Contents

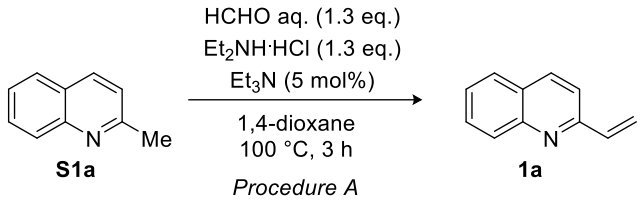
1. General Information

All reactions were carried out under nitrogen atmosphere in flame-dried glassware. Toluene (tol), dichloromethane (DCM) and tetrahydrofuran (THF) were supplied from KANTO Chemical Co., Inc. as “Dehydrated solvent system”. Other solvents and reagents were purchased from commercial suppliers (Wako Pure Chemical Industries, Ltd., Tokyo Chemical Industry Co., LTD., Aldrich Inc., and others) and used without further purification. Purification of reaction products was carried out by flash column chromatography using silica gel 60 N (Merck 40-63 μm). Analytical thin layer chromatography (TLC) was performed on Merck precoated TLC plates (silica gel 60 GF 254, 0.25 mm). ^{1}H NMR spectra were recorded on a JEOL ECA-600 (600 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane or solvent resonance as the internal standard ($CDCl_3$: 7.26 ppm, TMS: 0.00 ppm). ^{13}C NMR spectra were recorded on a JEOL ECA-600 (150 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from the solvent resonance as the internal standard ($CDCl_3$: 77.2 ppm). ^{19}F NMR spectra were recorded on JEOL ECA-600 (565 MHz) spectrometer with complete proton decoupling. Infrared spectra were recorded on a Jasco FT/IR-4100 spectrometer. Chiral stationary phase HPLC analysis was performed on a Jasco LC-2000 Plus Series system with DACIEL chiral analytical column (4.6 mmΦ* 250 mm length). Optical rotations were measured on a Jasco P-1020 digital polarimeter with a sodium lamp and reported as follows; $[\alpha]^{T\,^{\circ}C}D$ (*c* = g/100 mL, solvent, % ee). High resolution mass spectra analysis was performed on a Bruker Daltonics solariX 9.4T FT-ICR-MS spectrometer and a JEOL JMST100GCV Time-of-Flight Mass Spectrometer at the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University.

2. Preparation of substrates

Procedures for preparation of novel 2-vinylquinolines **1**.

1 was synthesized from corresponding 2-methylquinoline derivatives **S1**.

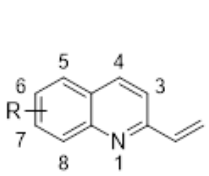


[Procedure A]

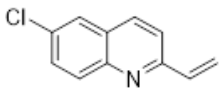
The representative procedure for **1a** was shown below as *Procedure A*. This procedure was slightly modified from Feng's method.[1]

To a frame-dried 50 mL round-bottom flask with a magnetic stirrer bar, 2-methylquinoline (**S1a**) (716 mg, 5.0 mmol), HCHO (30% in H_2O, 6.5 mmol, 1.3 eq.), $Et_2NH{\cdot}HCl$ (713 mg, 6.5 mmol, 1.3 eq.), Et_3N (35 uL, 0.25 mmol, 5 mol %) and 1,4-dioxane (10 mL) were added. This suspension was heated to 100 ℃ until the starting material **S1a** was fully consumed (checked by TLC). After cooling to room temperature, H_2O (15 mL) was added, and extracted with DCM (10 mL * 3 times). The combined organic layers were dried over $MgSO_4$, and the solvent was removed under reduced pressure. The residue was purified by column chromatography using hexane/ethyl acetate (14/1) as the eluent yielding the 2-vinyl quinoline **1a** (590 mg, 3.8 mmol, 76% yield) as a colorless oil. **1a** was stored at -20 ℃ under Ar atmosphere.

2-vinylquinolines **1a**, **1c** and **1g** were known compounds and their data are identical with the reported literature.[1]

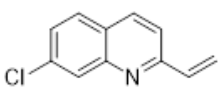


6-Chloro-2-vinylquinoline (1b)



64% yield [*Procedure A*]; white solid; R_f = 0.40 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.65-7.58 (m, 2H), 7.01 (dd, *J* = 17.4, 10.8 Hz, 1H), 6.29 (d, *J* = 17.4 Hz, 1H), 5.69 (d, *J* = 10.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.4, 146.5, 137.7, 135.6, 132.1, 131.1, 130.7, 128.1, 126.3, 120.5, 119.5; IR (ATR) 3089, 3053, 3020, 2990, 1849, 1592, 1556, 1493, 1421, 1382, 1308, 1192, 1073, 993, 924, 903, 831, 726 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{11}H_8ClN$ 189.03453, found: 189.03450.

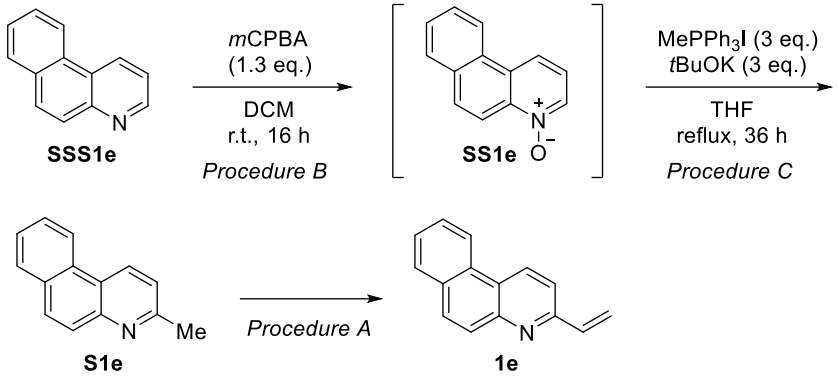
7-Chloro-2-vinylquinoline (1h)



60% yield [*Procedure A*]; white solid; R_f = 0.45 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 1H), 8.06 (d, *J* = 1.8 Hz, 1H), 7.71 (d, *J* = 9.0 Hz, 1H), 7.58 (d, *J* = 9.0 Hz, 1H), 7.45 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.01 (dd, *J* = 18.0, 10.8 Hz, 1H), 6.31 (dd, *J* = 18.0, 0.6 Hz, 1H), 5.69 (dd, *J* = 10.8, 0.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.1, 148.6, 137.7, 136.3, 135.6, 128.8, 128.5, 127.4, 125.9, 120.8, 118.9; IR (ATR) 3090, 3059, 3016, 2989, 1852, 1609, 1597, 1496, 1427, 1396,

1144, 1130, 1070, 993, 927, 873, 848, 777 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{11}H_8ClN$ 189.03453, found: 189.03449.

1d, **1e,** and **1f** were synthesized from corresponding quinoline derivatives **SSS1**.



The representative procedure for **1e** was shown below as *Procedure B* and *Procedure C*. These procedures were slightly modified from Kim's method.[2a]

[Procedure B]

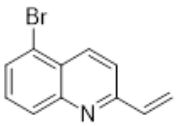
To a solution of **SSS1e** (1115 mg, 6.2 mmol) in dry-DCM (25 mL), *m*CPBA (60%, 1.8 g, 1.3 eq.) was added in three portions at room temperature under N_2 atmosphere. After 16 h, 1*N* NaOH aq. (20 mL) was added. The organic layer was separated, and the aqueous layer was extracted with DCM (20 mL * 2 times). The combined organic layers were dried over $MgSO_4$, and the solvent was removed under reduced pressure. This crude material including quinoline *n*-oxide **SS1e** was directly used for the next step without further purification.

[Procedure C]

To a corresponding crude material of **SS1e** in a frame-dried 100 mL round-bottom flask with a reflux condenser, $MePPh_3I$ (7.54 g, 18.7 mmol, 3.0 eq.), *t*BuOK (2.1 g, 18.7 mmol, 3.0 eq.) and dry-THF (16 mL) were added. This mixture was heated to 85 ℃ (reflux) for 36 h under N_2 atmosphere. After cooling to ambient temperature, this solution was filtered through Celite®, and the solvent removed under reduced pressure. The residue was purified by column chromatography using hexane/ethyl acetate (9/1 to 4/1) as the eluent yielding the 2-methyl quinoline derivative **S1e** (878 mg, 4.55 mmol, 76% yield) as a yellow solid.

2-methylquinoline derivative **S1d**[2b] and **S1e**[2a] were known compounds and their data are identical to the reported literature.

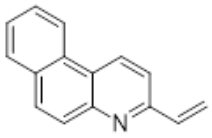
5-Bromo-2-vinylquinoline (1d)



29% yield [3 steps, *Procedure B, C and A*]; colorless oil; R_f = 0.44 (Hexane/EtOAc= 6/1); ^1H NMR (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.4 Hz, 1H), 8.03 (d, *J* = 7.8 Hz, 1H), 7.77 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.55 (dd, *J* = 8.4, 7.8 Hz, 1H), 7.04 (dd, *J* = 17.4, 10.8 Hz, 1H), 6.34 (d, *J* = 17.4 Hz, 1H), 5.72 (d, *J* = 10.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.9, 148.9, 136.0, 137.4,

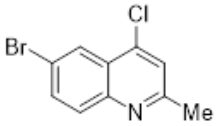
136.0, 130.1, 130.0, 129.4, 127.0, 121.9, 121.1, 119.8; IR (ATR) 3089, 3063, 3019, 2984, 2902, 1607, 1588, 1547, 1492, 1395 1305, 1125, 1089, 953, 927, 905, 835, 814, 771 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{11}H_8BrN$ 232.98401, found: 232.98394.

3-Vinylbenzo[f]quinoline (1e)



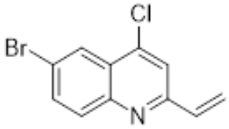
46% yield [3 steps, *Procedure B, C and A*]; pale yellow solid; R_f = 0.40 (Hexane/EtOAc= 6/1); ^1H NMR (600 MHz, $CDCl_3$) δ 8.87 (d, *J* = 9.0 Hz, 1H), 8.57 (d, *J* = 7.8 Hz, 1H), 7.96 (s, 2H), 7.91 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.67 (ddd, *J* = 7.8, 7.2, 1.2 Hz, 1H), 7.62 (ddd, *J* = 7.8, 7.2, 1.2 Hz, 1H), 7.07 (dd, *J* = 17.7, 10.8 Hz, 1H), 6.35 (dd, *J* = 17.7, 0.6 Hz, 1H), 5.66 (dd, *J* = 10.8, 0.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ155.7, 148.1, 137.7, 131.8, 131.2, 131.1, 129.7, 128.8, 128.4, 127.3, 127.2, 124.6, 122.7, 119.6, 118.8; IR (ATR) 3057, 3016, 2985, 2910, 2789, 1580, 1567, 1489, 1456, 1415, 1235, 1090, 925, 867, 832, 750 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{15}H_{11}N$ 205.08915, found: 205.08911.

6-Bromo-4-chloro-2-methylquinoline (S1f)



38% yield [2 steps, *Procedure B and C*]; pale orange solid; R_f = 0.28 (Hexane/EtOAc= 6/1); ^1H NMR (600 MHz, $CDCl_3$) δ 8.33 (d, *J* = 2.4 Hz, 1H), 7.88 (d, *J* = 9.0 Hz, 1H), 7.79 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.41 (s, 1H), 2.71 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.5, 147.4, 141.5, 134.0, 130.9, 126.4, 126.0, 122.8, 120.9, 25.3; IR (ATR) 3089, 3049, 3033, 2989, 2903, 1747, 1587, 1546, 1481, 1373, 1306, 1232, 1169, 1073, 979, 924, 837, 765, 657 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{10}H_7BrClN$ 254.94504, found: 254.94495.

6-Bromo-4-chloro-2-vinylquinoline (1f)



50% yield [*Procedure A*]; white pink solid; R_f = 0.46 (Hexane/EtOAc= 6/1); ^1H NMR (600 MHz, $CDCl_3$) δ 8.34 (d, *J* = 2.4 Hz, 1H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.81 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.68 (s, 1H), 6.94 (dd, *J* = 18.0, 10.8 Hz, 1H), 6.30 (d, *J* = 18.0 Hz, 1H), 5.73 (d, *J* = 10.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.4, 147.5, 141.8, 136.8, 134.2, 131.5, 126.8, 126.5, 121.7, 121.5, 119.5; IR (ATR) 3088, 3065, 3054, 3027, 3010, 2986, 2887, 1748, 1583, 1541, 1480, 1415, 1373, 1317, 1170, 1067, 1025, 984, 931, 913, 876, 824, 780 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{11}H_7BrClN$ 266.94504, found: 266.94499.

Procedures for preparation of novel dienylcarbamates **2**, **7b**, **8**, **9b**, **10b**.

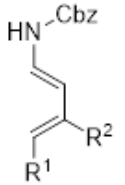
Dienylcarbamates were prepared following literature *procedure D* from corresponding carboxylic acids.[3a]

[Procedure D]

To a solution of corresponding carboxylic acid (1.0 eq.) in dry-DMF (0.5 M) was added NEt_3 (1.1 eq.) and diphenyl phosphoryl azido (1.1 eq.) dropwise at 0 °C and the reaction was allowed to stir for 1 h at the same temperature. Then corresponding benzyl alcohol (3.0 eq.) was added, and the reaction was heated to 85 °C for 4 h. The reaction was

quenched with water and extracted with hexane/AcOEt = 3/1. The combined organic layers were washed with water and brine, dried over Na_2SO_4, concentrated in vacuo, and purified by silica-gel chromatography (hexane/AcOEt = 40/1 to 20/1) to afford the dienylcarbamates in moderate yield.

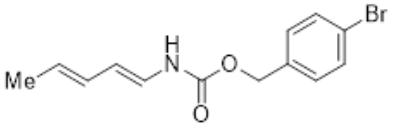
Dienylcarbamates **2a**,[3a] **2b**,[3a] **2c**,[3b] and **2d**[3a] were known compounds and their data are identical with the reported literatures.



2a : R^1 = H, R^2 = H
2b : R^1 = Me, R^2 = H
2c : R^1 = C_6H_{13}, R^2 = H
2d : R^1 = H, R^2 = Me

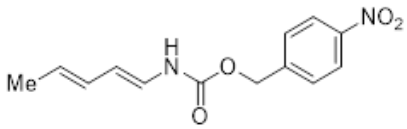
<u>In all cases, dienylcarbamates showed multiple resonance for the presence of different rotational isomers at 20 ℃. Therefore, we conducted ^{1}H NMR measurements at 50 ℃ for characterization.</u>

4-Bromobenzyl ((1*E*,3*E*)-penta-1,3-dien-1-yl)carbamate (7b)



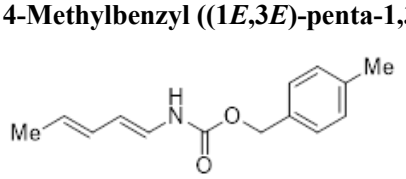
51% yield [*Procedure D*]; white solid; R_f = 0.14 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.49 (d, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 2H), 6.56 (dd, *J* = 12.6, 12.6 Hz, 1H), 6.29 (brs, 1H), 5.95 (dd, *J* = 12.6, 12.6 Hz, 1H), 5.64 (dd, *J* = 12.6, 12.6 Hz, 1H), 5.51 (qd, *J* = 12.6, 6.6 Hz, 1H), 5.09 (s, 2H), 1.72 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.3, 135.1, 131.9, 130.0, 128.5, 126.2, 124.1, 122.6, 112.4, 66.6, 18.3; IR (ATR) 3315, 3069, 3023, 2958, 2907, 2884, 1687, 1665, 1637, 1529, 1490, 1328, 1277, 1232, 1165, 1060, 1014, 974, 922, 811, 674 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{13}H_{14}BrNO_4$ 295.02079, found: 295.02075.

4-Nitrobenzyl ((1*E*,3*E*)-penta-1,3-dien-1-yl)carbamate (8b)



49% yield [*Procedure D*]; pale yellow solid; R_f = 0.18 (Hexane/EtOAc= 3/1); Mp: 122.4-124.9 ℃; ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.21 (d, *J* = 9.0 Hz, 2H), 7.50 (d, *J* = 9.0 Hz, 2H), 6.56 (dd, *J* = 12.0, 12.0 Hz, 1H), 6.38 (brs, 1H), 5.96 (dd, *J* = 12.0, 12.0 Hz, 1H), 5.68 (dd, *J* = 12.0, 10.8 Hz, 1H), 5.54 (qd, *J* = 12.0, 7.2 Hz, 1H), 5.24 (s, 2H), 1.73 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.0, 147.9, 143.4, 128.4, 128.3, 126.6, 124.0, 123.8, 112.9, 65.8, 18.3; IR (ATR) 3297, 3158, 3118, 3018, 2911, 2880, 1703, 1664, 1637, 1606, 1500, 1354, 1323, 1270, 1232, 1164, 1064, 972, 922, 846, 738, 686 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{13}H_{14}N_2O_4$ 262.09536, found: 262.09525.

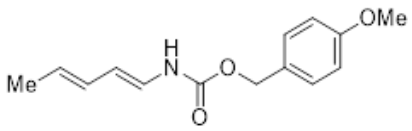
4-Methylbenzyl ((1*E*,3*E*)-penta-1,3-dien-1-yl)carbamate (9b)



78% yield [*Procedure D*]; white solid; R_f = 0.36 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.24 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.58 (t, *J* = 12.0 Hz, 1H), 6.28 (brs, 1H), 5.95 (t, *J* = 12.0 Hz, 1H), 5.61 (t, *J* = 12.0 Hz, 1H), 5.49 (qd, *J* = 12.0, 6.6 Hz, 1H), 5.10 (s, 2H), 2.34 (s, 3H), 1.72 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.5, 138.4, 133.0, 130.2, 129.4, 128.6, 125.9, 124.3, 112.0, 67.4, 21.4, 18.3; IR (ATR)

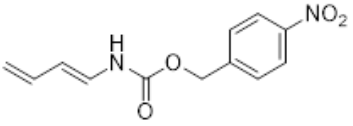
3300, 3062, 3013, 2952, 2910, 2880, 2848, 1688, 1663, 1637, 1523, 1461, 1376, 1326, 1274, 1228, 1166, 1058, 974, 924, 811, 784, 690 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{14}H_{17}NO_2$ 231.12593, found: 231.12584.

4-Methoxybenzyl ((1*E*,3*E*)-penta-1,3-dien-1-yl)carbamate (10b)



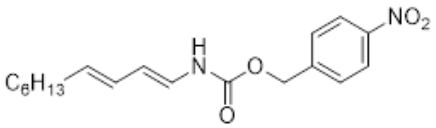
77% yield [*Procedure D*]; pale yellow solid; R_f = 0.18 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.28 (d, *J* = 8.4 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 2H), 6.58 (dd, *J* = 12.0, 12.0 Hz, 1H), 6.26 (brs, 1H), 5.95 (dd, *J* = 12.0, 12.0 Hz, 1H), 5.61 (dd, *J* = 12.0, 12.0 Hz, 1H), 5.49 (qd, *J* = 12.0, 6.6 Hz, 1H), 5.08 (s, 2H), 3.80 (s, 3H), 1.72 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.9, 153.5, 130.3, 128.6, 128.1, 125.9, 124.3, 114.1, 111.9, 67.3, 55.4, 18.3; IR (ATR) 3301, 3066, 3011, 2957, 2912, 2838, 1694, 1664, 1638, 1615, 1529, 1516, 1455, 1326, 1273, 1250, 1232, 1176, 1065, 1034, 972, 925, 813, 768 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{14}H_{17}NO_3$ 247.12084, found: 247.12080.

4-Nitrobenzyl (*E*)-buta-1,3-dien-1-ylcarbamate (8a)



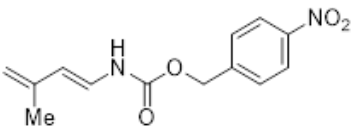
60% yield [*Procedure D*]; pale yellow solid; R_f = 0.12 (Hexane/EtOAc= 3/1); Mp: 111.3-113.8 ˚C; ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.21 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 6.70 (dd, *J* = 12.0, 12.0 Hz, 1H), 6.51 (brs, 1H), 6.29-6.23 (m, 1H), 5.74 (s, 1H), 5.25 (s, 2H), 5.06 (d, *J* = 16.8 Hz, 1H), 4.94 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.0, 147.9, 143.3, 134.3, 134.3, 128.5, 126.6, 124.0, 114.3, 113.1, 65.9; IR (ATR) 3301, 3116, 3090, 3061, 2979, 2938, 2882, 1702, 1660, 1606, 1530, 1509, 1354, 1294, 1282, 1240, 1175, 1066, 997, 926, 898, 842, 737, 687 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{12}H_{12}N_2O_4$ 248.07971, found: 248.07956.

4-Nitrobenzyl ((1*E*,3*E*)-deca-1,3-dien-1-yl)carbamate (8c)



66% yield [*Procedure D*]; pale yellow solid; R_f = 0.20 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.21 (d, *J* = 7.8 Hz, 2H), 7.50 (d, *J* = 7.8 Hz, 2H), 6.57 (dd, *J* = 12.0, 12.0 Hz, 1H), 6.37 (brs, 1H), 5.94 (dd, *J* = 15.6, 12.0 Hz, 1H), 5.69 (dd, *J* = 12.0, 12.0 Hz, 1H), 5.54 (td, *J* = 15.6, 7.2 Hz, 1H), 5.24 (s, 2H), 2.05 (q, *J* = 7.2 Hz, 2H), 1.39-1.34 (m, 2H), 1.31-1.23 (m, 6H), 0.88 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ153.0, 147.9, 143.4, 132.4, 128.4, 127.0, 124.0, 123.9, 113.0, 65.8, 32.9, 31.9, 29.5, 29.0, 22.8, 14.2; IR (ATR) 3330, 3066, 3019, 2957, 2925, 2853, 1698, 1661, 1633, 1610, 1522, 1457, 1347, 1277, 1229, 1054, 977, 848, 768, 738 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{18}H_{24}N_2O_4$ 332.17361, found: 332.17353.

4-Nitrobenzyl (*E*)-(3-methylbuta-1,3-dien-1-yl)carbamate (8d)



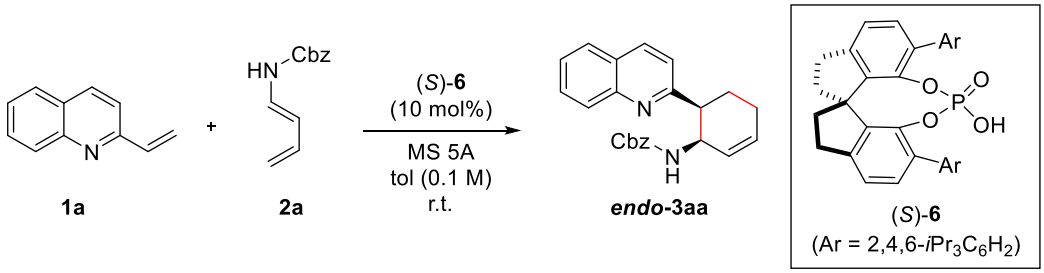
68% yield [*Procedure D*]; pale yellow solid; R_f = 0.32 (Hexane/EtOAc= 3/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.21 (d, *J* = 7.8 Hz, 2H), 7.51 (d, *J* = 7.8 Hz, 2H), 6.67 (dd, *J* = 12.6, 12.6 Hz, 1H), 6.50 (brs, 1H), 5.82 (d, *J* = 12.6 Hz, 1H), 5.25 (s, 2H), 4.82 (s, 2H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.2, 147.9, 143.3, 140.1, 128.5, 124.0, 123.6, 115.2, 114.1, 65.9, 18.8; IR (ATR) 3312, 3083, 2976, 2948, 2891, 1712, 1656, 1608, 1521, 1348, 1281, 1227,

1069, 1015, 947, 854, 767 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{13}H_{14}N_2O_4$ 262.09536, found: 262.09528.

3. Enantioselective Diels-Alder Reaction of 2-Vinyl Quinolines with Dienylcarbamates

3-1. General Procedure

Representative procedure for the enantioselective Diels-Alder reaction of 2-vinyl quinolines **1a** with dienylcarbamate **2a** catalyzed by chiral phosphoric acid (*S*)-**6**.

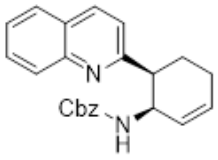


1a **2a** ***endo*-3aa** (*S*)-**6** (Ar = 2,4,6-*i*$Pr_3C_6H_2$)

To a solution of **1a** (15.5 mg, 0.1 mmol), **2a** (24.4 mg, 0.12 mmol) and pre-activated MS 5A (50 mg) in dry toluene (1.0 ml), (*S*)-**6** (7.2 mg, 10 mol %) was added. The reaction mixture was stirred at room temperature for 5 days. This suspension was directly charged into column chromatography (Hexane/ EtOAc = 3/1) and purified to give **3aa** (32.6 mg, 0.091 mmol, 91%) as colorless oil. The enantiomeric and diastereomeric excess were determined by chiral stationary phase HPLC analysis.

<u>In all cases, Diels-Alder adducts show multiple resonance for the presence of different rotational isomers at 20 ℃. Therefore, we conducted ^{1}H NMR measurements at 50 ℃ for product characterization.</u>

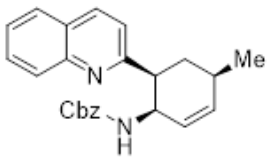
Benzyl (*1R,6S*)-6-(quinolin-2-yl)cyclohex-2-enylcarbamate (3aa)



91% yield (32.6 mg); colorless oil; $[\alpha]_D^{23.0}$ = -112.4 (*c* = 1.0, $CHCl_3$, 92% ee); R_f = 0.15 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.01 (t, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.21-7.16 (m, 3H), 7.05 (brs, 2H), 5.94-5.85 (m, 2H), 5.59 (brs, 1H), 4.86-4.74 (m, 2H), 4.68 (brs, 1H), 3.44 (s, 1H), 2.22-2.03 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 155.8, 147.6, 136.7, 136.1, 129.8, 129.4, 128.4, 127.9, 127.9, 127.6, 127.0, 126.0, 121.4, 66.3, 48.8, 45.9, 24.7, 23.5; IR (ATR) 3418, 3323, 3060, 3028, 2934, 2836, 1714, 1601, 1504, 1455, 1330, 1220, 1120, 1058, 1002, 829, 771, 697 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{22}N_2O_2$ 358.16813, found: 358.16806.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 ℃, 254 nm) 14.2 min (major), 39.8 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by chiral HPLC charts comparison (see, section 6).

Benzyl ((*1R,4R,6S*)-4-methyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (3ab)

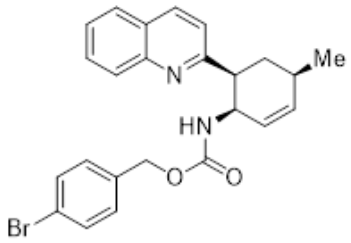


86% yield (32.0 mg); colorless oil; $[\alpha]_D^{23.0}$ = -115.0 (*c* = 1.0, $CHCl_3$, 91% ee); R_f = 0.18 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.03 (t, *J* = 7.8 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.65 (t, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.19-7.14 (m, 3H), 6.98 (brs, 2H), 5.89 (brs, 1H),

5.78 (d, *J* = 8.4 Hz, 1H), 5.17 (brs, 1H), 4.74-4.56 (m, 3H), 3.42-3.36 (m, 1H), 2.37 (brs, 1H), 2.12 (brs, 1H), 1.75 (q, *J* = 12.6 Hz, 1H), 1.11 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 155.6, 147.9, 136.9, 136.6, 136.0, 129.4, 129.3, 128.4, 127.9, 127.8, 127.7, 127.1, 126.3, 126.0, 121.6, 66.3, 48.5, 46.5, 31.9, 31.0, 21.5; IR (ATR) 3421, 3322, 3062, 3022, 2955, 2927, 2870, 1711, 1601, 1505, 1331, 1220, 1069, 828, 772, 697 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{24}H_{24}N_2O_2$ 372.18378, found: 372.18359.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 ℃, 254 nm) 11.2 min (major), 33.4 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 4R, 6S*) by analogy and NOESY experiment (see, section 6).

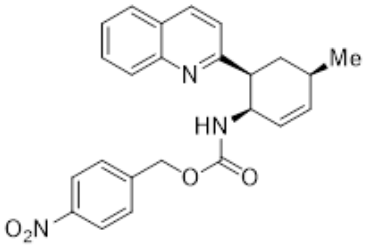
4-Bromobenzyl ((*1R,4R,6S*)-4-methyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (11ab)



98% yield (44.3 mg); colorless oil; $[\alpha]_D^{23.0}$ = -94.8 (*c* = 1.0, $CHCl_3$, 95% ee); R_f = 0.10 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.01 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 2H), 6.79 (brs, 2H), 5.88 (brs, 1H), 5.78 (d, *J* = 10.2 Hz, 1H), 5.20 (brs, 1H), 4.72-4.48 (m, 3H), 3.42-3.35 (m, 1H), 2.37 (brs, 1H), 2.11 (brs, 1H), 1.75 (q, *J* = 13.2 Hz, 1H), 1.12 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.1, 155.4, 147.8, 137.0, 136.0, 135.7, 131.4, 129.4, 129.3, 127.7, 127.1, 126.2, 126.1, 121.8, 121.6, 65.3, 48.5, 46.4, 31.9, 30.9, 21.4, one carbon was not found probably due to overlapping; IR (ATR) 3421, 3322, 3019, 2955, 2925, 2870, 1713, 1601, 1505, 1332, 1235, 1071, 1011, 887, 828, 771 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}BrN_2O_2$ 450.09429, found: 450.09427.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 ℃, 254 nm) 11.5 min (major), 29.6 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 4R, 6S*) by analogy.

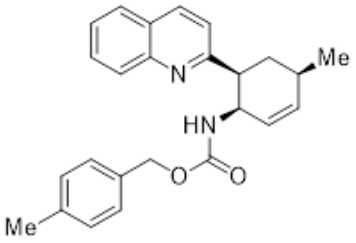
4-Nitrobenzyl ((*1R,4R,6S*)-4-methyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12ab)



98% yield (40.9 mg); colorless oil; $[\alpha]_D^{23.0}$ = -82.2 (*c* = 1.0, $CHCl_3$, 98% ee); R_f = 0.14 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.07-8.00 (m, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 7.2 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 7.2 Hz, 1H), 7.03-6.93 (m, 2H), 5.92-5.86 (m, 1H), 5.81 (d, *J* = 10.2 Hz, 1H), 5.33 (brs, 1H), 4.88 (d, *J* = 12.0 Hz, 1H), 4.68 (d, *J* = 12.0 Hz, 1H), 4.62 (brs, 1H), 3.42-3.37 (m, 1H), 2.38 (brs, 1H), 2.18-2.09 (m, 1H), 1.78 (q, *J* = 13.2 Hz, 1H), 1.13 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.1, 155.1, 147.8, 147.3, 144.2, 137.3, 136.0, 129.4, 129.2, 127.7, 127.5, 127.0, 126.2, 126.0, 123.5, 121.8, 64.6, 48.6, 46.3, 31.9, 30.9, 21.4; IR (ATR) 3414, 3315, 3020, 2956, 2927, 2871, 1716, 1604, 1520, 1347, 1232, 1110, 1076, 1013, 829, 755 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}N_3O_4$ 417.16886, found: 417.16856.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 ℃, 254 nm) 24.0 min (major), 63.9 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 4R, 6S*) by analogy.

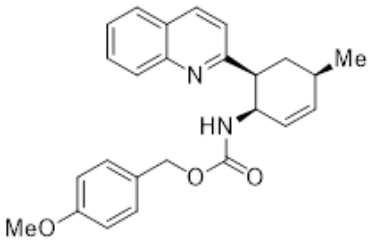
4-Methylbenzyl ((*1R,4R,6S*)-4-methyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (13ab)



85% yield (33.2 mg); colorless oil; $[\alpha]_D^{23.0}$ = -113.1 (*c* = 1.0, $CHCl_3$, 90% ee); R_f = 0.25 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.03 (d, *J* = 7.8 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.65 (t, *J* = 6.6 Hz, 1H), 7.47 (t, *J* = 6.6 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 6.95 (d, *J* = 7.2 Hz, 2H), 6.88 (brs, 2H), 5.89 (brs, 1H), 5.77 (d, *J* = 10.2 Hz, 1H), 5.13 (brs, 1H), 4.71-4.53 (m, 3H), 3.42-3.34 (m, 1H), 2.41-2.33 (m, 1H), 2.28 (s, 3H), 2.11 (brs, 1H), 1.74 (q, *J* = 13.2 Hz, 1H), 1.11 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 155.7, 147.8, 137.6, 136.8, 136.0, 133.6, 129.4, 129.2, 129.1, 128.0, 127.7, 127.1, 126.4, 125.9, 121.6, 66.2, 48.4, 46.5, 31.9, 31.0, 21.4, 21.3; IR (ATR) 3418, 3320, 3020, 2954, 2927, 2870, 1713, 1602, 1505, 1334, 1235, 1120, 1070, 1015, 829, 755 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{25}H_{26}N_2O_2$ 386.19943, found: 386.19936.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 °C, 254 nm) 10.2 min (major), 27.6 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 4R, 6S*) by analogy.

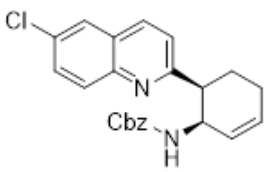
4-Methoxybenzyl ((*1R,4R,6S*)-4-methyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (14ab)



95% yield (38.3 mg); colorless oil; $[\alpha]_D^{23.0}$ = -109.5 (*c* = 1.0, $CHCl_3$, 90% ee); R_f = 0.12 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.03 (d, *J* = 7.8 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.66 (td, *J* = 7.8, 1.2 Hz, 1H), 7.48 (td, *J* = 7.8, 1.2 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 6.91 (brs, 2H), 6.67 (d, *J* = 8.4 Hz, 2H), 5.88 (brs, 1H), 5.77 (d, *J* = 10.2 Hz, 1H), 5.11 (brs, 1H), 4.68-4.54 (m, 3H), 3.75 (s, 3H), 3.41-3.35 (m, 1H), 2.41-2.33 (m, 1H), 2.11 (brs, 1H), 1.73 (q, *J* = 14.4 Hz, 1H), 1.11 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 159.4, 155.7, 147.9, 136.8, 136.0, 129.6, 129.4, 129.2, 128.8, 127.7, 127.1, 126.4, 126.0, 121.6, 113.8, 66.1, 55.4, 48.4, 46.5, 31.9, 31.0, 21.5; IR (ATR) 3312, 3015, 2955, 2925, 2870, 1714, 1614, 1515, 1466, 1334, 1303, 1236, 1175, 1089, 888, 829, 771 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{25}H_{26}N_2O_3$ 402.19434, found: 402.19427.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40 °C, 254 nm) 13.5 min (major), 33.8 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 4R, 6S*) by analogy.

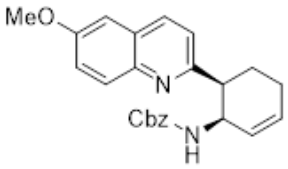
Benzyl (*1R,6S*)-6-(6-chloroquinolin-2-y)cyclohex-2-enylcarbamate (3ba)



95% yield (37.3 mg); colorless oil; $[\alpha]_D^{23.0}$ = -119.2 (*c* = 1.0, $CHCl_3$, 93% ee); R_f = 0.12 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.93 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.71 (s, 1H), 7.56 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.23-7.15 (m, 3H), 7.04 (brs, 2H), 5.89 (s, 2H), 5.36 (brs, 1H), 4.81-4.73 (m, 2H), 4.67 (brs, 1H), 3.46-3.34 (m, 1H), 2.20-2.04 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 156.7, 146.0, 136.6, 135.1, 131.6, 131.0, 130.1, 130.0, 128.4, 128.0, 127.9, 127.6, 127.5, 126.3, 122.3, 66.3, 48.7, 46.0, 24.8, 23.0; IR (ATR) 3421, 3332, 3029, 2937, 2836, 1719, 1599, 1493, 1455, 1335, 1307, 1234, 1058, 880, 834, 751, 697 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}ClN_2O_2$ 392.12915, found: 392.12919.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 °C, 254 nm) 16.4 min (major), 29.6 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

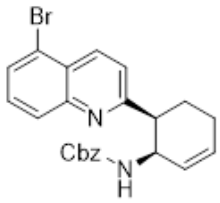
Benzyl ((*1R,6S*)-6-(6-methoxyquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (3ca)



72% yield (28.0 mg); colorless oil; $[\alpha]_D^{23.0}$ = -107.4 (*c* = 1.0, $CHCl_3$, 82% ee); R_f = 0.10 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.91 (d, *J* = 9.0 Hz, 2H), 7.32-7.26 (m, 2H), 7.22-7.16 (m, 3H), 7.07 (brs, 2H), 7.03 (d, *J* = 2.4 Hz, 1H), 5.94-5.84 (m, 2H), 5.58 (brs, 1H), 4.87-4.73 (m, 2H), 4.64 (brs, 1H), 3.91 (s, 3H), 3.44-3.36 (m, 1H), 2.18-2.04 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.6, 157.5, 155.8, 143.7, 136.7, 135.0, 130.8, 129.8, 128.4, 128.0, 127.9, 127.8, 121.9, 121.7, 105.3, 66.3, 55.7, 48.9, 45.6, 24.8, 23.5, one carbon was not found probably due to overlapping) ; IR (ATR) 3414, 3331, 3028, 2938, 2907, 2836, 1715, 1625, 1602, 1500, 1456, 1382, 1331, 1231, 1162, 1114, 1058, 1029, 856, 834, 738, 698 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{24}H_{24}N_2O_3$ 388.17869, found: 388.17867.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 °C, 254 nm) 17.2 min (major), 28.2 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

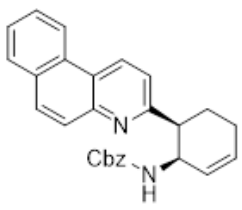
Benzyl ((*1R,6S*)-6-(5-bromoquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (3da)



97% yield (42.4 mg); colorless oil; $[\alpha]_D^{23.0}$ = -98.6 (*c* = 1.0, $CHCl_3$, 86% ee); R_f = 0.14 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.39 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 8.4 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.21-7.16 (m, 3H), 7.04 (brs, 2H), 5.89 (s, 2H), 5.40 (brs, 1H), 4.86-4.75 (m, 2H), 4.70 (brs, 1H), 3.51-3.40 (m, 1H), 2.21-2.05 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.0, 155.7, 148.3, 136.6, 135.5, 130.0, 129.8, 129.5, 129.3, 128.4, 128.0, 127.9, 127.7, 126.5, 122.6, 121.9, 66.4, 48.6, 45.9, 24.8, 23.2; IR (ATR) 3418, 3325, 3062, 3027, 2927, 1719, 1593, 1552, 1496, 1455, 1394, 1332, 1235, 1120, 1057, 999, 951, 815, 759, 697 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}BrN_2O_2$ 436.07864, found: 436.07846.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 °C, 254 nm) 11.1 min (major), 23.3 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

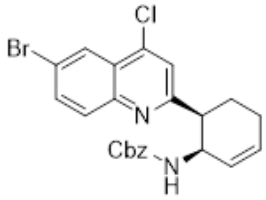
Benzyl ((*1R,6S*)-6-(benzo[f]quinolin-3-yl)cyclohex-2-en-1-yl)carbamate (3ea)



63% yield (25.7 mg); colorless oil; $[\alpha]_D^{23.0}$ = -124.5 (*c* = 1.0, $CHCl_3$, 85% ee); R_f = 0.12 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.79 (d, *J* = 8.4 Hz, 1H), 8.56 (d, *J* = 7.8 Hz, 1H), 7.96-7.89 (m, 3H), 7.67 (td, *J* = 7.2, 1.2 Hz, 1H), 7.62 (td, *J* = 7.2, 1.2 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.14-7.06 (m, 3H), 7.02 (brs, 2H), 5.96-5.88 (m, 2H), 5.55 (brs, 1H), 4.84-4.73 (m, 2H), 4.70 (brs, 1H), 3.55-3.41 (m, 1H), 2.28-2.07 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.7, 155.8, 147.5, 136.7, 131.7, 130.9, 130.6, 129.9, 129.8, 128.7, 128.5, 128.3, 127.9, 127.0, 123.8, 122.7, 121.3, 66.3, 48.9, 45.6, 24.9, 23.4, three carbons were not found probably due to overlapping ; IR (ATR) 3414, 3322, 3060, 3029, 2922, 2833, 1714, 1498, 1456, 1335, 1235, 1087, 1063, 874, 834, 752, 698 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{27}H_{24}N_2O_2$ 408.18378, found: 408.18359.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 °C, 254 nm) 17.7 min (major), 37.1 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

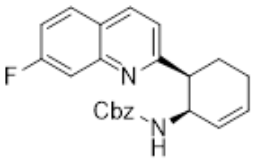
Benzyl ((*1R,6S*)-6-(6-bromo-4-chloroquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (3fa)



83% yield (39.2 mg); white solid; $[\alpha]^{23.0}_{D}$ = -115.4 (*c* = 1.0, $CHCl_3$, 91% ee); R_f = 0.20 (Hexane/EtOAc= 6/1); Mp: 253.2-255.4 ℃; ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.31 (brs, 1H), 7.86 (d, *J* = 9.0 Hz, 1H), 7.74 (dd, *J* = 9.0, 1.8 Hz, 1H), 7.45 (s, 1H), 7.23-7.17 (m, 3H), 7.06 (brs, 2H), 5.92-5.84 (m, 2H), 5.25 (brs, 1H), 4.83-4.74 (m, 2H), 4.66 (brs, 1H), 3.42-3.31 (m, 1H), 2.21-1.98 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.8, 155.6, 147.0, 141.2, 136.4, 133.7, 131.4, 130.1, 128.5, 128.0, 127.4, 126.4, 122.1, 121.2, 66.3, 48.5, 46.2, 24.8, 23.0, two carbons were not found probably due to overlapping ; IR (ATR) 3422, 3319, 3064, 3029, 2935, 2835, 1704, 1587, 1546, 1498, 1478, 1455, 1335, 1311, 1235, 1059, 988, 875, 828, 755, 698 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{20}BrClN_2O_2$ 470.03967, found: 470.03946.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 °C, 254 nm) 10.1 min (major), 20.3 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

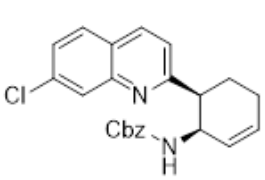
Benzyl ((*1R,6S*)-6-(7-fluoroquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (3ga)



96% yield (36.1 mg); colorless oil; $[\alpha]_D^{23.0}$ = -104.4 (*c* = 1.0, $CHCl_3$, 87% ee); R_f = 0.12 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.98 (d, *J* = 8.4 Hz, 1H), 7.72 (dd, *J* = 8.4, 6.0 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.26 (td, *J* = 8.4, 1.8 Hz, 1H), 7.22-7.16 (m, 3H), 7.05 (brs, 2H), 5.89 (s, 2H), 5.42 (brs, 1H), 4.86-4.73 (m, 2H), 4.67 (brs, 1H), 3.48-3.35 (m, 1H), 2.23-2.01 (m, 4H); ^{19}F NMR (565 MHz, $CDCl_3$, VT50) δ -110.4 (s, 1F); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.1 (d, C-F, $J_{C\text{-}F}$ = 250.0 Hz), 163.4, 155.7, 148.6 (d, C-F, $J_{C\text{-}F}$ = 13.0 Hz), 136.6, 135.9, 130.0, 129.6 (d, C-F, $J_{C\text{-}F}$ = 8.8 Hz), 128.4, 128.0, 127.9 127.7, 123.9, 120.9, 116.4 (d, C-F, $J_{C\text{-}F}$ = 24.6 Hz), 113.1 (d, C-F, $J_{C\text{-}F}$ = 20.2 Hz), 66.4, 48.7, 46.0, 24.8, 23.2; IR (ATR) 3414, 3324, 3066, 3029, 2924, 2835, 1713, 1627, 1602, 1510, 1455, 1433, 1335, 1236, 1212, 1165, 1086, 1059, 968, 871, 847, 751, 698 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}FN_2O_2$ 376.15871, found: 376.15870.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3, 1.0 mL/min, 40 °C, 254 nm) 12.6 min (major), 19.8 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

Benzyl (*1R,6S*)-6-(7-chloroquinolin-2-y)cyclohex-2-enylcarbamate (3ha)

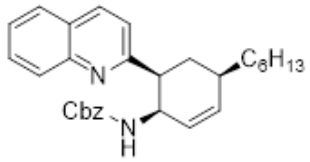


79% yield (31.0 mg); colorless oil; $[\alpha]_D^{23.0}$ = -51.9 (*c* = 1.0, $CHCl_3$, 49% ee); R_f = 0.10 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.02 (brs, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.23-7.17 (m, 3H), 7.05 (brs, 2H), 5.89 (s, 2H), 5.39 (brs, 1H), 4.84-4.71 (m, 2H), 4.67 (brs, 1H), 3.48-3.34 (m, 1H), 2.28-2.00 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ163.3, 155.7, 148.0, 136.5, 135.8, 135.1, 130.0, 128.9, 128.4, 128.3, 128.0, 127.7, 127.0, 125.3, 121.8, 66.4, 48.7, 46.0, 24.8, 23.2; IR (ATR) 3421, 3322, 3029, 2937, 2836, 1719, 1614, 1497, 1337, 1236, 1060, 883, 848, 735, 697 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}ClN_2O_2$ 392.12915, found: 392.12900.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 97/3,

1.0 mL/min, 40 °C, 254 nm) 15.8 min (major), 26.0 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

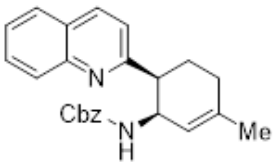
Benzyl ((*1R,4R,6S*)-4-hexyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (3ac)



89% yield (39.3 mg); colorless oil; $[\alpha]_D^{23.0}$ = -116.8 (*c* = 1.0, $CHCl_3$, 93% ee); R_f = 0.30 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.75 (t, *J* = 7.2 Hz, 1H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.21-7.09 (m, 3H), 6.98 (brs, 2H), 5.91 (brs, 1H), 5.83 (d, *J* = 9.6 Hz, 1H), 5.27-5.09 (m, 1H), 4.80-4.64 (m, 2H), 4.60 (brs, 1H), 3.41-3.34 (m, 1H), 2.26 (brs, 1H), 2.19-2.04 (m, 1H), 1.76 (q, *J* = 13.8 Hz, 1H), 1.51-1.36 (m, 4H), 1.35-1.25 (m, 6H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.4, 155.6, 147.9, 136.7, 136.0, 135.9, 129.4, 129.3, 128.4, 127.9, 127.8, 127.7, 127.1, 126.6, 126.0, 121.6, 66.3, 48.8, 46.5, 36.9, 36.0, 32.0, 29.6, 28.8, 26.8, 22.8, 14.2; IR (ATR) 3312, 3062, 3031, 2954, 2925, 2854, 1708, 1602, 1505, 1456, 1337, 1220, 1083, 828, 771, 697 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{29}H_{34}N_2O_2$ 442.26203, found: 442.26177.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 98/2, 1.0 mL/min, 40 °C, 254 nm) 12.0 min (major), 28.4 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 4R, 6S*) by analogy.

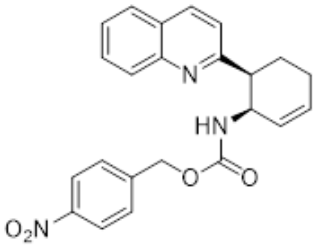
Benzyl ((*1R,6S*)-3-methyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (3ad)



87% yield (32.5 mg); colorless oil; $[\alpha]_D^{23.0}$ = -148.2 (*c* = 1.0, $CHCl_3$, 96% ee); R_f = 0.16 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.64 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.21-7.13 (m, 3H), 7.03 (brs, 2H), 5.64 (s, 1H), 5.42 (brs, 1H), 4.90-4.69 (m, 2H), 4.64 (brs, 1H), 3.39-3.32 (m, 1H), 2.22-2.00 (m, 4H), 1.73 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.4, 155.8, 147.7, 137.8, 136.8, 136.0, 129.4, 129.3, 128.4, 127.9, 127.8, 127.7, 127.0, 126.0, 122.2, 121.5, 66.2, 49.2, 45.8, 30.0, 23.6, 23.4; IR (ATR) 3418, 3331, 3038, 2930, 2910, 2829, 1719, 1601, 1504, 1454, 1334, 1234, 1057, 1026, 968, 830, 752, 698 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{24}H_{24}N_2O_2$ 372.18378, found: 372.18375.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40 °C, 254 nm) 11.6 min (major), 35.5 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

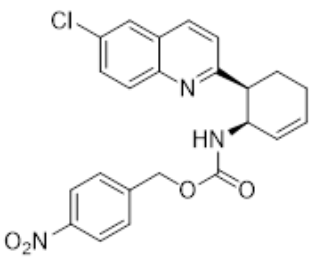
4-Nitrobenzyl ((*1R,6S*)-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12aa)



99% yield (40.0 mg); pale yellow oil; $[\alpha]_D^{23.0}$ = -107.8 (*c* = 1.0, $CHCl_3$, 98% ee); R_f = 0.22 (Hexane/EtOAc= 3/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.01 (d, *J* = 8.4 Hz, 2H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.07 (brs, 2H), 5.92 (s, 2H), 5.72 (brs, 1H), 4.93 (d, *J* = 12.6 Hz, 1H), 4.78 (d, *J* = 12.6 Hz, 1H), 4.68 (s, 1H), 3.48-3.40 (m, 1H), 2.32-1.96 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 155.3, 147.8, 147.6, 144.3, 136.1, 130.1, 129.4, 127.8, 127.6, 127.1, 126.3, 123.6, 121.6, 64.8, 49.0, 45.8, 24.9, 23.4, two carbons were not found probably due to overlapping; IR (ATR) 3411, 3322, 3062, 3026, 2934, 2876, 2836, 1715, 1603, 1520, 1428, 1346, 1234, 1114, 1062, 1002, 829, 756 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}N_3O_4$ 403.15321, found: 403.15312.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40℃, 254 nm) 23.7 min (major), 46.8 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

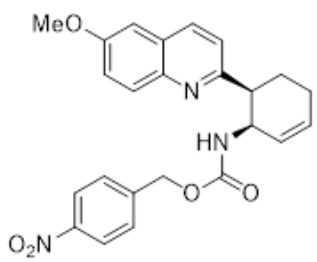
4-Nitrobenzyl ((*1R,6S*)-6-(6-chloroquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12ba)



99% yield (43.4 mg); colorless oil; $[\alpha]_D^{23.0}$ = -105.8 (*c* = 1.0, $CHCl_3$, 99% ee); R_f = 0.16 (Hexane/EtOAc= 3/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.99 (d, *J* = 8.4 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 2H), 7.74 (s, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.14 (brs, 2H), 5.97-5.87 (m, 2H), 5.55 (brs, 1H), 4.89-4.77 (m, 2H), 4.66 (brs, 1H), 3.47-3.37 (m, 1H), 2.40-1.96 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 155.2, 147.5, 146.0, 144.2, 135.2, 131.9, 130.9, 130.4, 130.3, 127.8, 127.5, 127.4, 126.3, 123.6, 122.5, 64.8, 48.9, 45.9, 24.9, 23.0; IR (ATR) 3240, 3026, 2937, 2877, 1719, 1600, 1521, 1492, 1346, 1238, 1176, 1062, 1009, 836, 752 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{20}ClN_3O_4$ 437.11423, found: 437.11427.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40 °C, 254 nm) 24.8 min (major), 36.2 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

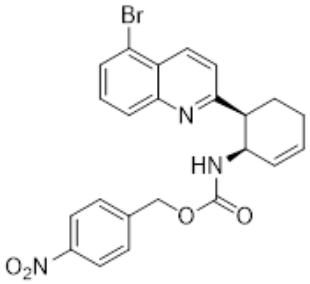
4-Nitrobenzyl ((*1R,6S*)-6-(6-methoxyquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12ca)



92% yield (39.7 mg); pale yellow oil; $[\alpha]_D^{23.0}$ = -89.0 (*c* = 1.0, $CHCl_3$, 96% ee); R_f = 0.10 (Hexane/EtOAc= 3/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 7.90 (dd, *J* = 9.0, 9.0 Hz, 4H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 7.11-6.93 (m, 3H), 5.91 (s, 2H), 5.70 (brs, 1H), 4.97 (d, *J* = 12.6 Hz, 1H), 4.78 (d, *J* = 12.6 Hz, 1H), 4.64 (brs, 1H), 3.94 (s, 3H), 3.43-3.36 (m, 1H), 2.30-1.95 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.5, 157.6, 155.3, 147.3, 144.5, 143.7, 135.0, 130.7, 130.2, 127.9, 127.5, 123.5, 122.1, 121.8, 105.1, 64.6, 55.7, 48.9, 45.5, 25.0, 23.1, one carbon was not found probably due to overlapping; IR (ATR) 3414, 3331, 3026, 2939, 2907, 2837, 1716, 1625, 1603, 1520, 1502, 1347, 1232, 1113, 1063, 1029, 856, 836, 738 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}N_3O_5$ 433.16377, found: 433.16372; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40 °C, 254 nm) 27.8 min (major), 44.5 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

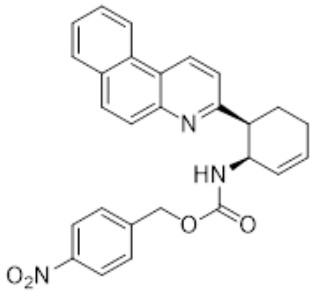
4-Nitrobenzyl ((*1R,6S*)-6-(5-bromoquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12da)



97% yield (46.7 mg); colorless oil; $[\alpha]_D^{23.0}$ = -102.7 (*c* = 1.0, $CHCl_3$, 98% ee); R_f = 0.14 (Hexane/EtOAc= 3/1); ^1H NMR (600 MHz, $CDCl_3$, VT50) δ 8.38 (d, *J* = 7.8 Hz, 1H), 8.01-7.90 (m, 3H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.10 (brs, 2H), 5.97-5.87 (m, 2H), 5.51 (brs, 1H), 4.93 (d, *J* = 13.2 Hz, 1H), 4.78 (d, *J* = 13.2 Hz, 1H), 4.70 (brs, 1H), 3.52-3.40 (m, 1H), 2.30-2.08 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.0, 155.2, 148.3, 147.4, 144.1, 135.4, 130.5, 129.9, 129.6, 129.2, 127.7, 127.3, 126.4, 123.6, 122.8, 122.0, 64.8, 48.8, 45.8, 24.9, 22.9; IR (ATR) 3414, 3325, 3026, 2922, 2833, 1720, 1608, 1553, 1521, 1394, 1347, 1235, 1087, 1063, 883, 858, 816, 761 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{20}BrN_3O_4$ 481.06372, found: 481.06361.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40 °C, 254 nm) 25.8 min (major), 57.5 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

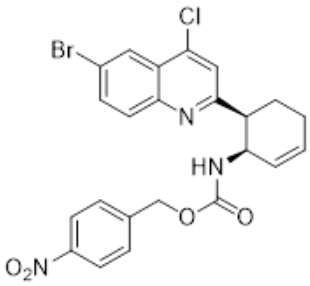
4-Nitrobenzyl ((*1R,6S*)-6-(benzo[f]quinolin-3-yl)cyclohex-2-en-1-yl)carbamate (12ea)



96% yield (43.6 mg); white solid; $[\alpha]_D^{23.0}$ = -141.3 (*c* = 1.0, $CHCl_3$, 98% ee); R_f = 0.16 (Hexane/EtOAc= 3/1); Mp: 160.7-162.5 ℃; ^1H NMR (600 MHz, $CDCl_3$, VT50) δ 8.79 (d, *J* = 7.8 Hz, 1H), 8.54 (d, *J* = 7.8 Hz, 1H), 7.96-7.86 (m, 3H), 7.84-7.73 (m, 2H), 7.68 (t, *J* = 7.8 Hz, 1H), 7.64 (t, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 7.2 Hz, 1H), 7.03 (brs, 2H), 5.94 (s, 2H), 5.68 (brs, 1H), 4.91 (d, *J* = 11.4 Hz, 1H), 4.74 (d, *J* = 11.4 Hz, 1H), 4.69 (s, 1H), 3.54-3.42 (m, 1H), 2.32-2.04 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.6, 155.3, 147.5,147.3, 144.2, 131.6, 130.9, 130.8, 130.3, 129.7, 128.8, 128.3, 127.6, 127.5, 127.3, 123.8, 123.5, 122.5, 121.5, 64.7, 49.0, 45.5, 25.0, 23.1, one carbon was not found probably due to overlapping; IR (ATR) 3411, 3326, 3060, 3027, 2922, 2836, 1719, 1606, 1520, 1346, 1235, 1087, 1063, 834, 752 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{27}H_{23}N_3O_4$ 453.16886, found: 453.16875.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40 °C, 254 nm) 37.0 min (major), 72.6 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

4-Nitrobenzyl ((*1R,6S*)-6-(6-bromo-4-chloroquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12fa)

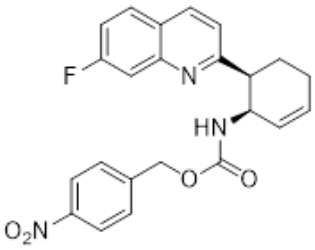


86% yield (44.3 mg); white solid; $[\alpha]_D^{23.0}$ = -121.1 (*c* = 1.0, $CHCl_3$, 99% ee); R_f = 0.30 (Hexane/EtOAc= 3/1); Mp: 131.6-133.9 ℃; ^1H NMR (600 MHz, $CDCl_3$, VT50) δ 8.31 (s, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.46 (s, 1H), 7.18 (brs, 2H), 5.97-5.85 (m, 2H), 5.40 (brs, 1H), 4.99-4.77 (m, 2H), 4.66 (brs, 1H), 3.44-3.32 (m, 1H), 2.34-1.95 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7, 155.1, 147.5, 146.9, 144.0, 141.2, 133.9, 131.3, 130.5, 127.9, 127.1, 126.4, 126.3, 123.6, 122.2, 121.3, 64.9, 48.7, 46.0, 24.8, 22.9; IR (ATR) 3418, 3322, 3080, 3027, 2940, 2836, 1720, 1606, 1587, 1520, 1477, 1346, 1234, 1063, 853, 829, 753 cm^{-1}; HRMS (FD+) m/z:

$[M+H]^+$ Calcd for $C_{23}H_{19}BrClN_3O_4$ 515.02475, found: 515.02440.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 95/5, 1.0 mL/min, 40 °C, 254 nm) 18.0 min (major), 33.2 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

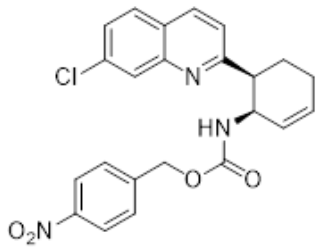
4-Nitrobenzyl ((*1R,6S*)-6-(7-fluoroquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12ga)



99% yield (41.5 mg); colorless oil; $[\alpha]_D^{23.0}$ = -95.4 (*c* = 1.0, $CHCl_3$, 98% ee); R_f = 0.20 (Hexane/EtOAc= 3/1); ^1H NMR (600 MHz, $CDCl_3$, VT50) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 2H), 7.73 (t, *J* = 7.2 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.34-7.26 (m, 2H), 7.13 (d, *J* = 7.2 Hz, 2H), 5.95-5.86 (m, 2H), 5.58 (brs, 1H), 4.91 (d, *J* = 13.2 Hz, 1H), 4.80 (d, *J* = 13.2 Hz, 1H), 4.66 (brs, 1H), 3.45-3.38 (m, 1H), 2.24-1.96 (m, 4H); ^{19}F NMR (565 MHz, $CDCl_3$, VT50) δ -109.9 (s, 1F); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.1 (d, C-F, $J_{C\text{-}F}$ = 247.0 Hz), 163.3, 155.2, 148.5 (d, C-F, $J_{C\text{-}F}$ = 12.9 Hz), 147.4, 144.2, 136.0, 130.3, 129.6 (d, C-F, $J_{C\text{-}F}$ = 8.6 Hz), 127.8, 127.4, 123.9 123.6, 121.0, 116.6 (d, C-F, $J_{C\text{-}F}$ = 18.8 Hz), 112.9 (d, C-F, $J_{C\text{-}F}$ = 18.8 Hz), 64.7, 48.8, 45.9, 24.9, 23.0; IR (ATR) 3405, 3324, 3027, 2925, 1714, 1626, 1604, 1511, 1432, 1346, 1235, 1165, 1110, 1086, 1062, 846, 754 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{20}FN_3O_4$ 421.14378, found: 421.14374; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40 °C, 254 nm) 23.3 min (major), 37.1 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

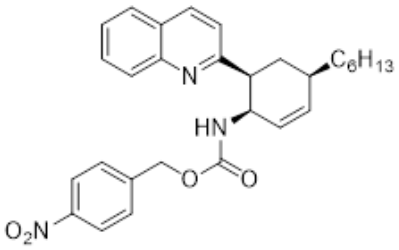
4-Nitrobenzyl ((*1R,6S*)-6-(7-chloroquinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12ha)



85% yield (37.1 mg); colorless oil; $[\alpha]_D^{23.0}$ = -68.1 (*c* = 1.0, $CHCl_3$, 92% ee); R_f = 0.15 (Hexane/EtOAc= 3/1); ^1H NMR (600 MHz, $CDCl_3$, VT50) δ 8.01 (brs, 1H), 7.99-7.94 (m, 3H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.19-7.05 (m, 2H), 5.95-5.87 (m, 2H), 5.55 (brs, 1H), 4.90 (d, *J* = 12.6 Hz, 1H), 4.78 (d, *J* = 12.6 Hz, 1H), 4.66 (s, 1H), 3.44-3.39 (m, 1H), 2.19-2.00 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.3, 155.2, 147.9, 147.4, 144.1, 135.9, 135.3, 130.4, 128.9, 128.3, 127.9, 127.3, 127.2, 125.3, 123.6, 122.0, 64.8, 48.8, 45.9, 24.8, 23.0 ; IR (ATR) 3422, 3333, 3079, 3026, 2929, 2836, 1719, 1612, 1520, 1498, 1347, 1235, 1086, 1065, 881, 847, 768 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{20}ClN_3O_4$ 437.11423, found: 437.11421.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40 °C, 254 nm) 27.7 min (major), 45.1 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

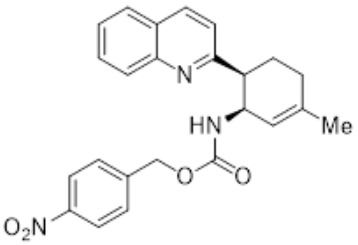
4-Nitrobenzyl ((*1R,4R,6S*)-4-hexyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12ac)



94% yield (45.6 mg); colorless oil; $[\alpha]^{23.0}_{D}$ = -90.9 (*c* = 1.0, $CHCl_3$, 95% ee); R_f = 0.20 (Hexane/EtOAc= 6/1); ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.07-8.00 (m, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 7.2 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 7.2 Hz, 1H), 6.99 (brs, 2H), 5.93-5.84 (m, 2H), 5.35 (brs, 1H), 4.88 (d, *J* = 12.6 Hz, 1H), 4.68 (d, *J* = 12.6 Hz, 1H), 4.61 (brs, 1H), 3.40-3.36 (m, 1H), 2.27 (brs, 1H), 2.18-2.09 (m, 1H), 1.78 (q, *J* = 12.6 Hz, 1H), 1.49-1.38 (m, 4H), 1.35-1.25 (m, 6H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 155.1, 147.8, 147.3, 144.2, 136.2, 136.0, 129.4, 129.2, 127.7, 127.5, 127.0, 126.2, 123.5, 123.4, 121.8, 64.6, 48.9, 46.3, 36.8, 36.0, 31.9, 29.6, 28.7, 26.8, 22.8, 14.2; IR (ATR) 3408, 3317, 3020, 2954, 2925, 2855, 1719, 1603, 1521, 1467, 1346, 1235, 1088, 887, 860, 830, 757 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{29}H_{33}N_3O_4$ 487.24711, found: 487.24666.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40℃, 254 nm) 12.7 min (major), 21.1 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 4R, 6S*) by analogy.

4-Nitrobenzyl ((*1R,6S*)-3-methyl-6-(quinolin-2-yl)cyclohex-2-en-1-yl)carbamate (12ad)

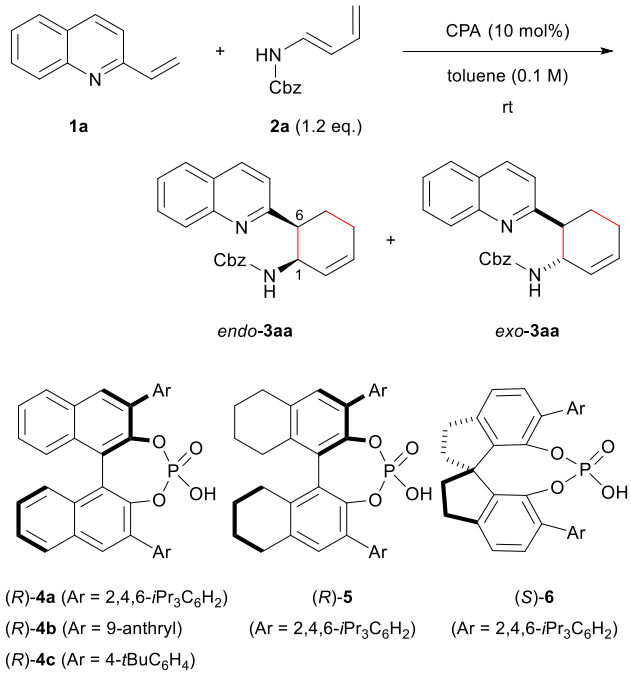


98% yield (40.9 mg); white solid; $[\alpha]^{23.0}_{D}$ = -94.9 (*c* = 1.0, $CHCl_3$, 99% ee); R_f = 0.22 (Hexane/EtOAc= 3/1); Mp: 59.2-63.1 ℃; ^{1}H NMR (600 MHz, $CDCl_3$, VT50) δ 8.03-7.97 (m, 2H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 7.2 Hz, 1H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 7.2 Hz, 1H), 7.05 (brs, 2H), 5.64 (s, 1H), 5.55 (brs, 1H), 4.92 (d, *J* = 12.0 Hz, 1H), 4.74 (d, *J* = 12.0 Hz, 1H), 4.64 (brs, 1H), 3.38-3.33 (m, 1H), 2.23-2.03 (m, 4H), 1.75 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.3, 155.2, 147.6, 147.3, 144.4, 138.3, 136.0, 129.4, 129.3, 127.7, 127.6, 127.0, 126.2, 123.5, 121.8, 64.6, 49.3, 45.7, 30.0, 23.6, 23.1, one carbon was not found probably due to overlapping; IR (ATR) 3410, 3333, 3044, 3013, 2934, 2909, 2832, 1720, 1603, 1520, 1429, 1347, 1227, 1106, 1061, 973, 831, 755 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}N_3O_4$ 417.16886, found: 417.16881.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 95/5, 1.0 mL/min, 40℃, 254 nm) 18.4 min (major), 38.0 min (minor).

Configuration Assignment: The absolute configuration was assigned as (*1R, 6S*) by analogy.

3-2. Screening of reaction conditions

Table S1. Screening of reaction conditions



Entry	CPA	Time (h)	yield of **3aa** (%)[b]	*endo*/*exo*[c]	ee (%)[c]
1	(*R*)-**4a**	12	95	81:19	71 / 88
2	(*R*)-**4b**	36	95	88:12	5 / -12
3	(*R*)-**4c**	36	67	87:13	5 / -3
4	(*R*)-**5**	20	95	74:26	71 / ND[d]
5	(*S*)-**6**	74	62	99:1	88 / ND[d]
6[e]	(*S*)-**6**	5 d	91	99:1	92 / ND[d]
7[f]	(*S*)-**6**	5 d	trace	-	-
8[g]	(*R*)-**4a**	12	90	76:24	72 / 86
9[h]	(*R*)-**4a**	48	85	77:23	73 / 83
10[i]	(*R*)-**4a**	48	84	80:20	72 / 82

[a] Unless otherwise noted, all reactions were carried out using 0.1 mmol of **1a**, 0.12 mmol of **2a**, and 0.010 mmol of CPA catalyst (10 mol %) in toluene (1 mL). [b] Isolated yield. [c] Diastereomeric and enantiomeric excess were determined by chiral stationary phase HPLC analysis. [d] ND: Not determined. [e] MS 5A (50 mg) was used as an additive. [f] conducted at 0°C. [g] C_6H_5Cl was used instead of toluene. [h] CH_2Cl_2 was used instead of toluene. [i] $C_2H_4Cl_2$ was used instead of toluene.

4. Computational study by DFT calculations

4-1. Method

All calculations were performed with the Gaussian 16 package.[4] Molecular geometries and transition state structures were optimized and characterized using frequency calculations in the gas phase at the M06-2X/6-31G(d) level of theory,[5] unless otherwise noted. A manual conformational search has been performed on possible catalyst substrate orientations. Transition state structures were verified by the presence of a single imaginary vibrational frequency. NBO version 7.0.7 were employed to calculate the energy of the proposed hydrogen bonding interactions.[6] CYLview was used for generation of molecular structures.[7]

4-2. Investigation of other transition state structures

Table S2. Summary of TS search

G=Trip-spinol	m062x/6-31g(d) in gas-phase		
TS	Hartree	kcal/mol	$\Delta\Delta G^{\ddagger}$(kcal/mol)
R_exo	-3615.906268	-2269017.342	8.92
R_exo2	-3615.903415	-2269015.552	10.71
S_exo	-3615.91317	-2269021.673	4.59
S_exo2	-3615.909697	-2269019.494	6.77
R_endo [**TS_R(H)**]	-3615.92049	-2269026.267	**0.00**
S_endo	-3615.91178	-2269020.801	5.47
S_endo2 [**TS_S(H)**]	-3615.917654	-2269024.487	**1.78**
R_exo_t-t	-3615.904635	-2269016.318	9.95
S_exo_t-t	-3615.905438	-2269016.821	9.45
R_endo_t-c	-3615.910534	-2269020.019	6.25
S_endo_t-c	-3615.910506	-2269020.002	6.27
↓ Rotational isomers of catalyst substituents [*i* Pr groups (at para-position)]			
r-r_R_endo	-3615.918406	-2269024.959	1.31
r-r_S_endo2	-3615.914482	-2269022.497	3.77
r-l_R_endo	-3615.916591	-2269023.82	2.45
r-l_S_endo2	-3615.911926	-2269020.893	5.37
l-l_R_endo	-3615.919252	-2269025.49	0.78
l-l_S_endo2	-3615.915464	-2269023.113	3.15

It is well known that the Diels-Alder reaction proceeds through a concerted fashion and hence the simultaneous formation of the two carbon-carbon bonds restricts the flexibility of the relative location between a dienophile and a diene. Therefore, structure searches were manually performed by primarily changing the conformation of the Cbz group, the orientation of the benzyl moiety and the geometry of the carbamate unit, i.e., *s-cis* and *s-trans*, and the initial structures were systematically generated by changing these parameters. In addition, several rotamers of the

catalyst were tested as the initial geometry in the optimizations. According to an exhaustive TS search, the predicted selectivity (95.4:4.6 er) at the m06-2x/6-31g(d) level of theory in gas phase was consistent with the observed selectivity (95.9:4.1 er), as shown in the next section 4-3.

4-3. Investigation of other calculation methods

Table S3. Summary of other calculation methods

Conditions	TS	Free Energy (Hartree)	$\Delta\Delta G^{\ddagger}$(kcal mol-1)	predicted e.r.
B3LYP-D3/6-31g(d) in gas phase	**TS_R(H)**	-3617.586897	0	97.5:2.5
	TS_S(H)	-3617.583479	2.14	
B3LYP-D3/6-31g(d)+cpcm(tol)//B3LYP-D3/6-31g(d)	**TS_R(H)**	-3617.598267	0	97.3:2.7
	TS_S(H)	-3617.594915	2.10	
B3LYP-D3/6-311g(d,p)+cpcm(tol)//B3LYP-D3/6-31g(d)	**TS_R(H)**	-3618.442786	0	97.5:2.5
	TS_S(H)	-3618.439397	2.13	
M062-X/6-31g(d)+cpcm(tol)//B3LYP-D3/6-31g(d)	**TS_R(H)**	-3615.931635	0	88.4:11.6
	TS_S(H)	-3615.929742	1.19	
B3LYP/6-31g(d) in gas phasae	**TS_R(H)**	-3617.327413	0	97.3:2.7
	TS_S(H)	-3617.324162	2.04	
M06-2X/6-31g(d)+cpcm(tol)//B3LYP/6-31g(d)	**TS_R(H)**	-3615.924636	0	99.8:0.2
	TS_S(H)	-3615.918823	3.65	
M06-2X/6-31g(d) in gas phasae	**TS_R(H)**	**-3615.92049**	**0**	**95.4:4.6**
	TS_S(H)	**-3615.917654**	**1.78**	
M06-2X/6-31g(d)+cpcm(tol)//M06-2X/6-31g(d)	**TS_R(H)**	-3615.933642	0	95.9:4.1
	TS_S(H)	-3615.930697	1.85	
M06-2X/6-31+g(d,p)//M06-2X/6-31g(d) in gas phase	**TS_R(H)**	-3616.104741	0	99.3:0.7
	TS_S(H)	-3616.100081	2.92	

Calculations using the M06-2X/6-31g(d) level in the gas phase reproduced the experimental values well. In addition, calculations that took into account the solvent effect of toluene also reproduced the experimental values.

M06-2X/6-31g(d) level in the gas phase does not necessarily guarantee accurate relative energies in all TSs. However, the energy values at the M06-2X/6-31g(d) level in the gas phase are adopted in the following calculations to reduce the computational cost as much as possible.

4-4. Energy profile

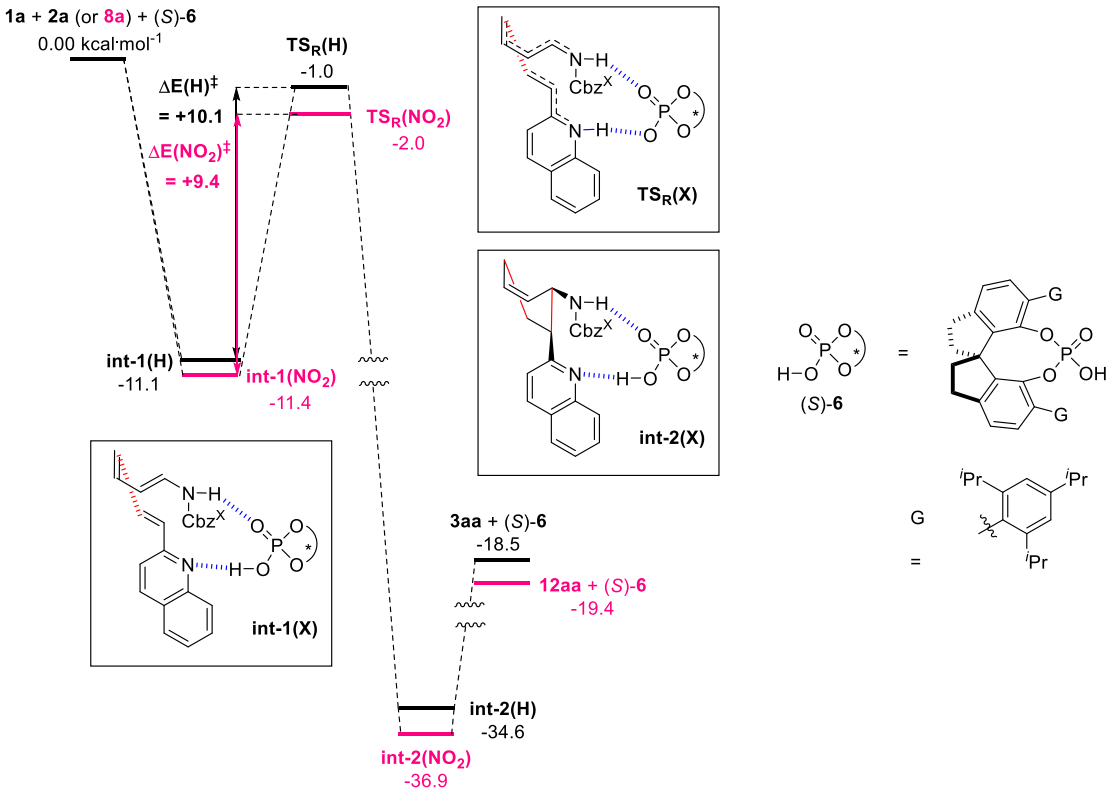


Figure S1. Energy profile of the Diels-Alder reaction

[Calculated at the m06-2x/6-31g(d) level of theory in gas phase.]

The activation free energies were calculated for the reactions using Cbz (**Figure S1**, **black-bars**) and Cbz-NO_2 groups (**Figure S1**, **pink-bars**). The results showed that the activation free energy was smaller when the Cbz-NO_2 group was used. This result indicates stabilization of TS in the rate-determining step and can be interpreted as a result of enhanced hydrogen bonding in the **$TS_R(NO_2)$**.

4-5. Distortion/Interaction analysis

Vinylquinoline (**1a**), dienylcarbamate (**2a**) and catalyst ((*S*)-**6**) were extracted from the transition state structures of R and S, respectively, and the free energies were calculated by single-point calculations.

Each was calculated as a neutral molecule at the m06-2x/6-31g(d) level of theory in gas phase. However, in the actual TS, the catalyst was present as a phosphate anion, and the dienophile was present as a vinylquinolinium cation. Therefore, the additional single-point calculations were performed at the m06-2x/6-31+g(d,p) level of theory in gas phase.

Comparing both calculation levels showed a marked difference in the catalyst distortion energy. However, it did not change the conclusion of distortion/interaction analysis that the difference in interaction energy was essential for enantioselectivity induction.

Table S4. Summary of distortion/interaction analysis

Trip-spinol		**m06-2x/6-31g(d)//m06-2x/6-31g(d) in gas phase**					
Origin of Enantioseletivity			**distortion**				
	$\Delta\Delta G^{\ddagger}$		phosphoric acid	dienylcarbamate	vinylquinoline	SUM	
TS_R(H)		Hartree	-2466.948293	-669.7857430	-478.9673730	-3615.70140900	
		kcal/mol	-1548034.723	-420297.2516	-300556.8162	-2268888.79	
TS_S(H)		Hartree	-2466.957728	-669.7871120	-478.9672350	-3615.71207500	
		kcal/mol	-1548040.644	-420298.1107	-300556.73	-2268895.48	**interaction**
TS_S(H)-TS_R(H)	**1.78**	kcal/mol	**-5.92**	**-0.86**	**0.09**	**-6.69**	**8.47**
Trip-spinol		**m06-2x/6-31+g(d,p)//m06-2x/6-31g(d) in gas phase**					
Origin of Enantioseletivity			**distortion**				
	$\Delta\Delta G^{\ddagger}$		phosphate	dienylcarbamate	vinylquinolinium	SUM	
TS_R(H)		Hartree	-2466.723484	-669.8275130	-479.3644710	-3615.91546800	
		kcal/mol	-1547893.653	-420323.4627	-300805.9992	-2269023.12	
TS_S(H)		Hartree	-2466.723958	-669.8286210	-479.3635520	-3615.91613100	
		kcal/mol	-1547893.951	-420324.158	-300805.42	-2269023.53	**interaction**
TS_S(H)-TS_R(H)	**2.92**	kcal/mol	**-0.30**	**-0.70**	**0.58**	**-0.42**	**3.34**

4-6. NCI plot[8]

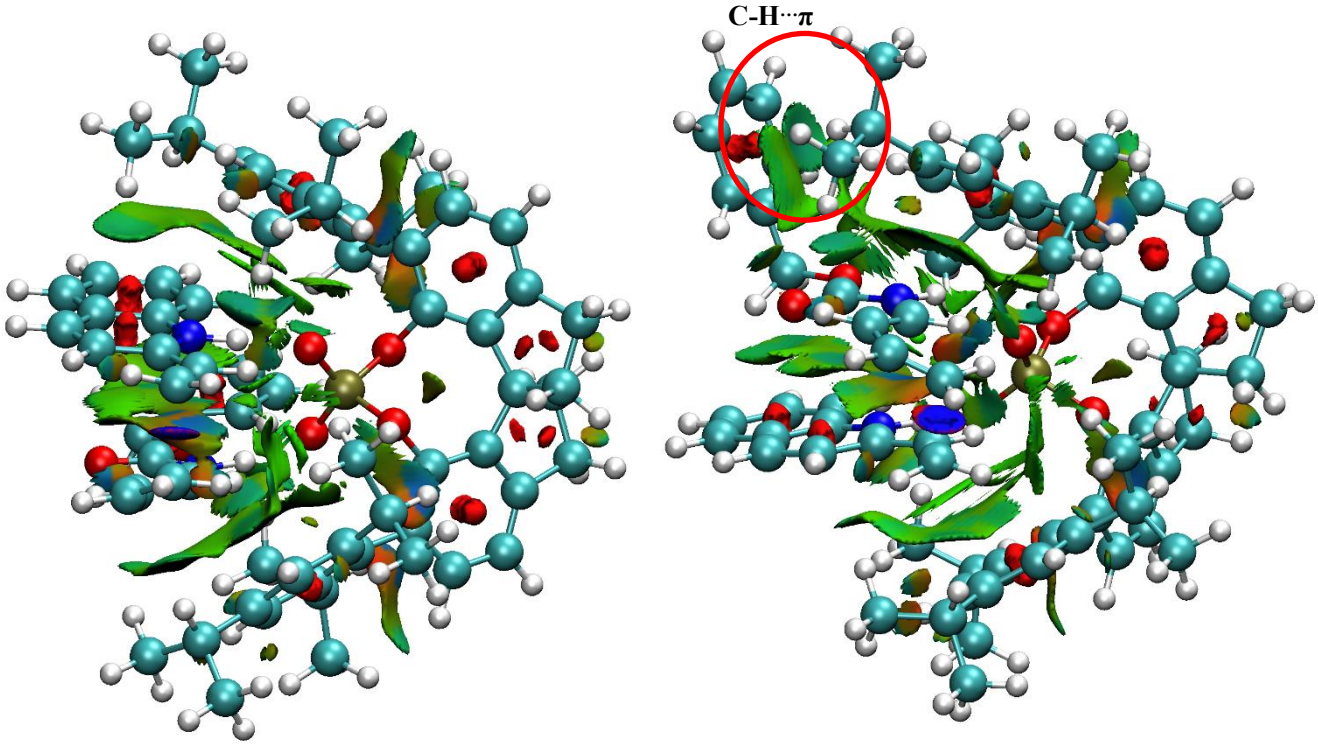


Figure S2. NCI analysis of $\mathbf{TS_R(H)}$ (left) and $\mathbf{TS_S(H)}$ (right) (The structure was fully optimized at the M06-2x/6-31G(d) level of theory in gas phase).

4-7. Investigation of substituent effect

Table S5. Summary of substituent effect

Trip-spinol	M06-2X/6-31g(d) in gas phase			
TS	Hartree	kcal·mol^{-1}	$\Delta\Delta G^{\ddagger}$	Note
TS_R(H) [**1a** with **2a**]	-3615.920490	-2269026.267	0.00	Fig. 2 left
TS_S(H) [**1a** with **2a**]	-3615.917654	-2269024.487	1.78	Fig. 2 right
TS_R(Br) [**1a** with **7a**]	-6187.117688	-3882478.220	0.00	Fig. S3 left
TS_S(Br) [**1a** with **7a**]	-6187.114515	-3882476.229	1.99	Fig. S3 right
$TS_R(NO_2)$ [**1a** with **8a**]	-3820.350334	-2397308.038	0.00	Fig. S4 left
$TS_S(NO_2)$ [**1a** with **8a**]	-3820.345497	-2397305.003	3.04	Fig. S4 right

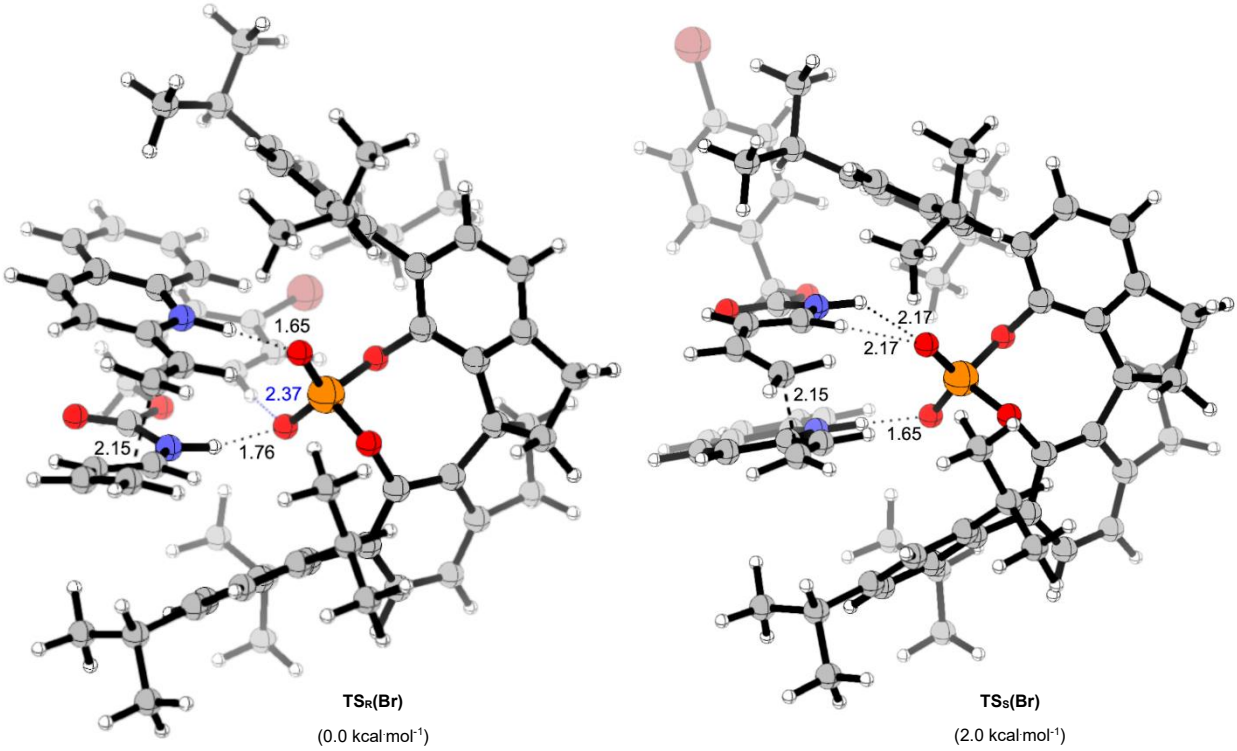


Figure S3. Optimized transition state structures for the Diels-Alder reaction of **1a** with **7a**.

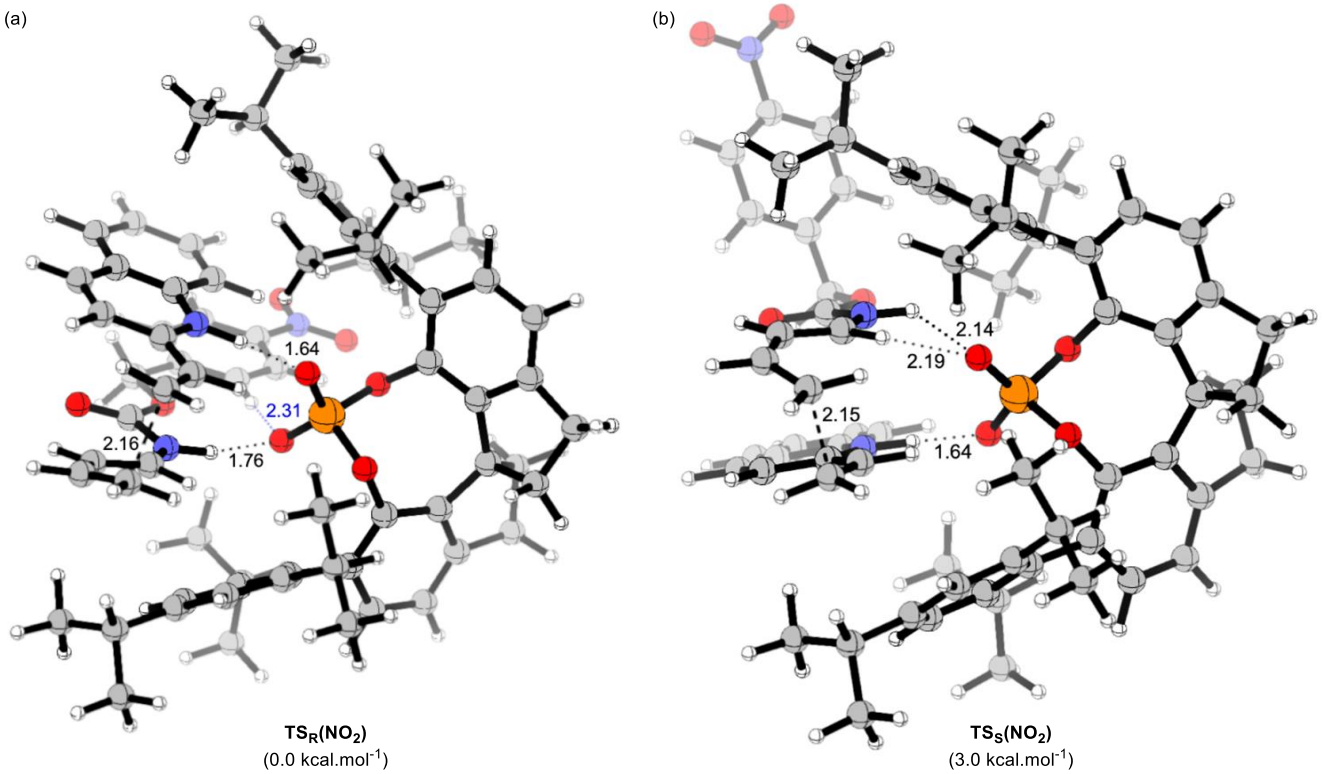


Figure S4. Optimized transition state structures for the Diels-Alder reaction of **1a** with **8a**.

4-8. Coordination

1a

M06-2X/6-31g(d) in gas phase
SCF Done: E(RM062X) = -479.121439 hartree
Sum of electronic and thermal Free Energies = -478.985687 hartree
The number of imaginary frequency = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.276695	0.292449	-0.000137
2	6	0	-2.266453	1.220984	0.000059
3	6	0	-0.912517	0.804693	0.000070
4	6	0	-0.607427	-0.582790	-0.000123
5	6	0	-1.672200	-1.521204	-0.000326
6	6	0	-2.974620	-1.091652	-0.000333
7	1	0	-0.008514	2.777670	0.000425
8	1	0	-4.313024	0.615095	-0.000145
9	1	0	-2.488648	2.285038	0.000210
10	6	0	0.182568	1.707346	0.000267
11	1	0	-1.412131	-2.574570	-0.000474
12	1	0	-3.784850	-1.814153	-0.000489
13	6	0	1.664345	-0.192089	0.000051
14	6	0	1.457400	1.220427	0.000262
15	1	0	2.306419	1.894590	0.000419
16	7	0	0.668889	-1.055927	-0.000129
17	6	0	3.015443	-0.785991	0.000047
18	1	0	3.004577	-1.872867	-0.000095
19	6	0	4.172485	-0.124171	0.000188
20	1	0	4.232471	0.960064	0.000325
21	1	0	5.116872	-0.657443	0.000162

2a

M06-2X/6-31g(d) in gas phase
SCF Done: E(RM062X) = -670.002606 hartree
Sum of electronic and thermal Free Energies = -669.814822 hartree
The number of imaginary frequency = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.247649	-1.068550	0.517449
2	1	0	6.413947	-0.728229	1.536110
3	1	0	7.064757	-1.591124	0.033208
4	6	0	5.086847	-0.850845	-0.107043
5	1	0	4.953262	-1.205518	-1.128619
6	6	0	3.952491	-0.157595	0.483261
7	1	0	4.060493	0.206547	1.504502
8	6	0	2.806846	0.038568	-0.182829
9	1	0	2.655055	-0.306338	-1.200806
10	1	0	1.717459	1.054767	1.282136
11	7	0	1.698469	0.693372	0.338097
12	6	0	0.548330	0.873431	-0.384325
13	8	0	-0.348164	1.552443	0.356962
14	8	0	0.375486	0.490132	-1.519336
15	6	0	-1.635499	1.735732	-0.260392
16	1	0	-2.051730	2.608853	0.245417
17	1	0	-1.489307	1.958410	-1.319186
18	6	0	-2.515438	0.527983	-0.069644
19	6	0	-2.596641	-0.457632	-1.055168
20	6	0	-3.240728	0.375170	1.113465
21	6	0	-3.398671	-1.578643	-0.859043
22	1	0	-2.016018	-0.344324	-1.965603
23	6	0	-4.039823	-0.746060	1.312090
24	1	0	-3.178156	1.142531	1.881510
25	6	0	-4.120299	-1.724198	0.323176
26	1	0	-3.459380	-2.340152	-1.630379
27	1	0	-4.602534	-0.855258	2.234057
28	1	0	-4.746096	-2.598543	0.473992

(*S*)-6

M06-2X/6-31g(d) in gas phase
SCF Done: E(RM062X) = -2468.005309 hartree
Sum of electronic and thermal Free Energies = -2467.118302 hartree
The number of imaginary frequency = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.473353	-0.586475	0.394417
2	1	0	-5.687322	-1.543254	0.893492
3	1	0	-6.427644	-0.057569	0.324066
4	6	0	-4.888697	-0.857732	-0.965307
5	1	0	-5.488696	-0.696773	-1.856354
6	6	0	-3.634675	-1.302945	-1.048733
7	1	0	-3.140246	-1.513793	-1.988462
8	6	0	-2.890513	-1.516433	0.242857
9	1	0	-3.389564	-2.337909	0.776575
10	1	0	-1.067851	-2.278672	0.926094
11	7	0	-1.511672	-1.957853	0.074187
12	6	0	-0.632598	-1.321748	-0.763977
13	8	0	0.639596	-1.589448	-0.386047
14	8	0	-0.914740	-0.647886	-1.729923
15	6	0	1.637527	-0.973637	-1.195941
16	1	0	1.644771	-1.450166	-2.183342
17	1	0	1.382088	0.082702	-1.342219
18	6	0	2.979969	-1.093550	-0.523265
19	6	0	3.150775	-1.726250	0.705454
20	6	0	4.082320	-0.500716	-1.143705
21	6	0	4.406594	-1.756006	1.310680
22	1	0	2.295303	-2.182205	1.191259
23	6	0	5.334838	-0.531799	-0.542061
24	1	0	3.950988	0.003721	-2.098756
25	6	0	5.500455	-1.158513	0.692674
26	1	0	4.527643	-2.248492	2.270968
27	1	0	6.182499	-0.064122	-1.033887

28	1	0	6.476890	-1.181780	1.166544
29	6	0	2.377177	2.843925	-0.236073
30	6	0	1.128177	3.062372	-0.763626
31	6	0	0.003882	2.361353	-0.258807
32	6	0	0.183396	1.440903	0.807187
33	6	0	1.479441	1.254177	1.351574
34	6	0	2.553743	1.931485	0.833144
35	1	0	-1.481866	3.189568	-1.604014
36	1	0	3.237721	3.368591	-0.639484
37	1	0	0.985300	3.760247	-1.584747
38	6	0	-1.304677	2.492994	-0.788432
39	1	0	1.590386	0.531775	2.153656
40	1	0	3.550400	1.747345	1.223781
41	6	0	-2.024494	0.783362	0.743281
42	6	0	-2.312318	1.711698	-0.298756
43	1	0	-3.305950	1.749126	-0.730812
44	7	0	-0.834338	0.675796	1.293847
45	6	0	-3.024814	-0.261698	1.186082
46	1	0	-2.683380	-0.589067	2.173170
47	6	0	-4.491496	0.224338	1.268363
48	1	0	-4.545217	1.273049	0.962654
49	1	0	-4.826976	0.196110	2.309161

Int-1(H)

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.205628 hartree

Sum of electronic and thermal Free Energies = -3615.936512 hartree

The number of imaginary frequency = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.065561	-1.516879	-4.018933
2	1	0	-3.544184	-0.622235	-3.692667
3	1	0	-4.711490	-1.420558	-4.885858
4	6	0	-3.947530	-2.684246	-3.368031
5	1	0	-4.498710	-3.539321	-3.758764
6	6	0	-3.154177	-2.965131	-2.175262
7	1	0	-3.052965	-4.001283	-1.876606
8	6	0	-2.563272	-2.010667	-1.426793
9	1	0	-2.684148	-0.955052	-1.664401
10	1	0	-1.330886	-1.351567	0.110255
11	7	0	-1.754991	-2.190010	-0.314931
12	6	0	-1.522110	-3.375634	0.321066
13	8	0	-0.611013	-3.177690	1.300215
14	8	0	-2.021756	-4.454093	0.073996
15	6	0	-0.504615	-4.226837	2.253245
16	1	0	-1.498271	-4.425333	2.674534
17	1	0	-0.168248	-5.143757	1.756868
18	6	0	0.462645	-3.804322	3.329426
19	6	0	0.800643	-2.465036	3.533454
20	6	0	1.017044	-4.784152	4.155265
21	6	0	1.673684	-2.118262	4.563404
22	1	0	0.402532	-1.700627	2.871297
23	6	0	1.892755	-4.436087	5.179150
24	1	0	0.762027	-5.829496	3.992801
25	6	0	2.222087	-3.098385	5.386870
26	1	0	1.925482	-1.073360	4.718290
27	1	0	2.318302	-5.208509	5.812663
28	1	0	2.903353	-2.822404	6.185908
29	1	0	0.803199	-0.688616	-1.754755
30	6	0	2.575562	-4.222467	0.876513
31	6	0	1.882967	-4.787411	-0.168265
32	6	0	1.278415	-3.960170	-1.142515
33	6	0	1.406001	-2.558582	-1.013006
34	6	0	2.121481	-1.983186	0.052191
35	6	0	2.694734	-2.817711	0.981484
36	1	0	0.374307	-5.526380	-2.331305
37	1	0	3.026063	-4.850825	1.638227
38	1	0	1.783297	-5.865265	-0.259927
39	6	0	0.514630	-4.453469	-2.234089
40	1	0	2.213570	-0.902176	0.117773
41	1	0	3.238626	-2.388388	1.817160
42	6	0	0.080556	-2.200001	-2.961186
43	6	0	-0.061043	-3.600330	-3.132514
44	1	0	-0.679764	-3.971380	-3.939547
45	7	0	0.797121	-1.751149	-1.936569
46	6	0	-0.543579	-1.186089	-3.813083
47	1	0	-0.483399	-0.166313	-3.437332
48	6	0	-1.148068	-1.453121	-4.972980
49	1	0	-1.226560	-2.454064	-5.385170
50	1	0	-1.588447	-0.654260	-5.559211
51	6	0	-0.621763	5.659651	2.999229
52	6	0	-1.541258	4.582400	2.471094
53	6	0	-1.016585	4.020537	1.303224
54	6	0	0.669523	5.401317	2.203064
55	1	0	-1.024137	6.659919	2.794153
56	1	0	-0.475740	5.588035	4.081214
57	1	0	1.263892	4.627502	2.702221
58	1	0	1.298070	6.288766	2.081986
59	6	0	0.174466	4.836356	0.841093
60	6	0	-0.260465	6.011747	-0.079075
61	6	0	1.327343	4.274358	0.034954
62	6	0	1.060658	6.544929	-0.663604
63	1	0	-0.840552	6.768297	0.457949
64	1	0	-0.886521	5.608126	-0.882866
65	6	0	1.913746	5.297426	-0.717162
66	1	0	0.934880	7.003915	-1.648828
67	1	0	1.509352	7.303787	-0.010110
68	6	0	-2.744882	4.132201	2.992511
69	6	0	-3.403586	3.091910	2.345471
70	6	0	-2.858626	2.444116	1.229475
71	6	0	-1.641222	2.922396	0.723907
72	1	0	-3.167732	4.579386	3.887693
73	1	0	-4.358307	2.737442	2.723184
74	6	0	1.876085	2.999406	0.009951
75	6	0	3.087625	2.757164	-0.654458
76	6	0	3.700796	3.826962	-1.315848
77	6	0	3.109787	5.085654	-1.386160
78	1	0	4.651192	3.647466	-1.810142
79	1	0	3.580575	5.883167	-1.953987
80	8	0	-1.066521	2.327112	-0.386963

81	8	0	-0.420994	0.077282	0.759677
82	8	0	0.555546	0.822513	-1.536046
83	15	0	0.058453	1.162282	-0.148757
84	8	0	1.231999	1.967728	0.670137
85	6	0	3.739524	1.413395	-0.659519
86	6	0	3.956629	0.733836	-1.878347
87	6	0	4.212715	0.851400	0.545758
88	6	0	4.622257	-0.494470	-1.860706
89	6	0	4.900129	-0.361934	0.502287
90	6	0	5.100633	-1.062917	-0.683515
91	1	0	4.775333	-1.016185	-2.802548
92	1	0	5.273019	-0.792590	1.431335
93	6	0	-3.607857	1.296422	0.634304
94	6	0	-3.891227	0.164518	1.426491
95	6	0	-4.148343	1.390787	-0.667365
96	6	0	-4.720833	-0.834146	0.910848
97	6	0	-4.980015	0.370002	-1.130781
98	6	0	-5.288991	-0.749081	-0.355689
99	1	0	-4.929580	-1.703527	1.528570
100	1	0	-5.412867	0.446226	-2.128337
101	6	0	-3.357799	-0.022474	2.842054
102	1	0	-2.682590	0.805196	3.071988
103	6	0	-4.499637	-0.014427	3.866924
104	1	0	-5.171361	-0.865435	3.707725
105	1	0	-4.100050	-0.089304	4.883768
106	1	0	-5.102366	0.896809	3.801228
107	6	0	-2.534691	-1.307094	2.966197
108	1	0	-2.171360	-1.430279	3.993176
109	1	0	-3.126751	-2.195575	2.711512
110	1	0	-1.672819	-1.256644	2.301239
111	6	0	-3.905332	2.592293	-1.569836
112	1	0	-3.273847	3.306793	-1.037463
113	6	0	-5.219185	3.309855	-1.902832
114	1	0	-5.895790	2.659586	-2.467862
115	1	0	-5.736465	3.621699	-0.990422
116	1	0	-5.025094	4.199949	-2.510850
117	6	0	-3.162355	2.188492	-2.848012
118	1	0	-2.909831	3.074305	-3.440847
119	1	0	-2.230849	1.665759	-2.604973
120	1	0	-3.788815	1.540038	-3.471937
121	6	0	-6.260154	-1.789031	-0.882016
122	1	0	-6.057079	-1.900076	-1.954094
123	6	0	-7.700065	-1.278446	-0.724252
124	1	0	-8.415691	-1.997874	-1.137014
125	1	0	-7.934838	-1.131716	0.336026
126	1	0	-7.840156	-0.320380	-1.234265
127	6	0	-6.108488	-3.161625	-0.224782
128	1	0	-6.457662	-3.143126	0.814224
129	1	0	-6.715996	-3.900790	-0.756910
130	1	0	-5.067202	-3.499546	-0.231148
131	6	0	3.542548	1.302302	-3.230527
132	1	0	2.933680	2.192854	-3.058416
133	6	0	2.679655	0.332275	-4.041388
134	1	0	2.433884	0.771514	-5.014247
135	1	0	3.186442	-0.621555	-4.226251
136	1	0	1.747048	0.142288	-3.511867
137	6	0	4.783554	1.704632	-4.040164
138	1	0	4.490202	2.183496	-4.980301
139	1	0	5.425527	2.397072	-3.487443
140	1	0	5.386756	0.822746	-4.284918
141	6	0	4.014770	1.508107	1.903996
142	1	0	3.461764	2.439900	1.767068
143	6	0	3.184769	0.608796	2.828649
144	1	0	2.976603	1.124723	3.773123
145	1	0	2.227645	0.344555	2.365646
146	1	0	3.727598	-0.313662	3.070742
147	6	0	5.360279	1.866666	2.546479
148	1	0	5.960609	0.970839	2.739661
149	1	0	5.941513	2.527712	1.896474
150	1	0	5.202489	2.375536	3.503196
151	6	0	5.826024	-2.394934	-0.667591
152	1	0	5.718021	-2.805050	0.346360
153	6	0	7.322265	-2.192825	-0.940151
154	1	0	7.861643	-3.144833	-0.891315
155	1	0	7.469128	-1.767228	-1.939172
156	1	0	7.765421	-1.504746	-0.214204
157	6	0	5.231007	-3.411914	-1.644735
158	1	0	5.684542	-4.396213	-1.489898
159	1	0	4.148394	-3.505700	-1.510503
160	1	0	5.423285	-3.124018	-2.683977

R_endo [TS$_R$(H)]

B3LYP/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -3618.575510 hartree

Sum of electronic and thermal Free Energies = -3617.327413 hartree

The number of imaginary frequency = 1

Imaginary frequency = -356.54

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.340122	-2.419102	-3.935136
2	1	0	-3.414042	-1.435040	-3.484604
3	1	0	-3.870860	-2.523244	-4.878301
4	6	0	-3.190472	-3.545869	-3.134824
5	1	0	-3.414158	-4.510305	-3.590317
6	6	0	-2.601022	-3.603491	-1.852082
7	1	0	-2.405253	-4.576269	-1.420814
8	6	0	-2.176221	-2.484509	-1.160636
9	1	0	-2.428559	-1.490581	-1.511454
10	1	0	-1.193302	-1.516289	0.379127
11	7	0	-1.462462	-2.449007	-0.000032
12	6	0	-0.989058	-3.552483	0.699835
13	8	0	-0.311327	-3.117901	1.777740
14	8	0	-1.147742	-4.720918	0.402603
15	6	0	0.253294	-4.135431	2.620346
16	1	0	-0.531078	-4.850296	2.891632
17	1	0	1.008906	-4.683157	2.044501
18	6	0	0.857342	-3.486056	3.843380
19	6	0	0.993234	-2.099210	3.966044
20	6	0	1.309873	-4.313911	4.879537
21	6	0	1.573847	-1.554572	5.115163

22	1	0	0.639239	-1.448684	3.172841
23	6	0	1.893553	-3.767583	6.021133
24	1	0	1.201357	-5.393831	4.794137
25	6	0	2.026767	-2.382146	6.142374
26	1	0	1.668485	-0.475720	5.201803
27	1	0	2.238070	-4.422244	6.817546
28	1	0	2.476825	-1.952878	7.033680
29	1	0	0.861465	-1.096000	-1.600062
30	6	0	3.646438	-4.415437	0.417547
31	6	0	3.038949	-4.964227	-0.698276
32	6	0	2.162581	-4.190820	-1.488301
33	6	0	1.926384	-2.837645	-1.126976
34	6	0	2.556488	-2.279960	0.001250
35	6	0	3.400162	-3.070468	0.762526
36	1	0	1.658211	-5.724541	-2.941912
37	1	0	4.314227	-5.016695	1.027178
38	1	0	3.219237	-5.999534	-0.975987
39	6	0	1.478602	-4.696159	-2.638657
40	1	0	2.372263	-1.244194	0.264848
41	1	0	3.875009	-2.641712	1.639249
42	6	0	0.353786	-2.560847	-2.949325
43	6	0	0.608227	-3.917971	-3.340668
44	1	0	0.090671	-4.314259	-4.205148
45	7	0	1.049644	-2.088290	-1.879869
46	6	0	-0.537687	-1.673725	-3.611808
47	1	0	-0.563545	-0.657781	-3.227520
48	6	0	-1.376844	-2.016373	-4.666761
49	1	0	-1.243698	-2.949055	-5.205411
50	1	0	-1.775234	-1.209996	-5.274899
51	6	0	-1.370144	5.665707	2.703589
52	6	0	-2.198699	4.510160	2.185739
53	6	0	-1.574430	3.901422	1.085582
54	6	0	-0.032598	5.474521	1.957966
55	1	0	-1.831105	6.633497	2.460503
56	1	0	-1.254928	5.639574	3.793613
57	1	0	0.612744	4.789034	2.519203
58	1	0	0.520716	6.406839	1.808263
59	6	0	-0.433590	4.790258	0.607982
60	6	0	-0.968762	5.879866	-0.381838
61	6	0	0.801044	4.318159	-0.151712
62	6	0	0.302594	6.523947	-0.969429
63	1	0	-1.637368	6.596557	0.104869
64	1	0	-1.535220	5.381342	-1.176878
65	6	0	1.291769	5.380335	-0.928605
66	1	0	0.153036	6.910027	-1.984669
67	1	0	0.642618	7.372067	-0.358345
68	6	0	-3.421812	4.045226	2.651450
69	6	0	-4.000104	2.945000	2.022761
70	6	0	-3.349265	2.236397	0.997615
71	6	0	-2.101046	2.723827	0.551669
72	1	0	-3.926660	4.531040	3.482938
73	1	0	-4.974511	2.594241	2.348467
74	6	0	1.504451	3.111082	-0.102447
75	6	0	2.784224	3.011529	-0.692806
76	6	0	3.284961	4.137332	-1.369888
77	6	0	2.539892	5.302035	-1.531959
78	1	0	4.280062	4.073928	-1.799464
79	1	0	2.935877	6.133028	-2.110679
80	8	0	-1.411069	2.073202	-0.464318
81	8	0	-0.558903	0.045730	0.951007
82	8	0	0.323788	0.541489	-1.453881
83	15	0	-0.163521	1.036939	-0.110954
84	8	0	0.961123	2.034608	0.589847
85	6	0	3.667191	1.800717	-0.623737
86	6	0	4.078272	1.154879	-1.818439
87	6	0	4.216968	1.382888	0.614836
88	6	0	5.020414	0.120495	-1.745570
89	6	0	5.148356	0.338763	0.626219
90	6	0	5.578324	-0.301712	-0.538774
91	1	0	5.330949	-0.358891	-2.669304
92	1	0	5.578942	0.030731	1.577609
93	6	0	-4.031690	1.025826	0.434419
94	6	0	-4.348089	-0.068770	1.280363
95	6	0	-4.476429	1.012053	-0.913241
96	6	0	-5.090450	-1.139198	0.762151
97	6	0	-5.206896	-0.087844	-1.375788
98	6	0	-5.538820	-1.173071	-0.558044
99	1	0	-5.328334	-1.966606	1.423518
100	1	0	-5.564147	-0.085751	-2.404300
101	6	0	-3.952163	-0.132763	2.759508
102	1	0	-3.355067	0.751080	2.991883
103	6	0	-5.196333	-0.106875	3.671387
104	1	0	-5.817001	-0.999746	3.528751
105	1	0	-4.895269	-0.077660	4.725614
106	1	0	-5.829065	0.766270	3.475772
107	6	0	-3.069979	-1.349926	3.088797
108	1	0	-2.837558	-1.364420	4.160782
109	1	0	-3.567074	-2.297577	2.847137
110	1	0	-2.126135	-1.298757	2.544105
111	6	0	-4.268129	2.190238	-1.866550
112	1	0	-3.697831	2.958147	-1.340408
113	6	0	-5.614461	2.829794	-2.262321
114	1	0	-6.244148	2.133434	-2.828952
115	1	0	-6.178336	3.143558	-1.376794
116	1	0	-5.448017	3.713751	-2.890227
117	6	0	-3.451596	1.801181	-3.112708
118	1	0	-3.291698	2.677727	-3.752647
119	1	0	-2.470257	1.411353	-2.825760
120	1	0	-3.972860	1.047374	-3.717129
121	6	0	-6.422818	-2.288161	-1.108768
122	1	0	-6.136035	-2.431875	-2.160376
123	6	0	-7.904335	-1.854989	-1.091333
124	1	0	-8.541563	-2.625000	-1.543780
125	1	0	-8.246925	-1.692917	-0.062119
126	1	0	-8.054250	-0.920395	-1.642565
127	6	0	-6.252455	-3.640024	-0.400399
128	1	0	-6.617267	-3.605160	0.633104
129	1	0	-6.830902	-4.412601	-0.920319
130	1	0	-5.204067	-3.954510	-0.380913
131	6	0	3.567206	1.553315	-3.206757
132	1	0	2.828160	2.347576	-3.083293
133	6	0	2.845980	0.396515	-3.920912
134	1	0	2.510760	0.718070	-4.914929
135	1	0	3.497167	-0.475485	-4.057228

136	1	0	1.967155	0.094256	-3.349044
137	6	0	4.704010	2.108034	-4.089185
138	1	0	4.306808	2.451145	-5.052349
139	1	0	5.213476	2.953434	-3.613497
140	1	0	5.461739	1.342872	-4.296705
141	6	0	3.894159	2.075048	1.939535
142	1	0	3.182446	2.878742	1.739668
143	6	0	3.225086	1.119957	2.944611
144	1	0	2.984040	1.654640	3.872194
145	1	0	2.294552	0.716366	2.535017
146	1	0	3.882641	0.282732	3.209317
147	6	0	5.148862	2.734027	2.547296
148	1	0	5.909374	1.990997	2.815320
149	1	0	5.605393	3.439977	1.844417
150	1	0	4.886906	3.284091	3.459482
151	6	0	6.672188	-1.361632	-0.460408
152	1	0	6.568958	-1.855260	0.516775
153	6	0	8.065479	-0.698366	-0.491422
154	1	0	8.858376	-1.447372	-0.372755
155	1	0	8.226340	-0.182266	-1.445717
156	1	0	8.171327	0.041842	0.308939
157	6	0	6.572779	-2.452795	-1.537562
158	1	0	7.320184	-3.233552	-1.353351
159	1	0	5.584139	-2.922724	-1.545176
160	1	0	6.766755	-2.051661	-2.539409

R_endo [TS$_R$(H)]

B3LYP-D/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -3618.847860 hartree

Sum of electronic and thermal Free Energies = -3617.586897 hartree

The number of imaginary frequency = 1

Imaginary frequency = -327.37

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.502506	-2.722189	-3.682142
2	1	0	-3.567382	-1.693959	-3.343135
3	1	0	-4.004655	-2.919904	-4.625782
4	6	0	-3.384919	-3.754449	-2.758188
5	1	0	-3.612554	-4.762679	-3.102521
6	6	0	-2.810909	-3.658287	-1.475349
7	1	0	-2.625376	-4.568502	-0.921322
8	6	0	-2.373070	-2.462209	-0.936595
9	1	0	-2.626690	-1.517579	-1.399710
10	1	0	-1.362100	-1.326888	0.463490
11	7	0	-1.648559	-2.291855	0.199896
12	6	0	-1.142674	-3.296041	1.012318
13	8	0	-0.360100	-2.715788	1.934677
14	8	0	-1.347654	-4.491098	0.917930
15	6	0	0.214013	-3.558734	2.938723
16	1	0	-0.593594	-4.072129	3.475090
17	1	0	0.831031	-4.323354	2.455489
18	6	0	1.031144	-2.691072	3.865366
19	6	0	1.029546	-1.294266	3.770581
20	6	0	1.807321	-3.313889	4.850304
21	6	0	1.784493	-0.538085	4.670838
22	1	0	0.461094	-0.798890	2.990166
23	6	0	2.567996	-2.554934	5.739145
24	1	0	1.817977	-4.400246	4.920634
25	6	0	2.555749	-1.160403	5.653501
26	1	0	1.773145	0.545138	4.591464
27	1	0	3.168519	-3.051292	6.497136
28	1	0	3.145897	-0.565045	6.345113
29	1	0	0.723167	-1.161500	-1.390568
30	6	0	3.309800	-4.202325	1.204042
31	6	0	2.664304	-4.915895	0.208496
32	6	0	1.832996	-4.252628	-0.718826
33	6	0	1.679954	-2.845359	-0.611805
34	6	0	2.340313	-2.124142	0.398076
35	6	0	3.143647	-2.805350	1.293972
36	1	0	1.230904	-5.989876	-1.874483
37	1	0	3.943024	-4.715984	1.921034
38	1	0	2.784611	-5.993049	0.128640
39	6	0	1.123190	-4.913273	-1.770964
40	1	0	2.216091	-1.049409	0.463899
41	1	0	3.644097	-2.250191	2.079791
42	6	0	0.140388	-2.805432	-2.480707
43	6	0	0.313864	-4.222233	-2.622740
44	1	0	-0.233557	-4.736257	-3.402586
45	7	0	0.848558	-2.198165	-1.495010
46	6	0	-0.701738	-1.992153	-3.289899
47	1	0	-0.722886	-0.936654	-3.037578
48	6	0	-1.482897	-2.437345	-4.349820
49	1	0	-1.340612	-3.428212	-4.769039
50	1	0	-1.825089	-1.697099	-5.066529
51	6	0	-1.134922	5.878394	2.357837
52	6	0	-2.008921	4.726956	1.909734
53	6	0	-1.413842	4.046168	0.838336
54	6	0	0.195590	5.586463	1.628093
55	1	0	-1.555361	6.845464	2.048621
56	1	0	-1.023076	5.917115	3.447430
57	1	0	0.806954	4.898855	2.223893
58	1	0	0.792928	6.481712	1.430162
59	6	0	-0.237013	4.852567	0.316654
60	6	0	-0.722052	5.902966	-0.737589
61	6	0	0.960715	4.267005	-0.418356
62	6	0	0.577904	6.437845	-1.370446
63	1	0	-1.349860	6.681679	-0.294230
64	1	0	-1.318616	5.380939	-1.494828
65	6	0	1.490845	5.235515	-1.285318
66	1	0	0.440754	6.786917	-2.400234
67	1	0	0.979889	7.286081	-0.798689
68	6	0	-3.235702	4.311144	2.413592
69	6	0	-3.837428	3.178412	1.866208
70	6	0	-3.207805	2.400883	0.878964
71	6	0	-1.976938	2.861277	0.373793
72	1	0	-3.719455	4.852160	3.222981
73	1	0	-4.802617	2.850129	2.238105
74	6	0	1.584870	3.023778	-0.309742
75	6	0	2.802342	2.774432	-0.973216
76	6	0	3.352026	3.806326	-1.751931

77	6	0	2.695404	5.020317	-1.942055
78	1	0	4.303806	3.625109	-2.240464
79	1	0	3.117750	5.778865	-2.596236
80	8	0	-1.316763	2.144739	-0.614713
81	8	0	-0.632421	0.176803	0.956786
82	8	0	0.319130	0.451062	-1.462646
83	15	0	-0.155382	1.059375	-0.164033
84	8	0	1.009437	2.037703	0.487022
85	6	0	3.542546	1.475068	-0.894150
86	6	0	3.696925	0.680160	-2.053040
87	6	0	4.189245	1.097392	0.310053
88	6	0	4.478341	-0.480994	-1.980093
89	6	0	4.969064	-0.060642	0.319926
90	6	0	5.121980	-0.871279	-0.809120
91	1	0	4.586133	-1.088230	-2.872937
92	1	0	5.473769	-0.356761	1.235057
93	6	0	-3.852976	1.125339	0.436905
94	6	0	-4.126930	0.112446	1.390185
95	6	0	-4.278219	0.949594	-0.904353
96	6	0	-4.842292	-1.024005	0.991522
97	6	0	-4.989659	-0.205418	-1.244029
98	6	0	-5.297418	-1.203069	-0.313278
99	1	0	-5.044878	-1.789093	1.733181
100	1	0	-5.337835	-0.327771	-2.267794
101	6	0	-3.701040	0.200243	2.857556
102	1	0	-3.094098	1.098276	2.987316
103	6	0	-4.928884	0.319918	3.781514
104	1	0	-5.549606	-0.582910	3.732832
105	1	0	-4.612446	0.451750	4.823224
106	1	0	-5.564453	1.169501	3.508541
107	6	0	-2.816389	-0.982581	3.285920
108	1	0	-2.545447	-0.884837	4.344392
109	1	0	-3.325654	-1.946625	3.163410
110	1	0	-1.896740	-0.996136	2.704442
111	6	0	-4.040856	1.992375	-1.994704
112	1	0	-3.513775	2.840685	-1.554631
113	6	0	-5.370693	2.534854	-2.551680
114	1	0	-5.951687	1.750367	-3.050968
115	1	0	-5.991349	2.950954	-1.750257
116	1	0	-5.182366	3.327419	-3.286082
117	6	0	-3.147507	1.439864	-3.121274
118	1	0	-2.939381	2.221089	-3.862409
119	1	0	-2.190871	1.091742	-2.721811
120	1	0	-3.640242	0.612186	-3.648238
121	6	0	-6.139354	-2.396915	-0.743725
122	1	0	-5.785779	-2.694717	-1.740443
123	6	0	-7.617706	-1.977956	-0.879135
124	1	0	-8.228661	-2.811936	-1.246112
125	1	0	-8.016941	-1.664349	0.093085
126	1	0	-7.731421	-1.137544	-1.572584
127	6	0	-6.009658	-3.620478	0.172954
128	1	0	-6.452220	-3.432482	1.158672
129	1	0	-6.538885	-4.475336	-0.263271
130	1	0	-4.962355	-3.904122	0.317251
131	6	0	3.102991	1.062700	-3.409112
132	1	0	2.410743	1.894136	-3.257211
133	6	0	2.291677	-0.071006	-4.055809
134	1	0	1.881557	0.263235	-5.016677
135	1	0	2.900639	-0.961609	-4.251571
136	1	0	1.460298	-0.348633	-3.412550
137	6	0	4.215229	1.528834	-4.370508
138	1	0	3.786185	1.858898	-5.324543
139	1	0	4.795715	2.358398	-3.954373
140	1	0	4.915225	0.710959	-4.581200
141	6	0	4.116429	1.978836	1.555978
142	1	0	3.114202	2.412353	1.601906
143	6	0	4.321487	1.211618	2.870320
144	1	0	4.091868	1.863410	3.721326
145	1	0	3.667711	0.336651	2.932367
146	1	0	5.357880	0.874905	2.994771
147	6	0	5.129722	3.136867	1.450637
148	1	0	6.153023	2.745060	1.396659
149	1	0	4.950020	3.743931	0.558305
150	1	0	5.061300	3.791376	2.328461
151	6	0	6.001991	-2.110451	-0.730683
152	1	0	5.940348	-2.480816	0.302521
153	6	0	7.472543	-1.739665	-1.007114
154	1	0	8.126238	-2.614159	-0.899039
155	1	0	7.583579	-1.354712	-2.028164
156	1	0	7.820025	-0.962016	-0.318119
157	6	0	5.545976	-3.252498	-1.650254
158	1	0	6.129698	-4.157969	-1.447846
159	1	0	4.488218	-3.486119	-1.498536
160	1	0	5.692391	-3.001141	-2.707455

R_endo [TS_R(H)]

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.192607 hartree

Sum of electronic and thermal Free Energies = -3615.920490 hartree

The number of imaginary frequency = 1

Imaginary frequency = -353.67

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.508844	-2.787733	-3.537639
2	1	0	-3.569356	-1.764208	-3.180565
3	1	0	-4.019225	-2.981278	-4.476733
4	6	0	-3.310556	-3.825521	-2.650706
5	1	0	-3.505305	-4.836706	-3.004741
6	6	0	-2.691241	-3.715650	-1.386441
7	1	0	-2.422830	-4.620608	-0.858396
8	6	0	-2.317761	-2.500483	-0.855352
9	1	0	-2.665868	-1.567800	-1.290927
10	1	0	-1.364897	-1.319187	0.556503
11	7	0	-1.565323	-2.294021	0.257823
12	6	0	-0.880038	-3.273786	0.948471
13	8	0	-0.154406	-2.688385	1.906264
14	8	0	-0.903961	-4.465459	0.733789
15	6	0	0.571642	-3.564986	2.759602
16	1	0	-0.139931	-4.187494	3.315453
17	1	0	1.192239	-4.231101	2.150587

18	6	0	1.410169	-2.729031	3.689835
19	6	0	1.300853	-1.338687	3.732406
20	6	0	2.321114	-3.377162	4.526840
21	6	0	2.088952	-0.613524	4.625956
22	1	0	0.618963	-0.824165	3.059731
23	6	0	3.114108	-2.647958	5.406176
24	1	0	2.411703	-4.460931	4.484846
25	6	0	2.997317	-1.259882	5.459421
26	1	0	1.995007	0.467780	4.658986
27	1	0	3.821654	-3.161710	6.050075
28	1	0	3.612484	-0.686295	6.146015
29	1	0	0.727610	-1.130864	-1.314429
30	6	0	3.632945	-4.086195	1.010813
31	6	0	2.953741	-4.811541	0.053469
32	6	0	2.016215	-4.176281	-0.786507
33	6	0	1.798696	-2.790766	-0.631345
34	6	0	2.489835	-2.051293	0.344513
35	6	0	3.394458	-2.703770	1.154965
36	1	0	1.412823	-5.920215	-1.930461
37	1	0	4.349588	-4.577081	1.661507
38	1	0	3.126596	-5.877467	-0.065795
39	6	0	1.263898	-4.851900	-1.799431
40	1	0	2.305903	-0.982904	0.441613
41	1	0	3.922142	-2.139669	1.919374
42	6	0	0.157980	-2.778625	-2.395999
43	6	0	0.371477	-4.185595	-2.576730
44	1	0	-0.208694	-4.705316	-3.329281
45	7	0	0.881175	-2.165669	-1.440728
46	6	0	-0.738343	-1.975064	-3.162504
47	1	0	-0.775218	-0.922569	-2.891877
48	6	0	-1.499435	-2.428860	-4.220288
49	1	0	-1.334960	-3.411255	-4.650519
50	1	0	-1.897783	-1.693950	-4.912604
51	6	0	-1.408857	5.819994	2.397651
52	6	0	-2.216399	4.611961	1.978151
53	6	0	-1.606586	3.972635	0.895627
54	6	0	-0.081292	5.603498	1.645679
55	1	0	-1.897031	6.752217	2.086403
56	1	0	-1.277596	5.873913	3.482578
57	1	0	0.577502	4.954330	2.233162
58	1	0	0.457496	6.531305	1.430368
59	6	0	-0.493826	4.844955	0.353192
60	6	0	-1.052327	5.860251	-0.685111
61	6	0	0.709901	4.315197	-0.404428
62	6	0	0.200728	6.455465	-1.347580
63	1	0	-1.706664	6.607182	-0.225680
64	1	0	-1.636387	5.306412	-1.428907
65	6	0	1.166481	5.294703	-1.292331
66	1	0	0.020756	6.798765	-2.370753
67	1	0	0.582066	7.314788	-0.781265
68	6	0	-3.392914	4.112173	2.517375
69	6	0	-3.928908	2.943817	1.983525
70	6	0	-3.282083	2.221685	0.972425
71	6	0	-2.102027	2.758758	0.439381
72	1	0	-3.887854	4.616215	3.342642
73	1	0	-4.857832	2.545473	2.381300
74	6	0	1.389769	3.104673	-0.300850
75	6	0	2.586234	2.900566	-1.004904
76	6	0	3.058350	3.938402	-1.818793
77	6	0	2.350103	5.122067	-1.993349
78	1	0	3.999669	3.788480	-2.339288
79	1	0	2.716060	5.889781	-2.669194
80	8	0	-1.422580	2.088888	-0.560432
81	8	0	-0.664479	0.206287	1.045259
82	8	0	0.288087	0.462679	-1.367789
83	15	0	-0.220449	1.074084	-0.090259
84	8	0	0.888122	2.115272	0.527471
85	6	0	3.388600	1.639862	-0.932997
86	6	0	3.533689	0.835927	-2.080002
87	6	0	4.101291	1.322707	0.245471
88	6	0	4.381455	-0.275860	-2.024692
89	6	0	4.947696	0.215957	0.241259
90	6	0	5.099244	-0.600398	-0.880372
91	1	0	4.484883	-0.895274	-2.911768
92	1	0	5.508030	-0.034381	1.139671
93	6	0	-3.871125	0.924811	0.518348
94	6	0	-4.076649	-0.113167	1.453226
95	6	0	-4.332464	0.766796	-0.808654
96	6	0	-4.766983	-1.262592	1.054042
97	6	0	-5.026919	-0.394660	-1.149558
98	6	0	-5.268779	-1.420004	-0.233738
99	1	0	-4.916952	-2.053150	1.784412
100	1	0	-5.410051	-0.503739	-2.164506
101	6	0	-3.616007	-0.034834	2.905438
102	1	0	-3.050733	0.889888	3.039346
103	6	0	-4.822191	-0.009948	3.854813
104	1	0	-5.373991	-0.955706	3.807968
105	1	0	-4.490103	0.131712	4.888543
106	1	0	-5.524310	0.792103	3.606513
107	6	0	-2.669250	-1.179661	3.279730
108	1	0	-2.426333	-1.128406	4.347202
109	1	0	-3.116676	-2.162652	3.087351
110	1	0	-1.738895	-1.097571	2.717996
111	6	0	-4.142401	1.826169	-1.885078
112	1	0	-3.638913	2.688120	-1.442597
113	6	0	-5.488352	2.318829	-2.430889
114	1	0	-6.036462	1.514633	-2.933770
115	1	0	-6.120746	2.704334	-1.625530
116	1	0	-5.331798	3.120752	-3.159989
117	6	0	-3.248553	1.302130	-3.016040
118	1	0	-3.056692	2.091597	-3.750594
119	1	0	-2.284310	0.964834	-2.621887
120	1	0	-3.736685	0.472677	-3.544437
121	6	0	-6.094400	-2.621539	-0.658541
122	1	0	-5.765677	-2.894932	-1.670546
123	6	0	-7.578025	-2.231754	-0.732640
124	1	0	-8.184713	-3.073780	-1.082787
125	1	0	-7.939504	-1.937292	0.258811
126	1	0	-7.735252	-1.387354	-1.410517
127	6	0	-5.912968	-3.844625	0.239020
128	1	0	-6.340503	-3.672191	1.233270
129	1	0	-6.429431	-4.707310	-0.193342
130	1	0	-4.855586	-4.100283	0.359169
131	6	0	2.858979	1.158965	-3.407557

132	1	0	2.119517	1.945126	-3.233305
133	6	0	2.106278	-0.036698	-3.995515
134	1	0	1.625604	0.250736	-4.937122
135	1	0	2.771474	-0.880984	-4.209489
136	1	0	1.331143	-0.361459	-3.304404
137	6	0	3.893499	1.666033	-4.423103
138	1	0	3.402835	1.949846	-5.360278
139	1	0	4.447406	2.532382	-4.051301
140	1	0	4.623637	0.880307	-4.649411
141	6	0	4.021520	2.215899	1.475942
142	1	0	2.994996	2.585266	1.555874
143	6	0	4.336471	1.479095	2.779197
144	1	0	4.082316	2.112659	3.635432
145	1	0	3.765157	0.549212	2.862308
146	1	0	5.402078	1.237139	2.861811
147	6	0	4.957844	3.422178	1.314680
148	1	0	5.994999	3.081575	1.216607
149	1	0	4.705324	4.009654	0.427462
150	1	0	4.894870	4.077714	2.190067
151	6	0	6.048714	-1.782474	-0.823811
152	1	0	6.025529	-2.162361	0.207269
153	6	0	7.482737	-1.325416	-1.124339
154	1	0	8.184942	-2.162597	-1.047160
155	1	0	7.542574	-0.920013	-2.140479
156	1	0	7.800885	-0.540964	-0.431176
157	6	0	5.643812	-2.929481	-1.750372
158	1	0	6.246507	-3.818693	-1.539334
159	1	0	4.587957	-3.189497	-1.622702
160	1	0	5.806543	-2.665737	-2.801361

Int-2(H)

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.253292 hartree

Sum of electronic and thermal Free Energies = -3615.973905 hartree

The number of imaginary frequency = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.231904	-3.064649	-3.455909
2	1	0	-3.846796	-2.180488	-3.228271
3	1	0	-3.579588	-3.453998	-4.416302
4	6	0	-3.385926	-4.073361	-2.350699
5	1	0	-3.924708	-5.000725	-2.525583
6	6	0	-2.844285	-3.797003	-1.163057
7	1	0	-2.885886	-4.474188	-0.318312
8	6	0	-2.140679	-2.477247	-1.004866
9	1	0	-2.879681	-1.675951	-1.122218
10	1	0	-1.464998	-1.303751	0.647289
11	7	0	-1.548804	-2.263127	0.293118
12	6	0	-0.775803	-3.184858	0.920454
13	8	0	-0.128712	-2.611607	1.955222
14	8	0	-0.641812	-4.356196	0.612075
15	6	0	0.704313	-3.461196	2.728782
16	1	0	0.080646	-4.132022	3.332419
17	1	0	1.310804	-4.087821	2.063189
18	6	0	1.580675	-2.595517	3.597559
19	6	0	1.449077	-1.206470	3.616827
20	6	0	2.567598	-3.207979	4.373152
21	6	0	2.302978	-0.446054	4.415711
22	1	0	0.696837	-0.720893	2.999010
23	6	0	3.422863	-2.444046	5.160339
24	1	0	2.672724	-4.291214	4.350579
25	6	0	3.292812	-1.055914	5.181993
26	1	0	2.194263	0.634595	4.427707
27	1	0	4.189252	-2.930347	5.756721
28	1	0	3.958487	-0.454385	5.793872
29	1	0	0.762485	-1.193938	-0.963086
30	6	0	4.083434	-3.952058	1.018835
31	6	0	3.397566	-4.717206	0.105432
32	6	0	2.345755	-4.143814	-0.650523
33	6	0	2.050434	-2.775423	-0.452964
34	6	0	2.780965	-1.983453	0.453634
35	6	0	3.773089	-2.581596	1.192140
36	1	0	1.758035	-5.915822	-1.742147
37	1	0	4.871248	-4.397531	1.617810
38	1	0	3.633558	-5.767900	-0.035357
39	6	0	1.537278	-4.866863	-1.564465
40	1	0	2.533357	-0.929860	0.567554
41	1	0	4.314678	-1.993779	1.928460
42	6	0	0.150285	-2.926972	-1.880752
43	6	0	0.454727	-4.279071	-2.162027
44	1	0	-0.220369	-4.850579	-2.785996
45	7	0	0.981872	-2.232570	-1.111443
46	6	0	-1.132351	-2.232335	-2.219376
47	1	0	-0.929639	-1.158313	-2.197514
48	6	0	-1.758484	-2.622342	-3.574726
49	1	0	-1.193816	-3.438272	-4.036278
50	1	0	-1.680289	-1.771068	-4.257938
51	6	0	-1.580601	5.781742	2.381448
52	6	0	-2.352907	4.551317	1.958076
53	6	0	-1.703467	3.912603	0.899315
54	6	0	-0.237667	5.599710	1.644956
55	1	0	-2.089593	6.700539	2.063958
56	1	0	-1.461994	5.840911	3.467575
57	1	0	0.436007	4.978913	2.245761
58	1	0	0.271589	6.542971	1.424142
59	6	0	-0.614352	4.815485	0.358537
60	6	0	-1.214925	5.798569	-0.689566
61	6	0	0.597449	4.312049	-0.404302
62	6	0	0.008753	6.414224	-1.384479
63	1	0	-1.882560	6.535099	-0.232724
64	1	0	-1.795491	5.216461	-1.414324
65	6	0	0.997790	5.274024	-1.336915
66	1	0	-0.200006	6.744633	-2.406361
67	1	0	0.384841	7.285488	-0.832876
68	6	0	-3.532631	4.031732	2.471341
69	6	0	-4.034574	2.851194	1.930294
70	6	0	-3.345443	2.128879	0.947047
71	6	0	-2.155978	2.678940	0.451549
72	1	0	-4.059436	4.532175	3.278888
73	1	0	-4.970287	2.443607	2.301573

74	6	0	1.313512	3.123437	-0.282725
75	6	0	2.469002	2.911670	-1.049751
76	6	0	2.880719	3.930633	-1.919420
77	6	0	2.150922	5.101306	-2.087069
78	1	0	3.796142	3.777256	-2.483326
79	1	0	2.472672	5.856011	-2.799051
80	8	0	-1.411115	1.990300	-0.489175
81	8	0	-0.667650	0.290805	1.312130
82	8	0	0.350750	0.326492	-1.086649
83	15	0	-0.206298	1.050182	0.115449
84	8	0	0.881451	2.170189	0.623173
85	6	0	3.303709	1.669725	-1.006362
86	6	0	3.353702	0.823716	-2.131762
87	6	0	4.153753	1.431005	0.095839
88	6	0	4.266176	-0.237063	-2.139072
89	6	0	5.058475	0.373265	0.029349
90	6	0	5.134210	-0.471254	-1.078877
91	1	0	4.303034	-0.884992	-3.011028
92	1	0	5.727948	0.186589	0.866738
93	6	0	-3.914905	0.829214	0.471878
94	6	0	-4.167225	-0.206853	1.396984
95	6	0	-4.336682	0.677758	-0.870632
96	6	0	-4.876731	-1.339966	0.978109
97	6	0	-5.063785	-0.457908	-1.225788
98	6	0	-5.367453	-1.473182	-0.316441
99	1	0	-5.065513	-2.125402	1.704895
100	1	0	-5.421783	-0.554796	-2.250880
101	6	0	-3.751209	-0.134610	2.863287
102	1	0	-3.179047	0.783337	3.014232
103	6	0	-4.989177	-0.093326	3.771316
104	1	0	-5.542123	-1.038210	3.718876
105	1	0	-4.690713	0.060386	4.813508
106	1	0	-5.680728	0.707144	3.490277
107	6	0	-2.834194	-1.291497	3.275252
108	1	0	-2.669798	-1.262840	4.358390
109	1	0	-3.268844	-2.267686	3.029354
110	1	0	-1.864025	-1.204362	2.785947
111	6	0	-4.056593	1.705851	-1.957715
112	1	0	-3.569627	2.572637	-1.505992
113	6	0	-5.348217	2.206662	-2.615879
114	1	0	-5.865661	1.404878	-3.153511
115	1	0	-6.038125	2.611682	-1.869492
116	1	0	-5.121533	2.996352	-3.339767
117	6	0	-3.094180	1.126485	-3.003658
118	1	0	-2.870821	1.871310	-3.775241
119	1	0	-2.150186	0.828896	-2.535898
120	1	0	-3.540465	0.254769	-3.500172
121	6	0	-6.253155	-2.624828	-0.762224
122	1	0	-5.886414	-2.953590	-1.744917
123	6	0	-7.696166	-2.128829	-0.938213
124	1	0	-8.342029	-2.934141	-1.304210
125	1	0	-8.092854	-1.780024	0.021587
126	1	0	-7.749778	-1.295433	-1.644942
127	6	0	-6.224411	-3.829587	0.175292
128	1	0	-6.678059	-3.586164	1.142649
129	1	0	-6.797083	-4.655954	-0.257113
130	1	0	-5.202221	-4.175090	0.353466
131	6	0	2.511348	1.061638	-3.380685
132	1	0	1.751619	1.810716	-3.141215
133	6	0	1.767941	-0.190130	-3.859686
134	1	0	1.208770	0.041402	-4.773082
135	1	0	2.452047	-1.013773	-4.093826
136	1	0	1.058643	-0.517233	-3.100492
137	6	0	3.392430	1.594016	-4.521014
138	1	0	2.783141	1.818735	-5.402885
139	1	0	3.928509	2.503094	-4.236620
140	1	0	4.139654	0.845241	-4.808922
141	6	0	4.144993	2.353858	1.306764
142	1	0	3.112213	2.677954	1.469203
143	6	0	4.611872	1.666765	2.592162
144	1	0	4.403735	2.309419	3.453954
145	1	0	4.098588	0.712623	2.748218
146	1	0	5.691711	1.480164	2.582100
147	6	0	5.005888	3.596234	1.036084
148	1	0	6.044360	3.299018	0.849937
149	1	0	4.647407	4.151658	0.165100
150	1	0	4.993025	4.268358	1.900929
151	6	0	6.161366	-1.588126	-1.094414
152	1	0	6.243562	-1.960952	-0.063393
153	6	0	7.534739	-1.039687	-1.505488
154	1	0	8.294806	-1.828018	-1.479891
155	1	0	7.489426	-0.639295	-2.524259
156	1	0	7.852278	-0.230520	-0.841205
157	6	0	5.766155	-2.766312	-1.984380
158	1	0	6.443153	-3.610709	-1.820182
159	1	0	4.743896	-3.097583	-1.774648
160	1	0	5.826975	-2.498855	-3.045189

3aa

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -1149.188720 hartree

Sum of electronic and thermal Free Energies = -1148.829908 hartree

The number of imaginary frequency = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.473353	-0.586475	0.394417
2	1	0	-5.687322	-1.543254	0.893492
3	1	0	-6.427644	-0.057569	0.324066
4	6	0	-4.888697	-0.857732	-0.965307
5	1	0	-5.488696	-0.696773	-1.856354
6	6	0	-3.634675	-1.302945	-1.048733
7	1	0	-3.140246	-1.513793	-1.988462
8	6	0	-2.890513	-1.516433	0.242857
9	1	0	-3.389564	-2.337909	0.776575
10	1	0	-1.067851	-2.278672	0.926094
11	7	0	-1.511672	-1.957853	0.074187
12	6	0	-0.632598	-1.321748	-0.763977
13	8	0	0.639596	-1.589448	-0.386047
14	8	0	-0.914740	-0.647886	-1.729923
15	6	0	1.637527	-0.973637	-1.195941

16	1	0	1.644771	-1.450166	-2.183342
17	1	0	1.382088	0.082702	-1.342219
18	6	0	2.979969	-1.093550	-0.523265
19	6	0	3.150775	-1.726250	0.705454
20	6	0	4.082320	-0.500716	-1.143705
21	6	0	4.406594	-1.756006	1.310680
22	1	0	2.295303	-2.182205	1.191259
23	6	0	5.334838	-0.531799	-0.542061
24	1	0	3.950988	0.003721	-2.098756
25	6	0	5.500455	-1.158513	0.692674
26	1	0	4.527643	-2.248492	2.270968
27	1	0	6.182499	-0.064122	-1.033887
28	1	0	6.476890	-1.181780	1.166544
29	6	0	2.377177	2.843925	-0.236073
30	6	0	1.128177	3.062372	-0.763626
31	6	0	0.003882	2.361353	-0.258807
32	6	0	0.183396	1.440903	0.807187
33	6	0	1.479441	1.254177	1.351574
34	6	0	2.553743	1.931485	0.833144
35	1	0	-1.481866	3.189568	-1.604014
36	1	0	3.237721	3.368591	-0.639484
37	1	0	0.985300	3.760247	-1.584747
38	6	0	-1.304677	2.492994	-0.788432
39	1	0	1.590386	0.531775	2.153656
40	1	0	3.550400	1.747345	1.223781
41	6	0	-2.024494	0.783362	0.743281
42	6	0	-2.312318	1.711698	-0.298756
43	1	0	-3.305950	1.749126	-0.730812
44	7	0	-0.834338	0.675796	1.293847
45	6	0	-3.024814	-0.261698	1.186082
46	1	0	-2.683380	-0.589067	2.173170
47	6	0	-4.491496	0.224338	1.268363
48	1	0	-4.545217	1.273049	0.962654
49	1	0	-4.826976	0.196110	2.309161

R_exo

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.178724 hartree

Sum of electronic and thermal Free Energies = -3615.906268 hartree

The number of imaginary frequency = 1

Imaginary frequency = -386.92

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.309844	-4.792850	-2.215096
2	1	0	-1.367793	-5.293984	-2.016860
3	1	0	-3.132316	-5.461528	-2.450253
4	6	0	-2.327938	-3.499500	-2.704248
5	1	0	-3.254735	-3.128807	-3.139117
6	6	0	-1.304301	-2.552341	-2.488140
7	1	0	-1.458779	-1.509989	-2.748928
8	6	0	-0.153921	-2.916728	-1.837758
9	1	0	0.086817	-3.957126	-1.647949
10	1	0	0.668390	-1.037726	-1.466043
11	7	0	0.831566	-2.068595	-1.448861
12	6	0	1.956576	-2.598976	-0.846820
13	8	0	2.813404	-1.625296	-0.520012
14	8	0	2.134063	-3.780204	-0.642736
15	6	0	3.998693	-2.068903	0.141350
16	1	0	4.333759	-1.195613	0.701743
17	1	0	3.740809	-2.867302	0.843804
18	6	0	5.071126	-2.537598	-0.811056
19	6	0	6.317592	-2.882078	-0.280596
20	6	0	4.866353	-2.642062	-2.184088
21	6	0	7.346262	-3.312634	-1.110646
22	1	0	6.479920	-2.806898	0.793708
23	6	0	5.897680	-3.072655	-3.017710
24	1	0	3.901776	-2.382405	-2.608194
25	6	0	7.138553	-3.407074	-2.485959
26	1	0	8.310418	-3.574226	-0.685358
27	1	0	5.725719	-3.147195	-4.087139
28	1	0	7.940232	-3.741373	-3.136962
29	1	0	-0.373509	-1.506668	1.106376
30	6	0	3.497650	-2.301997	3.697492
31	6	0	2.916601	-3.519812	3.415703
32	6	0	1.747020	-3.584404	2.630558
33	6	0	1.184275	-2.382269	2.154750
34	6	0	1.785717	-1.138318	2.427606
35	6	0	2.930052	-1.112264	3.194647
36	1	0	1.512035	-5.743009	2.629058
37	1	0	4.398318	-2.254126	4.301270
38	1	0	3.349957	-4.443909	3.787952
39	6	0	1.089864	-4.805087	2.278738
40	1	0	1.345366	-0.233347	2.017479
41	1	0	3.408206	-0.158643	3.397059
42	6	0	-0.610510	-3.566689	1.072244
43	6	0	-0.038976	-4.801917	1.524461
44	1	0	-0.536376	-5.729003	1.268466
45	7	0	0.036952	-2.433751	1.401700
46	6	0	-1.832890	-3.444251	0.353874
47	1	0	-2.201569	-2.428449	0.217247
48	6	0	-2.605113	-4.496923	-0.107284
49	1	0	-2.351918	-5.524187	0.141771
50	1	0	-3.658282	-4.312144	-0.267845
51	6	0	-3.301048	5.467352	1.784212
52	6	0	-3.728686	4.046735	1.495755
53	6	0	-2.906670	3.477586	0.519390
54	6	0	-1.914285	5.528692	1.120370
55	1	0	-3.993707	6.187400	1.329934
56	1	0	-3.270139	5.683969	2.856323
57	1	0	-1.155007	5.148429	1.813569
58	1	0	-1.617879	6.534946	0.809294
59	6	0	-2.017207	4.543920	-0.080008
60	6	0	-2.702601	5.255977	-1.279247
61	6	0	-0.649255	4.273865	-0.667164
62	6	0	-1.575767	6.089481	-1.917772
63	1	0	-3.568778	5.849940	-0.971777
64	1	0	-3.045533	4.490870	-1.985010
65	6	0	-0.347118	5.263761	-1.607548
66	1	0	-1.715013	6.237133	-2.993026
67	1	0	-1.508469	7.085904	-1.462896

68	6	0	-4.769278	3.319257	2.053598
69	6	0	-4.964576	2.010302	1.628059
70	6	0	-4.104843	1.385018	0.714466
71	6	0	-3.048268	2.136866	0.182221
72	1	0	-5.425320	3.761065	2.798206
73	1	0	-5.795829	1.431820	2.021565
74	6	0	0.302581	3.318510	-0.334584
75	6	0	1.620226	3.447501	-0.794830
76	6	0	1.916677	4.507368	-1.659508
77	6	0	0.938812	5.389350	-2.109975
78	1	0	2.943388	4.623095	-1.992168
79	1	0	1.186878	6.168962	-2.824687
80	8	0	-2.177284	1.575934	-0.730102
81	8	0	-0.989376	-0.010747	0.923013
82	8	0	-0.014374	0.532449	-1.443032
83	15	0	-0.749208	0.952271	-0.208021
84	8	0	-0.041735	2.264307	0.493163
85	6	0	2.726967	2.556022	-0.337635
86	6	0	3.464797	1.804292	-1.276371
87	6	0	3.124604	2.578364	1.015290
88	6	0	4.608677	1.129522	-0.847622
89	6	0	4.271909	1.877021	1.396016
90	6	0	5.045436	1.172371	0.476140
91	1	0	5.194037	0.559142	-1.569401
92	1	0	4.594846	1.933152	2.434338
93	6	0	-4.409123	-0.023429	0.325229
94	6	0	-4.508473	-1.014743	1.328889
95	6	0	-4.769970	-0.334804	-1.001320
96	6	0	-5.041131	-2.258751	0.994750
97	6	0	-5.275212	-1.607995	-1.287298
98	6	0	-5.467029	-2.566746	-0.297307
99	1	0	-5.145751	-3.015841	1.772105
100	1	0	-5.579099	-1.825643	-2.308615
101	6	0	3.090842	1.748612	-2.752070
102	1	0	2.111612	2.218730	-2.873666
103	6	0	4.118686	2.504419	-3.606577
104	1	0	5.100319	2.021303	-3.538729
105	1	0	3.815766	2.502718	-4.659041
106	1	0	4.241120	3.543411	-3.288554
107	6	0	2.966605	0.313198	-3.267011
108	1	0	2.632091	0.320043	-4.309898
109	1	0	3.929655	-0.207245	-3.227897
110	1	0	2.241854	-0.247290	-2.675596
111	6	0	2.419788	3.423414	2.069530
112	1	0	1.590614	3.952432	1.595023
113	6	0	3.366649	4.491595	2.632950
114	1	0	4.204747	4.038957	3.174229
115	1	0	3.779419	5.110535	1.830457
116	1	0	2.832029	5.143685	3.331714
117	6	0	1.827405	2.568106	3.193243
118	1	0	1.328793	3.204841	3.932244
119	1	0	1.086875	1.867066	2.798455
120	1	0	2.609461	2.007304	3.719634
121	6	0	6.383337	0.553950	0.844452
122	1	0	6.586117	-0.241025	0.114554
123	6	0	6.428066	-0.068056	2.242132
124	1	0	6.318582	0.693076	3.022932
125	1	0	5.638152	-0.813754	2.385762
126	1	0	7.392870	-0.560850	2.402844
127	6	0	7.489060	1.609995	0.703208
128	1	0	8.473428	1.176810	0.911077
129	1	0	7.500414	2.029826	-0.306677
130	1	0	7.318964	2.432195	1.407550
131	6	0	-4.730386	0.680528	-2.136609
132	1	0	-4.436956	1.649870	-1.728433
133	6	0	-6.117480	0.863826	-2.767405
134	1	0	-6.454108	-0.045629	-3.276691
135	1	0	-6.863535	1.122083	-2.009647
136	1	0	-6.089277	1.666877	-3.511142
137	6	0	-3.691835	0.296723	-3.196116
138	1	0	-3.707453	1.015417	-4.022602
139	1	0	-2.687254	0.297927	-2.765322
140	1	0	-3.905731	-0.695180	-3.614847
141	6	0	-6.209332	-3.868739	-0.549668
142	1	0	-5.772539	-4.633410	0.108786
143	6	0	-4.078583	-0.783058	2.773284
144	1	0	-3.707392	0.240151	2.863354
145	6	0	-5.253757	-0.954325	3.744416
146	1	0	-5.613500	-1.989372	3.751208
147	1	0	-4.942896	-0.704772	4.764162
148	1	0	-6.099361	-0.312679	3.477685
149	6	0	-2.919351	-1.705612	3.164512
150	1	0	-2.667902	-1.567827	4.221914
151	1	0	-3.170093	-2.761689	3.008946
152	1	0	-2.038813	-1.458332	2.568957
153	6	0	-7.681556	-3.704217	-0.144784
154	1	0	-8.155295	-2.933505	-0.762537
155	1	0	-8.231591	-4.641585	-0.280934
156	1	0	-7.770085	-3.397538	0.901401
157	6	0	-6.112238	-4.369358	-1.990566
158	1	0	-6.663848	-3.714932	-2.673908
159	1	0	-5.073316	-4.412049	-2.332174
160	1	0	-6.545606	-5.370462	-2.076382

R_exo2

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.176596 hartree

Sum of electronic and thermal Free Energies = -3615.903415 hartree

The number of imaginary frequency = 1

Imaginary frequency = -349.67

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.388170	-2.286545	4.411989
2	1	0	3.013688	-3.250908	4.080865
3	1	0	4.293070	-2.326480	5.010713
4	6	0	2.543680	-1.203715	4.525557
5	1	0	2.904201	-0.332805	5.069275
6	6	0	1.341124	-1.047536	3.802219
7	1	0	0.867119	-0.071566	3.748601
8	6	0	0.828566	-2.058264	3.029243

9	1	0	1.159476	-3.089568	3.114460
10	1	0	-0.487419	-0.902065	1.952561
11	7	0	-0.208408	-1.880374	2.169957
12	6	0	-0.854356	-2.946046	1.592936
13	8	0	-1.872723	-2.493741	0.837842
14	8	0	-0.555319	-4.109090	1.755103
15	6	0	-2.811517	-3.474203	0.394265
16	1	0	-2.333459	-4.457416	0.414054
17	1	0	-3.641927	-3.472245	1.112634
18	6	0	-3.297657	-3.161756	-0.997209
19	6	0	-3.932806	-4.180517	-1.712397
20	6	0	-3.089262	-1.923433	-1.602564
21	6	0	-4.327487	-3.982731	-3.031578
22	1	0	-4.091754	-5.147282	-1.238941
23	6	0	-3.462916	-1.734642	-2.933501
24	1	0	-2.607726	-1.120763	-1.047812
25	6	0	-4.076816	-2.759190	-3.651867
26	1	0	-4.814356	-4.784772	-3.578113
27	1	0	-3.265248	-0.780655	-3.410344
28	1	0	-4.362654	-2.603257	-4.687684
29	1	0	1.293151	-1.589382	-0.231199
30	6	0	-0.342783	-5.439134	-2.436021
31	6	0	0.643410	-5.834585	-1.559608
32	6	0	1.313976	-4.880866	-0.768086
33	6	0	0.954016	-3.522290	-0.888740
34	6	0	-0.066505	-3.122354	-1.767796
35	6	0	-0.694608	-4.078221	-2.537155
36	1	0	2.625037	-6.253659	0.281056
37	1	0	-0.859120	-6.173523	-3.045325
38	1	0	0.917421	-6.881305	-1.461732
39	6	0	2.339357	-5.211375	0.166533
40	1	0	-0.348047	-2.074008	-1.809364
41	1	0	-1.488429	-3.773954	-3.213462
42	6	0	2.577522	-2.872667	0.761353
43	6	0	2.950979	-4.247957	0.904492
44	1	0	3.728260	-4.503620	1.613925
45	7	0	1.603817	-2.584047	-0.120581
46	6	0	3.163868	-1.803582	1.494999
47	1	0	2.805424	-0.803630	1.255143
48	6	0	4.183529	-1.950377	2.413841
49	1	0	4.753818	-2.872514	2.485826
50	1	0	4.724798	-1.059392	2.706299
51	6	0	0.411989	5.625640	-2.789960
52	6	0	1.390975	4.524519	-2.452272
53	6	0	1.037453	3.909565	-1.248886
54	6	0	-0.747404	5.337126	-1.820029
55	1	0	0.851711	6.613991	-2.604457
56	1	0	0.104445	5.603012	-3.839829
57	1	0	-1.422282	4.593195	-2.259519
58	1	0	-1.337553	6.221769	-1.562301
59	6	0	-0.063260	4.699151	-0.576101
60	6	0	0.513375	5.818891	0.333802
61	6	0	-1.103327	4.101784	0.348596
62	6	0	-0.705478	6.330579	1.123901
63	1	0	1.024864	6.598599	-0.239001
64	1	0	1.239091	5.366489	1.019237
65	6	0	-1.579660	5.098892	1.206978
66	1	0	-0.437904	6.716160	2.112373
67	1	0	-1.216423	7.142061	0.590387
68	6	0	2.513032	4.107964	-3.154030
69	6	0	3.267085	3.059714	-2.637919
70	6	0	2.890192	2.369628	-1.477436
71	6	0	1.738343	2.795902	-0.801909
72	1	0	2.805779	4.593667	-4.080575
73	1	0	4.169296	2.737308	-3.151144
74	6	0	-1.686508	2.841312	0.352674
75	6	0	-2.870707	2.617138	1.076143
76	6	0	-3.384410	3.670595	1.839498
77	6	0	-2.724112	4.891601	1.959285
78	1	0	-4.338789	3.523305	2.334873
79	1	0	-3.120556	5.672339	2.602366
80	8	0	1.325515	2.166851	0.353663
81	8	0	0.519230	-0.086629	-0.628182
82	8	0	-0.182883	0.756330	1.741520
83	15	0	0.138016	1.029025	0.303830
84	8	0	-1.113893	1.830538	-0.406110
85	6	0	-3.708772	1.391222	0.884246
86	6	0	-3.830294	0.392887	1.875346
87	6	0	-4.479335	1.312047	-0.291828
88	6	0	-4.697348	-0.674124	1.637410
89	6	0	-5.332358	0.221463	-0.480681
90	6	0	-5.454365	-0.785697	0.469840
91	1	0	-4.795805	-1.453459	2.391321
92	1	0	-5.904320	0.161247	-1.402988
93	6	0	3.763170	1.251818	-1.008756
94	6	0	3.982237	0.136166	-1.846763
95	6	0	4.491232	1.369861	0.191889
96	6	0	4.922649	-0.819661	-1.466044
97	6	0	5.469823	0.416958	0.492243
98	6	0	5.708965	-0.685243	-0.322017
99	1	0	5.066453	-1.690542	-2.103677
100	1	0	6.051895	0.548016	1.400881
101	6	0	-3.082040	0.472668	3.201451
102	1	0	-2.120483	0.959474	3.005864
103	6	0	-3.856655	1.297485	4.242722
104	1	0	-4.869167	0.895029	4.364353
105	1	0	-3.351371	1.240404	5.213327
106	1	0	-3.934026	2.350082	3.970822
107	6	0	-2.814511	-0.908168	3.816949
108	1	0	-2.009055	-0.842046	4.555812
109	1	0	-3.703433	-1.287756	4.335016
110	1	0	-2.531445	-1.642265	3.061758
111	6	0	-4.452463	2.396506	-1.362074
112	1	0	-3.799955	3.205312	-1.024217
113	6	0	-5.845568	3.002176	-1.570950
114	1	0	-6.553513	2.257166	-1.949873
115	1	0	-6.243789	3.398056	-0.631609
116	1	0	-5.800327	3.819924	-2.298094
117	6	0	-3.879634	1.867917	-2.680358
118	1	0	-3.816233	2.672150	-3.421904
119	1	0	-2.875898	1.457530	-2.526574
120	1	0	-4.521730	1.081572	-3.094163
121	6	0	-6.396086	-1.967121	0.303299
122	1	0	-5.832865	-2.871799	0.577132

123	6	0	-6.899624	-2.154354	-1.126039
124	1	0	-7.578772	-1.342156	-1.410643
125	1	0	-6.073038	-2.180029	-1.842101
126	1	0	-7.455949	-3.093371	-1.209559
127	6	0	-7.580366	-1.841778	1.272256
128	1	0	-8.241972	-2.711068	1.192726
129	1	0	-7.244405	-1.758073	2.309969
130	1	0	-8.162962	-0.944688	1.035536
131	6	0	4.277404	2.504156	1.184172
132	1	0	3.551461	3.204247	0.764969
133	6	0	5.568381	3.291045	1.440330
134	1	0	6.331806	2.670290	1.921808
135	1	0	5.986718	3.674403	0.504791
136	1	0	5.368594	4.140448	2.101846
137	6	0	3.691520	1.964670	2.496383
138	1	0	3.497772	2.785871	3.195214
139	1	0	2.746040	1.441509	2.319287
140	1	0	4.395838	1.275805	2.981475
141	6	0	6.767306	-1.736893	-0.018698
142	1	0	6.241812	-2.699605	0.081602
143	6	0	3.262686	-0.060886	-3.175538
144	1	0	2.584238	0.780690	-3.330587
145	6	0	4.257339	-0.089085	-4.342864
146	1	0	4.923705	-0.956331	-4.273986
147	1	0	3.722931	-0.154281	-5.296358
148	1	0	4.884435	0.808107	-4.360991
149	6	0	2.394856	-1.320154	-3.160164
150	1	0	1.928295	-1.478647	-4.138777
151	1	0	2.975275	-2.218046	-2.914616
152	1	0	1.604836	-1.193460	-2.419993
153	6	0	7.759512	-1.860359	-1.184764
154	1	0	8.303170	-0.918152	-1.313309
155	1	0	8.489285	-2.652667	-0.988052
156	1	0	7.258219	-2.087330	-2.129003
157	6	0	7.545832	-1.486153	1.272482
158	1	0	8.100227	-0.542714	1.212836
159	1	0	6.895759	-1.440063	2.150698
160	1	0	8.271909	-2.288719	1.434077

S_exo

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.184958 hartree

Sum of electronic and thermal Free Energies = -3615.913170 hartree

The number of imaginary frequency = 1

Imaginary frequency = -392.60

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.434137	-3.348288	3.994076
2	1	0	1.929971	-4.215747	3.578288
3	1	0	2.904634	-3.517481	4.957914
4	6	0	2.939380	-2.366097	3.161300
5	1	0	3.653661	-1.659197	3.578631
6	6	0	2.448834	-2.075271	1.871951
7	1	0	2.764630	-1.165890	1.366415
8	6	0	1.514929	-2.873153	1.265001
9	1	0	1.239106	-3.847400	1.658072
10	1	0	0.991116	-1.645237	-0.359867
11	7	0	0.909814	-2.580180	0.089353
12	6	0	0.020450	-3.479190	-0.467549
13	8	0	-0.489071	-2.961190	-1.585340
14	8	0	-0.256017	-4.564936	-0.007179
15	6	0	-1.375724	-3.802125	-2.316067
16	1	0	-0.809456	-4.655402	-2.708077
17	1	0	-2.142596	-4.192655	-1.638672
18	6	0	-1.988366	-2.992547	-3.428041
19	6	0	-2.977037	-3.588492	-4.214269
20	6	0	-1.612802	-1.672096	-3.674494
21	6	0	-3.585890	-2.876669	-5.241616
22	1	0	-3.275446	-4.615765	-4.013871
23	6	0	-2.219589	-0.965182	-4.712770
24	1	0	-0.864984	-1.193123	-3.046885
25	6	0	-3.205555	-1.559425	-5.494829
26	1	0	-4.355525	-3.348661	-5.844961
27	1	0	-1.919769	0.061133	-4.901633
28	1	0	-3.676155	-1.001067	-6.298212
29	1	0	-1.083703	-0.963652	1.420688
30	6	0	-4.564998	-3.226181	-0.902915
31	6	0	-4.185857	-3.999717	0.174510
32	6	0	-3.164793	-3.559271	1.041445
33	6	0	-2.552898	-2.311629	0.791229
34	6	0	-2.938866	-1.524364	-0.307372
35	6	0	-3.933812	-1.988165	-1.141553
36	1	0	-3.158570	-5.272774	2.374285
37	1	0	-5.343476	-3.569011	-1.576911
38	1	0	-4.660879	-4.957346	0.368977
39	6	0	-2.700041	-4.309718	2.166873
40	1	0	-2.450953	-0.566918	-0.480572
41	1	0	-4.222730	-1.390843	-2.002230
42	6	0	-1.091242	-2.572635	2.689516
43	6	0	-1.703553	-3.840744	2.960868
44	1	0	-1.356296	-4.411794	3.813207
45	7	0	-1.547765	-1.882975	1.623909
46	6	0	-0.068296	-1.970626	3.469207
47	1	0	0.242570	-0.983516	3.139829
48	6	0	0.549088	-2.522602	4.578533
49	1	0	0.185892	-3.447062	5.020183
50	1	0	1.022319	-1.847771	5.281576
51	6	0	2.425889	5.356792	-2.518997
52	6	0	2.982104	3.993953	-2.175269
53	6	0	2.341693	3.472823	-1.045843
54	6	0	1.145933	5.409011	-1.667629
55	1	0	3.127146	6.152049	-2.235492
56	1	0	2.230032	5.468163	-3.589723
57	1	0	0.321861	4.927662	-2.206542
58	1	0	0.833141	6.423501	-1.402464
59	6	0	1.480823	4.547352	-0.416740
60	6	0	2.290797	5.399787	0.600366
61	6	0	0.233514	4.269481	0.392297
62	6	0	1.222362	6.232389	1.332728
63	1	0	3.063582	6.004065	0.115490

64	1	0	2.781464	4.720046	1.306481
65	6	0	0.017886	5.319092	1.289381
66	1	0	1.511979	6.489354	2.356204
67	1	0	1.022451	7.175818	0.809010
68	6	0	3.979840	3.277935	-2.817281
69	6	0	4.324763	2.027035	-2.315655
70	6	0	3.644963	1.444783	-1.240020
71	6	0	2.618524	2.177372	-0.624490
72	1	0	4.490839	3.685145	-3.685124
73	1	0	5.133891	1.464463	-2.771767
74	6	0	-0.693875	3.240552	0.285626
75	6	0	-1.920243	3.324578	0.961373
76	6	0	-2.146852	4.440068	1.778480
77	6	0	-1.178733	5.417544	1.983554
78	1	0	-3.106140	4.514689	2.283345
79	1	0	-1.364539	6.242935	2.664982
80	8	0	1.901872	1.636060	0.431414
81	8	0	0.638932	-0.056510	-1.064056
82	8	0	-0.114265	0.451173	1.374130
83	15	0	0.464290	0.912633	0.065123
84	8	0	-0.415437	2.164539	-0.537278
85	6	0	-3.003667	2.307045	0.823486
86	6	0	-3.494090	1.643072	1.967073
87	6	0	-3.628420	2.096973	-0.425991
88	6	0	-4.588473	0.783147	1.838542
89	6	0	-4.731532	1.246993	-0.493765
90	6	0	-5.229617	0.577760	0.622047
91	1	0	-4.950005	0.269242	2.725787
92	1	0	-5.222153	1.092040	-1.454783
93	6	0	4.102550	0.106421	-0.758019
94	6	0	3.950842	-1.033322	-1.572553
95	6	0	4.831566	0.019301	0.448347
96	6	0	4.523865	-2.237598	-1.152488
97	6	0	5.405509	-1.200623	0.808539
98	6	0	5.269449	-2.342093	0.017829
99	1	0	4.420807	-3.118328	-1.783893
100	1	0	5.984403	-1.257994	1.729942
101	6	0	5.058509	1.225963	1.348817
102	1	0	4.551572	2.087808	0.908308
103	6	0	6.549899	1.571253	1.436232
104	1	0	6.701280	2.467049	2.047781
105	1	0	7.120836	0.753974	1.890750
106	1	0	6.964997	1.758688	0.441186
107	6	0	4.458756	1.011845	2.742172
108	1	0	3.389398	0.785329	2.675517
109	1	0	4.965915	0.191891	3.265371
110	1	0	4.578262	1.914012	3.351683
111	6	0	3.291407	-0.978464	-2.945503
112	1	0	2.809851	-0.002935	-3.053125
113	6	0	4.355956	-1.128408	-4.042861
114	1	0	4.811021	-2.124860	-4.002847
115	1	0	3.903338	-1.005014	-5.032324
116	1	0	5.160929	-0.394882	-3.939994
117	6	0	2.199811	-2.033567	-3.133449
118	1	0	1.367441	-1.839892	-2.459819
119	1	0	1.815424	-1.993361	-4.159046
120	1	0	2.572993	-3.050079	-2.960764
121	6	0	5.946277	-3.648861	0.390293
122	1	0	5.757115	-4.354969	-0.428571
123	6	0	7.463928	-3.472137	0.514710
124	1	0	7.711948	-2.798388	1.342256
125	1	0	7.949337	-4.433892	0.710961
126	1	0	7.888007	-3.049332	-0.400568
127	6	0	5.365023	-4.252915	1.671901
128	1	0	5.858141	-5.202104	1.908294
129	1	0	5.509034	-3.575655	2.521796
130	1	0	4.290479	-4.431038	1.572456
131	6	0	-2.907700	1.834074	3.360729
132	1	0	-2.050352	2.506496	3.288655
133	6	0	-2.377280	0.517668	3.931085
134	1	0	-1.561150	0.164011	3.302401
135	1	0	-1.990393	0.667338	4.945223
136	1	0	-3.152537	-0.256605	3.976751
137	6	0	-3.934878	2.466472	4.308507
138	1	0	-3.480926	2.665055	5.285107
139	1	0	-4.325409	3.409642	3.913242
140	1	0	-4.788166	1.797368	4.466406
141	6	0	-3.179214	2.782537	-1.708167
142	1	0	-2.340908	3.444148	-1.479444
143	6	0	-2.692284	1.753863	-2.734506
144	1	0	-2.346136	2.259261	-3.643834
145	1	0	-1.860539	1.164100	-2.335331
146	1	0	-3.500753	1.070685	-3.023022
147	6	0	-4.298128	3.655005	-2.291106
148	1	0	-5.161551	3.051160	-2.590737
149	1	0	-4.641083	4.393984	-1.560525
150	1	0	-3.940872	4.187821	-3.178648
151	6	0	-6.449049	-0.313709	0.483869
152	1	0	-6.396691	-0.776213	-0.511740
153	6	0	-6.495559	-1.438518	1.518250
154	1	0	-6.721581	-1.048150	2.516878
155	1	0	-7.280270	-2.157788	1.262684
156	1	0	-5.540637	-1.971743	1.567316
157	6	0	-7.730337	0.529245	0.543487
158	1	0	-8.618006	-0.097755	0.406397
159	1	0	-7.808137	1.026197	1.516812
160	1	0	-7.730167	1.303795	-0.229269

S_exo2

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.182891 hartree

Sum of electronic and thermal Free Energies = -3615.909697 hartree

The number of imaginary frequency = 1

Imaginary frequency = -424.53

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.117482	-0.366116	5.201706
2	1	0	2.746862	-1.177214	4.847874
3	1	0	2.161175	-0.200603	6.273953
4	6	0	1.834692	0.707261	4.370448

5	1	0	1.450582	1.617774	4.826213
6	6	0	1.796713	0.639420	2.964049
7	1	0	1.370744	1.454165	2.385556
8	6	0	2.222815	-0.481019	2.296351
9	1	0	2.752491	-1.281657	2.803339
10	1	0	1.566940	-0.059579	0.341741
11	7	0	2.132457	-0.671147	0.960415
12	6	0	2.737510	-1.776580	0.392841
13	8	0	2.601444	-1.749638	-0.931116
14	8	0	3.310322	-2.640571	1.025857
15	6	0	3.314918	-2.772187	-1.651817
16	1	0	3.185199	-3.723562	-1.131013
17	1	0	2.808126	-2.811028	-2.618128
18	6	0	4.771859	-2.409920	-1.806099
19	6	0	5.192248	-1.653398	-2.902842
20	6	0	5.711727	-2.793393	-0.844673
21	6	0	6.523152	-1.264545	-3.029430
22	1	0	4.468862	-1.366567	-3.662410
23	6	0	7.044596	-2.409892	-0.972973
24	1	0	5.386496	-3.375673	0.011240
25	6	0	7.451568	-1.640847	-2.061109
26	1	0	6.834701	-0.671275	-3.883404
27	1	0	7.766041	-2.710088	-0.218934
28	1	0	8.489895	-1.338030	-2.156599
29	1	0	-0.719887	-1.455149	1.325243
30	6	0	0.423129	-4.929206	-1.721577
31	6	0	0.865319	-5.285434	-0.464277
32	6	0	0.649718	-4.428897	0.634020
33	6	0	-0.036126	-3.213180	0.423463
34	6	0	-0.487650	-2.848914	-0.857513
35	6	0	-0.249762	-3.705094	-1.911909
36	1	0	1.618832	-5.650759	2.145858
37	1	0	0.592497	-5.589362	-2.566134
38	1	0	1.386397	-6.225030	-0.301693
39	6	0	1.098133	-4.714526	1.963852
40	1	0	-0.992465	-1.897224	-1.000031
41	1	0	-0.595531	-3.425024	-2.902973
42	6	0	0.221918	-2.590802	2.739240
43	6	0	0.899977	-3.833824	2.976857
44	1	0	1.249381	-4.049505	3.979285
45	7	0	-0.227037	-2.365577	1.487218
46	6	0	-0.031279	-1.589694	3.710949
47	1	0	-0.603189	-0.737912	3.353318
48	6	0	0.402060	-1.584300	5.028850
49	1	0	0.866087	-2.465385	5.465555
50	1	0	-0.153451	-0.979485	5.735957
51	6	0	-2.848730	5.804760	-1.862076
52	6	0	-1.503934	5.227589	-1.492573
53	6	0	-1.648732	4.184680	-0.569007
54	6	0	-3.797015	4.686386	-1.411721
55	1	0	-3.043840	6.737169	-1.316544
56	1	0	-2.927733	6.031227	-2.929447
57	1	0	-3.847352	3.913617	-2.187189
58	1	0	-4.816192	5.024254	-1.203077
59	6	0	-3.107567	4.074037	-0.154306
60	6	0	-3.483091	4.920172	1.091336
61	6	0	-3.787845	2.765897	0.194444
62	6	0	-4.920872	4.467483	1.428158
63	1	0	-3.397668	5.995678	0.907510
64	1	0	-2.805404	4.656828	1.910499
65	6	0	-4.934209	3.031281	0.948079
66	1	0	-5.146603	4.543704	2.496202
67	1	0	-5.666206	5.075030	0.900085
68	6	0	-0.257855	5.588009	-1.979574
69	6	0	0.847827	4.845319	-1.582421
70	6	0	0.730628	3.743173	-0.728785
71	6	0	-0.532028	3.441725	-0.189429
72	1	0	-0.149436	6.413850	-2.676947
73	1	0	1.837048	5.101364	-1.950516
74	6	0	-3.501903	1.463938	-0.188093
75	6	0	-4.427594	0.431884	0.021687
76	6	0	-5.632569	0.759940	0.655182
77	6	0	-5.876114	2.034999	1.162732
78	1	0	-6.369853	-0.025493	0.796256
79	1	0	-6.787535	2.238155	1.718010
80	8	0	-0.679104	2.426991	0.743347
81	8	0	0.079196	0.364547	-0.629772
82	8	0	-1.453449	0.119804	1.436397
83	15	0	-1.022564	0.901473	0.227636
84	8	0	-2.286925	1.179990	-0.779297
85	6	0	-4.130604	-0.977878	-0.374842
86	6	0	-4.166816	-2.001991	0.597453
87	6	0	-3.843078	-1.309642	-1.719405
88	6	0	-3.921977	-3.322074	0.208427
89	6	0	-3.621429	-2.645288	-2.053491
90	6	0	-3.650753	-3.669131	-1.110143
91	1	0	-3.947130	-4.098690	0.968727
92	1	0	-3.407623	-2.901370	-3.091127
93	6	0	1.958808	2.937632	-0.445030
94	6	0	2.405224	1.993395	-1.397281
95	6	0	2.720678	3.203129	0.705797
96	6	0	3.590604	1.306977	-1.141606
97	6	0	3.885684	2.462459	0.933147
98	6	0	4.334133	1.508381	0.022348
99	1	0	3.952783	0.578937	-1.863666
100	1	0	4.471232	2.663134	1.829871
101	6	0	2.382605	4.368129	1.630547
102	1	0	1.463362	4.834488	1.264650
103	6	0	3.493774	5.424325	1.547645
104	1	0	3.226871	6.310896	2.132561
105	1	0	4.439196	5.032597	1.939158
106	1	0	3.662769	5.731468	0.510943
107	6	0	2.135176	3.960605	3.086204
108	1	0	1.199977	3.400207	3.180681
109	1	0	2.951190	3.342437	3.478406
110	1	0	2.053976	4.852211	3.717328
111	6	0	1.684436	1.781520	-2.724155
112	1	0	0.644184	2.096649	-2.594600
113	6	0	2.335055	2.648673	-3.813346
114	1	0	3.383102	2.356788	-3.950775
115	1	0	1.817069	2.514082	-4.769260
116	1	0	2.313615	3.711822	-3.562714
117	6	0	1.658594	0.324790	-3.198424
118	1	0	1.232315	-0.328414	-2.436811

119	1	0	1.051358	0.254684	-4.108241
120	1	0	2.665189	-0.029018	-3.453697
121	6	0	5.633290	0.751657	0.230468
122	1	0	5.713476	0.018696	-0.581575
123	6	0	6.834100	1.698643	0.118884
124	1	0	6.823834	2.438821	0.927444
125	1	0	7.773017	1.137506	0.183712
126	1	0	6.818459	2.239080	-0.832327
127	6	0	5.672390	-0.015873	1.555357
128	1	0	6.652299	-0.488234	1.688842
129	1	0	5.500751	0.651508	2.408146
130	1	0	4.919459	-0.809217	1.582515
131	6	0	-4.478827	-1.756420	2.069428
132	1	0	-4.550784	-0.680403	2.236937
133	6	0	-3.356383	-2.255219	2.981450
134	1	0	-2.444030	-1.704166	2.757239
135	1	0	-3.613987	-2.079000	4.031740
136	1	0	-3.162982	-3.327223	2.859180
137	6	0	-5.817731	-2.398690	2.455334
138	1	0	-6.069999	-2.164507	3.495066
139	1	0	-6.635401	-2.050639	1.816041
140	1	0	-5.768365	-3.489325	2.359359
141	6	0	-3.786513	-0.288513	-2.847578
142	1	0	-3.979833	0.704145	-2.435932
143	6	0	-2.397187	-0.260981	-3.499712
144	1	0	-2.347748	0.532270	-4.253910
145	1	0	-1.615584	-0.075462	-2.756558
146	1	0	-2.184803	-1.210205	-4.007424
147	6	0	-4.877002	-0.564479	-3.891134
148	1	0	-4.729986	-1.536907	-4.373834
149	1	0	-5.870462	-0.563845	-3.432212
150	1	0	-4.857690	0.202155	-4.673018
151	6	0	-3.418325	-5.103529	-1.544804
152	1	0	-2.716569	-5.071743	-2.390059
153	6	0	-2.791599	-5.971632	-0.453218
154	1	0	-3.510061	-6.181390	0.347084
155	1	0	-2.473971	-6.933662	-0.868143
156	1	0	-1.918851	-5.481918	-0.009358
157	6	0	-4.729567	-5.724941	-2.044681
158	1	0	-4.567965	-6.749009	-2.398428
159	1	0	-5.464755	-5.754434	-1.232832
160	1	0	-5.157486	-5.138344	-2.863145

S_endo

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.188305 hartree

Sum of electronic and thermal Free Energies = -3615.911780 hartree

The number of imaginary frequency = 1

Imaginary frequency = -376.87

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.079575	-3.339823	-4.439106
2	1	0	0.566866	-2.469780	-4.387225
3	1	0	-0.362994	-3.634044	-5.445401
4	6	0	-0.027751	-4.307029	-3.450755
5	1	0	-0.444638	-5.286913	-3.677710
6	6	0	0.341897	-4.079186	-2.106489
7	1	0	0.201331	-4.865109	-1.375634
8	6	0	0.748921	-2.831239	-1.693224
9	1	0	0.974925	-2.053265	-2.410425
10	1	0	1.288544	-1.418801	-0.367710
11	7	0	0.972389	-2.390110	-0.426595
12	6	0	0.703454	-3.064789	0.740985
13	8	0	0.952337	-2.257150	1.782275
14	8	0	0.290982	-4.202124	0.819055
15	6	0	0.777595	-2.823038	3.079805
16	1	0	-0.027138	-3.563560	3.042666
17	1	0	1.704652	-3.342322	3.355310
18	6	0	0.460192	-1.721334	4.060696
19	6	0	0.311538	-2.056335	5.408340
20	6	0	0.296100	-0.394959	3.658578
21	6	0	-0.012467	-1.080953	6.345818
22	1	0	0.445106	-3.089155	5.724374
23	6	0	-0.031039	0.579155	4.601279
24	1	0	0.405660	-0.121282	2.612004
25	6	0	-0.188336	0.242004	5.942565
26	1	0	-0.127368	-1.353161	7.390720
27	1	0	-0.164330	1.605902	4.273163
28	1	0	-0.443746	1.004104	6.672392
29	1	0	-1.591941	-0.994956	-0.101293
30	6	0	-3.217144	-3.945122	3.193129
31	6	0	-3.402446	-4.540531	1.963162
32	6	0	-3.003589	-3.881298	0.784028
33	6	0	-2.413415	-2.604925	0.889966
34	6	0	-2.205275	-2.009723	2.141826
35	6	0	-2.615620	-2.673914	3.278622
36	1	0	-3.640931	-5.395424	-0.637106
37	1	0	-3.529858	-4.456539	4.097393
38	1	0	-3.857906	-5.523595	1.883860
39	6	0	-3.176450	-4.419039	-0.527722
40	1	0	-1.711246	-1.046223	2.179210
41	1	0	-2.449928	-2.209505	4.247197
42	6	0	-2.133055	-2.443383	-1.489436
43	6	0	-2.765760	-3.727150	-1.621461
44	1	0	-2.881162	-4.143970	-2.613903
45	7	0	-2.017922	-1.938742	-0.246849
46	6	0	-1.622068	-1.698710	-2.588946
47	1	0	-1.095505	-0.774728	-2.358485
48	6	0	-1.740954	-2.120597	-3.902922
49	1	0	-2.483375	-2.859661	-4.184815
50	1	0	-1.506436	-1.403789	-4.684008
51	6	0	0.461302	6.182116	1.802597
52	6	0	-0.619723	5.378004	1.113691
53	6	0	-0.048688	4.392798	0.300763
54	6	0	1.721324	5.335916	1.530944
55	1	0	0.553153	7.187080	1.372321
56	1	0	0.259347	6.309689	2.870496
57	1	0	1.814864	4.549749	2.288244
58	1	0	2.647348	5.918606	1.528189
59	6	0	1.435009	4.668133	0.157568

60	6	0	1.673374	5.714710	-0.970398
61	6	0	2.474422	3.623769	-0.222186
62	6	0	3.193421	5.699625	-1.182587
63	1	0	1.270306	6.699436	-0.717079
64	1	0	1.169880	5.363370	-1.877934
65	6	0	3.525491	4.254364	-0.899134
66	1	0	3.488959	6.001972	-2.191655
67	1	0	3.702191	6.372886	-0.480846
68	6	0	-1.998066	5.503520	1.204777
69	6	0	-2.799429	4.569092	0.552230
70	6	0	-2.253623	3.475735	-0.129770
71	6	0	-0.856838	3.424232	-0.277368
72	1	0	-2.448765	6.298698	1.792031
73	1	0	-3.881615	4.641204	0.625079
74	6	0	2.520906	2.245813	-0.008134
75	6	0	3.636226	1.502908	-0.429103
76	6	0	4.708951	2.189481	-1.012668
77	6	0	4.662548	3.553333	-1.268320
78	1	0	5.582827	1.612762	-1.302040
79	1	0	5.485974	4.050676	-1.772951
80	8	0	-0.282560	2.427277	-1.037070
81	8	0	-0.773602	0.443909	0.585860
82	8	0	0.808765	0.218078	-1.457911
83	15	0	0.246695	1.042340	-0.341499
84	8	0	1.456437	1.616458	0.616538
85	6	0	3.742463	0.011542	-0.349012
86	6	0	3.810618	-0.733606	-1.550508
87	6	0	3.908298	-0.634084	0.892670
88	6	0	4.052569	-2.106062	-1.477439
89	6	0	4.135502	-2.013977	0.907787
90	6	0	4.226485	-2.764781	-0.260999
91	1	0	4.122237	-2.676812	-2.402718
92	1	0	4.275406	-2.521370	1.858601
93	6	0	-3.104818	2.335188	-0.577415
94	6	0	-3.865389	1.627508	0.378345
95	6	0	-3.101992	1.909845	-1.923481
96	6	0	-4.571993	0.489460	-0.024841
97	6	0	-3.827914	0.773988	-2.272346
98	6	0	-4.564921	0.041459	-1.341936
99	1	0	-5.140532	-0.057058	0.723694
100	1	0	-3.826574	0.443073	-3.310405
101	6	0	-3.983327	2.040800	1.842905
102	1	0	-3.375762	2.928835	2.010119
103	6	0	-3.436656	0.977985	2.795811
104	1	0	-3.539571	1.310936	3.835106
105	1	0	-3.966799	0.024743	2.694085
106	1	0	-2.375938	0.814779	2.587663
107	6	0	-5.433679	2.402924	2.186686
108	1	0	-5.503462	2.763658	3.218461
109	1	0	-5.818416	3.183147	1.521336
110	1	0	-6.093066	1.533096	2.091577
111	6	0	-2.420590	2.695843	-3.035362
112	1	0	-1.829612	3.496775	-2.585017
113	6	0	-3.482658	3.355061	-3.926653
114	1	0	-3.008819	3.964191	-4.703941
115	1	0	-4.102661	2.598353	-4.420903
116	1	0	-4.144279	3.998596	-3.338530
117	6	0	-1.469900	1.832699	-3.871671
118	1	0	-0.977677	2.447338	-4.633187
119	1	0	-0.695958	1.377808	-3.246193
120	1	0	-2.017441	1.039765	-4.396114
121	6	0	-5.360565	-1.162297	-1.816827
122	1	0	-4.688857	-1.758354	-2.453628
123	6	0	-6.542220	-0.707066	-2.685629
124	1	0	-7.098886	-1.568940	-3.069411
125	1	0	-7.227637	-0.092503	-2.091902
126	1	0	-6.206479	-0.106801	-3.536126
127	6	0	-5.859751	-2.056603	-0.684009
128	1	0	-6.646936	-1.554942	-0.109610
129	1	0	-6.283832	-2.981360	-1.088511
130	1	0	-5.056790	-2.323028	0.009775
131	6	0	3.725089	-0.089752	-2.932616
132	1	0	3.451313	0.960153	-2.808402
133	6	0	2.656732	-0.713499	-3.838334
134	1	0	2.728779	-0.285179	-4.844354
135	1	0	2.788846	-1.798869	-3.934144
136	1	0	1.661899	-0.492476	-3.442488
137	6	0	5.092412	-0.160659	-3.629881
138	1	0	5.065425	0.378114	-4.582940
139	1	0	5.888591	0.269040	-3.015395
140	1	0	5.364929	-1.201533	-3.839381
141	6	0	3.955391	0.166716	2.189498
142	1	0	3.137115	0.895217	2.160843
143	6	0	3.769255	-0.687837	3.443849
144	1	0	3.602532	-0.044759	4.313426
145	1	0	2.908524	-1.351447	3.351015
146	1	0	4.658044	-1.297127	3.645805
147	6	0	5.287566	0.925406	2.305894
148	1	0	6.120553	0.213020	2.312035
149	1	0	5.440196	1.623826	1.480410
150	1	0	5.318847	1.491608	3.243125
151	6	0	4.544791	-4.247627	-0.210514
152	1	0	4.668216	-4.518441	0.846319
153	6	0	3.407062	-5.097017	-0.785150
154	1	0	3.215373	-4.836177	-1.832313
155	1	0	3.664226	-6.161247	-0.744903
156	1	0	2.476879	-4.949290	-0.227921
157	6	0	5.864489	-4.550871	-0.929874
158	1	0	6.122505	-5.610686	-0.832912
159	1	0	5.785467	-4.322241	-1.998461
160	1	0	6.684209	-3.954409	-0.518946

S_endo2 [TSs(H)]

B3LYP/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -3618.572093 hartree

Sum of electronic and thermal Free Energies = -3617.324162 hartree

The number of imaginary frequency = 1

Imaginary frequency = -355.84

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.071298	-2.489566	4.440860
2	1	0	0.235909	-1.443423	4.204004
3	1	0	0.563759	-2.827782	5.348919
4	6	0	-1.099820	-3.122996	4.046204
5	1	0	-1.358399	-4.054510	4.549000
6	6	0	-1.895589	-2.785287	2.927147
7	1	0	-2.694828	-3.454189	2.637308
8	6	0	-1.613518	-1.692948	2.135674
9	1	0	-0.878951	-0.952072	2.422729
10	1	0	-1.865907	-0.477314	0.538059
11	7	0	-2.191389	-1.352709	0.942201
12	6	0	-3.061922	-2.130166	0.193966
13	8	0	-3.301444	-1.530975	-0.986818
14	8	0	-3.518711	-3.202516	0.548289
15	6	0	-4.122962	-2.275526	-1.934292
16	1	0	-3.728111	-1.972334	-2.904713
17	1	0	-3.933465	-3.339226	-1.781877
18	6	0	-5.592471	-1.953410	-1.821771
19	6	0	-6.170757	-0.998339	-2.667712
20	6	0	-6.404655	-2.617498	-0.891174
21	6	0	-7.531933	-0.701284	-2.582179
22	1	0	-5.551394	-0.488235	-3.401880
23	6	0	-7.765298	-2.321800	-0.804991
24	1	0	-5.959749	-3.357676	-0.233396
25	6	0	-8.331560	-1.362838	-1.648684
26	1	0	-7.966840	0.041403	-3.245578
27	1	0	-8.385594	-2.843786	-0.081187
28	1	0	-9.392212	-1.135696	-1.581616
29	1	0	0.555347	-1.747027	-0.629925
30	6	0	-1.392882	-4.680849	-3.799033
31	6	0	-1.190483	-5.386797	-2.626785
32	6	0	-0.623811	-4.754532	-1.499243
33	6	0	-0.271634	-3.383168	-1.589535
34	6	0	-0.483247	-2.663876	-2.783959
35	6	0	-1.034433	-3.318501	-3.872126
36	1	0	-0.626238	-6.469978	-0.164904
37	1	0	-1.824375	-5.174145	-4.664878
38	1	0	-1.460963	-6.437390	-2.558373
39	6	0	-0.366590	-5.418495	-0.258354
40	1	0	-0.200811	-1.616380	-2.822447
41	1	0	-1.189811	-2.771733	-4.798049
42	6	0	0.543408	-3.367806	0.690916
43	6	0	0.194908	-4.756883	0.792167
44	1	0	0.385094	-5.271204	1.725646
45	7	0	0.285633	-2.757103	-0.496206
46	6	0	1.165876	-2.610061	1.720334
47	1	0	1.378751	-1.570456	1.492390
48	6	0	1.516358	-3.089152	2.978755
49	1	0	1.496859	-4.151911	3.197308
50	1	0	2.274366	-2.537800	3.525822
51	6	0	3.402962	4.432069	-3.478525
52	6	0	3.877695	3.213442	-2.714277
53	6	0	3.089367	3.004822	-1.571536
54	6	0	2.072290	4.776321	-2.771177
55	1	0	4.121562	5.260642	-3.409753
56	1	0	3.270630	4.222716	-4.546764
57	1	0	1.247958	4.215995	-3.226754
58	1	0	1.819647	5.840492	-2.816150
59	6	0	2.275423	4.268689	-1.307139
60	6	0	3.162314	5.302578	-0.527081
61	6	0	0.996519	4.341395	-0.479279
62	6	0	2.177007	6.394791	-0.071892
63	1	0	3.991767	5.683390	-1.130396
64	1	0	3.590400	4.802750	0.349555
65	6	0	0.903179	5.605690	0.125732
66	1	0	2.499917	6.906517	0.842271
67	1	0	2.055258	7.170806	-0.841247
68	6	0	4.940718	2.366428	-3.002530
69	6	0	5.185364	1.287889	-2.154106
70	6	0	4.328619	0.961837	-1.087815
71	6	0	3.242961	1.829492	-0.832025
72	1	0	5.581689	2.543996	-3.862831
73	1	0	6.044301	0.649423	-2.336932
74	6	0	-0.028820	3.409860	-0.296827
75	6	0	-1.192395	3.760931	0.422815
76	6	0	-1.284422	5.069105	0.927955
77	6	0	-0.243896	5.986388	0.809555
78	1	0	-2.191273	5.350338	1.455325
79	1	0	-0.327234	6.974487	1.255638
80	8	0	2.354472	1.541282	0.193397
81	8	0	0.935893	-0.192234	-1.167135
82	8	0	0.238242	0.608839	1.211398
83	15	0	0.855644	0.902773	-0.125170
84	8	0	0.088546	2.159289	-0.886440
85	6	0	-2.336215	2.831511	0.701766
86	6	0	-2.642899	2.483516	2.044620
87	6	0	-3.190578	2.402636	-0.341039
88	6	0	-3.794985	1.733525	2.303375
89	6	0	-4.325052	1.643671	-0.023050
90	6	0	-4.658520	1.308274	1.290475
91	1	0	-4.029847	1.485675	3.335475
92	1	0	-4.987375	1.323274	-0.823875
93	6	0	4.613731	-0.272166	-0.283349
94	6	0	4.698196	-1.536620	-0.927897
95	6	0	4.893243	-0.187527	1.104725
96	6	0	5.048896	-2.664421	-0.177491
97	6	0	5.227353	-1.353407	1.804901
98	6	0	5.318405	-2.602186	1.190412
99	1	0	5.117369	-3.622772	-0.686139
100	1	0	5.452038	-1.279694	2.867284
101	6	0	4.431003	-1.744208	-2.422008
102	1	0	4.135627	-0.787143	-2.855116
103	6	0	3.257648	-2.707259	-2.668104
104	1	0	3.077193	-2.820932	-3.744249
105	1	0	3.446349	-3.705871	-2.255678
106	1	0	2.350208	-2.308547	-2.211836
107	6	0	5.694192	-2.221026	-3.166177
108	1	0	5.496097	-2.303469	-4.241958
109	1	0	6.532685	-1.528886	-3.028709
110	1	0	6.021979	-3.206233	-2.813131
111	6	0	4.922979	1.132965	1.875713
112	1	0	4.637146	1.936140	1.194330
113	6	0	6.349293	1.455364	2.366572
114	1	0	6.370038	2.433085	2.863654

115	1	0	6.709743	0.709792	3.085383
116	1	0	7.058858	1.483570	1.531840
117	6	0	3.917006	1.149848	3.042229
118	1	0	3.933559	2.126194	3.542273
119	1	0	2.899865	0.970811	2.682657
120	1	0	4.162847	0.392197	3.797353
121	6	0	5.755503	-3.827858	1.982931
122	1	0	5.709311	-3.555739	3.046926
123	6	0	7.218514	-4.198666	1.667416
124	1	0	7.548337	-5.047312	2.279638
125	1	0	7.331991	-4.479178	0.613314
126	1	0	7.889910	-3.355173	1.861142
127	6	0	4.830400	-5.040214	1.777377
128	1	0	4.875231	-5.410564	0.746470
129	1	0	5.126313	-5.866307	2.435385
130	1	0	3.787759	-4.783135	1.992770
131	6	0	-1.786401	2.914284	3.239839
132	1	0	-0.927079	3.471145	2.860617
133	6	0	-1.216117	1.712940	4.017545
134	1	0	-0.631513	2.065375	4.876934
135	1	0	-2.008821	1.059647	4.402938
136	1	0	-0.557357	1.133647	3.365891
137	6	0	-2.564990	3.854058	4.182581
138	1	0	-1.915744	4.204091	4.994497
139	1	0	-2.947824	4.733695	3.652836
140	1	0	-3.422724	3.346326	4.639926
141	6	0	-2.964292	2.802621	-1.799290
142	1	0	-2.055387	3.406589	-1.847712
143	6	0	-2.742963	1.583890	-2.713319
144	1	0	-2.550201	1.912227	-3.742556
145	1	0	-1.884864	0.994906	-2.377193
146	1	0	-3.623921	0.931502	-2.729154
147	6	0	-4.115055	3.686355	-2.321044
148	1	0	-5.068648	3.145027	-2.332635
149	1	0	-4.245271	4.576260	-1.695024
150	1	0	-3.908239	4.019260	-3.345810
151	6	0	-5.960988	0.577795	1.597375
152	1	0	-6.344732	0.185261	0.646887
153	6	0	-5.789216	-0.617533	2.550962
154	1	0	-5.426896	-0.301635	3.536374
155	1	0	-6.751494	-1.121352	2.702774
156	1	0	-5.084502	-1.355699	2.155215
157	6	0	-7.014552	1.561354	2.147476
158	1	0	-7.974388	1.054815	2.308615
159	1	0	-6.692448	1.986118	3.106109
160	1	0	-7.178833	2.393133	1.453682

S_endo2 [TSs(H)]

B3LYP-D/6-31g(d) in gas phase

SCF Done: E(RB3LYP) = -3618.847049 hartree

Sum of electronic and thermal Free Energies = -3617.583479 hartree

The number of imaginary frequency = 1

Imaginary frequency = -317.10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.137308	-2.322200	4.403660
2	1	0	0.095648	-1.285940	4.179807
3	1	0	0.308714	-2.695845	5.321724
4	6	0	-1.325725	-2.889496	3.959391
5	1	0	-1.651100	-3.812041	4.438988
6	6	0	-2.045369	-2.500748	2.808615
7	1	0	-2.853027	-3.129005	2.459007
8	6	0	-1.655230	-1.415509	2.052513
9	1	0	-0.917200	-0.715085	2.411015
10	1	0	-1.727608	-0.153397	0.485263
11	7	0	-2.121825	-1.027675	0.830960
12	6	0	-2.953358	-1.754519	0.002936
13	8	0	-3.122496	-1.100009	-1.159165
14	8	0	-3.442026	-2.837456	0.277810
15	6	0	-4.023865	-1.723537	-2.117952
16	1	0	-3.676882	-1.340096	-3.077542
17	1	0	-3.870366	-2.803325	-2.087783
18	6	0	-5.458661	-1.345085	-1.854238
19	6	0	-6.015165	-0.217562	-2.471152
20	6	0	-6.243307	-2.093724	-0.966909
21	6	0	-7.326719	0.169873	-2.194302
22	1	0	-5.413936	0.364703	-3.165570
23	6	0	-7.556644	-1.710335	-0.692894
24	1	0	-5.807179	-2.957729	-0.477062
25	6	0	-8.099360	-0.576007	-1.301371
26	1	0	-7.743228	1.051898	-2.672931
27	1	0	-8.154492	-2.293843	0.002021
28	1	0	-9.119809	-0.274428	-1.081103
29	1	0	0.467989	-1.630931	-0.668436
30	6	0	-1.891001	-4.361369	-3.730714
31	6	0	-1.728985	-5.072329	-2.554901
32	6	0	-1.064149	-4.492255	-1.453886
33	6	0	-0.570139	-3.168818	-1.575018
34	6	0	-0.755946	-2.437624	-2.766024
35	6	0	-1.400355	-3.042660	-3.830270
36	1	0	-1.229537	-6.175064	-0.089794
37	1	0	-2.399111	-4.814963	-4.576416
38	1	0	-2.110255	-6.085917	-2.462123
39	6	0	-0.854315	-5.161849	-0.207456
40	1	0	-0.393282	-1.416702	-2.819169
41	1	0	-1.537098	-2.486503	-4.753382
42	6	0	0.288186	-3.206499	0.687203
43	6	0	-0.210162	-4.546155	0.822564
44	1	0	-0.073571	-5.053962	1.768532
45	7	0	0.082436	-2.595504	-0.507934
46	6	0	0.989597	-2.497719	1.697944
47	1	0	1.301233	-1.488399	1.455818
48	6	0	1.307517	-2.997177	2.955238
49	1	0	1.220242	-4.055967	3.174582
50	1	0	2.097517	-2.492025	3.500479
51	6	0	4.119711	4.301912	-3.164119
52	6	0	4.379742	2.995657	-2.442947
53	6	0	3.492227	2.844633	-1.367114
54	6	0	2.776248	4.761519	-2.549734
55	1	0	4.916770	5.034114	-2.974790

56	1	0	4.065763	4.169902	-4.250906
57	1	0	1.938899	4.310421	-3.094252
58	1	0	2.640259	5.847466	-2.560475
59	6	0	2.799739	4.174725	-1.102921
60	6	0	3.707754	5.072358	-0.192116
61	6	0	1.470064	4.328265	-0.376645
62	6	0	2.790742	6.232505	0.240952
63	1	0	4.620913	5.396958	-0.699576
64	1	0	4.002745	4.485456	0.685669
65	6	0	1.442635	5.552766	0.309074
66	1	0	3.085503	6.678354	1.197637
67	1	0	2.795726	7.041838	-0.502939
68	6	0	5.325287	2.015056	-2.721145
69	6	0	5.342289	0.854866	-1.945339
70	6	0	4.373673	0.609083	-0.958125
71	6	0	3.438303	1.628064	-0.691348
72	1	0	6.039618	2.143306	-3.530661
73	1	0	6.089077	0.090169	-2.136869
74	6	0	0.365933	3.480185	-0.309530
75	6	0	-0.785153	3.850513	0.414015
76	6	0	-0.810671	5.127157	0.998824
77	6	0	0.294888	5.975125	0.968306
78	1	0	-1.708741	5.428069	1.529754
79	1	0	0.266757	6.935070	1.477774
80	8	0	2.464328	1.416747	0.270914
81	8	0	1.014828	-0.157642	-1.247715
82	8	0	0.206713	0.676704	1.082985
83	15	0	0.955954	0.923637	-0.192882
84	8	0	0.407590	2.266615	-0.980953
85	6	0	-1.947151	2.936599	0.644121
86	6	0	-2.263065	2.537527	1.970307
87	6	0	-2.778486	2.531135	-0.421994
88	6	0	-3.423474	1.791335	2.193711
89	6	0	-3.924327	1.777002	-0.140142
90	6	0	-4.278481	1.409109	1.156890
91	1	0	-3.669374	1.503970	3.212530
92	1	0	-4.571894	1.475828	-0.956941
93	6	0	4.324361	-0.712085	-0.258059
94	6	0	4.166057	-1.902807	-1.010596
95	6	0	4.461684	-0.797183	1.150836
96	6	0	4.147176	-3.135355	-0.345478
97	6	0	4.447938	-2.055329	1.757594
98	6	0	4.286337	-3.239039	1.036495
99	1	0	4.017557	-4.037168	-0.935656
100	1	0	4.567219	-2.118743	2.837477
101	6	0	4.019236	-1.925859	-2.532696
102	1	0	3.986369	-0.897066	-2.894630
103	6	0	2.697344	-2.572450	-2.973572
104	1	0	2.620766	-2.578257	-4.067928
105	1	0	2.600784	-3.608851	-2.628582
106	1	0	1.867093	-1.992009	-2.575164
107	6	0	5.226581	-2.616184	-3.194787
108	1	0	5.142340	-2.572428	-4.287525
109	1	0	6.171105	-2.141017	-2.905896
110	1	0	5.289206	-3.672492	-2.906538
111	6	0	4.664609	0.419859	2.051095
112	1	0	4.641582	1.319397	1.433454
113	6	0	6.047353	0.381765	2.729866
114	1	0	6.204203	1.286196	3.330368
115	1	0	6.145879	-0.482511	3.397593
116	1	0	6.849320	0.321464	1.985408
117	6	0	3.535515	0.551603	3.091670
118	1	0	3.665411	1.468221	3.679947
119	1	0	2.558091	0.596672	2.604227
120	1	0	3.542278	-0.291395	3.795279
121	6	0	4.317103	-4.575443	1.763663
122	1	0	3.916586	-4.399942	2.772849
123	6	0	5.770896	-5.063692	1.921617
124	1	0	5.813461	-5.999442	2.492969
125	1	0	6.221198	-5.243184	0.937830
126	1	0	6.383361	-4.315971	2.437024
127	6	0	3.449974	-5.660081	1.107711
128	1	0	3.865378	-5.978812	0.144547
129	1	0	3.401072	-6.548209	1.748755
130	1	0	2.430419	-5.303948	0.928863
131	6	0	-1.403291	2.905308	3.182273
132	1	0	-0.518253	3.437911	2.828454
133	6	0	-0.886868	1.668651	3.942707
134	1	0	-0.329949	1.981563	4.834836
135	1	0	-1.704556	1.016987	4.274428
136	1	0	-0.215007	1.099573	3.297088
137	6	0	-2.166499	3.848512	4.132539
138	1	0	-1.522188	4.163302	4.962519
139	1	0	-2.515375	4.747520	3.612532
140	1	0	-3.046433	3.354090	4.561382
141	6	0	-2.508358	2.925267	-1.871715
142	1	0	-1.609215	3.544762	-1.898973
143	6	0	-2.240338	1.694503	-2.757147
144	1	0	-2.000655	2.008655	-3.780719
145	1	0	-1.401018	1.109632	-2.372714
146	1	0	-3.120087	1.043310	-2.800036
147	6	0	-3.658602	3.776424	-2.442533
148	1	0	-4.597076	3.210134	-2.482480
149	1	0	-3.832846	4.666290	-1.827245
150	1	0	-3.423506	4.105136	-3.462382
151	6	0	-5.589198	0.681637	1.417440
152	1	0	-5.964210	0.328437	0.451122
153	6	0	-5.446879	-0.546486	2.331354
154	1	0	-5.075575	-0.271755	3.325578
155	1	0	-6.422353	-1.029598	2.464425
156	1	0	-4.764367	-1.289003	1.910558
157	6	0	-6.634347	1.661824	1.984789
158	1	0	-7.604872	1.165830	2.110855
159	1	0	-6.318083	2.046043	2.962480
160	1	0	-6.770306	2.519407	1.316633

S_endo2 [TSs(H)]

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.193091 hartree

Sum of electronic and thermal Free Energies = -3615.917654 hartree

The number of imaginary frequency = 1

Imaginary frequency = -344.52

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.147675	-2.258249	4.355129
2	1	0	0.144454	-1.246844	4.088176
3	1	0	0.302325	-2.639732	5.266875
4	6	0	-1.347618	-2.787935	3.928028
5	1	0	-1.701965	-3.692057	4.420447
6	6	0	-2.059430	-2.380039	2.774994
7	1	0	-2.881906	-2.987324	2.422399
8	6	0	-1.635592	-1.300411	2.038902
9	1	0	-0.879861	-0.621797	2.413165
10	1	0	-1.698255	0.000297	0.490954
11	7	0	-2.087607	-0.885390	0.820539
12	6	0	-2.897033	-1.615648	-0.016282
13	8	0	-3.088448	-0.959899	-1.167371
14	8	0	-3.353820	-2.711263	0.241451
15	6	0	-3.991251	-1.591080	-2.095424
16	1	0	-3.688936	-1.199332	-3.068514
17	1	0	-3.822704	-2.670591	-2.071383
18	6	0	-5.423789	-1.236672	-1.787238
19	6	0	-6.013868	-0.124946	-2.393654
20	6	0	-6.168260	-1.991005	-0.876098
21	6	0	-7.319193	0.244825	-2.081088
22	1	0	-5.441646	0.458433	-3.112590
23	6	0	-7.475822	-1.624890	-0.565830
24	1	0	-5.708248	-2.852344	-0.401765
25	6	0	-8.051184	-0.504852	-1.162522
26	1	0	-7.763848	1.115072	-2.553734
27	1	0	-8.045493	-2.214320	0.146341
28	1	0	-9.068901	-0.218436	-0.915475
29	1	0	0.391451	-1.615413	-0.694780
30	6	0	-2.028774	-4.271945	-3.771384
31	6	0	-1.920634	-4.975659	-2.590912
32	6	0	-1.254695	-4.412550	-1.483771
33	6	0	-0.710508	-3.118871	-1.606382
34	6	0	-0.842662	-2.387963	-2.803651
35	6	0	-1.485842	-2.974879	-3.872489
36	1	0	-1.513697	-6.074479	-0.108691
37	1	0	-2.534803	-4.712659	-4.623839
38	1	0	-2.341480	-5.972824	-2.497048
39	6	0	-1.089781	-5.081294	-0.228892
40	1	0	-0.430458	-1.383425	-2.853571
41	1	0	-1.581193	-2.424547	-4.803452
42	6	0	0.140302	-3.179154	0.644898
43	6	0	-0.427290	-4.490433	0.797452
44	1	0	-0.318261	-4.992577	1.751105
45	7	0	-0.040395	-2.567301	-0.540455
46	6	0	0.902937	-2.504582	1.639709
47	1	0	1.285200	-1.520547	1.376904
48	6	0	1.214533	-3.031268	2.877830
49	1	0	1.049981	-4.080255	3.103477
50	1	0	2.033765	-2.573301	3.423952
51	6	0	4.216871	4.162876	-3.187896
52	6	0	4.429405	2.848254	-2.468896
53	6	0	3.552133	2.741547	-1.385465
54	6	0	2.895300	4.667098	-2.572497
55	1	0	5.040234	4.862248	-2.996120
56	1	0	4.155085	4.032111	-4.272567
57	1	0	2.043981	4.236734	-3.111066
58	1	0	2.794512	5.756732	-2.586977
59	6	0	2.908517	4.092670	-1.129908
60	6	0	3.841962	4.968277	-0.240849
61	6	0	1.592775	4.280085	-0.394425
62	6	0	2.960975	6.151430	0.190407
63	1	0	4.756432	5.264518	-0.763202
64	1	0	4.127761	4.382636	0.640253
65	6	0	1.600830	5.501871	0.286787
66	1	0	3.278613	6.598288	1.137171
67	1	0	2.968571	6.949444	-0.563244
68	6	0	5.320496	1.824213	-2.757617
69	6	0	5.292430	0.669688	-1.978543
70	6	0	4.337655	0.480268	-0.972280
71	6	0	3.458921	1.538690	-0.697236
72	1	0	6.026443	1.914582	-3.578453
73	1	0	5.994599	-0.135071	-2.179705
74	6	0	0.474858	3.457218	-0.314053
75	6	0	-0.654333	3.850712	0.421224
76	6	0	-0.642927	5.119298	1.013309
77	6	0	0.475921	5.944520	0.966612
78	1	0	-1.528346	5.435963	1.557768
79	1	0	0.475256	6.903121	1.477718
80	8	0	2.503512	1.383846	0.284665
81	8	0	1.035113	-0.182325	-1.185016
82	8	0	0.238179	0.734285	1.111908
83	15	0	0.994493	0.921460	-0.161452
84	8	0	0.485181	2.247173	-0.980097
85	6	0	-1.840498	2.967681	0.639058
86	6	0	-2.184431	2.580802	1.957651
87	6	0	-2.661197	2.582121	-0.435919
88	6	0	-3.361862	1.863504	2.165467
89	6	0	-3.827776	1.857657	-0.172082
90	6	0	-4.206844	1.499286	1.116348
91	1	0	-3.629052	1.582393	3.182917
92	1	0	-4.470784	1.567655	-1.000125
93	6	0	4.247177	-0.823423	-0.246871
94	6	0	4.043535	-2.017426	-0.972853
95	6	0	4.401727	-0.884919	1.156741
96	6	0	3.999735	-3.235318	-0.287931
97	6	0	4.369729	-2.128578	1.786145
98	6	0	4.163905	-3.316426	1.090051
99	1	0	3.833112	-4.144971	-0.860114
100	1	0	4.508121	-2.176557	2.866375
101	6	0	3.868709	-2.063260	-2.486316
102	1	0	3.867868	-1.041656	-2.869973
103	6	0	2.517162	-2.665515	-2.875272
104	1	0	2.413870	-2.704308	-3.965539
105	1	0	2.387618	-3.683800	-2.489526
106	1	0	1.725589	-2.032339	-2.475575
107	6	0	5.024113	-2.822867	-3.150027
108	1	0	4.922648	-2.797080	-4.240164
109	1	0	5.995589	-2.393235	-2.884592
110	1	0	5.033391	-3.873810	-2.839690

111	6	0	4.634977	0.336640	2.034631
112	1	0	4.630331	1.229380	1.406264
113	6	0	6.008235	0.269716	2.715470
114	1	0	6.183446	1.173615	3.308497
115	1	0	6.077629	-0.590613	3.390280
116	1	0	6.809917	0.182132	1.975773
117	6	0	3.514437	0.490732	3.072071
118	1	0	3.646233	1.418025	3.640071
119	1	0	2.533334	0.523282	2.587885
120	1	0	3.531247	-0.338701	3.790654
121	6	0	4.165435	-4.637785	1.835018
122	1	0	3.817540	-4.430227	2.857065
123	6	0	5.594175	-5.189900	1.931218
124	1	0	5.616898	-6.124331	2.502466
125	1	0	5.986675	-5.390970	0.928242
126	1	0	6.261974	-4.470633	2.414400
127	6	0	3.227993	-5.680608	1.223836
128	1	0	3.607739	-6.040190	0.261412
129	1	0	3.142269	-6.549652	1.884334
130	1	0	2.227992	-5.267139	1.055169
131	6	0	-1.339731	2.932326	3.178722
132	1	0	-0.436804	3.445424	2.840421
133	6	0	-0.872029	1.688714	3.946535
134	1	0	-0.351622	1.989356	4.862924
135	1	0	-1.712032	1.045292	4.236280
136	1	0	-0.178926	1.118294	3.323737
137	6	0	-2.105569	3.879438	4.112884
138	1	0	-1.470347	4.189879	4.949204
139	1	0	-2.445946	4.777691	3.588229
140	1	0	-2.990860	3.386136	4.529857
141	6	0	-2.363520	2.960975	-1.878984
142	1	0	-1.440815	3.545441	-1.903200
143	6	0	-2.146954	1.716177	-2.746672
144	1	0	-1.874446	2.007714	-3.767067
145	1	0	-1.348793	1.087937	-2.339581
146	1	0	-3.064731	1.117849	-2.797261
147	6	0	-3.478784	3.840414	-2.458336
148	1	0	-4.430999	3.298643	-2.496739
149	1	0	-3.628104	4.737990	-1.850492
150	1	0	-3.229259	4.151812	-3.478370
151	6	0	-5.522262	0.783954	1.357379
152	1	0	-5.904031	0.471062	0.378444
153	6	0	-5.380074	-0.468274	2.227094
154	1	0	-4.979621	-0.225400	3.217933
155	1	0	-6.359840	-0.938204	2.369317
156	1	0	-4.719704	-1.210406	1.769056
157	6	0	-6.547394	1.747548	1.968393
158	1	0	-7.521079	1.256421	2.075270
159	1	0	-6.222068	2.080756	2.960802
160	1	0	-6.673619	2.634550	1.340395

R_exo_t-t

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.175954 hartree

Sum of electronic and thermal Free Energies = -3615.904635 hartree

The number of imaginary frequency = 1

Imaginary frequency = -369.23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.197034	-4.625063	-2.653573
2	1	0	-0.237319	-5.015098	-2.328185
3	1	0	-1.877086	-5.371140	-3.053750
4	6	0	-1.324299	-3.309091	-3.052847
5	1	0	-2.224274	-3.027896	-3.597207
6	6	0	-0.489219	-2.254574	-2.624388
7	1	0	-0.771614	-1.223237	-2.815479
8	6	0	0.612918	-2.499443	-1.843667
9	1	0	0.999734	-3.503242	-1.710172
10	1	0	0.953790	-0.555674	-1.224505
11	7	0	1.340541	-1.527239	-1.235128
12	6	0	2.472206	-1.749600	-0.486090
13	8	0	2.893413	-3.035191	-0.576463
14	8	0	3.017907	-0.904206	0.176461
15	6	0	4.169136	-3.278178	0.011619
16	1	0	4.191014	-2.859869	1.023203
17	1	0	4.236180	-4.368067	0.078718
18	6	0	5.306509	-2.709484	-0.806919
19	6	0	6.599983	-2.769834	-0.285205
20	6	0	5.102008	-2.118030	-2.051888
21	6	0	7.673047	-2.234362	-0.989499
22	1	0	6.764125	-3.222841	0.690454
23	6	0	6.175939	-1.576880	-2.757045
24	1	0	4.102171	-2.069116	-2.474058
25	6	0	7.462136	-1.629771	-2.227942
26	1	0	8.672473	-2.278713	-0.567437
27	1	0	6.000938	-1.107784	-3.720905
28	1	0	8.295988	-1.201286	-2.774843
29	1	0	-0.116114	-1.499267	1.187624
30	6	0	3.571151	-2.218858	4.068869
31	6	0	3.172068	-3.440854	3.575579
32	6	0	2.084429	-3.522602	2.680261
33	6	0	1.415027	-2.336195	2.316126
34	6	0	1.826953	-1.086323	2.815673
35	6	0	2.895164	-1.041763	3.681933
36	1	0	2.139230	-5.667812	2.351447
37	1	0	4.413457	-2.154486	4.749682
38	1	0	3.687746	-4.354134	3.860068
39	6	0	1.631176	-4.742739	2.090304
40	1	0	1.316502	-0.188470	2.479995
41	1	0	3.234658	-0.082141	4.058327
42	6	0	-0.104997	-3.545667	0.891702
43	6	0	0.582465	-4.758509	1.225986
44	1	0	0.236156	-5.688856	0.793341
45	7	0	0.364553	-2.405508	1.433628
46	6	0	-1.257914	-3.465729	0.062758
47	1	0	-1.724788	-2.484351	-0.010724
48	6	0	-1.843385	-4.535453	-0.589173
49	1	0	-1.520814	-5.555342	-0.397700
50	1	0	-2.876195	-4.431203	-0.889036
51	6	0	-3.976218	4.940662	2.186434

52	6	0	-4.225775	3.504511	1.784074
53	6	0	-3.342947	3.121427	0.770342
54	6	0	-2.619673	5.235851	1.520390
55	1	0	-4.763122	5.601305	1.800723
56	1	0	-3.953564	5.069332	3.272869
57	1	0	-1.804480	4.906677	2.174967
58	1	0	-2.464643	6.293842	1.287980
59	6	0	-2.615198	4.343862	0.247252
60	6	0	-3.429208	5.042187	-0.879782
61	6	0	-1.245812	4.302706	-0.395589
62	6	0	-2.443702	6.055647	-1.490714
63	1	0	-4.352927	5.495683	-0.507329
64	1	0	-3.696948	4.288727	-1.629364
65	6	0	-1.112816	5.365025	-1.294922
66	1	0	-2.652393	6.268279	-2.543565
67	1	0	-2.475429	7.013844	-0.956330
68	6	0	-5.167167	2.612112	2.276512
69	6	0	-5.203966	1.325283	1.749706
70	6	0	-4.271679	0.883224	0.801593
71	6	0	-3.313866	1.798647	0.342719
72	1	0	-5.870291	2.911438	3.048640
73	1	0	-5.958566	0.621524	2.090932
74	6	0	-0.173110	3.454173	-0.165852
75	6	0	1.085817	3.724890	-0.721685
76	6	0	1.206759	4.844363	-1.552323
77	6	0	0.114820	5.646867	-1.874871
78	1	0	2.184697	5.068204	-1.968956
79	1	0	0.228545	6.478949	-2.564088
80	8	0	-2.377074	1.403163	-0.588307
81	8	0	-0.927728	-0.074504	0.974513
82	8	0	-0.111657	0.732660	-1.374085
83	15	0	-0.868204	0.973817	-0.103479
84	8	0	-0.353649	2.342911	0.640595
85	6	0	2.283112	2.890425	-0.410608
86	6	0	2.990016	2.237806	-1.443971
87	6	0	2.759767	2.822871	0.914719
88	6	0	4.158341	1.548807	-1.124050
89	6	0	3.921584	2.096388	1.183251
90	6	0	4.636915	1.453309	0.179282
91	1	0	4.710340	1.037278	-1.912196
92	1	0	4.279797	2.046100	2.209986
93	6	0	-4.375028	-0.517698	0.294795
94	6	0	-4.347205	-1.596130	1.209084
95	6	0	-4.637778	-0.768973	-1.067991
96	6	0	-4.651009	-2.877552	0.751205
97	6	0	-4.915805	-2.076997	-1.477992
98	6	0	-4.969971	-3.138457	-0.580900
99	1	0	-4.646219	-3.707389	1.457898
100	1	0	-5.138480	-2.252133	-2.527753
101	6	0	2.559295	2.283365	-2.905457
102	1	0	1.581933	2.769154	-2.964005
103	6	0	3.563261	3.099857	-3.731889
104	1	0	4.540994	2.604291	-3.748642
105	1	0	3.219464	3.201661	-4.766902
106	1	0	3.712306	4.102256	-3.318717
107	6	0	2.394318	0.887147	-3.516665
108	1	0	2.179553	0.970823	-4.587947
109	1	0	3.304064	0.284618	-3.405308
110	1	0	1.562335	0.364166	-3.043768
111	6	0	2.109402	3.579921	2.066855
112	1	0	1.248344	4.132518	1.683236
113	6	0	3.081115	4.615039	2.649631
114	1	0	3.955814	4.131501	3.098227
115	1	0	3.437610	5.297478	1.872124
116	1	0	2.588484	5.206146	3.429257
117	6	0	1.595074	2.638883	3.160643
118	1	0	1.144638	3.212722	3.978289
119	1	0	0.835516	1.963019	2.758928
120	1	0	2.415904	2.048408	3.585785
121	6	0	5.907058	0.673544	0.455416
122	1	0	6.024038	-0.041112	-0.368113
123	6	0	5.844774	-0.130464	1.754426
124	1	0	5.816166	0.525096	2.633516
125	1	0	4.951013	-0.762030	1.767006
126	1	0	6.734005	-0.763934	1.849167
127	6	0	7.126944	1.602581	0.445760
128	1	0	8.051656	1.030293	0.583636
129	1	0	7.196633	2.148297	-0.500332
130	1	0	7.055224	2.339478	1.254332
131	6	0	-4.712159	0.324452	-2.125645
132	1	0	-4.556079	1.291552	-1.644429
133	6	0	-6.099867	0.370124	-2.779360
134	1	0	-6.310761	-0.544557	-3.343992
135	1	0	-6.885433	0.490396	-2.027033
136	1	0	-6.159954	1.211307	-3.477806
137	6	0	-3.612870	0.151452	-3.180080
138	1	0	-3.673674	0.949997	-3.927248
139	1	0	-2.624144	0.194805	-2.715689
140	1	0	-3.723179	-0.804822	-3.706916
141	6	0	-5.433315	-4.528201	-0.985266
142	1	0	-4.882417	-5.251445	-0.366787
143	6	0	-3.996365	-1.429586	2.683091
144	1	0	-3.805931	-0.371948	2.876769
145	6	0	-5.146287	-1.881163	3.591672
146	1	0	-5.331641	-2.956541	3.492309
147	1	0	-4.902861	-1.681909	4.640432
148	1	0	-6.079399	-1.361528	3.351598
149	6	0	-2.703102	-2.175363	3.027943
150	1	0	-2.489519	-2.090387	4.099179
151	1	0	-2.768920	-3.240824	2.776588
152	1	0	-1.872741	-1.731219	2.476002
153	6	0	-6.925555	-4.689086	-0.661818
154	1	0	-7.513858	-3.969264	-1.241225
155	1	0	-7.273618	-5.697634	-0.909644
156	1	0	-7.119499	-4.504808	0.398744
157	6	0	-5.173668	-4.863484	-2.455201
158	1	0	-5.817495	-4.270792	-3.113630
159	1	0	-4.134132	-4.666810	-2.740731
160	1	0	-5.391309	-5.918260	-2.649013

S_exo_t-t

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.177845 hartree

Sum of electronic and thermal Free Energies = -3615.905438
hartree
The number of imaginary frequency = 1
Imaginary frequency = -440.09

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.474309	-0.475079	4.865976
2	1	0	3.102396	-1.251553	4.438246
3	1	0	2.618442	-0.322950	5.931504
4	6	0	2.075949	0.602194	4.086062
5	1	0	1.690946	1.483374	4.594996
6	6	0	1.912670	0.557719	2.688865
7	1	0	1.390476	1.357220	2.170672
8	6	0	2.357826	-0.516378	1.955808
9	1	0	2.991301	-1.272542	2.405943
10	1	0	1.419849	-0.133829	0.118354
11	7	0	2.129001	-0.698700	0.636139
12	6	0	2.757325	-1.657144	-0.135894
13	8	0	3.699822	-2.329998	0.555648
14	8	0	2.481742	-1.863524	-1.292117
15	6	0	4.493378	-3.232099	-0.239000
16	1	0	4.902659	-3.938336	0.486257
17	1	0	3.834771	-3.754159	-0.937303
18	6	0	5.591225	-2.484289	-0.951165
19	6	0	5.391126	-1.970901	-2.236141
20	6	0	6.804388	-2.248243	-0.302006
21	6	0	6.391490	-1.224443	-2.854633
22	1	0	4.442127	-2.142669	-2.734710
23	6	0	7.804259	-1.501533	-0.919001
24	1	0	6.960954	-2.643450	0.699223
25	6	0	7.596590	-0.986077	-2.196877
26	1	0	6.226264	-0.824237	-3.850263
27	1	0	8.742412	-1.320149	-0.403075
28	1	0	8.372605	-0.398984	-2.678432
29	1	0	-0.729290	-1.534007	1.275013
30	6	0	0.473738	-4.635750	-2.114760
31	6	0	1.092238	-5.012161	-0.941707
32	6	0	0.879679	-4.274331	0.240179
33	6	0	0.019021	-3.155837	0.198993
34	6	0	-0.617686	-2.778059	-0.994104
35	6	0	-0.380318	-3.515601	-2.133642
36	1	0	2.164490	-5.441289	1.545506
37	1	0	0.643443	-5.199975	-3.025689
38	1	0	1.749177	-5.877671	-0.908997
39	6	0	1.507035	-4.576698	1.490854
40	1	0	-1.268009	-1.908223	-1.006606
41	1	0	-0.863947	-3.219086	-3.059757
42	6	0	0.456500	-2.646433	2.516833
43	6	0	1.304539	-3.802667	2.588750
44	1	0	1.789170	-4.032380	3.530322
45	7	0	-0.156708	-2.409428	1.338426
46	6	0	0.229152	-1.727187	3.569125
47	1	0	-0.424648	-0.896158	3.318077
48	6	0	0.809952	-1.747744	4.830494
49	1	0	1.353172	-2.624356	5.175326
50	1	0	0.302411	-1.205667	5.620160
51	6	0	-3.238698	5.644661	-1.785766
52	6	0	-1.853739	5.128539	-1.478359
53	6	0	-1.909199	4.093383	-0.537365
54	6	0	-4.117678	4.498574	-1.267341
55	1	0	-3.442063	6.578941	-1.246457
56	1	0	-3.382844	5.847710	-2.851059
57	1	0	-4.182294	3.712900	-2.028712
58	1	0	-5.135612	4.802093	-1.005974
59	6	0	-3.337036	3.930634	-0.043309
60	6	0	-3.672838	4.778055	1.212757
61	6	0	-3.942958	2.601451	0.358433
62	6	0	-5.067029	4.271559	1.642429
63	1	0	-3.643759	5.853434	1.011267
64	1	0	-2.936231	4.554575	1.992034
65	6	0	-5.050125	2.829710	1.179914
66	1	0	-5.230733	4.353980	2.721276
67	1	0	-5.867735	4.840152	1.153358
68	6	0	-0.647259	5.534369	-2.025725
69	6	0	0.507880	4.850549	-1.664155
70	6	0	0.479382	3.756996	-0.791877
71	6	0	-0.746442	3.403260	-0.201879
72	1	0	-0.605531	6.353720	-2.737799
73	1	0	1.467847	5.151049	-2.072929
74	6	0	-3.632840	1.308446	-0.035639
75	6	0	-4.508743	0.246120	0.230350
76	6	0	-5.679579	0.531862	0.942808
77	6	0	-5.936530	1.799845	1.461620
78	1	0	-6.378473	-0.278410	1.130747
79	1	0	-6.817540	1.972746	2.073370
80	8	0	-0.815681	2.388620	0.740960
81	8	0	-0.035247	0.388882	-0.702237
82	8	0	-1.431419	0.040158	1.451208
83	15	0	-1.111203	0.852750	0.228103
84	8	0	-2.447381	1.065670	-0.701205
85	6	0	-4.198867	-1.147675	-0.210325
86	6	0	-4.117147	-2.188357	0.741363
87	6	0	-4.020964	-1.446516	-1.581048
88	6	0	-3.849862	-3.490171	0.307730
89	6	0	-3.780740	-2.767166	-1.959384
90	6	0	-3.677163	-3.804019	-1.036075
91	1	0	-3.778297	-4.279909	1.051700
92	1	0	-3.650166	-2.998141	-3.016393
93	6	0	1.760713	3.033446	-0.521086
94	6	0	2.272318	2.124622	-1.475410
95	6	0	2.500080	3.344834	0.632490
96	6	0	3.495535	1.507978	-1.212591
97	6	0	3.716960	2.693018	0.854316
98	6	0	4.225537	1.764298	-0.050233
99	1	0	3.899774	0.795994	-1.930687
100	1	0	4.287041	2.933802	1.750848
101	6	0	2.060053	4.444428	1.592154
102	1	0	1.118392	4.860881	1.223548
103	6	0	3.090874	5.581134	1.596749
104	1	0	2.743385	6.412620	2.219093
105	1	0	4.053182	5.241241	1.995411
106	1	0	3.261732	5.955803	0.582857

107	6	0	1.806093	3.937744	3.014955
108	1	0	0.944181	3.263036	3.039357
109	1	0	2.679517	3.404977	3.409692
110	1	0	1.593657	4.778556	3.684229
111	6	0	1.579132	1.886411	-2.811900
112	1	0	0.527688	2.167678	-2.696868
113	6	0	2.217638	2.779997	-3.887487
114	1	0	3.272742	2.512582	-4.020025
115	1	0	1.710123	2.642075	-4.848430
116	1	0	2.172510	3.840591	-3.628207
117	6	0	1.609710	0.432151	-3.289248
118	1	0	1.177280	-0.239151	-2.548359
119	1	0	1.035237	0.351142	-4.219413
120	1	0	2.630701	0.097292	-3.510108
121	6	0	5.575797	1.103730	0.162540
122	1	0	5.680398	0.325150	-0.602920
123	6	0	6.707093	2.116877	-0.049621
124	1	0	6.666558	2.908623	0.707586
125	1	0	7.683164	1.623626	0.022722
126	1	0	6.629362	2.588353	-1.033938
127	6	0	5.704634	0.428626	1.530700
128	1	0	6.721027	0.041680	1.666246
129	1	0	5.497160	1.127581	2.348761
130	1	0	5.012982	-0.414842	1.614725
131	6	0	-4.339598	-1.978237	2.234720
132	1	0	-4.430896	-0.907543	2.426548
133	6	0	-3.154420	-2.463582	3.071165
134	1	0	-2.270466	-1.881561	2.814283
135	1	0	-3.359653	-2.319620	4.137701
136	1	0	-2.937174	-3.525974	2.912656
137	6	0	-5.635157	-2.666031	2.686022
138	1	0	-5.834136	-2.455611	3.742268
139	1	0	-6.497976	-2.333783	2.100059
140	1	0	-5.558448	-3.752989	2.568124
141	6	0	-4.096866	-0.404055	-2.688131
142	1	0	-4.281372	0.574353	-2.239847
143	6	0	-2.773995	-0.321371	-3.461992
144	1	0	-2.812780	0.493512	-4.193074
145	1	0	-1.931725	-0.136163	-2.788299
146	1	0	-2.587059	-1.249656	-4.015917
147	6	0	-5.268958	-0.695403	-3.634240
148	1	0	-5.138783	-1.655727	-4.145204
149	1	0	-6.216618	-0.730862	-3.088077
150	1	0	-5.341549	0.083152	-4.401068
151	6	0	-3.407182	-5.218133	-1.513644
152	1	0	-2.842132	-5.135028	-2.452621
153	6	0	-2.561143	-6.034658	-0.535344
154	1	0	-3.126745	-6.278967	0.370665
155	1	0	-2.257276	-6.980476	-0.995463
156	1	0	-1.659338	-5.488972	-0.239763
157	6	0	-4.728187	-5.936852	-1.818908
158	1	0	-4.545550	-6.946144	-2.203509
159	1	0	-5.329808	-6.021311	-0.906973
160	1	0	-5.315957	-5.384533	-2.558199

R_endo_t-c

M06-2X/6-31g(d) in gas phase
SCF Done: E(RM062X) = -3617.184342 hartree
Sum of electronic and thermal Free Energies = -3615.910534 hartree
The number of imaginary frequency = 1
Imaginary frequency = -411.53

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.815435	-2.034686	3.675663
2	1	0	-1.836065	-2.299139	3.291309
3	1	0	-3.036872	-2.418327	4.667735
4	6	0	-3.865272	-1.792788	2.807321
5	1	0	-4.869083	-1.778965	3.230043
6	6	0	-3.752398	-1.353636	1.475019
7	1	0	-4.651239	-1.006184	0.985930
8	6	0	-2.548340	-1.246819	0.811053
9	1	0	-1.639510	-1.665439	1.238591
10	1	0	-1.311962	-0.546386	-0.661518
11	7	0	-2.310929	-0.644145	-0.384335
12	6	0	-3.211439	-0.090402	-1.278935
13	8	0	-4.442123	-0.630903	-1.155173
14	8	0	-2.908880	0.734527	-2.104863
15	6	0	-5.458594	-0.047976	-1.979659
16	1	0	-5.026684	0.235636	-2.940813
17	1	0	-6.181517	-0.854177	-2.125139
18	6	0	-6.099710	1.131612	-1.294030
19	6	0	-6.774002	0.948127	-0.082599
20	6	0	-6.045533	2.404117	-1.857165
21	6	0	-7.394095	2.019247	0.550838
22	1	0	-6.821860	-0.046981	0.354491
23	6	0	-6.682814	3.477527	-1.233851
24	1	0	-5.494774	2.553466	-2.782228
25	6	0	-7.355952	3.287935	-0.030384
26	1	0	-7.920386	1.865790	1.487973
27	1	0	-6.649394	4.463582	-1.688425
28	1	0	-7.852287	4.123381	0.453690
29	1	0	-0.203141	1.267335	1.086054
30	6	0	-2.150753	4.150880	-2.136904
31	6	0	-3.088687	3.898413	-1.158926
32	6	0	-2.775264	3.053756	-0.076659
33	6	0	-1.478204	2.508104	0.000727
34	6	0	-0.520985	2.765456	-0.991778
35	6	0	-0.870263	3.572056	-2.053039
36	1	0	-4.727617	3.057474	0.877947
37	1	0	-2.396119	4.795655	-2.974572
38	1	0	-4.080395	4.336937	-1.206451
39	6	0	-3.710344	2.676285	0.940132
40	1	0	0.472673	2.332140	-0.907739
41	1	0	-0.135529	3.768693	-2.828009
42	6	0	-2.020436	1.312251	2.024835
43	6	0	-3.352004	1.842659	1.954235
44	1	0	-4.071655	1.541401	2.706492
45	7	0	-1.164380	1.685939	1.055500
46	6	0	-1.522844	0.418049	3.013890
47	1	0	-0.488569	0.107175	2.880735

48	6	0	-2.228113	-0.074279	4.099656
49	1	0	-3.193531	0.342938	4.369871
50	1	0	-1.654924	-0.446641	4.943401
51	6	0	5.567744	-3.311043	-2.282261
52	6	0	4.143286	-3.617438	-1.879458
53	6	0	3.735489	-2.766820	-0.847804
54	6	0	5.800875	-1.938920	-1.625042
55	1	0	6.261202	-4.065093	-1.888275
56	1	0	5.698235	-3.290404	-3.368383
57	1	0	5.424042	-1.145883	-2.280966
58	1	0	6.851852	-1.728614	-1.404510
59	6	0	4.921661	-1.971664	-0.341955
60	6	0	5.680856	-2.720829	0.788888
61	6	0	4.805429	-0.593581	0.276146
62	6	0	6.644452	-1.665094	1.362878
63	1	0	6.182625	-3.623523	0.426876
64	1	0	4.955368	-3.016675	1.555173
65	6	0	5.876043	-0.379899	1.149961
66	1	0	6.883071	-1.836755	2.416851
67	1	0	7.595553	-1.653603	0.815437
68	6	0	3.274430	-4.565749	-2.398628
69	6	0	1.979879	-4.632531	-1.892545
70	6	0	1.514349	-3.735293	-0.923753
71	6	0	2.416632	-2.791950	-0.412396
72	1	0	3.592502	-5.242005	-3.187064
73	1	0	1.288426	-5.379664	-2.271442
74	6	0	3.887883	0.422904	0.047999
75	6	0	4.095712	1.704186	0.578721
76	6	0	5.228510	1.910965	1.373173
77	6	0	6.101602	0.874867	1.695659
78	1	0	5.406034	2.908528	1.763551
79	1	0	6.942706	1.051665	2.360139
80	8	0	2.007485	-1.895592	0.557114
81	8	0	0.383050	-0.575012	-0.979023
82	8	0	1.191509	0.347535	1.314059
83	15	0	1.454837	-0.432149	0.055641
84	8	0	2.769442	0.170420	-0.725860
85	6	0	3.169088	2.841038	0.295333
86	6	0	2.470975	3.469897	1.348502
87	6	0	3.051689	3.341870	-1.019130
88	6	0	1.672556	4.580470	1.063716
89	6	0	2.262671	4.470130	-1.243011
90	6	0	1.553768	5.098202	-0.222642
91	1	0	1.129633	5.053110	1.878351
92	1	0	2.175779	4.863341	-2.255843
93	6	0	0.096258	-3.836104	-0.465112
94	6	0	-0.954513	-3.681341	-1.392827
95	6	0	-0.194476	-4.204563	0.867648
96	6	0	-2.265609	-3.941789	-0.981328
97	6	0	-1.520339	-4.447218	1.227793
98	6	0	-2.572144	-4.342530	0.315251
99	1	0	-3.067119	-3.823865	-1.706146
100	1	0	-1.746440	-4.751203	2.250420
101	6	0	-0.728229	-3.294964	-2.850910
102	1	0	0.332817	-3.074710	-2.988444
103	6	0	-1.105862	-4.460650	-3.776841
104	1	0	-2.182131	-4.662586	-3.727659
105	1	0	-0.858423	-4.218676	-4.815722
106	1	0	-0.586082	-5.384874	-3.505980
107	6	0	-1.495887	-2.032228	-3.258415
108	1	0	-1.393946	-1.869319	-4.337034
109	1	0	-2.567933	-2.120322	-3.040702
110	1	0	-1.096338	-1.154164	-2.748808
111	6	0	0.889073	-4.412043	1.916740
112	1	0	1.859809	-4.211996	1.459554
113	6	0	0.910462	-5.865371	2.406383
114	1	0	-0.028340	-6.131899	2.904389
115	1	0	1.056171	-6.557018	1.571092
116	1	0	1.724223	-6.014976	3.123932
117	6	0	0.728728	-3.439886	3.090339
118	1	0	1.577453	-3.525856	3.777158
119	1	0	0.686204	-2.404318	2.734226
120	1	0	-0.179856	-3.666376	3.661804
121	6	0	-3.977761	-4.714790	0.752466
122	1	0	-4.125201	-4.285382	1.752937
123	6	0	-4.098875	-6.241003	0.872661
124	1	0	-5.094200	-6.526162	1.230434
125	1	0	-3.938478	-6.709405	-0.104644
126	1	0	-3.354140	-6.646480	1.564070
127	6	0	-5.073749	-4.169152	-0.162700
128	1	0	-5.058655	-4.673486	-1.135822
129	1	0	-6.058150	-4.348014	0.281894
130	1	0	-4.955263	-3.094450	-0.335223
131	6	0	2.584135	3.018282	2.799443
132	1	0	3.098457	2.054059	2.817938
133	6	0	1.220399	2.805317	3.462165
134	1	0	1.357732	2.467752	4.495325
135	1	0	0.626588	3.725635	3.492262
136	1	0	0.659337	2.039872	2.927838
137	6	0	3.399343	4.034168	3.612925
138	1	0	3.537320	3.681468	4.640651
139	1	0	4.386188	4.214850	3.177255
140	1	0	2.877656	4.997480	3.654242
141	6	0	3.750572	2.711243	-2.215071
142	1	0	4.335583	1.856060	-1.868628
143	6	0	2.729529	2.190084	-3.234352
144	1	0	3.240112	1.674387	-4.054912
145	1	0	2.033119	1.485674	-2.769186
146	1	0	2.157518	3.017574	-3.672015
147	6	0	4.728823	3.695346	-2.867959
148	1	0	4.205476	4.570044	-3.269499
149	1	0	5.470796	4.049321	-2.145657
150	1	0	5.257196	3.213591	-3.697441
151	6	0	0.693549	6.308960	-0.530546
152	1	0	0.388312	6.223756	-1.582960
153	6	0	1.511849	7.597855	-0.377583
154	1	0	0.910844	8.476796	-0.634966
155	1	0	1.851670	7.707028	0.658462
156	1	0	2.396975	7.581879	-1.020583
157	6	0	-0.579278	6.371441	0.316292
158	1	0	-1.243412	7.158308	-0.055921
159	1	0	-1.120739	5.420338	0.288972
160	1	0	-0.349134	6.605738	1.361529

S_endo_t-c

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.183543 hartree

Sum of electronic and thermal Free Energies = -3615.910506 hartree

The number of imaginary frequency = 1

Imaginary frequency = -355.37

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.016499	0.713405	4.175635
2	1	0	1.075238	0.197839	4.010355
3	1	0	2.104637	1.203227	5.140835
4	6	0	3.165246	0.319210	3.518516
5	1	0	4.116434	0.681642	3.905137
6	6	0	3.208129	-0.340049	2.268503
7	1	0	4.158396	-0.416187	1.759068
8	6	0	2.047990	-0.744331	1.650105
9	1	0	1.109903	-0.741130	2.191685
10	1	0	0.880919	-1.522045	0.216847
11	7	0	1.846974	-1.233318	0.394468
12	6	0	2.681074	-1.289643	-0.700641
13	8	0	3.911353	-0.816352	-0.432221
14	8	0	2.337210	-1.702711	-1.782350
15	6	0	4.842928	-0.948171	-1.515801
16	1	0	4.926523	-2.012492	-1.765193
17	1	0	4.454066	-0.427588	-2.396530
18	6	0	6.161138	-0.375929	-1.069405
19	6	0	6.624311	-0.565078	0.234538
20	6	0	6.958512	0.319197	-1.978696
21	6	0	7.853547	-0.044416	0.627298
22	1	0	6.021394	-1.130950	0.939340
23	6	0	8.193253	0.833208	-1.589703
24	1	0	6.604099	0.461227	-2.996309
25	6	0	8.639706	0.659554	-0.282570
26	1	0	8.201868	-0.194306	1.644614
27	1	0	8.804252	1.372140	-2.307457
28	1	0	9.598768	1.064719	0.024675
29	1	0	0.680109	1.192100	-0.738545
30	6	0	4.033468	1.884649	-4.014734
31	6	0	4.506134	2.359024	-2.809378
32	6	0	3.730351	2.228838	-1.640445
33	6	0	2.454256	1.637199	-1.734654
34	6	0	1.985987	1.119708	-2.958292
35	6	0	2.775358	1.251331	-4.080768
36	1	0	5.176473	3.050408	-0.242946
37	1	0	4.631614	1.989293	-4.914233
38	1	0	5.483586	2.827850	-2.736623
39	6	0	4.173044	2.644808	-0.344360
40	1	0	1.018205	0.626728	-2.984293
41	1	0	2.421231	0.858572	-5.028179
42	6	0	2.037845	1.987410	0.608709
43	6	0	3.365434	2.522918	0.740041
44	1	0	3.706606	2.823456	1.723315
45	7	0	1.664151	1.561027	-0.612356
46	6	0	1.097233	1.895732	1.673016
47	1	0	0.127468	1.463817	1.436855
48	6	0	1.339337	2.341768	2.959041
49	1	0	2.177805	2.995112	3.179333
50	1	0	0.480390	2.475424	3.610267
51	6	0	-6.187918	-0.014659	-3.060676
52	6	0	-5.407682	0.999625	-2.252191
53	6	0	-4.672275	0.356839	-1.252400
54	6	0	-5.569329	-1.351688	-2.601253
55	1	0	-7.260150	0.029707	-2.832208
56	1	0	-6.083684	0.150555	-4.137351
57	1	0	-4.674945	-1.572764	-3.193739
58	1	0	-6.254383	-2.200976	-2.685507
59	6	0	-5.136783	-1.082962	-1.134165
60	6	0	-6.389487	-1.159381	-0.210801
61	6	0	-4.297666	-2.201337	-0.535967
62	6	0	-6.565755	-2.658729	0.072832
63	1	0	-7.267393	-0.687425	-0.661763
64	1	0	-6.161873	-0.632885	0.723020
65	6	0	-5.134115	-3.139243	0.078809
66	1	0	-7.077385	-2.858358	1.019051
67	1	0	-7.146133	-3.148995	-0.719432
68	6	0	-5.342402	2.378672	-2.395771
69	6	0	-4.491283	3.102659	-1.562962
70	6	0	-3.642825	2.472350	-0.644839
71	6	0	-3.750613	1.080343	-0.508605
72	1	0	-5.936237	2.889377	-3.148675
73	1	0	-4.437229	4.184156	-1.655822
74	6	0	-2.918815	-2.392994	-0.516739
75	6	0	-2.363416	-3.532098	0.088391
76	6	0	-3.239265	-4.488452	0.617675
77	6	0	-4.617015	-4.301257	0.631228
78	1	0	-2.808923	-5.383262	1.059081
79	1	0	-5.269426	-5.037810	1.091602
80	8	0	-2.935165	0.422095	0.386990
81	8	0	-0.838266	0.715725	-1.116387
82	8	0	-0.830659	-0.754402	1.028535
83	15	0	-1.539650	-0.225969	-0.175700
84	8	0	-2.104884	-1.447499	-1.112047
85	6	0	-0.892144	-3.761831	0.246513
86	6	0	-0.331172	-3.781396	1.545246
87	6	0	-0.090687	-4.059790	-0.872090
88	6	0	1.010572	-4.132991	1.690818
89	6	0	1.252442	-4.393416	-0.671579
90	6	0	1.818124	-4.449043	0.598364
91	1	0	1.436851	-4.165592	2.692646
92	1	0	1.877626	-4.618345	-1.531320
93	6	0	-2.625329	3.253769	0.122386
94	6	0	-1.663661	4.021613	-0.570283
95	6	0	-2.619780	3.249648	1.535723
96	6	0	-0.727383	4.762864	0.156902
97	6	0	-1.672595	4.018541	2.210511
98	6	0	-0.714361	4.779998	1.546842
99	1	0	0.010475	5.343763	-0.391449
100	1	0	-1.679914	4.027498	3.300612
101	6	0	-1.586236	4.104027	-2.090437
102	1	0	-2.331299	3.430292	-2.516328

103	6	0	-0.231626	3.622907	-2.613837
104	1	0	-0.189305	3.711949	-3.705248
105	1	0	0.605452	4.196935	-2.198301
106	1	0	-0.108358	2.573602	-2.347445
107	6	0	-1.893920	5.525868	-2.576876
108	1	0	-1.901157	5.562789	-3.671412
109	1	0	-2.866080	5.875525	-2.214113
110	1	0	-1.136679	6.234620	-2.223043
111	6	0	-3.622564	2.475787	2.379887
112	1	0	-4.283339	1.914350	1.716514
113	6	0	-4.504263	3.432308	3.193438
114	1	0	-5.251033	2.869957	3.764085
115	1	0	-3.908611	4.014437	3.905326
116	1	0	-5.028474	4.136041	2.539569
117	6	0	-2.914865	1.468066	3.295560
118	1	0	-3.651027	0.854927	3.826610
119	1	0	-2.266593	0.802213	2.717864
120	1	0	-2.311813	1.984761	4.052798
121	6	0	0.261173	5.622609	2.346898
122	1	0	0.439390	5.094039	3.294410
123	6	0	-0.367826	6.981813	2.682790
124	1	0	0.308069	7.586952	3.296842
125	1	0	-0.581265	7.533726	1.760735
126	1	0	-1.310337	6.856258	3.223790
127	6	0	1.611818	5.815029	1.656140
128	1	0	1.520076	6.465796	0.779817
129	1	0	2.324814	6.288511	2.339077
130	1	0	2.028417	4.859387	1.320661
131	6	0	-1.140508	-3.493468	2.806261
132	1	0	-2.132361	-3.145676	2.506762
133	6	0	-0.530206	-2.385567	3.675170
134	1	0	-1.089319	-2.299714	4.613735
135	1	0	0.515844	-2.593990	3.932296
136	1	0	-0.593157	-1.431547	3.147155
137	6	0	-1.305013	-4.776118	3.634619
138	1	0	-1.948800	-4.593932	4.501621
139	1	0	-1.743610	-5.587247	3.045973
140	1	0	-0.333799	-5.125063	4.004233
141	6	0	-0.696918	-4.139221	-2.266682
142	1	0	-1.477570	-3.376967	-2.336395
143	6	0	0.302715	-3.861514	-3.391345
144	1	0	-0.232858	-3.774507	-4.342231
145	1	0	0.857196	-2.937640	-3.210475
146	1	0	1.023091	-4.680300	-3.501796
147	6	0	-1.350524	-5.514731	-2.464499
148	1	0	-0.594985	-6.305115	-2.386827
149	1	0	-2.121325	-5.703835	-1.711295
150	1	0	-1.813932	-5.581689	-3.454916
151	6	0	3.263144	-4.871275	0.791680
152	1	0	3.692045	-5.034970	-0.205799
153	6	0	4.094660	-3.790071	1.491062
154	1	0	3.683032	-3.551991	2.478357
155	1	0	5.128125	-4.127568	1.628747
156	1	0	4.112138	-2.862543	0.910475
157	6	0	3.344594	-6.193850	1.563579
158	1	0	4.383149	-6.530234	1.651979
159	1	0	2.941463	-6.074899	2.575433
160	1	0	2.766892	-6.975996	1.062853

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r-r_R_endo

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.190876 hartree

Sum of electronic and thermal Free Energies = -3615.918406 hartree

The number of imaginary frequency = 1

Imaginary frequency = -340.28

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.509480	-2.825036	-3.442878
2	1	0	-3.552616	-1.796900	-3.096509
3	1	0	-4.033838	-3.022923	-4.373693
4	6	0	-3.305442	-3.855687	-2.550778
5	1	0	-3.512836	-4.868044	-2.894011
6	6	0	-2.665092	-3.740454	-1.296301
7	1	0	-2.385515	-4.643239	-0.770413
8	6	0	-2.283934	-2.523836	-0.776629
9	1	0	-2.649573	-1.592155	-1.202217
10	1	0	-1.305975	-1.338232	0.613628
11	7	0	-1.501108	-2.314598	0.315511
12	6	0	-0.782369	-3.288750	0.977598
13	8	0	-0.036664	-2.700452	1.919372
14	8	0	-0.794548	-4.479299	0.755022
15	6	0	0.716512	-3.575971	2.749975
16	1	0	0.023623	-4.215450	3.310157
17	1	0	1.336491	-4.225996	2.123228
18	6	0	1.558952	-2.739821	3.676378
19	6	0	1.424973	-1.352823	3.745861
20	6	0	2.499263	-3.384858	4.482792
21	6	0	2.218394	-0.628236	4.635308
22	1	0	0.719369	-0.840087	3.096838
23	6	0	3.296798	-2.656202	5.358372
24	1	0	2.609236	-4.465788	4.419321
25	6	0	3.155656	-1.271657	5.438390
26	1	0	2.105258	0.450355	4.689554
27	1	0	4.027022	-3.167618	5.978365
28	1	0	3.774220	-0.698600	6.122325
29	1	0	0.746272	-1.138743	-1.294812
30	6	0	3.761319	-4.034424	0.964901
31	6	0	3.074607	-4.774168	0.024244
32	6	0	2.104436	-4.158677	-0.793495
33	6	0	1.863905	-2.777438	-0.634277
34	6	0	2.563519	-2.023030	0.324127
35	6	0	3.498904	-2.656707	1.114025
36	1	0	1.505050	-5.916041	-1.918649
37	1	0	4.502521	-4.510296	1.599019
38	1	0	3.265787	-5.836577	-0.098329
39	6	0	1.340298	-4.850225	-1.786330
40	1	0	2.360874	-0.958260	0.423913
41	1	0	4.032563	-2.081878	1.866172
42	6	0	0.185978	-2.798177	-2.362744
43	6	0	0.417902	-4.201732	-2.543762

44	1	0	-0.169772	-4.733232	-3.282054
45	7	0	0.916166	-2.171126	-1.422512
46	6	0	-0.731511	-2.008375	-3.119571
47	1	0	-0.775004	-0.954815	-2.854217
48	6	0	-1.500010	-2.475450	-4.163906
49	1	0	-1.341020	-3.463149	-4.583827
50	1	0	-1.916999	-1.750756	-4.855820
51	6	0	-1.475428	5.782486	2.416360
52	6	0	-2.262677	4.555632	2.013406
53	6	0	-1.658382	3.928243	0.920817
54	6	0	-0.156656	5.594085	1.641876
55	1	0	-1.989947	6.702607	2.111515
56	1	0	-1.326648	5.842227	3.498712
57	1	0	0.526493	4.961089	2.219101
58	1	0	0.357467	6.533189	1.415469
59	6	0	-0.574082	4.823497	0.358110
60	6	0	-1.170403	5.823448	-0.674025
61	6	0	0.628500	4.317415	-0.416862
62	6	0	0.058993	6.442299	-1.359182
63	1	0	-1.832400	6.558345	-0.206184
64	1	0	-1.755085	5.255065	-1.406278
65	6	0	1.050286	5.302750	-1.315257
66	1	0	-0.145024	6.777451	-2.380548
67	1	0	0.431056	7.311928	-0.802519
68	6	0	-3.417303	4.030300	2.575027
69	6	0	-3.937845	2.850427	2.051232
70	6	0	-3.294933	2.142432	1.027850
71	6	0	-2.135641	2.703265	0.474567
72	1	0	-3.907655	4.523968	3.409260
73	1	0	-4.851131	2.433254	2.465410
74	6	0	1.335668	3.122478	-0.318418
75	6	0	2.525628	2.940614	-1.039304
76	6	0	2.963258	3.985022	-1.864049
77	6	0	2.227113	5.152449	-2.032919
78	1	0	3.899721	3.853043	-2.398039
79	1	0	2.566672	5.924904	-2.717084
80	8	0	-1.457206	2.044371	-0.533729
81	8	0	-0.640095	0.197024	1.082430
82	8	0	0.276267	0.443726	-1.346385
83	15	0	-0.227838	1.059318	-0.069193
84	8	0	0.868072	2.127746	0.522940
85	6	0	3.355208	1.697237	-0.975419
86	6	0	3.502214	0.894220	-2.122799
87	6	0	4.089537	1.397122	0.194032
88	6	0	4.375348	-0.198091	-2.077475
89	6	0	4.959990	0.309149	0.180291
90	6	0	5.115374	-0.504960	-0.942448
91	1	0	4.480553	-0.816476	-2.965066
92	1	0	5.537375	0.072939	1.071768
93	6	0	-3.873461	0.838313	0.579168
94	6	0	-4.032730	-0.214567	1.511760
95	6	0	-4.382051	0.687363	-0.726203
96	6	0	-4.726920	-1.358783	1.122126
97	6	0	-5.101206	-0.469756	-1.053873
98	6	0	-5.310197	-1.498907	-0.139399
99	1	0	-4.838026	-2.166803	1.842790
100	1	0	-5.525596	-0.546051	-2.051576
101	6	0	-3.541023	-0.134117	2.953989
102	1	0	-2.983637	0.797151	3.076609
103	6	0	-4.732348	-0.120930	3.923033
104	1	0	-5.271061	-1.074945	3.888288
105	1	0	-4.386156	0.030359	4.950760
106	1	0	-5.450313	0.669099	3.682104
107	6	0	-2.578116	-1.268095	3.318028
108	1	0	-2.337573	-1.222620	4.386275
109	1	0	-3.010674	-2.255954	3.116850
110	1	0	-1.648018	-1.167469	2.759618
111	6	0	-4.225617	1.752994	-1.801839
112	1	0	-3.712081	2.613573	-1.368251
113	6	0	-5.584201	2.247727	-2.312932
114	1	0	-6.143551	1.447974	-2.810330
115	1	0	-6.198157	2.626530	-1.490295
116	1	0	-5.444679	3.055678	-3.038828
117	6	0	-3.358020	1.235078	-2.955813
118	1	0	-3.181840	2.028174	-3.690390
119	1	0	-2.385337	0.895268	-2.584458
120	1	0	-3.858343	0.408350	-3.476832
121	6	0	-6.150177	-2.731645	-0.445320
122	1	0	-5.484146	-3.603757	-0.370588
123	6	0	-6.767351	-2.728439	-1.843150
124	1	0	-7.342739	-3.646355	-1.998169
125	1	0	-7.452125	-1.880764	-1.963405
126	1	0	-6.007576	-2.672566	-2.627037
127	6	0	-7.268812	-2.894276	0.595204
128	1	0	-7.950586	-2.037891	0.550524
129	1	0	-7.847115	-3.802345	0.395652
130	1	0	-6.880568	-2.959092	1.614730
131	6	0	2.799094	1.196506	-3.440395
132	1	0	2.045972	1.967618	-3.257671
133	6	0	2.062828	-0.018969	-4.008352
134	1	0	1.554349	0.253285	-4.939808
135	1	0	2.743758	-0.847368	-4.234508
136	1	0	1.311763	-0.360409	-3.298815
137	6	0	3.804566	1.720639	-4.476109
138	1	0	3.292031	1.986463	-5.406836
139	1	0	4.343577	2.602470	-4.119031
140	1	0	4.549380	0.950928	-4.709532
141	6	0	4.006763	2.290282	1.424148
142	1	0	2.976552	2.647078	1.510898
143	6	0	4.338543	1.558109	2.725813
144	1	0	4.082070	2.189051	3.583272
145	1	0	3.778467	0.621635	2.812252
146	1	0	5.407258	1.328294	2.802498
147	6	0	4.926354	3.508041	1.254124
148	1	0	5.967231	3.180983	1.149557
149	1	0	4.659805	4.089616	0.366968
150	1	0	4.860712	4.165085	2.128178
151	6	0	6.092043	-1.665194	-0.898263
152	1	0	6.093624	-2.043253	0.133735
153	6	0	7.510540	-1.176526	-1.221913
154	1	0	8.232597	-1.997494	-1.154376
155	1	0	7.545410	-0.771778	-2.239477
156	1	0	7.821596	-0.383766	-0.535009
157	6	0	5.698779	-2.823114	-1.816360

158	1	0	6.324386	-3.698172	-1.612925
159	1	0	4.651056	-3.106473	-1.672098
160	1	0	5.839518	-2.558170	-2.870207

r-r_S_endo2

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.189831 hartree

Sum of electronic and thermal Free Energies = -3615.914482 hartree

The number of imaginary frequency = 1

Imaginary frequency = -348.89

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.334140	-2.178769	4.405510
2	1	0	0.010955	-1.182809	4.144766
3	1	0	0.087458	-2.584775	5.320269
4	6	0	-1.557540	-2.643019	3.968326
5	1	0	-1.963205	-3.528169	4.455612
6	6	0	-2.236649	-2.197628	2.810168
7	1	0	-3.083552	-2.764354	2.447250
8	6	0	-1.757255	-1.139926	2.074729
9	1	0	-0.975170	-0.492229	2.452224
10	1	0	-1.752060	0.144759	0.511769
11	7	0	-2.187892	-0.713981	0.853110
12	6	0	-3.015658	-1.423602	0.010729
13	8	0	-3.181461	-0.753465	-1.137568
14	8	0	-3.500600	-2.507423	0.255431
15	6	0	-4.024607	-1.396151	-2.113416
16	1	0	-3.717948	-0.945444	-3.059791
17	1	0	-3.797798	-2.464658	-2.129565
18	6	0	-5.482057	-1.148522	-1.828928
19	6	0	-6.065508	0.074517	-2.168035
20	6	0	-6.248788	-2.114316	-1.175367
21	6	0	-7.391743	0.338507	-1.838344
22	1	0	-5.475544	0.824486	-2.691055
23	6	0	-7.577798	-1.854702	-0.851601
24	1	0	-5.783942	-3.054329	-0.893908
25	6	0	-8.147809	-0.625711	-1.173924
26	1	0	-7.835643	1.294313	-2.100136
27	1	0	-8.165729	-2.608415	-0.336862
28	1	0	-9.181274	-0.419361	-0.912938
29	1	0	0.275906	-1.608609	-0.667612
30	6	0	-2.210972	-4.205261	-3.732314
31	6	0	-2.164156	-4.886796	-2.534686
32	6	0	-1.495993	-4.332450	-1.424527
33	6	0	-0.889953	-3.067968	-1.560477
34	6	0	-0.961145	-2.357296	-2.775216
35	6	0	-1.604762	-2.937894	-3.847365
36	1	0	-1.856414	-5.954371	-0.024588
37	1	0	-2.717466	-4.640563	-4.587264
38	1	0	-2.633650	-5.860982	-2.430293
39	6	0	-1.383101	-4.985114	-0.155477
40	1	0	-0.498775	-1.375403	-2.836162
41	1	0	-1.652300	-2.404657	-4.791779
42	6	0	-0.072484	-3.130137	0.703533
43	6	0	-0.706449	-4.409055	0.869898
44	1	0	-0.635445	-4.898816	1.833549
45	7	0	-0.210352	-2.529527	-0.493582
46	6	0	0.714483	-2.481281	1.696393
47	1	0	1.137216	-1.515125	1.429902
48	6	0	0.997204	-3.013052	2.939903
49	1	0	0.789376	-4.053371	3.170167
50	1	0	1.834289	-2.587878	3.485683
51	6	0	4.330324	3.784399	-3.450105
52	6	0	4.500702	2.498919	-2.668715
53	6	0	3.649326	2.490934	-1.559792
54	6	0	3.060942	4.393087	-2.817247
55	1	0	5.196150	4.446981	-3.327824
56	1	0	4.219385	3.599320	-4.522905
57	1	0	2.167840	3.987707	-3.304912
58	1	0	3.021989	5.484830	-2.882829
59	6	0	3.095826	3.888731	-1.349899
60	6	0	4.122688	4.741089	-0.543605
61	6	0	1.830227	4.189118	-0.564166
62	6	0	3.337801	5.993262	-0.125716
63	1	0	5.027467	4.956495	-1.119376
64	1	0	4.414254	4.176068	0.348993
65	6	0	1.950740	5.430210	0.070949
66	1	0	3.731127	6.462949	0.780671
67	1	0	3.350015	6.753814	-0.917142
68	6	0	5.334702	1.419048	-2.922670
69	6	0	5.270128	0.308459	-2.083736
70	6	0	4.327514	0.214342	-1.052669
71	6	0	3.509002	1.328544	-0.813187
72	1	0	6.024376	1.432234	-3.762015
73	1	0	5.928803	-0.538352	-2.257723
74	6	0	0.669800	3.440761	-0.392752
75	6	0	-0.378463	3.921731	0.407098
76	6	0	-0.256641	5.205135	0.952560
77	6	0	0.899427	5.962893	0.801489
78	1	0	-1.084526	5.588533	1.542173
79	1	0	0.987159	6.936400	1.275500
80	8	0	2.563106	1.268084	0.188454
81	8	0	0.992649	-0.235518	-1.238469
82	8	0	0.286090	0.722177	1.068199
83	15	0	1.024550	0.873133	-0.220560
84	8	0	0.556832	2.220561	-1.030282
85	6	0	-1.589348	3.120412	0.763814
86	6	0	-1.801705	2.779802	2.118810
87	6	0	-2.559295	2.792913	-0.202161
88	6	0	-3.019433	2.204509	2.480300
89	6	0	-3.752399	2.187197	0.208799
90	6	0	-4.021395	1.928946	1.552461
91	1	0	-3.205839	1.975164	3.528613
92	1	0	-4.502111	1.937814	-0.541093
93	6	0	4.176806	-1.049758	-0.269288
94	6	0	3.904670	-2.261818	-0.941140
95	6	0	4.330128	-1.057790	1.136177
96	6	0	3.789634	-3.442915	-0.202172
97	6	0	4.221757	-2.267312	1.821217
98	6	0	3.945879	-3.471146	1.178645

99	1	0	3.570077	-4.366159	-0.733152
100	1	0	4.356190	-2.274473	2.903001
101	6	0	3.723967	-2.367744	-2.450941
102	1	0	3.785787	-1.367836	-2.882963
103	6	0	2.334695	-2.897806	-2.808922
104	1	0	2.222628	-2.981003	-3.895863
105	1	0	2.138977	-3.885482	-2.374287
106	1	0	1.589822	-2.194618	-2.437759
107	6	0	4.826987	-3.228472	-3.078903
108	1	0	4.723154	-3.247283	-4.168965
109	1	0	5.824290	-2.848023	-2.834688
110	1	0	4.772326	-4.262348	-2.719939
111	6	0	4.643875	0.184531	1.958291
112	1	0	4.689743	1.047335	1.290918
113	6	0	6.015928	0.062047	2.633973
114	1	0	6.251438	0.978060	3.186169
115	1	0	6.037186	-0.771090	3.345155
116	1	0	6.804870	-0.107054	1.894710
117	6	0	3.543432	0.453597	2.993881
118	1	0	3.732511	1.399174	3.513750
119	1	0	2.562068	0.517205	2.513912
120	1	0	3.518868	-0.338521	3.753000
121	6	0	3.868594	-4.755605	1.981921
122	1	0	3.517657	-4.484755	2.987979
123	6	0	5.265680	-5.374396	2.126356
124	1	0	5.232115	-6.282377	2.738291
125	1	0	5.661957	-5.639409	1.139893
126	1	0	5.962283	-4.668998	2.588905
127	6	0	2.888062	-5.776709	1.402312
128	1	0	3.265756	-6.202133	0.466273
129	1	0	2.744626	-6.606844	2.101712
130	1	0	1.914475	-5.320612	1.193180
131	6	0	-0.777970	3.046302	3.217762
132	1	0	0.135360	3.427320	2.753930
133	6	0	-0.387648	1.768459	3.972670
134	1	0	0.294526	2.014027	4.794557
135	1	0	-1.261737	1.266030	4.405264
136	1	0	0.123259	1.085447	3.289947
137	6	0	-1.295555	4.103256	4.203208
138	1	0	-0.531465	4.334625	4.952822
139	1	0	-1.569139	5.032865	3.695338
140	1	0	-2.184611	3.740697	4.731526
141	6	0	-2.379898	3.151239	-1.670600
142	1	0	-1.426042	3.673383	-1.780825
143	6	0	-2.326204	1.905469	-2.559169
144	1	0	-2.141805	2.191922	-3.600529
145	1	0	-1.531066	1.225111	-2.239056
146	1	0	-3.277165	1.363593	-2.515989
147	6	0	-3.483311	4.106884	-2.141573
148	1	0	-4.468616	3.628628	-2.093293
149	1	0	-3.517051	5.006384	-1.519345
150	1	0	-3.309242	4.410889	-3.179272
151	6	0	-5.352982	1.364712	2.012925
152	1	0	-5.387053	1.474097	3.104877
153	6	0	-6.536470	2.139463	1.425356
154	1	0	-6.583004	2.012747	0.338398
155	1	0	-7.479646	1.766088	1.838451
156	1	0	-6.459171	3.208945	1.642776
157	6	0	-5.467462	-0.123789	1.677641
158	1	0	-6.432002	-0.528452	2.004197
159	1	0	-5.399156	-0.267820	0.594567
160	1	0	-4.669928	-0.703310	2.154666

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r-l_R_endo

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.188702 hartree

Sum of electronic and thermal Free Energies = -3615.916591 hartree

The number of imaginary frequency = 1

Imaginary frequency = -346.93

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.590314	-2.846484	-3.436725
2	1	0	-3.633982	-1.818386	-3.089471
3	1	0	-4.124387	-3.044848	-4.361896
4	6	0	-3.379711	-3.877247	-2.545427
5	1	0	-3.589362	-4.889661	-2.886804
6	6	0	-2.727098	-3.760878	-1.297982
7	1	0	-2.440639	-4.663102	-0.774850
8	6	0	-2.342959	-2.543134	-0.782361
9	1	0	-2.715985	-1.612312	-1.203103
10	1	0	-1.357574	-1.357302	0.601870
11	7	0	-1.552388	-2.333030	0.304095
12	6	0	-0.814653	-3.304920	0.949540
13	8	0	-0.083015	-2.719245	1.903196
14	8	0	-0.802596	-4.490849	0.704145
15	6	0	0.700915	-3.590312	2.709229
16	1	0	0.031336	-4.254169	3.269237
17	1	0	1.326418	-4.216137	2.063219
18	6	0	1.538258	-2.748458	3.635485
19	6	0	1.411359	-1.359932	3.688037
20	6	0	2.473639	-3.388567	4.451339
21	6	0	2.208438	-0.628572	4.568555
22	1	0	0.709171	-0.851156	3.032104
23	6	0	3.275124	-2.653215	5.317778
24	1	0	2.577527	-4.470832	4.402167
25	6	0	3.142228	-1.266934	5.379788
26	1	0	2.101331	0.451284	4.608661
27	1	0	4.001888	-3.160893	5.944854
28	1	0	3.764236	-0.688684	6.056206
29	1	0	0.661003	-1.131008	-1.325297
30	6	0	3.753934	-3.963255	0.899877
31	6	0	3.093819	-4.710798	-0.053451
32	6	0	2.096351	-4.118017	-0.855046
33	6	0	1.810380	-2.748642	-0.673886
34	6	0	2.482486	-1.985647	0.297095
35	6	0	3.437646	-2.599946	1.077007
36	1	0	1.538110	-5.881018	-1.992177
37	1	0	4.514306	-4.421845	1.524333
38	1	0	3.322002	-5.763770	-0.193221
39	6	0	1.341328	-4.822469	-1.845597

40	1	0	2.243958	-0.930097	0.415188
41	1	0	3.943962	-2.021397	1.844837
42	6	0	0.119911	-2.801321	-2.389281
43	6	0	0.386906	-4.196620	-2.582934
44	1	0	-0.193653	-4.739136	-3.318876
45	7	0	0.842301	-2.163018	-1.451436
46	6	0	-0.818208	-2.024792	-3.134936
47	1	0	-0.869691	-0.971226	-2.870488
48	6	0	-1.593401	-2.498925	-4.171719
49	1	0	-1.431003	-3.486923	-4.589906
50	1	0	-2.016469	-1.778437	-4.864345
51	6	0	-1.387959	5.770391	2.450594
52	6	0	-2.200068	4.559989	2.047011
53	6	0	-1.616632	3.930379	0.944592
54	6	0	-0.079786	5.564802	1.662187
55	1	0	-1.889396	6.701286	2.156911
56	1	0	-1.227863	5.820147	3.531833
57	1	0	0.597790	4.916334	2.228679
58	1	0	0.448104	6.496635	1.437439
59	6	0	-0.522164	4.810448	0.377097
60	6	0	-1.112011	5.827630	-0.641906
61	6	0	0.664313	4.289856	-0.414306
62	6	0	0.120428	6.431204	-1.334960
63	1	0	-1.757112	6.569820	-0.162146
64	1	0	-1.713248	5.274346	-1.372288
65	6	0	1.092802	5.274957	-1.310012
66	1	0	-0.088355	6.777708	-2.351556
67	1	0	0.512686	7.290078	-0.775461
68	6	0	-3.358133	4.049325	2.615480
69	6	0	-3.901941	2.880686	2.089876
70	6	0	-3.279967	2.168744	1.056201
71	6	0	-2.118565	2.716841	0.494970
72	1	0	-3.832993	4.545203	3.457339
73	1	0	-4.817046	2.474877	2.511281
74	6	0	1.353453	3.082999	-0.333030
75	6	0	2.532365	2.886726	-1.068458
76	6	0	2.978117	3.930343	-1.889584
77	6	0	2.259066	5.110885	-2.041528
78	1	0	3.907183	3.788378	-2.433702
79	1	0	2.603914	5.883117	-2.723296
80	8	0	-1.461290	2.056547	-0.525659
81	8	0	-0.651261	0.173765	1.055771
82	8	0	0.235650	0.445841	-1.381259
83	15	0	-0.242969	1.048375	-0.087830
84	8	0	0.878712	2.088982	0.505620
85	6	0	3.346340	1.631201	-1.022240
86	6	0	3.448440	0.816654	-2.170490
87	6	0	4.117743	1.333170	0.117999
88	6	0	4.313330	-0.277106	-2.140622
89	6	0	5.000581	0.249526	0.080922
90	6	0	5.115163	-0.570832	-1.038491
91	1	0	4.379620	-0.915425	-3.019796
92	1	0	5.608328	0.043332	0.955728
93	6	0	-3.877341	0.872080	0.609808
94	6	0	-4.039758	-0.180198	1.542805
95	6	0	-4.395532	0.725611	-0.692269
96	6	0	-4.747646	-1.317586	1.157941
97	6	0	-5.128037	-0.424613	-1.015020
98	6	0	-5.341307	-1.451723	-0.099328
99	1	0	-4.860968	-2.124830	1.879093
100	1	0	-5.559498	-0.496716	-2.009997
101	6	0	-3.533214	-0.107914	2.980255
102	1	0	-2.964830	0.817081	3.099443
103	6	0	-4.713919	-0.084604	3.961882
104	1	0	-5.263967	-1.032197	3.929521
105	1	0	-4.355136	0.058910	4.986399
106	1	0	-5.425192	0.714573	3.731436
107	6	0	-2.578265	-1.252799	3.330168
108	1	0	-2.320114	-1.209564	4.394384
109	1	0	-3.025409	-2.235594	3.136568
110	1	0	-1.656133	-1.164087	2.756751
111	6	0	-4.234942	1.787820	-1.770594
112	1	0	-3.711081	2.644460	-1.341462
113	6	0	-5.591532	2.294109	-2.275763
114	1	0	-6.160146	1.499155	-2.770318
115	1	0	-6.198534	2.678739	-1.450668
116	1	0	-5.448119	3.100393	-3.002730
117	6	0	-3.378335	1.258589	-2.927803
118	1	0	-3.205796	2.045655	-3.669715
119	1	0	-2.403802	0.918406	-2.562059
120	1	0	-3.885373	0.429303	-3.438372
121	6	0	-6.195137	-2.676279	-0.399820
122	1	0	-5.537163	-3.554822	-0.329875
123	6	0	-6.821528	-2.666700	-1.793492
124	1	0	-7.407287	-3.578668	-1.944621
125	1	0	-7.498263	-1.811986	-1.909326
126	1	0	-6.066600	-2.619022	-2.582569
127	6	0	-7.308246	-2.828104	0.648184
128	1	0	-7.981991	-1.965162	0.607970
129	1	0	-7.896624	-3.730559	0.452671
130	1	0	-6.913770	-2.896544	1.665079
131	6	0	2.721429	1.131620	-3.472149
132	1	0	1.975211	1.904371	-3.268464
133	6	0	1.971473	-0.072036	-4.045252
134	1	0	1.459698	0.213294	-4.970951
135	1	0	2.643240	-0.904340	-4.284182
136	1	0	1.221430	-0.413063	-3.335271
137	6	0	3.714564	1.661519	-4.517411
138	1	0	3.189738	1.942095	-5.436916
139	1	0	4.266097	2.534733	-4.158777
140	1	0	4.449785	0.888490	-4.770309
141	6	0	4.073012	2.226385	1.350255
142	1	0	3.053463	2.610538	1.447434
143	6	0	4.395484	1.482119	2.647825
144	1	0	4.163371	2.117506	3.509051
145	1	0	3.809346	0.561916	2.736742
146	1	0	5.457669	1.221746	2.716686
147	6	0	5.021949	3.419910	1.172902
148	1	0	6.052747	3.066529	1.054740
149	1	0	4.759396	4.009551	0.289732
150	1	0	4.984181	4.076873	2.048702
151	6	0	6.058807	-1.763692	-1.104142
152	1	0	5.437993	-2.649314	-1.308784
153	6	0	6.828269	-2.022940	0.190189

154	1	0	7.446672	-2.919640	0.084096
155	1	0	7.494694	-1.184239	0.422389
156	1	0	6.161796	-2.172493	1.044338
157	6	0	7.056075	-1.602675	-2.261086
158	1	0	7.700410	-2.484552	-2.340666
159	1	0	6.551844	-1.462953	-3.220867
160	1	0	7.692743	-0.728181	-2.087884

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r-l_S_endo2

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.187002 hartree

Sum of electronic and thermal Free Energies = -3615.911926 hartree

The number of imaginary frequency = 1

Imaginary frequency = -348.44

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.403777	-1.966393	4.486777
2	1	0	-0.103454	-0.965143	4.194471
3	1	0	0.009926	-2.312588	5.429328
4	6	0	-1.586003	-2.514133	4.033455
5	1	0	-1.960880	-3.398485	4.546217
6	6	0	-2.249256	-2.153001	2.836971
7	1	0	-3.057246	-2.773983	2.473997
8	6	0	-1.794283	-1.105153	2.073374
9	1	0	-1.048433	-0.413054	2.444420
10	1	0	-1.800903	0.120621	0.462995
11	7	0	-2.206305	-0.743943	0.824820
12	6	0	-2.997007	-1.506921	-0.006334
13	8	0	-3.166014	-0.877163	-1.177188
14	8	0	-3.449903	-2.598081	0.264959
15	6	0	-3.973310	-1.573746	-2.145614
16	1	0	-3.657236	-1.150141	-3.101592
17	1	0	-3.722703	-2.636540	-2.118205
18	6	0	-5.440956	-1.349270	-1.899200
19	6	0	-6.040120	-0.146641	-2.281058
20	6	0	-6.202251	-2.314285	-1.238570
21	6	0	-7.378691	0.097573	-1.988461
22	1	0	-5.452307	0.602698	-2.807577
23	6	0	-7.543449	-2.074398	-0.951542
24	1	0	-5.724778	-3.237048	-0.922745
25	6	0	-8.130437	-0.865925	-1.317851
26	1	0	-7.835698	1.037409	-2.283453
27	1	0	-8.127796	-2.827032	-0.431172
28	1	0	-9.173695	-0.674768	-1.085856
29	1	0	0.302366	-1.605354	-0.590500
30	6	0	-2.027636	-4.461022	-3.546915
31	6	0	-1.946863	-5.087914	-2.321710
32	6	0	-1.314238	-4.451203	-1.235283
33	6	0	-0.777835	-3.161958	-1.423467
34	6	0	-0.892598	-2.504908	-2.664641
35	6	0	-1.497054	-3.165724	-3.712814
36	1	0	-1.592974	-6.029368	0.231088
37	1	0	-2.505120	-4.959642	-4.383786
38	1	0	-2.361722	-6.081497	-2.176703
39	6	0	-1.174417	-5.041114	0.061111
40	1	0	-0.495484	-1.498044	-2.764219
41	1	0	-1.575328	-2.673615	-4.677366
42	6	0	0.022262	-3.079752	0.846812
43	6	0	-0.539234	-4.384211	1.064264
44	1	0	-0.448757	-4.827394	2.048505
45	7	0	-0.131250	-2.543288	-0.379539
46	6	0	0.749596	-2.341755	1.822567
47	1	0	1.122533	-1.367826	1.517720
48	6	0	1.013689	-2.789550	3.102678
49	1	0	0.845644	-3.822847	3.384209
50	1	0	1.810250	-2.297035	3.652401
51	6	0	4.262453	3.992437	-3.334960
52	6	0	4.446279	2.680443	-2.603956
53	6	0	3.585928	2.609799	-1.503788
54	6	0	2.973764	4.548203	-2.696427
55	1	0	5.113238	4.665811	-3.172290
56	1	0	4.171038	3.849034	-4.415959
57	1	0	2.095697	4.141727	-3.209890
58	1	0	2.909760	5.640374	-2.720488
59	6	0	3.002247	3.988637	-1.248704
60	6	0	3.996502	4.834428	-0.397191
61	6	0	1.716548	4.243313	-0.482311
62	6	0	3.180770	6.062848	0.034112
63	1	0	4.910278	5.079937	-0.946090
64	1	0	4.277133	4.250300	0.486480
65	6	0	1.796676	5.475658	0.175518
66	1	0	3.540909	6.510674	0.965076
67	1	0	3.204847	6.847190	-0.733356
68	6	0	5.304262	1.630145	-2.896521
69	6	0	5.250676	0.484322	-2.108439
70	6	0	4.301289	0.326159	-1.090340
71	6	0	3.462815	1.414308	-0.803986
72	1	0	6.001589	1.693537	-3.727180
73	1	0	5.923746	-0.343840	-2.313056
74	6	0	0.567717	3.469588	-0.356963
75	6	0	-0.515497	3.921203	0.413017
76	6	0	-0.436117	5.201780	0.973800
77	6	0	0.711161	5.981000	0.874587
78	1	0	-1.289953	5.562667	1.540280
79	1	0	0.764605	6.949348	1.364032
80	8	0	2.522550	1.301047	0.199047
81	8	0	0.939648	-0.202790	-1.213730
82	8	0	0.250073	0.768374	1.093224
83	15	0	0.979623	0.910814	-0.201564
84	8	0	0.503740	2.254644	-1.011278
85	6	0	-1.716138	3.090698	0.735085
86	6	0	-1.965716	2.762727	2.087288
87	6	0	-2.644048	2.722118	-0.257695
88	6	0	-3.177246	2.155405	2.415800
89	6	0	-3.833313	2.088926	0.122521
90	6	0	-4.139906	1.840149	1.459857
91	1	0	-3.391396	1.933079	3.460344
92	1	0	-4.550815	1.810042	-0.648141
93	6	0	4.191469	-0.992424	-0.393512
94	6	0	3.996843	-2.159966	-1.163877

95	6	0	4.364886	-1.107474	1.004710
96	6	0	4.028065	-3.404258	-0.530864
97	6	0	4.378161	-2.376510	1.587397
98	6	0	4.241937	-3.542023	0.834968
99	1	0	3.901305	-4.303384	-1.131630
100	1	0	4.537323	-2.454711	2.662369
101	6	0	3.742103	-2.151413	-2.666478
102	1	0	3.719940	-1.117238	-3.013587
103	6	0	2.362656	-2.735194	-2.974668
104	1	0	2.159450	-2.704640	-4.051238
105	1	0	2.268721	-3.776011	-2.642669
106	1	0	1.612677	-2.132904	-2.463194
107	6	0	4.842839	-2.890811	-3.435735
108	1	0	4.664196	-2.822895	-4.514058
109	1	0	5.833896	-2.475700	-3.225778
110	1	0	4.867197	-3.953130	-3.168870
111	6	0	4.615652	0.089064	1.912764
112	1	0	4.611039	0.996399	1.306062
113	6	0	5.996809	-0.004174	2.574771
114	1	0	6.190126	0.888530	3.179066
115	1	0	6.066474	-0.875567	3.235230
116	1	0	6.787242	-0.089124	1.822800
117	6	0	3.511811	0.232468	2.967655
118	1	0	3.676941	1.131097	3.572051
119	1	0	2.526608	0.317343	2.497706
120	1	0	3.514436	-0.626531	3.650861
121	6	0	4.368340	-4.919245	1.459429
122	1	0	4.320473	-5.649172	0.640969
123	6	0	3.217046	-5.222970	2.420727
124	1	0	3.303298	-6.238456	2.822576
125	1	0	3.226814	-4.523534	3.264701
126	1	0	2.251958	-5.127512	1.912119
127	6	0	5.719476	-5.091522	2.162371
128	1	0	5.809811	-4.401427	3.008391
129	1	0	5.827673	-6.110471	2.548852
130	1	0	6.547295	-4.890384	1.476613
131	6	0	-0.992246	3.074631	3.219770
132	1	0	-0.083495	3.500824	2.788758
133	6	0	-0.565586	1.812644	3.980792
134	1	0	0.063998	2.085051	4.835530
135	1	0	-1.429354	1.257266	4.367431
136	1	0	0.012785	1.167714	3.314462
137	6	0	-1.590880	4.101881	4.190501
138	1	0	-0.859819	4.372623	4.959610
139	1	0	-1.899439	5.016091	3.674495
140	1	0	-2.473207	3.693934	4.696309
141	6	0	-2.427376	3.062303	-1.725410
142	1	0	-1.486286	3.610912	-1.813901
143	6	0	-2.308711	1.803495	-2.589571
144	1	0	-2.099253	2.078044	-3.629376
145	1	0	-1.503674	1.152783	-2.233926
146	1	0	-3.244174	1.233626	-2.567282
147	6	0	-3.542280	3.976827	-2.248253
148	1	0	-4.514185	3.470224	-2.224899
149	1	0	-3.623392	4.884827	-1.642974
150	1	0	-3.342273	4.269154	-3.284618
151	6	0	-5.469056	1.244262	1.885733
152	1	0	-5.543492	1.372394	2.973628
153	6	0	-6.654827	1.971054	1.244338
154	1	0	-6.660252	1.824154	0.159008
155	1	0	-7.599626	1.575164	1.631995
156	1	0	-6.618175	3.046034	1.444697
157	6	0	-5.525877	-0.252902	1.575828
158	1	0	-6.486452	-0.682873	1.880987
159	1	0	-5.420253	-0.414095	0.498270
160	1	0	-4.724914	-0.797280	2.087319

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l-l_R_endo

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.191584 hartree

Sum of electronic and thermal Free Energies = -3615.919252 hartree

The number of imaginary frequency = 1

Imaginary frequency = -396.154

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.632779	-1.627206	-4.047740
2	1	0	-3.478932	-0.665308	-3.568426
3	1	0	-4.154091	-1.587681	-4.999891
4	6	0	-3.723135	-2.778725	-3.286622
5	1	0	-4.133714	-3.665528	-3.767608
6	6	0	-3.163403	-2.971470	-2.007022
7	1	0	-3.159926	-3.968523	-1.586869
8	6	0	-2.525238	-1.962908	-1.319624
9	1	0	-2.582610	-0.930079	-1.653983
10	1	0	-1.314337	-1.250663	0.196201
11	7	0	-1.789485	-2.095027	-0.184897
12	6	0	-1.607356	-3.262722	0.531277
13	8	0	-0.646765	-3.056429	1.442024
14	8	0	-2.208302	-4.303822	0.388151
15	6	0	-0.547136	-4.037845	2.469402
16	1	0	-1.543257	-4.192735	2.902497
17	1	0	-0.219492	-4.987823	2.034229
18	6	0	0.427732	-3.544768	3.507147
19	6	0	0.768096	-2.194979	3.615409
20	6	0	0.985644	-4.468024	4.392914
21	6	0	1.649621	-1.782239	4.613201
22	1	0	0.369776	-1.475494	2.903693
23	6	0	1.868608	-4.052952	5.384978
24	1	0	0.729540	-5.521698	4.301914
25	6	0	2.201656	-2.705018	5.498088
26	1	0	1.907070	-0.730608	4.692770
27	1	0	2.298343	-4.781402	6.065934
28	1	0	2.890257	-2.376566	6.270532
29	1	0	0.720873	-0.885692	-1.701329
30	6	0	2.491260	-4.318652	1.026246
31	6	0	1.794411	-4.909403	-0.006099
32	6	0	1.198858	-4.113168	-1.005533
33	6	0	1.341313	-2.713384	-0.928241
34	6	0	2.084615	-2.111802	0.100695
35	6	0	2.638689	-2.917537	1.070603

36	1	0	0.299265	-5.712800	-2.167320
37	1	0	2.929963	-4.926900	1.810850
38	1	0	1.681221	-5.989093	-0.058670
39	6	0	0.413888	-4.635317	-2.083832
40	1	0	2.197722	-1.030433	0.119806
41	1	0	3.190096	-2.463608	1.888258
42	6	0	-0.103129	-2.389052	-2.830501
43	6	0	-0.200683	-3.813697	-2.974172
44	1	0	-0.819109	-4.215009	-3.767808
45	7	0	0.691724	-1.927603	-1.848641
46	6	0	-0.793842	-1.426620	-3.620030
47	1	0	-0.641172	-0.388096	-3.333854
48	6	0	-1.626930	-1.711489	-4.688034
49	1	0	-1.649088	-2.704241	-5.126293
50	1	0	-1.837071	-0.910856	-5.390505
51	6	0	-0.466758	5.539274	3.129896
52	6	0	-1.434191	4.529291	2.554520
53	6	0	-0.922924	3.983659	1.373783
54	6	0	0.814986	5.260711	2.322004
55	1	0	-0.823136	6.565242	2.973148
56	1	0	-0.325690	5.410269	4.207259
57	1	0	1.378938	4.445243	2.788654
58	1	0	1.476908	6.127772	2.235776
59	6	0	0.296886	4.771528	0.940430
60	6	0	-0.116373	6.000343	0.080223
61	6	0	1.416186	4.208022	0.085747
62	6	0	1.208281	6.516669	-0.506779
63	1	0	-0.663677	6.749356	0.660388
64	1	0	-0.768777	5.651568	-0.728340
65	6	0	2.009912	5.242861	-0.645235
66	1	0	1.078562	7.032181	-1.463093
67	1	0	1.699499	7.221981	0.175683
68	6	0	-2.667462	4.121633	3.041881
69	6	0	-3.364204	3.133454	2.352853
70	6	0	-2.828333	2.489355	1.230046
71	6	0	-1.584559	2.930570	0.755657
72	1	0	-3.084268	4.560052	3.944190
73	1	0	-4.339777	2.813296	2.707755
74	6	0	1.922042	2.917192	-0.013026
75	6	0	3.083980	2.661181	-0.756181
76	6	0	3.707809	3.739013	-1.394277
77	6	0	3.167711	5.021343	-1.374542
78	1	0	4.629836	3.548318	-1.934262
79	1	0	3.644972	5.828578	-1.922943
80	8	0	-1.017857	2.340224	-0.357580
81	8	0	-0.461844	0.097235	0.829167
82	8	0	0.485615	0.730727	-1.517501
83	15	0	0.057955	1.124514	-0.129453
84	8	0	1.285195	1.884518	0.652501
85	6	0	3.698296	1.303693	-0.881502
86	6	0	3.789248	0.692607	-2.149785
87	6	0	4.302992	0.690551	0.236155
88	6	0	4.520096	-0.490981	-2.273841
89	6	0	5.021971	-0.493710	0.057768
90	6	0	5.165996	-1.088019	-1.195535
91	1	0	4.617386	-0.950525	-3.255746
92	1	0	5.501173	-0.951689	0.922483
93	6	0	-3.595315	1.371969	0.600229
94	6	0	-3.958940	0.252120	1.378558
95	6	0	-4.055999	1.470742	-0.732860
96	6	0	-4.792215	-0.723061	0.822537
97	6	0	-4.890802	0.472052	-1.236301
98	6	0	-5.284763	-0.629464	-0.474485
99	1	0	-5.062041	-1.580569	1.433065
100	1	0	-5.267172	0.559913	-2.255972
101	6	0	-3.507310	0.047425	2.820788
102	1	0	-2.832951	0.861343	3.094563
103	6	0	-4.703818	0.068801	3.780931
104	1	0	-5.375559	-0.775283	3.588490
105	1	0	-4.360996	-0.007238	4.818087
106	1	0	-5.292017	0.986443	3.679849
107	6	0	-2.707480	-1.248169	2.982460
108	1	0	-2.427878	-1.395168	4.032233
109	1	0	-3.283539	-2.126413	2.661857
110	1	0	-1.792992	-1.187244	2.392416
111	6	0	-3.726946	2.649832	-1.637873
112	1	0	-3.104488	3.354254	-1.082862
113	6	0	-4.998045	3.400401	-2.054730
114	1	0	-5.661059	2.764080	-2.651120
115	1	0	-5.557624	3.740427	-1.178112
116	1	0	-4.741768	4.275744	-2.660920
117	6	0	-2.927551	2.199544	-2.866495
118	1	0	-2.617158	3.066199	-3.459893
119	1	0	-2.025379	1.655407	-2.566840
120	1	0	-3.540272	1.560902	-3.515534
121	6	0	-6.259203	-1.637305	-1.056626
122	1	0	-5.957250	-1.810131	-2.098431
123	6	0	-7.675463	-1.043419	-1.069987
124	1	0	-8.385519	-1.741368	-1.526569
125	1	0	-8.007194	-0.837723	-0.046308
126	1	0	-7.708377	-0.102761	-1.628043
127	6	0	-6.256924	-2.983878	-0.333119
128	1	0	-6.696800	-2.893195	0.666709
129	1	0	-6.858701	-3.710066	-0.888602
130	1	0	-5.243904	-3.384154	-0.223845
131	6	0	3.174212	1.296895	-3.406076
132	1	0	2.503578	2.104879	-3.101616
133	6	0	2.331920	0.281859	-4.183295
134	1	0	1.839844	0.773398	-5.029549
135	1	0	2.941521	-0.535147	-4.585019
136	1	0	1.561237	-0.140368	-3.541052
137	6	0	4.259053	1.867279	-4.331108
138	1	0	3.803886	2.325938	-5.215517
139	1	0	4.873539	2.622588	-3.834661
140	1	0	4.927967	1.068890	-4.672732
141	6	0	4.242336	1.301641	1.628309
142	1	0	3.675320	2.233808	1.572623
143	6	0	3.509955	0.382875	2.611382
144	1	0	3.409686	0.876738	3.584704
145	1	0	2.505624	0.138124	2.247605
146	1	0	4.065792	-0.549190	2.773213
147	6	0	5.644327	1.652422	2.140996
148	1	0	6.264193	0.755845	2.251189
149	1	0	6.154354	2.331147	1.450581

150	1	0	5.582839	2.138773	3.120313
151	6	0	6.017633	-2.327172	-1.402876
152	1	0	6.072857	-2.499248	-2.485726
153	6	0	5.386768	-3.567517	-0.765286
154	1	0	5.990913	-4.457639	-0.972717
155	1	0	5.319308	-3.450876	0.322358
156	1	0	4.373236	-3.736140	-1.142814
157	6	0	7.446832	-2.120596	-0.889746
158	1	0	8.066584	-2.994582	-1.115919
159	1	0	7.907738	-1.240420	-1.347179
160	1	0	7.456347	-1.978897	0.196489

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l-l_S_endo2

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3617.190555 hartree

Sum of electronic and thermal Free Energies = -3615.915464 hartree

The number of imaginary frequency = 1

Imaginary frequency = -346.07

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.248072	-2.058655	4.423409
2	1	0	0.006632	-1.044400	4.131476
3	1	0	0.184021	-2.387023	5.364048
4	6	0	-1.405584	-2.659472	3.973364
5	1	0	-1.737612	-3.560301	4.487016
6	6	0	-2.090332	-2.326595	2.780388
7	1	0	-2.875949	-2.978304	2.422998
8	6	0	-1.678154	-1.259301	2.020956
9	1	0	-0.954752	-0.546308	2.393657
10	1	0	-1.737292	-0.009550	0.430392
11	7	0	-2.101609	-0.899249	0.775484
12	6	0	-2.884152	-1.666223	-0.053804
13	8	0	-3.076513	-1.037583	-1.220149
14	8	0	-3.317914	-2.766678	0.221594
15	6	0	-3.954901	-1.704691	-2.145774
16	1	0	-3.644809	-1.330735	-3.123692
17	1	0	-3.770730	-2.780456	-2.093715
18	6	0	-5.396449	-1.366056	-1.864907
19	6	0	-5.990977	-0.267053	-2.489806
20	6	0	-6.144447	-2.122620	-0.958872
21	6	0	-7.306196	0.086919	-2.201554
22	1	0	-5.414656	0.318378	-3.203795
23	6	0	-7.461994	-1.772512	-0.673165
24	1	0	-5.679530	-2.972790	-0.469113
25	6	0	-8.042852	-0.665811	-1.289071
26	1	0	-7.755096	0.947127	-2.688336
27	1	0	-8.035081	-2.363669	0.034811
28	1	0	-9.068492	-0.391848	-1.061428
29	1	0	0.412277	-1.619421	-0.627924
30	6	0	-1.886348	-4.506334	-3.593075
31	6	0	-1.743012	-5.156101	-2.385935
32	6	0	-1.103302	-4.518366	-1.304405
33	6	0	-0.619148	-3.206640	-1.479546
34	6	0	-0.795776	-2.528884	-2.702080
35	6	0	-1.410310	-3.188278	-3.745281
36	1	0	-1.290196	-6.132789	0.136482
37	1	0	-2.371260	-5.004264	-4.426065
38	1	0	-2.116706	-6.167173	-2.250479
39	6	0	-0.914195	-5.125809	-0.022626
40	1	0	-0.442885	-1.504842	-2.791392
41	1	0	-1.537498	-2.678304	-4.695278
42	6	0	0.215388	-3.131463	0.778009
43	6	0	-0.289064	-4.461158	0.981719
44	1	0	-0.164297	-4.917381	1.956192
45	7	0	0.025592	-2.582879	-0.437733
46	6	0	0.920096	-2.376637	1.757391
47	1	0	1.264161	-1.390624	1.457176
48	6	0	1.200229	-2.822764	3.034350
49	1	0	1.067168	-3.862760	3.309722
50	1	0	1.978478	-2.306023	3.587751
51	6	0	4.168595	4.336505	-3.058371
52	6	0	4.388079	2.994949	-2.394712
53	6	0	3.506866	2.830824	-1.321273
54	6	0	2.834624	4.794801	-2.437878
55	1	0	4.980471	5.036668	-2.824798
56	1	0	4.122441	4.252697	-4.148442
57	1	0	1.995694	4.372593	-3.001834
58	1	0	2.715291	5.882206	-2.409829
59	6	0	2.842100	4.162828	-1.018967
60	6	0	3.747148	5.019706	-0.084610
61	6	0	1.511017	4.310884	-0.304498
62	6	0	2.843710	6.181096	0.361272
63	1	0	4.669222	5.341075	-0.577892
64	1	0	4.020252	4.410609	0.784446
65	6	0	1.486664	5.518515	0.400885
66	1	0	3.131873	6.598493	1.330681
67	1	0	2.864890	7.004255	-0.364419
68	6	0	5.291493	1.995602	-2.726389
69	6	0	5.267999	0.806363	-2.003997
70	6	0	4.311368	0.559997	-1.011018
71	6	0	3.425189	1.597451	-0.683953
72	1	0	6.000467	2.131537	-3.538274
73	1	0	5.975292	0.016104	-2.240289
74	6	0	0.403032	3.472151	-0.271423
75	6	0	-0.752955	3.840134	0.435194
76	6	0	-0.776071	5.101229	1.043149
77	6	0	0.334757	5.938596	1.048914
78	1	0	-1.682015	5.399322	1.563957
79	1	0	0.306092	6.888115	1.575931
80	8	0	2.479285	1.396412	0.299383
81	8	0	0.991286	-0.161423	-1.158536
82	8	0	0.214655	0.768985	1.140459
83	15	0	0.963315	0.945953	-0.138581
84	8	0	0.452378	2.272477	-0.954521
85	6	0	-1.928548	2.935729	0.619550
86	6	0	-2.302258	2.548309	1.930337
87	6	0	-2.711856	2.528953	-0.475862
88	6	0	-3.469571	1.806861	2.108607
89	6	0	-3.871078	1.782736	-0.240500
90	6	0	-4.278191	1.421915	1.038711

91	1	0	-3.758591	1.523943	3.119537
92	1	0	-4.485238	1.476584	-1.084570
93	6	0	4.248312	-0.792751	-0.376834
94	6	0	4.094270	-1.930124	-1.198937
95	6	0	4.429541	-0.963183	1.014435
96	6	0	4.175139	-3.199671	-0.622755
97	6	0	4.494033	-2.255437	1.539517
98	6	0	4.399939	-3.390240	0.735190
99	1	0	4.081413	-4.075180	-1.263156
100	1	0	4.660488	-2.375815	2.609605
101	6	0	3.842949	-1.860183	-2.700460
102	1	0	3.769701	-0.811777	-2.994976
103	6	0	2.498392	-2.500139	-3.050684
104	1	0	2.305583	-2.430594	-4.127307
105	1	0	2.457218	-3.558895	-2.768769
106	1	0	1.711829	-1.962734	-2.522205
107	6	0	4.984201	-2.504081	-3.496709
108	1	0	4.807779	-2.393368	-4.571857
109	1	0	5.951875	-2.050364	-3.259807
110	1	0	5.060785	-3.575451	-3.280357
111	6	0	4.634966	0.202512	1.972395
112	1	0	4.591346	1.133714	1.404643
113	6	0	6.021002	0.137270	2.627307
114	1	0	6.180085	1.009811	3.269823
115	1	0	6.128386	-0.758727	3.248668
116	1	0	6.811448	0.117626	1.870852
117	6	0	3.530415	0.257741	3.034641
118	1	0	3.660639	1.138211	3.673132
119	1	0	2.539924	0.319711	2.571600
120	1	0	3.573003	-0.626019	3.684112
121	6	0	4.586576	-4.787779	1.296390
122	1	0	4.551293	-5.482938	0.447582
123	6	0	3.465746	-5.177000	2.262852
124	1	0	3.600883	-6.203245	2.621555
125	1	0	3.461716	-4.512437	3.134618
126	1	0	2.488664	-5.102393	1.774145
127	6	0	5.955983	-4.938169	1.968623
128	1	0	6.035904	-4.280468	2.841113
129	1	0	6.109014	-5.967415	2.310078
130	1	0	6.762969	-4.677530	1.278091
131	6	0	-1.503822	2.924089	3.175515
132	1	0	-0.610535	3.469827	2.865363
133	6	0	-1.012049	1.694043	3.949507
134	1	0	-0.539241	2.006271	4.887589
135	1	0	-1.833190	1.010983	4.200820
136	1	0	-0.271588	1.162548	3.346574
137	6	0	-2.326944	3.840081	4.091732
138	1	0	-1.723510	4.173096	4.942764
139	1	0	-2.688124	4.725554	3.559163
140	1	0	-3.202777	3.314197	4.488149
141	6	0	-2.384192	2.908375	-1.912304
142	1	0	-1.471964	3.509512	-1.915026
143	6	0	-2.123469	1.664645	-2.769576
144	1	0	-1.833554	1.958050	-3.784576
145	1	0	-1.321981	1.053564	-2.343045
146	1	0	-3.027803	1.047698	-2.838776
147	6	0	-3.500364	3.765500	-2.522671
148	1	0	-4.440907	3.205848	-2.584555
149	1	0	-3.682262	4.661528	-1.921436
150	1	0	-3.230083	4.079161	-3.536684
151	6	0	-5.585270	0.681934	1.247904
152	1	0	-5.931483	0.351981	0.261585
153	6	0	-5.442922	-0.558625	2.133946
154	1	0	-5.079215	-0.297990	3.134389
155	1	0	-6.415998	-1.049137	2.250076
156	1	0	-4.752079	-1.289658	1.703715
157	6	0	-6.647528	1.630071	1.818329
158	1	0	-7.613461	1.119567	1.902405
159	1	0	-6.358139	1.980466	2.815944
160	1	0	-6.773897	2.507513	1.177025

TS_R(Br)

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -6188.378498 hartree

Sum of electronic and thermal Free Energies = -6187.117688 hartree

The number of imaginary frequency = 1

Imaginary frequency = -353.25

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.697231	-2.954938	-2.596543
2	1	0	-4.645887	-1.899921	-2.344266

3	1	0	-5.412831	-3.210251	-3.372733
4	6	0	-4.333866	-3.912651	-1.672248
5	1	0	-4.634935	-4.941098	-1.865282
6	6	0	-3.438970	-3.714367	-0.597807
7	1	0	-3.084026	-4.575987	-0.048267
8	6	0	-2.916149	-2.474736	-0.302985
9	1	0	-3.327457	-1.572922	-0.747686
10	1	0	-1.626126	-1.213209	0.718636
11	7	0	-1.920859	-2.198996	0.581149
12	6	0	-1.112902	-3.136389	1.193436
13	8	0	-0.171954	-2.483288	1.881973
14	8	0	-1.207718	-4.341206	1.123500
15	6	0	0.738737	-3.270962	2.634561
16	1	0	0.194976	-3.773463	3.443774
17	1	0	1.173291	-4.043368	1.990087
18	6	0	1.797234	-2.342091	3.169758
19	6	0	1.703383	-0.959947	2.998721
20	6	0	2.906499	-2.882375	3.822012
21	6	0	2.711135	-0.129132	3.482163
22	1	0	0.863064	-0.525751	2.461730
23	6	0	3.925647	-2.061705	4.292734
24	1	0	2.987453	-3.959667	3.950439
25	6	0	3.816588	-0.686871	4.111892
26	1	0	2.645740	0.945034	3.345453
27	1	0	4.796413	-2.478019	4.786907
28	1	0	0.009988	-1.338578	-1.581769
29	6	0	3.284600	-4.229216	0.283502
30	6	0	2.358774	-5.001991	-0.387474
31	6	0	1.269406	-4.394298	-1.044458
32	6	0	1.152272	-2.988621	-1.001198
33	6	0	2.096935	-2.200255	-0.321287
34	6	0	3.149238	-2.825968	0.312922
35	1	0	0.337968	-6.200173	-1.809332
36	1	0	4.121968	-4.698086	0.790475
37	1	0	2.453941	-6.083706	-0.420394
38	6	0	0.267881	-5.116685	-1.767969
39	1	0	1.993319	-1.116476	-0.316516
40	1	0	3.878922	-2.221684	0.845431
41	6	0	-0.865527	-3.045199	-2.316035
42	6	0	-0.757097	-4.473765	-2.385246
43	1	0	-1.520770	-5.026210	-2.918848
44	7	0	0.087138	-2.389473	-1.628629
45	6	0	-1.886027	-2.263485	-2.936429
46	1	0	-1.817509	-1.189646	-2.778398
47	6	0	-2.885691	-2.767540	-3.743396
48	1	0	-2.857557	-3.792627	-4.097732
49	1	0	-3.405723	-2.077315	-4.400061
50	6	0	-0.814705	6.017134	1.845392
51	6	0	-1.766090	4.846988	1.728866
52	6	0	-1.456205	4.079833	0.603086
53	6	0	0.290069	5.643270	0.838077
54	1	0	-1.306444	6.958229	1.568575
55	1	0	-0.434965	6.141825	2.863916
56	1	0	1.029440	4.993975	1.319953
57	1	0	0.815520	6.508553	0.422636
58	6	0	-0.450733	4.820589	-0.252999
59	6	0	-1.180663	5.791822	-1.225066
60	6	0	0.512715	4.145933	-1.213326
61	6	0	-0.087893	6.239543	-2.208226
62	1	0	-1.667921	6.617912	-0.698548
63	1	0	-1.951826	5.227299	-1.761463
64	6	0	0.797212	5.016994	-2.270085
65	1	0	-0.483604	6.517116	-3.189785
66	1	0	0.463373	7.107763	-1.825018
67	6	0	-2.818950	4.484525	2.556365
68	6	0	-3.528894	3.323446	2.264409
69	6	0	-3.169540	2.474601	1.209163
70	6	0	-2.111771	2.876787	0.381689
71	1	0	-3.085520	5.088450	3.419082
72	1	0	-4.365960	3.031289	2.891986
73	6	0	1.134102	2.900266	-1.157038
74	6	0	2.116227	2.555394	-2.097693
75	6	0	2.431854	3.487911	-3.094671
76	6	0	1.767327	4.702911	-3.209448
77	1	0	3.215263	3.230194	-3.801000
78	1	0	2.001465	5.386366	-4.020683
79	8	0	-1.713672	2.083695	-0.678148
80	8	0	-0.716707	0.288915	0.891375
81	8	0	-0.333954	0.267279	-1.687335
82	15	0	-0.495461	1.021833	-0.395155
83	8	0	0.787665	2.015684	-0.148206
84	6	0	2.856706	1.254745	-2.100319
85	6	0	2.668235	0.347841	-3.161171
86	6	0	3.840737	0.998508	-1.117123
87	6	0	3.453461	-0.809345	-3.210171
88	6	0	4.608560	-0.159217	-1.224628
89	6	0	4.426864	-1.080574	-2.257351
90	1	0	3.297940	-1.509027	-4.027045
91	1	0	5.373255	-0.366208	-0.479185
92	6	0	-3.915674	1.191774	1.026557
93	6	0	-3.967108	0.260075	2.086656
94	6	0	-4.666929	0.950356	-0.146774
95	6	0	-4.790637	-0.864549	1.967091
96	6	0	-5.483156	-0.180065	-0.206799
97	6	0	-5.573231	-1.097709	0.841136
98	1	0	-4.818515	-1.572579	2.791008
99	1	0	-6.087507	-0.349342	-1.098393
100	6	0	-3.191061	0.428437	3.389221
101	1	0	-2.564682	1.318944	3.306901
102	6	0	-4.150574	0.618038	4.572329
103	1	0	-4.745501	-0.286728	4.741084
104	1	0	-3.588304	0.823423	5.489146
105	1	0	-4.849313	1.443811	4.405596
106	6	0	-2.242903	-0.744958	3.655546
107	1	0	-1.761392	-0.620688	4.632202
108	1	0	-2.771500	-1.706171	3.664600
109	1	0	-1.462690	-0.777183	2.895063
110	6	0	-4.661292	1.888510	-1.345371
111	1	0	-4.028277	2.747826	-1.114642
112	6	0	-6.065965	2.427311	-1.643338
113	1	0	-6.751661	1.623964	-1.933931
114	1	0	-6.487837	2.928990	-0.767309
115	1	0	-6.029141	3.146811	-2.467981
116	6	0	-4.064326	1.195385	-2.576770

117	1	0	-4.007878	1.892255	-3.419864
118	1	0	-3.051683	0.837117	-2.365295
119	1	0	-4.691652	0.350061	-2.889421
120	6	0	-6.537344	-2.265671	0.730327
121	1	0	-6.454215	-2.654518	-0.293867
122	6	0	-7.977130	-1.770981	0.932458
123	1	0	-8.691511	-2.592173	0.810443
124	1	0	-8.095462	-1.360394	1.941283
125	1	0	-8.232192	-0.982397	0.218134
126	6	0	-6.232279	-3.412773	1.692234
127	1	0	-6.421409	-3.118684	2.730860
128	1	0	-6.878213	-4.268503	1.472394
129	1	0	-5.190354	-3.737625	1.610928
130	6	0	1.694615	0.604669	-4.305388
131	1	0	1.046706	1.438701	-4.022780
132	6	0	0.782951	-0.590306	-4.592477
133	1	0	0.084353	-0.340700	-5.398579
134	1	0	1.346560	-1.475418	-4.908539
135	1	0	0.202389	-0.837186	-3.706366
136	6	0	2.460571	0.978359	-5.583349
137	1	0	1.761772	1.210338	-6.394205
138	1	0	3.113361	1.842971	-5.437678
139	1	0	3.089300	0.141463	-5.909083
140	6	0	4.117307	1.997796	-0.000322
141	1	0	3.151155	2.377305	0.350610
142	6	0	4.833945	1.384267	1.204382
143	1	0	4.823839	2.083708	2.046147
144	1	0	4.356915	0.455838	1.533056
145	1	0	5.884663	1.166213	0.980982
146	6	0	4.942021	3.181932	-0.528162
147	1	0	5.905647	2.823865	-0.908198
148	1	0	4.429453	3.709761	-1.336082
149	1	0	5.139102	3.897056	0.277798
150	6	0	5.301831	-2.318746	-2.318427
151	1	0	5.524368	-2.604402	-1.280498
152	6	0	6.632139	-1.995303	-3.012053
153	1	0	7.289046	-2.871734	-3.027528
154	1	0	6.450196	-1.684517	-4.046823
155	1	0	7.154660	-1.179418	-2.503855
156	6	0	4.618878	-3.509778	-2.991827
157	1	0	5.211517	-4.418781	-2.847045
158	1	0	3.618753	-3.679801	-2.579645
159	1	0	4.521301	-3.351608	-4.071670
160	35	0	5.218327	0.443312	4.699741

TSs(Br)

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -6188.377458 hartree

Sum of electronic and thermal Free Energies = -6187.114515 hartree

The number of imaginary frequency = 1

Imaginary frequency = -344.29

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.473628	-2.222668	4.364956
2	1	0	0.757919	-1.214297	4.078649
3	1	0	0.947297	-2.593341	5.269104
4	6	0	-0.735896	-2.758855	3.974959
5	1	0	-1.075829	-3.657737	4.486706
6	6	0	-1.478926	-2.364988	2.836597
7	1	0	-2.310982	-2.976342	2.514629
8	6	0	-1.076647	-1.293801	2.076482
9	1	0	-0.309104	-0.611805	2.419591
10	1	0	-1.169522	-0.020013	0.508327
11	7	0	-1.561812	-0.893719	0.865309
12	6	0	-2.408010	-1.626370	0.067460
13	8	0	-2.595626	-1.005386	-1.106545
14	8	0	-2.892505	-2.698510	0.366055
15	6	0	-3.500586	-1.664446	-2.013044
16	1	0	-3.218652	-1.280170	-2.994974
17	1	0	-3.317560	-2.741210	-1.977330
18	6	0	-4.927992	-1.319542	-1.677648
19	6	0	-5.503337	-0.158088	-2.197664
20	6	0	-5.661424	-2.096710	-0.777779
21	6	0	-6.767800	0.258007	-1.793266
22	1	0	-4.945760	0.445896	-2.910571
23	6	0	-6.931302	-1.698927	-0.369788
24	1	0	-5.215791	-2.995638	-0.364837
25	6	0	-7.462314	-0.514679	-0.868784
26	1	0	-7.206640	1.172421	-2.176523
27	1	0	-7.498020	-2.288208	0.342706
28	1	0	0.908732	-1.604044	-0.696977
29	6	0	-1.557479	-4.268836	-3.729150
30	6	0	-1.441739	-4.964624	-2.544608
31	6	0	-0.762728	-4.396667	-1.447663
32	6	0	-0.213479	-3.106452	-1.584399
33	6	0	-0.355555	-2.382644	-2.784984
34	6	0	-1.010767	-2.974426	-3.843824
35	1	0	-1.012596	-6.049586	-0.059506
36	1	0	-2.071741	-4.713942	-4.574369
37	1	0	-1.864361	-5.960026	-2.440309
38	6	0	-0.583598	-5.060092	-0.191444
39	1	0	0.060701	-1.380369	-2.845823
40	1	0	-1.111821	-2.430347	-4.777872
41	6	0	0.675833	-3.163300	0.652514
42	6	0	0.101104	-4.469976	0.820350
43	1	0	0.222951	-4.969066	1.774042
44	7	0	0.475379	-2.553411	-0.531025
45	6	0	1.461871	-2.492086	1.630334
46	1	0	1.845776	-1.511310	1.358089
47	6	0	1.793800	-3.017325	2.863967
48	1	0	1.624913	-4.064025	3.096854
49	1	0	2.628141	-2.564813	3.391330
50	6	0	4.735524	4.153419	-3.224596
51	6	0	4.947420	2.834692	-2.512961
52	6	0	4.083306	2.730233	-1.418612
53	6	0	3.426807	4.666162	-2.589324
54	1	0	5.567128	4.845449	-3.042072
55	1	0	4.657673	4.026679	-4.308705
56	1	0	2.564567	4.244981	-3.117697
57	1	0	3.334913	5.756623	-2.598248

58	6	0	3.455246	4.086006	-1.149311
59	6	0	4.408891	4.949976	-0.270301
60	6	0	2.151938	4.282333	-0.395022
61	6	0	3.544560	6.139267	0.177577
62	1	0	5.318511	5.240077	-0.804391
63	1	0	4.701888	4.358598	0.604586
64	6	0	2.180069	5.501542	0.290299
65	1	0	3.879212	6.579514	1.121561
66	1	0	3.548873	6.940168	-0.573006
67	6	0	5.827881	1.805944	-2.816803
68	6	0	5.802912	0.649528	-2.040595
69	6	0	4.859835	0.463039	-1.022880
70	6	0	3.989977	1.525129	-0.734038
71	1	0	6.523717	1.894597	-3.646395
72	1	0	6.498003	-0.158642	-2.252355
73	6	0	1.028252	3.469038	-0.302588
74	6	0	-0.087595	3.870231	0.449010
75	6	0	-0.057099	5.136462	1.045439
76	6	0	1.068343	5.951836	0.986610
77	1	0	-0.932101	5.458470	1.603555
78	1	0	1.083134	6.908532	1.501025
79	8	0	3.044489	1.370785	0.258150
80	8	0	1.546259	-0.171587	-1.207127
81	8	0	0.781972	0.728656	1.104567
82	15	0	1.526489	0.924719	-0.174543
83	8	0	1.019166	2.261900	-0.974626
84	6	0	-1.275126	2.993464	0.679908
85	6	0	-1.604527	2.601841	1.999014
86	6	0	-2.103321	2.603235	-0.389471
87	6	0	-2.770828	1.865687	2.218036
88	6	0	-3.255051	1.864741	-0.114757
89	6	0	-3.615300	1.489307	1.175880
90	1	0	-3.015421	1.567401	3.235301
91	1	0	-3.899525	1.562486	-0.937542
92	6	0	4.774758	-0.841196	-0.298000
93	6	0	4.556684	-2.033629	-1.022268
94	6	0	4.952172	-0.904887	1.102809
95	6	0	4.520216	-3.252272	-0.338255
96	6	0	4.928368	-2.149418	1.730796
97	6	0	4.707071	-3.335661	1.036695
98	1	0	4.341690	-4.160713	-0.908793
99	1	0	5.085120	-2.199379	2.808433
100	6	0	4.358812	-2.076656	-2.532949
101	1	0	4.356294	-1.054481	-2.915130
102	6	0	2.999065	-2.672966	-2.901890
103	1	0	2.879483	-2.711427	-3.990501
104	1	0	2.870782	-3.690608	-2.513979
105	1	0	2.216427	-2.035998	-2.490773
106	6	0	5.500879	-2.840014	-3.215159
107	1	0	5.383164	-2.811882	-4.303588
108	1	0	6.478013	-2.414867	-2.963706
109	1	0	5.510472	-3.891519	-2.906777
110	6	0	5.200476	0.315295	1.978428
111	1	0	5.188767	1.208649	1.351053
112	6	0	6.582818	0.245349	2.640215
113	1	0	6.767832	1.148493	3.231374
114	1	0	6.660105	-0.615541	3.313430
115	1	0	7.373986	0.156949	1.889401
116	6	0	4.094535	0.470660	3.031250
117	1	0	4.235030	1.397694	3.597541
118	1	0	3.106925	0.504680	2.560466
119	1	0	4.120226	-0.358869	3.749529
120	6	0	4.715531	-4.658053	1.779737
121	1	0	4.388664	-4.450018	2.808640
122	6	0	6.142535	-5.218739	1.847582
123	1	0	6.170641	-6.154436	2.416473
124	1	0	6.514741	-5.420005	0.836951
125	1	0	6.823593	-4.504391	2.319410
126	6	0	3.760151	-5.694235	1.185115
127	1	0	4.119361	-6.054828	0.215232
128	1	0	3.681406	-6.563629	1.845975
129	1	0	2.759752	-5.274237	1.035734
130	6	0	-0.749476	2.952004	3.213092
131	1	0	0.145345	3.475350	2.869265
132	6	0	-0.262492	1.705940	3.964884
133	1	0	0.276646	2.003604	4.871344
134	1	0	-1.094559	1.059217	4.269691
135	1	0	0.417966	1.139708	3.324283
136	6	0	-1.512621	3.886050	4.162173
137	1	0	-0.871895	4.193465	4.995400
138	1	0	-1.862822	4.786466	3.647620
139	1	0	-2.391238	3.383955	4.582566
140	6	0	-1.822836	2.976300	-1.837475
141	1	0	-0.901387	3.561959	-1.876308
142	6	0	-1.615026	1.726225	-2.700728
143	1	0	-1.356367	2.011641	-3.726393
144	1	0	-0.809820	1.102500	-2.300769
145	1	0	-2.531206	1.123742	-2.736579
146	6	0	-2.946968	3.850752	-2.407064
147	1	0	-3.899311	3.307983	-2.427567
148	1	0	-3.088889	4.752167	-1.803274
149	1	0	-2.712925	4.155353	-3.432761
150	6	0	-4.900075	0.711257	1.385157
151	1	0	-5.078170	0.157376	0.457552
152	6	0	-4.829859	-0.310148	2.519957
153	1	0	-4.733071	0.176143	3.496993
154	1	0	-5.749269	-0.905427	2.539563
155	1	0	-3.983729	-0.994178	2.394275
156	6	0	-6.086211	1.664969	1.577489
157	1	0	-7.029239	1.109038	1.627229
158	1	0	-5.970693	2.240736	2.503084
159	1	0	-6.154202	2.373106	0.744862
160	35	0	-9.151380	0.072471	-0.254078

$TS_R(NO_2)$

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3821.623046 hartree

Sum of electronic and thermal Free Energies = -3820.350334 hartree

The number of imaginary frequency = 1

Imaginary frequency = -350.22

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.325183	-3.083021	-2.818907
2	1	0	-4.315119	-2.021405	-2.589700
3	1	0	-4.968084	-3.371373	-3.645454
4	6	0	-4.021018	-4.011080	-1.844710
5	1	0	-4.285673	-5.049860	-2.035548
6	6	0	-3.221410	-3.767812	-0.705666
7	1	0	-2.897251	-4.607590	-0.105374
8	6	0	-2.747293	-2.510771	-0.404943
9	1	0	-3.137608	-1.629849	-0.906433
10	1	0	-1.567758	-1.195395	0.683734
11	7	0	-1.830944	-2.190785	0.547723
12	6	0	-1.053901	-3.091919	1.244899
13	8	0	-0.177281	-2.396816	1.979674
14	8	0	-1.117809	-4.300065	1.209433
15	6	0	0.676787	-3.137240	2.833958
16	1	0	0.074596	-3.655032	3.590549
17	1	0	1.214003	-3.896621	2.254619
18	6	0	1.626908	-2.159283	3.474882
19	6	0	1.517267	-0.784809	3.244805
20	6	0	2.632658	-2.651534	4.312580
21	6	0	2.400714	0.091811	3.867198
22	1	0	0.756013	-0.397540	2.571023
23	6	0	3.526808	-1.787454	4.927911
24	1	0	2.718303	-3.722110	4.482049
25	6	0	3.389735	-0.424342	4.692205
26	1	0	2.337408	1.161341	3.705146
27	1	0	4.317077	-2.143144	5.577268
28	1	0	0.271481	-1.374878	-1.459565
29	6	0	3.407507	-4.201668	0.720817
30	6	0	2.539211	-4.995094	-0.000953
31	6	0	1.501586	-4.409353	-0.754321
32	6	0	1.373200	-3.004108	-0.752216
33	6	0	2.256790	-2.194648	-0.016773
34	6	0	3.261741	-2.799204	0.708850
35	1	0	0.645902	-6.239031	-1.551088
36	1	0	4.207713	-4.653783	1.298044
37	1	0	2.642679	-6.076501	-0.002909
38	6	0	0.566248	-5.155500	-1.539922
39	1	0	2.147251	-1.111763	-0.045617
40	1	0	3.948689	-2.178406	1.277541
41	6	0	-0.530364	-3.104708	-2.224630
42	6	0	-0.408346	-4.533774	-2.252575
43	1	0	-1.123268	-5.103487	-2.833401
44	7	0	0.359289	-2.426256	-1.477226
45	6	0	-1.503996	-2.347111	-2.942492
46	1	0	-1.461522	-1.269771	-2.800528
47	6	0	-2.426703	-2.880345	-3.819100
48	1	0	-2.355225	-3.910529	-4.151639
49	1	0	-2.902588	-2.209320	-4.527107
50	6	0	-0.875166	6.027958	1.771304
51	6	0	-1.814778	4.858464	1.578930
52	6	0	-1.403183	4.078592	0.495050
53	6	0	0.317370	5.641987	0.874172
54	1	0	-1.336441	6.967319	1.441397
55	1	0	-0.590588	6.161524	2.819248
56	1	0	1.007320	4.996653	1.429031
57	1	0	0.881268	6.502127	0.500719
58	6	0	-0.321871	4.810116	-0.272424
59	6	0	-0.958894	5.773213	-1.315609
60	6	0	0.723068	4.125176	-1.135570
61	6	0	0.219159	6.210237	-2.199884
62	1	0	-1.489689	6.604918	-0.842879
63	1	0	-1.679859	5.204975	-1.914249
64	6	0	1.102969	4.985476	-2.170995
65	1	0	-0.085470	6.479892	-3.215531
66	1	0	0.735888	7.080599	-1.775735
67	6	0	-2.940205	4.505336	2.309375
68	6	0	-3.619593	3.339387	1.968219
69	6	0	-3.163146	2.476899	0.962833
70	6	0	-2.035879	2.872330	0.229409
71	1	0	-3.285433	5.119536	3.136179
72	1	0	-4.510390	3.053924	2.520200
73	6	0	1.334711	2.879668	-1.013044
74	6	0	2.392649	2.522038	-1.861946
75	6	0	2.799318	3.444834	-2.834712
76	6	0	2.152051	4.660914	-3.017293
77	1	0	3.640204	3.177870	-3.467787
78	1	0	2.459927	5.337071	-3.809774
79	8	0	-1.541516	2.064349	-0.778320
80	8	0	-0.690116	0.309224	0.915100
81	8	0	-0.081651	0.223360	-1.617972
82	15	0	-0.355635	1.010912	-0.365023
83	8	0	0.902426	2.007323	-0.026564
84	6	0	3.123033	1.217544	-1.793212
85	6	0	3.022778	0.305302	-2.861763
86	6	0	4.019057	0.964165	-0.729353
87	6	0	3.812165	-0.849898	-2.842369
88	6	0	4.801885	-0.187705	-0.773797
89	6	0	4.709617	-1.112178	-1.814998
90	1	0	3.724185	-1.553765	-3.665840
91	1	0	5.505052	-0.389310	0.031296
92	6	0	-3.883343	1.185955	0.737131
93	6	0	-4.027921	0.274267	1.806511
94	6	0	-4.522715	0.916585	-0.494818
95	6	0	-4.834258	-0.856135	1.635331
96	6	0	-5.326632	-0.218759	-0.606053
97	6	0	-5.510960	-1.115016	0.448005
98	1	0	-4.935998	-1.547140	2.467784
99	1	0	-5.846337	-0.408193	-1.545656
100	6	0	-3.375564	0.472135	3.171594
101	1	0	-2.742042	1.360313	3.127775
102	6	0	-4.440501	0.687605	4.256172
103	1	0	-5.049093	-0.213990	4.389400
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157	1	0	5.545520	-4.454041	-2.303027
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$TS_S(NO_2)$

M06-2X/6-31g(d) in gas phase

SCF Done: E(RM062X) = -3821.619857 hartree

Sum of electronic and thermal Free Energies = -3820.345497 hartree

The number of imaginary frequency = 1

Imaginary frequency = -348.09

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116	6	0	3.915523	0.489701	3.024697
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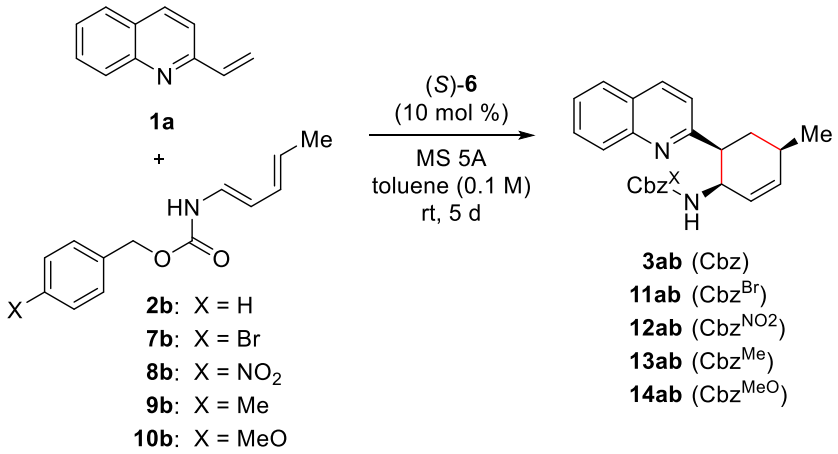
122	6	0	5.998059	-5.180125	1.832335
123	1	0	6.034492	-6.116137	2.400193
124	1	0	6.373471	-5.376613	0.821962
125	1	0	6.671539	-4.459767	2.305860
126	6	0	3.621499	-5.678201	1.166171
127	1	0	3.985598	-6.034083	0.196376
128	1	0	3.550529	-6.549120	1.825883
129	1	0	2.617109	-5.268158	1.015834
130	6	0	-0.933896	2.921311	3.231030
131	1	0	-0.039146	3.438785	2.878134
132	6	0	-0.448012	1.675004	3.983015
133	1	0	0.090748	1.972477	4.889677
134	1	0	-1.280782	1.028926	4.287415
135	1	0	0.233117	1.108784	3.343279
136	6	0	-1.684693	3.861411	4.184210
137	1	0	-1.034197	4.170079	5.009263
138	1	0	-2.038082	4.760902	3.670488
139	1	0	-2.560031	3.363470	4.616313
140	6	0	-2.052859	2.968521	-1.806699
141	1	0	-1.130924	3.553156	-1.846640
142	6	0	-1.852430	1.728262	-2.684762
143	1	0	-1.601449	2.024826	-3.709104
144	1	0	-1.045752	1.098521	-2.297259
145	1	0	-2.770774	1.129050	-2.720056
146	6	0	-3.179566	3.850627	-2.359097
147	1	0	-4.132851	3.309635	-2.381030
148	1	0	-3.316892	4.744955	-1.743913
149	1	0	-2.950822	4.167294	-3.382278
150	6	0	-5.139832	0.760814	1.474295
151	1	0	-5.515697	0.432857	0.498046
152	6	0	-4.981053	-0.480644	2.356352
153	1	0	-4.582679	-0.221603	3.343561
154	1	0	-5.954741	-0.960262	2.508165
155	1	0	-4.310278	-1.218789	1.906382
156	6	0	-6.181026	1.715310	2.072256
157	1	0	-7.146693	1.209659	2.187573
158	1	0	-5.860296	2.066330	3.059793
159	1	0	-6.322150	2.591998	1.433152
160	8	0	-9.528933	-0.730609	0.331327
161	8	0	-9.503788	0.817735	-1.173498
162	7	0	-8.999789	-0.113519	-0.574501

---

5. Hammett plot

Table S6. Summary of substituent effect



X	product	σ_m	$\Delta\Delta G^{\ddagger}_{(exp.)}$
H (**2b**)	**3ab** (Cbz)	0.115	1.80 [91% ee]
Br (**7b**)	**11ab** (Cbz^{Br})	-0.070	2.15 [95% ee]
NO_2 (**8b**)	**12ab** (Cbz^{NO2})	0.000	2.70 [98% ee]
Me (**9b**)	**13ab** (Cbz^{Me})	0.393	1.73 [90% ee]
MeO (**10b**)	**14ab** (Cbz^{MeO})	0.710	1.73 [90% ee]

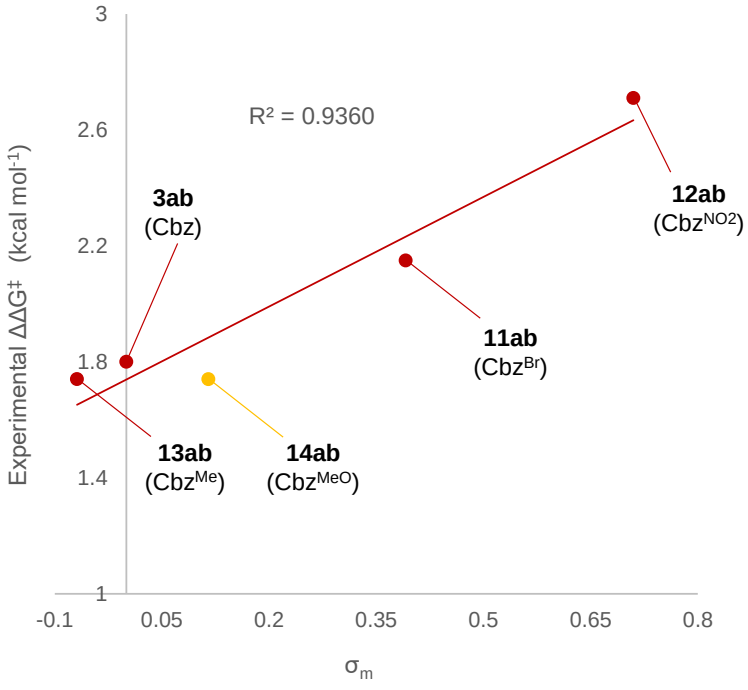
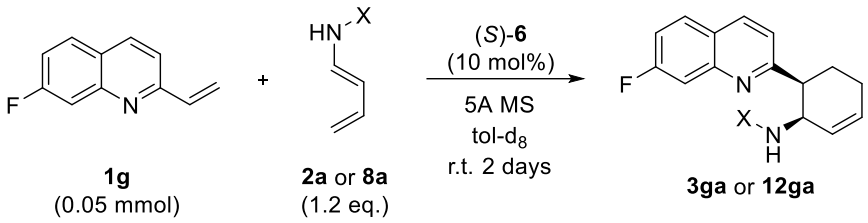


Figure S5. Hammett plot of $\Delta\Delta G^{\ddagger}$ vs. σ_m constants.

6. NMR experiment

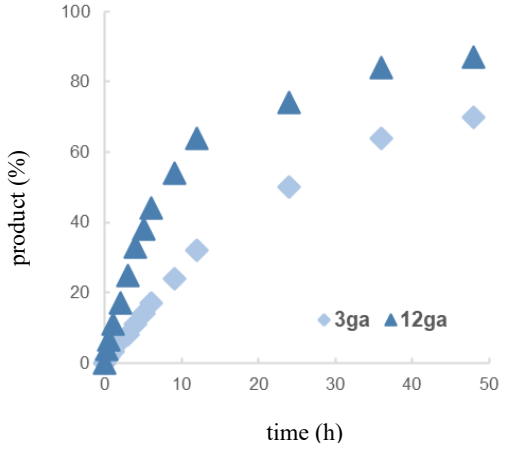


1g (0.05 mmol) + **2a** or **8a** (1.2 eq.) → **3ga** or **12ga**

To a dried NMR tube was added **1g** (0.05 mmol), **2a** or **8a** (0.06 mmol), activated MS 5A (10 mg), CH_2Br_2 (0.05 mmol as an internal standard), $C_6H_5CF_3$ (0.05 mmol as an internal standard) and toluene-d_8 (0.6 mL). The atmosphere was replaced with nitrogen and catalyst (*S*)-**6** (0.005 mmol) was added. The reaction mixture was monitored for 48 h by ^{1}H NMR and ^{19}F NMR.

Table S7 and **Figure S6.** Summary of NMR experiments.

Cbz	2a		Cbz^{NO2}	8a
time (h)	3ga (%)		time (h)	12ga (%)
0	0		0	0
0.25	1.2		0.25	4.0
0.5	1.7		0.5	6.7
1	3.2		1	11
2	6.3		2	17
3	8.1		3	25
4	11		4	33
5	14		5	38
6	17		6	44
9	24		9	54
12	32		12	64
24	50		24	74
36	64		36	84
48	70		48	87



7. Determination of relative and absolute configurations

7-1. Relative configurations

The NOESY experiment determined the relative configuration of **3ab**. Each substituent (quinoline, amide and methyl group) on a cyclohexene ring was in the same direction.

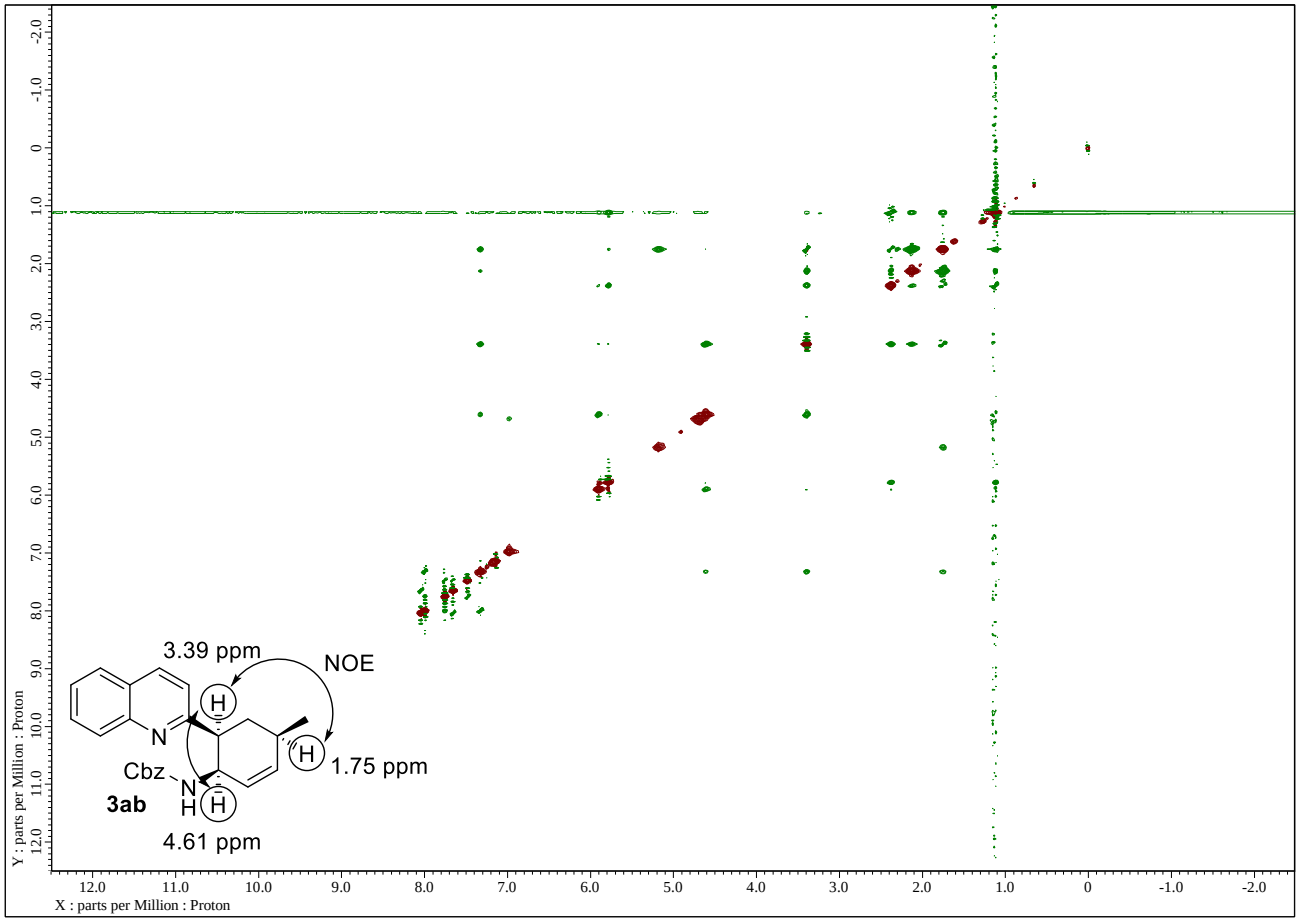
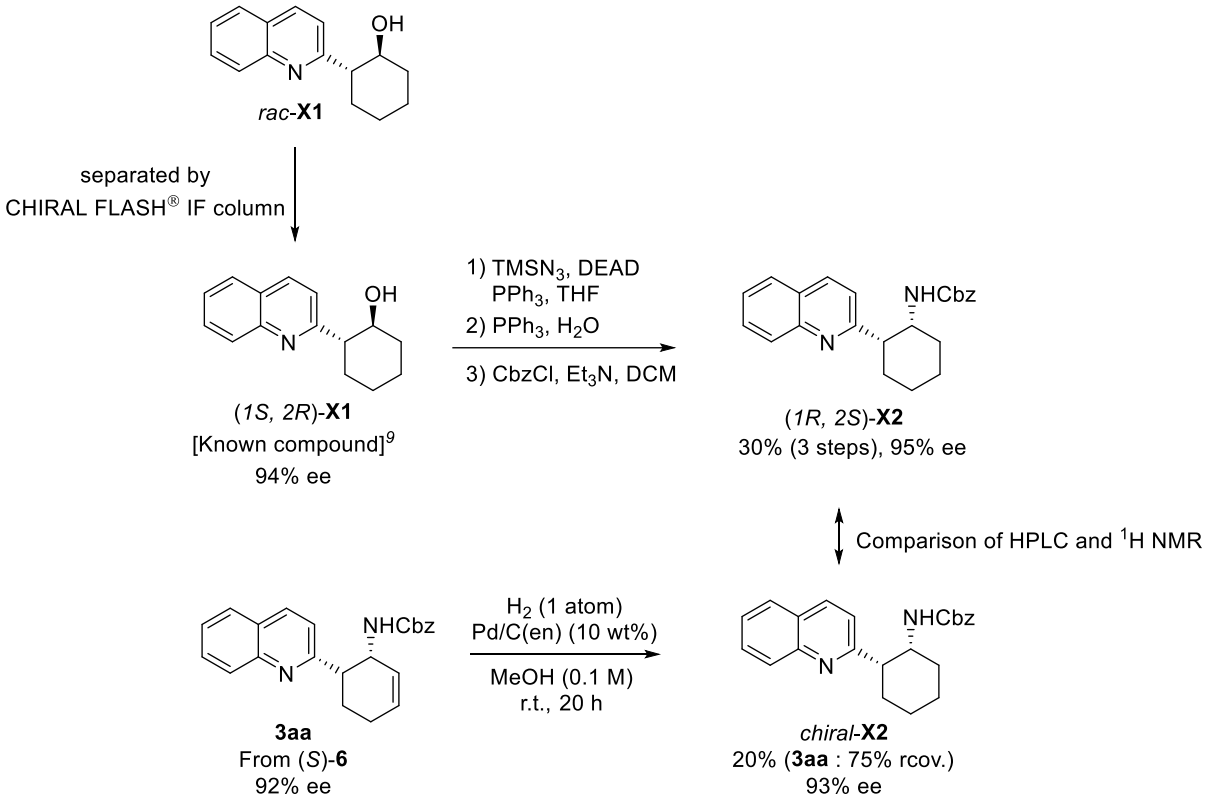


Figure S7. NOESY spectra of **3ab**.

7-2. Absolute configurations

The structure of **3aa** was determined by HPLC and ^{1}H NMR comparison of the chiral compound **X2** obtained from the derivatization of the known alcohol **X1**[9].



Scheme S1. Method for determination of absolute configuration of **3aa**.

[Synthesis of (*1R, 2S*)-**X2** from (*1S, 2R*)-**X1**]

To a frame-dried 5 mL glass tube with a magnetic stirrer bar, (*1S,2R*)-cyclohexyl alcohol **X1**[9] (68 mg, 0.3 mmol, 94% ee), PPh_3 (120 mg, 0.45 mmol, 1.5 eq.) and dry-THF (2 mL) were added. After cooling to -78 ℃, DEAD (2.2 *M* in toluene,180 µL, 0.39 mmol, 1.3 eq.) and DPPA (98 µL, 0.45 mmol, 1.5 eq.) were added, and gradually heated to room temperature. After 16 h, the solvent was removed under reduced pressure. The residue was filtered through short column chromatography using hexane/AcOEt (29/1) as the eluent. This crude material including corresponding chiral azide was directly used for the next step without further purification.

To the crude material containing azide compound, THF (3 mL), H_2O (80 µL) and PPh_3 (236 mg) were added. After stirring for 5 hours at 70 ℃, H_2O (10 mL) was added, and extracted with AcOEt (10 mL * 3 times). The combined organic layers were dried over $MgSO_4$, and the solvent was removed under reduced pressure. The residue was filtered through short column chromatography using MeOH as the eluent. This crude material including corresponding chiral amine was directly used for the next step without further purification.

To a frame-dried 5 mL glass tube with a magnetic stirrer bar, the crude material containing a corresponding chiral amine (~23 mg), NEt_3 (38 µL mg, 0.27 mmol) and dry-DCM (1 mL) were added. After cooling to 0 ℃, CbzCl (26 µL, 0.18 mmol) was added, and heated to room temperature. After 24 h, H_2O (10 mL) was carefully added, and

extracted with DCM (5 mL * 3 times). The combined organic layers were dried over $MgSO_4$, and the solvent was removed under reduced pressure. The residue was purified by column chromatography using hexane/AcOEt (4/1) as eluent, and the target product (*1R, 2S*)-**X2** was obtained in 30% yield (32.4 mg, 0.09 mmol) over 3steps.

[Synthesis of *chiral*-**X2** from **3aa**]

To a solution of **3aa** (63 mg, 0.17 mmol) in MeOH (1.7 mL), Pd/C(en) (7.0 mg, 10 wt%) was added under Ar atmosphere. The mixture was replaced three times with hydrogen gas (1 atom) and stirred at room temperature for 20 hours. This suspension was carefully filtered through Celite® (washed with MeOH), and concentrated in *vacuo*. The crude material was purified by using silica gel column chromatography (Hexane/AcOEt = 4/1) to afford *Chiral*-**X2** (12.3 mg, 0.034 mmol, 20% yield) with 75% recovery of **3aa**.

→ The ^{1}H NMR charts of (*1R,2S*)-**X2** and *Chiral*-**X2** synthesized by a different route were in perfect agreement. According to HPLC comparison (**Figure S8**), the absolute configuration of the product **3aa** was determined to be (1*R*, 6*S*). This result was also consistent with the calculation results.

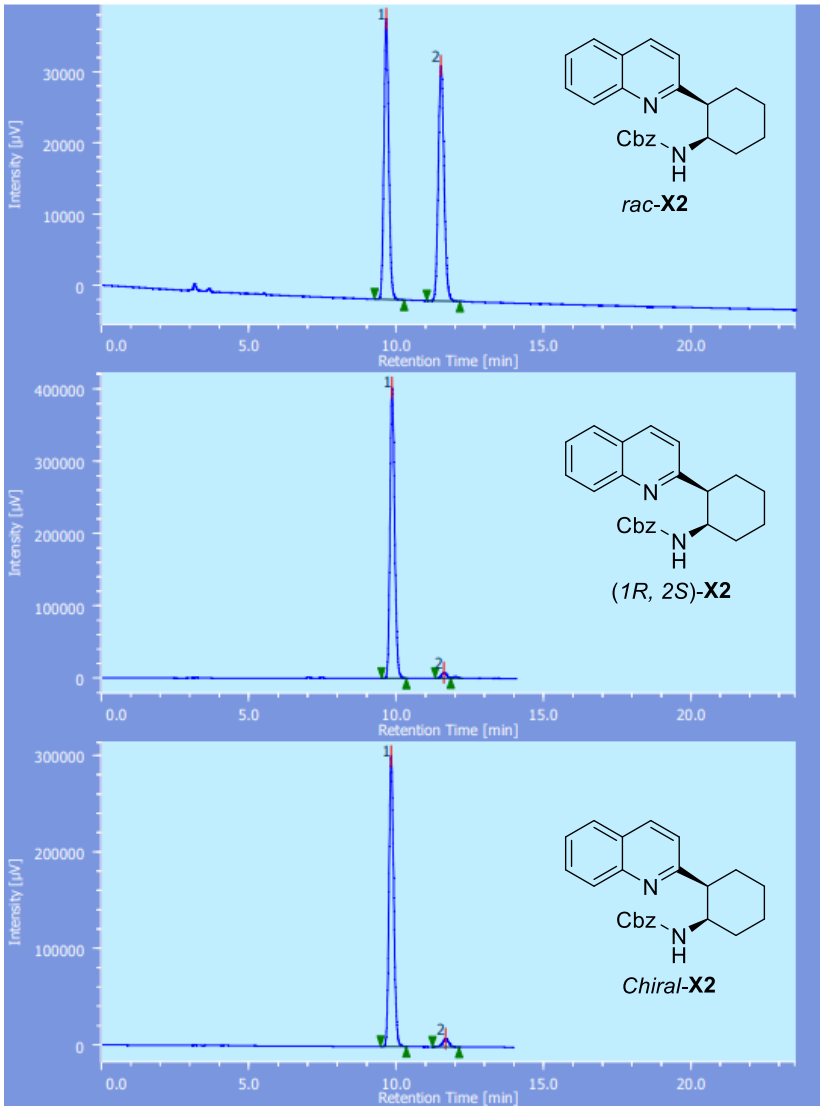
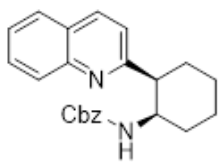


Figure S8. Comparison of HPLC chart of **X2**.

Benzyl ((*1R,2S*)-2-(quinolin-2-yl)cyclohexyl)carbamate (X2)



colorless oil; $[\alpha]_D^{23.0}$ = +62.9 (*c* = 0.82, $CHCl_3$, 93% ee); R_f = 0.20 (Hexane/EtOAc= 6/1); ^1H NMR (600 MHz, $CDCl_3$, VT50) δ 8.03 (t, *J* = 7.2 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.66 (t, *J* = 8.4 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 7.24-7.20 (m, 3H), 7.18 (brs, 2H), 6.24 (brs, 1H), 4.98-4.90 (m, 2H), 4.18-4.13 (m, 1H), 3.32-3.27 (m, 1H), 2.33 (brs, 1H), 2.19-2.11 (m, 1H), 1.93-1.87 (m, 1H), 1.75-1.55 (m, 4H), 1.48-1.40 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.2, 156.2, 147.6, 137.2, 136.5, 129.5, 129.4, 128.5, 127.9, 127.6, 127.0, 126.1, 121.5, 66.3, 51.5, 47.1, 30.7, 28.1, 24.1, 22.3, one carbon was not found probably due to overlapping; IR (ATR) 3401, 3348, 3061, 3034, 2932, 2857, 1715, 1600, 1503, 1454, 1310, 1231, 1094, 1051, 830, 759, 697 cm^{-1}; HRMS (FD+) m/z: $[M+H]^+$ Calcd for $C_{23}H_{24}N_2O_2$ 360.18378, found: 360.18375.; HPLC analysis CHIRALCEL OD-3 (Hexane:*i*PrOH = 96/4, 1.0 mL/min, 40℃, 254 nm) 10.4 min (major), 12.4 min (minor).

8. References

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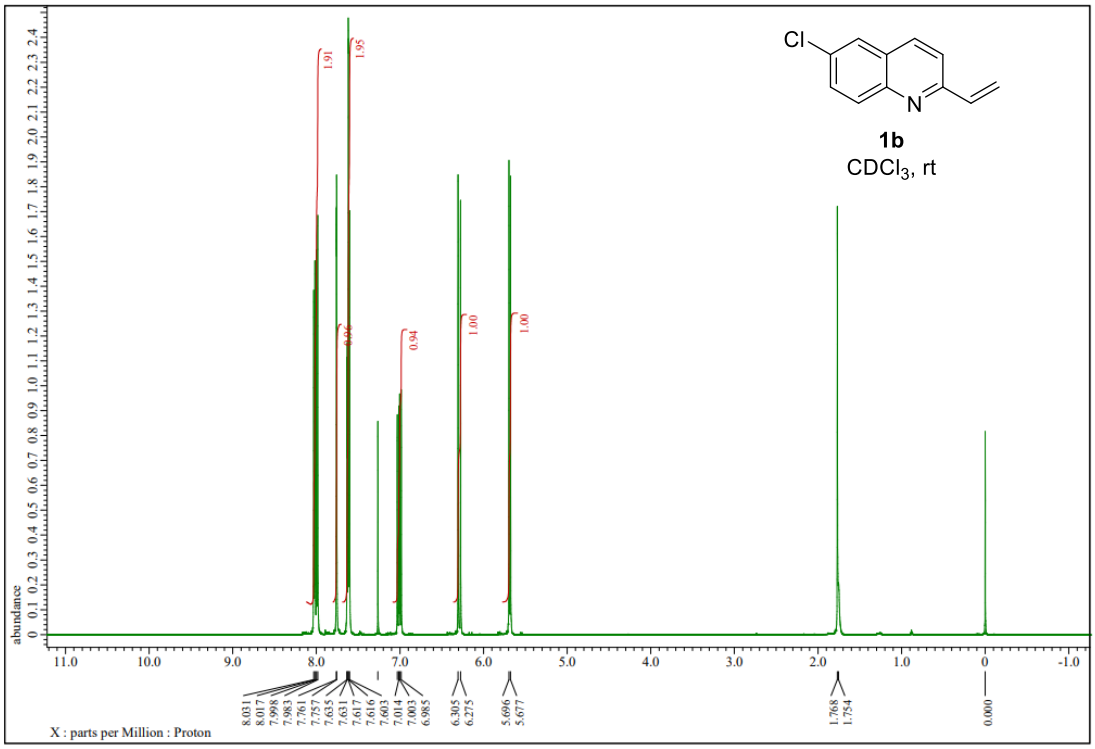
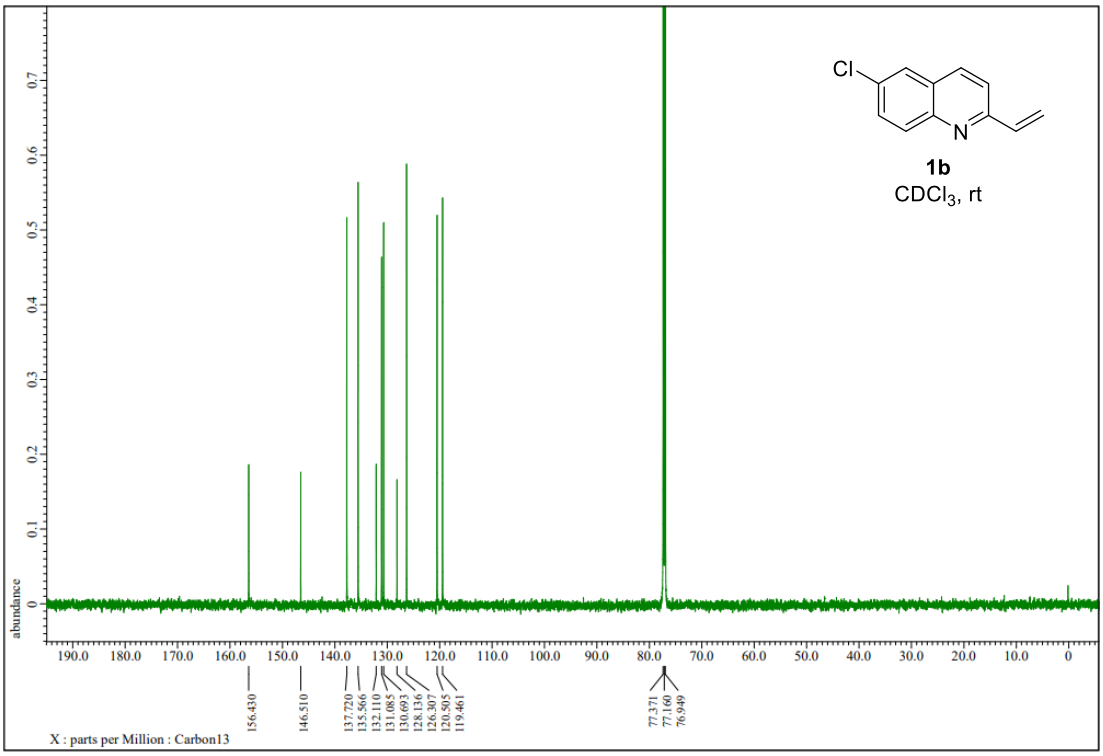
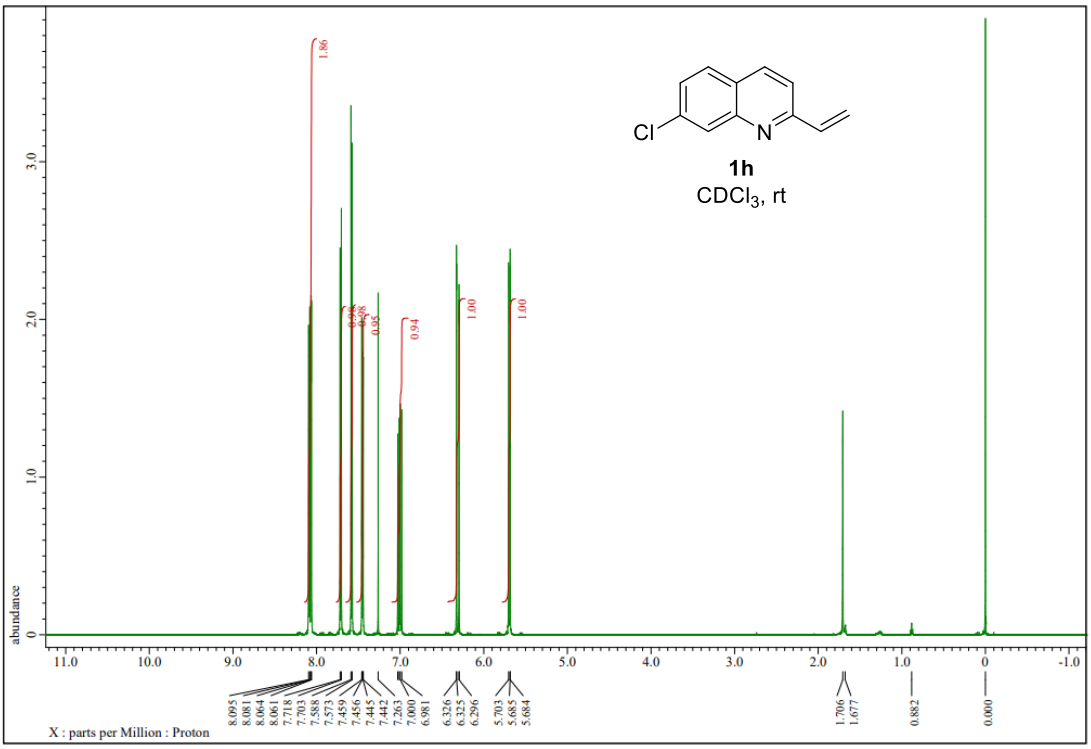
9. NMR spectra

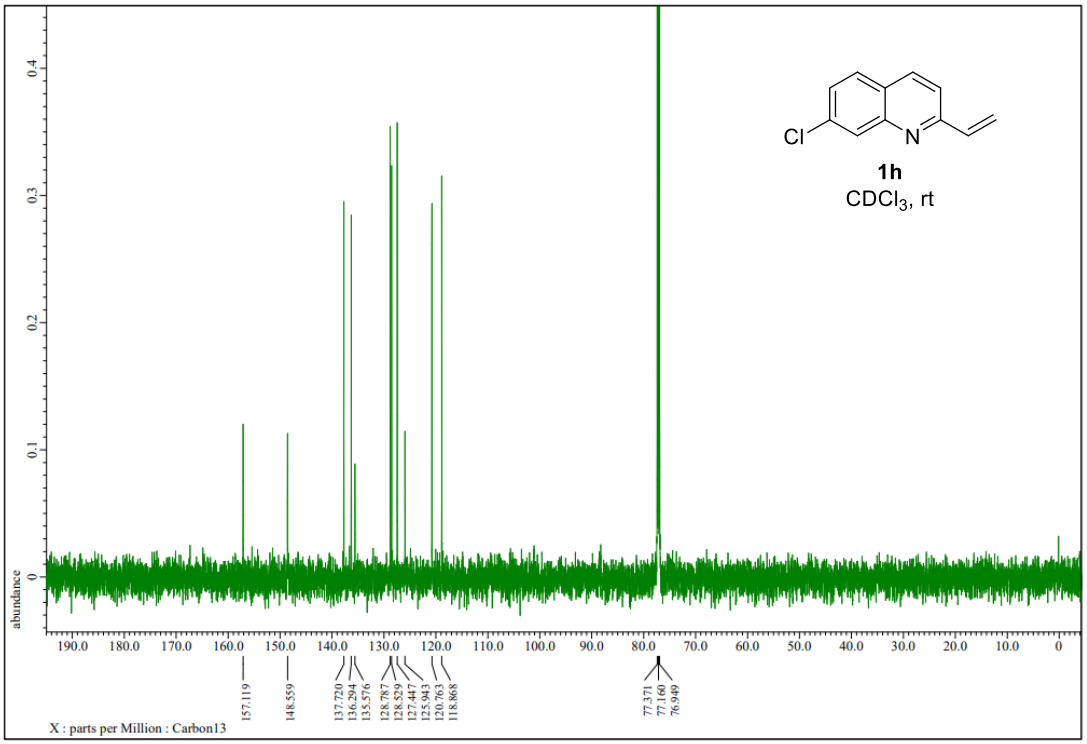
^{1}H and ^{13}C NMR charts of **1b**.



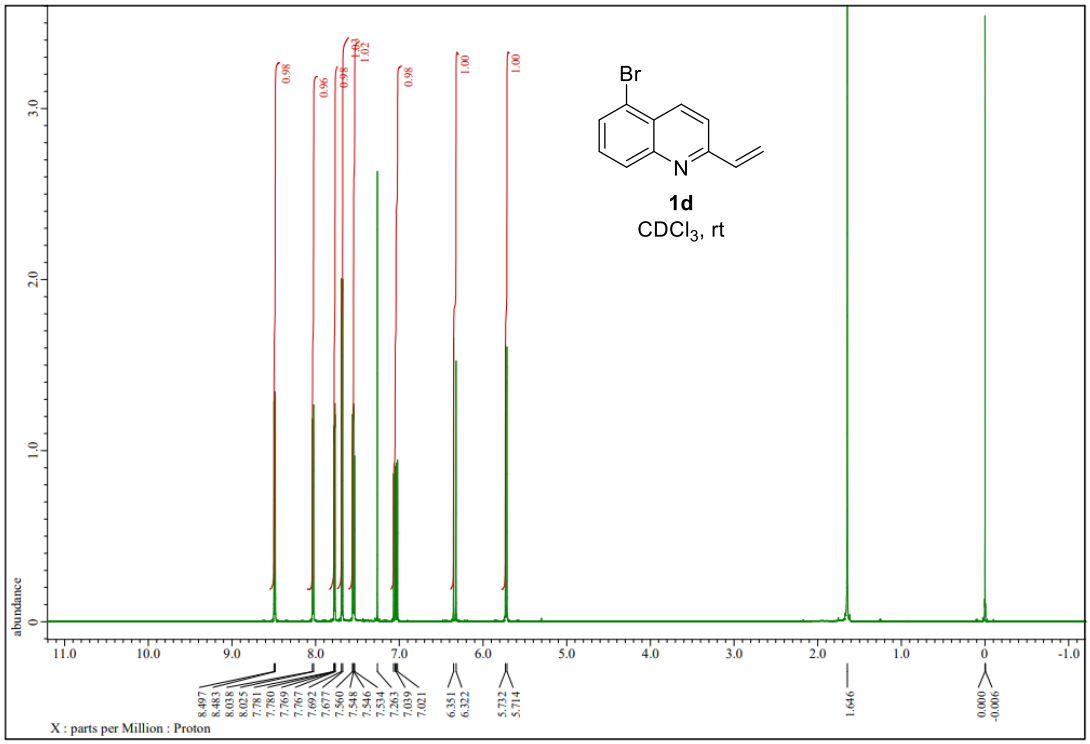


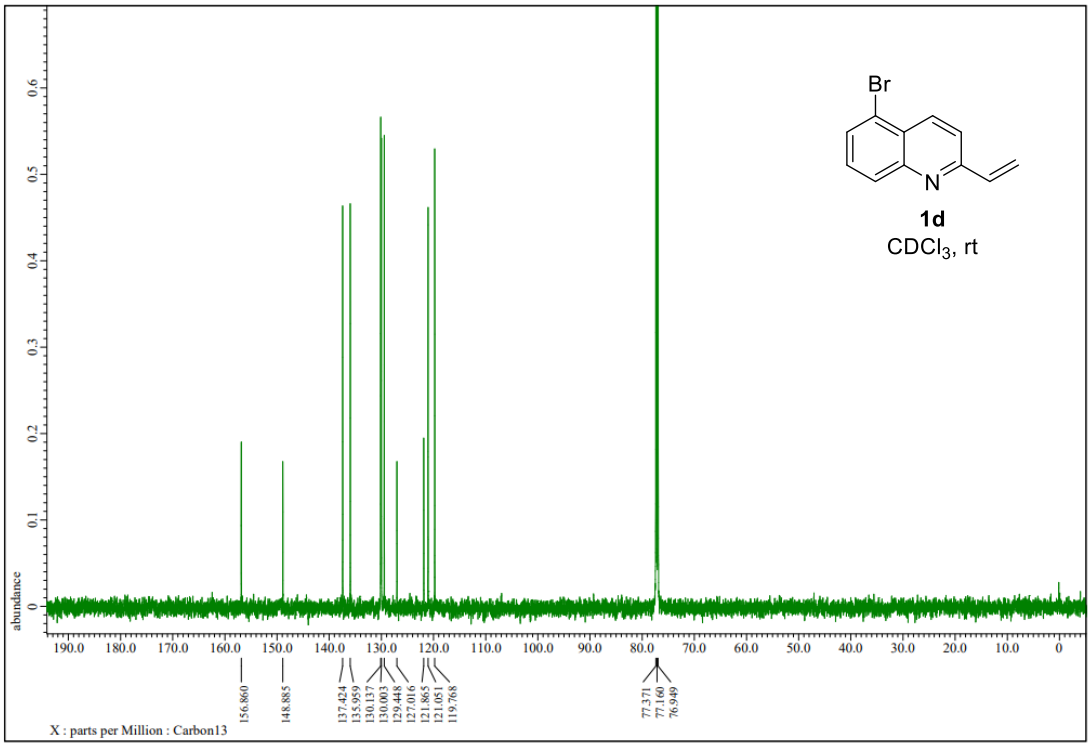
^{1}H and ^{13}C NMR charts of **1h**.



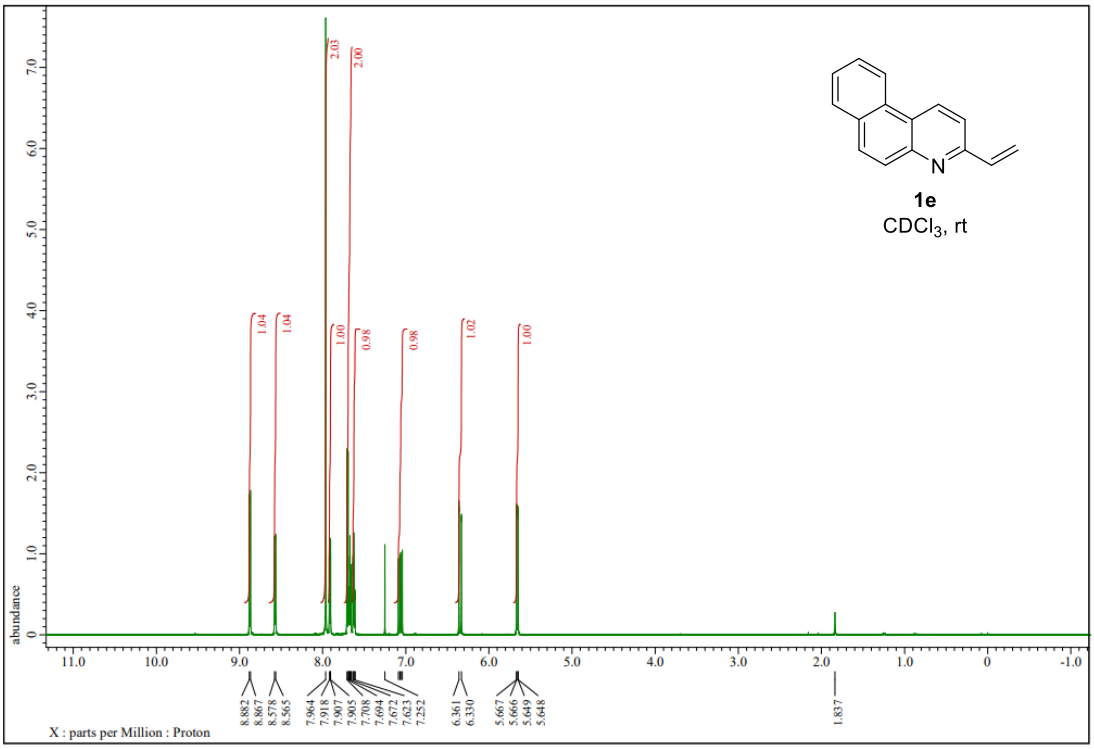


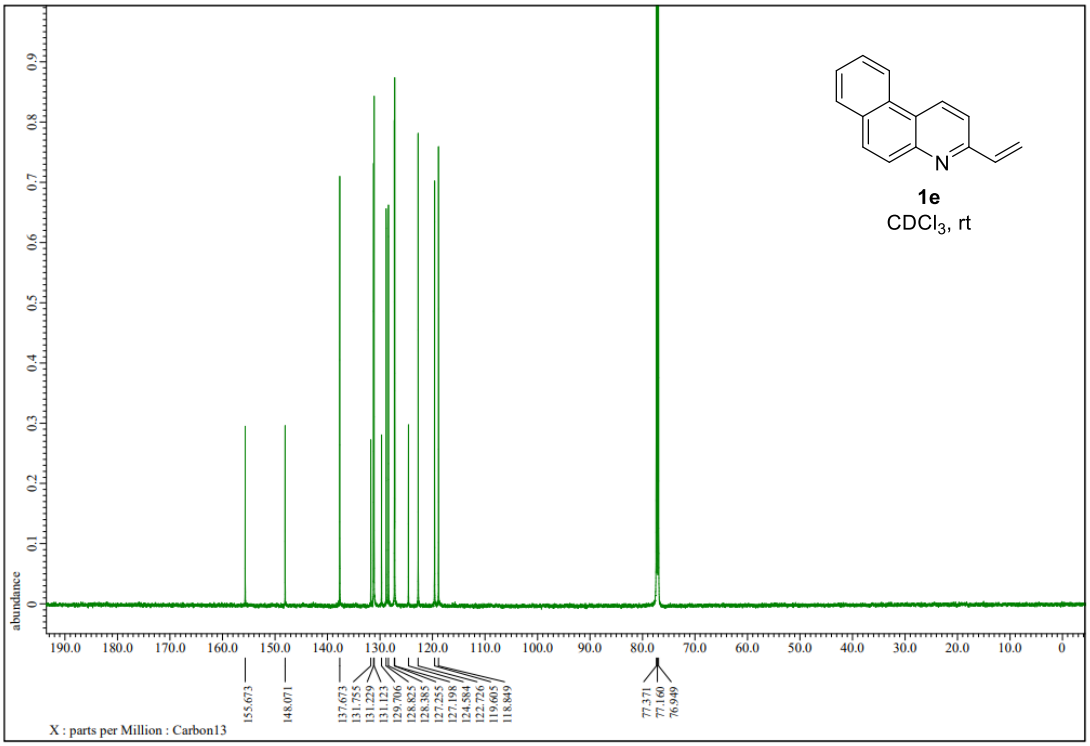
^{1}H and ^{13}C NMR charts of **1d**.



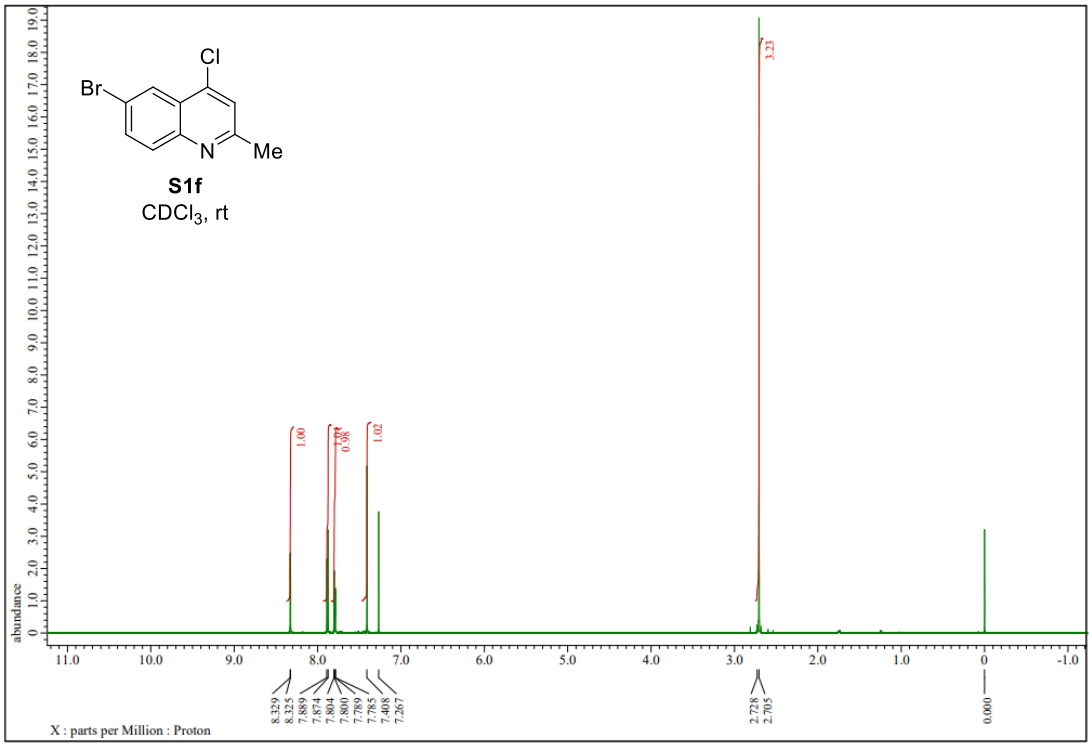


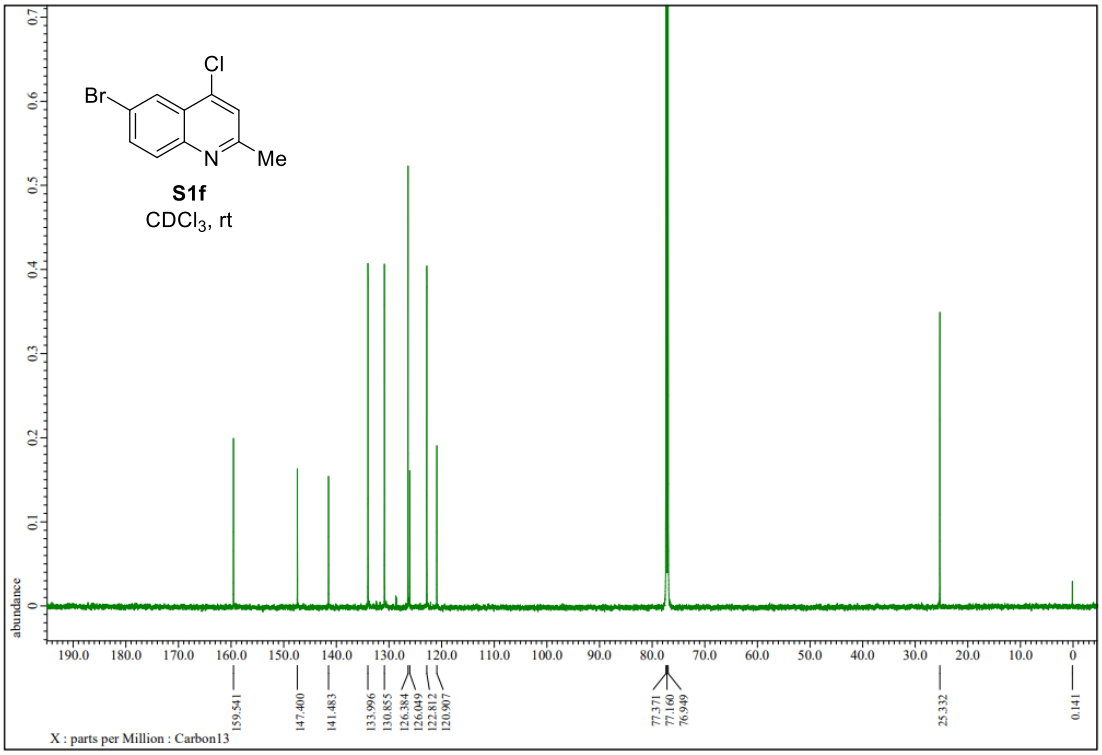
^{1}H and ^{13}C NMR charts of **1e**.





^{1}H and ^{13}C NMR charts of **S1f**.





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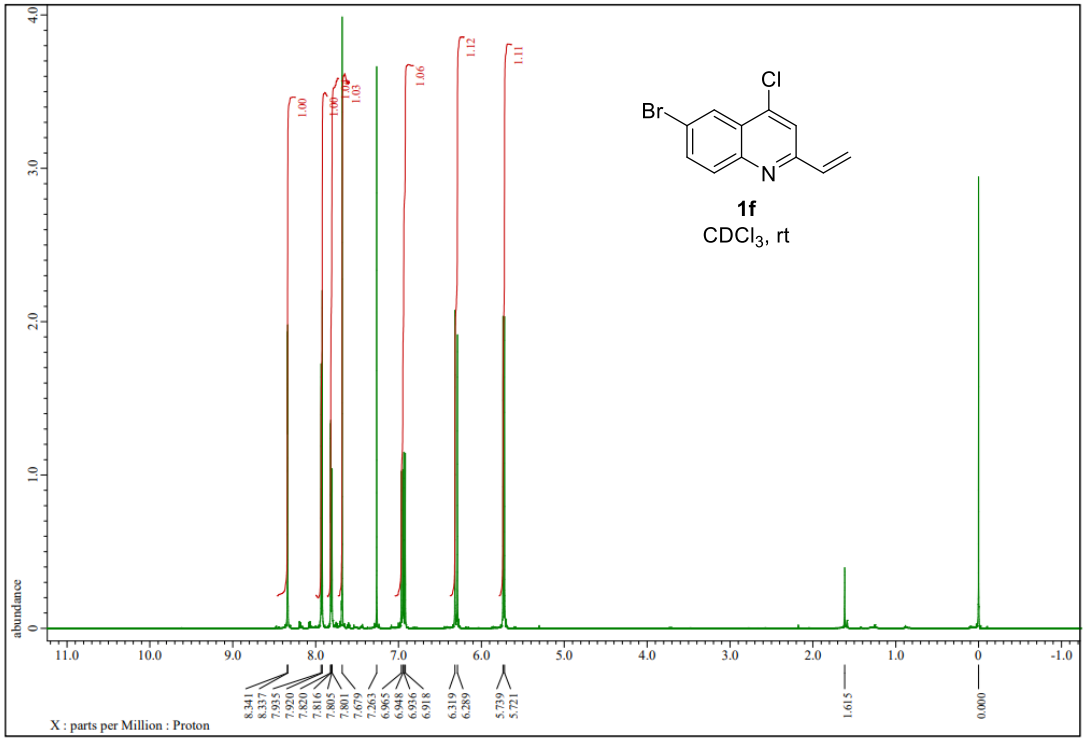
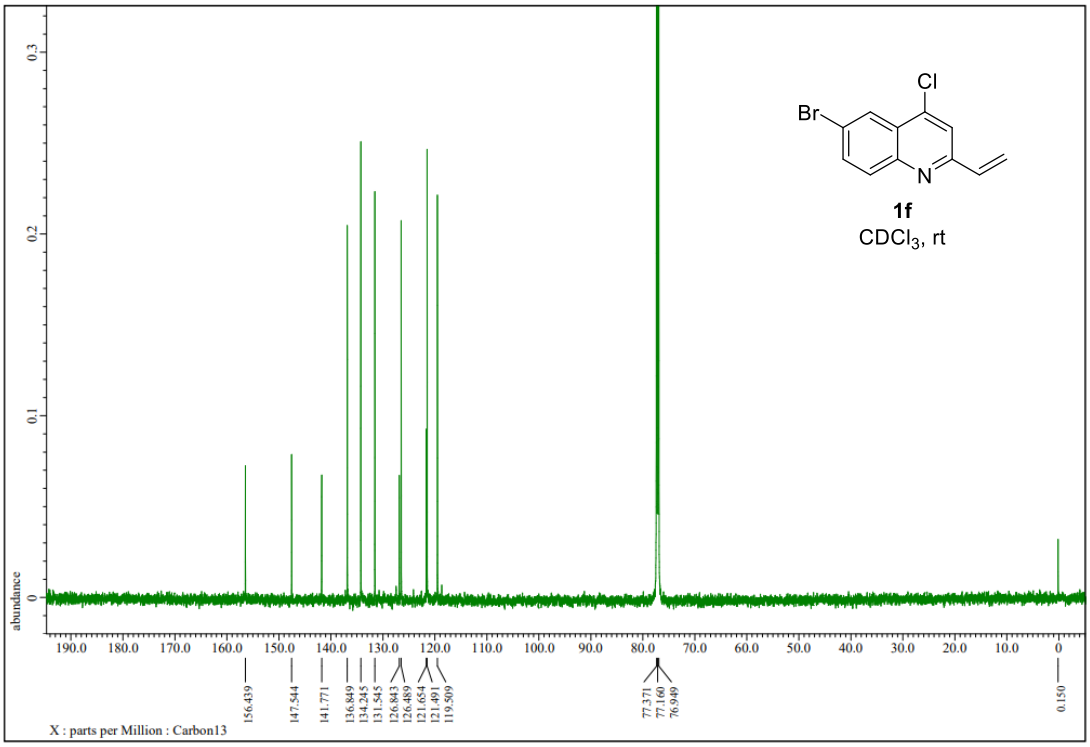
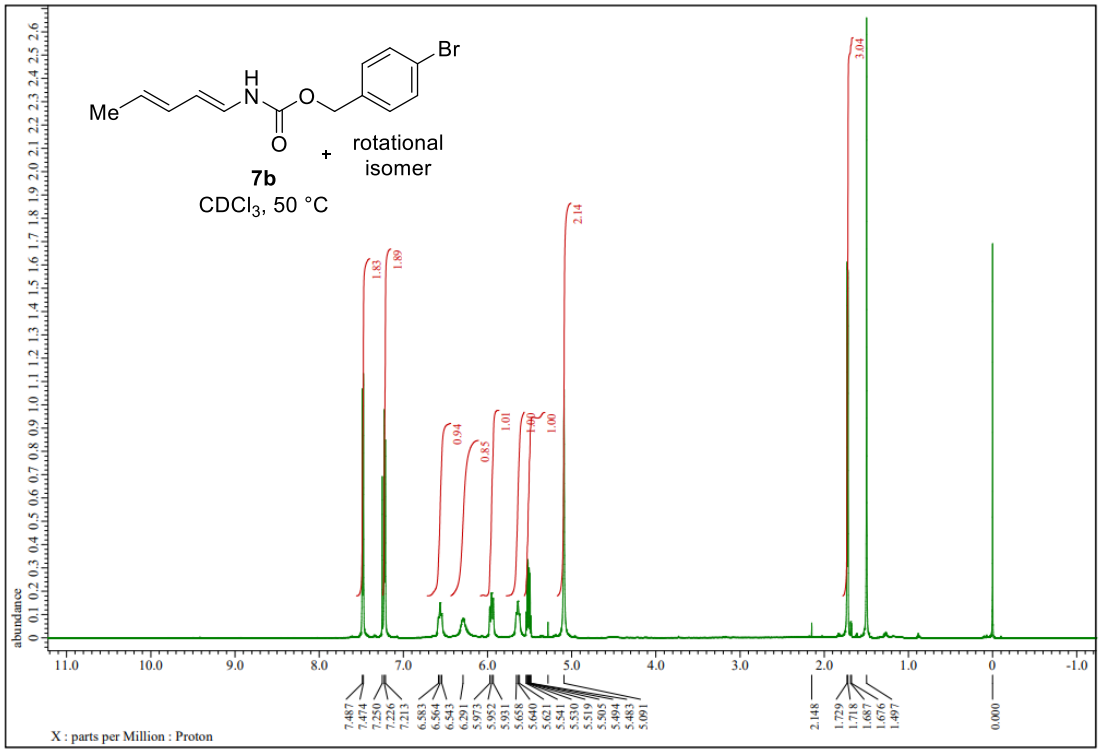
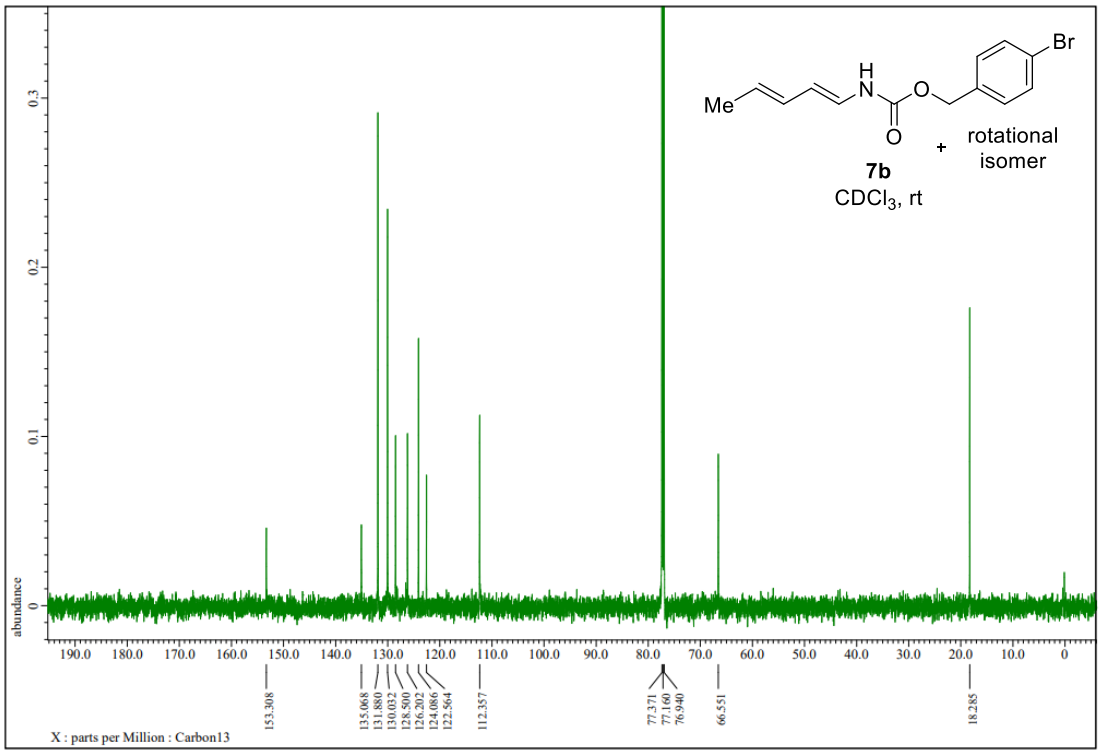


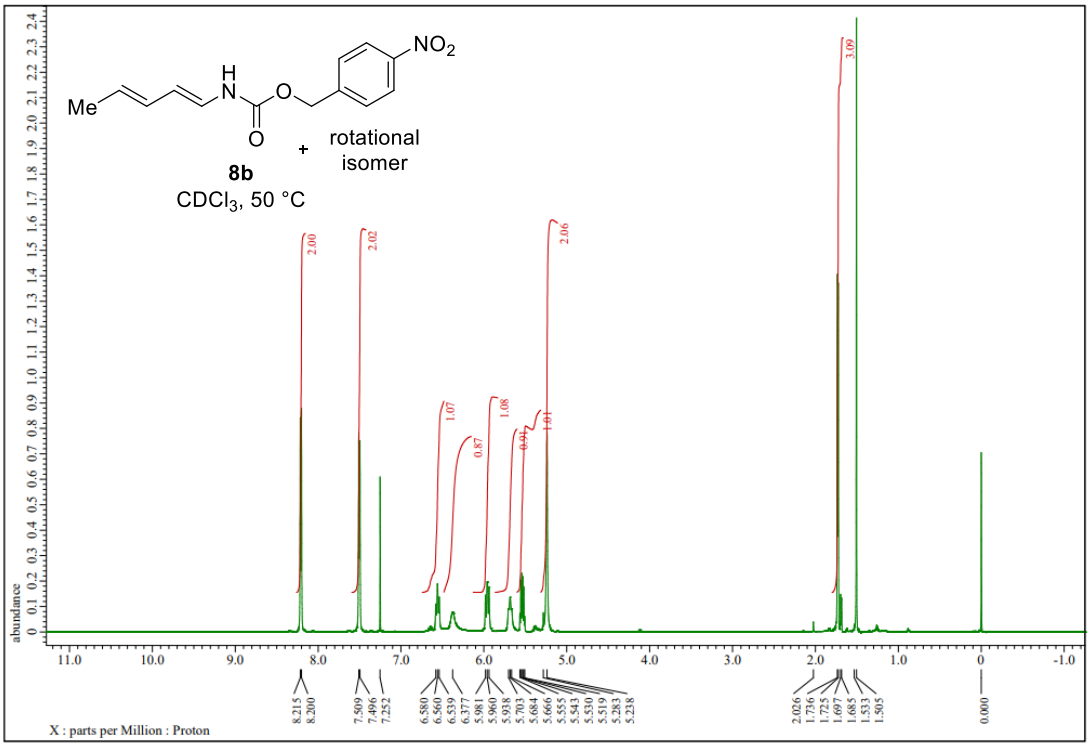


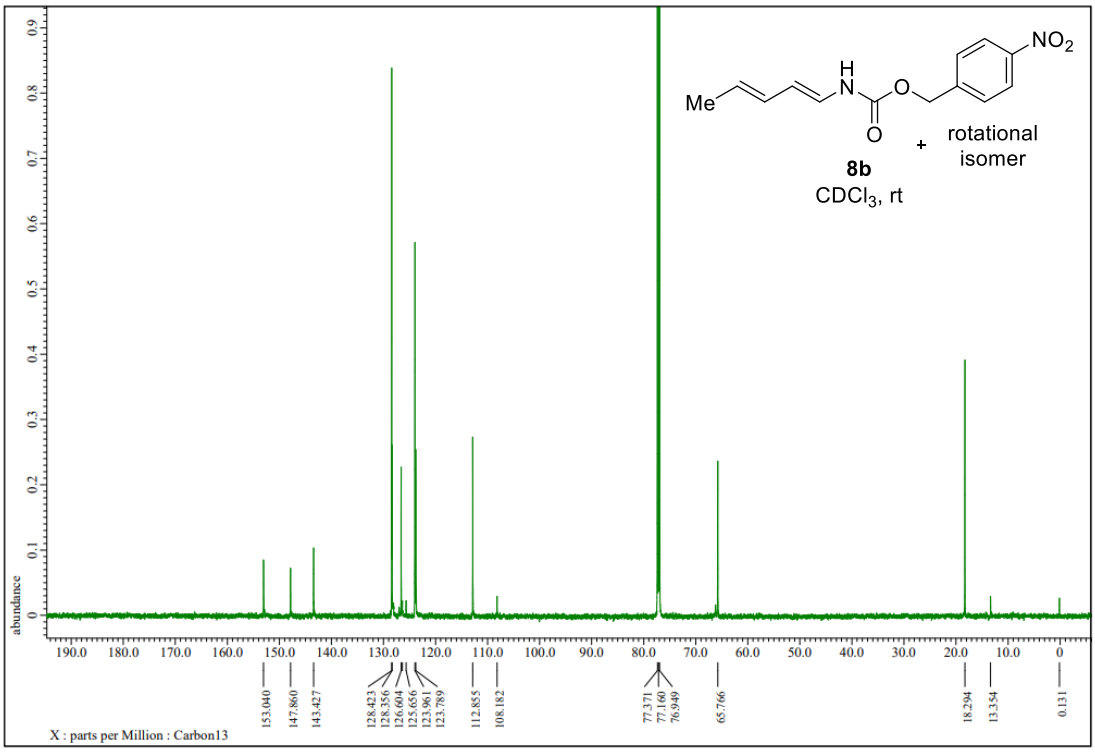
^{1}H and ^{13}C NMR charts of **7b**.



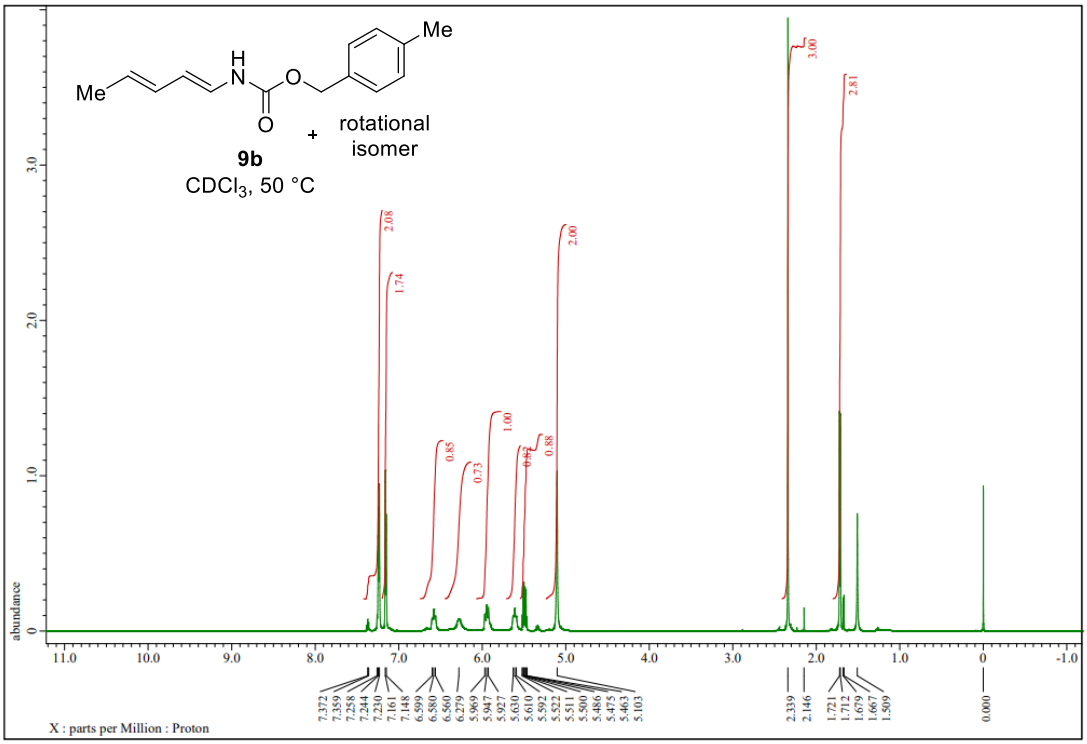


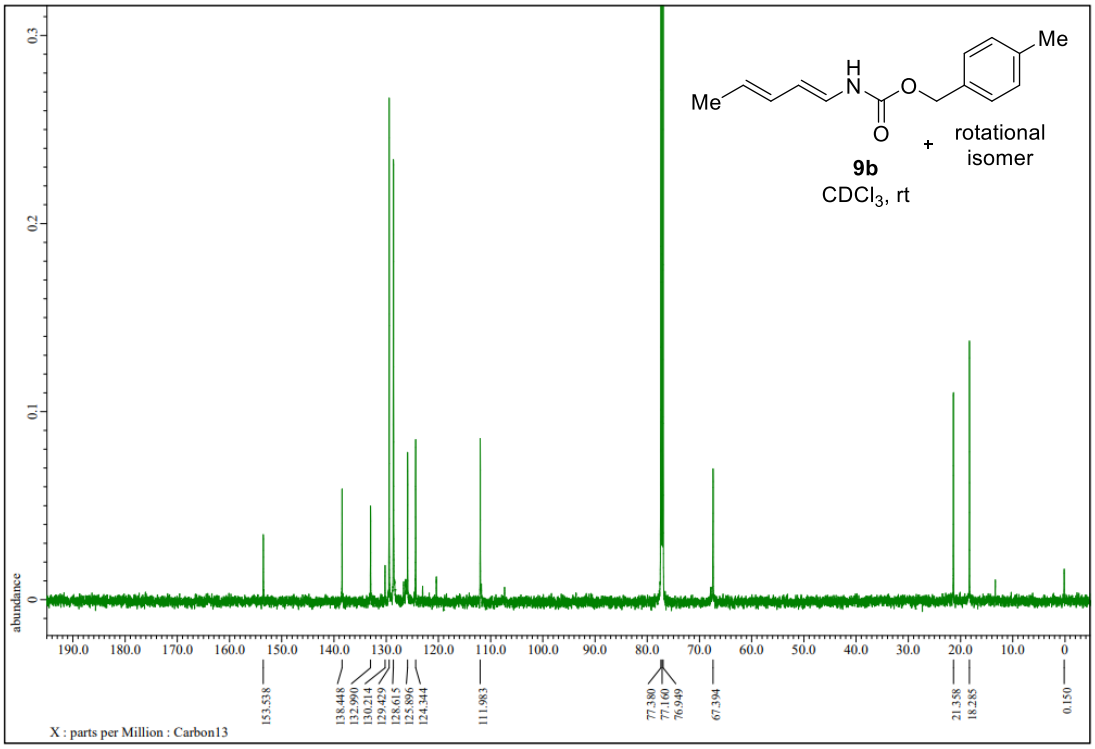
^{1}H and ^{13}C NMR charts of **8b**.





^{1}H and ^{13}C NMR charts of **9b**.





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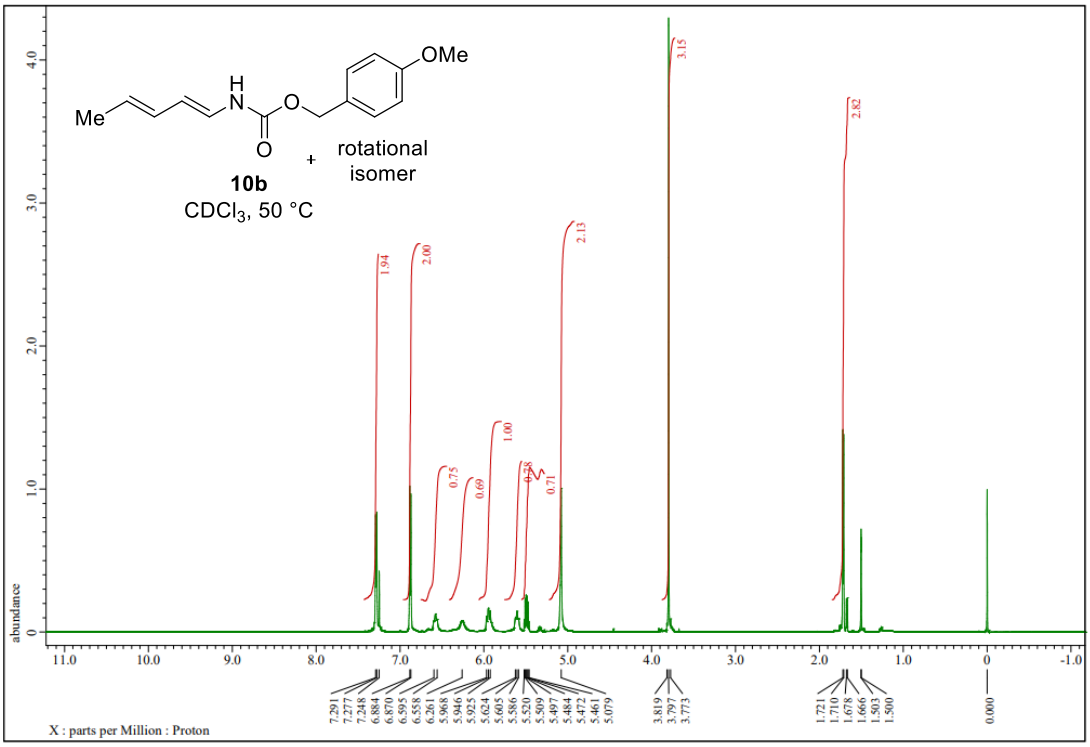

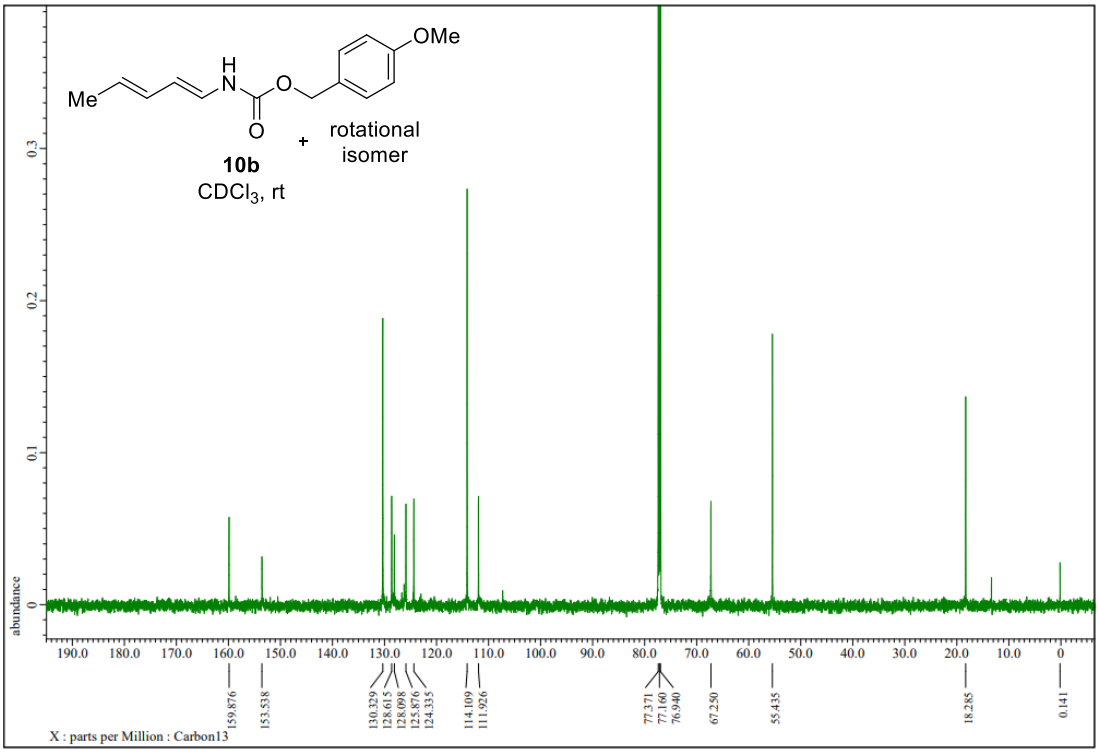

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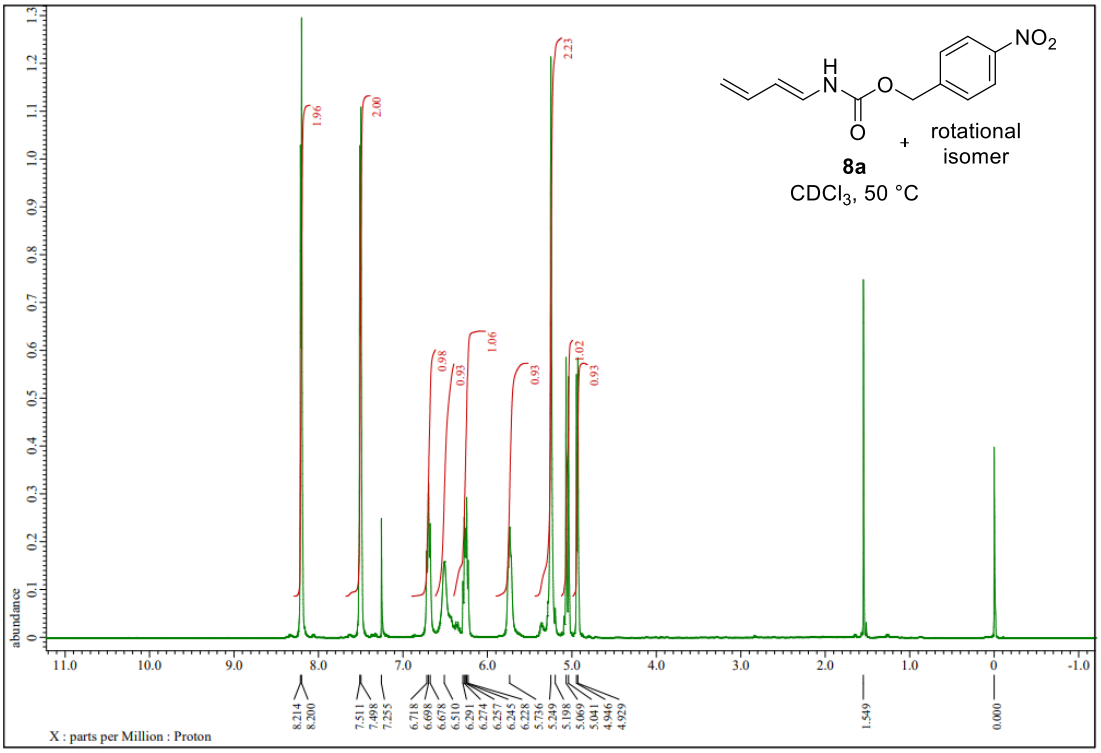
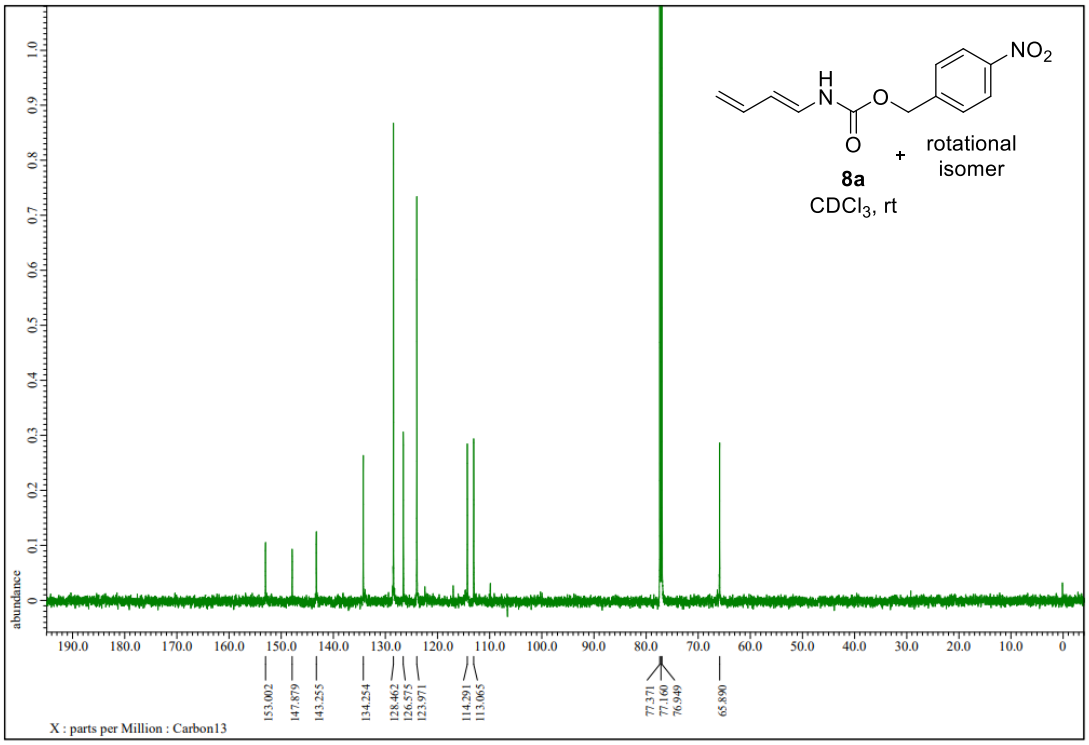
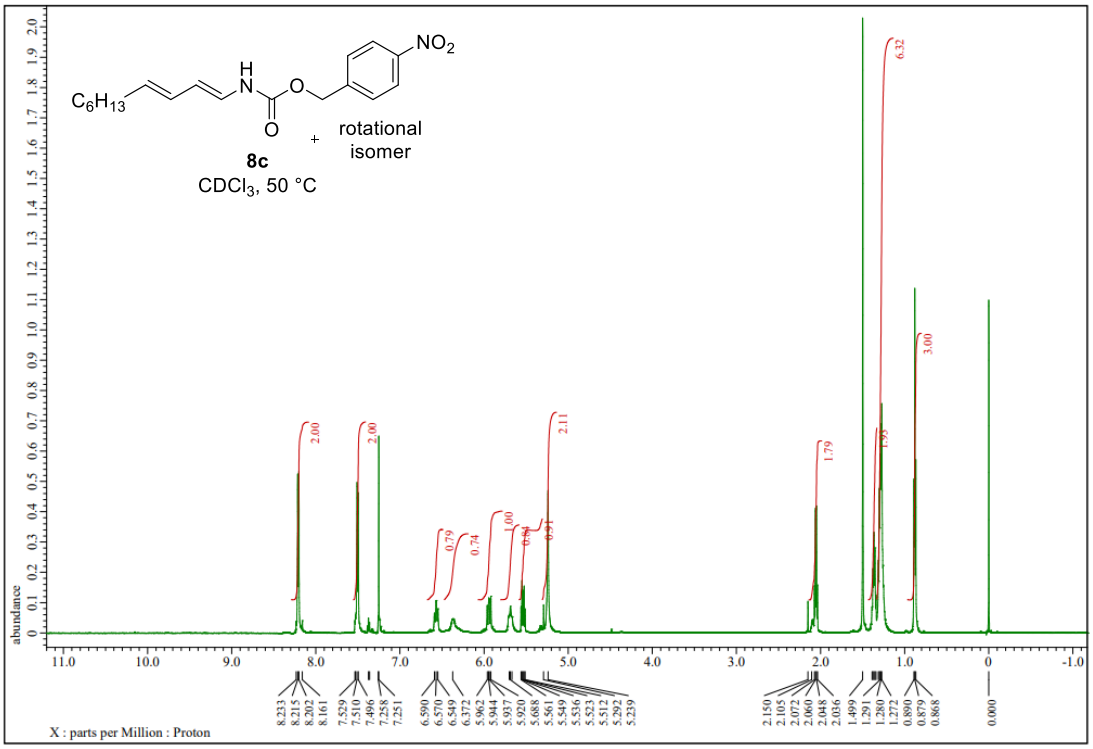
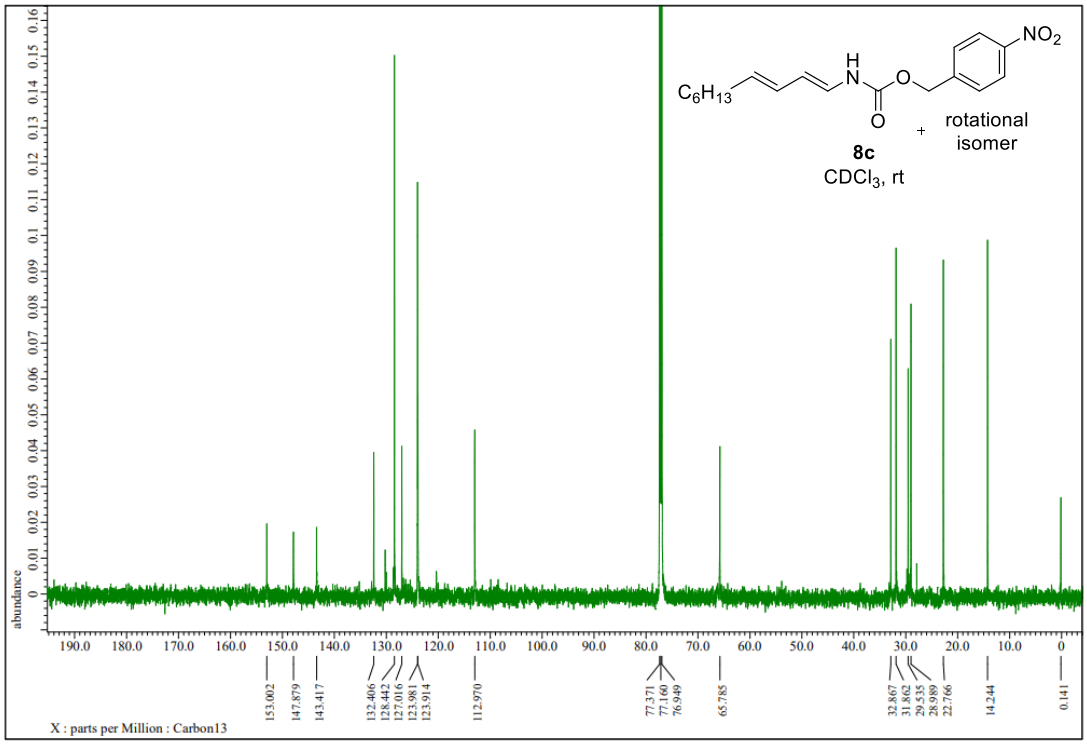


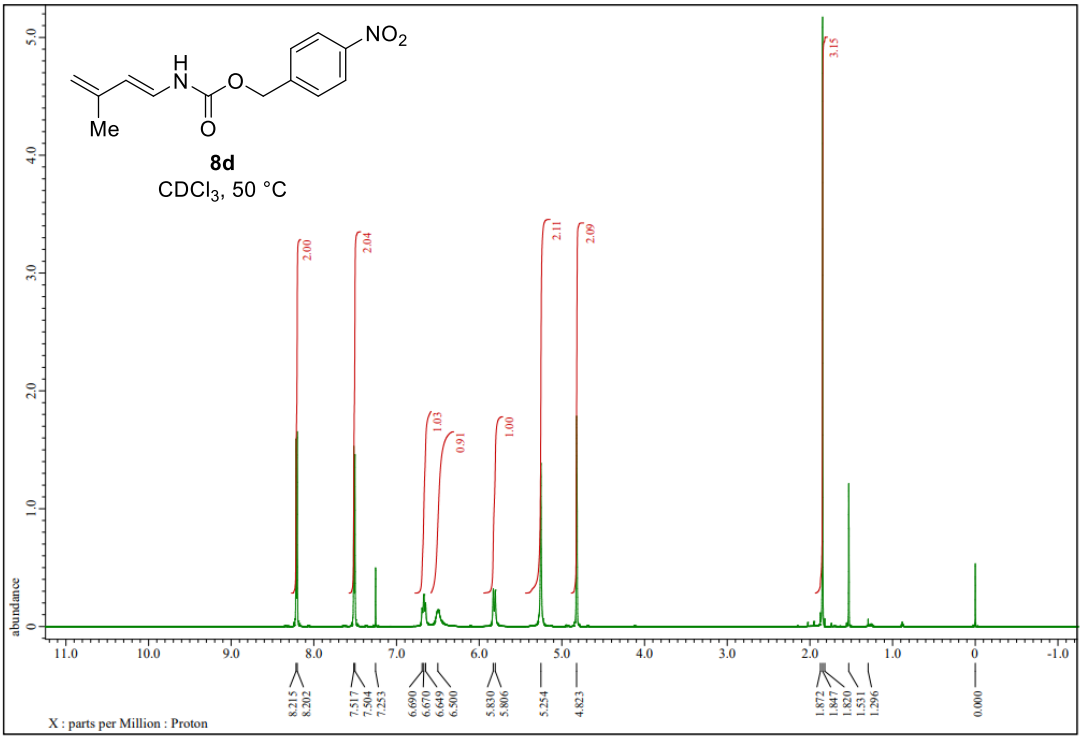


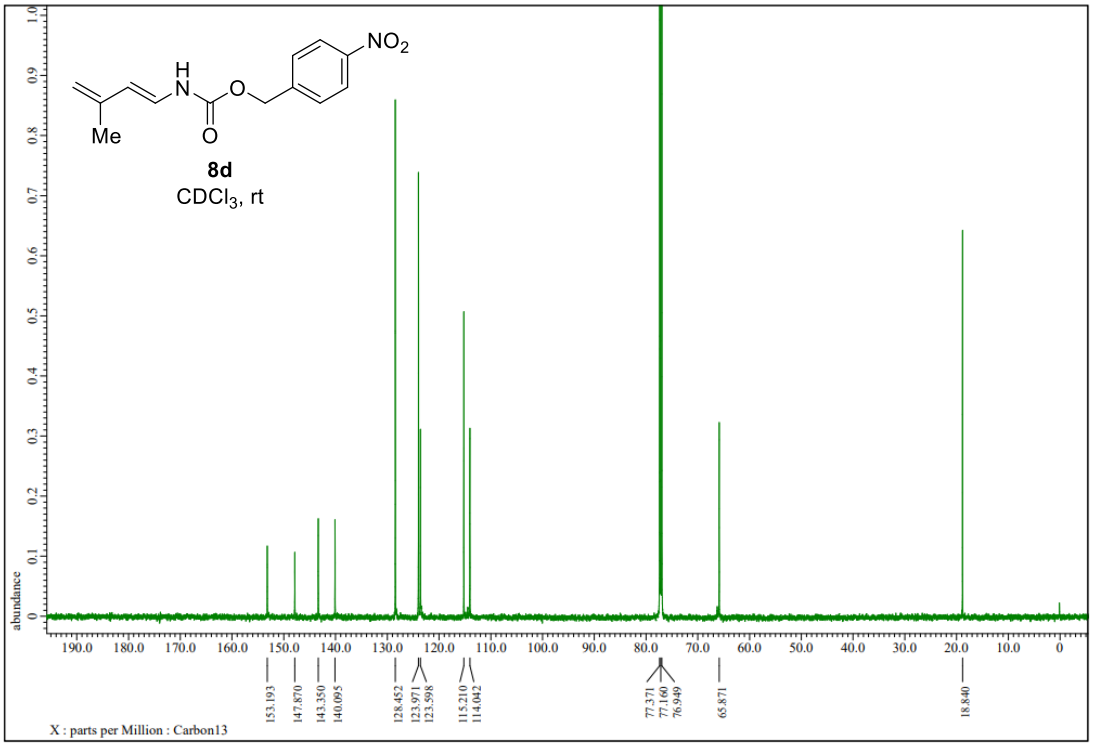
^{1}H and ^{13}C NMR charts of **8c**.



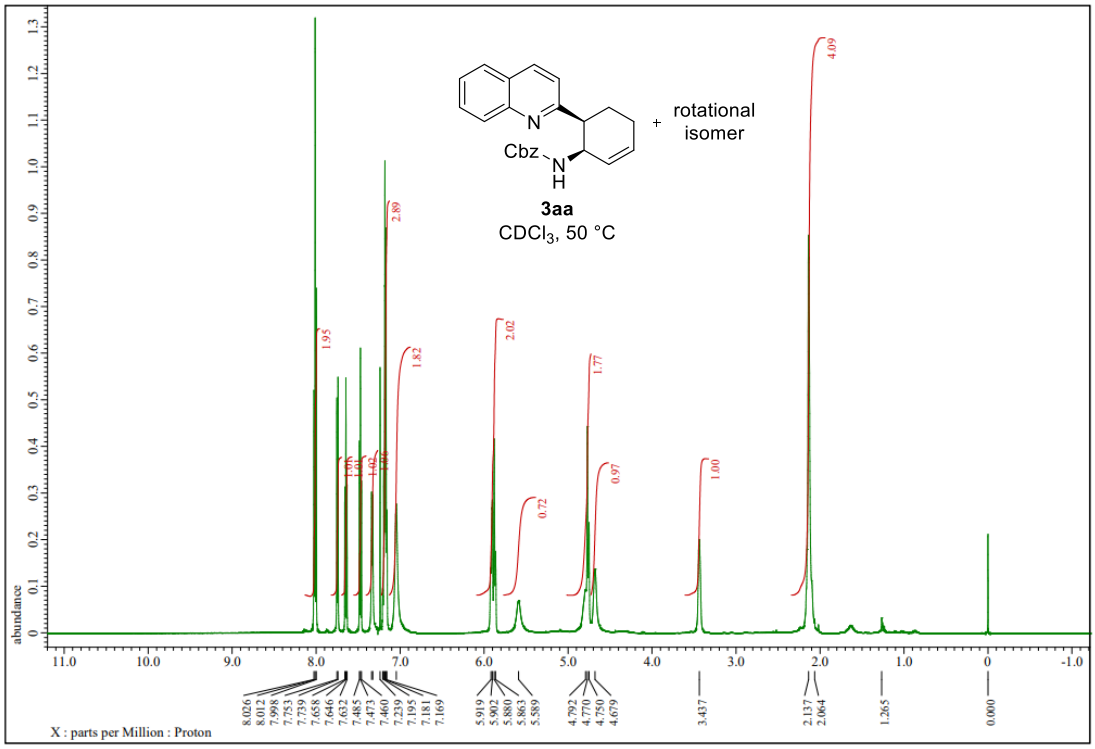


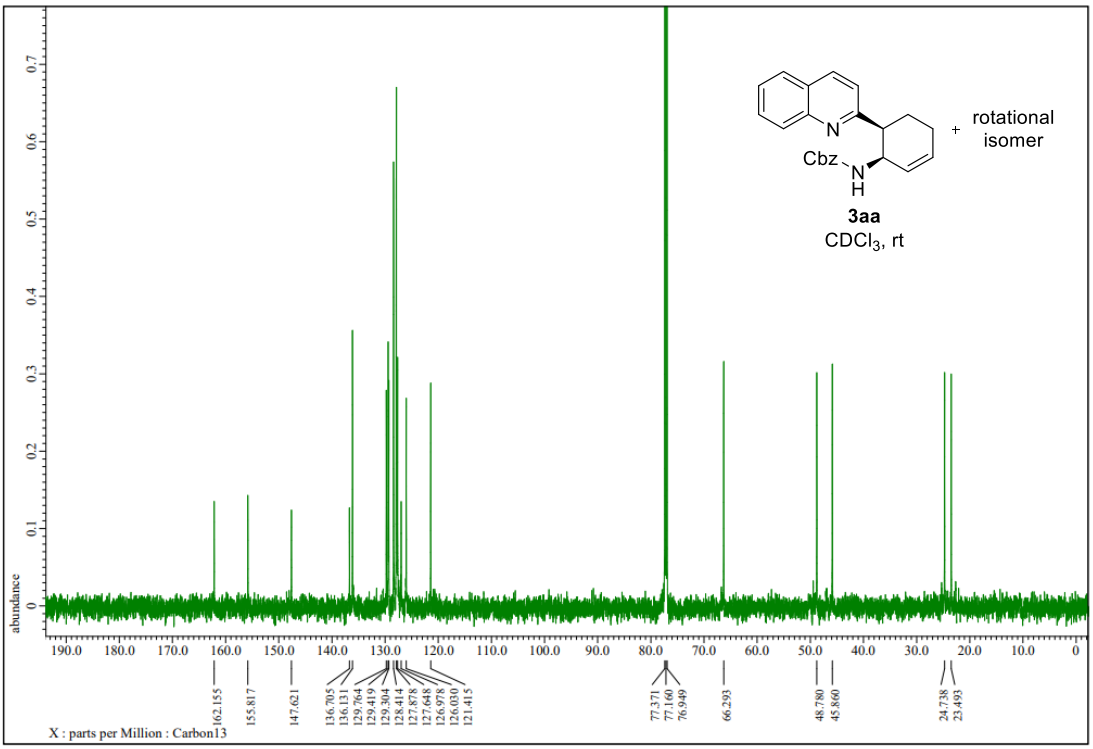
^{1}H and ^{13}C NMR charts of **8d**.





^{1}H and ^{13}C NMR charts of **3aa**.





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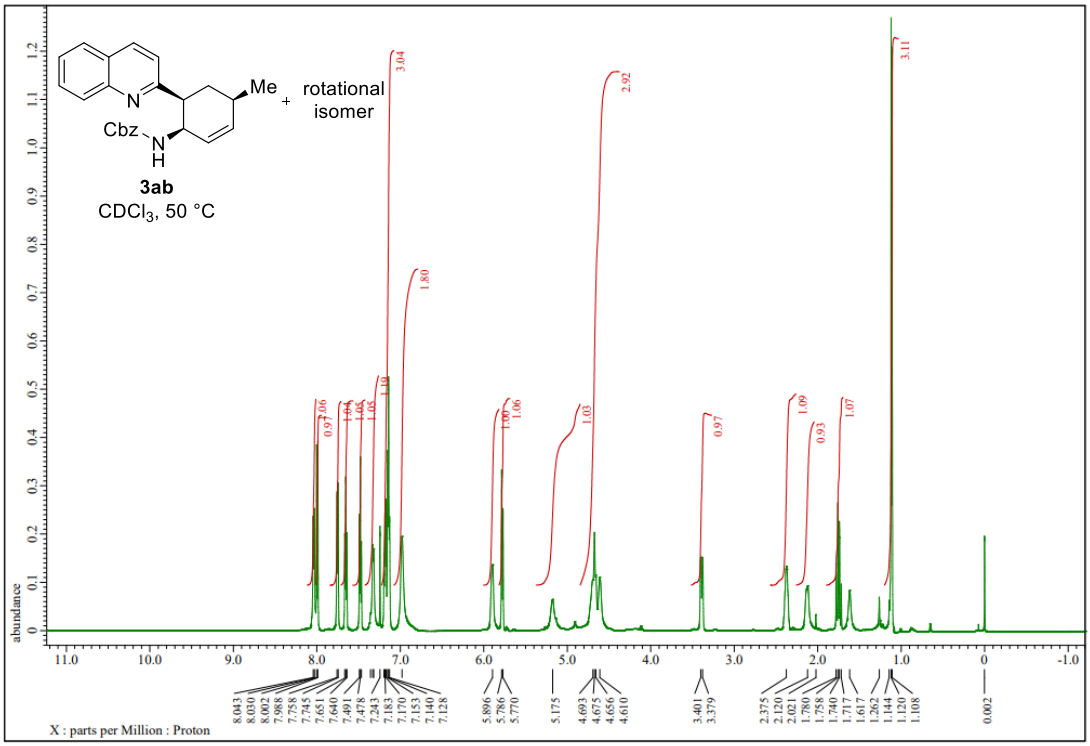

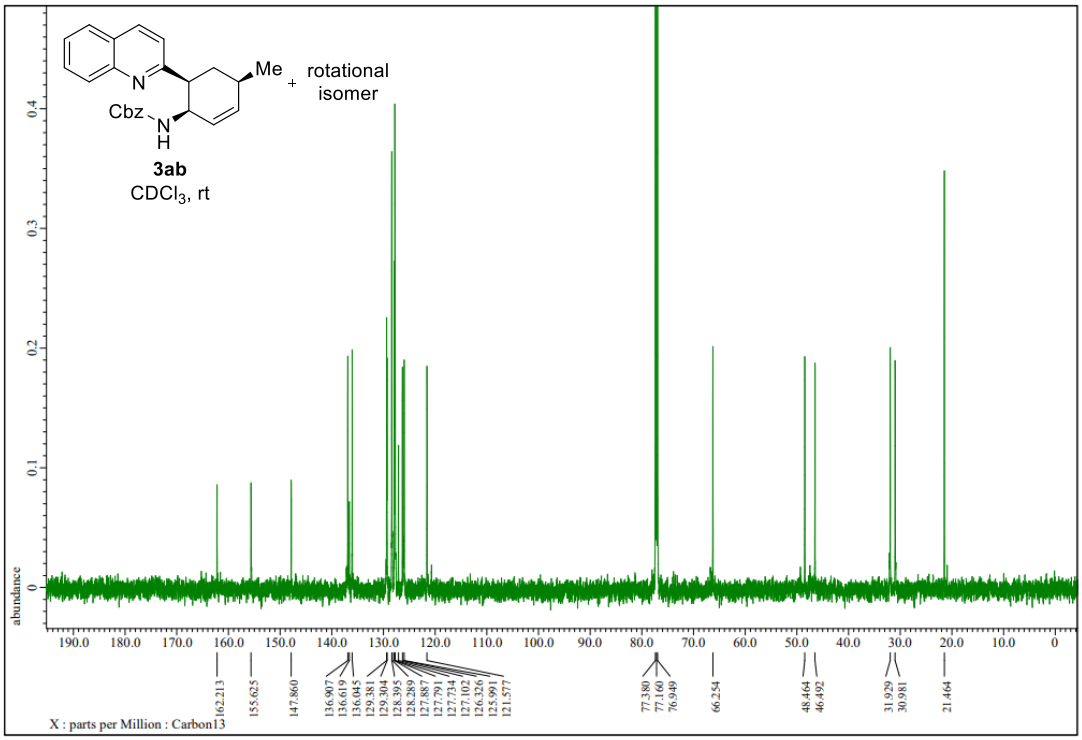

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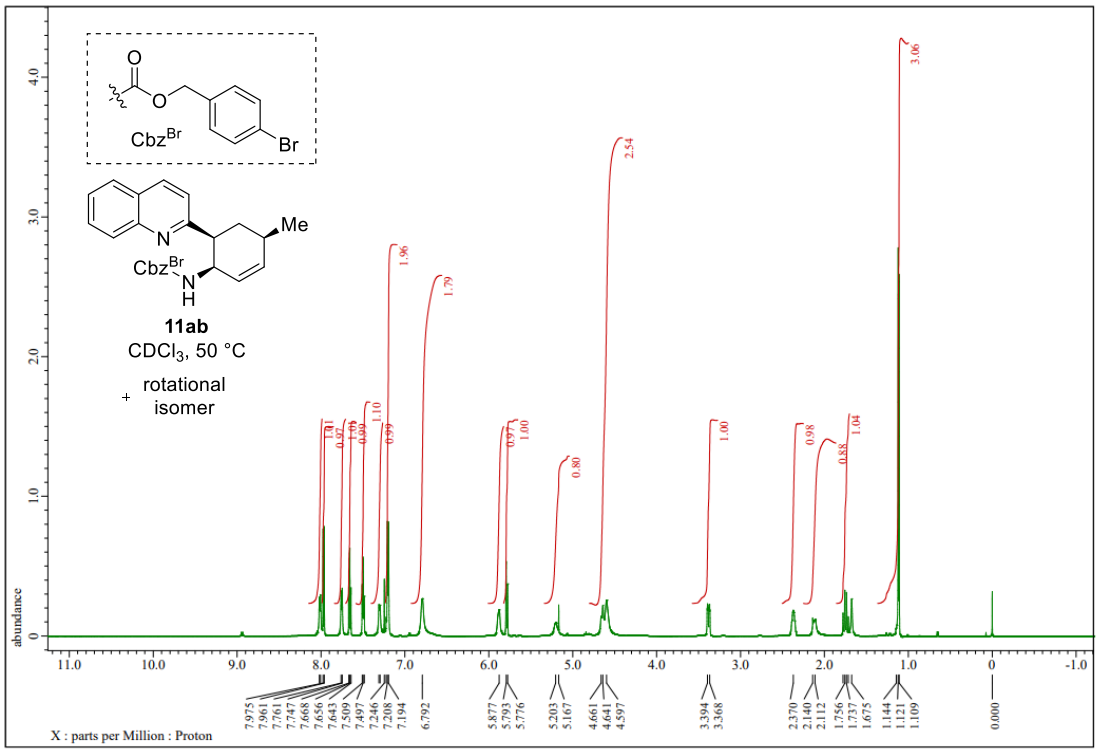

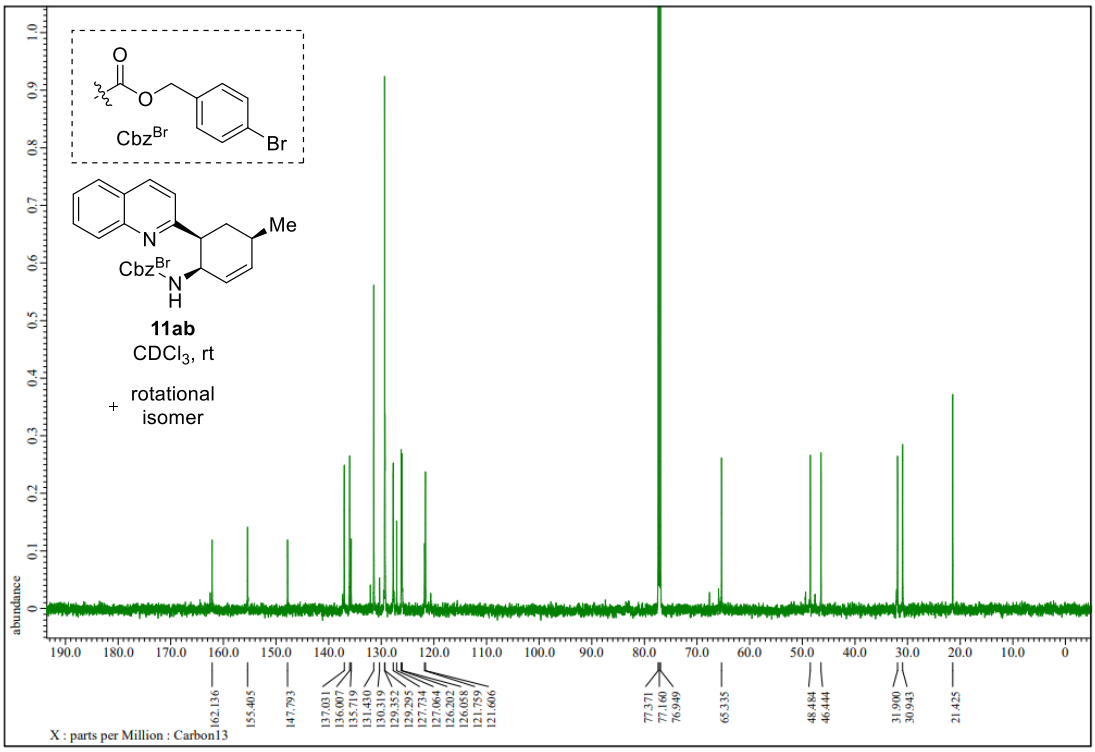

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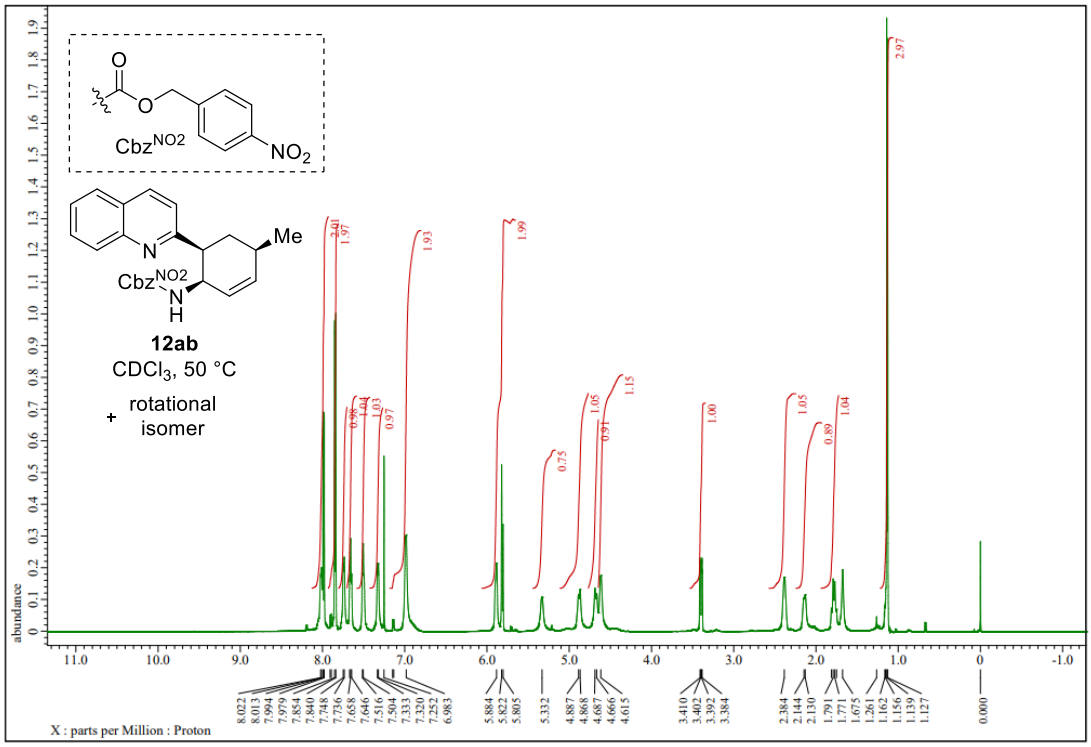

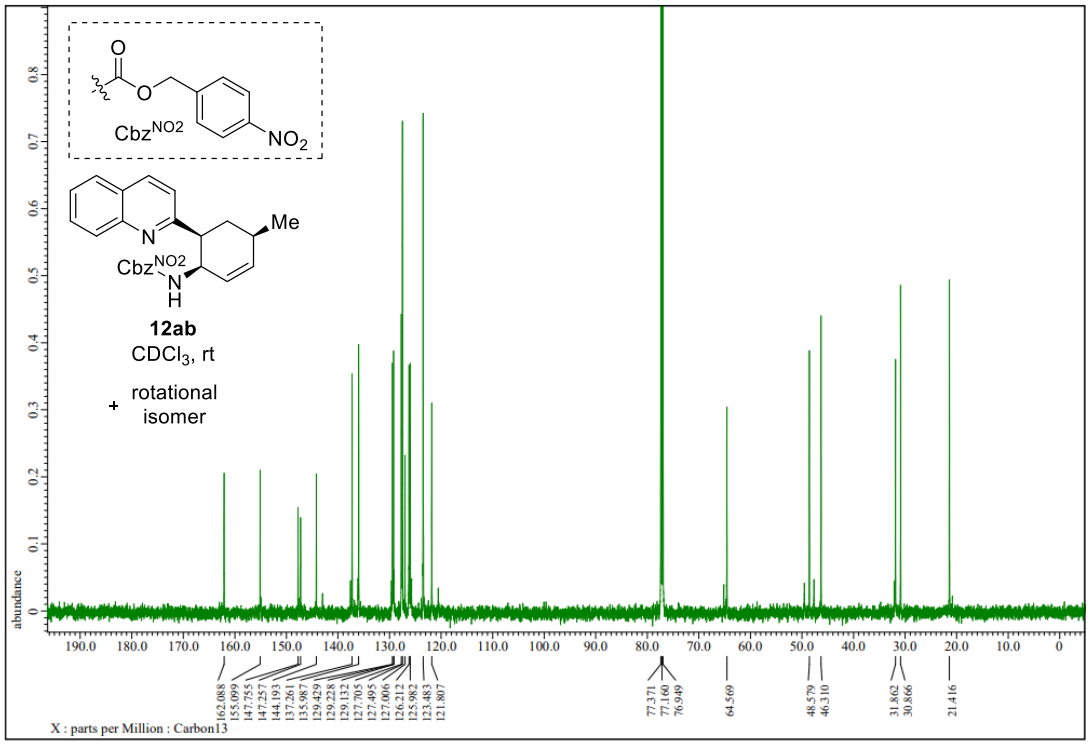

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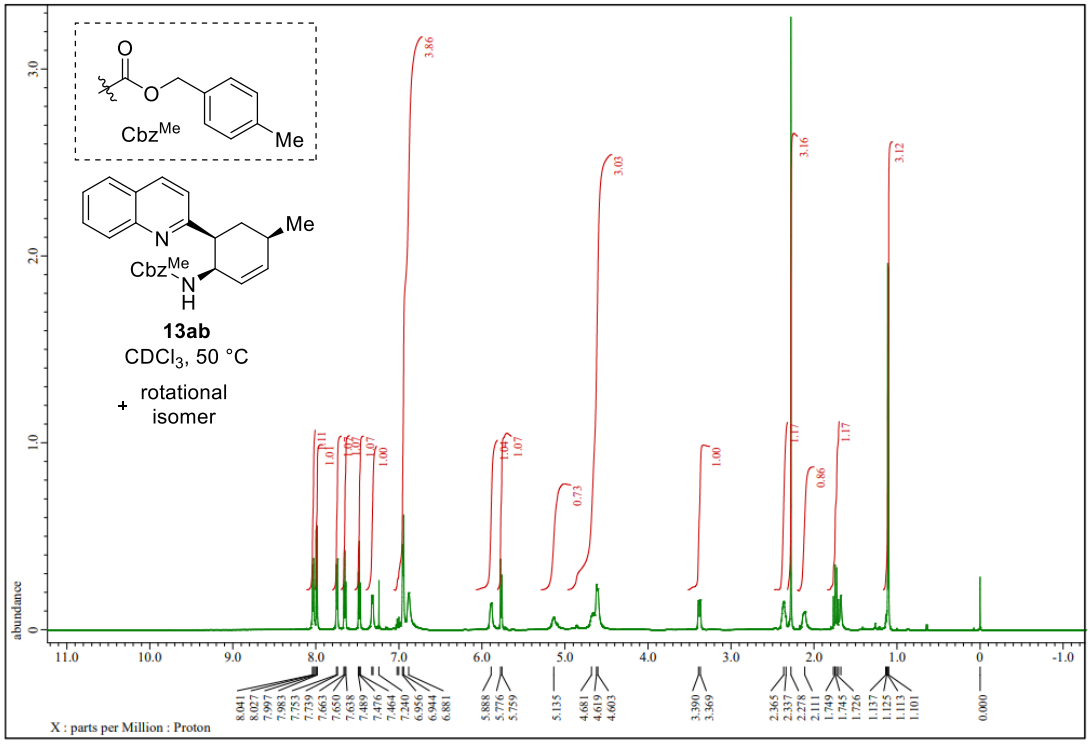
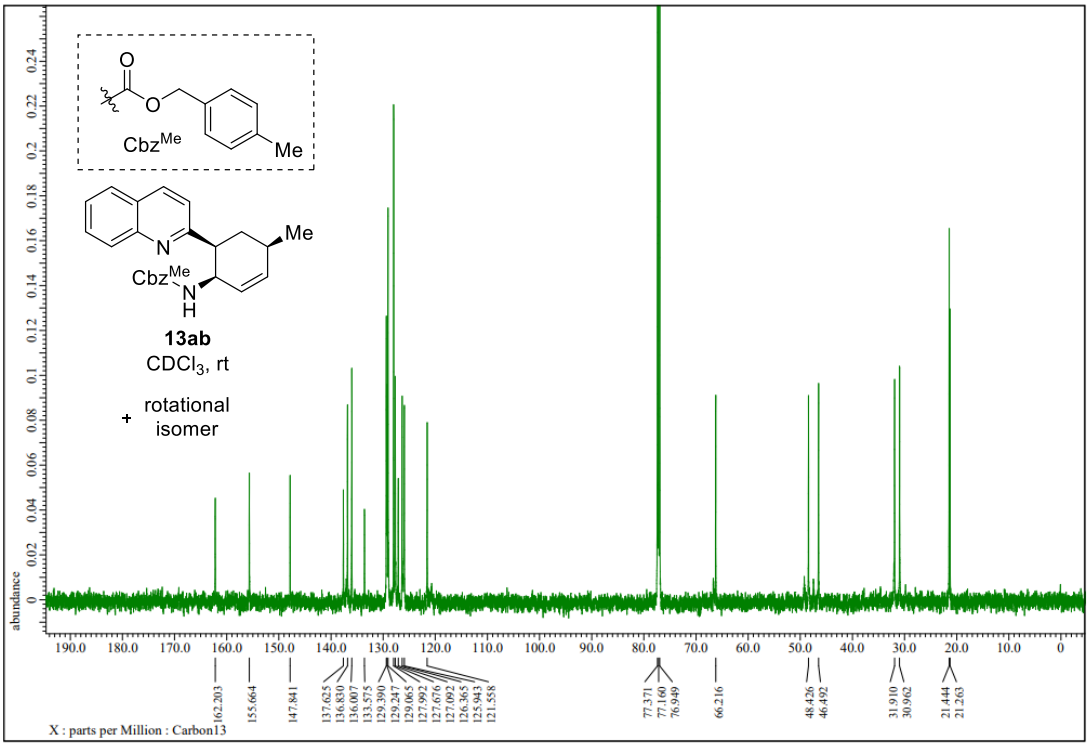
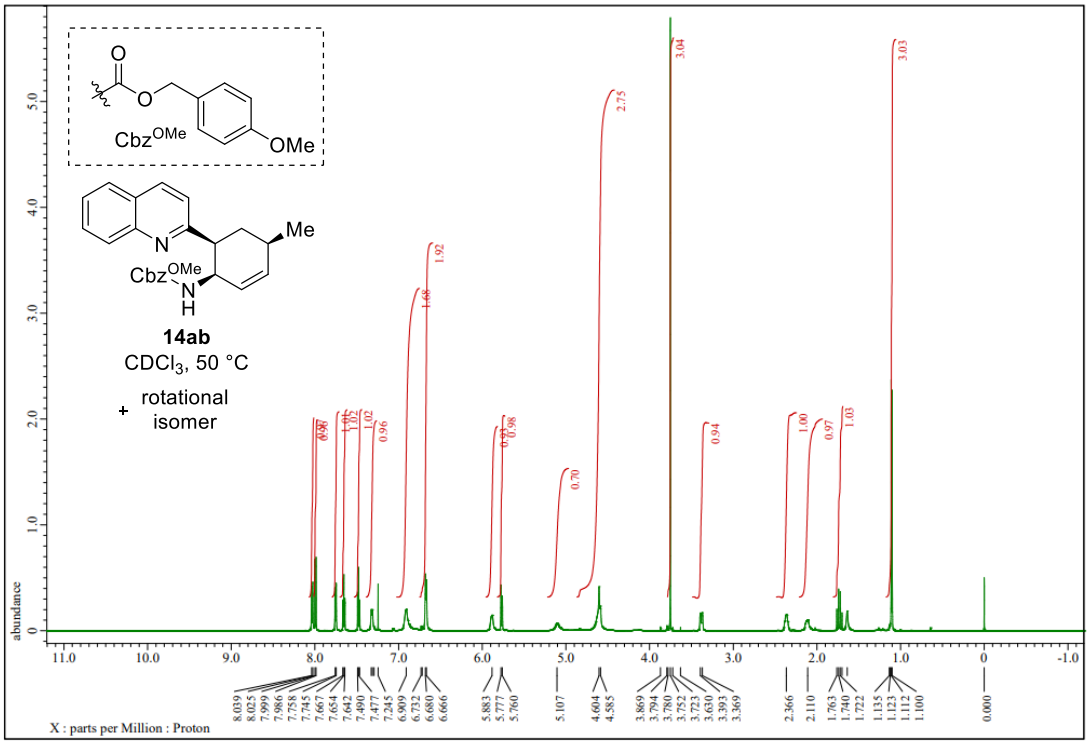
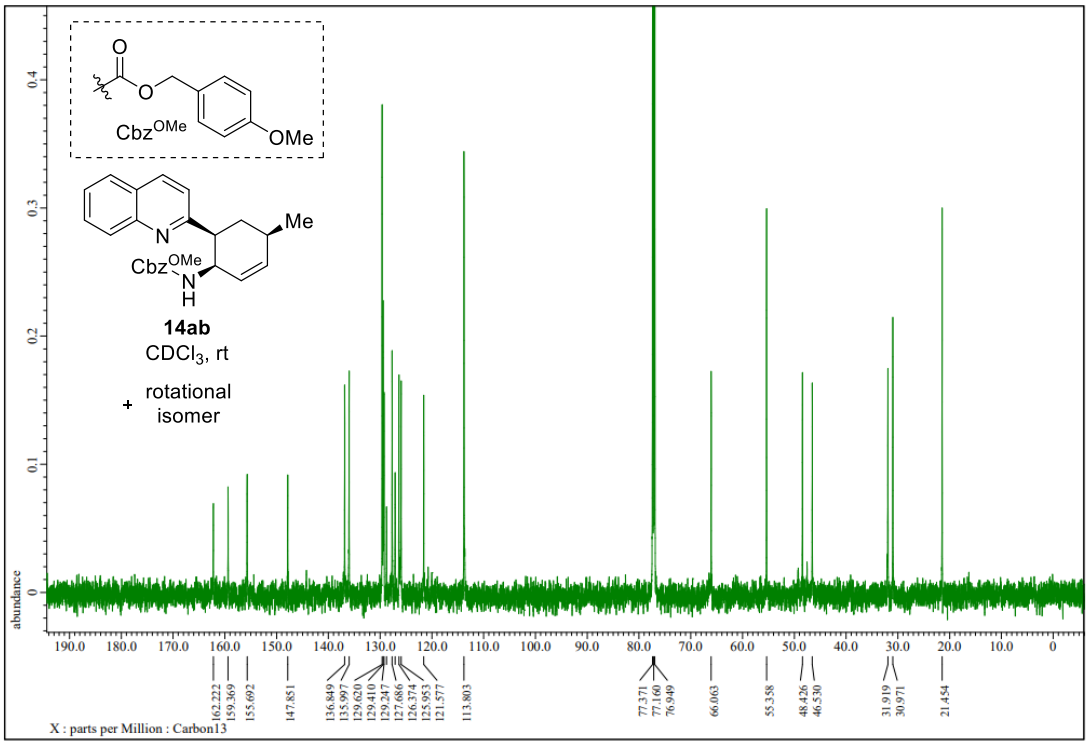




^{1}H and ^{13}C NMR charts of **14ab**.





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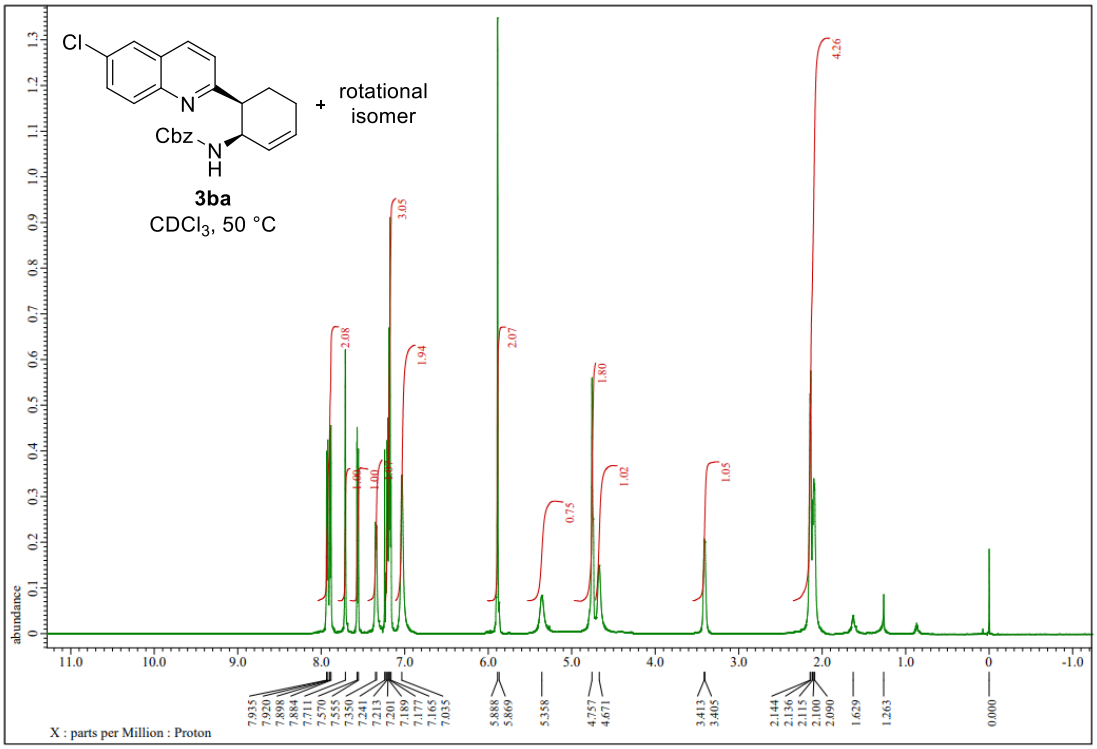
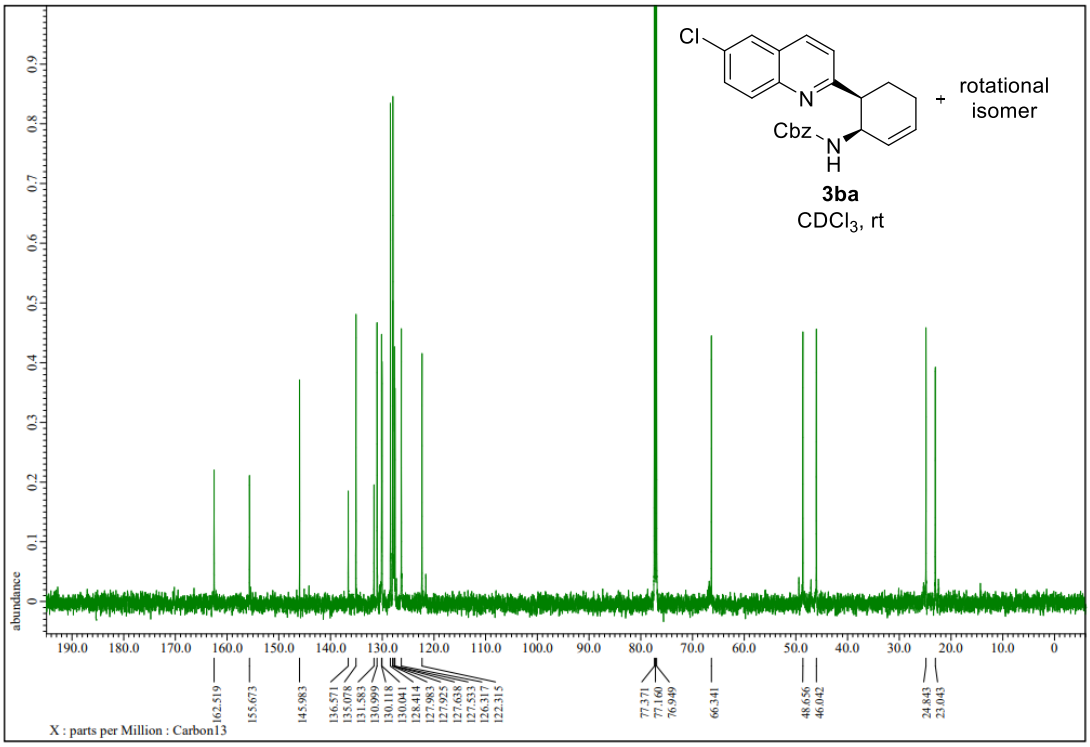
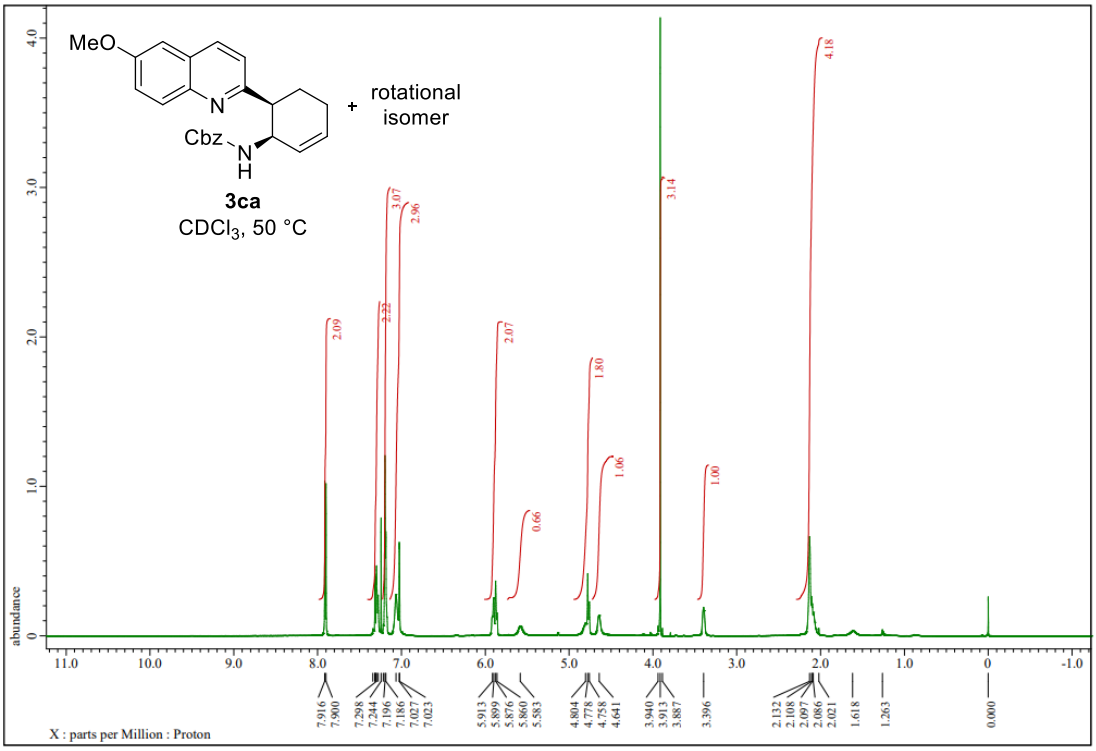
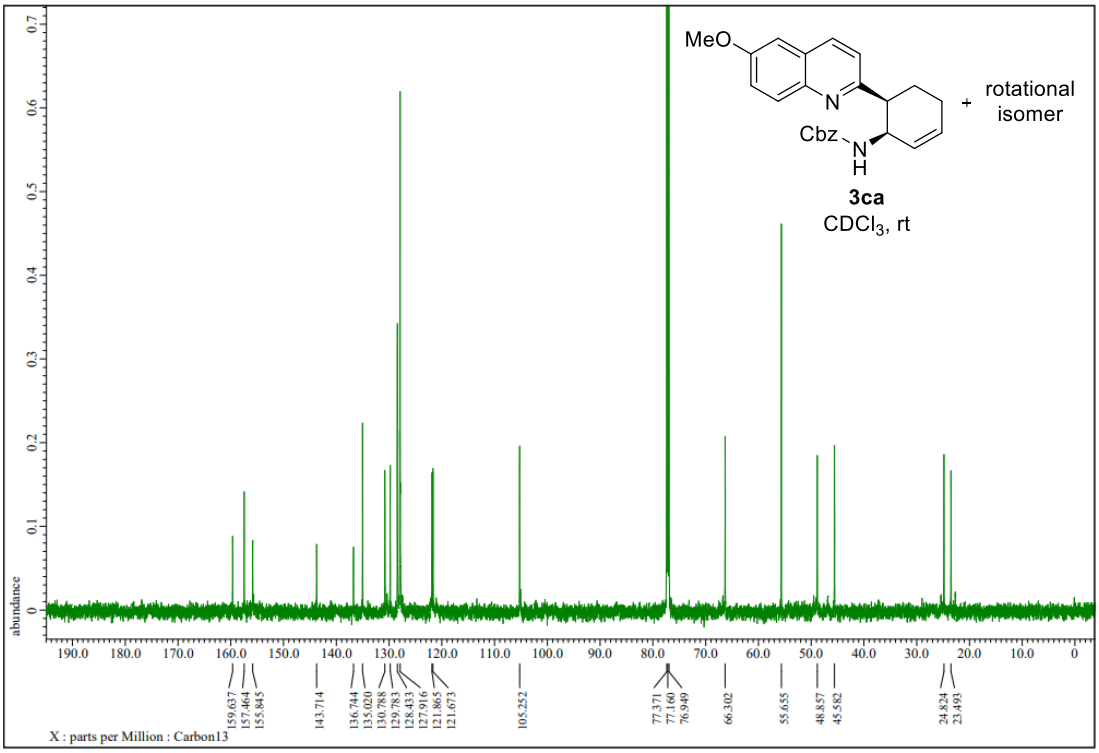


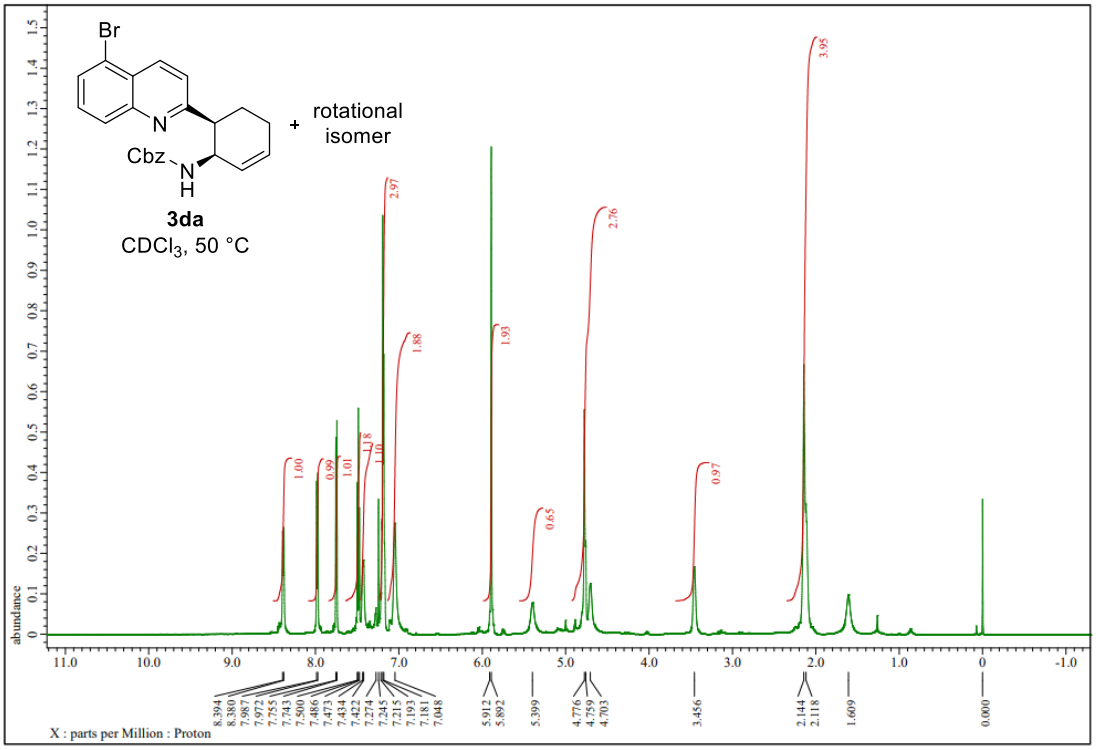


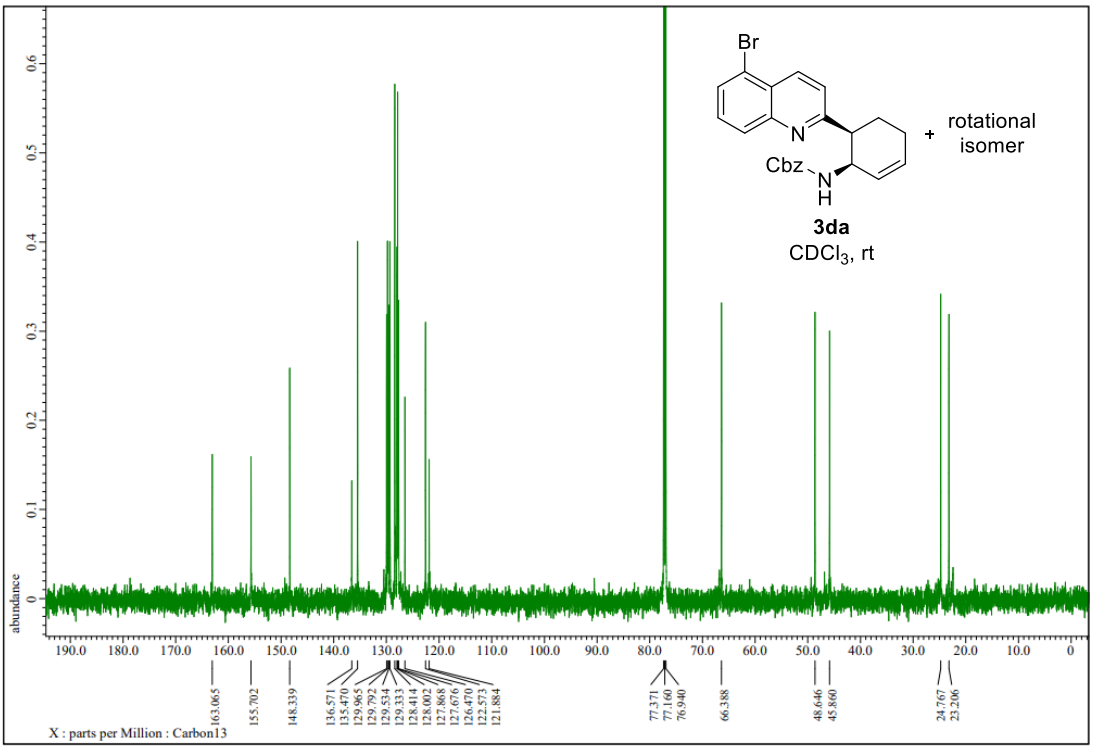
^{1}H and ^{13}C NMR charts of **3ca**.



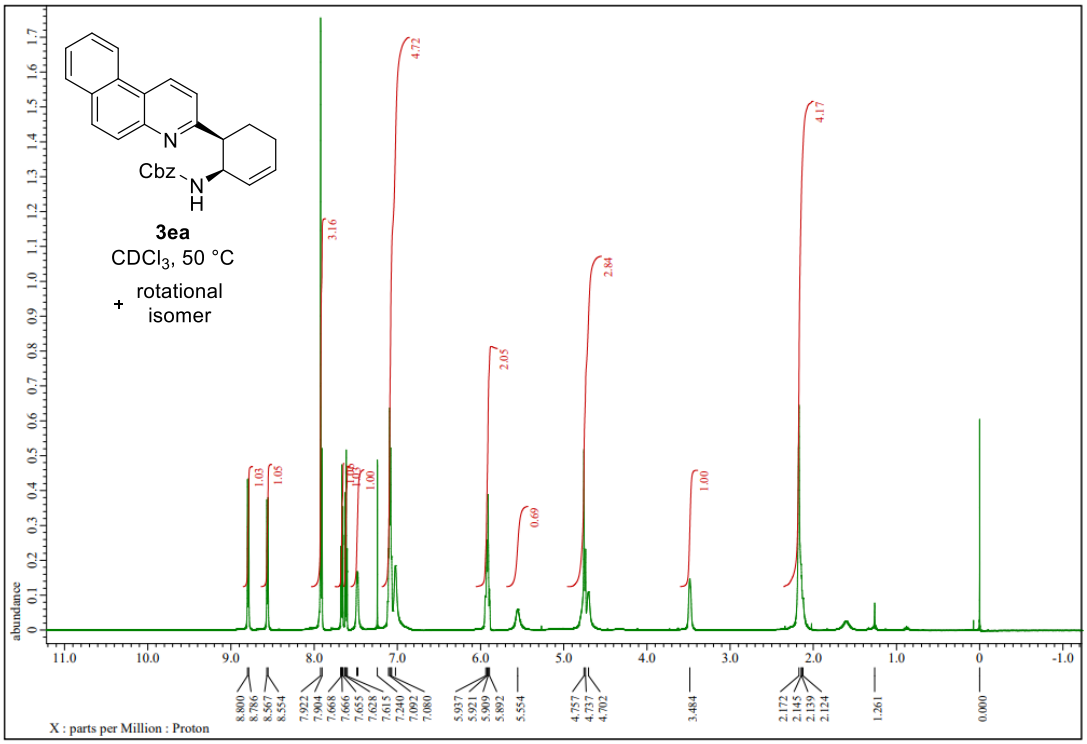


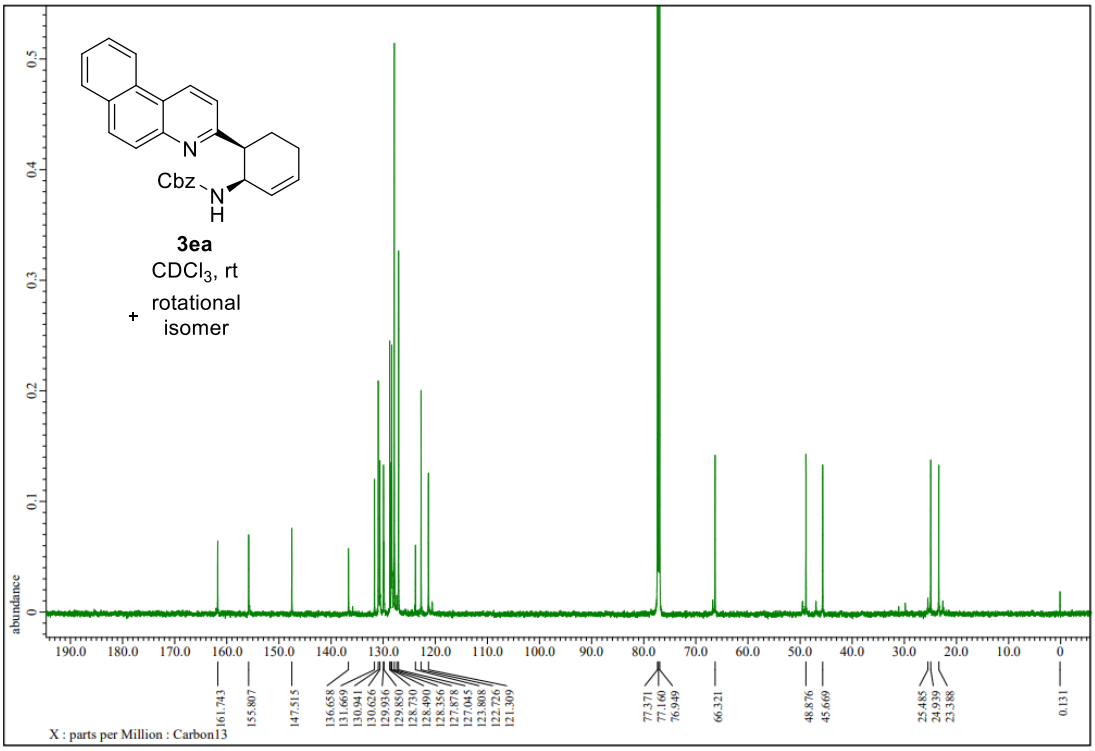
^{1}H and ^{13}C NMR charts of **3da**.



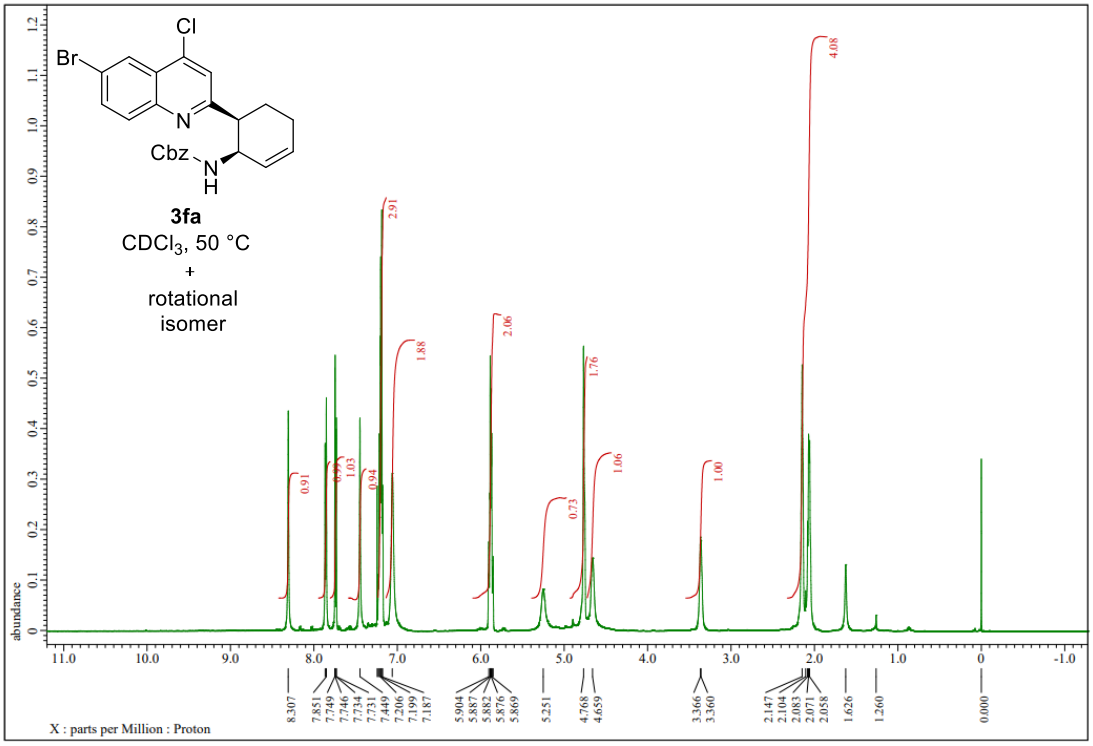


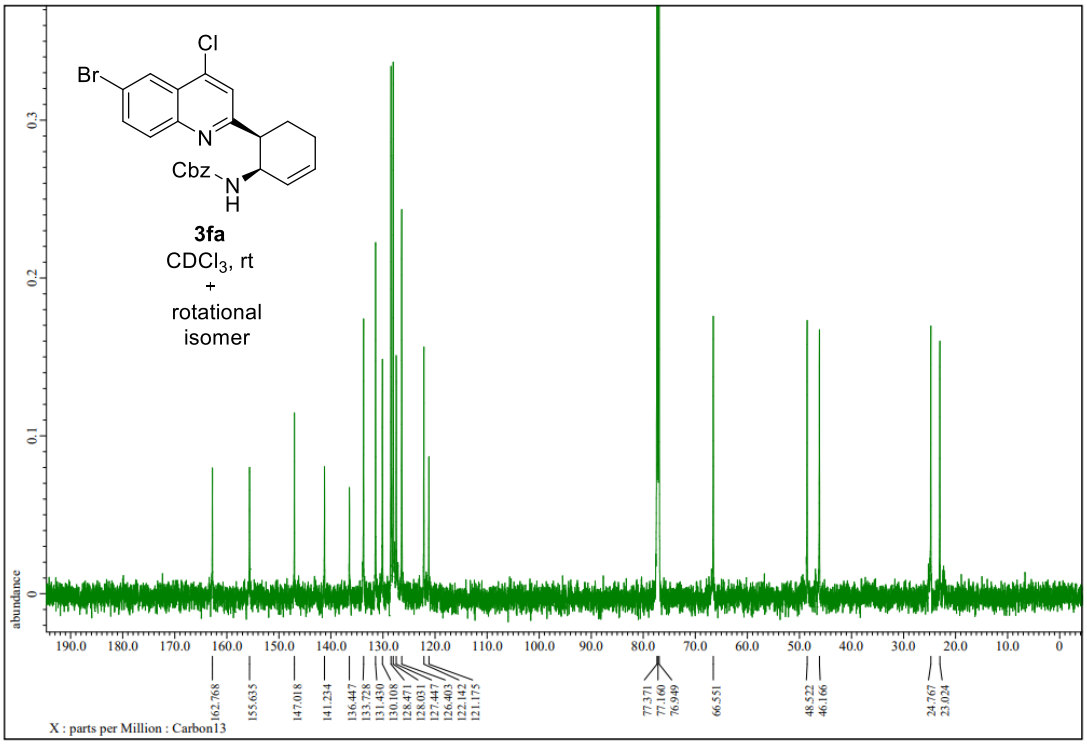
^{1}H and ^{13}C NMR charts of **3ea**.



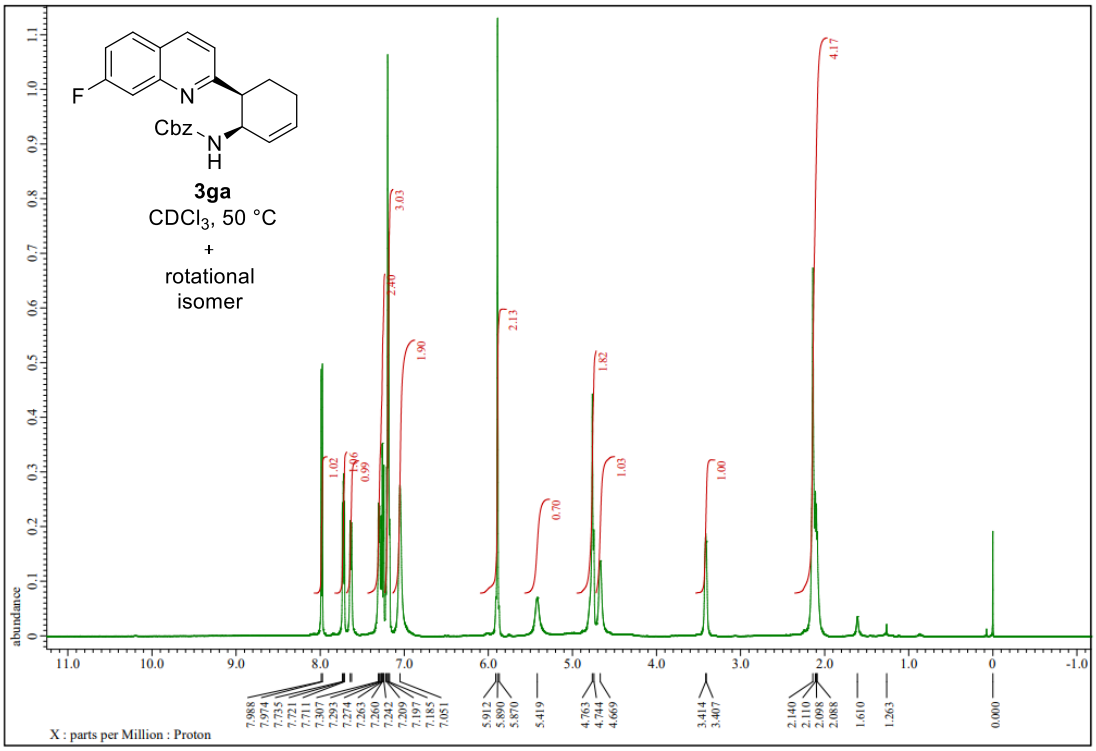


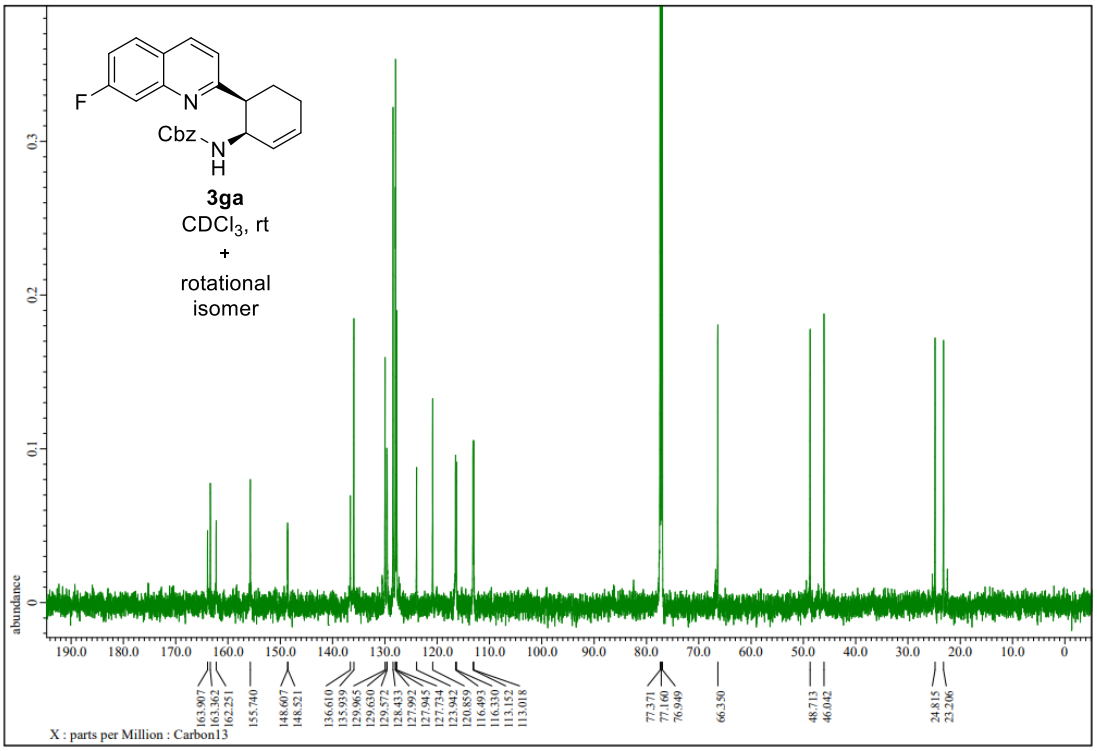
^{1}H and ^{13}C NMR charts of **3fa**.

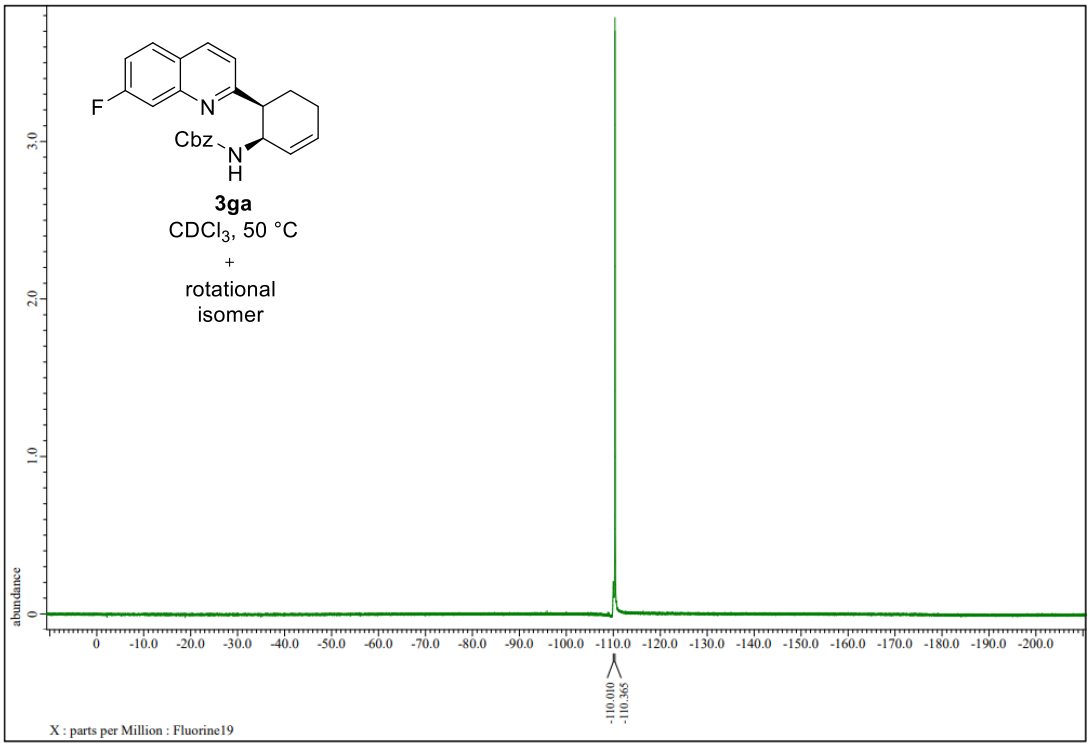




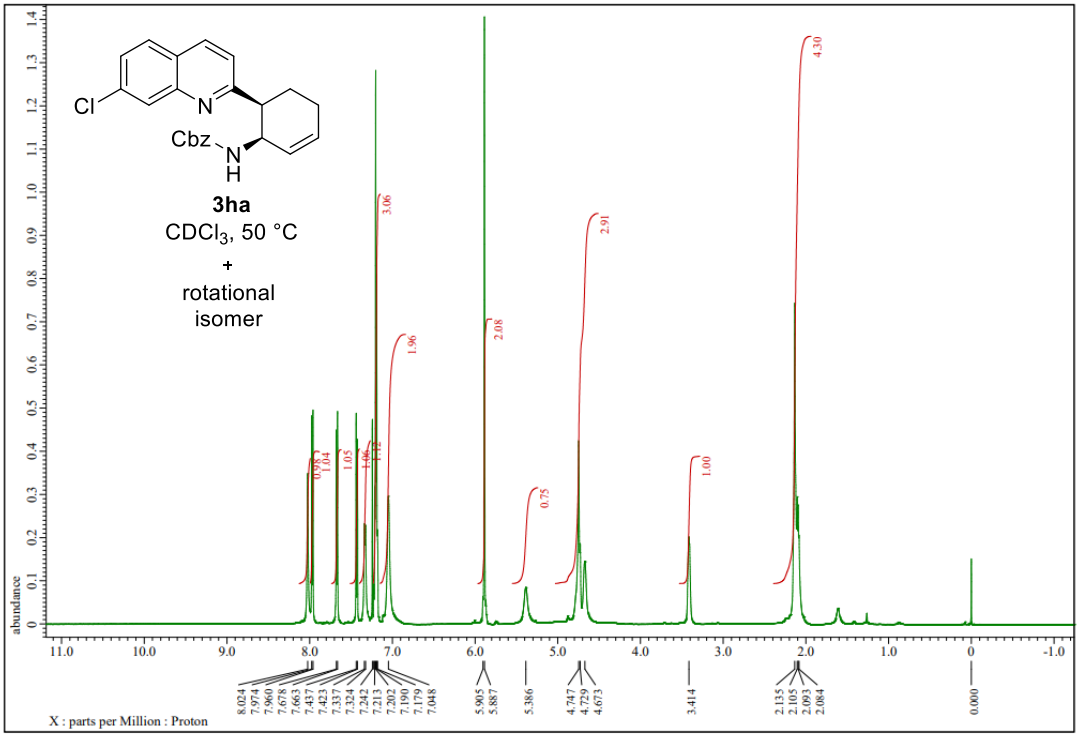
^{1}H, ^{13}C and ^{19}F NMR charts of **3ga**.

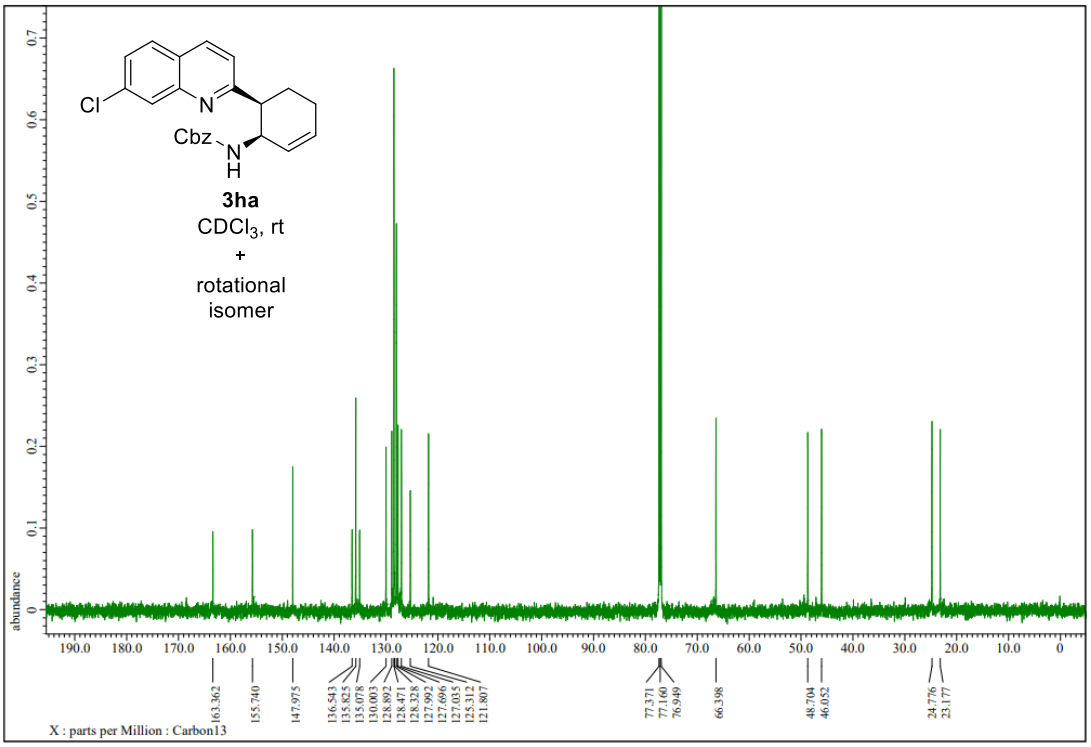




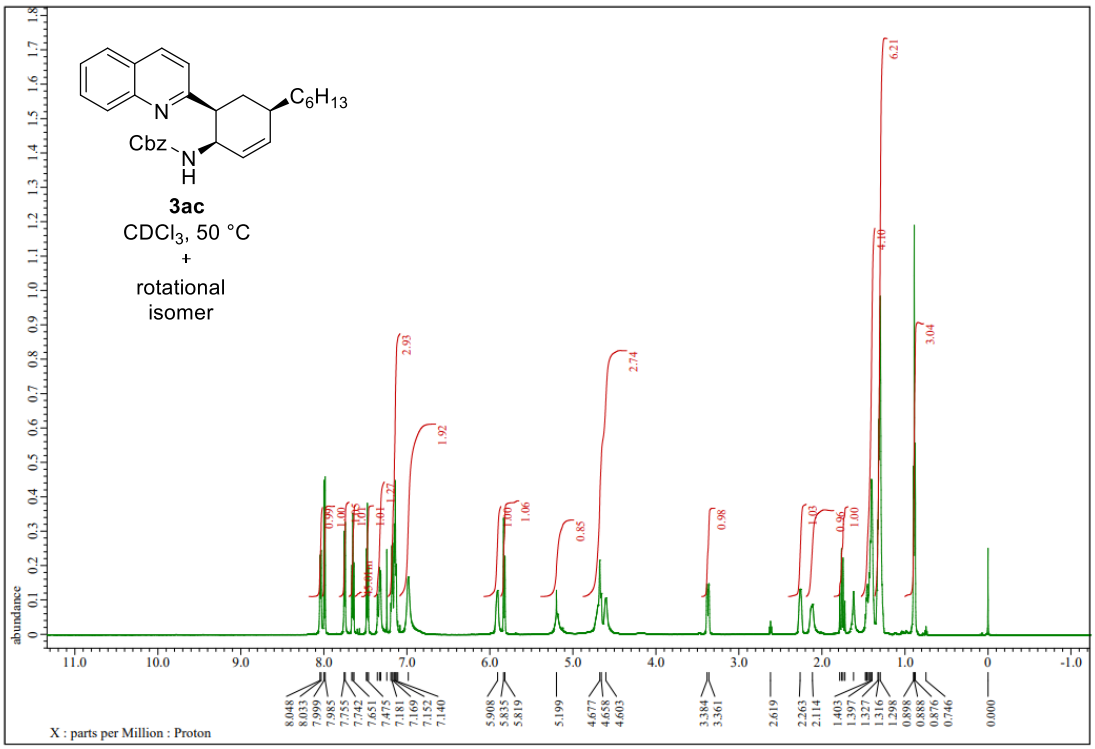

F
N
Cbz
N
H
3ga
CDCl3, 50 °C
+
rotational
isomer
abundance
3.0
2.0
1.0
0
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-190.0
-200.0
-110.010
-110.365
X : parts per Million : Fluorine19

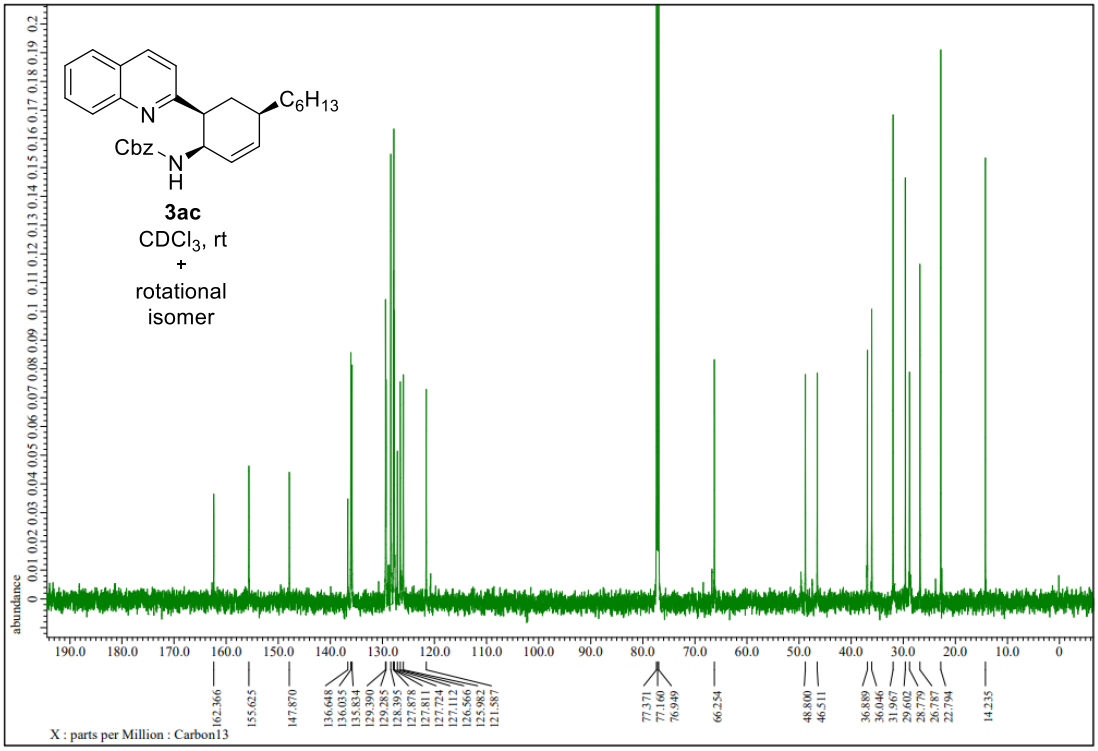
^{1}H and ^{13}C NMR charts of **3ha**.



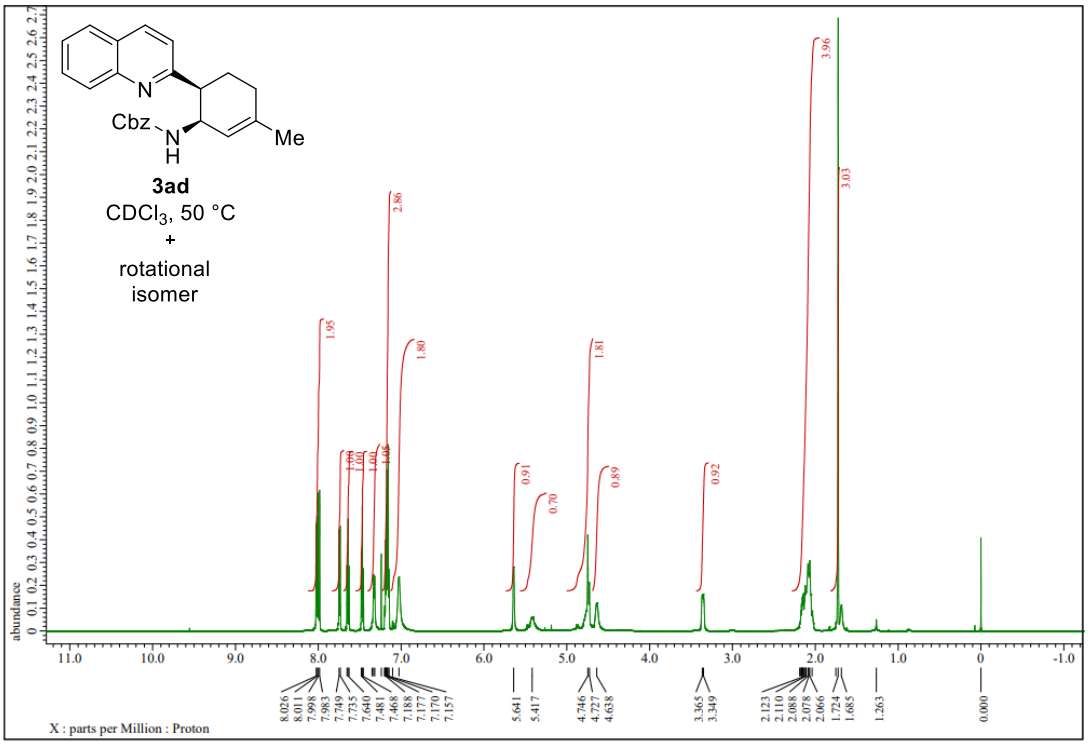


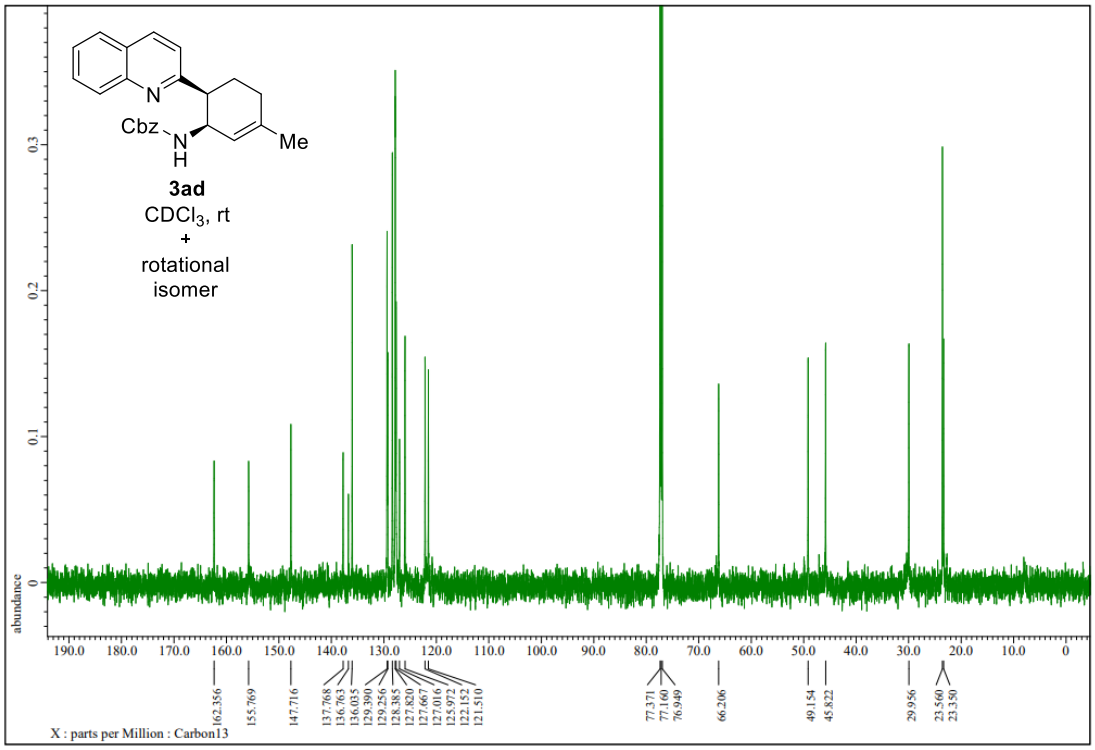
^{1}H and ^{13}C NMR charts of **3ac**.



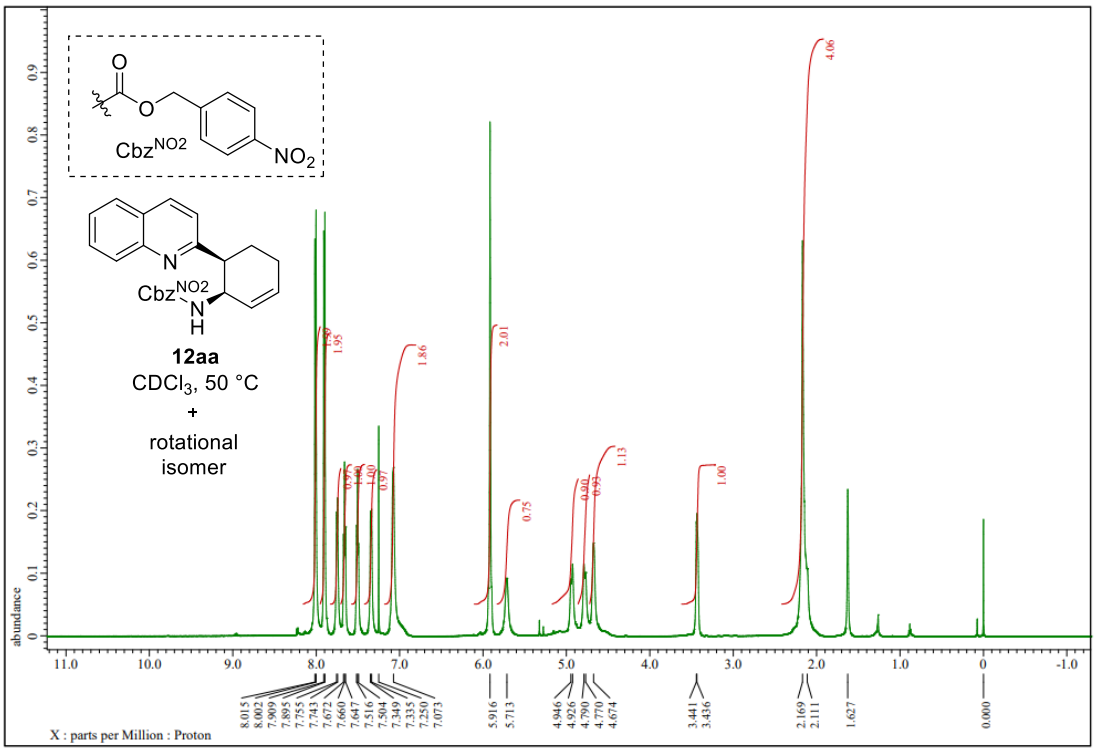


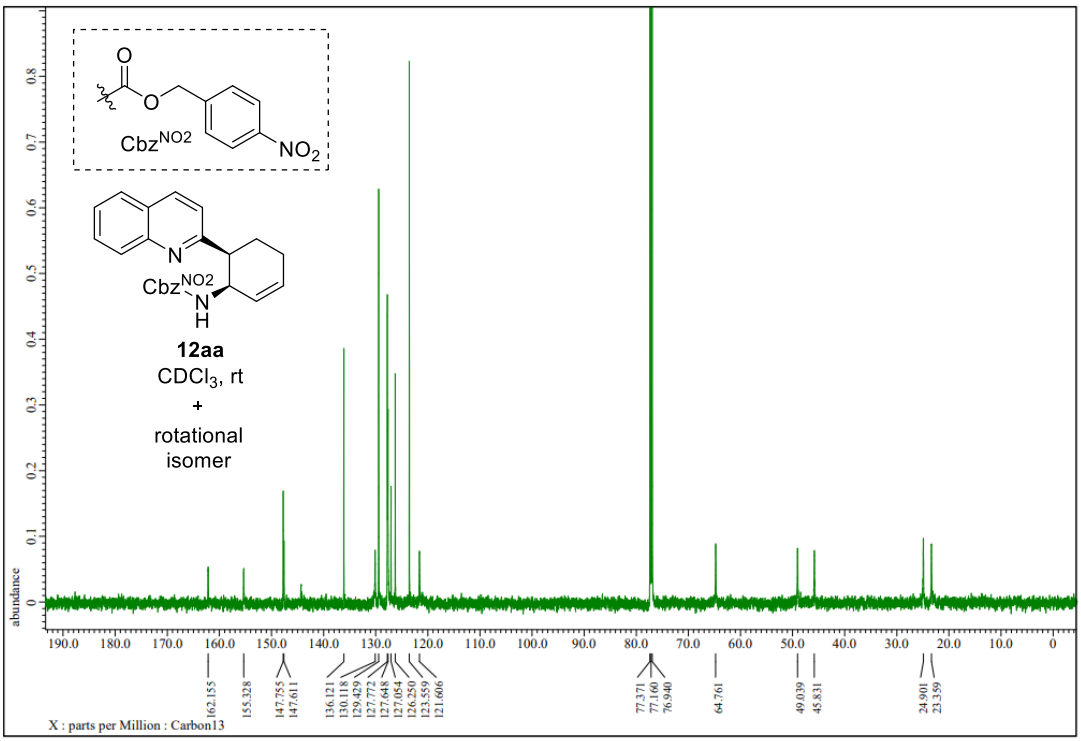
^{1}H and ^{13}C NMR charts of **3ad**.



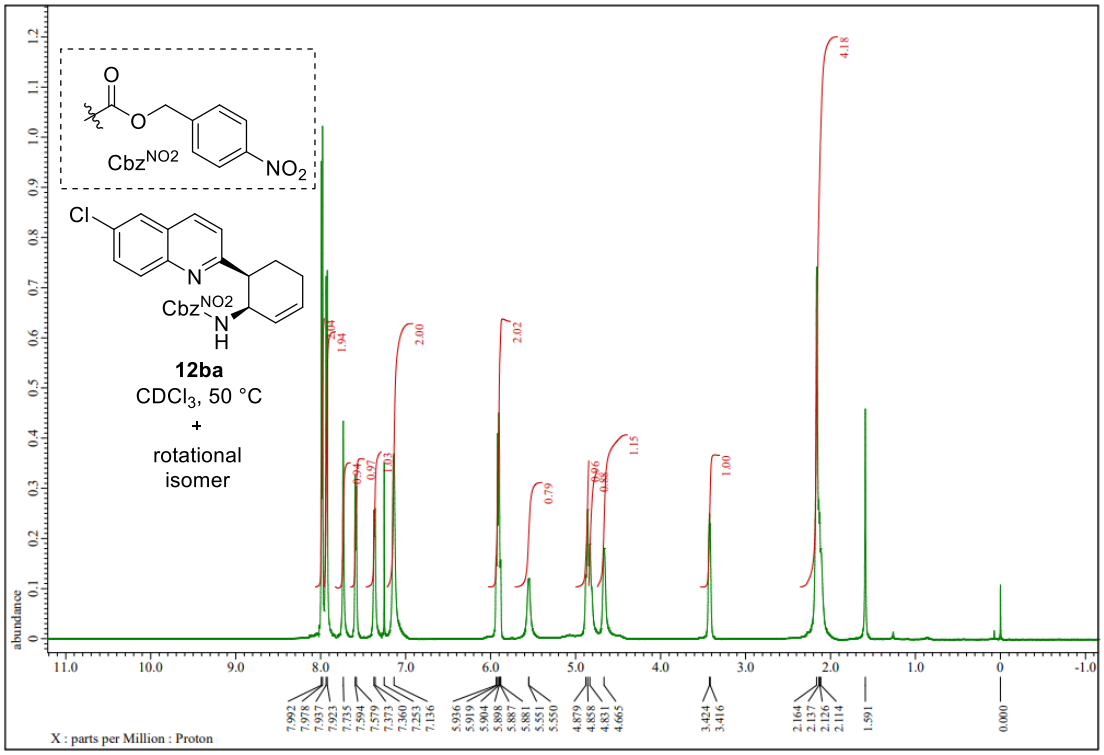


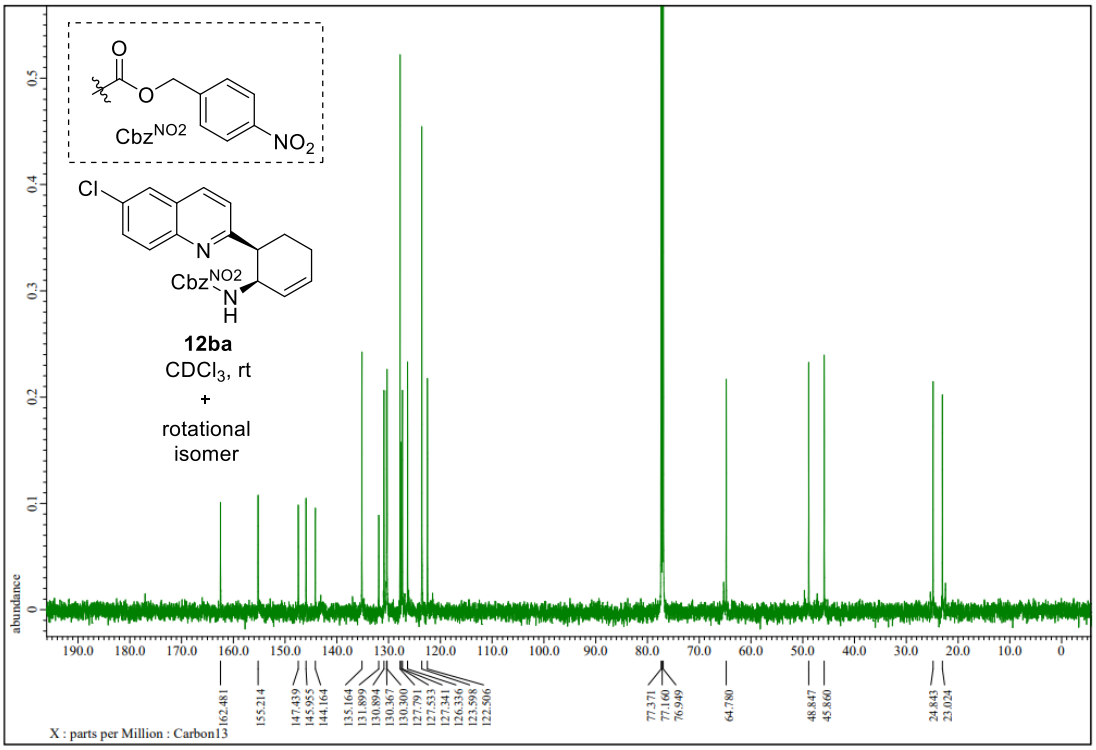
^{1}H and ^{13}C NMR charts of **12aa**.



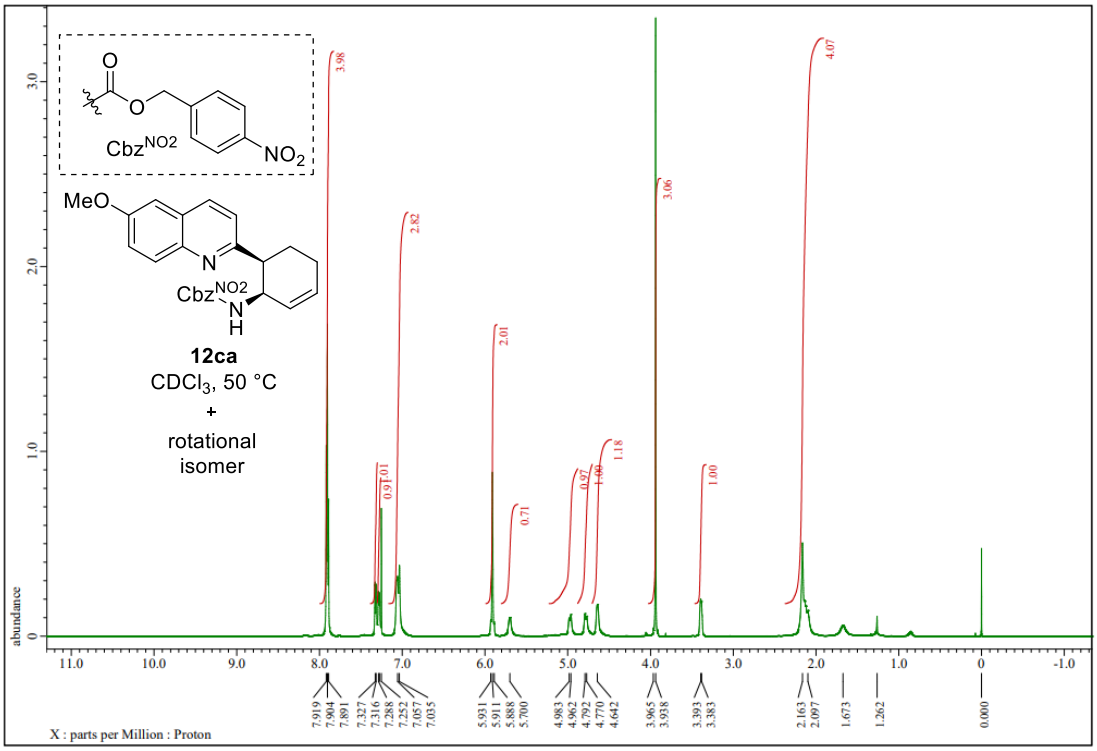


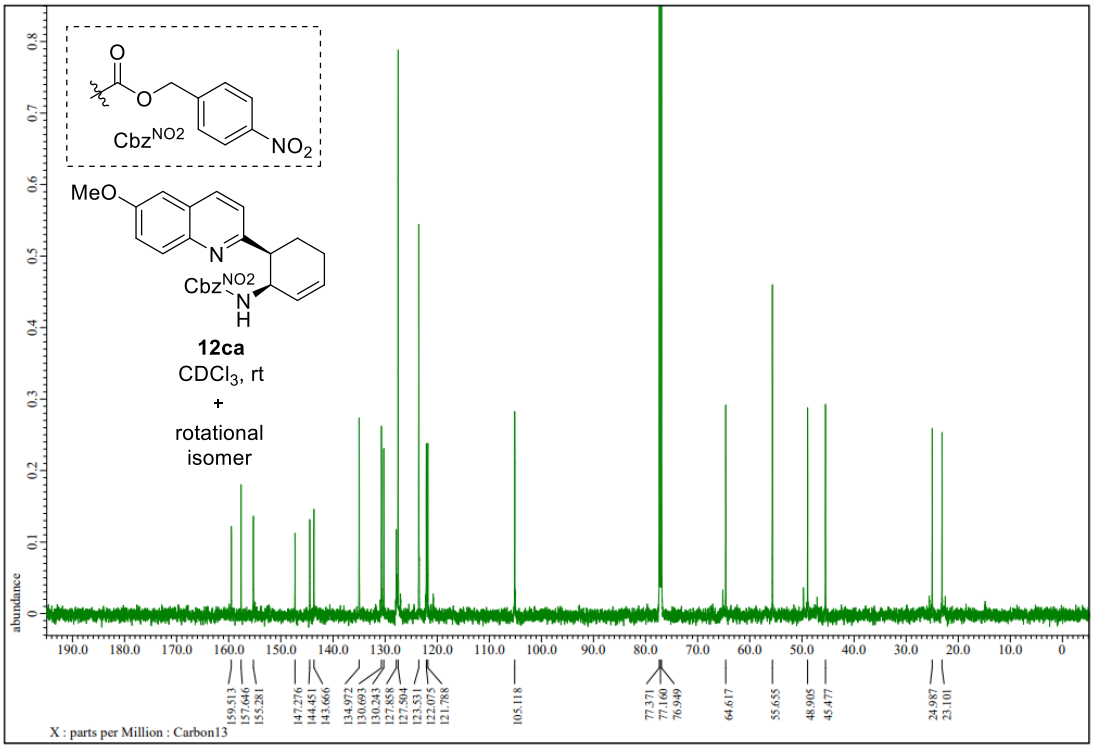
^{1}H and ^{13}C NMR charts of **12ba**.



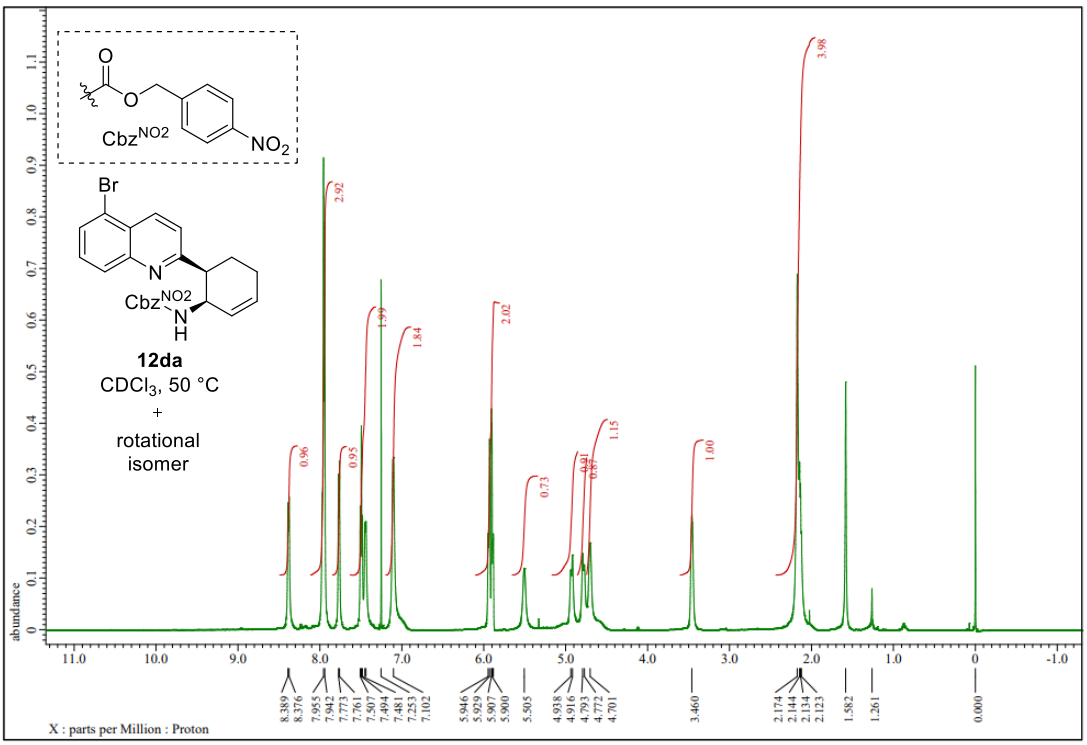


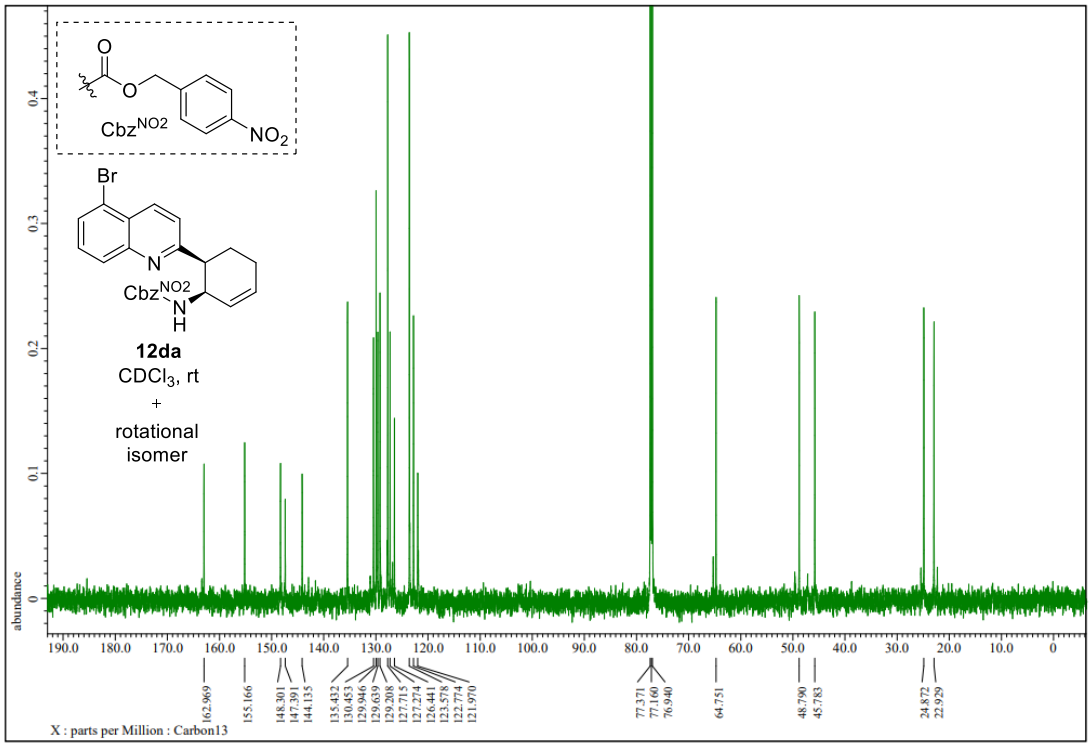
^{1}H and ^{13}C NMR charts of **12ca**.



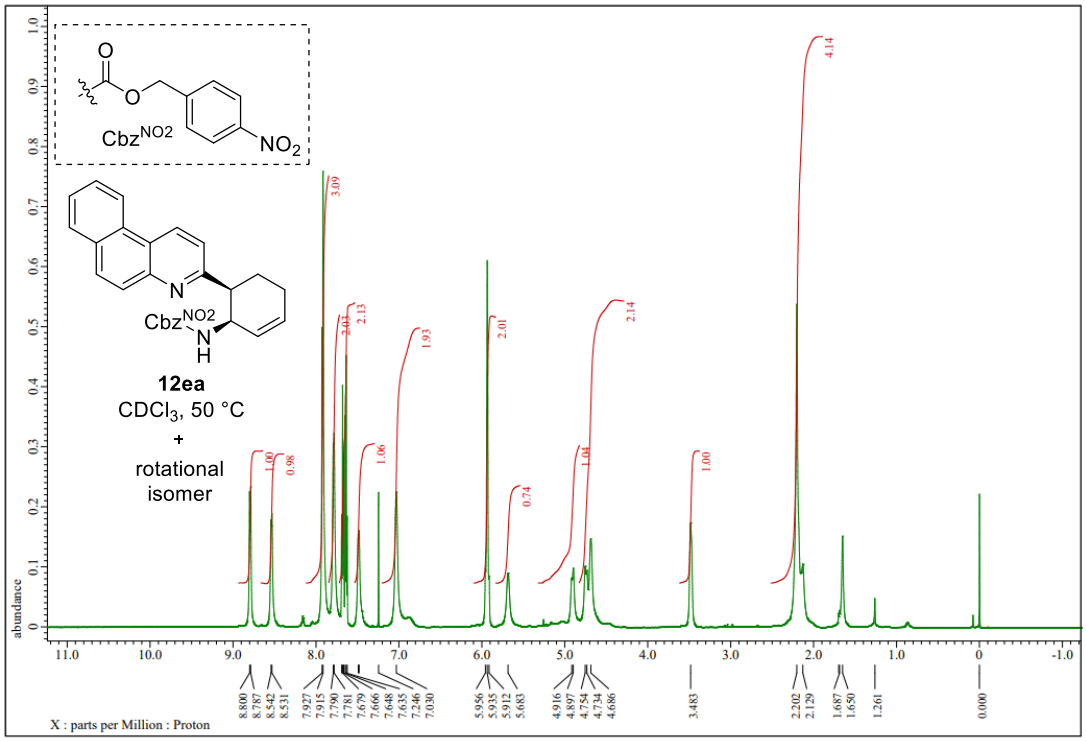


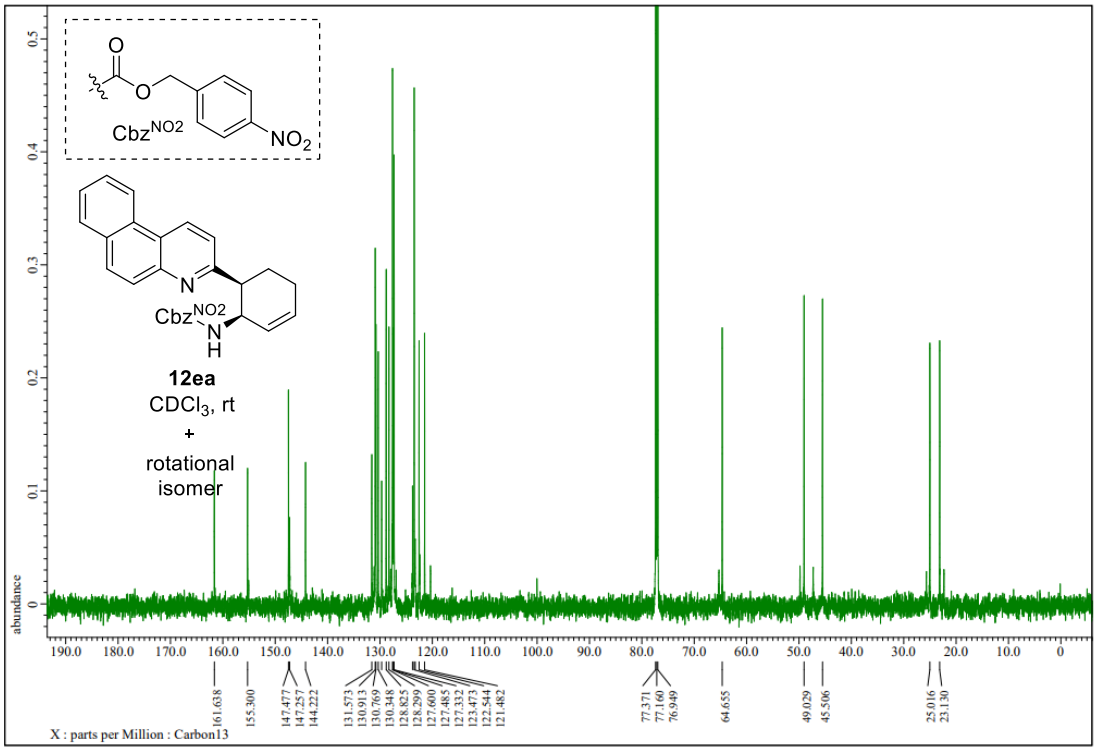
^{1}H and ^{13}C NMR charts of **12da**.



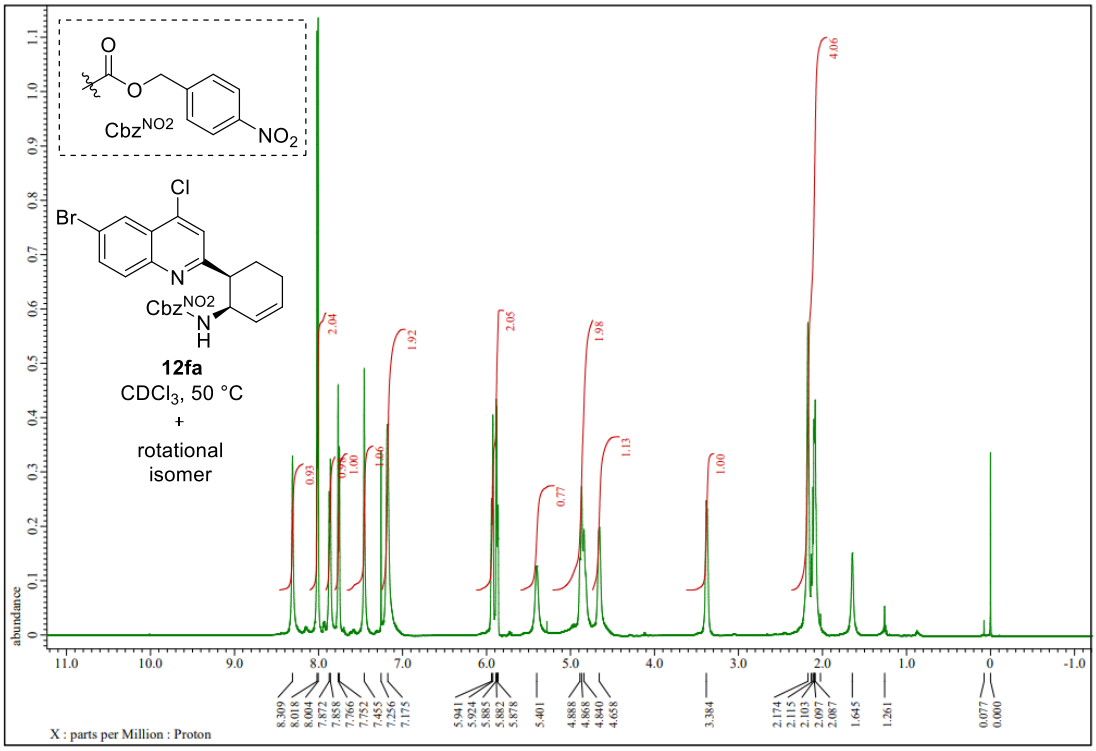


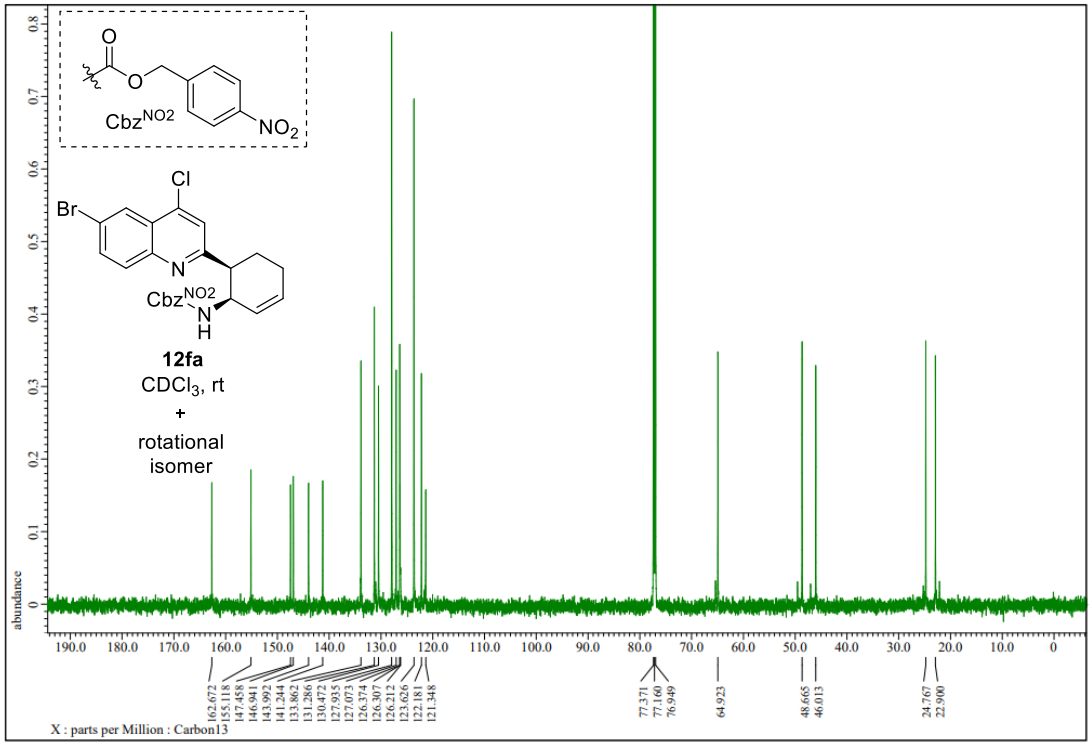
^{1}H and ^{13}C NMR charts of **12ea**.



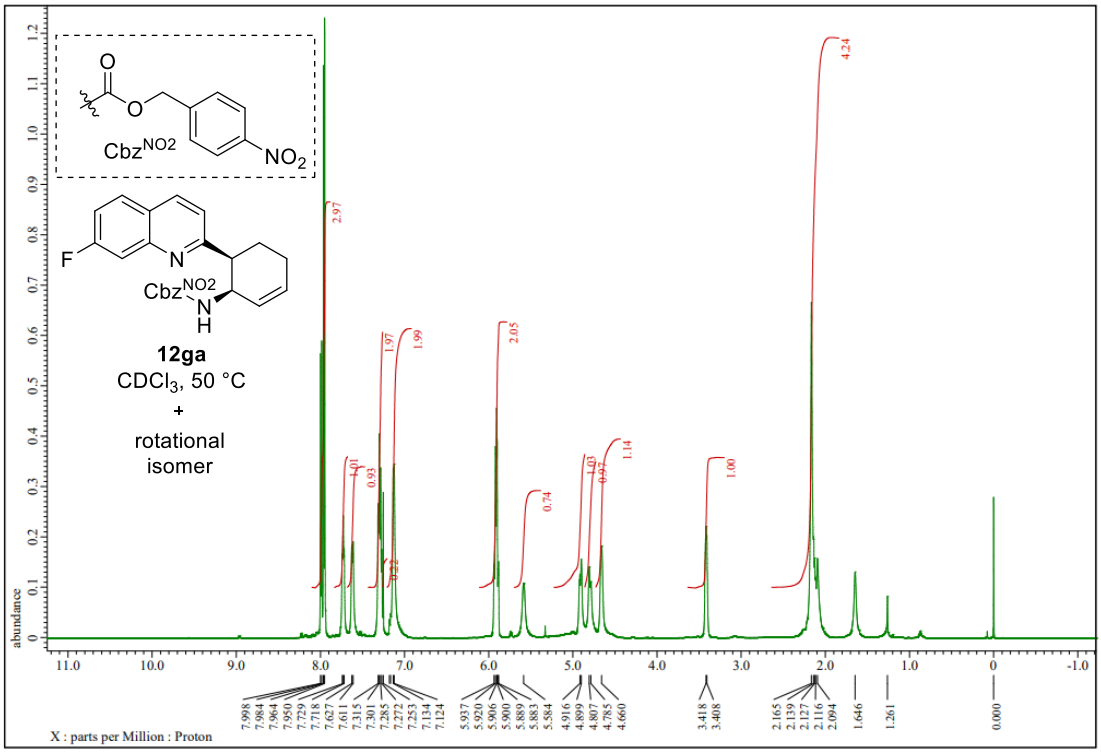


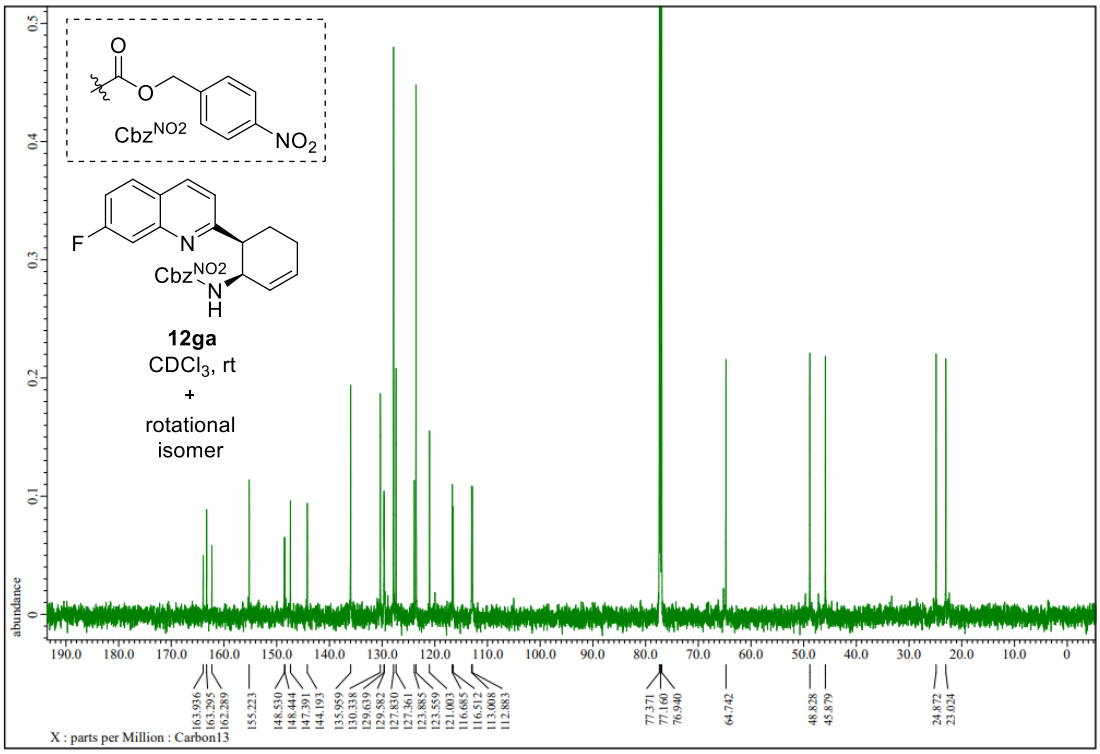
^{1}H and ^{13}C NMR charts of **12fa**.

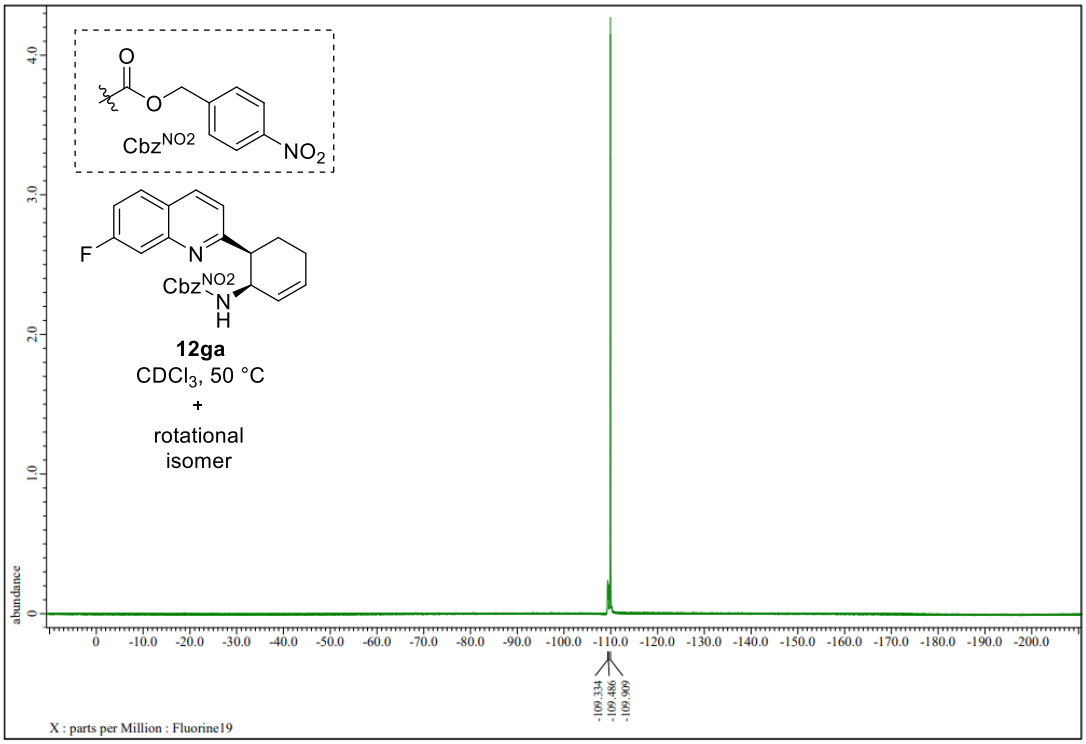




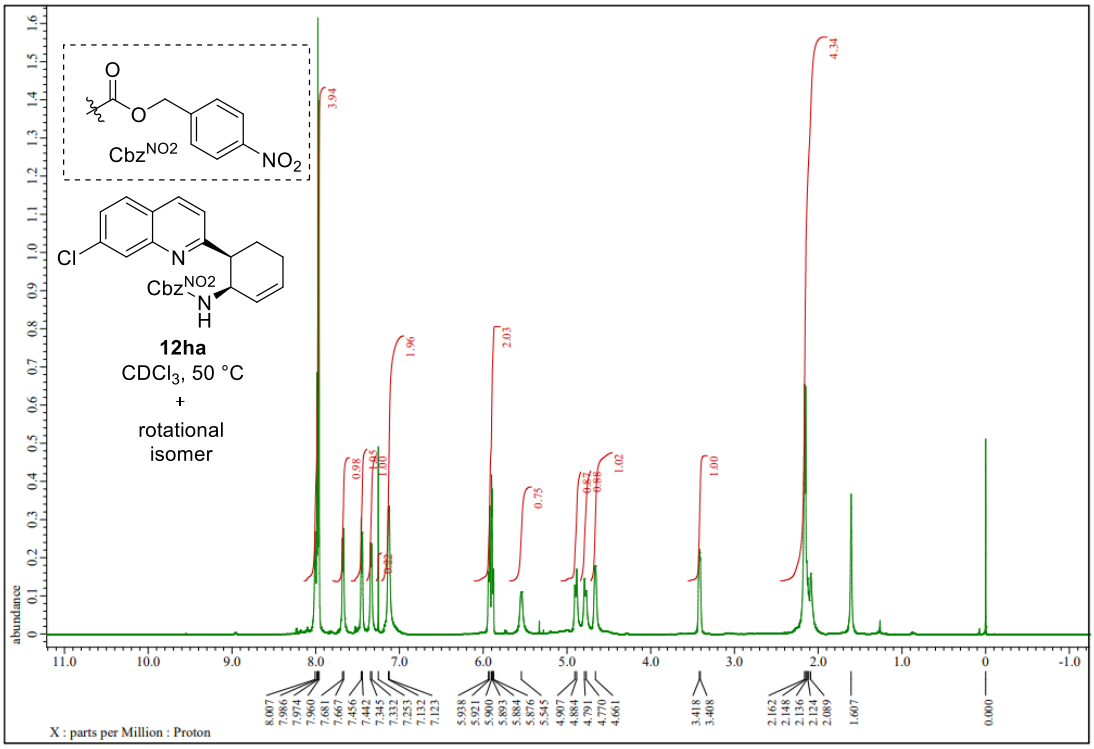
^{1}H, ^{13}C and ^{19}F NMR charts of **12ga**.

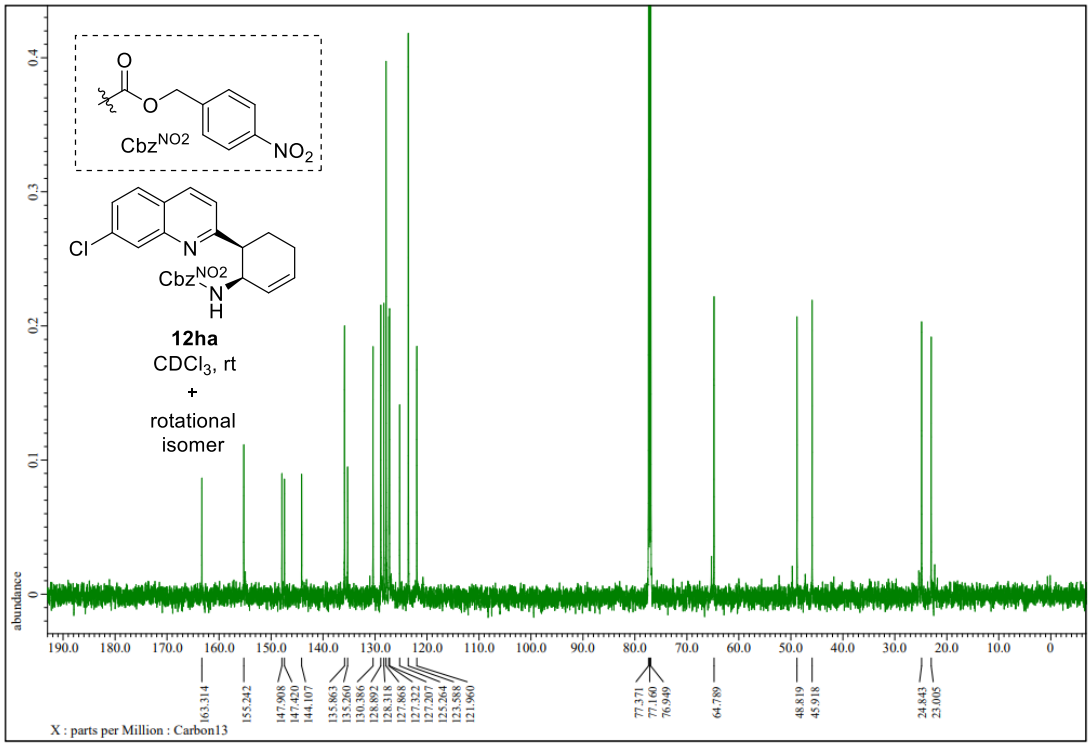




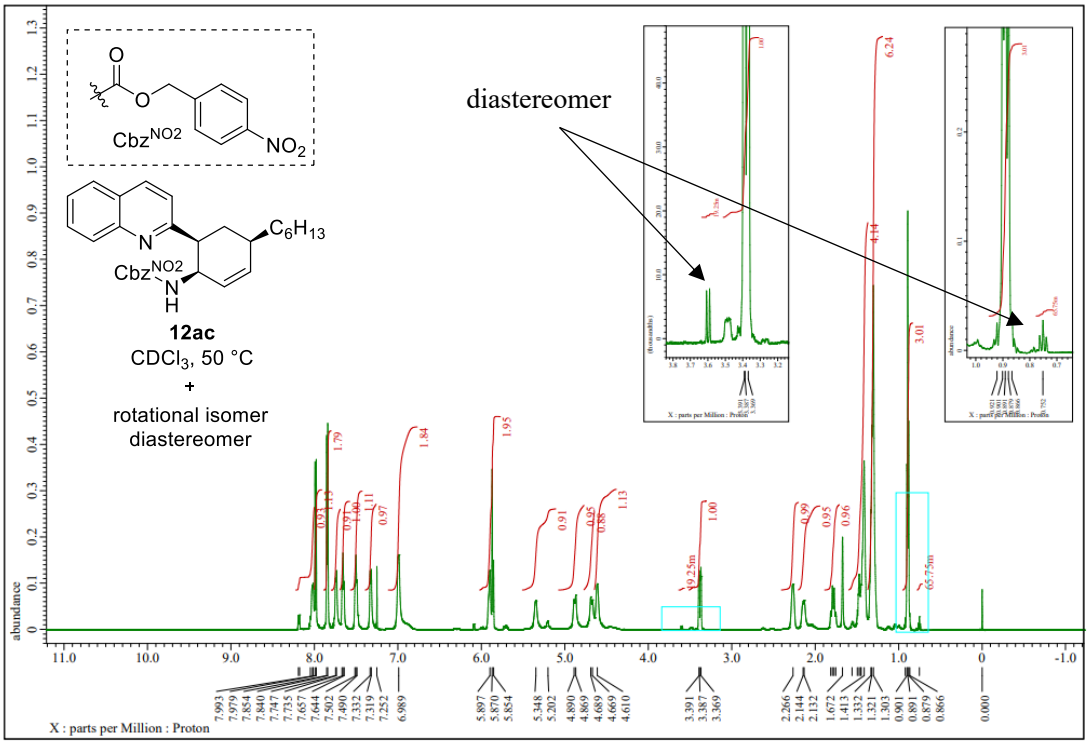

O
O
Cbz
NO2
NO2
F
N
Cbz
NO2
N
H
12ga
CDCl3, 50 °C
+
rotational
isomer
abundance
4.0
3.0
2.0
1.0
0
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-190.0
-200.0
-109.334
-109.486
-109.909
X : parts per Million : Fluorine19

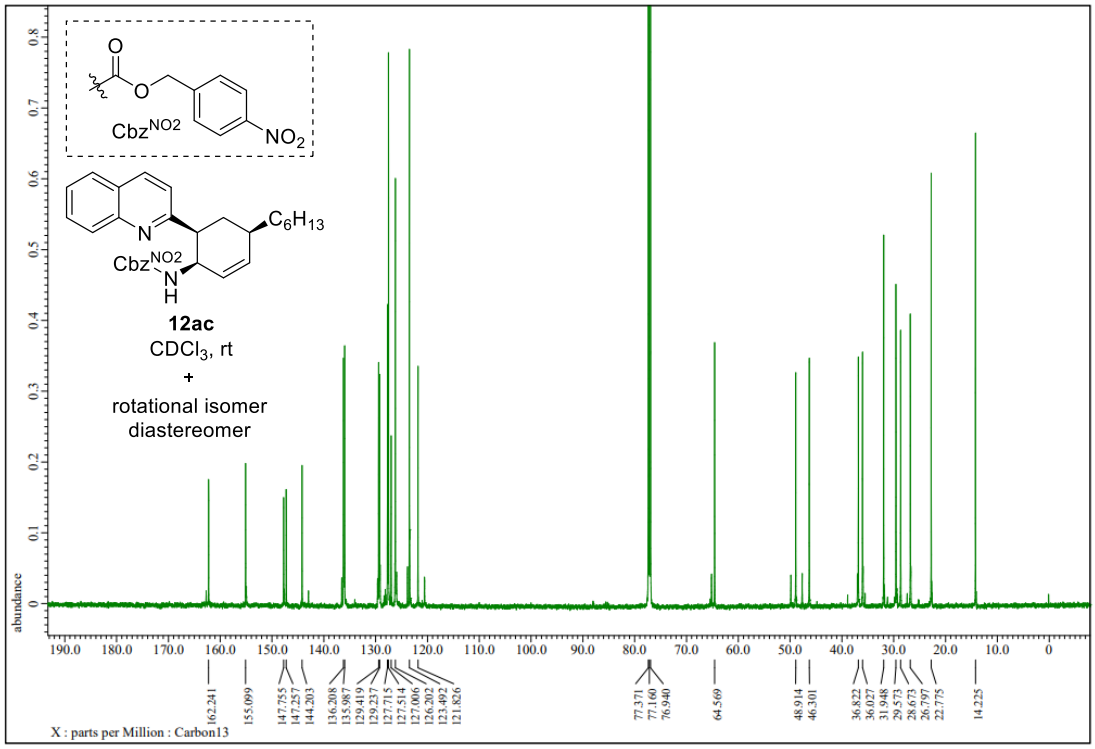
^{1}H and ^{13}C NMR charts of **12ha**.



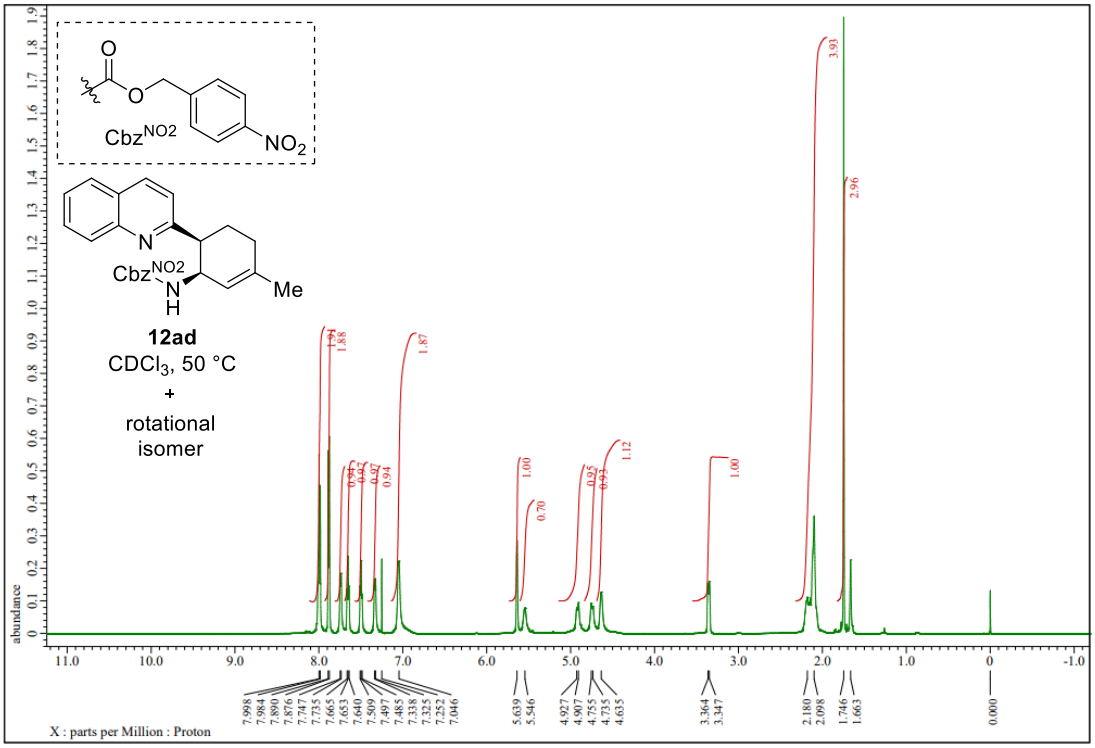


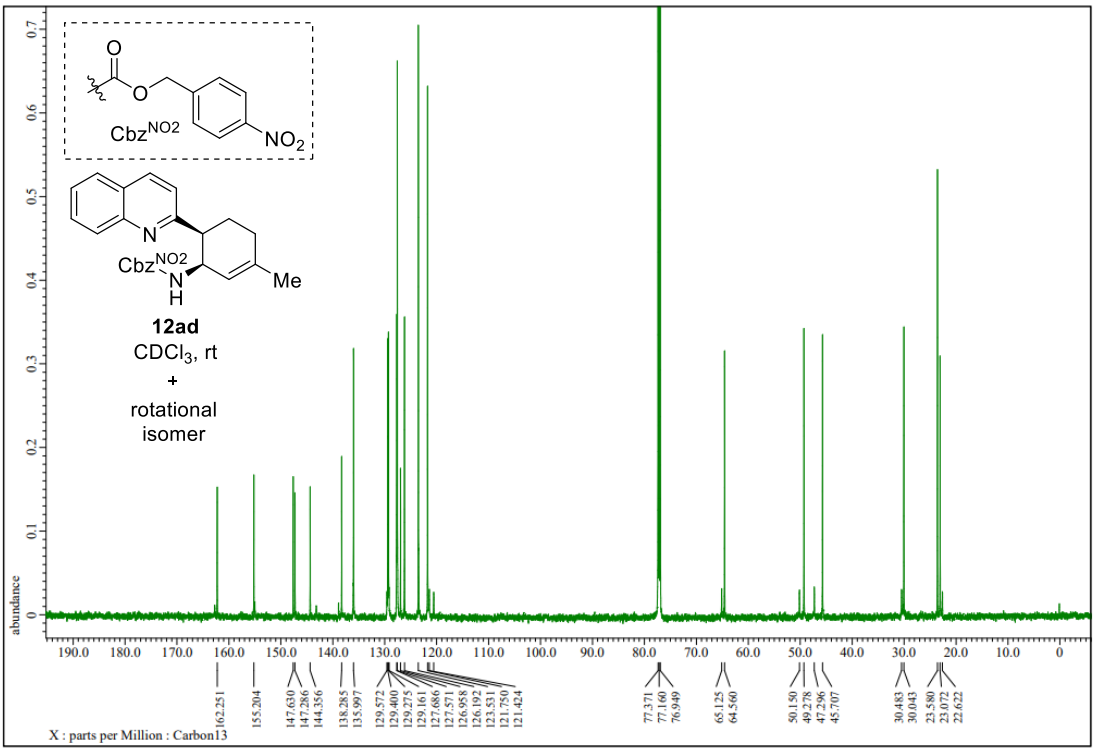
^{1}H and ^{13}C NMR charts of **12ac**.



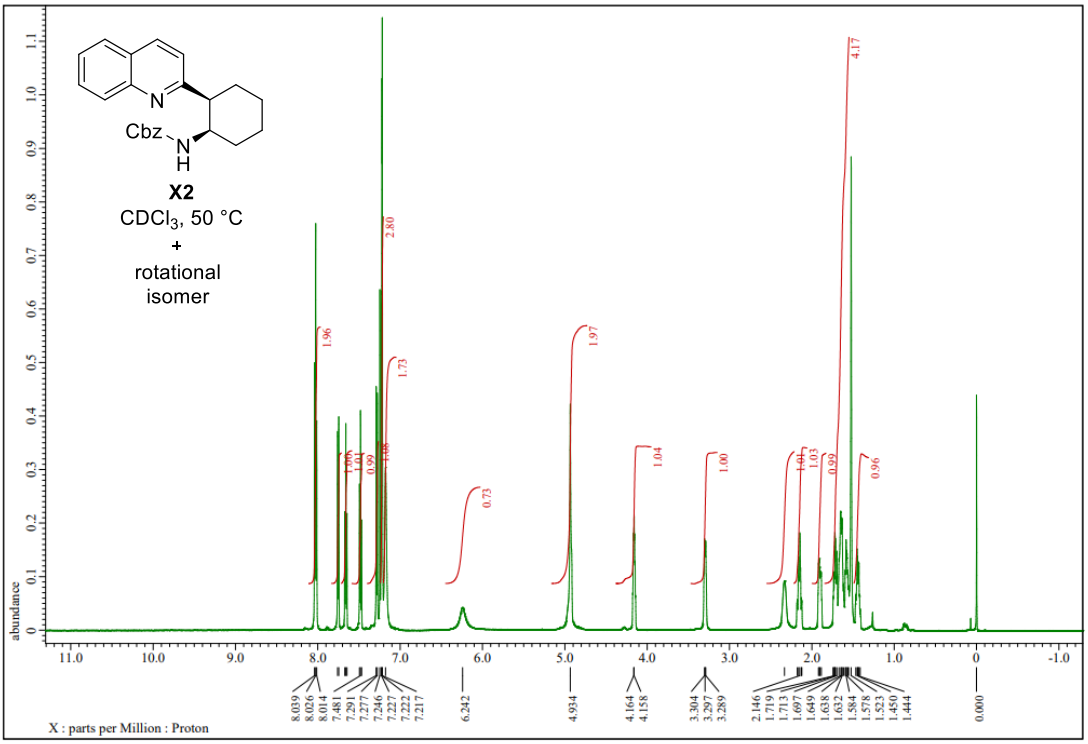


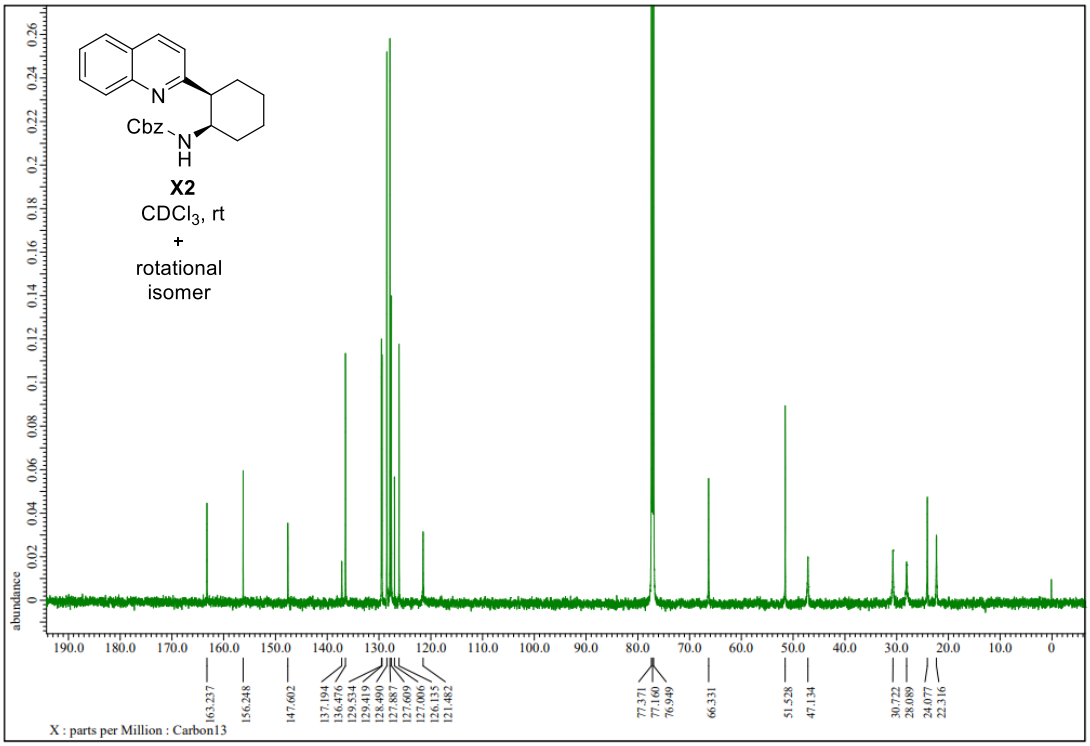
^{1}H and ^{13}C NMR charts of **12ad**.



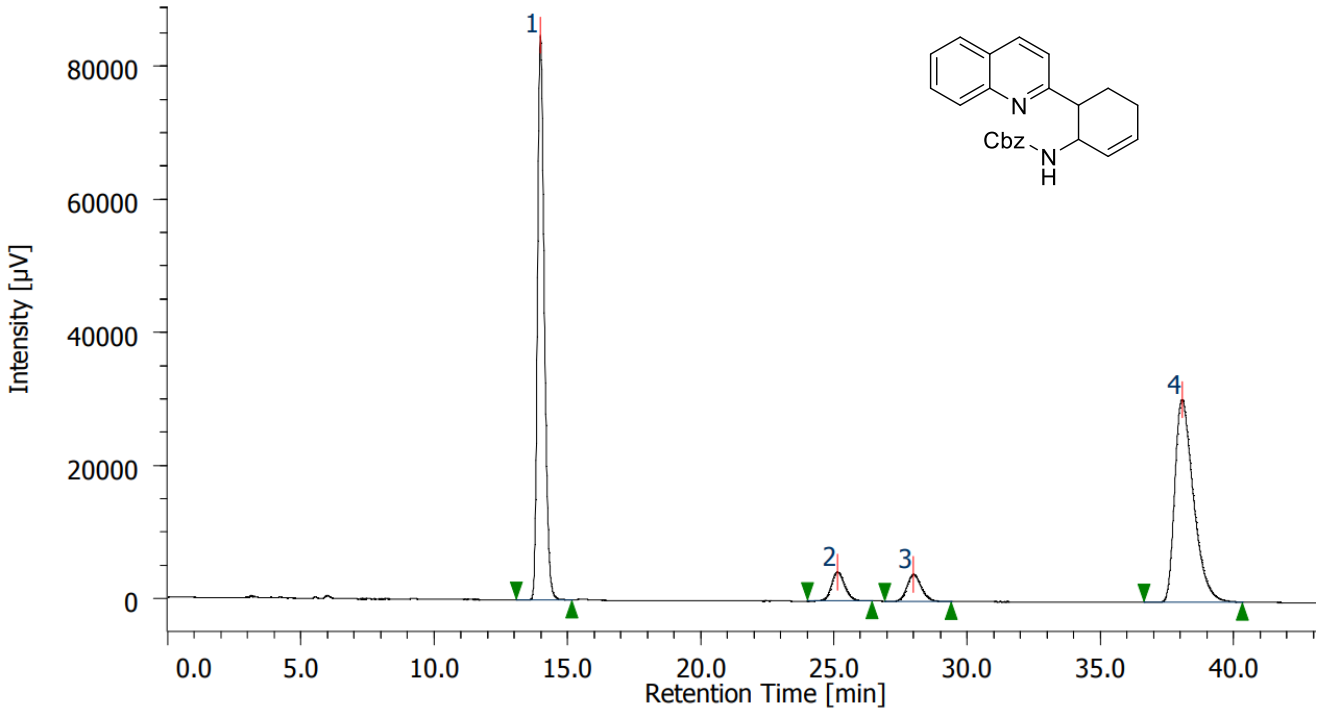


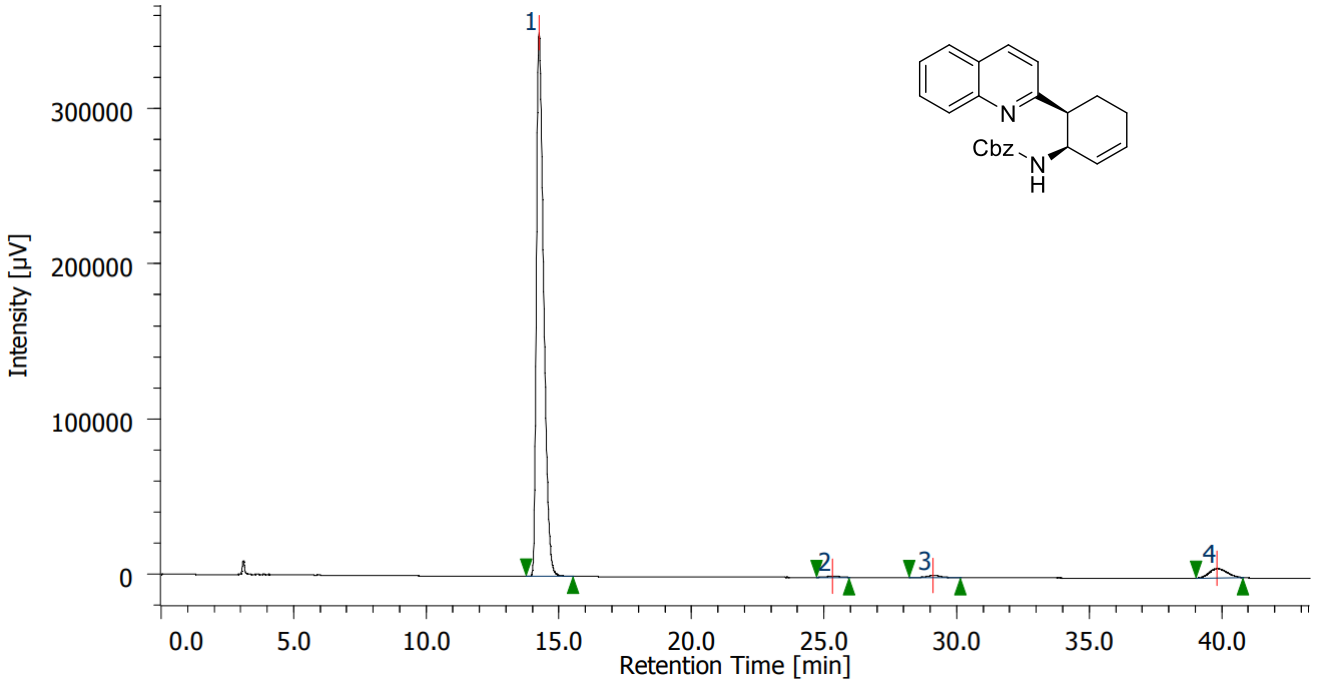
^{1}H and ^{13}C NMR charts of **X2**.





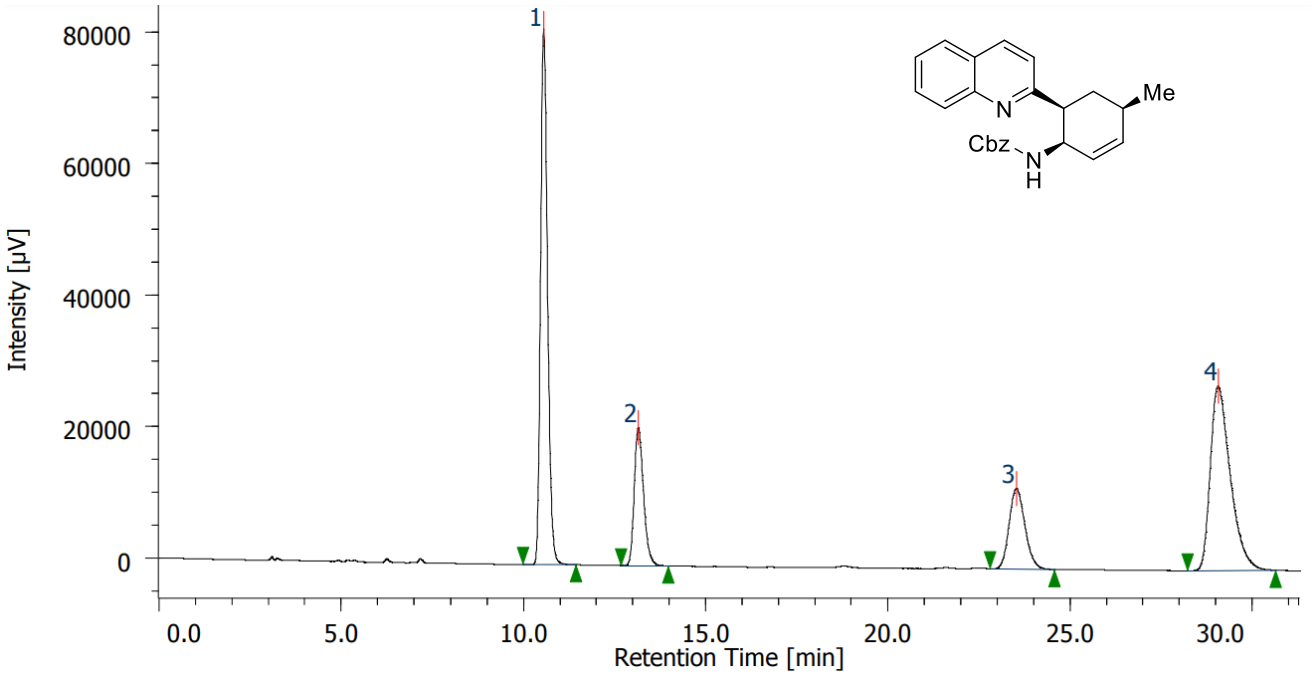
10. HPLC chart

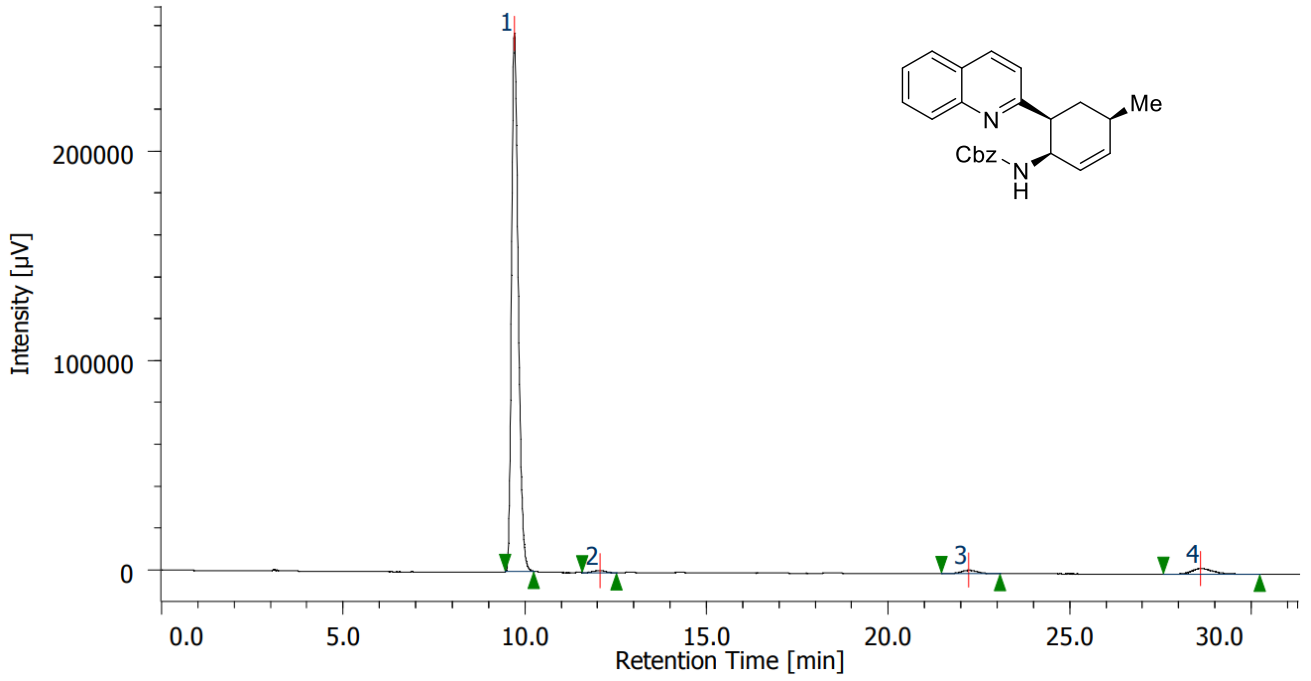




3aa

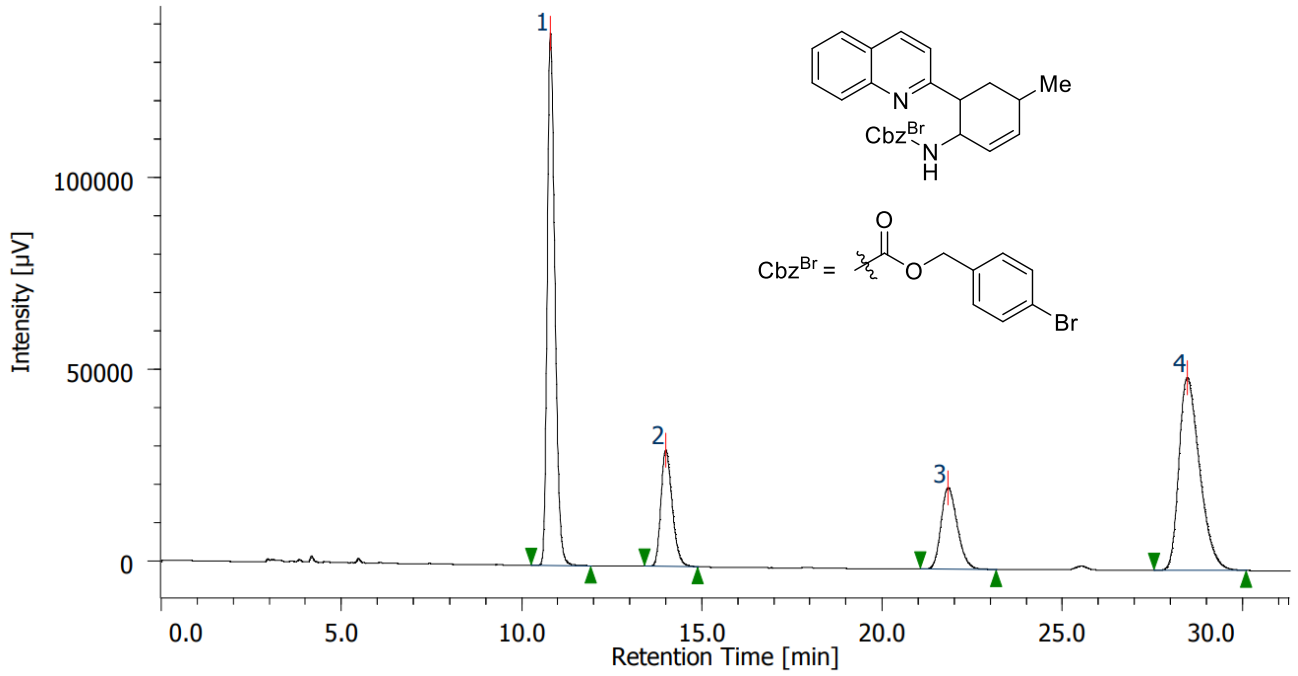
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	14.2	25.3	29.1	39.8
Area (%)	94.8	0.4	0.8	4.0

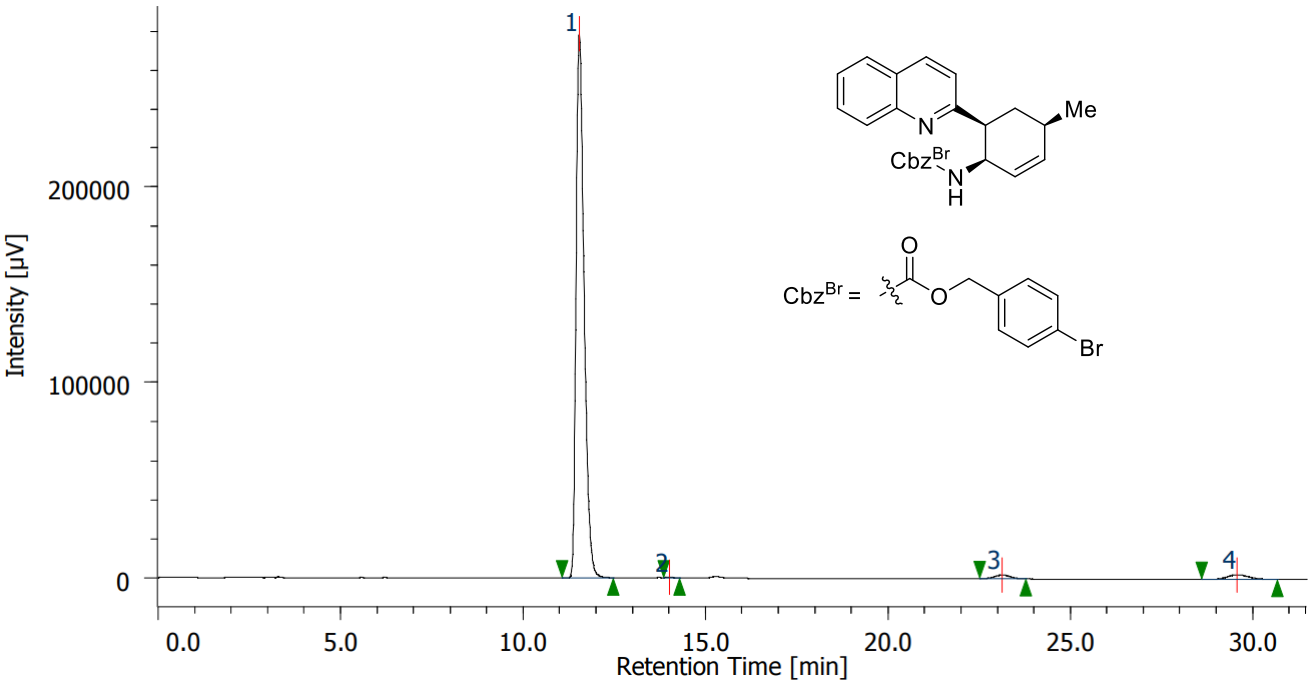




3ab

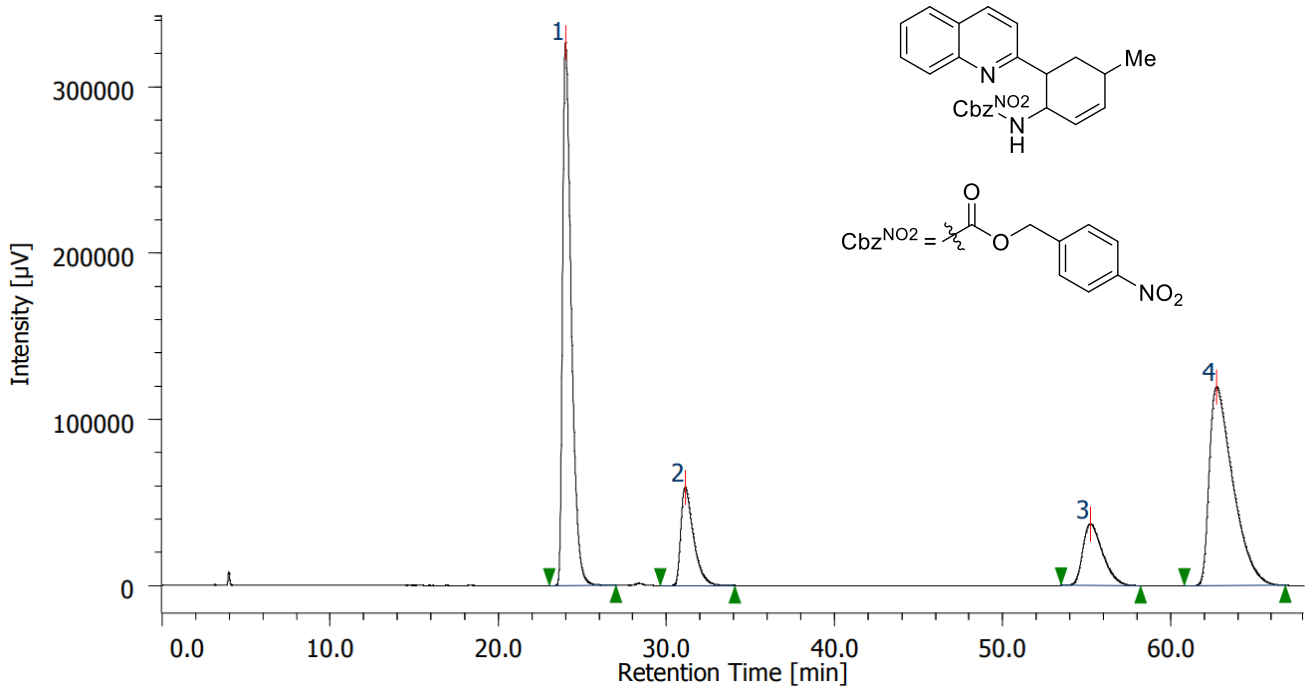
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	9.7	12.1	22.2	28.6
Area (%)	94.1	0.6	1.1	4.2

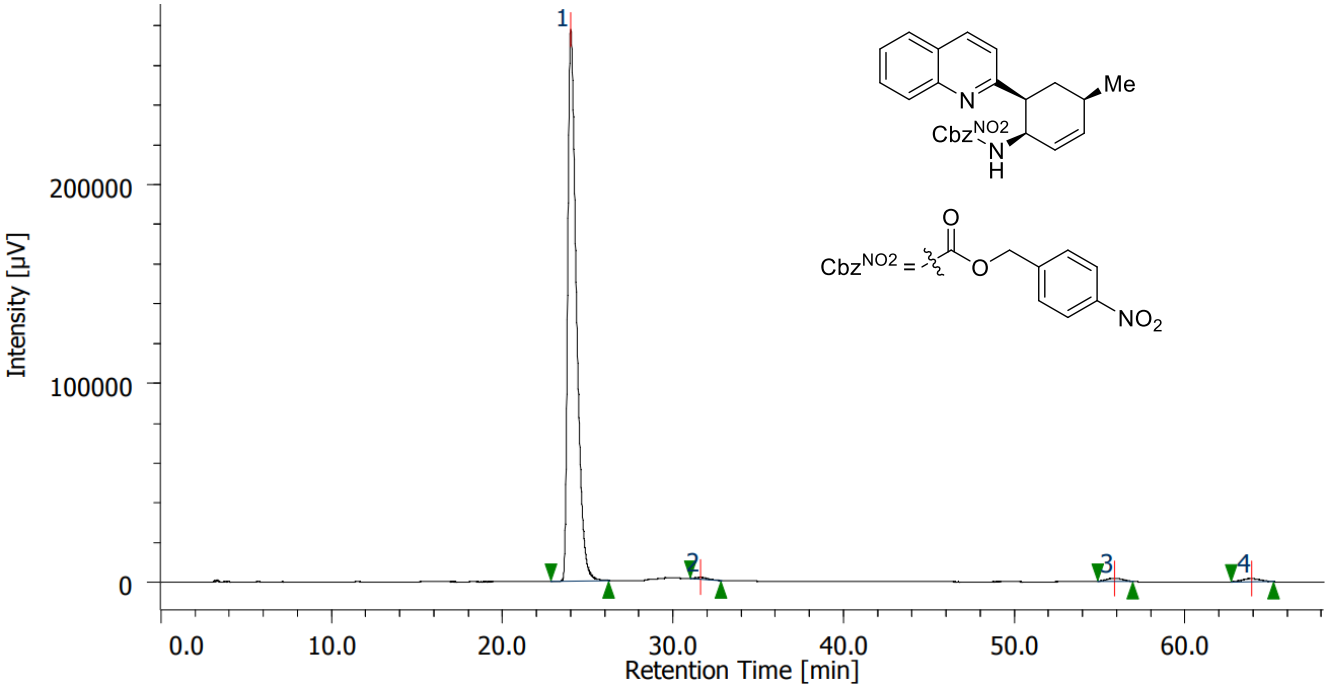




11ab

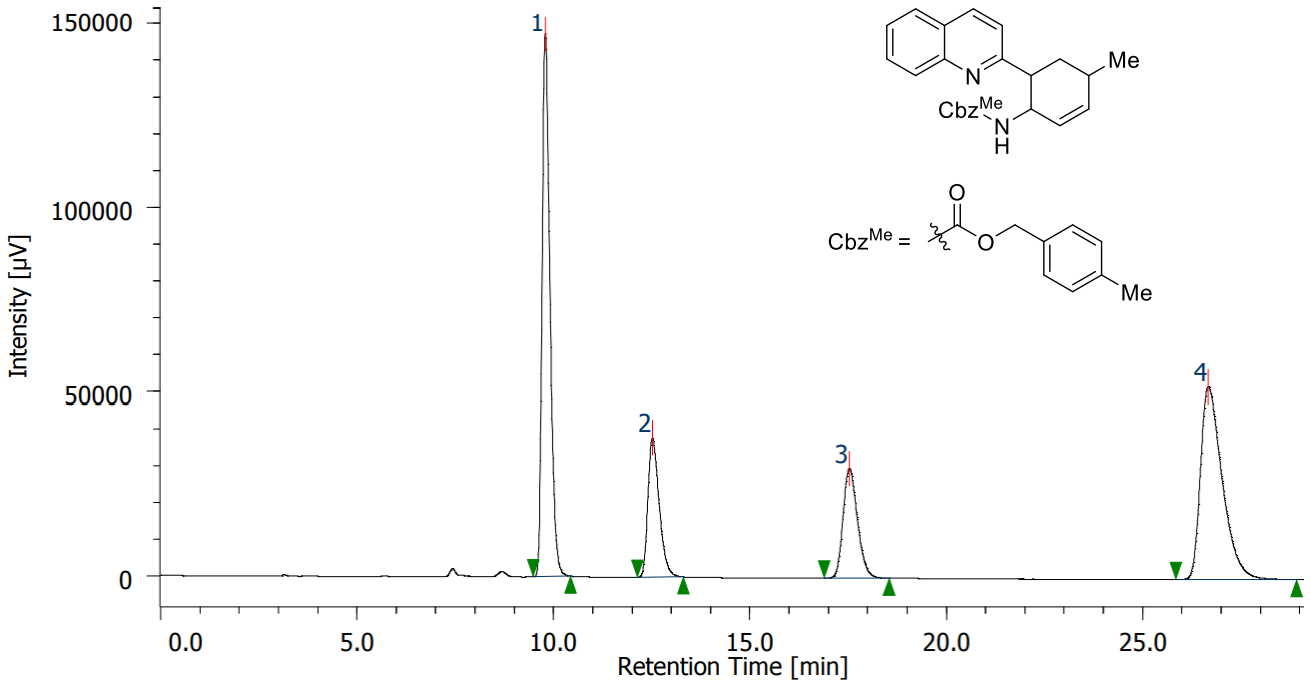
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	11.5	14.0	23.1	29.6
Area (%)	96.3	0.1	1.4	2.2

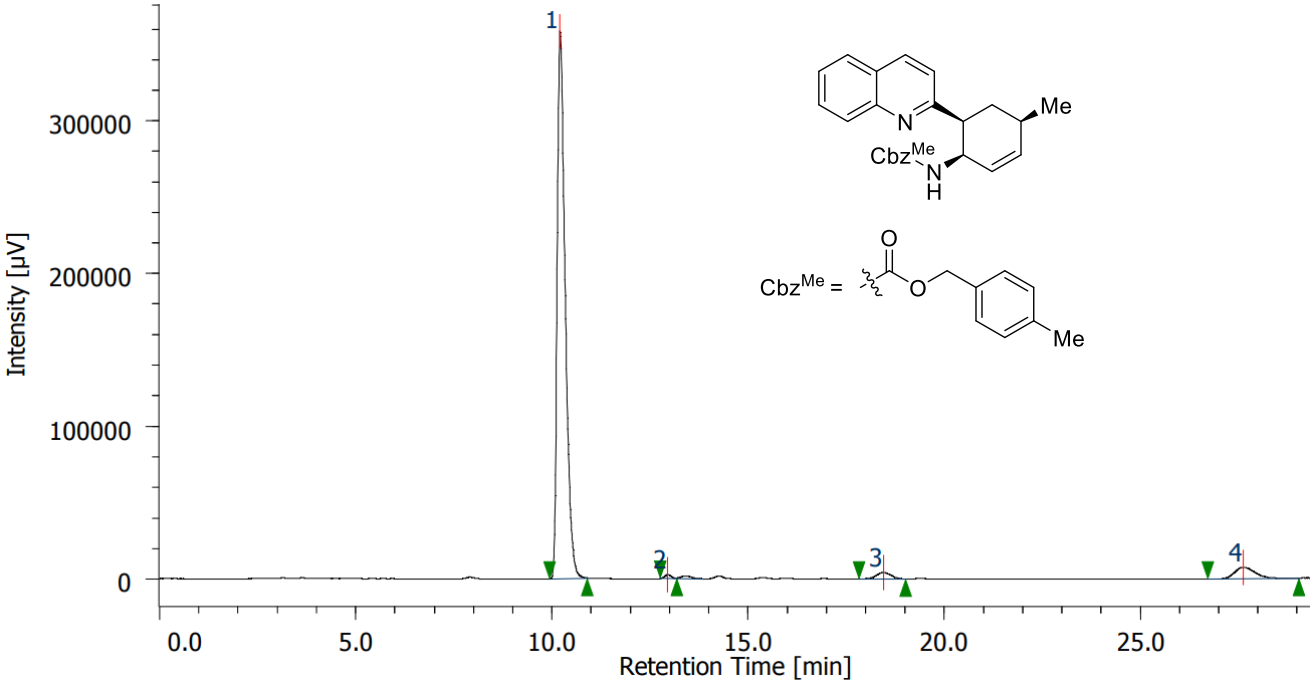




12ab

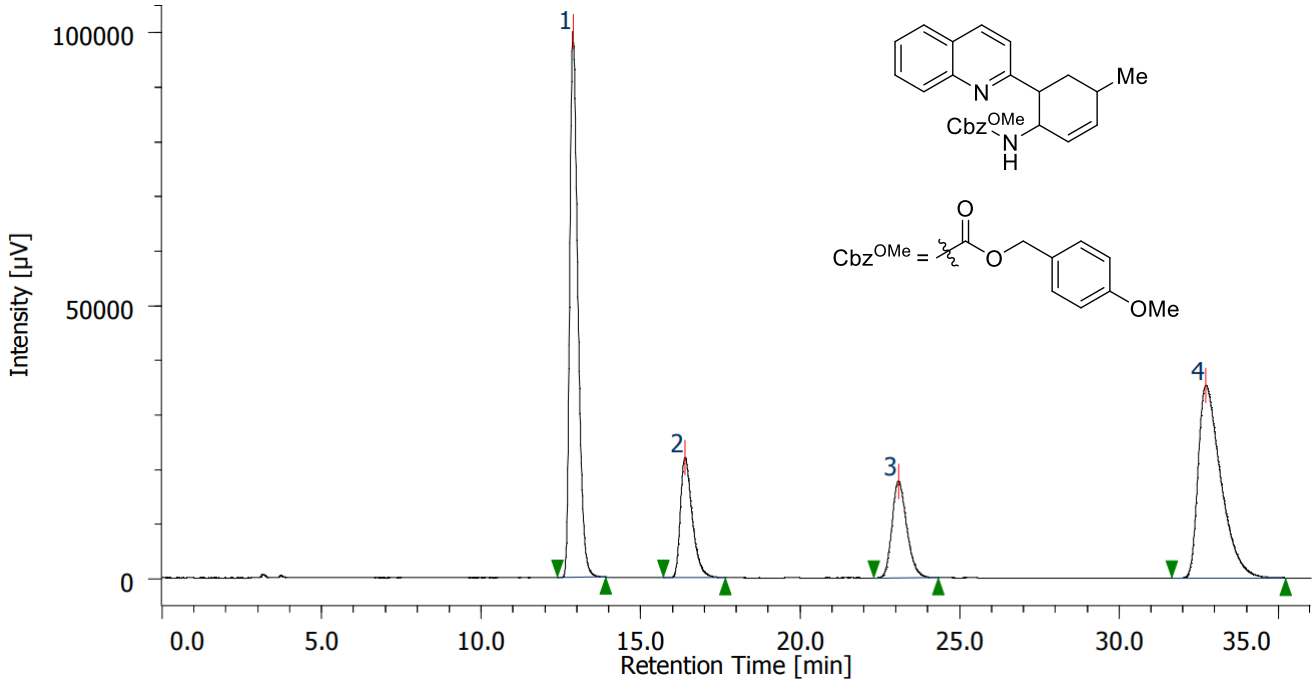
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	24.0	31.6	55.9	63.9
Area (%)	97.3	0.4	1.0	1.2

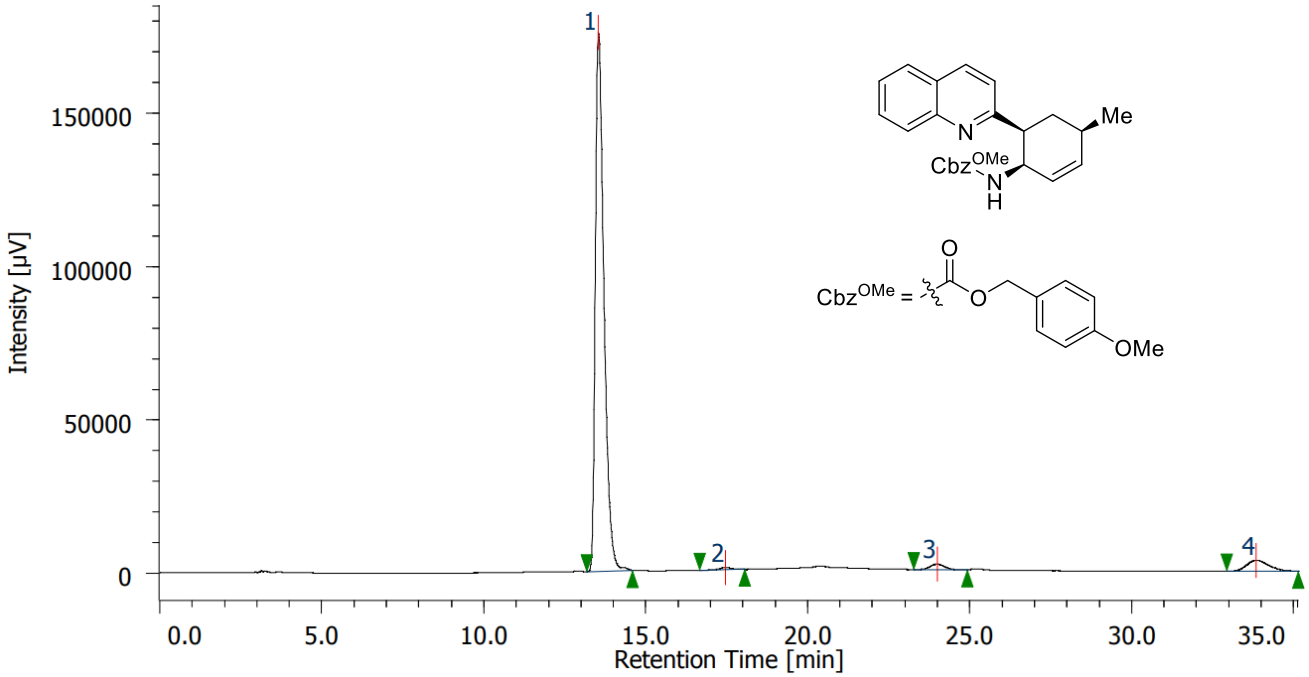




13ab

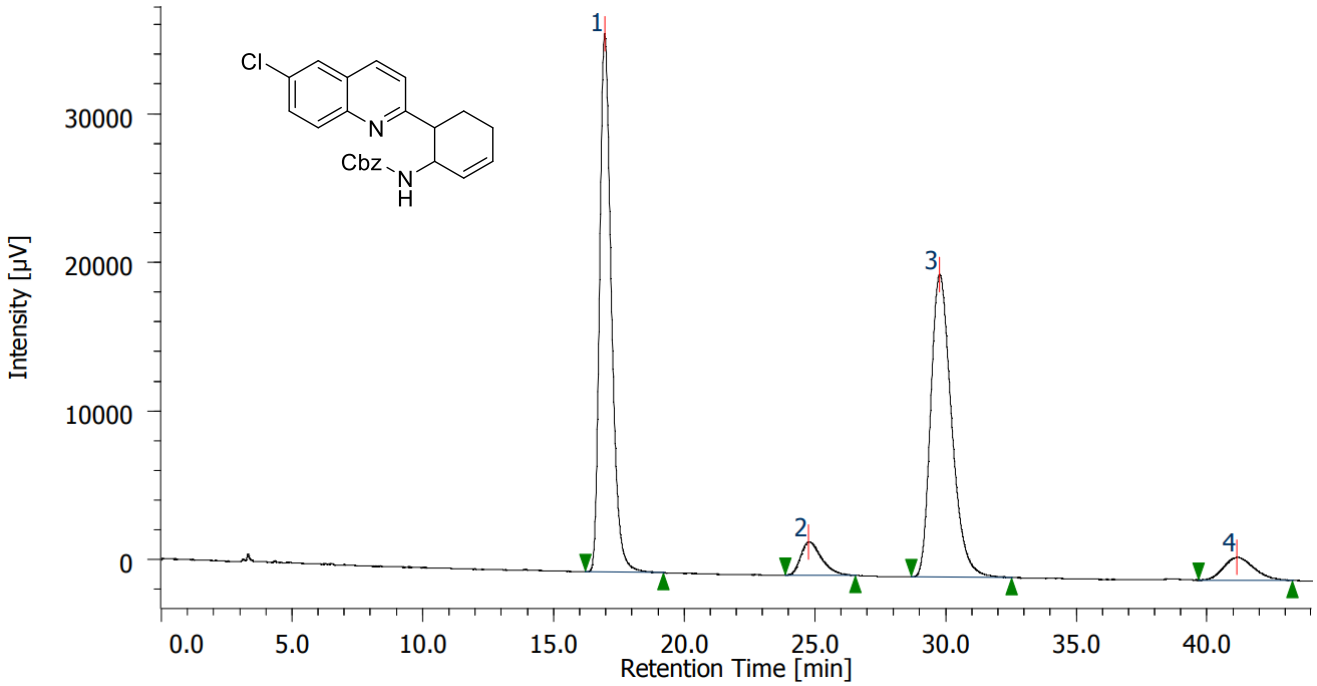
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	10.2	12.9	18.5	27.6
Area (%)	92.6	0.6	1.9	4.9

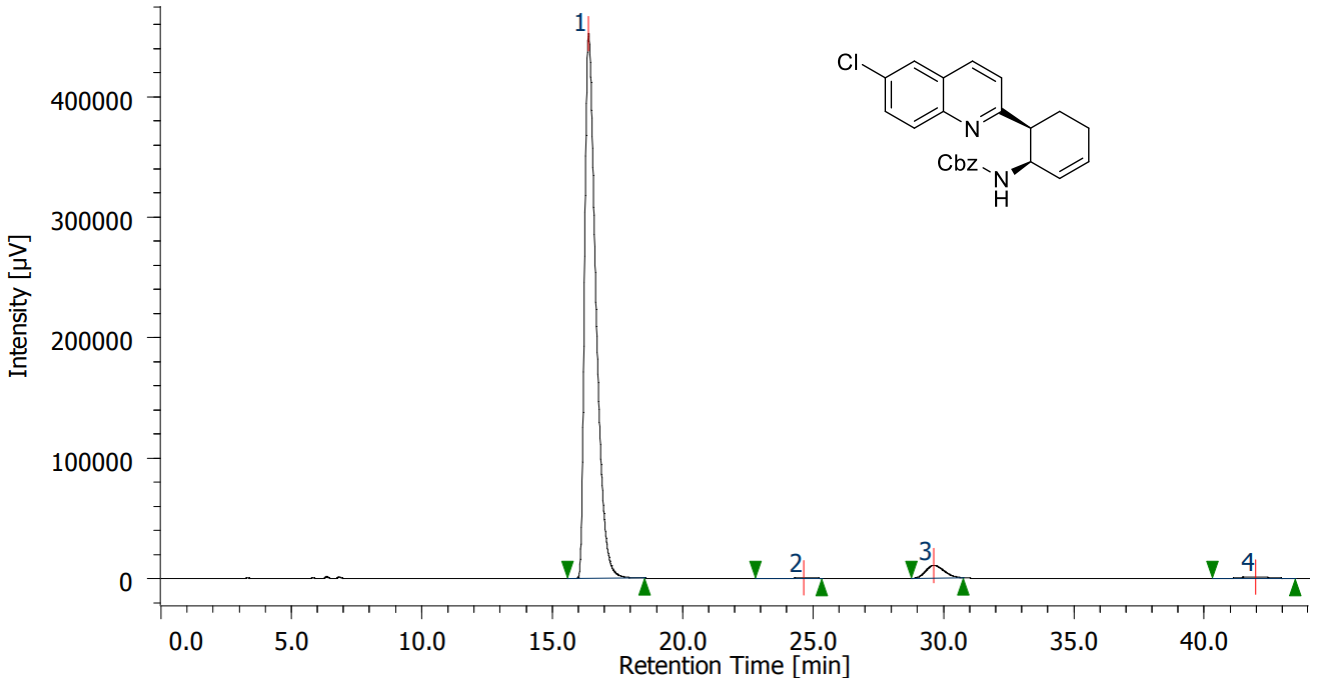




14ab

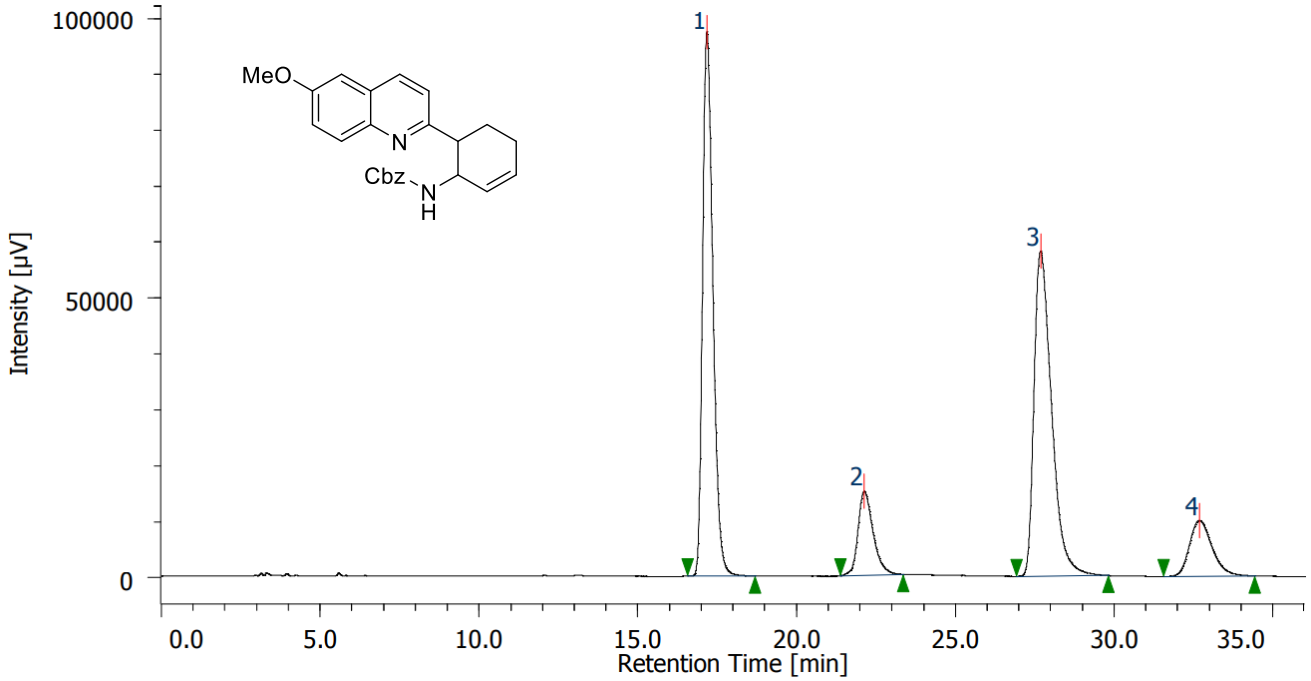
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	13.5	17.5	24.0	33.8
Area (%)	92.9	0.6	1.6	4.9

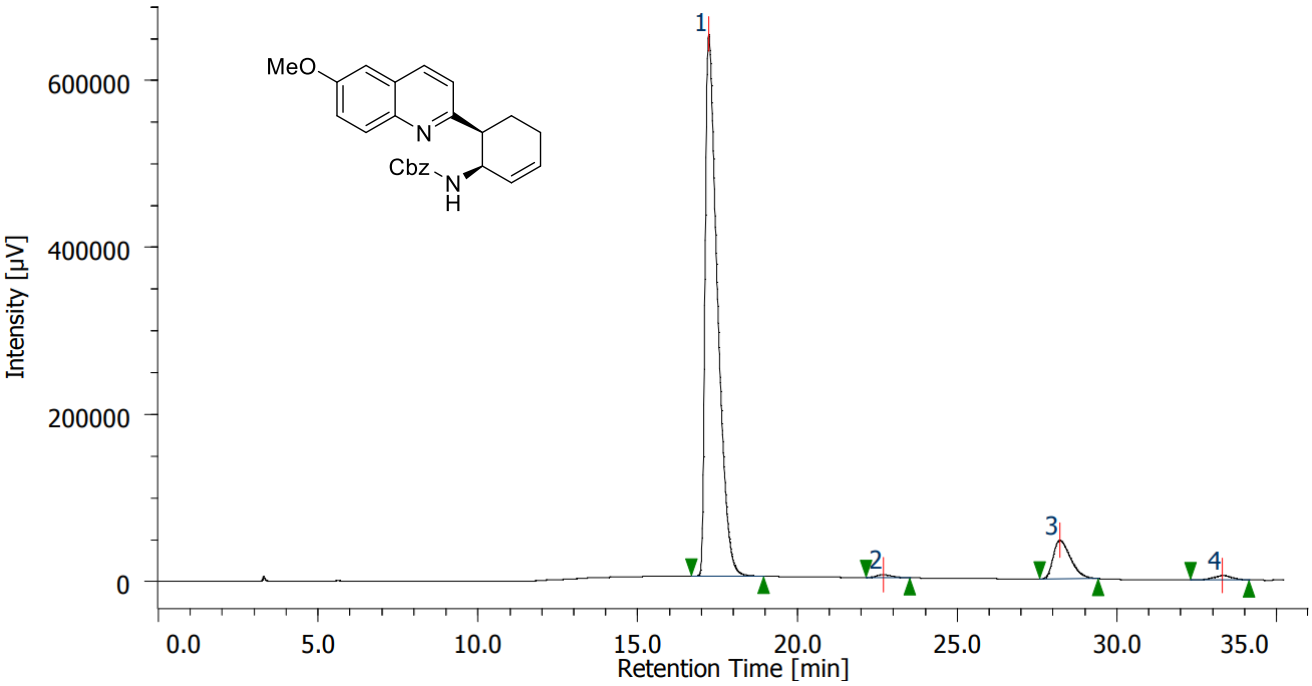




3ba

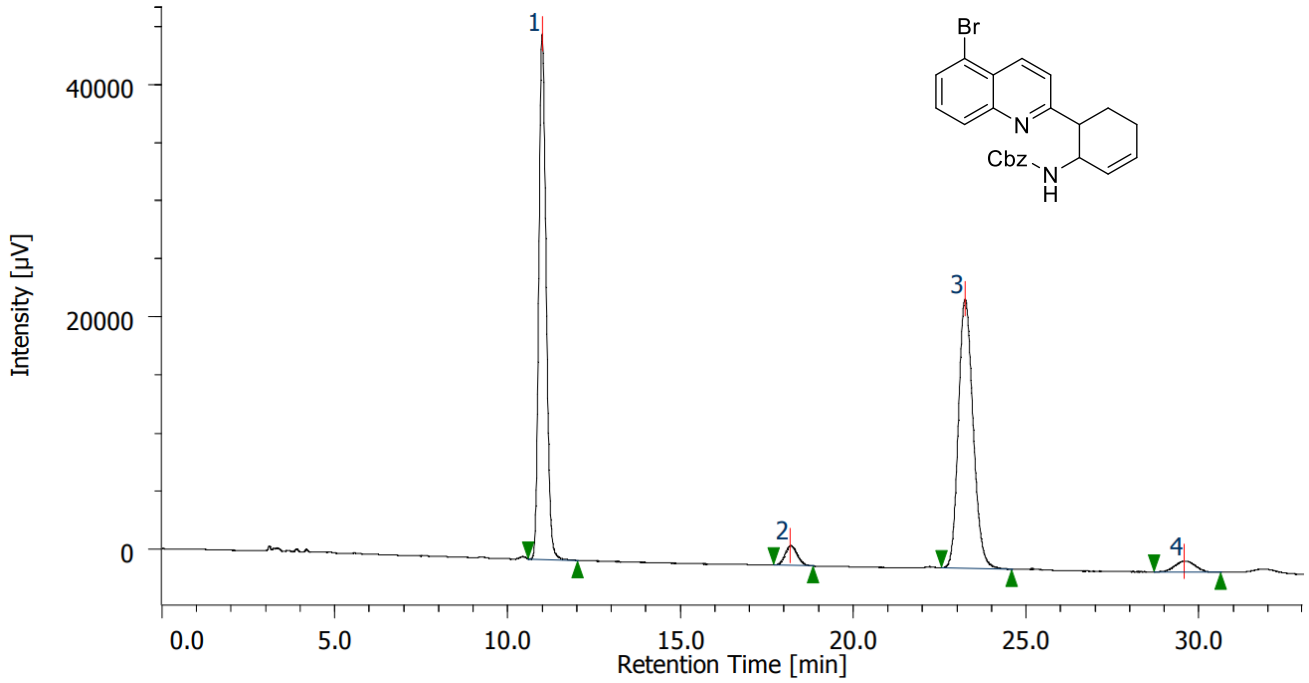
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	16.4	24.6	29.6	42.0
Area (%)	95.4	0.2	3.7	0.8

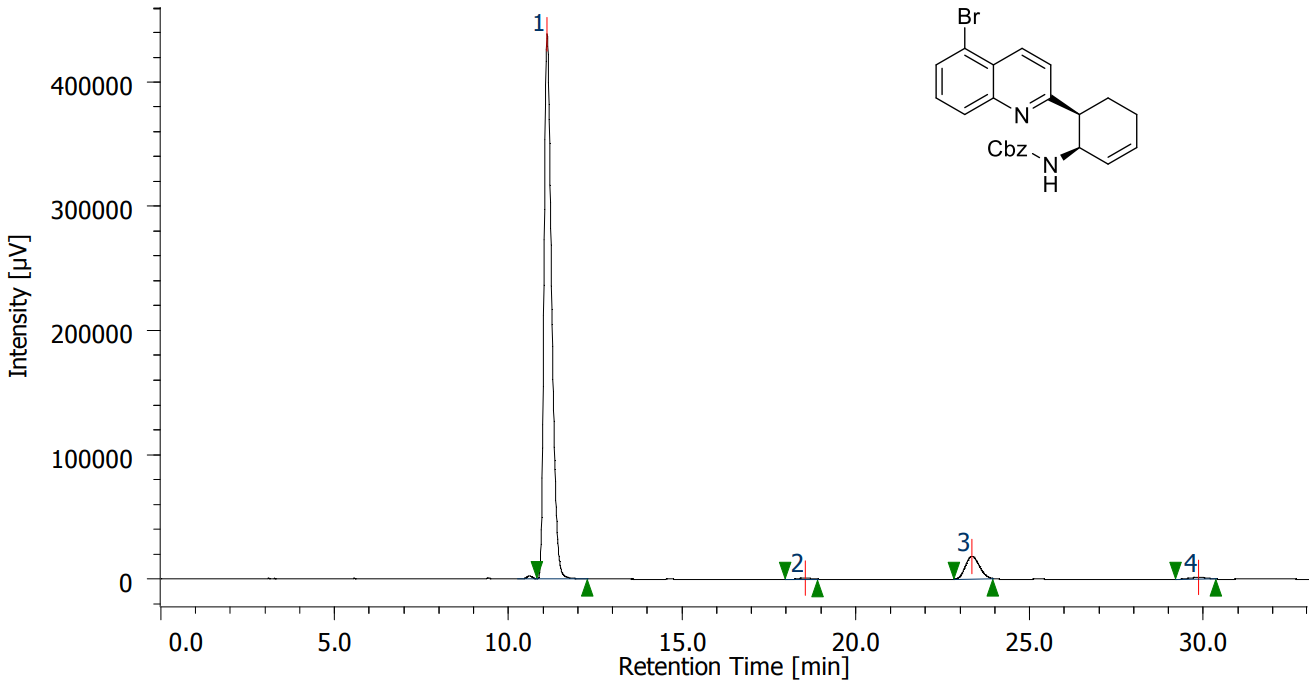




3ca

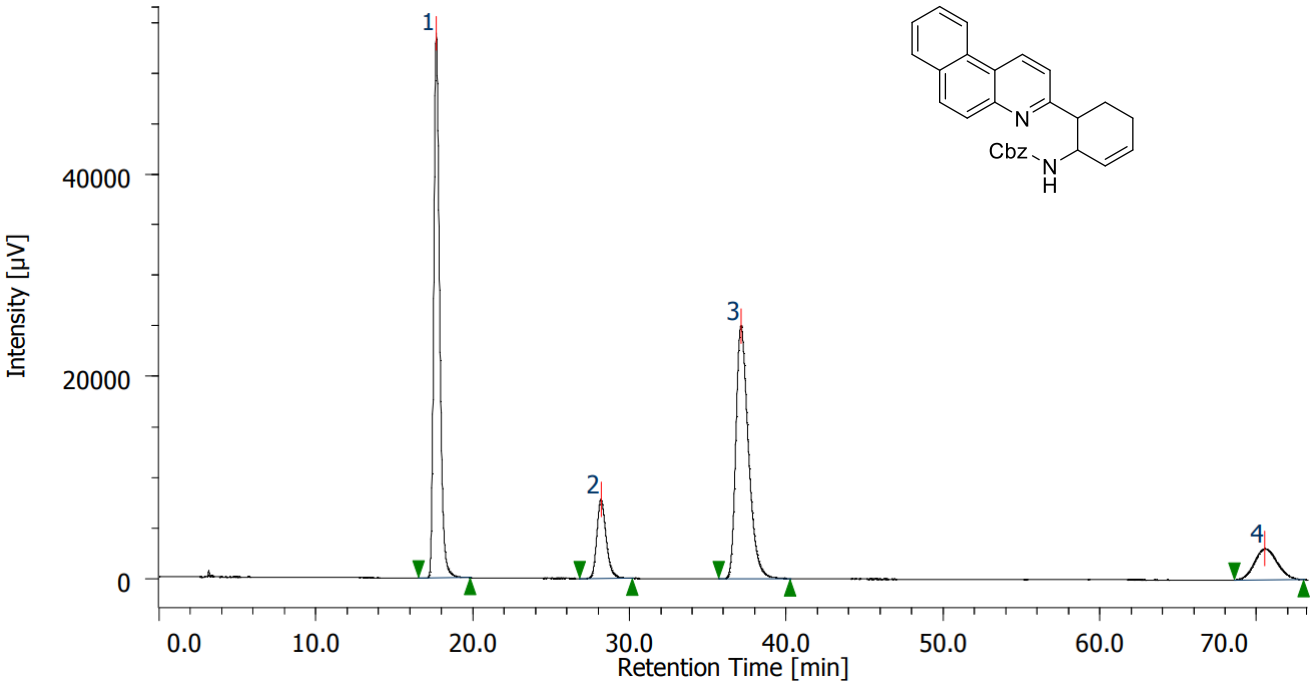
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	17.2	22.7	28.2	33.3
Area (%)	89.4	0.6	9.0	1.0

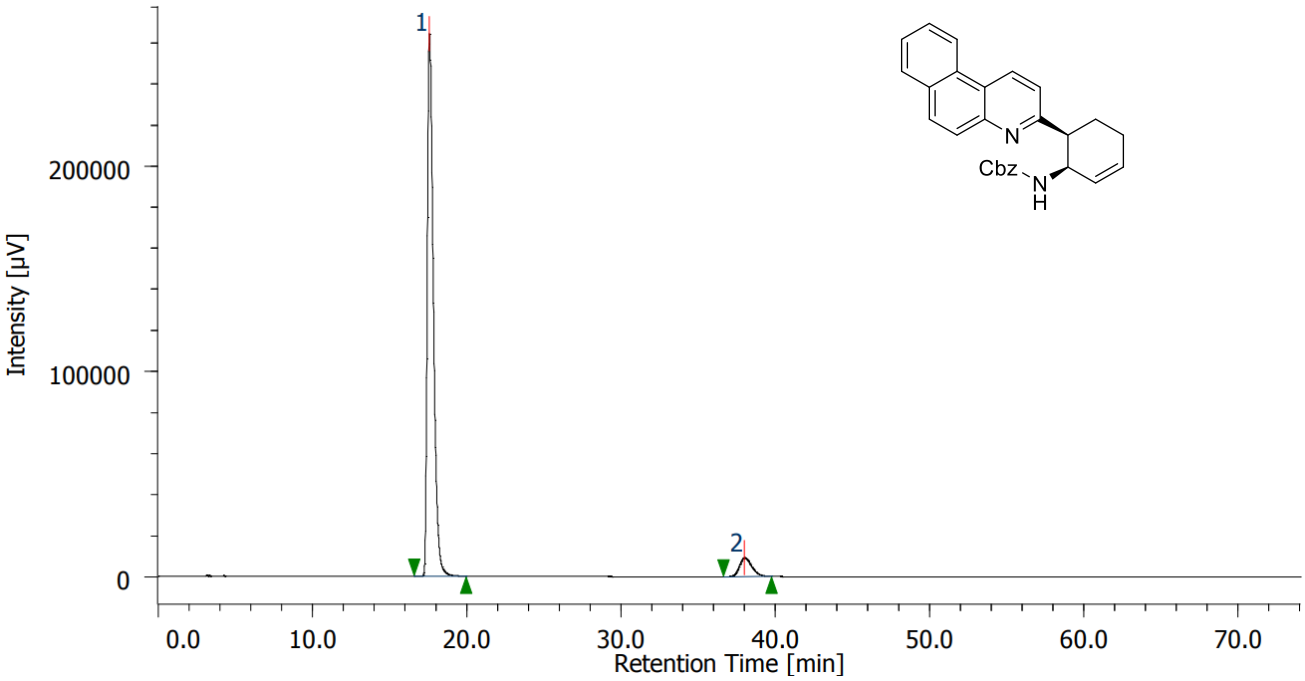




3da

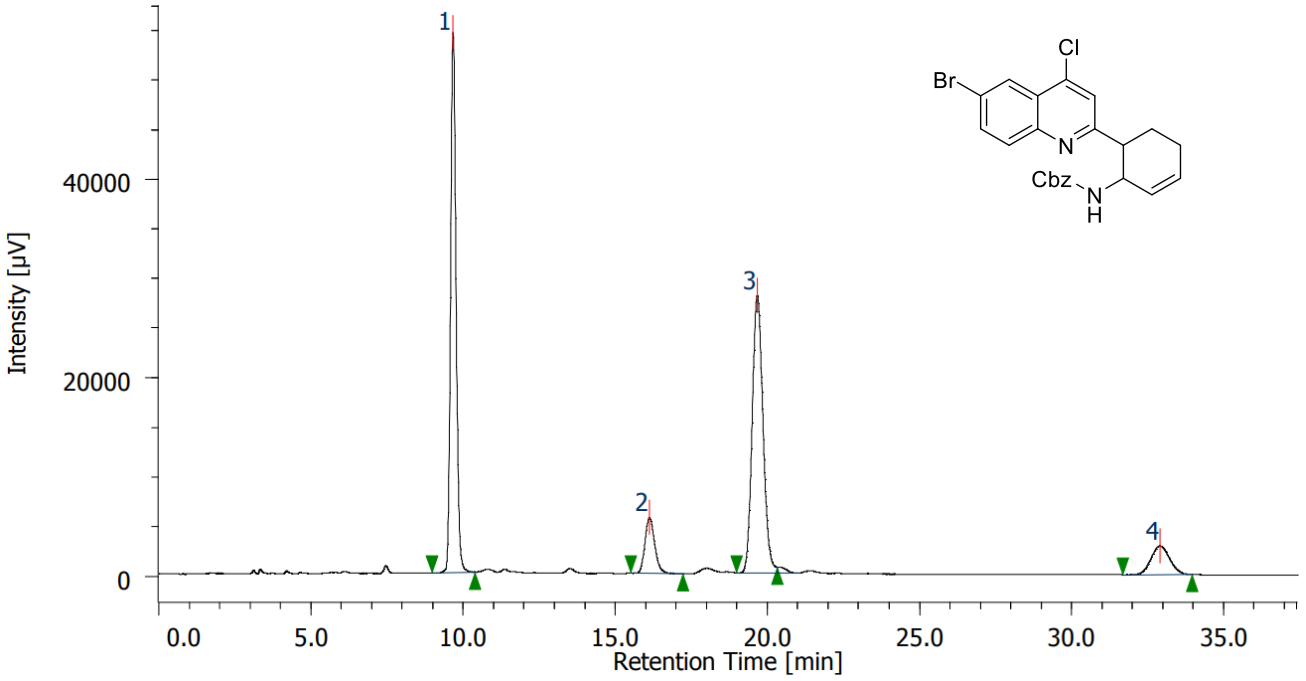
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	11.1	18.5	23.3	29.8
Area (%)	91.9	0.3	7.1	0.7

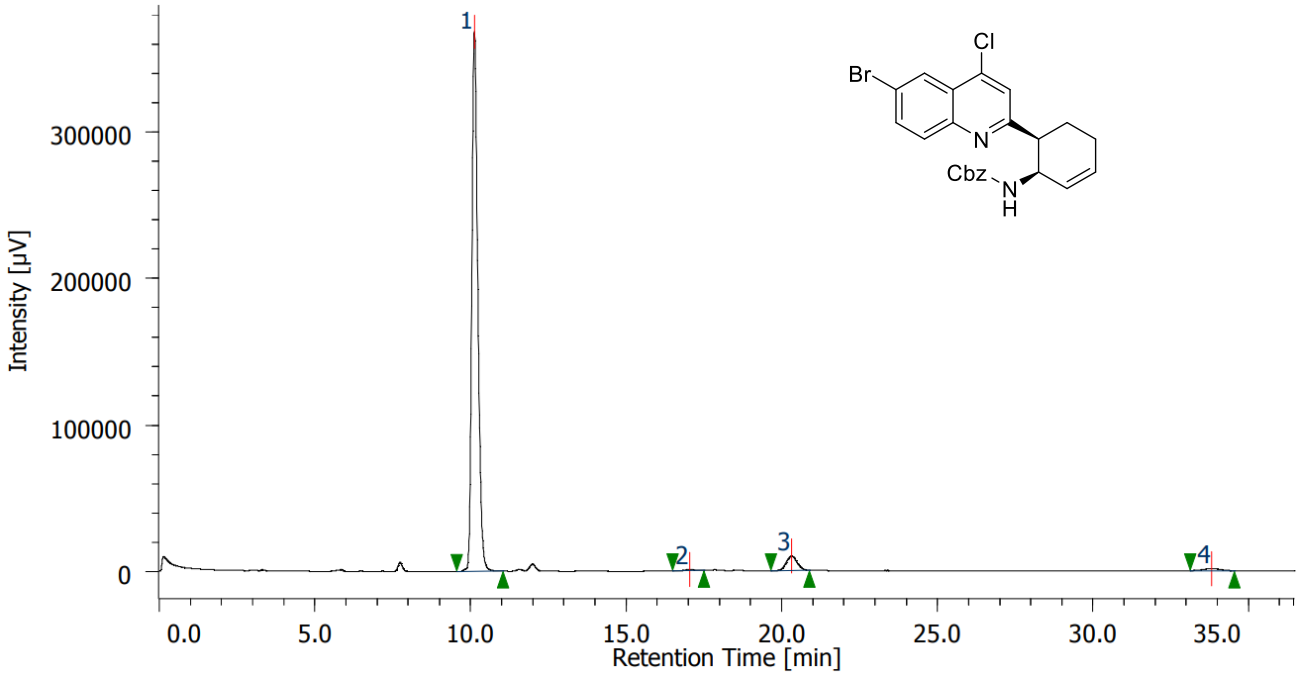




3ea

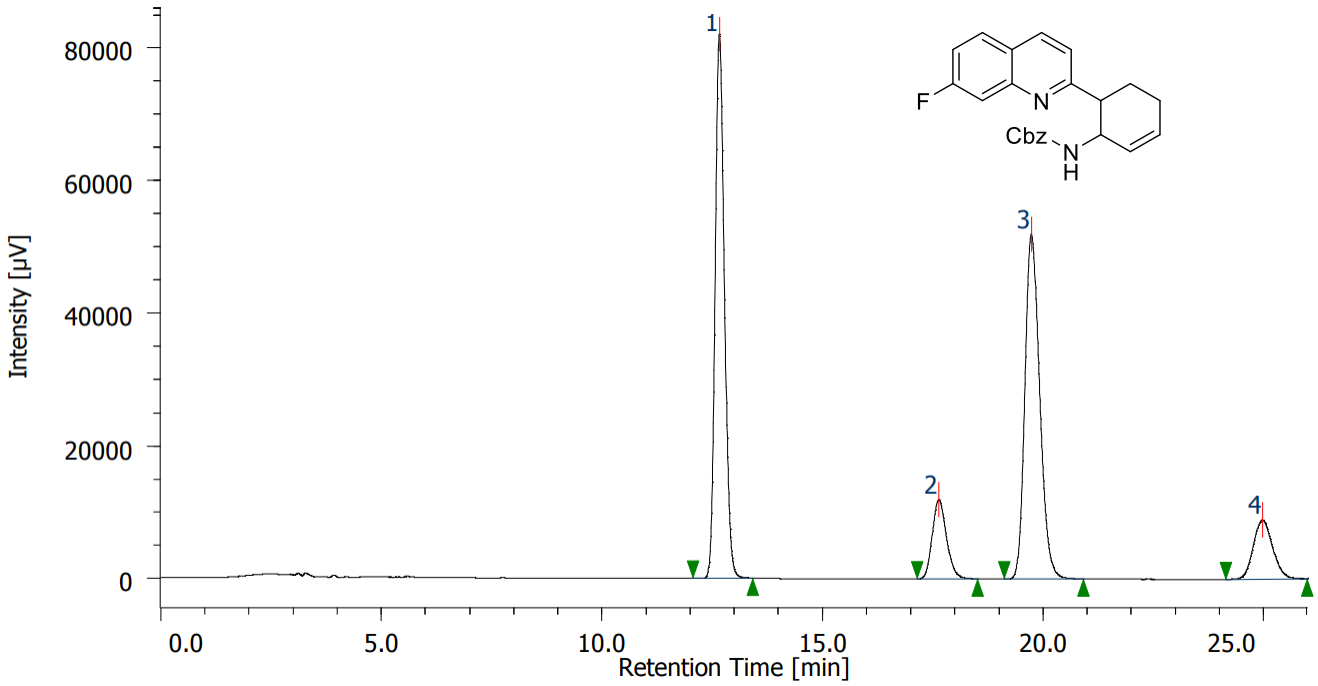
Peak	1 (*endo*)	2 (*exo*)	3(2) (*endo*)	4 (*exo*)
Retention Time (min)	17.7	28.2	37.1	70.5
Area (%)	93.1	-	6.9	-

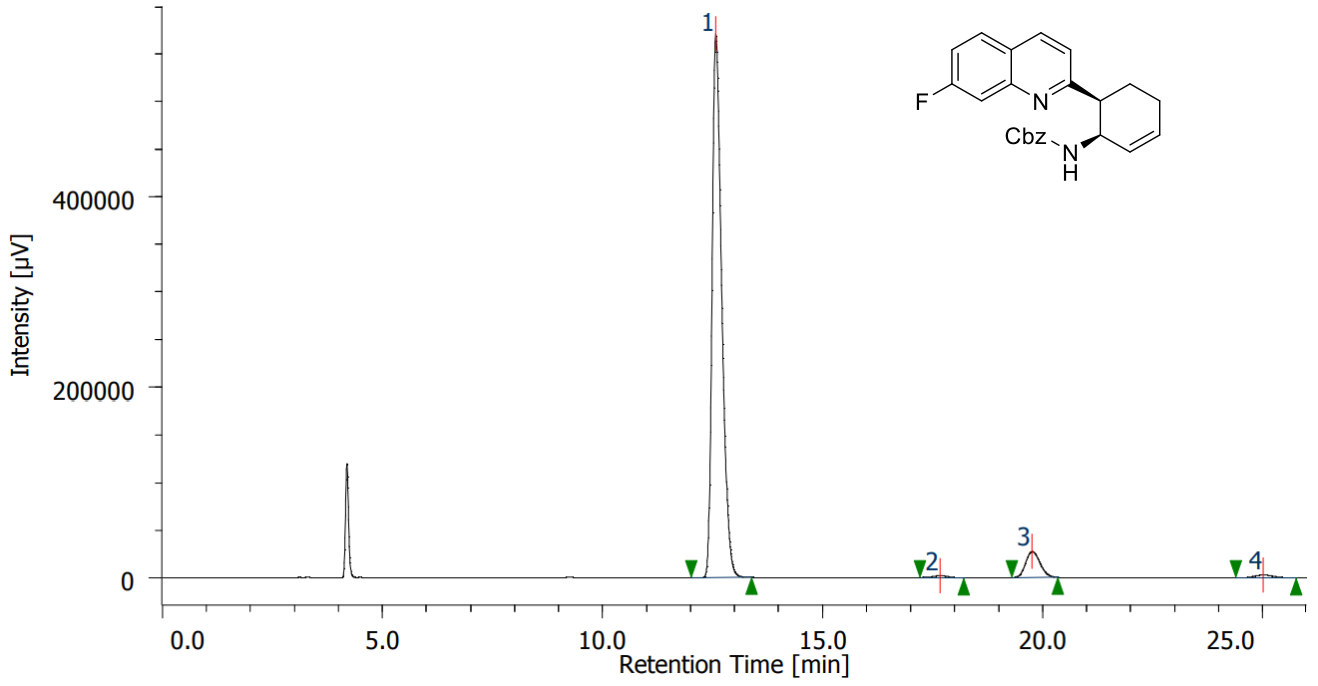




3fa

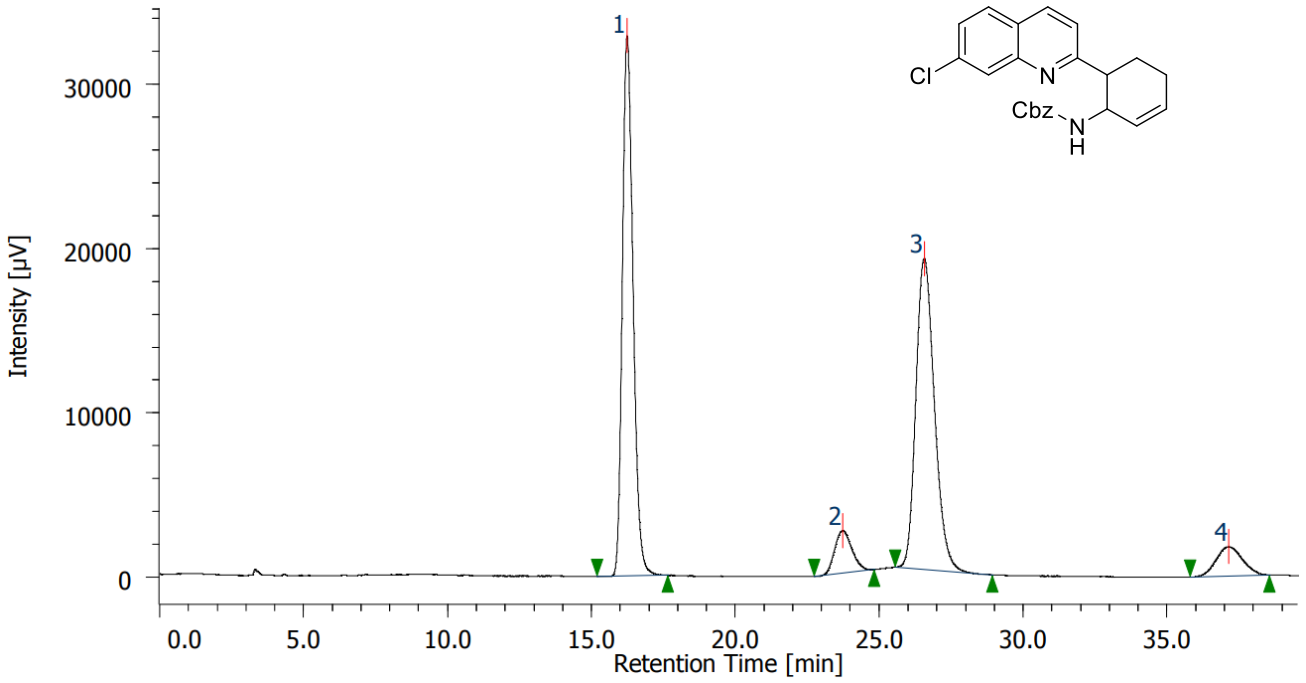
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	10.1	17.0	20.3	33.8
Area (%)	94.1	0.4	4.5	1.0

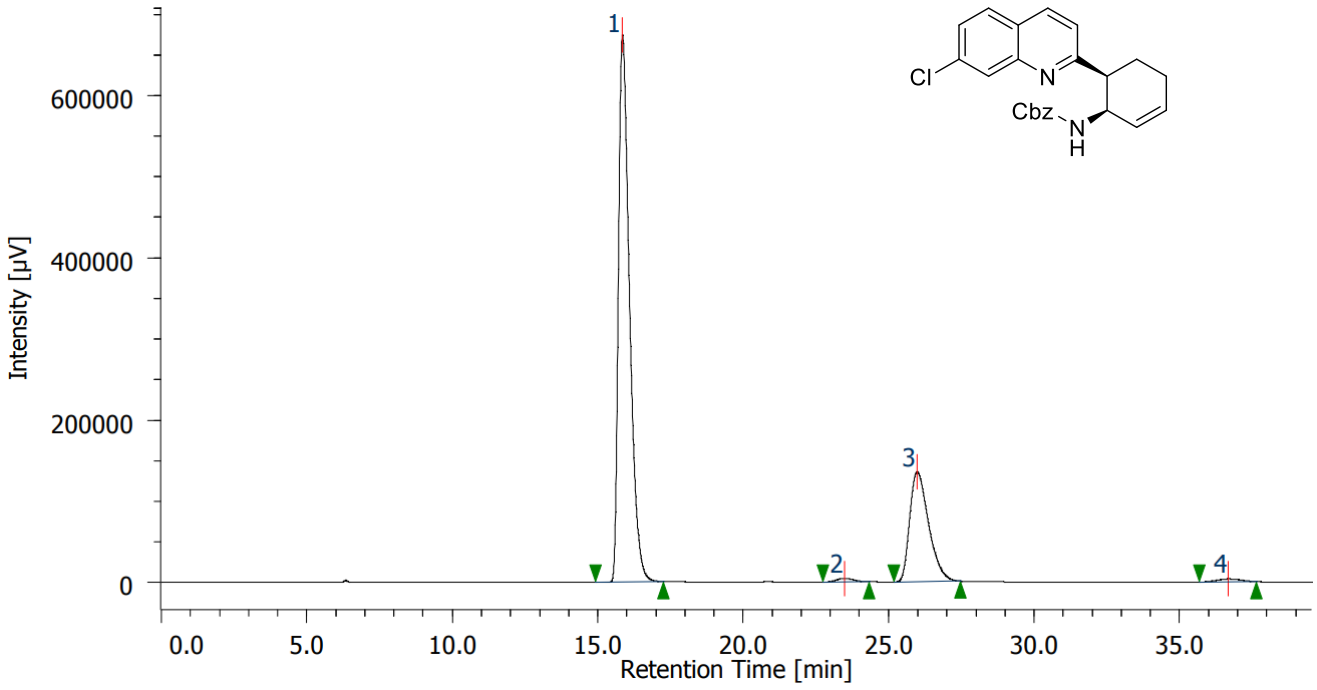




3ga

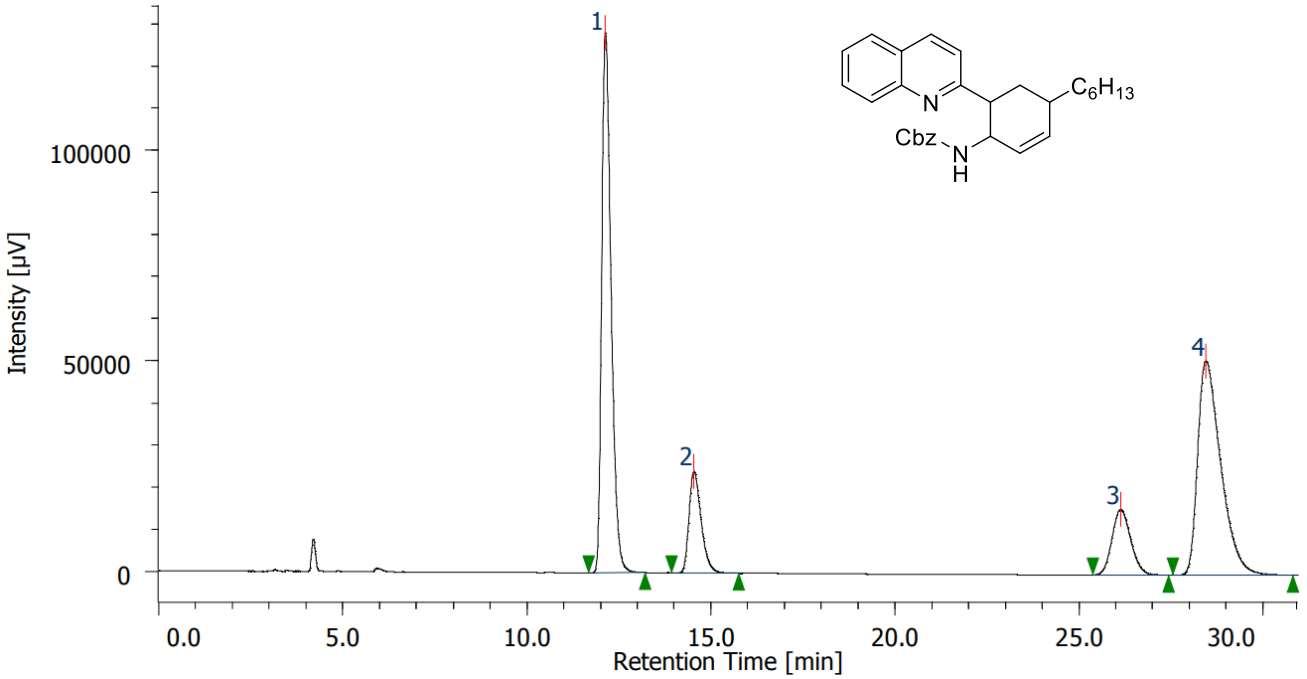
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	12.6	17.7	19.8	25.0
Area (%)	91.9	0.5	6.6	1.0

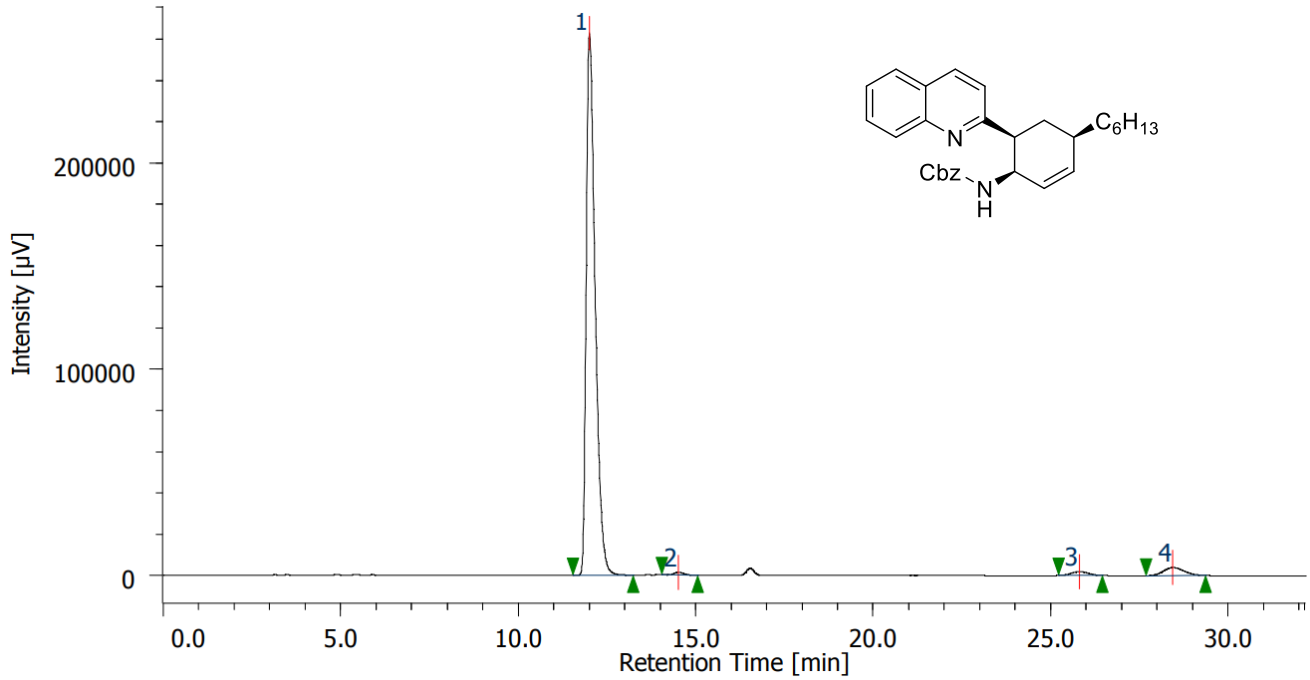




3ha

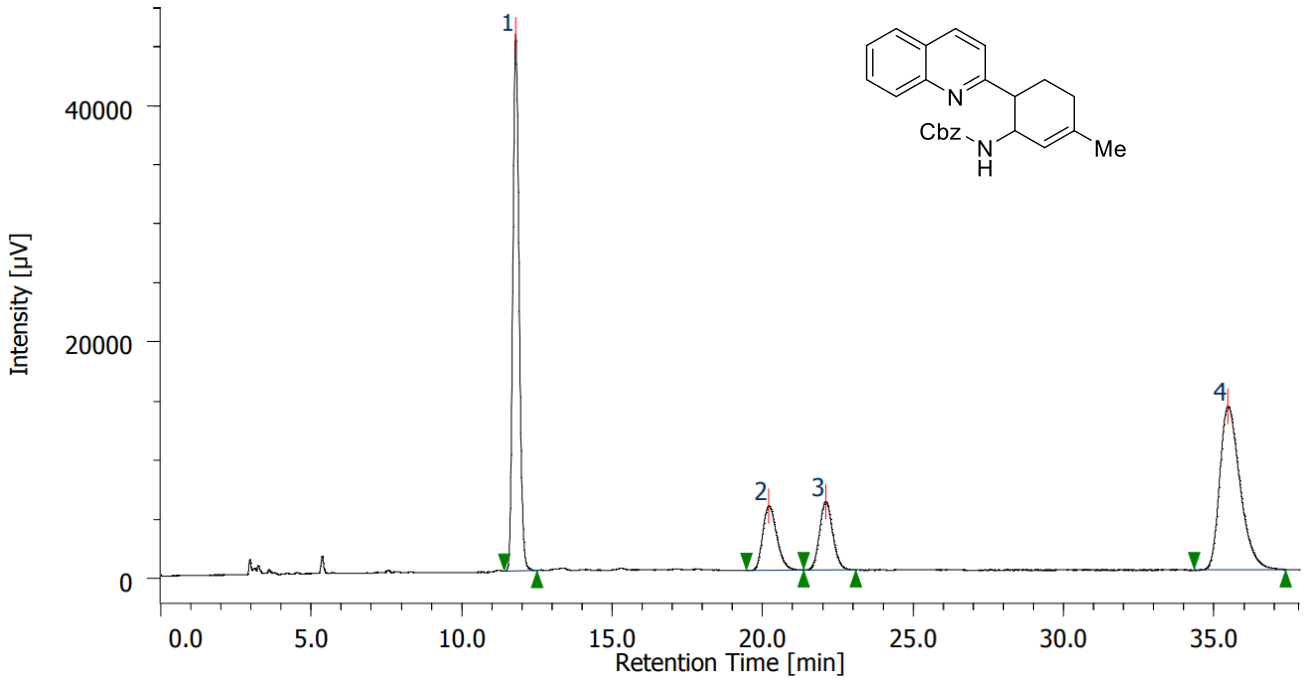
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	15.8	23.5	26.0	36.7
Area (%)	73.2	0.7	25.2	0.8

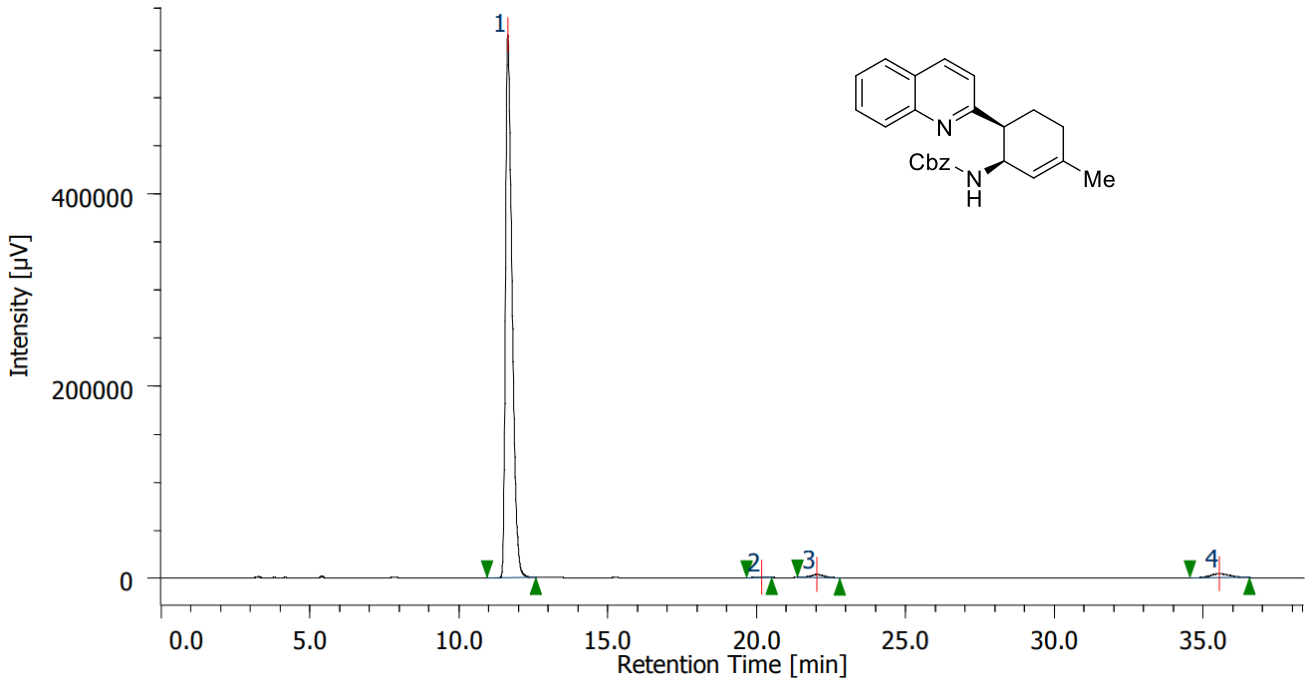




3ac

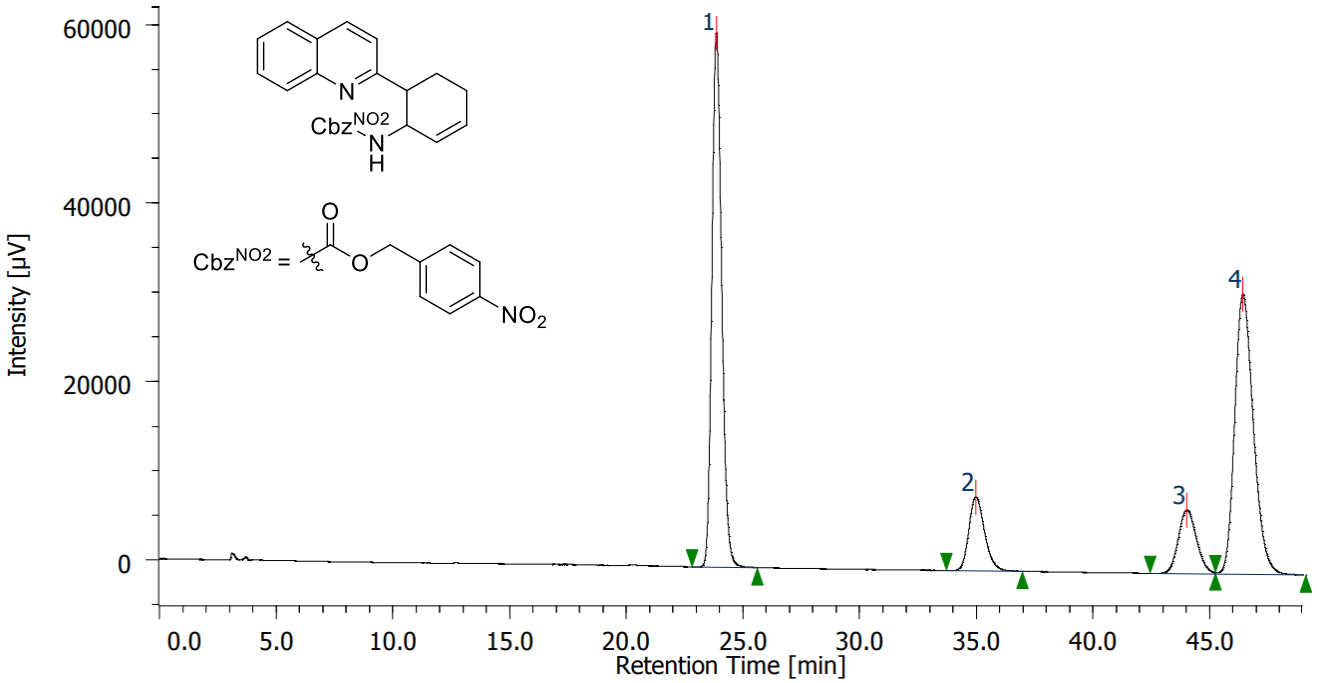
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	12.0	14.5	25.8	28.4
Area (%)	94.9	0.5	1.3	3.3

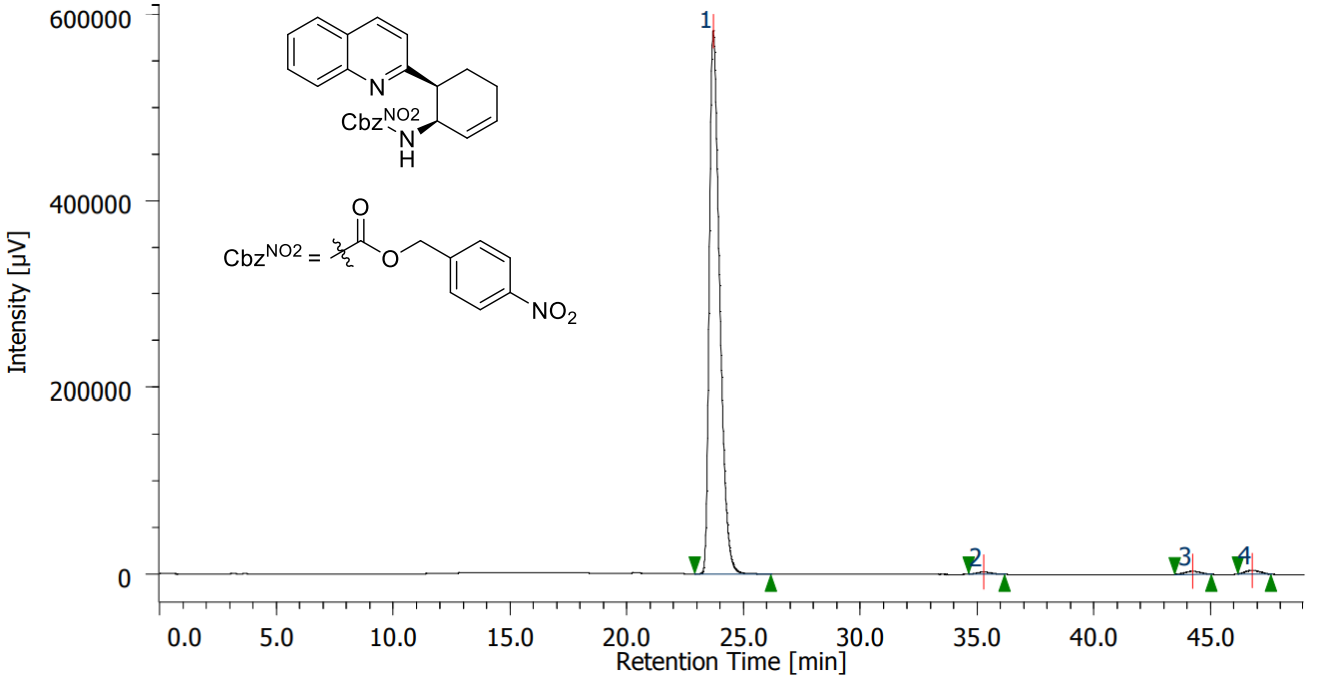




3ad

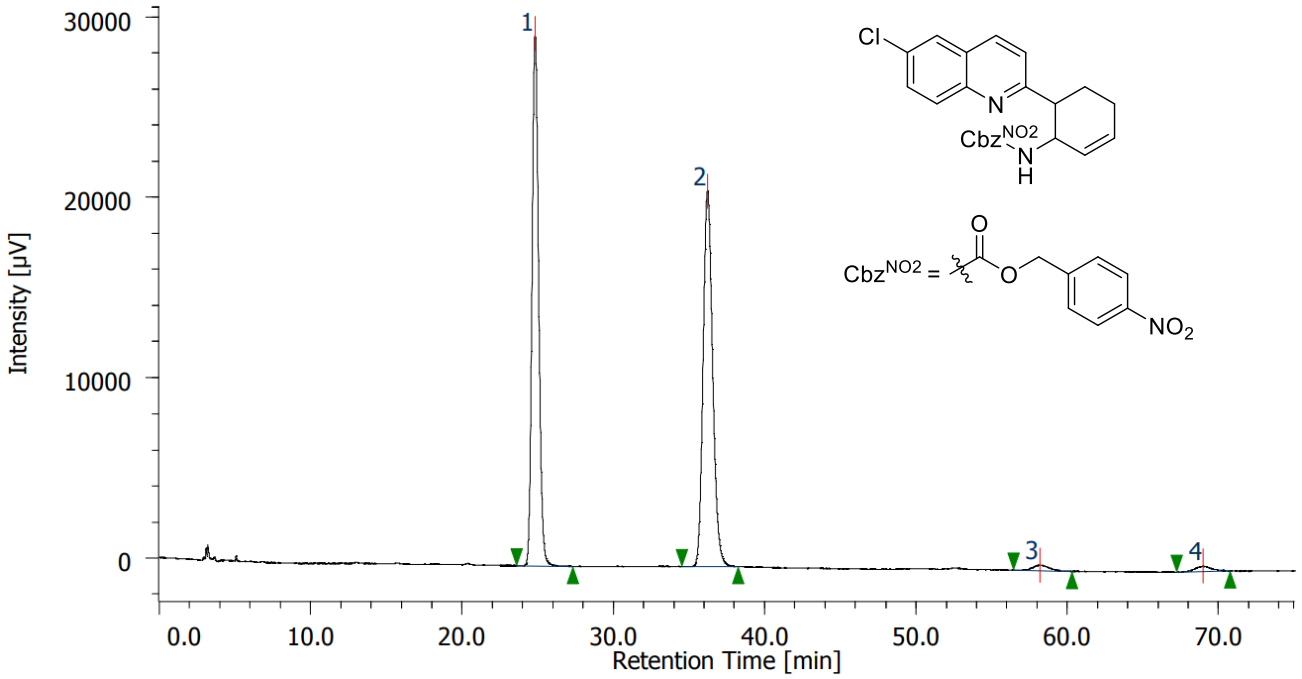
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	11.6	20.2	22.0	35.5
Area (%)	96.6	0.2	1.1	2.1

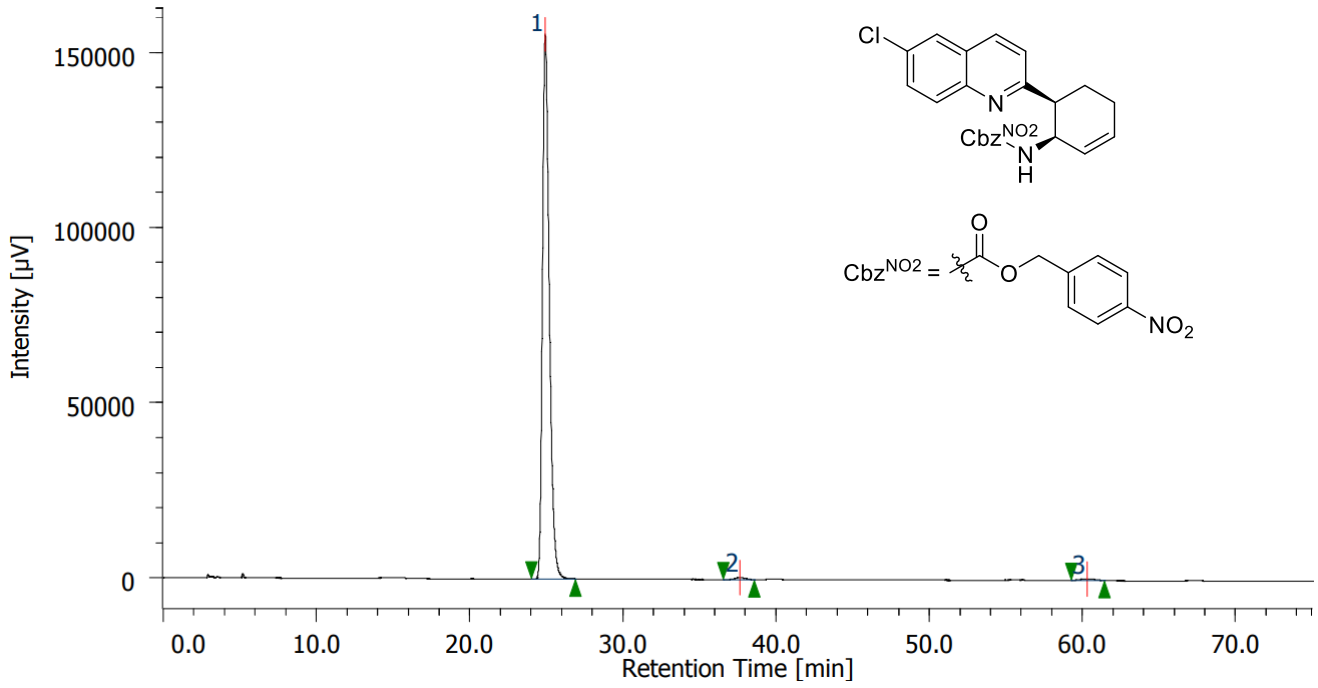




12aa

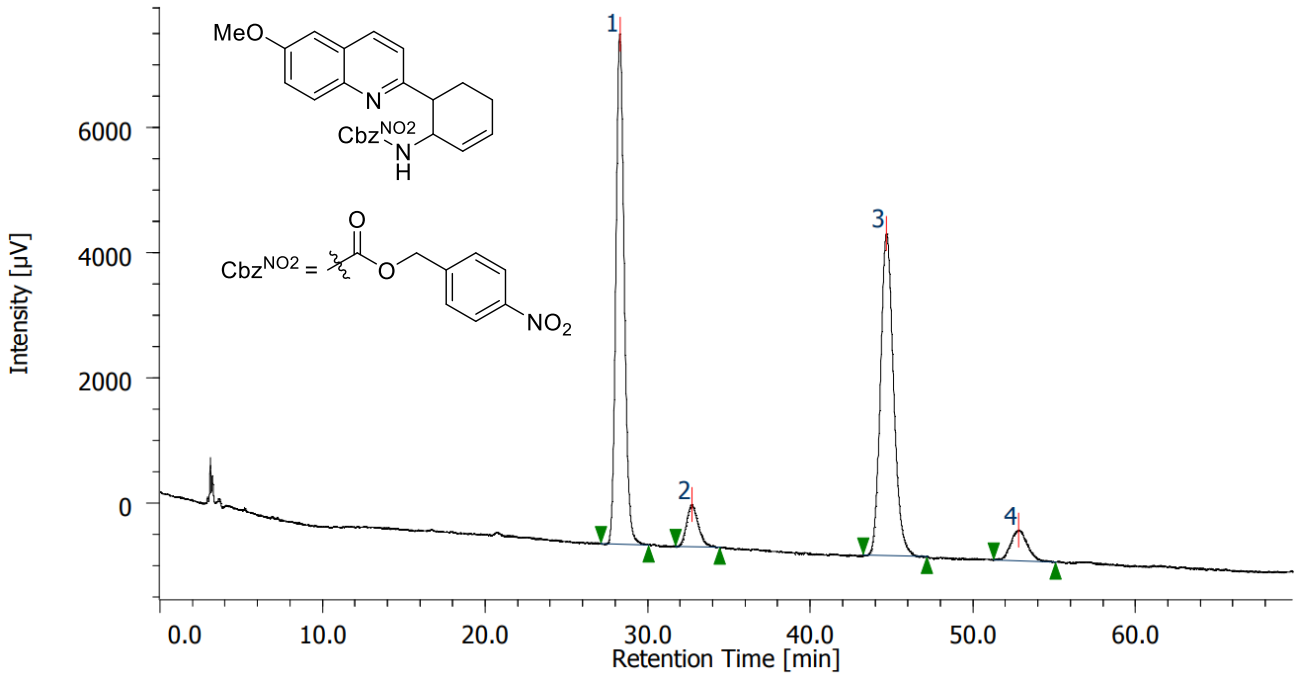
Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	23.7	35.3	44.2	46.8
Area (%)	97.6	0.6	0.8	1.0

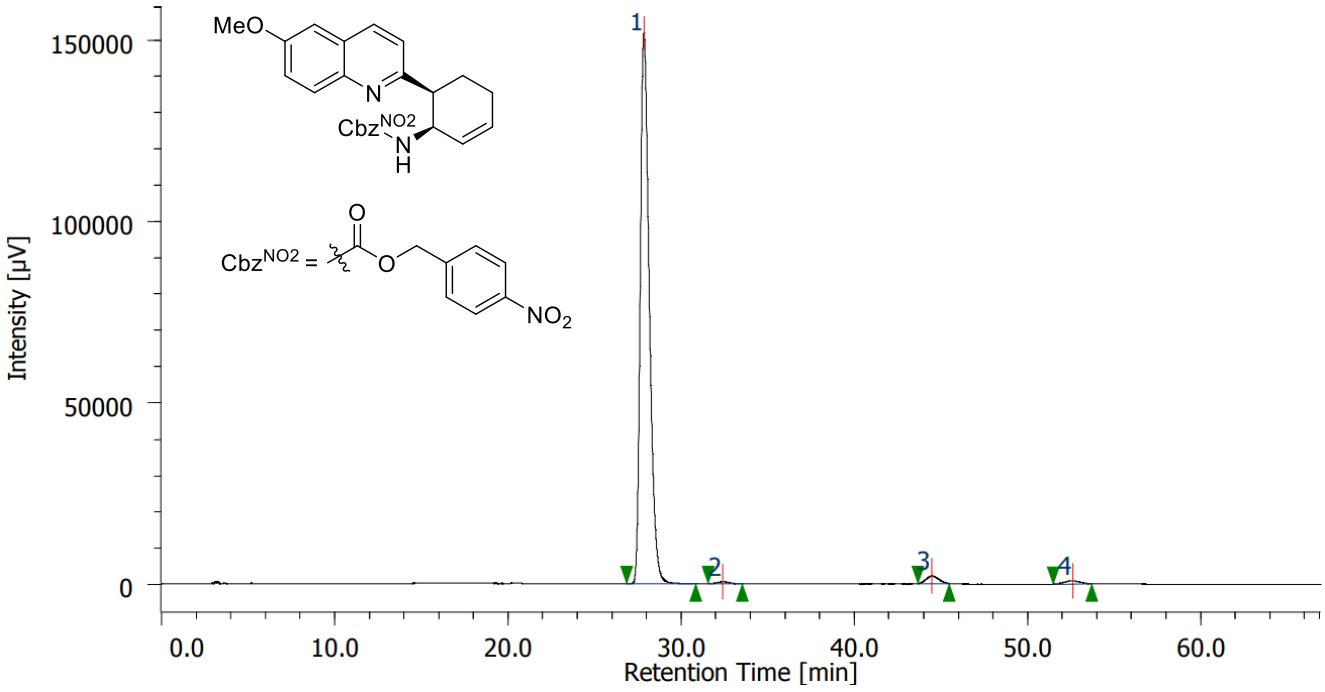




12ba

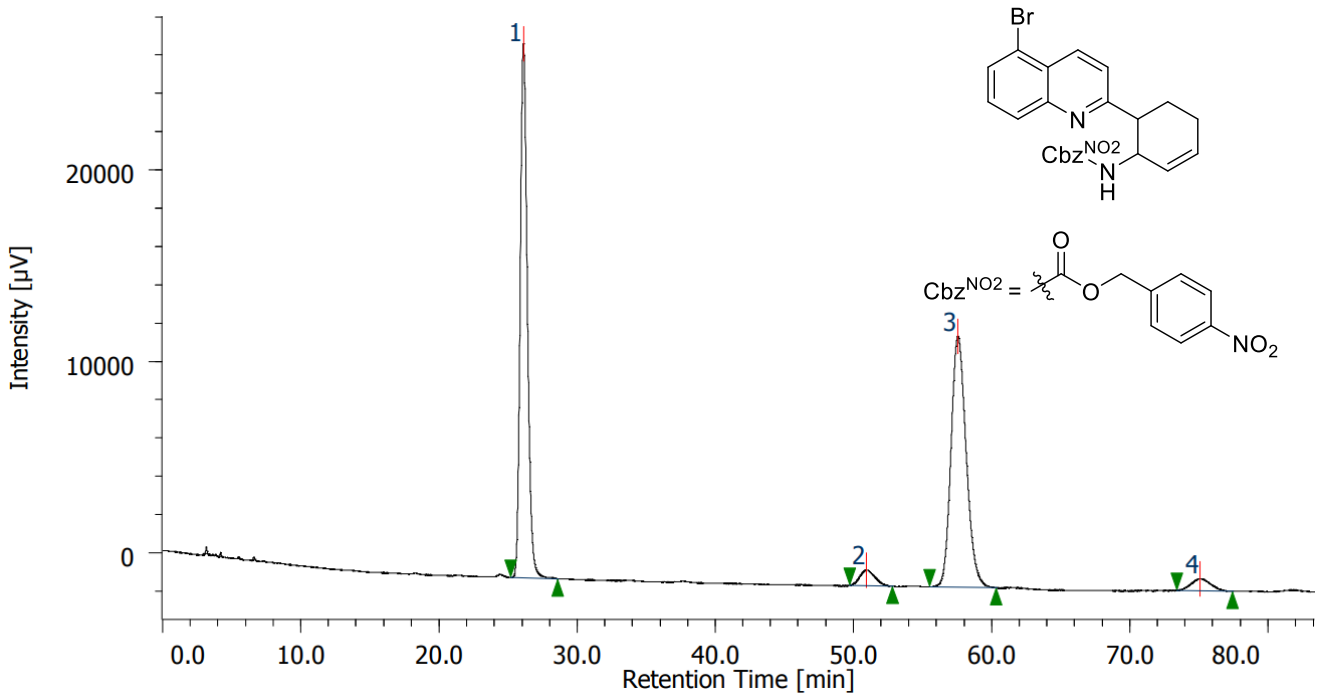
Peak	1 (*endo*)	2 (*endo*)	3 (*exo*)	4 (*exo*)
Retention Time (min)	24.8	36.2	58.2	68.9
Area (%)	98.8	0.5	0.7	-

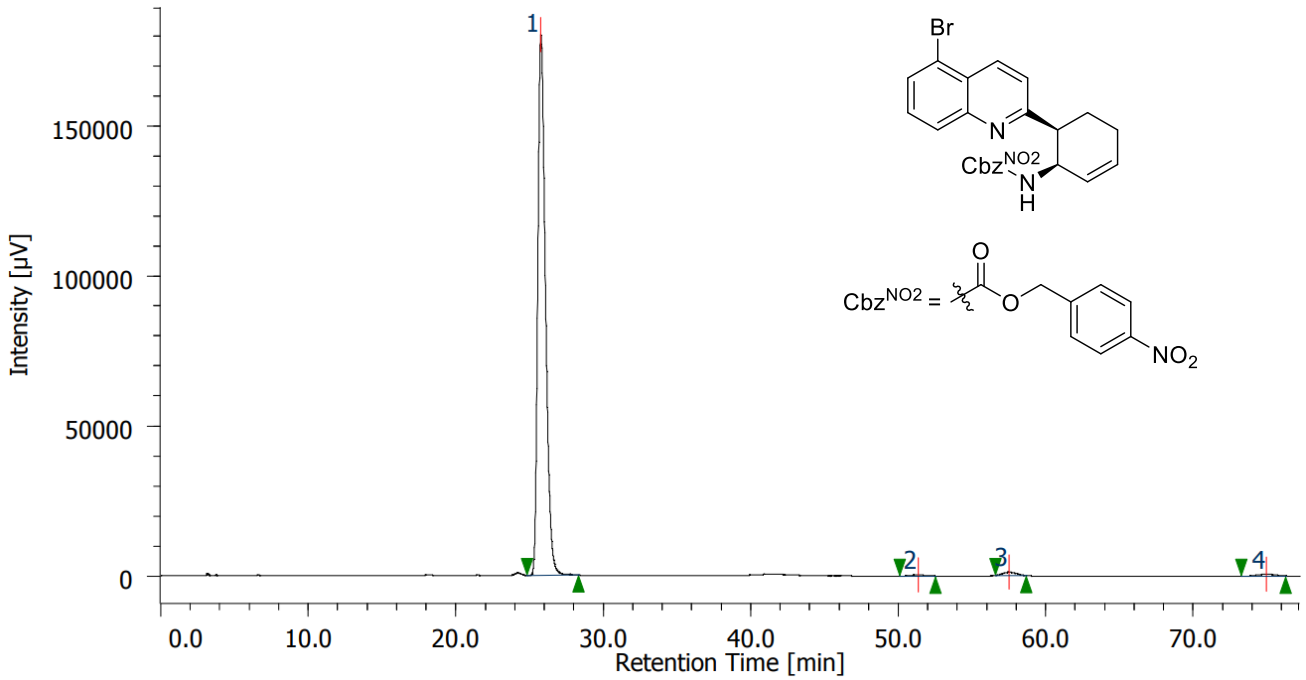




12ca

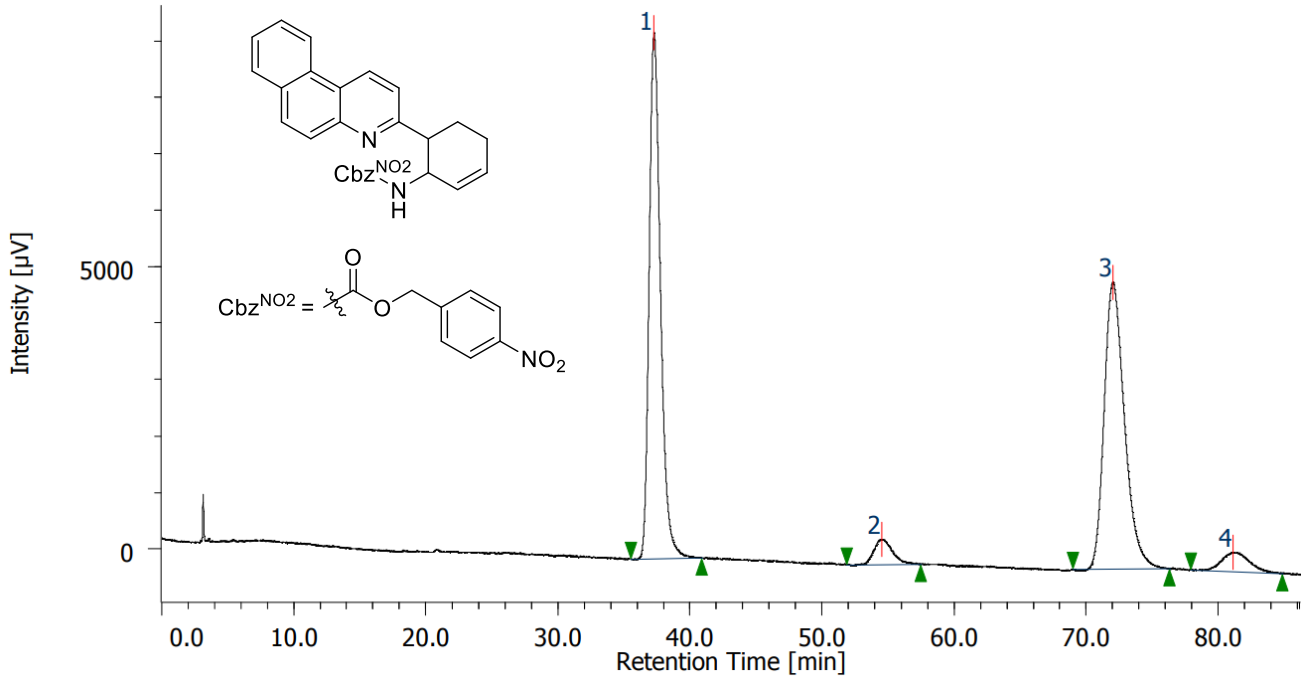
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	27.8	32.4	44.5	52.6
Area (%)	96.7	0.5	1.9	1.0

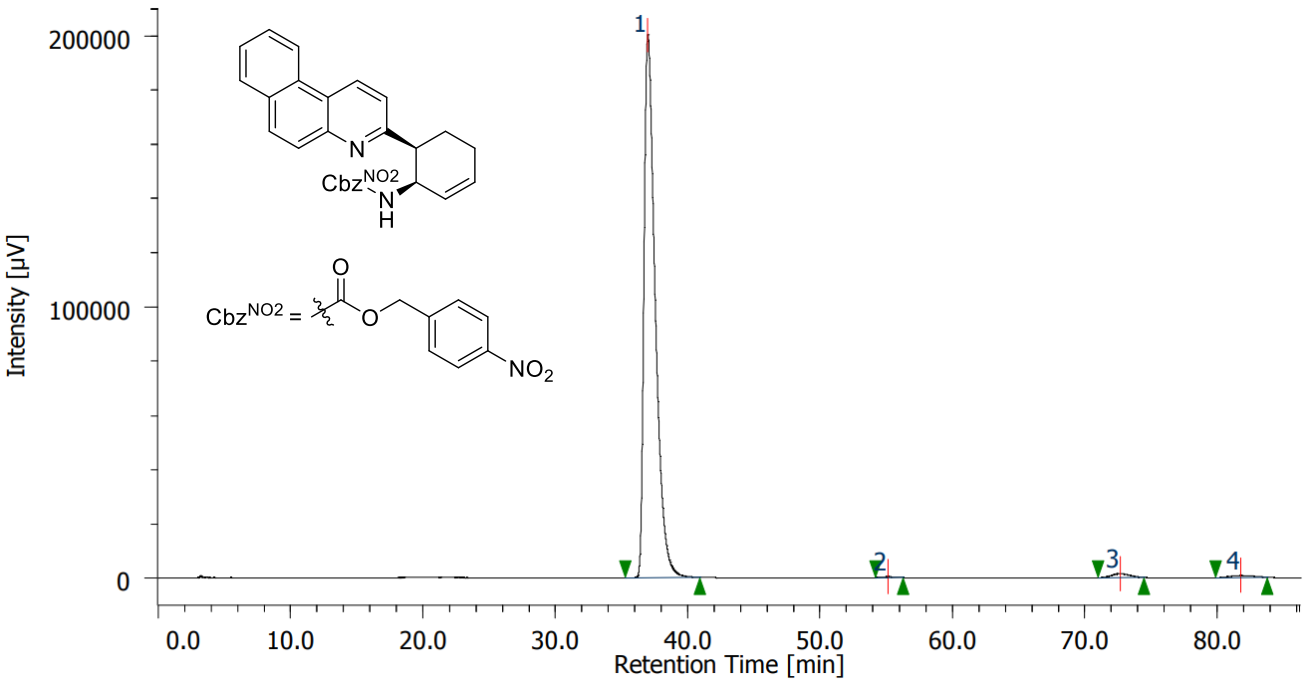




12da

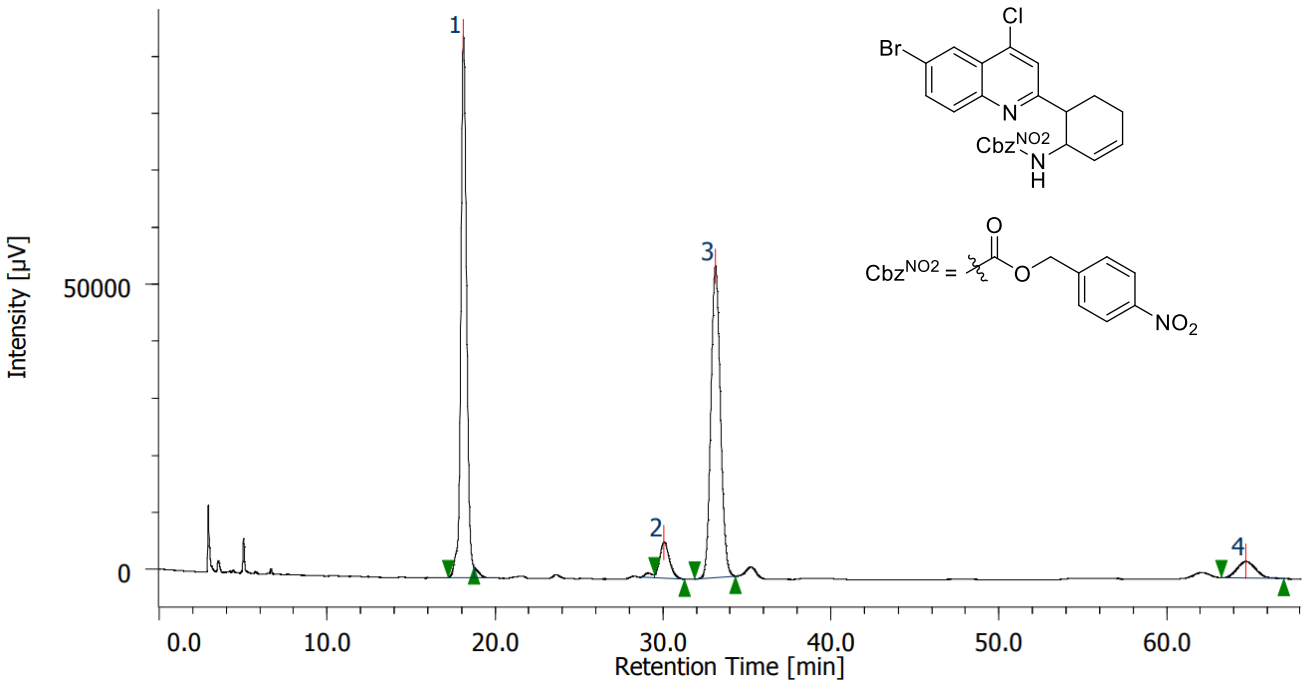
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	25.8	51.3	57.5	75.0
Area (%)	97.7	0.4	1.1	0.8

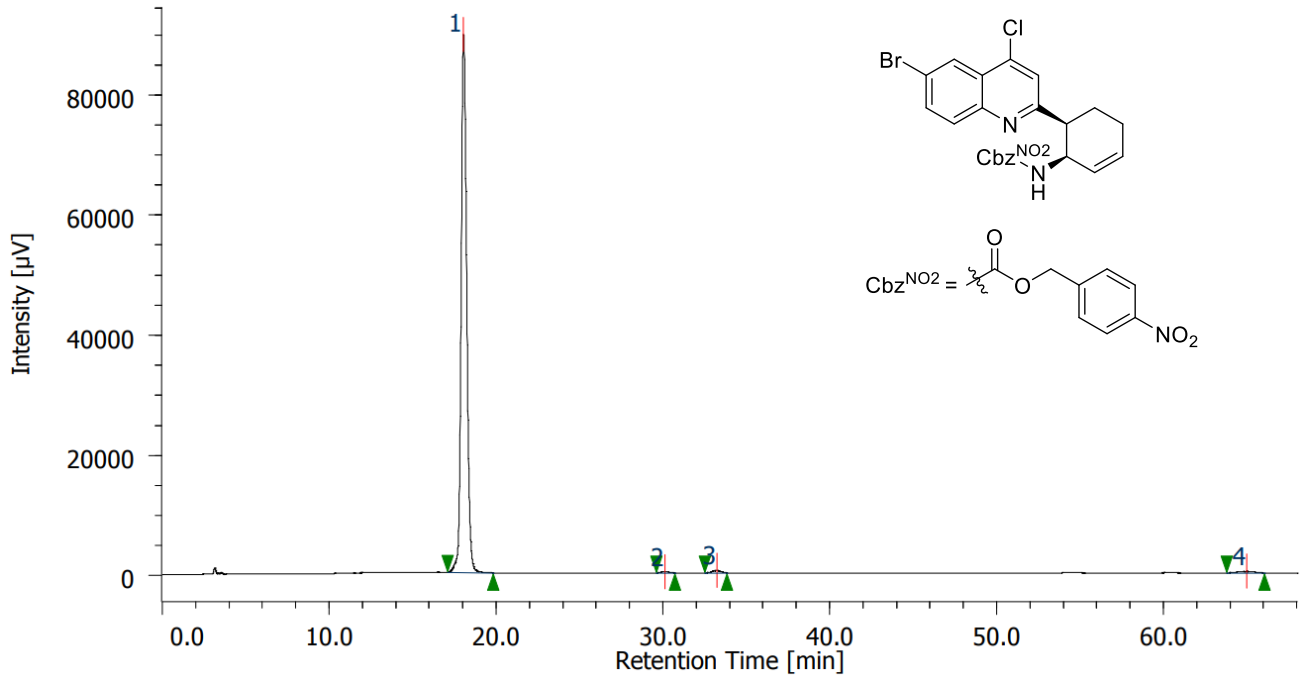




12ea

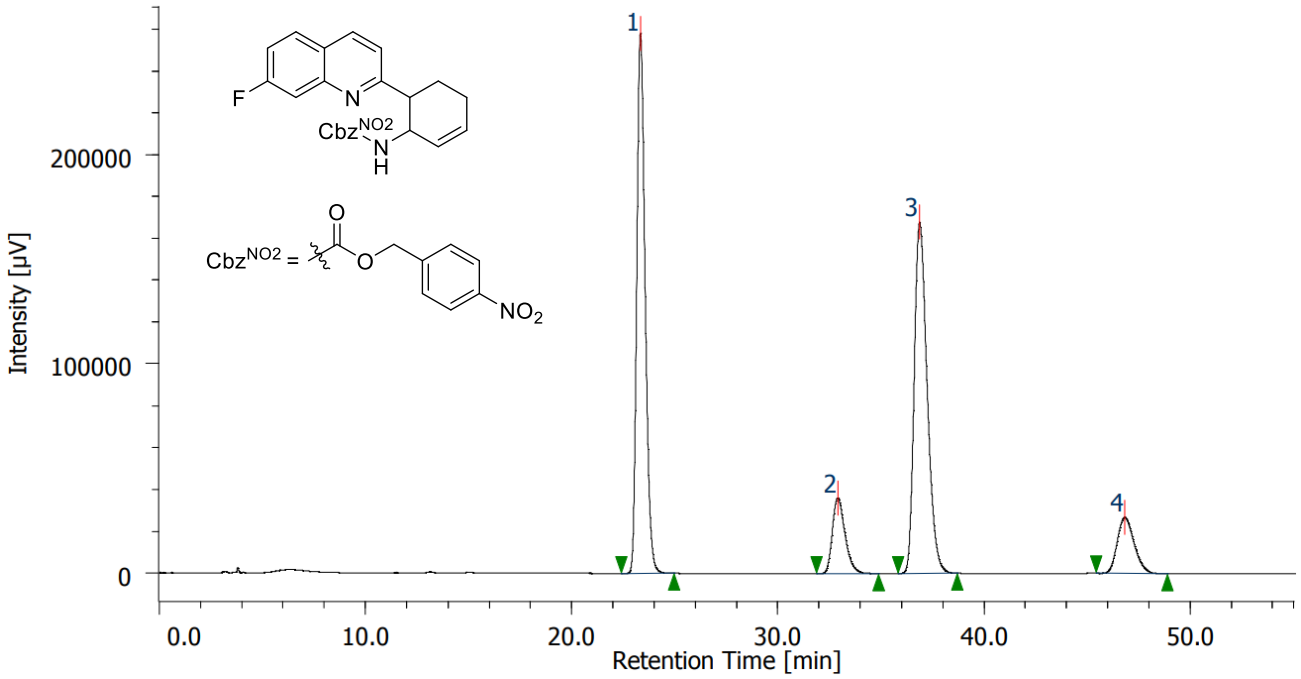
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	37.0	55.1	72.6	81.7
Area (%)	97.9	0.2	1.2	0.8

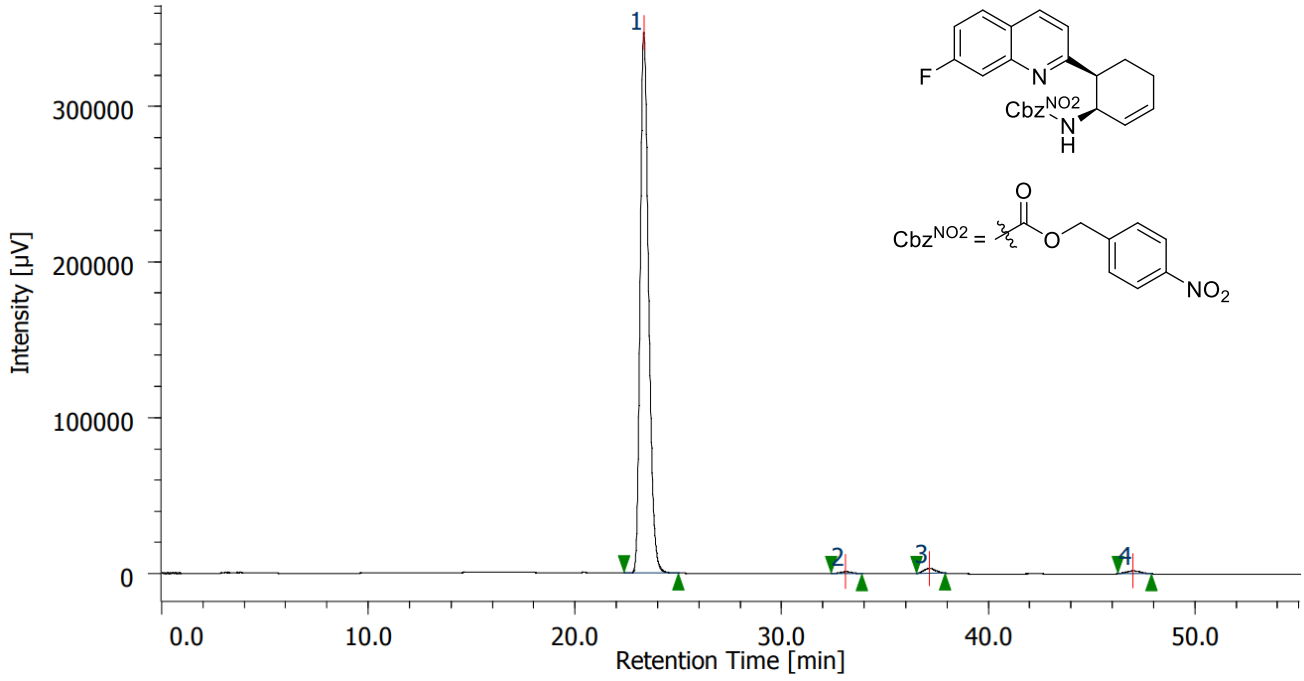




12fa

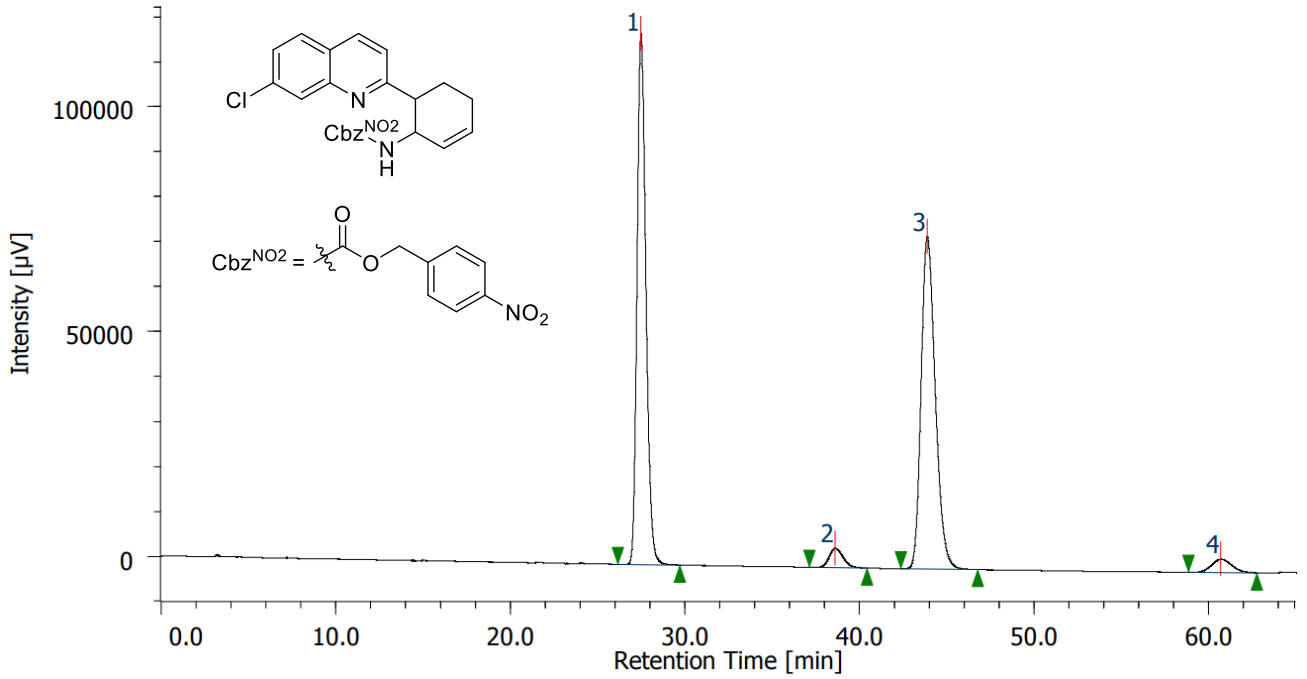
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	18.0	30.1	33.2	65.0
Area (%)	98.1	0.4	0.7	0.8

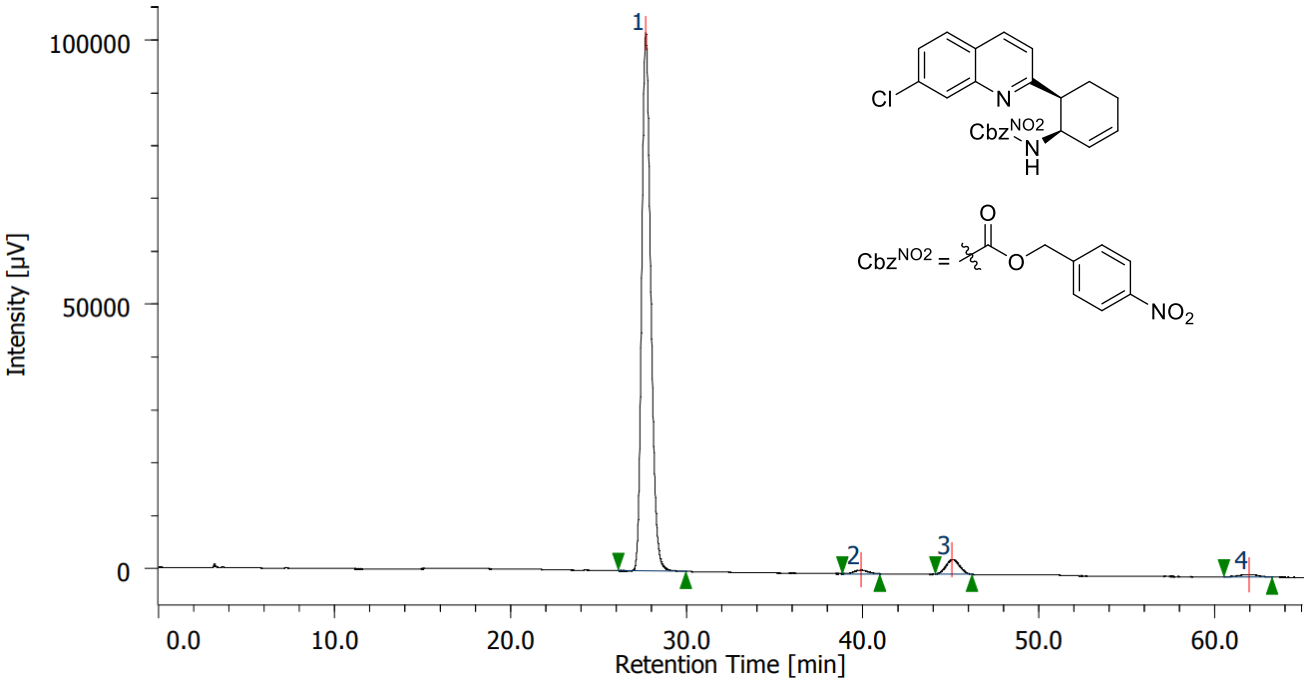




12ga

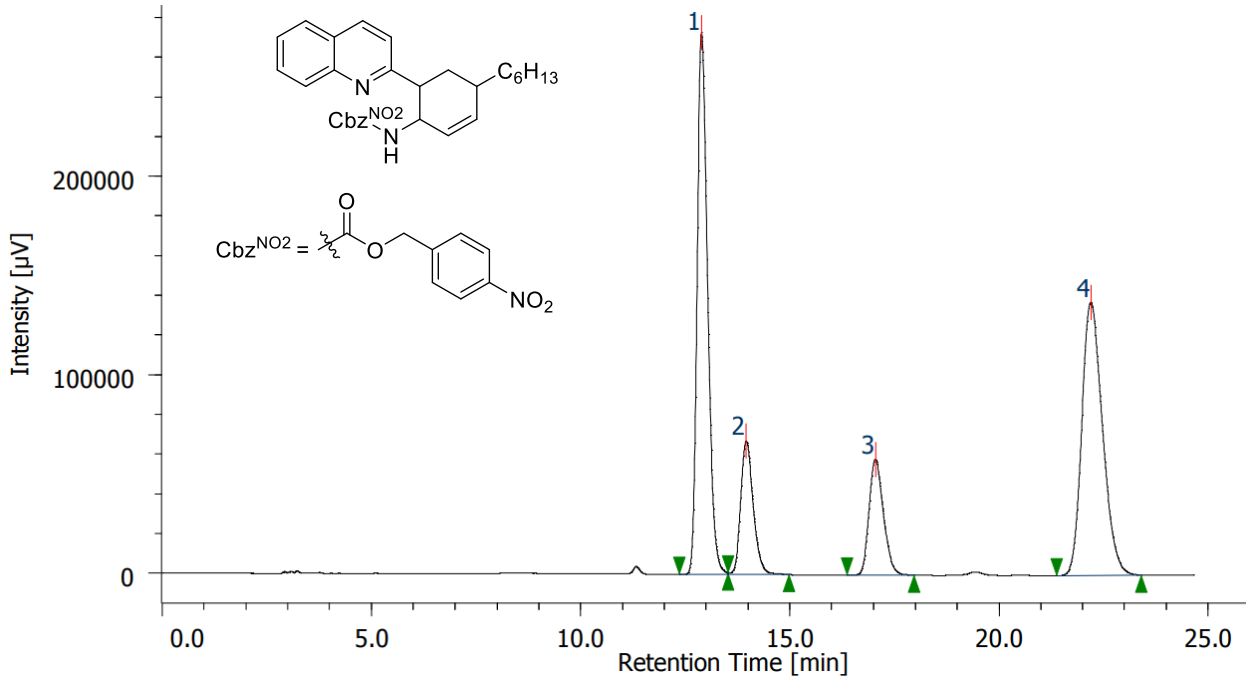
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	23.3	33.1	37.1	47.0
Area (%)	97.4	0.5	1.2	0.9

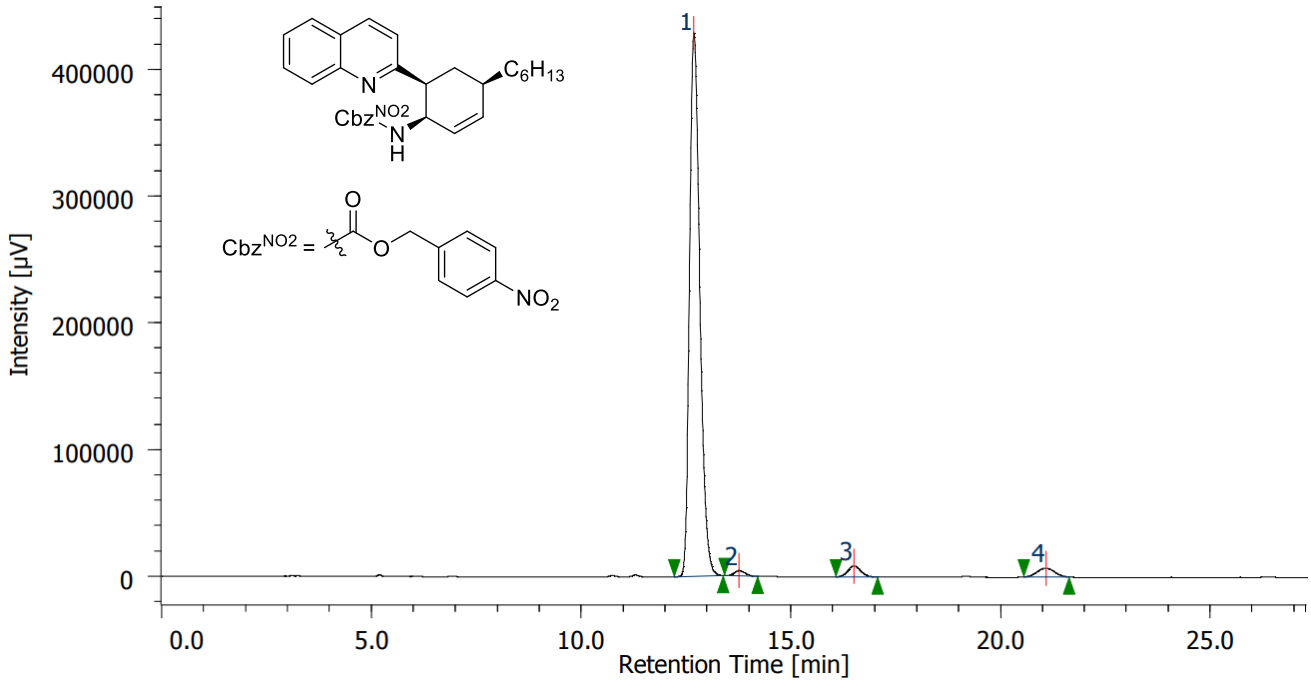




12ha

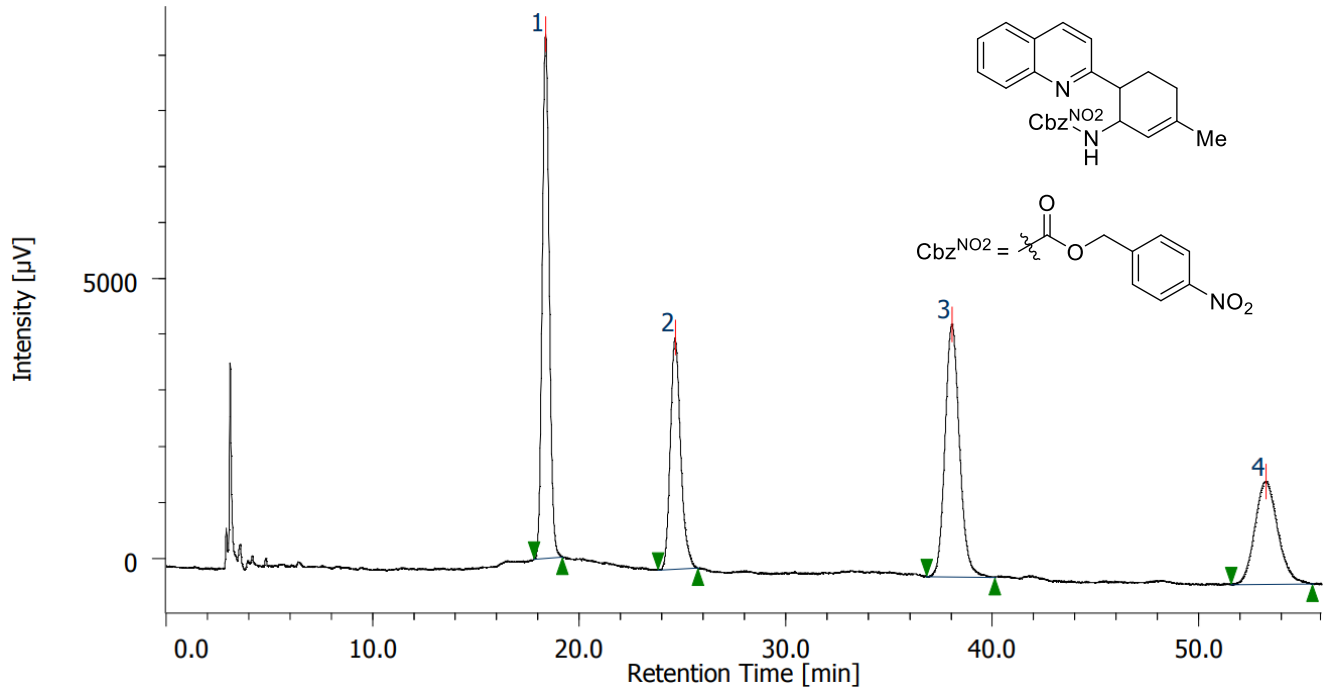
Peak	1 (*endo*)	2 (*exo*)	3 (*endo*)	4 (*exo*)
Retention Time (min)	27.7	39.9	45.1	62.0
Area (%)	94.2	1.0	3.9	0.9

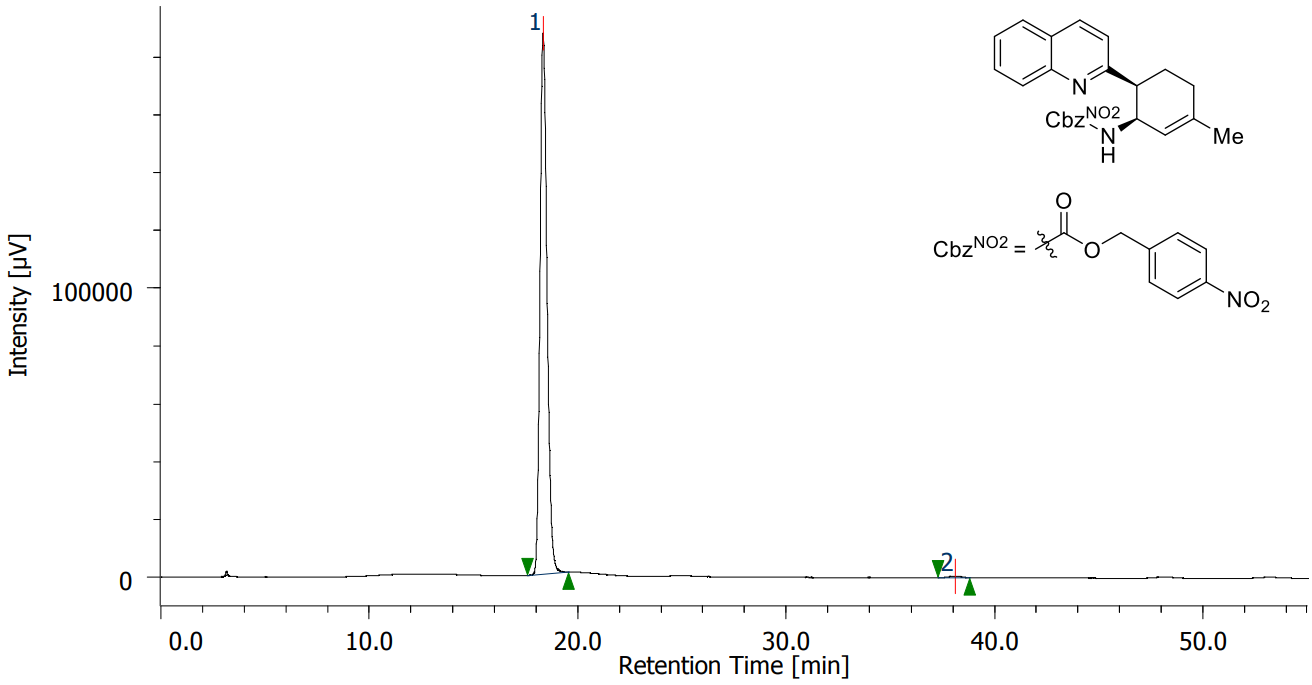




12ac

Peak	1 (*endo*)	2 (*exo*)	3 (*exo*)	4 (*endo*)
Retention Time (min)	12.7	13.8	16.5	21.1
Area (%)	94.0	1.0	2.4	2.6





12ad

Peak	1 (*endo*)	2 (*exo*)	3(2) (*endo*)	4 (*exo*)
Retention Time (min)	18.4	24.6	38.0	53.2
Area (%)	99.4	-	0.6	-