526830	-2.7400352492	-0.2353679457
C	0.8369656941	1.7095119091	0.3212031247
H	0.4365783759	2.4860345987	-0.3440627855

C	2.0212374252	2.1616497660	1.0697411675
H	2.0452319017	2.1226061595	2.1651376976
C	3.2507828865	2.6533530415	-0.9986552578
C	4.3245628487	3.0094655325	1.1728518407
C	4.6676003479	3.2022991249	-1.1861982131
H	3.1430064995	1.6212021145	-1.3652279224
H	2.4562446602	3.2657483802	-1.4475728965
C	5.3898573350	2.7837473479	0.1023412582
H	4.2371380432	4.0745320429	1.4423723063
H	4.4436007054	2.4146435951	2.0877676554
H	4.6452847954	4.2994141106	-1.2768655441
H	5.1370397465	2.8020897901	-2.0942561265
H	6.2998362187	3.3652702416	0.3002966381
H	5.6633212871	1.7172046355	0.0669252661
N	3.0719993166	2.6090815417	0.4800299257