Supporting Information for

Enantioselective Synthesis of Hexahydrofuro[3,2-*c*]quinolines through a Multicatalytic and Multicomponent Process. A New "Aromatic Sandwich" Model for BINOL-Phosphoric Acid Catalyzed Reactions

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Contents

General.

^{1}H NMR spectra were recorded on a Bruker AV-600 (600 MHz), Bruker NAV-400 (400 MHz), Bruker AV-400 (400 MHz), Bruker AV-300 (300 MHz) or Bruker DPX-300 (300 MHz). Chemical shifts are reported in ppm from tetramethylsilane with the residual solvent resonance as the internal standard ($CHCl_3$: δ 7.26, C_6H_6: δ 7.40). Data are reported as follows: chemical shift, multiplicity (s: singlet, d: doublet, dd: doublet of doublet, dt: doublet of triplet, ddd: doublet of doublet of doublet, dddd: doublet of doublet of doublet of doublet, ddt: doublet of doublet of triplet, td: triplet of doublet, tdd: triplet of doublet of doublet, t: triplet, q: quartet, dq: doublet of quartet, qd: quartet of doublet, qdd: quartet of doublet of doublet, ddq: doublet of doublet of quartet, qt: quartet of triplet, br: broad, m: multiplet), coupling constants (*J* in Hz), integration and assignment. ^{13}C NMR spectra were recorded on a Bruker Bruker AV-600 (150 MHz), Bruker NAV-400 (100 MHz), Bruker AV-400 (100 MHz), Bruker AV-300 (75 MHz) or Bruker DPX-300 (75 MHz) with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 76.95, C_6D_6: δ 128.62). High-resolution mass spectrometry was carried out on a Finnigan-Mat 95 spectrometer. Optical rotations were measured using a 2 mL cell with a 1 dm path length on an Autopol IV Rudolph Research Analytical polarimeter at 589 nm, and are reported as $[\alpha]^{T}_{D}$ (concentration in grams/mL). Chiral HPLC analysis was performed using a Waters LC Module 1 Plus instrument. Solvents were dried and deoxygenated with a PureSolv® column system before use. All reactions were conducted in dried glassware under an inert atmosphere of argon. The alkynols **1** were prepared according to the methods reported in the literature.[1]

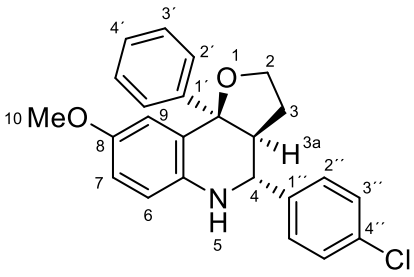
General Procedure for the Synthesis of Hexahydrofuro[3,2-*c*]quinoline Derivatives 4.

The corresponding alkynol **1** (0.2 mmol), aldehyde **2** (0.2 mmol), aniline **3** (0.2 mmol), (*R*) or (*S*)-TRIP (22 mg; 15 mol%) and 4 Å powder molecular sieves (50 mg), were placed in a carrousel tube under argon. Then, dichloromethane (2 mL) was added. The slurry was cooled to 0ºC and AuMe(JohnPhos) (10 mg; 10 mol%) was added portionwise. The mixture was stirred at 0ºC for 72 h. Then, the reaction was allowed to warm to room temperature and the resulting slurry was filtered through a path of celite, the solvent was removed at reduced pressure and the crude was purified by flash column chromatography on silica gel using mixtures of hexane and diethyl ether as eluent to give pure **4**.

[1] Belting, V.; Krause, N. *Org. Lett.* **2006**, *8*, 4489.

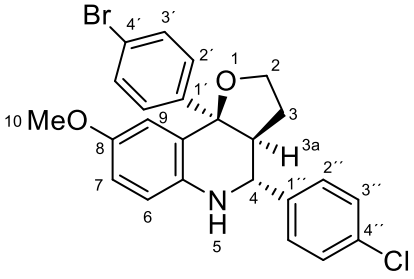
CHARACTERIZATION DATA

(3a*R*,4*S*,9b*S*)-4-(4-Chlorophenyl)-8-methoxy-9b-phenyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4a)



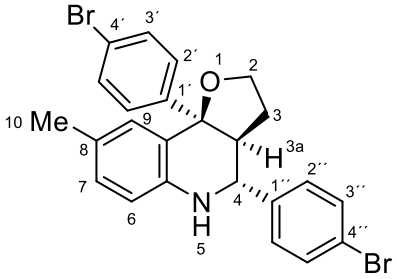
Brown solid. R_f = 0.25 (hexane:diethyl ether, 2:1). $[\alpha]^{25}_D$= –65º (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, $CDCl_3$) δ= 7.34 (d, *J*= 8.3 Hz, 2H, $H_{3''}$), 7.29 (d, *J*= 7.5 Hz, 2H, $H_{2'}$), 7.26 (d, *J*= 8.3 Hz, 2H, $H_{2''}$), 7.20 (t, *J*= 7.5 Hz, 2H, $H_{3'}$), 7.11 (t, *J*= 7.5 Hz, 1H, $H_{4'}$), 6.59 (dd, *J*= 8.7, 2.3 Hz, 1H, H_7), 6.51 (d, *J*= 8.7 Hz, 1H, H_6), 6.40 (d, *J*= 2.3 Hz, 1H, H_9), 4.11–3.94 (m, 2H, H_2), 3.87 (d containing br s, *J*= 11.0 Hz, 2H, H_4, H_5), 3.48 (s, 3H, H_{10}), 2.63 (dd, *J*= 11.0, 7.2 Hz, 1H, H_{3a}), 1.79–1.65 (m, 1H, H_{3A}), 1.63–1.39 (m, 1H, H_{3B}). ^{13}C NMR (75 MHz, $CDCl_3$) δ= 152.9, 146.8, 140.3, 138.9, 133.8, 129.4, 128.7, 127.9, 127.3, 126.5, 125.6, 115.9, 115.4, 115.1, 85.3, 65.1, 58.8, 55.5, 52.9, 27.4. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:*i*-PrOH= 90:10, 0.5 mL/min]. Retention times 18.1 (minor), 31.8 (major). HRMS calcd for $C_{24}H_{22}ClNO_2$ (M^+): 391.1334, found 391.1339.

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-chlorophenyl)-8-methoxy-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4b)



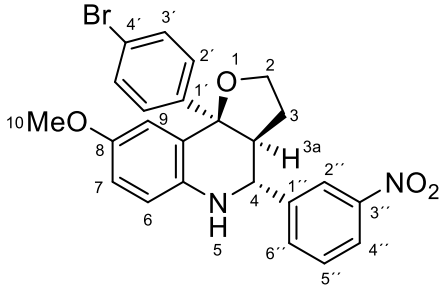
White solid. R_f = 0.25 (hexane:diethyl ether, 2:1). $[\alpha]^{25}_D$= –70º (*c* 0.1, DCM). ^{1}H NMR (300 MHz, $CDCl_3$) δ= 7.44 (d, *J*= 8.5 Hz, 2H, $H_{3'}$), 7.43 (d, *J*= 8.6 Hz, 2H, $H_{3''}$), 7.38 (d, *J*= 8.5 Hz, 2H, $H_{2'}$), 7.27 (d, *J*= 8.6 Hz, 2H, $H_{2''}$), 6.72 (dd, *J*= 8.7, 2.7 Hz, 1H, H_7), 6.64 (d, *J*= 8.7 Hz, 1H, H_6), 6.47 (d, *J*= 2.7 Hz, 1H, H_9), 4.13 (dd, *J*= 9.4, 5.3 Hz, 2H, H_2), 3.98 (d containing br s, *J*= 10.9 Hz, 2H, H_4, H_5), 3.62 (s, 3H, H_{10}), 2.68 (dd, *J*= 10.9, 6.8 Hz, 1H, H_{3a}), 1.95–1.74 (m, 1H, H_{3A}), 1.72–1.57 (m, 1H, H_{3B}). ^{13}C NMR (75 MHz, $CDCl_3$) δ= 153.0, 146.2, 140.0, 138.8, 134.0, 131.1, 129.4, 128.8, 127.5, 126.9, 120.5, 116.1, 115.6, 114.9, 85.1, 65.3, 58.9, 55.6, 53.1, 27.4. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:*i*-PrOH= 90:10, 0.5 mL/min]. Retention times 20.5 (minor), 30.7 (major). HRMS calcd for $C_{24}H_{21}BrClNO_2$ (M^+): 469.0439, found 469.0443.

(3a*R*,4*S*,9b*S*)-4,9b-Bis(4-bromophenyl)-8-methyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4c)



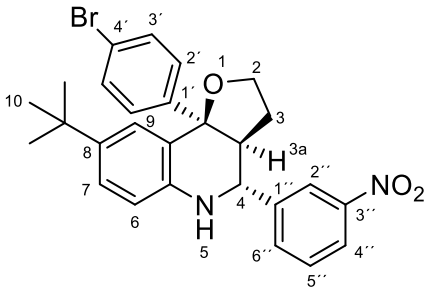
White solid. R_f = 0.25 (hexane:diethyl ether, 2:1). $[\alpha]^{25}_D$= –72º (*c* 0.1, DCM). ^{1}H-NMR (400 MHz, $CDCl_3$) δ= 7.53 (d, *J*= 8.3 Hz, 2H, $H_{3''}$), 7.43 (d, *J*= 8.5 Hz, 2H, $H_{3'}$), 7.37 (d, *J*= 8.3 Hz, 2H, $H_{2''}$), 7.26 (d, *J*= 8.5 Hz, 2H, $H_{2'}$), 6.89 (dd, *J*= 8.1, 1.4 Hz, 1H, H_7), 6.70 (br s, 1H, H_9), 6.59 (d, *J*= 8.1 Hz, 1H, H_6), 4.11 (dd, *J*= 9.6, 5.1 Hz, 2H, H_2), 4.04 (s, 1H, H_5), 3.96 (d, *J*= 11.2 Hz, 1H, H_4), 2.65 (dd, *J*= 11.2, 7.0 Hz, 1H, H_{3a}), 2.12 (s, 3H, H_{10}), 1.87–1.72 (m, 1H, H_{3A}), 1.63 (dt, *J*= 12.9, 5.1 Hz, 1H, H_{3B}). ^{13}C-NMR (100 MHz, $CDCl_3$) δ= 146.3, 142.4, 140.6, 131.8, 131.0, 130.7, 129.7, 129.2, 128.7, 127.5, 125.8, 122.0, 120.3, 115.0, 84.9, 65.1, 58.5, 53.0, 27.3, 20.4. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:*i*-PrOH= 90:10, 0.5 mL/min]. Retention times 16.9 (minor), 19.1 (major). HRMS calcd for $C_{24}H_{21}Br_2NO$ (M^+): 496.9984, found 496.9981.

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-methoxy-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4d)



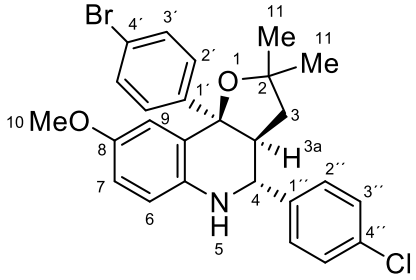
Orange solid. R_f = 0.25 (hexane:diethyl ether, 1:1). $[\alpha]^{25}_D$= –78º (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 8.20 (br s, 1H, $H_{2''}$), 7.96 (dd, *J*= 8.5, 1.9 Hz, 1H, $H_{4''}$), 7.34 (d, *J*= 8.3 Hz, 2H, $H_{3'}$), 7.19 (d, *J*= 8.3 Hz, 2H, $H_{2'}$), 7.23–7.14 (m, 1H, $H_{6''}$), 7.03–6.67 (m, 3H, H_7, H_9, $H_{5''}$), 6.47 (d, *J*= 8.5 Hz, 1H, H_6), 3.84 (apparent dd, *J*= 9.2, 5.0 Hz, 2H, H_2), 3.59 (d, *J*= 11.0 Hz, 1H, H_4), 3.38 (s, 1H, H_5), 3.31 (s, 3H, H_{10}), 2.46 (dd, *J*= 11.0, 7.3 Hz, 1H, H_{3a}), 1.60–1.37 (m, 1H, H_{3A}), 1.29–1.10 (m, 1H, H_{3B}). ^{13}C-NMR (75 MHz, C_6D_6) δ= 153.9, 148.8, 147.0, 144.3, 138.9, 133.8, 131.6, 129.4, 123.2, 123.1, 120.9, 116.5, 115.9, 115.4, 85.1, 65.2, 58.9, 55.1, 53.7, 27.7. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:*i*-PrOH= 90:10, 0.5 mL/min]. Retention times 39.7 (minor), 55.9 (major). HRMS calcd for $C_{24}H_{21}BrN_2O_4$ (M^+): 480.0679, found 480.0681.

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-*tert*-butyl-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4e)



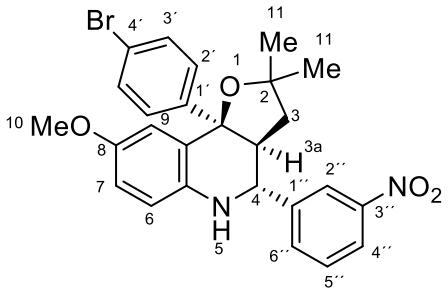
Orange solid. R_f = 0.25 (hexane:diethyl ether, 1:1). $[\alpha]^{25}_D$= –68º (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 8.19 (br s, 1H, $H_{2''}$), 7.95 (brd, *J*= 7.9 Hz, 1H, $H_{4''}$), 7.36–7.33 (m, 3H, $H_{3'}$, H_9), 7.24–7.15 (m, 4H, $H_{2'}$, H_7, $H_{6''}$), 6.88 (t, *J*= 7.9 Hz, 1H, $H_{5''}$), 6.53 (d, *J*= 8.4 Hz, 1H, H_6), 3.96–3.75 (m, 2H, H_2), 3.62 (d, *J*= 10.6 Hz, 1H, H_4), 3.47 (s, 1H, H_5), 2.45 (dd, *J*= 10.6, 7.1 Hz, 1H, H_{3a}), 1.49–1.34 (m, 2H, H_3), 1.24 (s, 9H, H_{10}). ^{13}C-NMR (75 MHz, C_6D_6) δ= 148.9, 147.1, 144.3, 142.6, 133.8, 131.4, 129.4, 126.3, 125.7, 123.2, 123.0, 120.9, 115.1, 85.1, 65.0, 58.4, 53.4, 34.2, 31.5, 27.6. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:*i*-PrOH= 90:10, 0.5 mL/min]. Retention times 16.8 (major), 20.0 (minor). HRMS calcd for $C_{27}H_{27}BrN_2O_3$ (M^+): 506.1200, found 506.1211.

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-chlorophenyl)-8-methoxy-2,2-dimethyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4f)



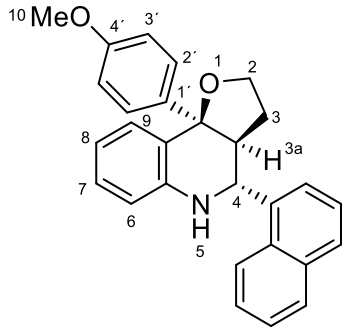
White solid. R_f = 0.20 (hexane:diethyl ether, 3:1). $[\alpha]^{25}_D$= –82º (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 7.45 (d, *J*= 8.6 Hz, 2H, $H_{3'}$), 7.30 (d, *J*= 8.6 Hz, 2H, $H_{2'}$), 7.21 (d, *J*= 8.4 Hz, 2H, $H_{3''}$), 7.15 (d, *J*= 2.9 Hz, 1H, H_9), 7.01 (d, *J*= 8.4 Hz, 2H, $H_{2''}$), 6.83 (dd, *J*= 8.6, 2.9 Hz, 1H, H_7), 6.40 (d, *J*= 8.6 Hz, 1H, H_7), 3.94 (d, *J*= 9.2 Hz, 1H, H_4), 3.36 (s, 4H, H_5, H_{10}), 2.96 (dt, *J*= 9.2, 6.8 Hz, 1H, H_{3a}), 1.69 (d, *J*= 6.8 Hz, 2H, H_3), 1.36 and 1.35 (2s, 6H, H_{11}). ^{13}C-NMR (75 MHz, C_6D_6) δ= 154.1, 149.1, 141.4, 138.1, 133.7, 131.2, 130.5, 129.2, 128.9, 128.2, 120.7, 116.4, 115.4, 114.3, 84.9, 81.4, 60.5, 56.9, 55.1, 42.5, 31.0, 30.7. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:EtOH= 98:2, 0.5 mL/min]. Retention times 21.3 (minor), 23.0 (major). HRMS calcd for $C_{26}H_{25}BrClNO_2$ (M^+): 497.0752, found 497.0754.

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-methoxy-2,2-dimethyl-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4g)



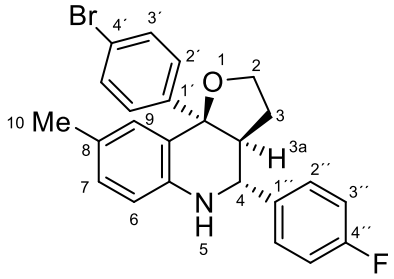
Yellow solid. R_f = 0.25 (hexane:diethyl ether, 2:1). $[\alpha]^{25}_D$= –91º (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 8.08 (br s, 1H, $H_{2''}$), 7.87 (dd, *J*= 8.0, 1.9 Hz, 1H, $H_{4''}$), 7.23 (d, *J*= 8.6 Hz, 2H, $H_{3'}$), 7.17 (d, *J*= 8.6 Hz, 2H, $H_{2'}$), 7.12 (d, *J*= 2.9 Hz, 1H, H_9), 7.09 (brd, *J*= 8.0 Hz 1H, $H_{6''}$), 6.89 (dd, *J*= 8.7, 2.9 Hz, 1H, H_7), 6.77 (t, *J*= 8.0 Hz, 1H, $H_{5''}$), 6.44 (d, *J*= 8.7 Hz, 1H, H_6), 3.92 (d, *J*= 7.4 Hz, 1H, H_4), 3.35 (s, 3H, H_{10}), 3.31 (s, 1H, H_5), 2.85 (apparent q, *J*= 7.0 Hz, 1H, H_{3a}), 1.73 (dd, *J*= 13.1, 7.0 Hz, 1H, H_{3A}), 1.69 (dd, *J*= 13.1, 7.5 Hz, 1H, H_{3B}), 1.33 y 1.29 (2s, 6H, H_{11}).^{13}C-NMR (75 MHz, C_6D_6) δ= 153.8, 147.5, 144.8, 136.7, 132.6, 130.8, 128.9, 128.7, 128.4, 122.1, 122.1, 120.6, 116.0, 115.8, 113.9, 83.9, 80.7, 58.3, 55.0, 54.8, 42.6, 30.6, 30.2. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:*i*-PrOH= 85:15, 0.5 mL/min]. Retention times 14.3 (major), 16.5 (minor). HRMS calcd for $C_{26}H_{25}BrN_2O_4$ (M^+): 508.0992, found 508.0995.

(3a*R*,4*S*,9b*S*)-9b-(4-Methoxyphenyl)-4-(naphthalen-1-yl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4h)



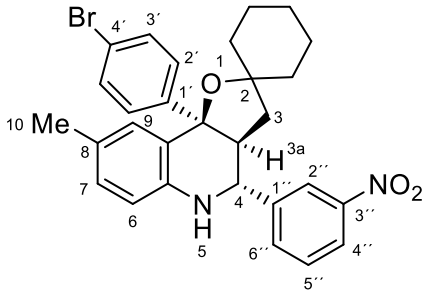
White solid. R_f = 0.28 (hexane:diethyl ether, 3:1). $[\alpha]^{25}_D$= –59º (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 7.80 (dd, *J*= 6.3, 3.3 Hz, 1H, H_{Nf}), 7.75 (d, *J*= 8.2 Hz, 1H, H_{Nf}), 7.68 (m, 1H, H_{Nf}), 7.54 (d, *J*= 8.6 Hz, 2H, $H_{2'}$), 7.49 (d, *J*= 7.8 Hz, 1H, H_9) 7.43–7.33 (m, 3H, H_{Nf}), 7.19–7.05 (t, *J*= 7.5 Hz, 1H, H_7), 6.89 (d, *J*= 8.6 Hz, 2H, $H_{3'}$), 6.82 (t, *J*= 7.5 Hz, 1H, H_8), 6.48 (d, *J*= 7.5 Hz, 1H, H_6), 4.84 (d, *J*= 10.8 Hz, 1H, H_4), 4.10 (apparent q, *J*= 8.5 Hz, 1H, H_{2A}), 4.01 (td, *J*= 8.5, 2.7 Hz, 1H, H_{2B}), 3.85 (s, 1H, H_5), 3.42 (s, 3H, H_{10}), 3.21 (dd, *J*= 10.8, 7.4 Hz, 1H, H_{3a}), 1.91–1.58 (m, 1H, H_{3A}), 1.58–1.21 (m, 1H, H_{3B}). ^{13}C NMR (75 MHz, C_6D_6) δ= 158.9, 145.9, 140.1, 138.2, 134.5, 132.9, 132.3, 129.4, 128.7, 127.4, 126.6, 125.9, 125.9, 119.3, 115.1, 113.9, 85.8, 65.3, 54.8, 53.1, 27.9. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:*i*-PrOH= 95:5, 0.5 mL/min]. Retention times 21.3 (minor), 43.9 (major). HRMS calcd for $C_{28}H_{25}NO_2$ (M^+): 407.1880, found 407.1882.

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-fluorophenyl)-8-methyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4i)



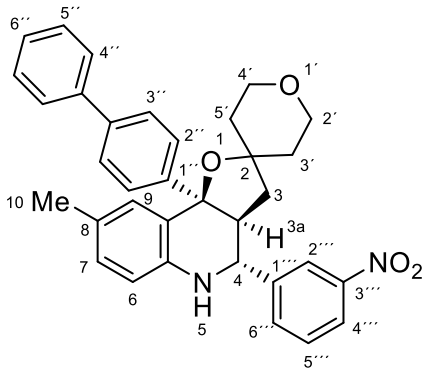
White solid. R_f= 0.25 (hexane:diethyl ether, 2:1). $[\alpha]^{25}_D$= –74º (*c* 0.1, DCM). ^{1}H-NMR (400 MHz, $CDCl_3$) δ= 7.38 (d, *J*= 8.6 Hz, 2H, $H_{3'}$), 7.30 (d, *J*= 8.6 Hz, 2H, $H_{2'}$), 7.15 (d, *J*= 1.3 Hz, 1H, H_9), 7.06 (dd, *J*= 8.8, J_{HF}= 5.7 Hz, 2H, $H_{2''}$), 6.93 (t, *J*= 8.8 Hz, J_{HF}= 8.8 Hz, 2H, $H_{3''}$), 6.92 (d, *J*= 8.1 Hz, 1H, H_7), 6.41 (d, *J*= 8.1 Hz, 1H, H_6), 3.97–3.85 (m, 2H, H_2), 3.68 (d, *J*= 11.2 Hz, 1H, H_4), 3.52 (s, 1H, H_5), 2.55 (dd, *J*= 11.2, 6.1 Hz, 1H, H_{3a}), 2.07 (s, 3H, H_{10}), 1.60–1.46 (m, 1H, H_{3A}), 1.35 (ddd, *J*= 10.0, 6.1, 3.5 Hz, 1H, H_{3B}). ^{13}C-NMR (75 MHz, C_6D_6) δ= 142.0, 141.9, 141.3, 135.1, 131.7, 130.8, 130.0, 129.1, 129.0, 126.1, 125.7, 125.1, 124.8, 124.4, 121.8, 114.9, 85.5, 63.8, 58.2, 49.8, 27.5, 20.2. ^{19}F-NMR (282 MHz, C_6D_6) δ= –113.8. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:EtOH= 95:5, 0.3 mL/min]. Retention times 28.1 (minor), 49.8 (major). HRMS calcd for $C_{24}H_{21}BrFNO$ (M^+): 437.0785, found 437.0786.

(3a'*R*,4'*S*,9b'*S*)-9b'-(4-Bromophenyl)-8'-methyl-4'-(3-nitrophenyl)-3a',4',5',9b'-tetrahydro-3'*H*-spiro[cyclohexane-1,2'-furo[3,2-*c*]quinoline] (4j)



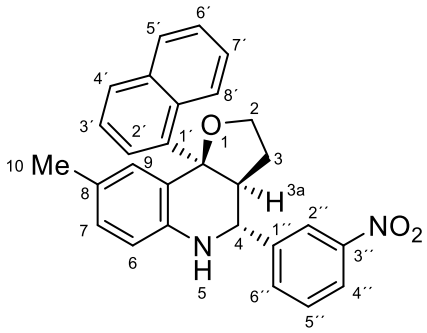
Yellow solid. R_f = 0.20 (hexane:diethyl ether, 1:1). $[\alpha]^{25}_D$= –106º (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 8.05 (t, *J*= 1.8 Hz, 1H, $H_{2''}$), 7.83 (dd, *J*= 8.1, 1.8 Hz, 1H, $H_{4''}$), 7.34 (d, *J*= 2.1 Hz, 1H, H_9), 7.18 (d, *J*= 8.9 Hz, 2H, $H_{3'}$), 7.14 (d, *J*= 8.9 Hz, 2H, $H_{2'}$), 7.07 (d, *J*= 8.1 Hz, 1H, $H_{6''}$), 6.97 (dd, *J*= 8.1, 2.1 Hz, 1H, H_7), 6.74 (t, *J*= 8.1 Hz, 1H, $H_{5''}$), 6.47 (d, *J*= 8.1 Hz, 1H, H_6), 3.97 (d, *J*= 6.9 Hz, 1H, H_4), 3.45 (s, 1H, H_5), 2.81 (apparent q, *J*= 7.0 Hz, 1H, H_{3a}), 2.15 (s, 3H, H_{10}), 1.97–1.54 and 1.59–1.16 (2m, 12H, H_3, H_{cy}). ^{13}C-NMR (75 MHz, C_6D_6) δ = 148.6, 147.6, 145.0, 140.7, 132.8, 131.2, 130.9, 129.4, 129.1, 128.9, 128.6, 127.5, 122.4, 122.2, 120.7, 114.9, 83.4, 82.6, 57.6, 54.0, 40.2, 39.7, 25.7, 24.2, 23.9, 20.7. The enantiomeric excess was determined by HPLC [Chiracel ODH, 250 x 4.6 mm, hexane:*i*-PrOH= 95:5, 0.3 mL/min]. Retention times 74.9 (major), 90.9 (minor). HRMS calcd for $C_{29}H_{29}BrN_2O_3$ (M^+): 532.1356, found 532.1360.

(3a*R*,4*S*,9b*S*)-9b-(Biphenyl-4-yl)-8-methyl-4-(3-nitrophenyl)-2',3a,3',4,5,5',6',9b-octahydro-3*H*-spiro[furo[3,2-*c*]quinoline-2,4'-pyran] (4k)



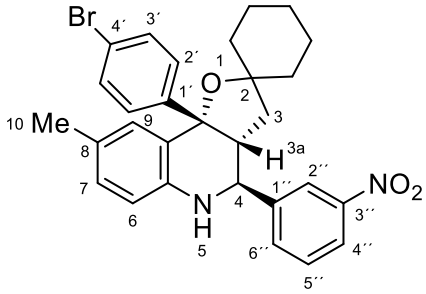
Yellow solid. R_f = 0.20 (hexane:diethyl ether, 1:2). $[\alpha]^{25}_D$= –102° (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 8.09 (apparent t, *J*= 1.9 Hz, 1H, $H_{2'''}$), 7.77 (apparent dd, *J*= 8.0, 1.9 Hz , 1H, $H_{4'''}$), 7.55 (d, *J*= 7.6 Hz, 2H, $H_{4''}$), 7.42 (br s, 1H, H_9), 7.40 (d, *J*= 8.3 Hz, 2H, $H_{2''}$), 7.32 (d, *J*= 8.3 Hz, 2H, $H_{3''}$), 7.31 (t, *J*= 7.6 Hz, 2H, $H_{5''}$), 7.20 (t, *J*= 7.6 Hz, 1H, $H_{6''}$), 7.12 (d, *J*= 8.0, 1H, $H_{6'''}$), 7.00 (dd, *J*= 8.1, 1.6 Hz, 1H, H_7), 6.73 (t, *J*= 8.0 Hz, 1H, $H_{5'''}$), 6.51 (d, *J*= 8.1 Hz, 1H, H_6), 4.16 (ddd, *J*= 11.7, 8.6, 3.1 Hz, 1H, $H_{2'A}$), 4.08–3.93 (m, 2H, H_4, $H_{5'A}$), 3.74 (dt, *J*= 11.7, 5.2 Hz, 1H, $H_{2'B}$), 3.59 (dt, *J*= 11.7, 5.2 Hz, $H_{5'B}$), 3.53 (s, 1H, H_5), 2.96 (apparent q, *J*= 7.6 Hz, 1H, H_{3a}), 2.15 (s, 3H, H_{10}), 1.96 (m, 1H, $H_{3'A}$), 1.88–1.60 (m, 4H, H_{3A}, H_{3B}, $H_{3'B}$, $H_{4'A}$), 1.57–1.45 (m, 1H, $H_{4'B}$). ^{13}C-NMR (75 MHz, C_6D_6) δ= 148.3, 146.5, 144.8, 141.1, 140.4, 139.78, 132.5, 131.0, 129.2, 128.8, 128.8, 127.2, 127.1, 126.4, 122.1, 121.8, 114.6, 83.6, 79.4, 65.3, 65.1, 57.0, 53.3, 41.0, 40.4, 39.8, 20.5. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:*i*-PrOH= 95:5, 0.5 mL/min]. Retention times 67.8 (major), 79.7 (minor). HRMS calcd for $C_{34}H_{32}N_2O_4$ (M^+): 532.2357, found 532.2358.

(3a*R*,4*S*,9b*S*)-8-Methyl-9b-(naphthalen-1-yl)-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4l)



Yellow solid. R_f = 0.25 (hexane:diethyl ether, 1:1). $[\alpha]^{25}_D$= –94° (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 8.35 (d, *J*= 8.8 Hz, 1H, $H_{8'}$), 8.30 (d, *J*= 7.30 Hz, 1H, $H_{2'}$) 8.25 (t, *J*= 1.4 Hz, 1H, $H_{2''}$), 7.93 (dd, *J*= 7.9, 1.4 Hz, 1H, $H_{4''}$), 7.72 (d, *J*= 7.30 Hz, 1H, $H_{4'}$), 7.67 (d, *J*= 8.8 Hz, 1H, $H_{5'}$), 7.55 (t, *J*= 7.3 Hz, 1H, $H_{3'}$), 7.35–7.30 (m, 1H, $H_{6''}$), 7.28 (m, 1H, $H_{7'}$), 7.23 (br s, 1H, H_9), 7.17 (t, *J*= 8.8 Hz, 1H, $H_{6'}$), 6.94 (dd, *J*= 8.1, 1.9 Hz, 1H, H_7), 6.85 (t, *J*= 7.9 Hz, 1H, $H_{5'}$), 6.57 (d, *J*= 8.1 Hz, 1H, H_6), 4.09 (ddd, *J*= 10.2, 8.4, 2.0 Hz, 1H, H_{2A}), 3.93 (dt, *J*= 10.2, 7.5 Hz, 1H, H_{2B}), 3.79 (d, *J*= 11.4, 1H, H_4), 3.71 (br s, 1H, H_5), 3.12 (dd, *J*= 11.4, 6.7 Hz, 1H, H_{3a}), 1.84 (s, 3H, H_{10}), 1.49–1.27 (m, 1H, H_{3A}), 1.17–1.04 (m, 1H, H_{3B}). ^{13}C-NMR (75 MHz, C_6D_6) δ= 148.5, 144.3, 141.6, 141.5, 135.1, 133.6, 130.8, 130.0, 129.1, 128.9, 128.6, 127.0, 125.9, 125.2, 124.8, 124.4, 123.2, 122.8, 115.1, 85.3, 63.7, 58.0, 49.7, 27.4, 20.2. The enantiomeric excess was determined by HPLC [Chiracel ADH, 250 x 4.6 mm, hexane:EtOH= 95:5, 0.5 mL/min]. Retention times 15.4 (minor), 26.5 (major). HRMS calcd for $C_{28}H_{24}N_2O_3$ (M^+): 436.1781, found 436.1785.

(3a'*S*,4'*R*,9b'*R*)-9b'-(4-Bromophenyl)-8'-methyl-4'-(3-nitrophenyl)-3a',4',5',9b'-tetrahydro-3'*H*-spiro[cyclohexane-1,2'-furo[3,2-*c*]quinoline] (*ent*-4j)



Yellow solid. R_f = 0.20 (hexane:diethyl ether, 1:1). $[\alpha]^{25}_D$= +106º (*c* 0.1, DCM). ^{1}H-NMR (300 MHz, C_6D_6) δ= 8.05 (t, *J*= 1.8 Hz, 1H, $H_{2''}$), 7.83 (dd, *J*= 8.1, 1.8 Hz, 1H, $H_{4''}$), 7.34 (d, *J*= 2.1 Hz, 1H, H_9), 7.18 (d, *J*= 8.9 Hz, 2H, $H_{3'}$), 7.14 (d, *J*= 8.9 Hz, 2H, $H_{2'}$), 7.07 (d, *J*= 8.1 Hz, 1H, $H_{6''}$), 6.97 (dd, *J*= 8.1, 2.1 Hz, 1H, H_7), 6.74 (t, *J*= 8.1 Hz, 1H, $H_{5''}$), 6.47 (d, *J*= 8.1 Hz, 1H, H_6), 3.97 (d, *J*= 6.9 Hz, 1H, H_4), 3.45 (s, 1H, H_5), 2.81 (apparent q, *J*= 7.0 Hz, 1H, H_{3a}), 2.15 (s, 3H, H_{10}), 1.97–1.54 and 1.59–1.16 (2m, 12H, H_3, H_{cy}). ^{13}C-NMR (75 MHz, C_6D_6) δ= 148.6, 147.6, 145.0, 140.7, 132.8, 131.2, 130.9, 129.4, 129.1, 128.9, 128.6, 127.5, 122.4, 122.2, 120.7, 114.9, 83.4, 82.6, 57.6, 54.0, 40.2, 39.7, 25.7, 24.2, 23.9, 20.7. The enantiomeric excess was determined by HPLC [Chiracel ODH, 250 x 4.6 mm, hexane:*i*-PrOH= 95:5, 0.3 mL/min]. Retention times 73.6 (minor), 87.6 (major). HRMS calcd for $C_{29}H_{29}BrN_2O_3$ (M^+): 532.1356, found 532.1364.

DETERMINATION OF THE ABSOLUTE CONFIGURATION

The four most stable conformations of the A enantiomer of compound **4j** (enclosed in a 3 kcal/mol window) were subjected to minimization by DFT calculations, in gas phase, at the B3LYP/6-31G* level to evaluate the free energy and the population percentages on ΔG assuming Boltzmann statistical distribution at T = 298 K.[2]

Conformer	ΔE_{zpve}	ΔG	Pop % (ΔG)
I	1.16	2.07	1.4
II	0.93	1.46	4.0
III	0.00	0.00	47.6
IV	0.18	0.01	46.8

Then, electronic excitation energies, oscillator strengths and rotational strengths were calculated for the first 50 excited states at the TD-DFT-OPBE/PCM (CH_3CN)/6-31G level.[3] The final simulated ECD spectrum of **4j** was obtained taking into account the populations ratios determined assuming Boltzmann statistical distribution.

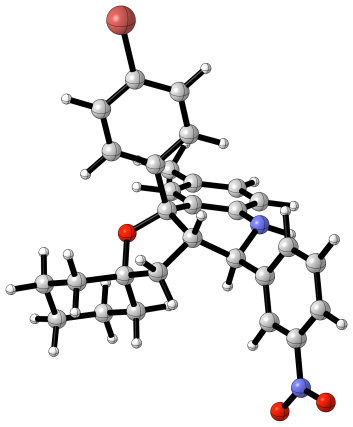


Figure 1. Most stable conformation (**III**) computed (B3LYP/6-31G*) for the A-enantiomer.

[2] Gaussian 09, Revision **A.1**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[3] a) L. Onsager, *J. Am. Chem. Soc.* **1936**, *58*, 1486-1493. b) A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648-5652. c) J. Tomasi, M. Persico, *Chem. Rev.* **1994**, *94*, 2027 –2094; d) J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev.* **2005**, *105*, 2999 –3094.

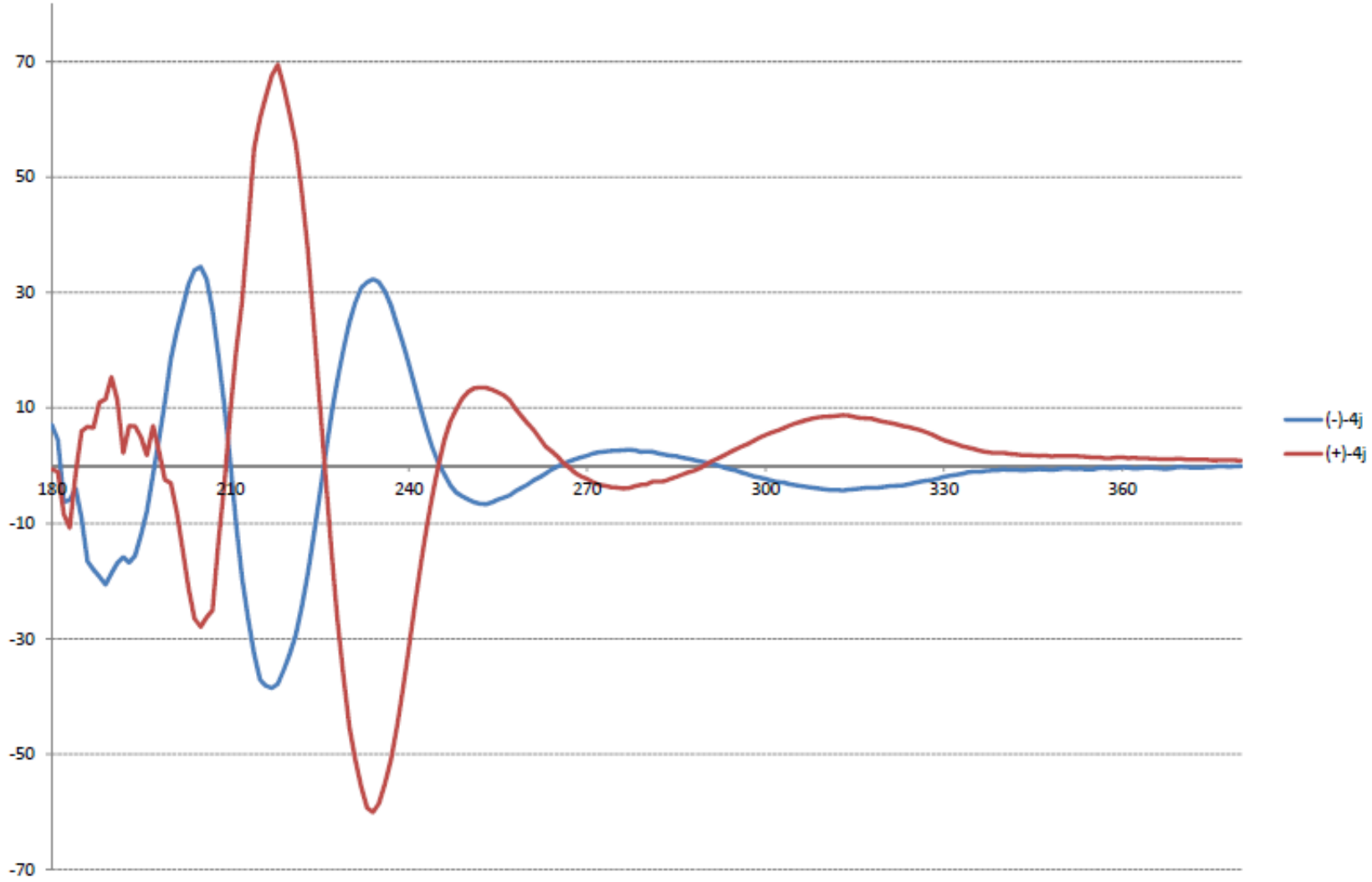


Figure 2. Experimental CD spectra of (+)-**4j** (4.42×10^{-4}M, obtained with (*S*)-TRIP-PA (**7d**) and (-)-**4j** (2.35×10^{-4}M, obtained with (*R*)-TRIP-PA (**7d**) in CH_3CN.

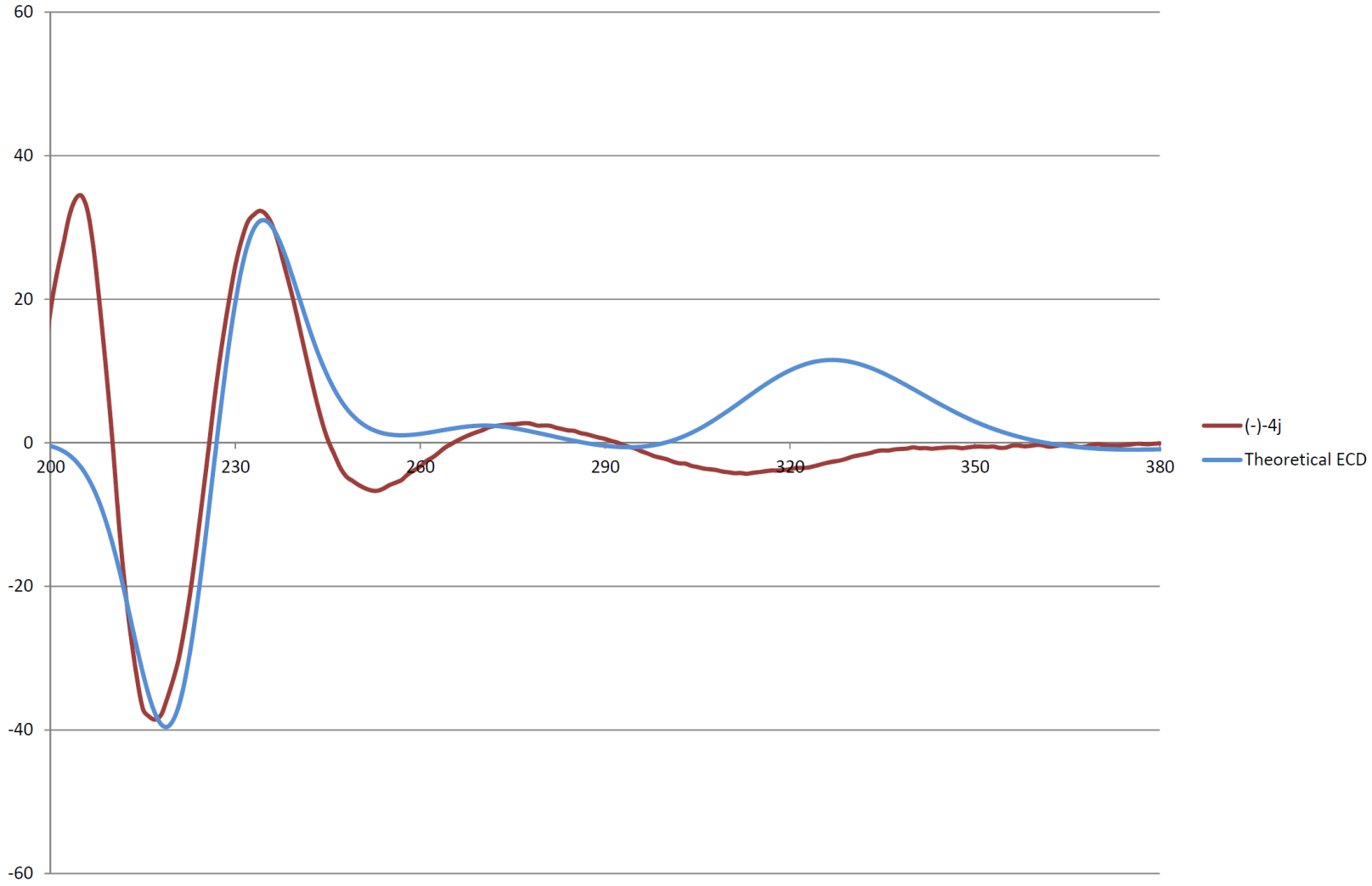


Figure 3. Experimental ((-)-**4j**, in CH_3CN) versus TD-DFT (*A-ent*) simulated CD spectra computed at the OPBE/PCM (CH_3CN)/6-31G//B3LYP/6-31G* level. The calculations overestimate electronic transition energies resulting in a blue shift of the calculated spectra, and the measured ECD was corrected by parallel shift towards longer wavelengths (20 nm).

CARTESIAN COORDINATES

Cartesian Coordinates (OPBE/PCM (CH_3CN)/6-31G//B3LYP/6-31G*), determination of excited states and rotatory strenghts for the conformations of 4j

Î-conf
SCF Energy:
Num. Imaginary Frequencies: 0

C	-1.571490	-2.345036	1.480571
C	-1.117260	-2.439881	0.160195
C	-2.064568	-2.493538	-0.867717
C	-3.419293	-2.435214	-0.558759
C	-3.881567	-2.331170	0.752025
C	-2.937410	-2.288005	1.773007
C	0.372454	-2.549554	-0.198002
C	0.924465	-1.333089	-0.973549
C	1.248764	-0.077910	-0.111658
C	1.898472	-0.487995	1.209476
C	1.835605	-1.813491	1.678897
N	1.247099	-2.829023	0.925154
C	2.273844	-1.621354	-1.654974
C	2.937184	-0.236907	-1.815701
O	2.188348	0.646288	-0.931015
C	2.795945	0.322543	-3.244472
C	3.417576	1.719166	-3.389946
C	4.894143	1.714085	-2.965647
C	5.059574	1.159666	-1.542682
C	4.418909	-0.228497	-1.395314
C	2.440835	-2.125762	2.912436
C	3.098847	-1.151295	3.648674
C	3.189017	0.173517	3.190473
C	2.579846	0.470554	1.971659
C	0.045141	0.856883	0.079888
C	-0.416780	1.610943	-1.009203
C	-1.519748	2.453384	-0.893287
C	-2.172977	2.550904	0.334280
C	-1.734261	1.823074	1.435072
C	-0.626491	0.983411	1.300202
Br	-3.686842	3.708129	0.507694
C	3.924443	1.226583	3.986655
N	-4.399236	-2.499303	-1.657313
O	-5.592590	-2.456608	-1.361250
O	-3.966802	-2.593673	-2.806143
H	4.583562	1.843075	-0.828317
H	4.956517	-0.953789	-2.024488
H	4.499227	-0.579757	-0.360390
H	3.296504	-0.372928	-3.933856
H	1.734861	0.338490	-3.526427
H	3.317411	2.063891	-4.426885
H	2.859034	2.425175	-2.762651
H	5.471163	1.093240	-3.667986
H	5.311117	2.727120	-3.029314
H	6.122167	1.107504	-1.273719
H	0.186272	-1.042898	-1.727283
H	2.140943	-2.126710	-2.617709
H	2.881426	-2.273437	-1.018574
H	0.453671	-3.405492	-0.883105
H	1.067922	-3.692444	1.419956
H	2.628154	1.484225	1.581934
H	3.554570	-1.424619	4.598204
H	2.398540	-3.149351	3.280426
H	5.003152	1.025179	4.025873
H	3.791782	2.220341	3.547308
H	3.569742	1.271121	5.023975
H	-1.769470	-2.587323	-1.907060
H	-4.945880	-2.290431	0.946138
H	-3.265485	-2.209597	2.805302
H	-0.850650	-2.310271	2.291112
H	-0.282343	0.429316	2.166327
H	-2.244102	1.912794	2.388259
H	-1.864188	3.033269	-1.742862
H	0.107841	1.553947	-1.956717

Excited states

Excited State 1:	Singlet-A	0.9377 eV	1322.27 nm	f=0.0032	<S**2>=0.000
Excited State 2:	Singlet-A	1.8345 eV	675.86 nm	f=0.0002	<S**2>=0.000
Excited State 3:	Singlet-A	2.4017 eV	516.23 nm	f=0.0009	<S**2>=0.000
Excited State 4:	Singlet-A	2.6635 eV	465.50 nm	f=0.0002	<S**2>=0.000
Excited State 5:	Singlet-A	2.9744 eV	416.83 nm	f=0.0047	<S**2>=0.000
Excited State 6:	Singlet-A	3.0566 eV	405.63 nm	f=0.0200	<S**2>=0.000
Excited State 7:	Singlet-A	3.1375 eV	395.17 nm	f=0.0076	<S**2>=0.000
Excited State 8:	Singlet-A	3.2727 eV	378.84 nm	f=0.0021	<S**2>=0.000
Excited State 9:	Singlet-A	3.2923 eV	376.59 nm	f=0.0020	<S**2>=0.000
Excited State 10:	Singlet-A	3.3759 eV	367.26 nm	f=0.0017	<S**2>=0.000
Excited State 11:	Singlet-A	3.3868 eV	366.08 nm	f=0.0006	<S**2>=0.000
Excited State 12:	Singlet-A	3.4989 eV	354.36 nm	f=0.0017	<S**2>=0.000
Excited State 13:	Singlet-A	3.6460 eV	340.06 nm	f=0.0004	<S**2>=0.000
Excited State 14:	Singlet-A	3.6729 eV	337.57 nm	f=0.0008	<S**2>=0.000
Excited State 15:	Singlet-A	3.6903 eV	335.97 nm	f=0.0023	<S**2>=0.000
Excited State 16:	Singlet-A	3.7177 eV	333.49 nm	f=0.0000	<S**2>=0.000
Excited State 17:	Singlet-A	3.7380 eV	331.69 nm	f=0.0022	<S**2>=0.000
Excited State 18:	Singlet-A	3.9422 eV	314.50 nm	f=0.0067	<S**2>=0.000
Excited State 19:	Singlet-A	3.9517 eV	313.75 nm	f=0.1247	<S**2>=0.000
Excited State 20:	Singlet-A	4.0506 eV	306.09 nm	f=0.0483	<S**2>=0.000
Excited State 21:	Singlet-A	4.1158 eV	301.24 nm	f=0.0099	<S**2>=0.000
Excited State 22:	Singlet-A	4.1489 eV	298.84 nm	f=0.0508	<S**2>=0.000
Excited State 23:	Singlet-A	4.1741 eV	297.03 nm	f=0.0158	<S**2>=0.000
Excited State 24:	Singlet-A	4.2108 eV	294.45 nm	f=0.0127	<S**2>=0.000
Excited State 25:	Singlet-A	4.2374 eV	292.59 nm	f=0.0206	<S**2>=0.000
Excited State 26:	Singlet-A	4.2840 eV	289.41 nm	f=0.0035	<S**2>=0.000
Excited State 27:	Singlet-A	4.5098 eV	274.92 nm	f=0.0033	<S**2>=0.000
Excited State 28:	Singlet-A	4.5462 eV	272.72 nm	f=0.0202	<S**2>=0.000
Excited State 29:	Singlet-A	4.5492 eV	272.54 nm	f=0.0002	<S**2>=0.000
Excited State 30:	Singlet-A	4.5769 eV	270.89 nm	f=0.0021	<S**2>=0.000
Excited State 31:	Singlet-A	4.6476 eV	266.77 nm	f=0.0056	<S**2>=0.000
Excited State 32:	Singlet-A	4.6681 eV	265.60 nm	f=0.0023	<S**2>=0.000
Excited State 33:	Singlet-A	4.7034 eV	263.60 nm	f=0.0004	<S**2>=0.000
Excited State 34:	Singlet-A	4.7782 eV	259.48 nm	f=0.0046	<S**2>=0.000
Excited State 35:	Singlet-A	4.8707 eV	254.55 nm	f=0.0093	<S**2>=0.000
Excited State 36:	Singlet-A	4.9219 eV	251.90 nm	f=0.0045	<S**2>=0.000
Excited State 37:	Singlet-A	4.9479 eV	250.58 nm	f=0.0271	<S**2>=0.000
Excited State 38:	Singlet-A	4.9983 eV	248.05 nm	f=0.0004	<S**2>=0.000
Excited State 39:	Singlet-A	5.0528 eV	245.38 nm	f=0.0002	<S**2>=0.000
Excited State 40:	Singlet-A	5.0720 eV	244.45 nm	f=0.0512	<S**2>=0.000
Excited State 41:	Singlet-A	5.0991 eV	243.15 nm	f=0.1828	<S**2>=0.000
Excited State 42:	Singlet-A	5.1429 eV	241.08 nm	f=0.0360	<S**2>=0.000
Excited State 43:	Singlet-A	5.1527 eV	240.62 nm	f=0.0743	<S**2>=0.000
Excited State 44:	Singlet-A	5.2206 eV	237.49 nm	f=0.0185	<S**2>=0.000
Excited State 45:	Singlet-A	5.2373 eV	236.73 nm	f=0.0072	<S**2>=0.000
Excited State 46:	Singlet-A	5.2624 eV	235.60 nm	f=0.0588	<S**2>=0.000
Excited State 47:	Singlet-A	5.2940 eV	234.20 nm	f=0.0017	<S**2>=0.000
Excited State 48:	Singlet-A	5.3051 eV	233.71 nm	f=0.0076	<S**2>=0.000
Excited State 49:	Singlet-A	5.3493 eV	231.78 nm	f=0.0094	<S**2>=0.000
Excited State 50:	Singlet-A	5.3532 eV	231.61 nm	f=0.0055	<S**2>=0.000

Rotatory Strengths (R) in cgs (10-40 erg-esu-cm/Gauss)**

state	XX	YY	ZZ	R(length)
1	-5.2924	3.4866	7.3691	1.8545
2	0.3130	-0.1876	-1.0265	-0.3004
3	-4.8753	1.2610	0.5465	-1.0226
4	1.0835	-0.0237	-0.9608	0.0330
5	-8.1035	8.8497	1.9389	0.8950
6	-30.2966	0.2964	34.0360	1.3453
7	16.1947	3.2472	-15.9404	1.1672
8	-0.0015	0.0883	-3.6566	-1.1899
9	-10.1829	5.6786	0.7236	-1.2602
10	-10.8529	0.1897	-6.6713	-5.7782
11	-2.6397	0.3376	-1.1857	-1.1626
12	-1.4033	-1.6691	-1.0162	-1.3629
13	0.9040	-2.0912	-0.4352	-0.5408
14	-0.5749	-2.1788	0.2684	-0.8284
15	-8.8356	-8.2317	-4.3539	-7.1404
16	-0.0247	-0.3752	-4.6323	-1.6774
17	1.9556	1.3286	-0.4644	0.9399
18	-7.4255	8.6675	-6.5334	-1.7638
19	-284.7239	81.0423	249.7863	15.3682
20	76.7426	130.9086	-159.6302	16.0070
21	-33.4266	5.0139	37.9113	3.1662
22	49.3070	24.7776	-46.1892	9.2985
23	-157.8823	11.0086	153.2048	2.1104
24	-44.2828	1.7835	58.3529	5.2845
25	-16.4782	-25.5123	4.4280	-12.5208
26	-2.5818	8.5344	19.2173	8.3900
27	-6.4705	1.6607	6.2753	0.4885
28	11.4919	20.0963	-20.5056	3.6942
29	0.4622	0.1037	0.1873	0.2511
30	-1.5141	-0.0907	3.5367	0.6440
31	6.7229	7.2180	3.7920	5.9110
32	-7.6980	0.9866	-5.3351	-4.0155
33	-0.9490	0.3335	0.8993	0.0946
34	-3.0896	0.0940	1.7116	-0.4280
35	-15.3707	2.5790	18.7892	1.9992
36	11.7719	-4.3318	-7.9833	-0.1811
37	-5.9407	9.4050	7.5367	3.6670
38	-0.8733	0.4422	-0.2420	-0.2244
39	-0.9762	0.1471	0.0520	-0.2590
40	-77.6282	54.5225	133.9394	36.9446
41	-484.8531	-16.4478	335.4618	-55.2797
42	-163.6003	-5.6703	11.1666	-52.7013
43	-129.4611	-6.1850	148.3622	4.2387
44	-3.1324	19.1085	57.7625	24.5795
45	7.6506	-19.1047	19.6082	2.7180
46	-49.4874	-19.4474	118.2128	16.4260
47	-1.8158	-3.4451	1.9064	-1.1182
48	2.5730	-2.9812	-2.8213	-1.0765
49	-35.7097	-6.2239	3.3674	-12.8554
50	5.4634	-9.5874	19.5232	5.1331

II-conf
SCF Energy:
Num. Imaginary Frequencies: 0

C	-0.970885	0.488265	0.979718
C	0.064719	0.911151	0.139537
C	-0.021020	2.194391	-0.420442
C	-1.108880	3.026202	-0.165618
C	-2.130337	2.571510	0.666588
C	-2.070194	1.307982	1.244721
C	1.266837	0.019707	-0.205763
C	1.225788	-0.526510	-1.662709
C	0.457827	-1.853630	-1.850297
N	0.962041	-2.823969	-0.897223
C	1.271202	-2.465553	0.417420
C	1.465531	-1.122799	0.790143
O	2.419214	0.887222	-0.215810
C	3.409319	0.468154	-1.197898
C	2.719189	-0.646071	-2.014624
C	1.460783	-3.472963	1.383517
C	1.841859	-3.153532	2.678092
C	2.057012	-1.821035	3.067984
C	1.860985	-0.833474	2.103737
C	4.669815	-0.025107	-0.463166
C	5.345178	1.086254	0.354230

C	5.664563	2.314161	-0.511544
C	4.407730	2.822148	-1.233864
C	3.750878	1.702429	-2.054637
C	-1.070178	-1.694976	-1.859263
C	-1.880087	-2.286961	-0.890216
C	-3.264124	-2.142708	-0.973106
C	-3.883397	-1.430344	-1.995234
C	-3.072448	-0.848862	-2.968357
C	-1.686350	-0.985612	-2.902193
H	-3.524660	-0.291893	-3.783479
C	2.485481	-1.480482	4.476484
Br	-3.628794	3.706254	1.026605
H	4.671859	1.381485	1.168762
H	5.373452	-0.412337	-1.215558
H	4.397138	-0.865794	0.184524
H	4.438367	1.383750	-2.851800
H	2.839550	2.065255	-2.548429
H	4.656444	3.666445	-1.889336
H	3.686947	3.192994	-0.494269
H	6.429064	2.046601	-1.256986
H	6.096198	3.112311	0.105605
H	6.259326	0.698878	0.821511
H	0.758851	0.236003	-2.293626
H	2.891964	-0.531786	-3.090384
H	3.093192	-1.632539	-1.721441
H	0.728897	-2.221924	-2.850413
H	0.625033	-3.770161	-1.017424
H	2.019098	0.209510	2.366360
H	1.975390	-3.954627	3.402078
H	1.311838	-4.513590	1.101712
H	3.482592	-1.879645	4.704274
H	2.521553	-0.397152	4.629090
H	1.795986	-1.898386	5.220693
H	-1.072073	-0.535465	-3.678959
H	-4.962515	-1.346293	-2.017869
N	-4.101886	-2.773490	0.061817
H	-1.459632	-2.850989	-0.067760
H	-0.925794	-0.489806	1.445256
H	-2.865081	0.966702	1.898976
H	-1.159801	4.018800	-0.600294
H	0.786713	2.555677	-1.047584
O	-5.322314	-2.651904	-0.037630
O	-3.532398	-3.386457	0.965189

Excited states:

Excited State 1:	Singlet-A	0.9622 eV	1288.52 nm	f=0.0042	<S**2>=0.000
Excited State 2:	Singlet-A	1.8443 eV	672.26 nm	f=0.0002	<S**2>=0.000
Excited State 3:	Singlet-A	2.3975 eV	517.13 nm	f=0.0005	<S**2>=0.000
Excited State 4:	Singlet-A	2.6681 eV	464.69 nm	f=0.0003	<S**2>=0.000
Excited State 5:	Singlet-A	2.9622 eV	418.56 nm	f=0.0019	<S**2>=0.000
Excited State 6:	Singlet-A	3.1407 eV	394.76 nm	f=0.0043	<S**2>=0.000
Excited State 7:	Singlet-A	3.2069 eV	386.62 nm	f=0.0089	<S**2>=0.000
Excited State 8:	Singlet-A	3.2753 eV	378.54 nm	f=0.0008	<S**2>=0.000
Excited State 9:	Singlet-A	3.2811 eV	377.87 nm	f=0.0068	<S**2>=0.000
Excited State 10:	Singlet-A	3.3892 eV	365.82 nm	f=0.0011	<S**2>=0.000
Excited State 11:	Singlet-A	3.4396 eV	360.47 nm	f=0.0039	<S**2>=0.000
Excited State 12:	Singlet-A	3.4840 eV	355.87 nm	f=0.0048	<S**2>=0.000
Excited State 13:	Singlet-A	3.6335 eV	341.22 nm	f=0.0064	<S**2>=0.000
Excited State 14:	Singlet-A	3.6387 eV	340.74 nm	f=0.0066	<S**2>=0.000
Excited State 15:	Singlet-A	3.6736 eV	337.50 nm	f=0.0022	<S**2>=0.000
Excited State 16:	Singlet-A	3.7067 eV	334.49 nm	f=0.0001	<S**2>=0.000
Excited State 17:	Singlet-A	3.7475 eV	330.84 nm	f=0.0031	<S**2>=0.000
Excited State 18:	Singlet-A	3.9640 eV	312.77 nm	f=0.1056	<S**2>=0.000
Excited State 19:	Singlet-A	4.0308 eV	307.59 nm	f=0.0234	<S**2>=0.000
Excited State 20:	Singlet-A	4.0621 eV	305.22 nm	f=0.0314	<S**2>=0.000
Excited State 21:	Singlet-A	4.1136 eV	301.40 nm	f=0.0018	<S**2>=0.000
Excited State 22:	Singlet-A	4.1282 eV	300.34 nm	f=0.0304	<S**2>=0.000
Excited State 23:	Singlet-A	4.1723 eV	297.16 nm	f=0.0248	<S**2>=0.000
Excited State 24:	Singlet-A	4.1779 eV	296.76 nm	f=0.0026	<S**2>=0.000
Excited State 25:	Singlet-A	4.2159 eV	294.09 nm	f=0.0105	<S**2>=0.000
Excited State 26:	Singlet-A	4.3544 eV	284.73 nm	f=0.0199	<S**2>=0.000
Excited State 27:	Singlet-A	4.5083 eV	275.02 nm	f=0.0017	<S**2>=0.000
Excited State 28:	Singlet-A	4.5220 eV	274.18 nm	f=0.0010	<S**2>=0.000
Excited State 29:	Singlet-A	4.5706 eV	271.26 nm	f=0.0002	<S**2>=0.000
Excited State 30:	Singlet-A	4.6190 eV	268.42 nm	f=0.0054	<S**2>=0.000
Excited State 31:	Singlet-A	4.6321 eV	267.66 nm	f=0.0079	<S**2>=0.000
Excited State 32:	Singlet-A	4.6726 eV	265.34 nm	f=0.0044	<S**2>=0.000
Excited State 33:	Singlet-A	4.7073 eV	263.39 nm	f=0.0003	<S**2>=0.000
Excited State 34:	Singlet-A	4.8185 eV	257.31 nm	f=0.0191	<S**2>=0.000
Excited State 35:	Singlet-A	4.8794 eV	254.10 nm	f=0.0189	<S**2>=0.000
Excited State 36:	Singlet-A	4.9050 eV	252.77 nm	f=0.0057	<S**2>=0.000
Excited State 37:	Singlet-A	4.9904 eV	248.44 nm	f=0.0040	<S**2>=0.000
Excited State 38:	Singlet-A	4.9940 eV	248.27 nm	f=0.0004	<S**2>=0.000
Excited State 39:	Singlet-A	5.0683 eV	244.63 nm	f=0.0218	<S**2>=0.000
Excited State 40:	Singlet-A	5.0834 eV	243.90 nm	f=0.0098	<S**2>=0.000
Excited State 41:	Singlet-A	5.0889 eV	243.63 nm	f=0.0050	<S**2>=0.000
Excited State 42:	Singlet-A	5.1201 eV	242.15 nm	f=0.2451	<S**2>=0.000
Excited State 43:	Singlet-A	5.2064 eV	238.14 nm	f=0.0700	<S**2>=0.000
Excited State 44:	Singlet-A	5.2325 eV	236.95 nm	f=0.0010	<S**2>=0.000
Excited State 45:	Singlet-A	5.2518 eV	236.08 nm	f=0.0054	<S**2>=0.000
Excited State 46:	Singlet-A	5.2682 eV	235.34 nm	f=0.0554	<S**2>=0.000
Excited State 47:	Singlet-A	5.2709 eV	235.23 nm	f=0.0051	<S**2>=0.000
Excited State 48:	Singlet-A	5.2978 eV	234.03 nm	f=0.0102	<S**2>=0.000
Excited State 49:	Singlet-A	5.3343 eV	232.43 nm	f=0.0011	<S**2>=0.000
Excited State 50:	Singlet-A	5.3872 eV	230.15 nm	f=0.0037	<S**2>=0.000

Rotatory Strengths (R) in cgs (10-40 erg-esu-cm/Gauss)**

state	XX	YY	ZZ	R(length)
1	-5.8517	0.3062	6.6640	0.3728
2	0.0179	-0.5454	-0.1366	-0.2213
3	-3.4248	0.1239	0.1556	-1.0484
4	0.8096	-0.5885	-0.3826	-0.0538
5	-3.2849	-1.8511	-0.0887	-1.7416
6	-14.2038	7.7337	-1.3487	-2.6063
7	13.1148	-9.2749	3.9808	2.6069
8	0.8783	-2.5980	0.0609	-0.5529
9	1.0321	4.1660	10.0546	5.0842
10	0.3999	-1.2119	0.1266	-0.2285
11	-17.3756	0.3710	2.1524	-4.9508
12	-2.1861	-0.5764	-0.0357	-0.9327
13	-15.0049	-0.9436	13.9233	-0.6751
14	-13.9047	-4.4871	1.5407	-5.6170
15	0.7240	-2.5979	0.0787	-0.5984
16	3.3194	2.4130	8.0889	4.6071
17	2.7633	-4.7980	0.0970	-0.6459
18	195.6982	-302.0124	-5.9961	-37.4368
19	5.6159	-25.7300	5.2251	-4.9630
20	-12.6898	80.5246	-20.7886	15.6821
21	-21.2241	3.9812	27.5395	3.4322
22	-17.8002	-50.5624	46.0504	-7.4374
23	163.9585	-103.3383	-66.3481	-1.9093
24	7.8792	-6.1581	-11.8143	-3.3644
25	1.0099	-16.5027	11.9351	-1.1859
26	-0.8676	6.5324	0.0358	1.9002
27	2.2816	-3.0682	-0.8519	-0.5462
28	0.3857	-0.7736	7.5002	2.3707
29	2.5664	-0.3471	-0.9300	0.4298
30	1.7037	-8.8292	7.2471	0.0405
31	-4.3310	-23.0285	8.9650	-6.1315
32	-6.5930	0.8056	-7.2550	-4.3474
33	1.3257	-0.7573	-0.2992	0.0897
34	42.9364	17.9642	3.7247	21.5418
35	-2.4001	-55.3346	9.9606	-15.9247
36	4.0093	-4.3453	-0.7229	-0.3530
37	-16.0886	0.2110	7.5524	-2.7751
38	0.3792	1.5165	-0.3227	0.5243
39	-26.4000	-4.7837	30.1460	-0.3459
40	-32.0008	-6.4869	9.8891	-9.5329
41	1.0279	-28.6400	4.5391	-7.6910
42	-549.6378	-74.5593	503.1793	-40.3393
43	-18.9228	-61.8763	144.1914	21.1308
44	3.7317	-15.1894	9.2823	-0.7251
45	-1.9587	-1.7796	1.8988	-0.6132
46	-31.6923	66.3714	2.6747	12.4512
47	3.9258	-3.7914	-0.1642	-0.0099
48	-4.1839	-6.7977	2.3455	-2.8787
49	-5.2665	-2.1059	1.9713	-1.8004
50	11.3745	-1.1642	-4.2133	1.9990

III-conf

SCF Energy:

Num. Imaginary Frequencies: 0

C	0.596683	4.616577	-2.682795
C	1.019034	4.263785	-1.249878
C	1.614515	2.849872	-1.168609
C	0.652148	1.774103	-1.720847
C	0.220396	2.151150	-3.149135
C	-0.371581	3.565275	-3.243172
C	1.215621	0.341551	-1.643511
C	0.731117	-0.228589	-0.296817
C	-0.537275	0.642792	0.035131
O	-0.541676	1.728360	-0.903913
C	1.810120	-0.225106	0.814613
N	1.145070	-0.425751	2.109641
C	0.259310	0.616262	2.457334
C	-0.540044	1.196695	1.461855
C	0.153597	1.074666	3.779040
C	-0.726906	2.100679	4.099827
C	-1.516882	2.714172	3.115183
C	-1.408487	2.237939	1.807333
C	-2.444585	3.855826	3.461803
C	-1.821033	-0.184451	-0.177546
C	-2.749186	0.149987	-1.166381
C	-3.910536	-0.606142	-1.348778
C	-4.140972	-1.707129	-0.531626
C	-3.232655	-2.061411	0.465723
C	-2.082171	-1.296108	0.637962
C	2.848135	-1.311678	0.595023
C	4.136997	-0.983355	0.169792
C	5.068042	-1.999050	-0.041365
C	4.765363	-3.341646	0.166963
C	3.480826	-3.664970	0.601616
C	2.532997	-2.662878	0.812208
H	3.218697	-4.704137	0.776666
Br	-5.726918	-2.752284	-0.774056
H	0.771583	0.623407	4.553057
H	-0.793483	2.439741	5.131392
H	-1.888903	4.782777	3.657247
H	-3.145619	4.060303	2.646272
H	-2.018348	2.679414	1.023836
H	-3.032408	3.638240	4.361473
H	0.414684	-1.267465	-0.417086
H	1.819027	-0.608410	2.847853
H	2.328028	0.747347	0.798608
H	1.537719	-2.921679	1.160755
H	5.522326	-4.096341	-0.006155
N	6.422867	-1.635204	-0.491427
H	4.433346	0.046133	0.005549
H	-3.425573	-2.920111	1.099806
H	-4.626052	-0.338451	-2.119109
H	-2.563895	1.012477	-1.795283
H	-1.379000	-1.567122	1.421287
H	2.305453	0.318076	-1.745080
H	0.802710	-0.254909	-2.464167
H	1.876233	2.619504	-0.129891
H	2.546291	2.808955	-1.751573
H	1.104275	2.078634	-3.799567
H	-0.500860	1.406102	-3.506886
H	1.748689	4.992092	-0.874442
H	0.146420	4.316434	-0.586888

H	0.134373	5.611393	-2.709228
H	1.489428	4.668969	-3.324416
H	-0.623448	3.791510	-4.286914
H	-1.310448	3.596737	-2.675406
O	7.231859	-2.546215	-0.662422
O	6.664789	-0.441631	-0.670280

Excited states

Excited State 1:	Singlet-A	1.0755 eV	1152.82 nm	f=0.0048	<S**2>=0.000
Excited State 2:	Singlet-A	1.9844 eV	624.78 nm	f=0.0002	<S**2>=0.000
Excited State 3:	Singlet-A	2.2816 eV	543.40 nm	f=0.0001	<S**2>=0.000
Excited State 4:	Singlet-A	2.6299 eV	471.45 nm	f=0.0005	<S**2>=0.000
Excited State 5:	Singlet-A	2.9592 eV	418.98 nm	f=0.0015	<S**2>=0.000
Excited State 6:	Singlet-A	3.0259 eV	409.75 nm	f=0.0028	<S**2>=0.000
Excited State 7:	Singlet-A	3.2114 eV	386.08 nm	f=0.0012	<S**2>=0.000
Excited State 8:	Singlet-A	3.2844 eV	377.49 nm	f=0.0037	<S**2>=0.000
Excited State 9:	Singlet-A	3.3814 eV	366.66 nm	f=0.0050	<S**2>=0.000
Excited State 10:	Singlet-A	3.4835 eV	355.92 nm	f=0.0010	<S**2>=0.000
Excited State 11:	Singlet-A	3.5392 eV	350.32 nm	f=0.0015	<S**2>=0.000
Excited State 12:	Singlet-A	3.5863 eV	345.71 nm	f=0.0273	<S**2>=0.000
Excited State 13:	Singlet-A	3.6125 eV	343.21 nm	f=0.0006	<S**2>=0.000
Excited State 14:	Singlet-A	3.6639 eV	338.40 nm	f=0.0216	<S**2>=0.000
Excited State 15:	Singlet-A	3.6752 eV	337.36 nm	f=0.0035	<S**2>=0.000
Excited State 16:	Singlet-A	3.7014 eV	334.97 nm	f=0.0001	<S**2>=0.000
Excited State 17:	Singlet-A	3.9075 eV	317.30 nm	f=0.0014	<S**2>=0.000
Excited State 18:	Singlet-A	3.9822 eV	311.35 nm	f=0.0740	<S**2>=0.000
Excited State 19:	Singlet-A	4.0369 eV	307.13 nm	f=0.0536	<S**2>=0.000
Excited State 20:	Singlet-A	4.1177 eV	301.10 nm	f=0.0073	<S**2>=0.000
Excited State 21:	Singlet-A	4.1202 eV	300.92 nm	f=0.0579	<S**2>=0.000
Excited State 22:	Singlet-A	4.1263 eV	300.47 nm	f=0.0316	<S**2>=0.000
Excited State 23:	Singlet-A	4.1433 eV	299.24 nm	f=0.0035	<S**2>=0.000
Excited State 24:	Singlet-A	4.2445 eV	292.11 nm	f=0.0501	<S**2>=0.000
Excited State 25:	Singlet-A	4.3970 eV	281.97 nm	f=0.0005	<S**2>=0.000
Excited State 26:	Singlet-A	4.4278 eV	280.01 nm	f=0.0054	<S**2>=0.000
Excited State 27:	Singlet-A	4.4536 eV	278.39 nm	f=0.0064	<S**2>=0.000
Excited State 28:	Singlet-A	4.4993 eV	275.56 nm	f=0.0010	<S**2>=0.000
Excited State 29:	Singlet-A	4.5718 eV	271.19 nm	f=0.0006	<S**2>=0.000
Excited State 30:	Singlet-A	4.6783 eV	265.02 nm	f=0.0046	<S**2>=0.000
Excited State 31:	Singlet-A	4.7180 eV	262.79 nm	f=0.0011	<S**2>=0.000
Excited State 32:	Singlet-A	4.7651 eV	260.19 nm	f=0.0073	<S**2>=0.000
Excited State 33:	Singlet-A	4.7929 eV	258.68 nm	f=0.0143	<S**2>=0.000
Excited State 34:	Singlet-A	4.7967 eV	258.48 nm	f=0.0007	<S**2>=0.000
Excited State 35:	Singlet-A	4.8414 eV	256.09 nm	f=0.0019	<S**2>=0.000
Excited State 36:	Singlet-A	4.8526 eV	255.50 nm	f=0.0013	<S**2>=0.000
Excited State 37:	Singlet-A	4.9031 eV	252.87 nm	f=0.0080	<S**2>=0.000
Excited State 38:	Singlet-A	4.9165 eV	252.18 nm	f=0.0044	<S**2>=0.000
Excited State 39:	Singlet-A	4.9315 eV	251.41 nm	f=0.0971	<S**2>=0.000
Excited State 40:	Singlet-A	5.0281 eV	246.58 nm	f=0.1939	<S**2>=0.000
Excited State 41:	Singlet-A	5.0507 eV	245.48 nm	f=0.0047	<S**2>=0.000
Excited State 42:	Singlet-A	5.0876 eV	243.70 nm	f=0.0082	<S**2>=0.000
Excited State 43:	Singlet-A	5.1121 eV	242.53 nm	f=0.0261	<S**2>=0.000
Excited State 44:	Singlet-A	5.1810 eV	239.30 nm	f=0.0545	<S**2>=0.000
Excited State 45:	Singlet-A	5.1862 eV	239.07 nm	f=0.0020	<S**2>=0.000
Excited State 46:	Singlet-A	5.2040 eV	238.25 nm	f=0.0273	<S**2>=0.000
Excited State 47:	Singlet-A	5.2261 eV	237.24 nm	f=0.0231	<S**2>=0.000
Excited State 48:	Singlet-A	5.2541 eV	235.98 nm	f=0.0008	<S**2>=0.000
Excited State 49:	Singlet-A	5.3205 eV	233.03 nm	f=0.0474	<S**2>=0.000
Excited State 50:	Singlet-A	5.3374 eV	232.29 nm	f=0.0252	<S**2>=0.000

Rotatory Strengths (R) in cgs (10-40 erg-esu-cm/Gauss)**

state	XX	YY	ZZ	R(length)
1	17.3114	-5.0280	-3.8066	2.8256
2	-0.0087	-0.0315	-0.2185	-0.0862
3	-0.0256	-0.0224	0.0922	0.0147
4	-0.2057	-1.0755	-1.2676	-0.8496
5	-0.0154	0.7251	-1.0540	-0.1148
6	0.2243	2.2843	-2.4715	0.0123
7	-0.1897	0.1512	-7.2936	-2.4440
8	0.4163	2.1195	-1.5824	0.3178
9	-5.6051	-0.2952	-3.7799	-3.2267
10	2.8099	4.5567	8.1242	5.1636
11	2.4921	-0.2270	-0.4976	0.5892
12	53.9259	19.7801	-14.1384	19.8559
13	1.0694	-0.6080	-0.8660	-0.1349
14	89.7097	-28.3153	-11.7922	16.5340
15	21.7956	-10.4435	1.8910	4.4144
16	-14.9086	-0.4511	-2.1375	-5.8324
17	-5.8996	-1.0515	-1.5644	-2.8385
18	100.7360	2.0265	-100.2851	0.8258
19	48.2201	22.4095	-68.2793	0.7835
20	2.0914	0.9196	-12.1583	-3.0491
21	46.8189	25.0760	-74.3405	-0.8152
22	53.6801	1.7407	-45.2875	3.3778
23	-18.0739	15.2715	-1.7958	-1.5328
24	84.1475	-4.9895	-53.1010	8.6857
25	2.4489	-0.0147	-0.6006	0.6112
26	-4.5385	-2.3053	-1.5666	-2.8035
27	9.5628	-6.1322	1.4356	1.6221
28	0.4027	0.0659	-0.9697	-0.1671
29	-1.0450	0.1684	-0.1231	-0.3333
30	4.9429	0.7098	-3.5108	0.7140
31	-1.9324	-0.7434	-0.0315	-0.9024
32	-15.3983	3.3349	-2.4593	-4.8409
33	45.1924	5.5237	-3.2878	15.8094
34	1.9459	1.6074	-1.9262	0.5424
35	-0.0300	-1.0613	7.2195	2.0427
36	2.5940	-7.8302	5.4617	0.0752
37	-26.3824	-10.0565	8.8219	-9.2057
38	7.1498	-0.7946	-0.3593	1.9986
39	316.9056	-19.5156	-27.9570	89.8110
40	362.6243	-513.5773	68.1094	-27.6146
41	-2.6712	2.5669	-2.2114	-0.7719
42	1.7247	8.6868	-16.9980	-2.1955
43	36.9079	-42.7376	6.8845	0.3516
44	-62.3765	-47.9699	-32.8883	-47.7449
45	0.3176	-0.5044	-0.1386	-0.1085
46	6.4852	-54.1256	-24.0138	-23.8847
47	40.3716	-54.0654	2.5941	-3.6999
48	-0.1860	-0.4018	-0.3810	-0.3229
49	30.0311	-31.6961	49.1145	15.8165
50	3.4222	-33.7857	-34.3898	-21.5844

IV-conf

SCF Energy:

Num. Imaginary Frequencies: 0

C	-0.431080	1.126851	1.660040
C	-1.533565	1.751547	2.255425
C	-1.594189	2.014690	3.624250
C	-0.504250	1.612396	4.412494
C	0.659014	0.759892	2.462999
H	1.447061	0.707833	4.470584
H	-0.522410	1.788211	5.485997
H	-2.545893	3.746797	4.522319
H	-3.628767	2.748903	3.544931
H	-2.370907	2.032469	1.622071
H	-3.123042	2.202275	5.150611
C	-0.455724	0.798329	0.167023
C	0.912797	0.282950	-0.389010
H	0.882653	-0.806301	-0.472094
C	2.111270	0.612258	0.533740
N	1.780283	0.138882	1.880873
H	2.586903	0.149524	2.497556
H	2.267972	1.703291	0.535719
C	3.392852	-0.048048	0.056439
C	4.404790	0.702946	-0.556426
C	5.577799	0.098159	-1.016056
C	5.767750	-1.272197	-0.862162
C	4.759505	-2.008311	-0.241885
C	3.582172	-1.425609	0.216665
H	2.833304	-2.039103	0.702204
N	4.948351	-3.459853	-0.061728
O	5.993924	-3.954958	-0.481194
O	4.050604	-4.088587	0.496804
H	6.666559	-1.771554	-1.201531
H	6.348824	0.699476	-1.488281
H	4.275822	1.776379	-0.670177
C	-1.563708	-0.243601	-0.091218
C	-2.703797	0.069963	-0.835080
C	-3.710605	-0.876288	-1.046514
C	-3.572586	-2.148845	-0.503499
C	-2.451488	-2.485827	0.254695
C	-1.459442	-1.530278	0.458993
H	-2.358069	-3.478833	0.680916
Br	-4.939758	-3.456382	-0.793430
H	-4.591367	-0.622704	-1.627022
H	-2.809643	1.066661	-1.246429
H	-0.596325	-1.791512	1.066181
O	-0.745168	2.007053	-0.557420
C	0.977190	0.927556	-1.784517
C	0.127214	2.213047	-1.698642
C	0.960549	3.488230	-1.441752
C	-2.784560	2.712316	4.240871
C	0.606116	1.001555	3.845221
H	2.002493	1.130699	-2.109354
H	0.537950	0.243739	-2.518918
C	0.086140	4.746971	-1.342185
H	1.545816	3.368947	-0.522968
H	1.677706	3.602213	-2.268315
C	-0.739072	2.418621	-2.956698
C	-1.613835	3.678789	-2.881393
H	-0.064294	2.492220	-3.822505
H	-1.357732	1.527386	-3.114087
H	0.721209	5.626692	-1.178174
C	-0.773013	4.932565	-2.600733
H	-0.563816	4.653751	-0.463196
H	-1.423279	5.809738	-2.492411
H	-0.118181	5.132459	-3.462629
H	-2.175660	3.794937	-3.816741
H	-2.354158	3.553733	-2.080237

Excited states

Excited State 1:	Singlet-A	1.0666 eV	1162.39 nm	f=0.0046	<S**2>=0.000
Excited State 2:	Singlet-A	1.9653 eV	630.86 nm	f=0.0001	<S**2>=0.000
Excited State 3:	Singlet-A	2.2876 eV	541.97 nm	f=0.0001	<S**2>=0.000
Excited State 4:	Singlet-A	2.6655 eV	465.15 nm	f=0.0007	<S**2>=0.000
Excited State 5:	Singlet-A	2.9711 eV	417.30 nm	f=0.0012	<S**2>=0.000
Excited State 6:	Singlet-A	3.0583 eV	405.41 nm	f=0.0030	<S**2>=0.000
Excited State 7:	Singlet-A	3.1499 eV	393.61 nm	f=0.0034	<S**2>=0.000
Excited State 8:	Singlet-A	3.3155 eV	373.96 nm	f=0.0029	<S**2>=0.000
Excited State 9:	Singlet-A	3.3600 eV	369.00 nm	f=0.0064	<S**2>=0.000
Excited State 10:	Singlet-A	3.4591 eV	358.43 nm	f=0.0034	<S**2>=0.000
Excited State 11:	Singlet-A	3.5410 eV	350.14 nm	f=0.0330	<S**2>=0.000
Excited State 12:	Singlet-A	3.5547 eV	348.79 nm	f=0.0006	<S**2>=0.000
Excited State 13:	Singlet-A	3.6237 eV	342.15 nm	f=0.0001	<S**2>=0.000
Excited State 14:	Singlet-A	3.6797 eV	336.94 nm	f=0.0026	<S**2>=0.000
Excited State 15:	Singlet-A	3.7060 eV	334.55 nm	f=0.0021	<S**2>=0.000
Excited State 16:	Singlet-A	3.7127 eV	333.94 nm	f=0.0001	<S**2>=0.000
Excited State 17:	Singlet-A	3.8899 eV	318.74 nm	f=0.0007	<S**2>=0.000
Excited State 18:	Singlet-A	4.0165 eV	308.68 nm	f=0.0996	<S**2>=0.000
Excited State 19:	Singlet-A	4.0416 eV	306.77 nm	f=0.0637	<S**2>=0.000
Excited State 20:	Singlet-A	4.0468 eV	306.37 nm	f=0.0116	<S**2>=0.000
Excited State 21:	Singlet-A	4.1091 eV	301.73 nm	f=0.0330	<S**2>=0.000
Excited State 22:	Singlet-A	4.1150 eV	301.30 nm	f=0.0033	<S**2>=0.000
Excited State 23:	Singlet-A	4.1623 eV	297.88 nm	f=0.0003	<S**2>=0.000
Excited State 24:	Singlet-A	4.2756 eV	289.98 nm	f=0.0545	<S**2>=0.000
Excited State 25:	Singlet-A	4.3629 eV	284.18 nm	f=0.0010	<S**2>=0.000
Excited State 26:	Singlet-A	4.3782 eV	283.19 nm	f=0.0037	<S**2>=0.000
Excited State 27:	Singlet-A	4.3958 eV	282.05 nm	f=0.0048	<S**2>=0.000
Excited State 28:	Singlet-A	4.5075 eV	275.06 nm	f=0.0013	<S**2>=0.000
Excited State 29:	Singlet-A	4.5992 eV	269.58 nm	f=0.0015	<S**2>=0.000
Excited State 30:	Singlet-A	4.6321 eV	267.66 nm	f=0.0006	<S**2>=0.000

Excited State 31:	Singlet-A	4.6886 eV	264.44 nm	f=0.0042	<S**2>=0.000
Excited State 32:	Singlet-A	4.7458 eV	261.25 nm	f=0.0045	<S**2>=0.000
Excited State 33:	Singlet-A	4.7653 eV	260.18 nm	f=0.0112	<S**2>=0.000
Excited State 34:	Singlet-A	4.8111 eV	257.70 nm	f=0.0008	<S**2>=0.000
Excited State 35:	Singlet-A	4.8689 eV	254.65 nm	f=0.0142	<S**2>=0.000
Excited State 36:	Singlet-A	4.8908 eV	253.51 nm	f=0.0007	<S**2>=0.000
Excited State 37:	Singlet-A	4.8998 eV	253.04 nm	f=0.0598	<S**2>=0.000
Excited State 38:	Singlet-A	4.9384 eV	251.06 nm	f=0.0525	<S**2>=0.000
Excited State 39:	Singlet-A	4.9443 eV	250.76 nm	f=0.0022	<S**2>=0.000
Excited State 40:	Singlet-A	5.0297 eV	246.50 nm	f=0.1581	<S**2>=0.000
Excited State 41:	Singlet-A	5.0714 eV	244.48 nm	f=0.0675	<S**2>=0.000
Excited State 42:	Singlet-A	5.0818 eV	243.98 nm	f=0.0078	<S**2>=0.000
Excited State 43:	Singlet-A	5.0976 eV	243.22 nm	f=0.0034	<S**2>=0.000
Excited State 44:	Singlet-A	5.1753 eV	239.57 nm	f=0.0315	<S**2>=0.000
Excited State 45:	Singlet-A	5.2024 eV	238.32 nm	f=0.0608	<S**2>=0.000
Excited State 46:	Singlet-A	5.2156 eV	237.72 nm	f=0.0008	<S**2>=0.000
Excited State 47:	Singlet-A	5.2496 eV	236.18 nm	f=0.0018	<S**2>=0.000
Excited State 48:	Singlet-A	5.2946 eV	234.17 nm	f=0.0375	<S**2>=0.000
Excited State 49:	Singlet-A	5.3085 eV	233.56 nm	f=0.0836	<S**2>=0.000
Excited State 50:	Singlet-A	5.3386 eV	232.24 nm	f=0.0125	<S**2>=0.000

Rotatory Strengths (R) in cgs (10-40 erg-esu-cm/Gauss)**

state	XX	YY	ZZ	R(length)
1	4.1239	-7.6506	5.8352	0.7695
2	0.0287	0.4917	0.2941	0.2715
3	0.1589	0.1254	-0.0189	0.0885
4	-0.2749	0.2901	-0.9503	-0.3117
5	-0.3083	2.7783	-2.0146	0.1518
6	-3.6695	7.1672	-4.2224	-0.2416
7	4.0921	-8.8939	-15.3795	-6.7271
8	0.2521	8.3947	-5.1399	1.1690
9	-2.6953	0.0587	5.9034	1.0889
10	18.0847	-1.6450	15.0725	10.5041
11	60.2983	22.9027	-23.1107	20.0301
12	-1.2913	-0.2647	2.6293	0.3578
13	-0.0093	0.0165	0.2051	0.0708
14	-6.8548	2.6826	8.1415	1.3231
15	-2.1057	1.3998	3.2185	0.8375
16	-1.8298	-9.1518	-0.4702	-3.8173
17	-1.4643	-2.4957	-0.3826	-1.4476
18	-54.0488	60.5113	-21.4962	-5.0113
19	12.8853	25.0260	-9.2387	9.5575
20	0.1601	11.5456	-11.2792	0.1422
21	47.6098	-9.0260	-52.9084	-4.7749
22	27.3163	-21.2703	-11.9924	-1.9821
23	-16.3547	4.4779	-0.7354	-4.2041
24	-21.0680	77.8582	-45.0265	3.9212
25	1.0785	2.9907	-0.1116	1.3192
26	-4.2104	-6.0671	1.1024	-3.0584
27	3.6380	-5.8916	5.4868	1.0777
28	0.3790	2.9360	-2.1962	0.3729
29	1.1000	0.7052	-0.2136	0.5305
30	0.4441	2.0606	-0.4398	0.6883
31	1.0524	-1.6201	-3.2220	-1.2632
32	-6.7705	10.8541	0.2735	1.4523
33	6.8547	10.8173	4.0719	7.2480
34	-1.9465	-2.0696	5.4874	0.4905
35	-31.0104	-5.8966	18.6284	-6.0929
36	-3.8422	0.6015	0.0123	-1.0761
37	70.2971	45.3506	-30.3287	28.4396
38	129.7303	39.3893	-9.1885	53.3104
39	1.4374	2.6772	0.5446	1.5531
40	167.2136	-374.7130	58.7796	-49.5733
41	62.3742	-118.9261	87.6911	10.3797
42	6.7343	7.3129	-28.1601	-4.7043
43	0.3395	10.4465	-13.1758	-0.7966
44	-48.6291	-2.0979	-19.5352	-23.4207
45	5.3979	-138.5468	19.5916	-37.8525
46	0.7867	-0.4781	-0.2578	0.0169
47	1.4268	0.1011	-0.2119	0.4386
48	28.3841	4.6098	11.8481	14.9474
49	2.5621	-97.9151	73.9626	-7.1301
50	-0.1288	-21.9657	-22.2736	-14.7893

COMPUTATIONAL STUDY OF THE POVAROV REACTION

CARTESIAN COORDINATES

Cartesian Coordinates (wB97XD-PCM(CH_2Cl_2)/6-31G*//wB97XD/6-31G*) for the Povarov reaction by thermal activation between *N*-phenylaldimine 6b and 2,3-dihydrofuran 5b (DHF) and 5-phenyl-2,3-dihydrofuran 5a (DHFPh)

1+2_DHFRe_exo
SCF Energy: -787.714852506
Num. Imaginary Frequencies: 0

N	0.462161	-0.934453	0.470940
C	1.839389	-0.926125	0.173561
C	2.693295	-1.587119	1.061154
C	4.060620	-1.629942	0.819073
C	4.596314	-0.989968	-0.296801
C	3.752540	-0.303678	-1.166148
C	2.380590	-0.270297	-0.938980
C	-0.374969	-1.026934	-0.484496
C	-1.828600	-1.023382	-0.258122
C	-2.692731	-1.009003	-1.356437
C	-4.070964	-0.979682	-1.169058
C	-4.594972	-0.972918	0.120209
C	-3.738387	-0.998907	1.221477
C	-2.363474	-1.024970	1.035568
C	0.575711	2.644913	1.232943
C	1.156205	2.578723	0.039827
O	0.311140	2.338346	-1.006323
C	-1.025654	2.435279	-0.473727
C	-0.898647	2.368471	1.059950
H	-0.054814	-1.123075	-1.531828
H	-2.279468	-1.013004	-2.362458
H	-4.735167	-0.963544	-2.027845
H	-5.670412	-0.950410	0.269491
H	-4.148522	-1.000459	2.226959
H	-1.679956	-1.049955	1.878487
H	2.261656	-2.070418	1.931937
H	4.712263	-2.159681	1.507797
H	5.666399	-1.014793	-0.479481
H	4.164520	0.215119	-2.027147
H	1.730317	0.305706	-1.590650
H	-1.545882	3.105086	1.547271
H	-1.164291	1.379203	1.452074
H	-1.619123	1.626276	-0.903156
H	-1.441321	3.396134	-0.800254
H	1.081763	2.788838	2.176818
H	2.200211	2.656611	-0.233975

TS_DHFRe_exo
SCF Energy: -787.667044377
Num. Imaginary Frequencies: 1

N	-0.241837	-1.357976	0.163389
C	-1.573034	-1.206907	0.303625
C	-2.418075	-2.232949	-0.218600
C	-3.777264	-2.074739	-0.269736
C	-4.386744	-0.887721	0.207814
C	-3.607685	0.105494	0.746817
C	-2.199454	-0.022431	0.777582
C	0.528465	-0.295575	0.440638
C	2.001328	-0.490400	0.284089
C	2.901111	0.204227	1.093616
C	4.275018	0.041062	0.932205
C	4.761007	-0.822610	-0.043565
C	3.867725	-1.527520	-0.850175
C	2.498332	-1.363442	-0.687110
C	0.078106	1.041552	-0.911983
C	-1.297548	1.346140	-0.924429
O	-1.595128	2.572253	-0.448875
C	-0.395366	3.106139	0.139257
C	0.750419	2.361793	-0.550738
H	0.290675	0.352957	1.296657
H	2.523557	0.867347	1.869624
H	4.962926	0.585231	1.572735
H	5.831363	-0.952720	-0.173138
H	4.243013	-2.211318	-1.606152
H	1.789881	-1.921552	-1.291466
H	-1.934722	-3.130153	-0.592712
H	-4.398247	-2.864566	-0.683455
H	-5.466051	-0.777941	0.161835
H	-4.060954	1.011063	1.139691
H	-1.643395	0.680219	1.388607
H	1.074338	2.884472	-1.457877
H	1.622916	2.248999	0.097575
H	-0.420427	2.901663	1.217006
H	-0.406730	4.185738	-0.017147
H	0.471224	0.465080	-1.741612
H	-2.063525	0.910616	-1.548749

3_DHFRe_exo
SCF Energy: -787.732725787
Num. Imaginary Frequencies: 0

N	0.207571	-1.337670	-0.218156
C	1.483210	-1.191697	-0.232899
C	2.346163	-2.358798	-0.092631
C	3.683793	-2.225061	-0.036668
C	4.330579	-0.918840	-0.118686
C	3.610838	0.199209	-0.275793
C	2.117960	0.175396	-0.364436
C	-0.553059	-0.103716	-0.339479
C	-2.037431	-0.373536	-0.221742
C	-2.952774	0.284105	-1.042638
C	-4.321999	0.075616	-0.894618
C	-4.789750	-0.802723	0.077009
C	-3.881239	-1.473536	0.893558
C	-2.515637	-1.260815	0.743931
C	-0.077387	0.922860	0.726520
C	1.458940	1.120789	0.676417
O	1.709516	2.476751	0.344241
C	0.535714	3.012112	-0.244086
C	-0.610504	2.348307	0.512082
H	-0.367622	0.340468	-1.333660
H	-2.591620	0.961358	-1.814148
H	-5.020689	0.594796	-1.544285
H	-5.856291	-0.970439	0.194345
H	-4.239064	-2.170508	1.646006
H	-1.803163	-1.800896	1.360535
H	1.854963	-3.323759	-0.021417
H	4.311686	-3.104292	0.078248
H	5.413405	-0.872148	-0.049587
H	4.083300	1.175627	-0.335340
H	1.826503	0.584263	-1.347446
H	-0.755365	2.846181	1.475413
H	-1.561002	2.372866	-0.026768
H	0.491971	2.774082	-1.319707
H	0.575579	4.098470	-0.135273
H	-0.378028	0.527378	1.700439
H	1.921794	0.938208	1.650754

1+2_DHFRe_endo
SCF Energy: -787.716608303
Num. Imaginary Frequencies: 0

N	-0.692395	-0.778072	-0.656569
C	-2.068613	-0.732243	-0.357851
C	-2.803258	0.385906	-0.765823
C	-4.160937	0.464034	-0.482771
C	-4.808152	-0.579407	0.178247
C	-4.083484	-1.703565	0.560982
C	-2.718383	-1.781756	0.299675
C	0.117119	-1.054039	0.286548
C	1.570253	-1.144706	0.077044
C	2.414715	-1.249601	1.184258
C	3.795549	-1.275088	1.017530
C	4.340729	-1.200565	-0.261185
C	3.501823	-1.109558	-1.372821
C	2.124090	-1.084917	-1.206436
C	1.884811	2.304539	0.317865
C	0.943840	2.374743	-0.901991
O	-0.389441	2.571979	-0.386869
C	-0.336848	2.269260	0.938272
C	0.885085	2.073390	1.428133
H	1.160126	3.198267	-1.585465
H	-0.230921	-1.207953	1.317983
H	1.984742	-1.294329	2.181940
H	4.445821	-1.348508	1.883959
H	5.418364	-1.217965	-0.394537
H	3.927773	-1.057987	-2.370360
H	1.455292	-1.013406	-2.058544
H	-2.282973	1.195180	-1.266984
H	-4.719992	1.344414	-0.786625
H	-5.872547	-0.518406	0.383994
H	-4.580741	-2.528746	1.062853
H	-2.154810	-2.668273	0.577439
H	1.128058	1.854856	2.458537
H	2.442188	3.238896	0.468293
H	0.939291	1.431227	-1.456661
H	2.615789	1.496327	0.211891
H	-1.303191	2.228527	1.425171

TS_DHFRe_endo
SCF Energy: -787.669599937
Num. Imaginary Frequencies: 1

N	-0.144933	-1.085551	-0.212958
C	-1.466806	-1.089393	0.060780
C	-2.351081	-1.538946	-0.965642
C	-3.709674	-1.401741	-0.843856
C	-4.274993	-0.833208	0.319853
C	-3.453718	-0.446824	1.353617
C	-2.053888	-0.545733	1.236569
C	0.640476	-0.388978	0.629171
C	2.111766	-0.428165	0.341267
C	3.023249	0.042293	1.288642
C	4.389131	0.033071	1.027805
C	4.859994	-0.450288	-0.190608
C	3.957646	-0.927780	-1.138183
C	2.591848	-0.917279	-0.874826
C	0.325538	1.811057	-1.037790
C	-1.132259	1.835673	-1.514555
O	-1.917582	2.057893	-0.321110
C	-1.172113	1.722733	0.728509
C	0.179653	1.440374	0.438846

H	-1.373655	2.643021	-2.207747
H	0.452756	-0.431776	1.712208
H	2.658124	0.414426	2.244697
H	5.086912	0.397713	1.776070
H	5.926344	-0.461557	-0.396645
H	4.321233	-1.317102	-2.084992
H	1.873344	-1.304674	-1.589944
H	-1.899025	-1.965601	-1.856176
H	-4.361073	-1.730795	-1.648943
H	-5.352271	-0.729104	0.405021
H	-3.882176	-0.048894	2.270070
H	-1.450807	-0.398367	2.126466
H	0.905538	1.835297	1.144477
H	0.794156	2.795242	-1.141958
H	-1.446049	0.878074	-1.938638
H	0.919887	1.085497	-1.597896
H	-1.606655	1.973105	1.685931

3_DHFRe_endo
SCF Energy: -787.731510302
Num. Imaginary Frequencies: 0

N	0.117798	-1.155473	-0.071658
C	1.388620	-1.033787	-0.209249
C	2.274371	-2.013162	0.409518
C	3.610752	-1.873413	0.346112
C	4.233642	-0.747157	-0.340943
C	3.491073	0.178619	-0.959160
C	1.996769	0.111524	-0.994956
C	-0.668801	-0.103860	-0.687138
C	-2.148069	-0.264722	-0.390575
C	-3.082573	0.471080	-1.122929
C	-4.441468	0.373546	-0.846117
C	-4.886067	-0.467011	0.171943
C	-3.961922	-1.207286	0.902168
C	-2.600944	-1.107924	0.622417
C	-0.215482	1.526269	1.278914
C	1.255216	1.558045	1.703490
O	1.961621	2.020338	0.562917
C	1.348887	1.469663	-0.580794
C	-0.152271	1.290746	-0.248930
H	1.464842	2.253987	2.519209
H	-0.543193	-0.156431	-1.784290
H	-2.743543	1.125352	-1.924164
H	-5.154019	0.950803	-1.428357
H	-5.947206	-0.548460	0.388539
H	-4.300481	-1.871238	1.692624
H	-1.873170	-1.694656	1.172701
H	1.800107	-2.836274	0.934212
H	4.255645	-2.605239	0.824731
H	5.316740	-0.670884	-0.335146
H	3.957629	1.025112	-1.456468
H	1.687614	-0.037982	-2.045498
H	-0.739704	2.048927	-0.772815
H	-0.694005	2.485780	1.490917
H	1.608896	0.559488	1.997510
H	-0.780838	0.746704	1.795416
H	1.516739	2.183600	-1.393489

1+2_DHFPhRe_exo
SCF Energy: -1018.70761100
Num. Imaginary Frequencies: 0

N	0.894612	1.214101	-0.908014
C	2.284079	1.011232	-0.829011
C	2.837986	-0.023766	-1.589287
C	4.197356	-0.296494	-1.516556
C	5.029905	0.479819	-0.710845
C	4.490473	1.536745	0.016022
C	3.125616	1.804791	-0.040608
C	0.258094	1.462393	0.168030
C	-1.193126	1.684556	0.195864
C	-1.829369	1.869950	1.425196
C	-3.208153	2.040653	1.485485
C	-3.957537	2.028834	0.312530
C	-3.326665	1.844884	-0.917628
C	-1.951521	1.672496	-0.978462
C	0.040001	-1.175648	2.271555
C	-0.012413	-1.582440	0.997313
O	1.194949	-1.967274	0.490195
C	2.199124	-1.675139	1.478385
C	1.450642	-1.317886	2.780389
H	0.762206	1.486245	1.144496
H	-1.238368	1.869846	2.338326
H	-3.696865	2.182882	2.444768
H	-5.034848	2.160809	0.356390
H	-3.913123	1.824612	-1.831196
H	-1.445618	1.505294	-1.923237
H	2.178580	-0.620766	-2.209670
H	4.611501	-1.117738	-2.094018
H	6.094326	0.271221	-0.662378
H	5.134233	2.162446	0.627619
H	2.710626	2.645989	0.507338
H	1.535421	-2.105682	3.540862
H	1.843410	-0.396805	3.226325
H	2.799720	-0.838402	1.108100
H	2.838142	-2.556240	1.567284
H	-0.797417	-0.822356	2.856752
C	-1.144036	-1.649528	0.064593
C	-2.460198	-1.541048	0.526247
C	-0.912988	-1.784945	-1.306482
C	-3.521842	-1.558601	-0.366850
C	-1.979396	-1.807802	-2.199093
C	-3.285383	-1.693796	-1.733367
H	-2.652759	-1.437378	1.589375
H	0.107053	-1.866127	-1.663175
H	-4.537401	-1.461916	0.004955
H	-1.787686	-1.913132	-3.262880
H	-4.116899	-1.708884	-2.432018

TS_DHFPhRe_exo
SCF Energy: -1018.65919222
Num. Imaginary Frequencies: 1

N	0.587657	-0.786067	1.197768
C	-0.628638	-0.383294	1.631875
C	-1.597192	-1.390307	1.918246
C	-2.910960	-1.071634	2.142406
C	-3.337597	0.275560	2.132982
C	-2.407515	1.277038	1.946802
C	-1.067166	0.963078	1.691430
C	1.411233	0.189905	0.728195
C	2.805144	-0.278546	0.407639
C	3.905462	0.552865	0.612356
C	5.190548	0.128141	0.281045
C	5.385464	-1.137439	-0.260940
C	4.291242	-1.979530	-0.457850
C	3.011888	-1.553620	-0.124053
C	0.796701	0.845263	-0.855485
C	-0.618096	1.049516	-0.939498
O	-0.971037	2.341059	-1.028307
C	0.198017	3.145223	-0.801892
C	1.377353	2.231052	-1.139910
H	1.451000	1.143735	1.277961
H	3.761095	1.535707	1.056486
H	6.038079	0.785353	0.453309
H	6.385804	-1.472066	-0.519852
H	4.439466	-2.974161	-0.868809
H	2.154334	-2.209876	-0.239869
H	-1.261888	-2.422304	1.882760
H	-3.637169	-1.861671	2.312579
H	-4.382654	0.515301	2.304312
H	-2.712677	2.319851	1.974221
H	-0.351716	1.775124	1.632338
H	1.654612	2.321996	-2.195329
H	2.263164	2.461181	-0.542794
H	0.201205	3.449863	0.251040
H	0.108172	4.032841	-1.429353
H	1.167813	0.051203	-1.497939
C	-1.629037	0.050492	-1.209238
C	-1.256438	-1.291571	-1.400209
C	-2.988089	0.399376	-1.259319
C	-2.224795	-2.257445	-1.620971
C	-3.948654	-0.573926	-1.493710
C	-3.572027	-1.903075	-1.670031
H	-0.213769	-1.580086	-1.337487
H	-3.276475	1.432107	-1.100492
H	-1.929412	-3.293329	-1.755847
H	-4.997879	-0.296736	-1.526874
H	-4.327477	-2.662763	-1.847494

3_DHFPhRe_exo
SCF Energy: -1018.71292112
Num. Imaginary Frequencies: 0

N	0.879671	1.648629	0.058905
C	-0.336754	1.855094	-0.297835
C	-1.063864	2.996067	0.242868
C	-2.354501	3.203907	-0.075461
C	-3.080145	2.310608	-0.971938
C	-2.480005	1.247021	-1.519739
C	-1.046778	0.917311	-1.246903
C	1.501157	0.470430	-0.523884
C	2.885618	0.263562	0.052641
C	3.953804	-0.121166	-0.756339
C	5.212004	-0.361784	-0.208506
C	5.414197	-0.215026	1.159563
C	4.353797	0.178137	1.974103
C	3.100039	0.415938	1.423498
C	0.613688	-0.785419	-0.292288
C	-0.855031	-0.561484	-0.760437
O	-1.063590	-1.410783	-1.884953
C	0.186036	-1.884509	-2.355451
C	1.042655	-2.014027	-1.104132
H	1.602300	0.617191	-1.613782
H	3.803673	-0.225979	-1.829023
H	6.034279	-0.657279	-0.853800
H	6.394214	-0.397841	1.590304
H	4.507224	0.305413	3.041850
H	2.277085	0.745960	2.050859
H	-0.516488	3.649788	0.914133
H	-2.884390	4.054423	0.344374
H	-4.123703	2.523884	-1.182369
H	-3.016074	0.571502	-2.179905
H	-0.501611	0.954323	-2.205311
H	0.774527	-2.928890	-0.567132
H	2.116147	-2.039672	-1.307238
H	0.626067	-1.170856	-3.070644
H	0.009268	-2.827838	-2.877659
H	0.638306	-0.995944	0.779172
C	-1.874296	-0.910288	0.316811
C	-1.812808	-0.299622	1.572956
C	-2.898518	-1.820498	0.060491
C	-2.760871	-0.588438	2.547381
C	-3.845748	-2.112402	1.038593
C	-3.782488	-1.497123	2.284070
H	-1.019107	0.407354	1.796448
H	-2.944662	-2.299750	-0.910303
H	-2.696583	-0.104633	3.517569
H	-4.635134	-2.826943	0.823109
H	-4.521427	-1.726080	3.046260

1+2_DHFPhRe_endo
SCF Energy: -1018.70800334

Num. Imaginary Frequencies: 0

N	0.445969	-1.443779	-0.984637
C	1.845927	-1.315311	-0.907587
C	2.488408	-1.921797	0.176217
C	3.858846	-1.777831	0.348569
C	4.612062	-1.057149	-0.577190
C	3.982845	-0.489617	-1.681551
C	2.607754	-0.617131	-1.850506
C	-0.234365	-0.426953	-1.344375
C	-1.702383	-0.443609	-1.398706
C	-2.383639	0.745502	-1.664624
C	-3.774476	0.781550	-1.634094
C	-4.491420	-0.375627	-1.344526
C	-3.815507	-1.571064	-1.094325
C	-2.428813	-1.606556	-1.121081
C	-2.128655	-1.244586	2.532102
C	-0.689438	-1.785544	2.465076
O	0.163232	-0.643013	2.297186
C	-0.627457	0.364130	1.807940
C	-1.936623	0.107017	1.895917
H	-0.363935	-2.316230	3.361953
H	0.240572	0.536825	-1.573565
H	-1.817549	1.650991	-1.869047
H	-4.297370	1.712200	-1.833421
H	-5.576909	-0.349482	-1.316399
H	-4.375494	-2.475600	-0.875211
H	-1.885479	-2.523458	-0.915772
H	1.887559	-2.469404	0.893992
H	4.342642	-2.232977	1.207796
H	5.684520	-0.951081	-0.445271
H	4.565059	0.054319	-2.419904
H	2.123451	-0.186041	-2.721889
H	-2.738602	0.739457	1.542456
H	-2.504403	-1.167547	3.561902
H	-0.553726	-2.428293	1.586172
H	-2.822616	-1.879724	1.971958
C	0.086705	1.495384	1.204723
C	-0.608485	2.615297	0.731777
C	1.470378	1.426536	1.014929
C	0.063266	3.629523	0.061815
C	2.139740	2.442035	0.339651
C	1.440275	3.543407	-0.143337
H	-1.681462	2.688144	0.881732
H	2.011925	0.558092	1.370771
H	-0.488268	4.491769	-0.301970
H	3.210490	2.358023	0.180908
H	1.962275	4.334936	-0.673110

TS_DHFPhRe_endo

SCF Energy: -1018.66142932

Num. Imaginary Frequencies: 1

N	1.076254	1.497412	-0.681783
C	-0.189978	1.918594	-0.890353
C	-0.475268	3.294835	-0.642576
C	-1.765744	3.768195	-0.650750
C	-2.845124	2.905228	-0.927469
C	-2.592515	1.583580	-1.241204
C	-1.286254	1.082862	-1.228618
C	1.262964	0.155536	-0.557216
C	2.709993	-0.259808	-0.453851
C	3.070617	-1.595239	-0.642631
C	4.395071	-2.001141	-0.517004
C	5.379058	-1.068554	-0.198738
C	5.028994	0.267173	-0.018006
C	3.703200	0.669916	-0.146524
C	0.919763	0.572246	2.110210
C	-0.376713	1.351445	2.356327
O	-1.427429	0.504647	1.845825
C	-0.902424	-0.394770	1.019543
C	0.528407	-0.387128	0.983678
H	-0.604340	1.536200	3.407312
H	0.730178	-0.523693	-1.244356
H	2.306279	-2.326726	-0.902298
H	4.659111	-3.043186	-0.672875
H	6.414682	-1.380496	-0.099203
H	5.793796	1.001406	0.218811
H	3.414506	1.709927	-0.035966
H	0.366263	3.942435	-0.413680
H	-1.957326	4.815812	-0.434131
H	-3.861761	3.286752	-0.919854
H	-3.410818	0.914172	-1.494134
H	-1.113648	0.076469	-1.589591
H	0.965409	-1.381914	1.042222
H	1.221780	0.016889	3.003254
H	-0.416974	2.290309	1.797180
H	1.733930	1.236471	1.813298
C	-1.808274	-1.396903	0.476531
C	-1.316596	-2.471926	-0.277931
C	-3.190736	-1.284479	0.686324
C	-2.190869	-3.407823	-0.815778
C	-4.056956	-2.225948	0.150412
C	-3.561953	-3.289025	-0.604001
H	-0.249221	-2.579467	-0.444804
H	-3.570445	-0.444997	1.257583
H	-1.799131	-4.235102	-1.399447
H	-5.125309	-2.128344	0.317190
H	-4.243296	-4.023171	-1.022902

3_DHFPhRe_endo

SCF Energy: -1018.71161860

Num. Imaginary Frequencies: 0

N	1.269589	1.585656	-0.449574
C	0.074806	2.045337	-0.553201
C	-0.158664	3.471872	-0.377950
C	-1.404662	3.976665	-0.407861
C	-2.570023	3.125499	-0.617942
C	-2.440580	1.805185	-0.792729
C	-1.106177	1.126002	-0.793039
C	1.389006	0.153967	-0.633774
C	2.816614	-0.321509	-0.451966
C	3.191103	-1.579297	-0.928938
C	4.479623	-2.062529	-0.729210
C	5.414570	-1.288529	-0.045965
C	5.050580	-0.031336	0.426717
C	3.759739	0.450807	0.224424
C	0.763900	-0.683395	1.763534
C	0.012342	0.515315	2.322213
O	-1.177587	0.605615	1.548748
C	-1.012495	-0.011335	0.277953
C	0.406048	-0.648769	0.271565
H	-0.279004	0.398498	3.369871
H	1.095054	-0.086710	-1.671608
H	2.467205	-2.186986	-1.468825
H	4.755183	-3.041360	-1.111093
H	6.421866	-1.662762	0.111691
H	5.775681	0.581192	0.955234
H	3.470095	1.435819	0.574770
H	0.716838	4.090802	-0.210537
H	-1.562474	5.042156	-0.265898
H	-3.552585	3.587543	-0.629214
H	-3.312316	1.175084	-0.945263
H	-0.969597	0.643401	-1.776467
H	0.360427	-1.664424	-0.128018
H	0.376445	-1.606678	2.206092
H	0.596217	1.438475	2.217795
H	1.840090	-0.639439	1.945203
C	-2.107713	-1.048962	0.067637
C	-2.139545	-1.813300	-1.102633
C	-3.100553	-1.244416	1.025244
C	-3.139251	-2.756962	-1.309016
C	-4.101986	-2.190774	0.820425
C	-4.125914	-2.949647	-0.344797
H	-1.371954	-1.677487	-1.861983
H	-3.077799	-0.646241	1.928680
H	-3.146445	-3.343496	-2.223169
H	-4.867545	-2.333127	1.577861
H	-4.906419	-3.688102	-0.502231

Cartesian Coordinates (wB97XD-PCM(CH_2Cl_2)/6-31G*//wB97XD/6-31G*) for the Povarov reaction by Brønsted acid activation between *N*-phenylaldimine 6b and 2,3-dihydrofuran 5b (DHF) and 5-phenyl-2,3-dihydrofuran 5a (DHFPh)

1+2_DHFRe_exo_H
SCF Energy: -788.111454736
Num. Imaginary Frequencies: 0

N	0.995412	-0.938709	0.333818
C	2.370964	-0.597024	0.132368
C	3.339796	-1.390634	0.741816
C	4.679400	-1.080522	0.545612
C	5.036653	0.008459	-0.247635
C	4.054319	0.799687	-0.836750
C	2.707405	0.508715	-0.645108
C	0.046990	-0.820026	-0.549095
C	-1.344530	-1.089624	-0.303218
C	-2.186893	-1.213077	-1.421255
C	-3.540033	-1.459506	-1.248978
C	-4.061836	-1.574877	0.038806
C	-3.234573	-1.445112	1.156499
C	-1.881433	-1.200566	0.991878
C	-1.517528	2.195771	1.441002
C	-0.316185	1.947835	0.930110
O	-0.294750	1.795444	-0.433866
C	-1.593363	2.227270	-0.913087
C	-2.522503	2.255712	0.314945
H	0.753806	-1.293915	1.254210
H	0.364063	-0.541504	-1.549242
H	-1.772146	-1.121664	-2.421393
H	-4.188461	-1.560428	-2.112254
H	-5.121952	-1.762154	0.175654
H	-3.653326	-1.523876	2.153742
H	-1.263645	-1.053098	1.872472
H	3.054536	-2.249256	1.343505
H	5.444656	-1.694002	1.008518
H	6.084500	0.244668	-0.398879
H	4.333355	1.659766	-1.435956
H	1.934551	1.153608	-1.052838
H	-3.125988	3.167452	0.336445
H	-3.213632	1.403591	0.338850
H	-1.909009	1.530639	-1.691909
H	-1.460115	3.220480	-1.351389
H	-1.740133	2.350021	2.487512
H	0.649153	1.842189	1.409691

TS_DHFRe_exo_H
SCF Energy: -788.096674749
Num. Imaginary Frequencies: 1

N	-0.476904	-1.213606	0.043136
C	-1.872510	-1.068928	0.165111
C	-2.691088	-1.914945	-0.589910
C	-4.069772	-1.780447	-0.520785
C	-4.642250	-0.802644	0.292800
C	-3.825575	0.032347	1.046185
C	-2.439819	-0.095617	0.990992
C	0.440238	-0.282021	0.350457
C	1.868292	-0.627733	0.248362
C	2.735122	-0.190753	1.255254
C	4.085893	-0.518609	1.205811
C	4.578591	-1.272890	0.145488
C	3.721695	-1.699988	-0.869155
C	2.373282	-1.376798	-0.821835
C	0.320572	1.267217	-1.113657
C	-0.939345	1.790996	-0.907568
O	-0.979821	2.881929	-0.181058
C	0.389805	3.261744	0.162303
C	1.289337	2.363377	-0.700019
H	-0.161093	-2.011579	-0.494138
H	0.175821	0.381864	1.166063
H	2.349415	0.389481	2.089586
H	4.751656	-0.185789	1.994894
H	5.633284	-1.523871	0.102967
H	4.109551	-2.277112	-1.701737
H	1.724455	-1.688728	-1.637726
H	-2.249101	-2.672569	-1.232096
H	-4.700249	-2.438398	-1.109274
H	-5.720640	-0.699079	0.343452
H	-4.262380	0.786441	1.692239
H	-1.826132	0.546712	1.613804
H	1.665645	2.892210	-1.581170
H	2.154446	1.992395	-0.144100
H	0.502108	3.084349	1.234949
H	0.479044	4.328961	-0.035606
H	0.516716	0.603432	-1.946522
H	-1.900470	1.425247	-1.248072

3_DHFRe_exo_H
SCF Energy: -788.140335994
Num. Imaginary Frequencies: 0

N	0.163880	-1.228417	-0.252134
C	1.477778	-1.223919	-0.227466
C	2.252456	-2.405421	-0.078485
C	3.609587	-2.294886	-0.010587
C	4.303196	-1.033057	-0.087183
C	3.606326	0.106237	-0.247612
C	2.124341	0.111143	-0.339996
C	-0.614144	0.015532	-0.352359
C	-2.085062	-0.280742	-0.191391
C	-2.986303	0.087191	-1.189463
C	-4.346335	-0.164844	-1.033157
C	-4.809784	-0.795637	0.117071
C	-3.913258	-1.172132	1.114892
C	-2.556286	-0.911020	0.964309
C	-0.071202	1.023482	0.686446
C	1.476272	1.113452	0.694854
O	1.838239	2.421254	0.357538
C	0.745717	3.030099	-0.326856
C	-0.493844	2.468212	0.363989
H	-0.346514	-2.103560	-0.194199
H	-0.442102	0.422489	-1.359191
H	-2.627066	0.571361	-2.094196
H	-5.042225	0.128274	-1.812245
H	-5.869675	-0.993416	0.238618
H	-4.273003	-1.661517	2.014026
H	-1.865924	-1.194246	1.756740
H	1.761346	-3.370508	-0.007598
H	4.198132	-3.199229	0.114122
H	5.384559	-1.024052	-0.013764
H	4.091722	1.074998	-0.307691
H	1.848503	0.523026	-1.325937
H	-0.689877	3.015428	1.288661
H	-1.394793	2.516320	-0.253798
H	0.769646	2.771342	-1.397052
H	0.862422	4.109730	-0.231526
H	-0.431011	0.710303	1.669057
H	1.896055	0.890007	1.678582

1+2_DHFRe_endo_H
SCF Energy: -788.108717091
Num. Imaginary Frequencies: 0

N	0.156976	-1.102590	0.303655
C	1.568251	-1.154175	0.095064
C	2.387143	-0.996140	1.209976
C	3.766493	-1.010078	1.043392
C	4.315930	-1.176623	-0.225631
C	3.483895	-1.347974	-1.329839
C	2.102202	-1.350275	-1.175757
C	-0.743657	-0.712245	-0.549767
C	-2.156381	-0.665967	-0.279534
C	-2.949766	0.108238	-1.142348
C	-4.309166	0.239225	-0.902553
C	-4.885487	-0.411943	0.186084
C	-4.107512	-1.199310	1.038736
C	-2.748131	-1.327353	0.812461
C	1.967772	2.429919	0.235688
C	1.040388	2.320026	-0.990736
O	-0.249763	1.873071	-0.499638
C	-0.221171	2.029925	0.862147
C	0.970622	2.331347	1.365889
H	0.882627	3.287590	-1.475378
H	-0.146877	-1.301494	1.252140
H	-0.384700	-0.403638	-1.524285
H	-2.487457	0.628576	-1.975109
H	-4.919861	0.846895	-1.560951
H	-5.950462	-0.313624	0.369835
H	-4.568847	-1.717340	1.872310
H	-2.164774	-1.975184	1.461899
H	1.953716	-0.835061	2.192985
H	4.411205	-0.884957	1.906523
H	5.392973	-1.186257	-0.353567
H	3.910864	-1.502002	-2.314888
H	1.463008	-1.535359	-2.033450
H	1.190962	2.501512	2.410486
H	2.512431	3.378385	0.238606
H	1.381424	1.598691	-1.736901
H	2.711640	1.624884	0.272289
H	-1.177149	1.882354	1.349355

TS_DHFRe_endo_H
SCF Energy: -788.095496754
Num. Imaginary Frequencies: 1

N	0.231677	-0.930112	0.423605
C	1.623750	-1.020393	0.228631
C	2.449933	-0.967684	1.355577
C	3.827684	-0.998407	1.200199
C	4.390312	-1.081903	-0.072935
C	3.564595	-1.155896	-1.188747
C	2.179755	-1.131034	-1.047634
C	-0.657009	-0.510299	-0.492074
C	-2.096719	-0.539485	-0.179972
C	-2.995356	-0.632363	-1.249745
C	-4.363449	-0.669056	-1.018756
C	-4.849701	-0.604997	0.285060
C	-3.964419	-0.506596	1.355950
C	-2.594936	-0.470992	1.127303
C	-0.444119	2.258524	0.540116
C	1.043221	2.429734	0.897885
O	1.771657	2.176830	-0.339697
C	0.936202	1.712323	-1.230926
C	-0.371678	1.564542	-0.810204
H	1.321875	3.430323	1.226636
H	-0.079074	-0.990682	1.384091
H	-0.406682	-0.737897	-1.521025
H	-2.618626	-0.687907	-2.268199
H	-5.050861	-0.751296	-1.853814
H	-5.918799	-0.634562	0.467460
H	-4.342144	-0.457491	2.371660
H	-1.932080	-0.391487	1.985683
H	2.013456	-0.900642	2.349514
H	4.465777	-0.956540	2.076578

H	5.468072	-1.104791	-0.191333
H	3.996606	-1.249897	-2.179541
H	1.554674	-1.244068	-1.927622
H	-1.180426	1.616169	-1.529075
H	-0.952029	3.223227	0.452044
H	1.409808	1.694724	1.618437
H	-0.983512	1.677897	1.294662
H	1.370578	1.504942	-2.202175

3_DHFRe_endo_H
SCF Energy: -788.135309546
Num. Imaginary Frequencies: 0

N	0.113313	-1.098016	-0.064873
C	1.425636	-1.065881	-0.128598
C	2.245802	-2.010304	0.546203
C	3.599673	-1.878178	0.469511
C	4.246370	-0.823498	-0.270382
C	3.506229	0.072305	-0.945911
C	2.020701	0.011629	-0.971305
C	-0.713998	-0.071491	-0.703098
C	-2.174219	-0.243712	-0.351243
C	-3.129730	0.096339	-1.310139
C	-4.485649	-0.009256	-1.023631
C	-4.901785	-0.468944	0.223170
C	-3.956447	-0.814628	1.182836
C	-2.598335	-0.696633	0.900281
C	-0.179300	1.709711	1.140402
C	1.291818	1.730603	1.559710
O	2.002076	2.061980	0.374083
C	1.375699	1.429318	-0.699390
C	-0.133618	1.319901	-0.356127
H	1.532053	2.487131	2.306992
H	-0.350900	-1.857301	0.421639
H	-0.610108	-0.207212	-1.789833
H	-2.813126	0.443301	-2.290961
H	-5.217644	0.258296	-1.778375
H	-5.960015	-0.560907	0.443890
H	-4.273418	-1.173096	2.156772
H	-1.881659	-0.955317	1.677287
H	1.788822	-2.803822	1.128834
H	4.223183	-2.592000	1.000019
H	5.328669	-0.767639	-0.267681
H	3.971056	0.880157	-1.502255
H	1.720210	-0.235063	-2.006408
H	-0.697544	2.037648	-0.955411
H	-0.617953	2.703614	1.247439
H	1.624151	0.752105	1.941452
H	-0.777237	1.025384	1.744791
H	1.568583	2.031296	-1.590472

1+2_DHFPhRe_exo_H
SCF Energy: -1019.10470317
Num. Imaginary Frequencies: 0

N	-0.245418	-1.103507	-0.515276
C	-1.659152	-1.301775	-0.615184
C	-2.322344	-0.738255	-1.700474
C	-3.689595	-0.944092	-1.832832
C	-4.379256	-1.697950	-0.884748
C	-3.704791	-2.236974	0.208320
C	-2.336426	-2.034912	0.354661
C	0.606599	-1.997558	-0.115880
C	2.024937	-1.823495	0.013773
C	2.752370	-2.887570	0.578594
C	4.124043	-2.780254	0.743836
C	4.777595	-1.618076	0.337240
C	4.064925	-0.562680	-0.237160
C	2.694994	-0.657724	-0.400354
C	-1.176126	1.238859	2.126163
C	-0.978894	1.716463	0.892917
O	-2.113522	1.810876	0.140685
C	-3.232163	1.507420	1.000301
C	-2.644659	0.967373	2.322170
H	0.092984	-0.169836	-0.764862
H	0.180882	-2.967041	0.133793
H	2.236833	-3.791506	0.891059
H	4.683695	-3.597839	1.184256
H	5.852135	-1.533335	0.464013
H	4.579671	0.336121	-0.558263
H	2.164868	0.168933	-0.863239
H	-1.774967	-0.159279	-2.437301
H	-4.215173	-0.516230	-2.679423
H	-5.446588	-1.857851	-0.994160
H	-4.244826	-2.805901	0.957513
H	-1.816554	-2.413808	1.229488
H	-3.057722	1.487231	3.192429
H	-2.849389	-0.102085	2.459413
H	-3.864059	0.788291	0.475684
H	-3.790957	2.435837	1.146323
H	-0.412588	1.065794	2.871988
C	0.259139	2.099531	0.197915
C	1.443360	2.345673	0.905288
C	0.262967	2.226764	-1.198913
C	2.599499	2.716536	0.231219
C	1.430635	2.584272	-1.872520
C	2.599820	2.834116	-1.159759
H	1.448526	2.279098	1.988663
H	-0.667215	2.095226	-1.743390
H	3.503493	2.928291	0.793802
H	1.416309	2.695049	-2.952332
H	3.501882	3.138228	-1.681438

TS1_DHFPhRe_exo_H
SCF Energy: -1019.09664014
Num. Imaginary Frequencies: 1

N	0.349405	-0.809098	1.049859
C	-0.956232	-0.533019	1.522820
C	-1.878413	-1.579722	1.519370
C	-3.180855	-1.349291	1.937801
C	-3.568330	-0.079603	2.359367
C	-2.638355	0.955480	2.373781
C	-1.329229	0.735917	1.962319
C	1.318066	0.070985	0.809671
C	2.675007	-0.395123	0.501743
C	3.759888	0.355813	0.965278
C	5.060837	-0.064922	0.711651
C	5.285687	-1.231026	-0.012748
C	4.207836	-1.978576	-0.488814
C	2.908962	-1.563418	-0.236513
C	0.984778	1.177319	-1.143938
C	-0.388819	1.291854	-1.185498
O	-0.833259	2.494637	-0.827613
C	0.295993	3.336685	-0.488745
C	1.546668	2.565224	-0.943411
H	0.523204	-1.774537	0.799362
H	1.231493	1.024621	1.315898
H	3.587171	1.258619	1.544788
H	5.897545	0.516586	1.083667
H	6.300668	-1.558552	-0.211807
H	4.384020	-2.882906	-1.061518
H	2.080674	-2.138780	-0.645169
H	-1.585457	-2.564992	1.166565
H	-3.897011	-2.163968	1.927523
H	-4.587891	0.099836	2.683019
H	-2.929070	1.944619	2.711838
H	-0.625268	1.560309	1.983541
H	1.955547	2.963410	-1.878080
H	2.349882	2.608929	-0.199356
H	0.261183	3.492254	0.594165
H	0.147002	4.294082	-0.987296
H	1.518297	0.418698	-1.698218
C	-1.381059	0.274396	-1.492881
C	-0.972785	-0.992862	-1.934524
C	-2.743426	0.533235	-1.289863
C	-1.912718	-1.990663	-2.150247
C	-3.677152	-0.468115	-1.507032
C	-3.264129	-1.730959	-1.929996
H	0.076611	-1.193691	-2.128626
H	-3.055946	1.510668	-0.940806
H	-1.596081	-2.966953	-2.503162
H	-4.730434	-0.268075	-1.341690
H	-3.999207	-2.511255	-2.100303

int_DHFPhRe_exo_H
SCF Energy: -1019.11603128
Num. Imaginary Frequencies: 0

N	0.446344	-1.047271	0.469673
C	-0.766342	-1.041149	1.175639
C	-1.669038	-2.093750	0.961064
C	-2.920443	-2.075599	1.552689
C	-3.309703	-1.006871	2.364559
C	-2.412958	0.024932	2.597592
C	-1.145192	0.009350	2.016238
C	1.336713	0.076912	0.479292
C	2.754060	-0.347940	0.160195
C	3.791201	-0.042579	1.040200
C	5.097902	-0.427407	0.750758
C	5.375292	-1.124813	-0.420133
C	4.343121	-1.438526	-1.302089
C	3.039973	-1.049421	-1.014742
C	0.901946	1.199170	-0.571772
C	-0.558869	1.494114	-0.583641
O	-0.846071	2.603563	0.013235
C	0.360121	3.243495	0.544310
C	1.497678	2.571982	-0.217308
H	0.896171	-1.947096	0.380680
H	1.351813	0.568678	1.460322
H	3.579033	0.487793	1.965408
H	5.896249	-0.185543	1.444749
H	6.393272	-1.425060	-0.645911
H	4.554691	-1.983991	-2.216158
H	2.241578	-1.301517	-1.710246
H	-1.385208	-2.910154	0.302503
H	-3.607029	-2.896744	1.371354
H	-4.293554	-0.994661	2.820983
H	-2.687847	0.849413	3.248436
H	-0.459081	0.817386	2.247340
H	1.742541	3.134555	-1.121405
H	2.406404	2.484396	0.382201
H	0.363343	3.049156	1.619445
H	0.239870	4.310298	0.364551
H	1.219865	0.846292	-1.554057
C	-1.603563	0.728356	-1.181294
C	-1.282257	-0.346310	-2.033815
C	-2.951249	1.003694	-0.866487
C	-2.293405	-1.132483	-2.557243
C	-3.950133	0.202580	-1.383767
C	-3.621007	-0.862712	-2.226413
H	-0.250452	-0.559042	-2.284018
H	-3.190021	1.815684	-0.189235
H	-2.053176	-1.955022	-3.221734
H	-4.986661	0.395978	-1.131563
H	-4.410732	-1.488555	-2.630231

TS2_DHFPhRe_exo_H
SCF Energy: -1019.10722113
Num. Imaginary Frequencies: 1

N	0.779345	-0.322969	1.434310
C	-0.490802	-0.003312	1.763221
C	-1.357288	-0.932055	2.381434
C	-2.683147	-0.614408	2.532507

C	-3.205438	0.641249	2.124080
C	-2.363449	1.571995	1.584858
C	-0.999990	1.253355	1.336894
C	1.514051	0.479829	0.486641
C	2.885605	-0.107240	0.241674
C	4.028157	0.626708	0.556160
C	5.292984	0.087141	0.338133
C	5.423102	-1.192457	-0.191591
C	4.285872	-1.933524	-0.505719
C	3.023759	-1.391511	-0.293017
C	0.713759	0.634745	-0.860419
C	-0.793124	0.855193	-0.778922
O	-1.123086	2.042651	-1.275287
C	0.047712	2.874595	-1.407079
C	1.175798	1.877400	-1.646588
H	1.148919	-1.230698	1.680085
H	1.645588	1.486307	0.903042
H	3.932452	1.621492	0.984099
H	6.176236	0.666084	0.587586
H	6.408499	-1.614599	-0.359153
H	4.383489	-2.930901	-0.922012
H	2.143999	-1.979157	-0.551618
H	-0.977341	-1.900598	2.691939
H	-3.352842	-1.345581	2.974512
H	-4.256099	0.859623	2.276739
H	-2.727161	2.554440	1.301937
H	-0.304605	2.078874	1.224491
H	1.258893	1.647060	-2.711035
H	2.146205	2.247724	-1.306883
H	0.169665	3.451560	-0.483029
H	-0.146806	3.559507	-2.231061
H	0.888005	-0.275661	-1.435369
C	-1.786957	-0.207763	-0.996378
C	-1.425592	-1.559681	-0.918249
C	-3.112756	0.132204	-1.294235
C	-2.370631	-2.550024	-1.142310
C	-4.053733	-0.862784	-1.522259
C	-3.685519	-2.203617	-1.446809
H	-0.405297	-1.843571	-0.681077
H	-3.397048	1.176688	-1.355972
H	-2.080966	-3.594171	-1.087540
H	-5.076728	-0.591526	-1.760638
H	-4.422024	-2.979536	-1.629069

3_DHFPhRe_exo_H
SCF Energy: -1019.12346408
Num. Imaginary Frequencies: 0

N	0.885429	1.537157	0.078108
C	-0.366202	1.853337	-0.171251
C	-1.031929	2.930548	0.468621
C	-2.343355	3.158083	0.172281
C	-3.088951	2.361226	-0.767693
C	-2.488277	1.338473	-1.402088
C	-1.063334	0.996577	-1.165284
C	1.535128	0.384883	-0.560469
C	2.894323	0.161918	0.057613
C	4.039185	0.177426	-0.737650
C	5.290945	-0.039768	-0.168607
C	5.404781	-0.263442	1.199780
C	4.264638	-0.276127	2.000631
C	3.013564	-0.069405	1.431384
C	0.606962	-0.847514	-0.448213
C	-0.878002	-0.547837	-0.813063
O	-1.166904	-1.260830	-1.989961
C	0.046100	-1.665851	-2.614423
C	0.994339	-1.941592	-1.454219
H	1.433711	2.088430	0.729602
H	1.663486	0.634362	-1.623533
H	3.955532	0.361629	-1.805827
H	6.176996	-0.028571	-0.794908
H	6.380695	-0.428566	1.644325
H	4.350728	-0.453907	3.067598
H	2.127397	-0.097409	2.063244
H	-0.500306	3.546640	1.186660
H	-2.853713	3.976779	0.671516
H	-4.131627	2.596867	-0.945432
H	-3.019468	0.710387	-2.109440
H	-0.523857	1.118544	-2.120012
H	0.789991	-2.926559	-1.028385
H	2.050372	-1.904696	-1.735158
H	0.423207	-0.867143	-3.272196
H	-0.177865	-2.538185	-3.229298
H	0.665266	-1.215091	0.577437
C	-1.867357	-0.931786	0.278913
C	-1.703641	-0.457784	1.583404
C	-2.973610	-1.724574	-0.022859
C	-2.637338	-0.760868	2.567682
C	-3.905796	-2.030499	0.965129
C	-3.744203	-1.547100	2.259082
H	-0.836484	0.142070	1.849849
H	-3.096930	-2.107224	-1.029269
H	-2.495238	-0.390197	3.577952
H	-4.760480	-2.652763	0.719194
H	-4.471997	-1.788799	3.026810

1+2_DHFPhRe_endo_H
SCF Energy: -1019.10218563
Num. Imaginary Frequencies: 0

N	-1.255336	1.608586	-0.365771
C	-2.517672	0.983759	-0.614535
C	-3.610894	1.428096	0.124338
C	-4.849873	0.829236	-0.070988
C	-4.988696	-0.198986	-1.000134
C	-3.888766	-0.620546	-1.744262
C	-2.646109	-0.026309	-1.563445
C	-0.075399	1.090500	-0.552819
C	1.176673	1.759057	-0.334942
C	2.328285	1.124143	-0.831000
C	3.570753	1.723271	-0.678174
C	3.672497	2.945947	-0.023096
C	2.533158	3.580722	0.484812
C	1.290999	2.996074	0.329984
C	-1.516069	-0.528288	2.535716
C	-2.105371	-1.595186	1.594429
O	-1.079365	-1.884895	0.623207
C	0.104070	-1.443365	1.149632
C	-0.047997	-0.653095	2.221766
H	-2.321467	-2.525058	2.129842
H	-1.309701	2.552661	0.004743
H	-0.054975	0.077445	-0.943724
H	2.244785	0.167330	-1.337773
H	4.455728	1.230831	-1.065216
H	4.644246	3.412850	0.101650
H	2.625610	4.529595	1.001540
H	0.422057	3.495843	0.750304
H	-3.495968	2.219475	0.860622
H	-5.704792	1.167044	0.504531
H	-5.956000	-0.665549	-1.151976
H	-3.998519	-1.408793	-2.480966
H	-1.803200	-0.345758	-2.166458
H	0.746656	-0.167573	2.770870
H	-1.752548	-0.737500	3.583103
H	-2.998120	-1.278076	1.053387
H	-1.896654	0.480427	2.317240
C	1.312034	-1.834969	0.413755
C	2.583351	-1.620944	0.959474
C	1.202360	-2.381276	-0.870510
C	3.721865	-1.928940	0.226272
C	2.346596	-2.679499	-1.606421
C	3.607773	-2.450225	-1.062263
H	2.682302	-1.222415	1.964274
H	0.218575	-2.584759	-1.281394
H	4.702101	-1.770629	0.664800
H	2.251495	-3.107970	-2.599242
H	4.499254	-2.695428	-1.630945

TS1_DHFPhRe_endo_H
SCF Energy: -1019.09689327
Num. Imaginary Frequencies: 1

N	0.312952	-1.822129	-0.630923
C	1.696972	-1.593775	-0.825960
C	2.571117	-2.650383	-0.567360
C	3.940655	-2.460737	-0.704413
C	4.440224	-1.220153	-1.092850
C	3.560115	-0.173984	-1.355653
C	2.187429	-0.353123	-1.231037
C	-0.631495	-0.892852	-0.503903
C	-2.041438	-1.283568	-0.407380
C	-2.998085	-0.456752	-1.007181
C	-4.345139	-0.795934	-0.951931
C	-4.743932	-1.952694	-0.288568
C	-3.795909	-2.773120	0.323428
C	-2.449995	-2.441230	0.268122
C	0.539376	-0.973867	2.366649
C	1.914121	-0.282832	2.265035
O	1.672229	0.993235	1.622850
C	0.392682	1.086403	1.285138
C	-0.349238	-0.035547	1.589456
H	2.376453	-0.070383	3.229442
H	0.044713	-2.784915	-0.467329
H	-0.429070	0.073317	-0.949397
H	-2.683697	0.442685	-1.529642
H	-5.082094	-0.158717	-1.429102
H	-5.795737	-2.215026	-0.241847
H	-4.110095	-3.667771	0.850381
H	-1.727837	-3.069822	0.784599
H	2.183505	-3.616282	-0.252458
H	4.617389	-3.284312	-0.502939
H	5.509416	-1.071358	-1.196942
H	3.941960	0.792324	-1.667819
H	1.525080	0.478767	-1.445625
H	-1.421087	-0.007010	1.720953
H	0.206232	-1.083085	3.403064
H	2.622115	-0.823261	1.632887
H	0.570076	-1.980031	1.927329
C	-0.015732	2.290070	0.570117
C	-1.371372	2.520174	0.291185
C	0.948569	3.204246	0.124152
C	-1.752805	3.646119	-0.425160
C	0.559467	4.327647	-0.593160
C	-0.788398	4.549605	-0.868765
H	-2.129545	1.830439	0.649822
H	1.995454	3.026555	0.344837
H	-2.803348	3.827212	-0.627400
H	1.307493	5.035413	-0.934409
H	-1.088996	5.431998	-1.424496

int_DHFPhRe_endo_H
SCF Energy: -1019.11610657
Num. Imaginary Frequencies: 0

N	-0.700613	-1.580074	-0.788153
C	0.620431	-1.995833	-0.925481
C	0.960522	-3.342250	-0.716170
C	2.284251	-3.749538	-0.797572
C	3.297087	-2.827891	-1.071244
C	2.960765	-1.500069	-1.302588
C	1.632720	-1.081960	-1.245006
C	-1.040447	-0.284622	-0.288045
C	-2.543775	-0.100744	-0.265331
C	-3.136546	0.812399	-1.136684

C	-4.517157	0.991341	-1.138761
C	-5.315927	0.254912	-0.270091
C	-4.731632	-0.659893	0.602672
C	-3.352010	-0.835307	0.606635
C	-0.223834	-1.193608	2.103771
C	1.294786	-1.322770	2.240570
O	1.818761	-0.036998	1.783719
C	0.927997	0.633169	1.144614
C	-0.422674	0.017541	1.169323
H	1.660476	-1.450027	3.258144
H	-1.388780	-2.303033	-0.634403
H	-0.627810	0.480407	-0.953318
H	-2.517940	1.378492	-1.828899
H	-4.967440	1.701929	-1.824328
H	-6.392362	0.391987	-0.272504
H	-5.351121	-1.237870	1.280831
H	-2.912551	-1.549255	1.299754
H	0.181057	-4.064278	-0.484899
H	2.529079	-4.794456	-0.635036
H	4.331080	-3.150870	-1.124632
H	3.732224	-0.778270	-1.553322
H	1.387379	-0.054945	-1.494930
H	-1.106153	0.751600	1.607953
H	-0.693987	-1.015942	3.072715
H	1.735677	-2.071193	1.578877
H	-0.645187	-2.105493	1.678606
C	1.303332	1.880957	0.539656
C	0.313613	2.763238	0.065138
C	2.666259	2.208635	0.400566
C	0.687269	3.953145	-0.538625
C	3.026908	3.395517	-0.211745
C	2.039400	4.265355	-0.679759
H	-0.740891	2.533777	0.186609
H	3.422192	1.518061	0.758166
H	-0.070820	4.641375	-0.895549
H	4.074900	3.647837	-0.329873
H	2.327140	5.196327	-1.157714

TS2_DHFPhRe_endo_H
SCF Energy: -1019.10305154
Num. Imaginary Frequencies: 1

N	1.111271	1.413612	-0.848202
C	-0.129889	1.938623	-0.904080
C	-0.364101	3.327521	-0.762603
C	-1.657185	3.786519	-0.720264
C	-2.767969	2.909805	-0.831902
C	-2.553254	1.575875	-1.029293
C	-1.231691	1.039712	-1.026445
C	1.296100	0.021730	-0.517417
C	2.757225	-0.349239	-0.367215
C	3.153204	-1.632751	-0.748424
C	4.470969	-2.046240	-0.591707
C	5.415558	-1.173468	-0.058833
C	5.033255	0.109142	0.319002
C	3.710513	0.517253	0.171782
C	0.842343	0.529362	2.012947
C	-0.414200	1.356459	2.273568
O	-1.481633	0.573475	1.708330
C	-1.034814	-0.173906	0.711546
C	0.481008	-0.327152	0.779682
H	-0.656250	1.499691	3.325770
H	1.905670	2.034661	-0.799356
H	0.886041	-0.594311	-1.327330
H	2.425697	-2.316583	-1.180503
H	4.761549	-3.046573	-0.895645
H	6.446557	-1.490494	0.058199
H	5.763942	0.797027	0.731832
H	3.446716	1.523232	0.490997
H	0.473940	4.012398	-0.671670
H	-1.834169	4.849768	-0.590288
H	-3.773244	3.313996	-0.797832
H	-3.384409	0.891931	-1.169681
H	-1.062433	0.134289	-1.599760
H	0.686507	-1.383814	0.970143
H	1.061762	-0.116334	2.865532
H	-0.406559	2.324934	1.764433
H	1.715443	1.160671	1.846484
C	-1.938703	-1.276569	0.317589
C	-1.472920	-2.334435	-0.472451
C	-3.275686	-1.260182	0.731491
C	-2.333268	-3.358074	-0.846605
C	-4.130587	-2.289100	0.357904
C	-3.663483	-3.336033	-0.433412
H	-0.436400	-2.373075	-0.795324
H	-3.636989	-0.445090	1.348863
H	-1.964646	-4.176548	-1.455799
H	-5.164243	-2.274826	0.687317
H	-4.334845	-4.137137	-0.724771

3_DHFPhRe_endo_H
SCF Energy: -1019.11980250
Num. Imaginary Frequencies: 0

N	1.230297	1.493801	-0.412631
C	0.050361	2.064353	-0.474281
C	-0.129221	3.453159	-0.240275
C	-1.392358	3.960257	-0.237437
C	-2.562648	3.151108	-0.471393
C	-2.433840	1.836237	-0.715073
C	-1.105192	1.164442	-0.768253
C	1.423061	0.065554	-0.682157
C	2.859568	-0.330240	-0.440178
C	3.483120	-1.198975	-1.335384
C	4.796435	-1.604918	-1.122755
C	5.501271	-1.137077	-0.017603
C	4.886993	-0.267686	0.879333
C	3.569723	0.129763	0.672810
C	0.655134	-1.151590	1.535436
C	0.073235	0.022615	2.310247
O	-0.996101	0.524988	1.506763
C	-0.996170	-0.059390	0.215125
C	0.364263	-0.790500	0.074394
H	-0.328326	-0.259533	3.286181
H	2.055033	2.058437	-0.238909
H	1.211293	-0.069448	-1.752312
H	2.943339	-1.559211	-2.207612
H	5.271525	-2.280347	-1.826588
H	6.528083	-1.447823	0.144459
H	5.429930	0.097378	1.744999
H	3.096309	0.788862	1.398370
H	0.732531	4.083000	-0.043836
H	-1.529155	5.020189	-0.043819
H	-3.538371	3.621935	-0.444696
H	-3.299450	1.207577	-0.895484
H	-0.974141	0.766697	-1.789804
H	0.248738	-1.699445	-0.518713
H	0.108136	-2.067699	1.776042
H	0.807697	0.826035	2.457877
H	1.711832	-1.328232	1.740256
C	-2.171136	-1.007726	0.023920
C	-2.338339	-1.682126	-1.188974
C	-3.097720	-1.198398	1.045968
C	-3.415152	-2.540528	-1.375159
C	-4.173510	-2.064195	0.860544
C	-4.335728	-2.734282	-0.347282
H	-1.622029	-1.548755	-1.998109
H	-2.971741	-0.665962	1.982004
H	-3.534714	-3.059939	-2.320516
H	-4.888191	-2.211305	1.664103
H	-5.174499	-3.408065	-0.489023

Cartesian Coordinates (wB97XD-PCM(CH_2Cl_2)/6-31G*//wB97XD/6-31G*) for the Povarov reaction between *N*-phenylaldimine 6b and 5-phenyl-2,3-dihydrofuran 5a, catalyzed by (*R*)-TRIP 7d

(R)-BINOL-TRIP-PA 7d
SCF Energy: -2581.39706884
Num. Imaginary Frequencies: 1

C	4.059670	-0.484459	1.365696
C	3.694686	-0.197156	0.039231
C	4.012669	-1.106074	-0.997657
C	4.674651	-2.287971	-0.667042
C	5.036321	-2.597715	0.643814
C	4.729511	-1.677977	1.638611
C	2.897753	1.027300	-0.275345
C	1.542029	1.100310	0.139826
C	0.678381	2.108615	-0.217091
C	1.164080	3.125688	-1.104609
C	2.541379	3.124811	-1.460770
C	3.382076	2.071943	-1.017782
C	0.323317	4.120400	-1.670794
C	0.833817	5.084157	-2.501814
C	2.211345	5.110056	-2.814987
C	3.042666	4.146165	-2.309125
C	-0.728362	2.074990	0.267404
C	-1.489490	0.940060	0.084675
C	-2.868479	0.854321	0.403779
C	-3.459055	1.964896	0.948187
C	-2.715856	3.130119	1.261514
C	-1.330883	3.185927	0.945065
C	-3.327792	4.235053	1.908647
C	-2.595416	5.338227	2.258326
C	-1.209776	5.378029	1.983061
C	-0.593827	4.332825	1.344509
C	-3.636768	-0.395648	0.124346
C	-3.992742	-1.253936	1.179304
C	-4.736124	-2.397286	0.882392
C	-5.114651	-2.720030	-0.415727
C	-4.736413	-1.858515	-1.442789
C	-4.002327	-0.701427	-1.199280
C	-3.618917	-0.959931	2.626328
C	-3.061384	-2.185003	3.360651
C	-3.632022	0.195762	-2.371959
C	-4.884010	0.790985	-3.029885
C	-5.896680	-3.987895	-0.706687
C	-7.258654	-3.685644	-1.344396
O	-0.912289	-0.179731	-0.505299
P	0.108773	-1.032370	0.398019
O	-0.406104	-1.883284	1.473399
O	1.092063	0.102383	0.987963
C	3.701336	-0.822907	-2.464705
C	3.129927	-2.026886	-3.225349
C	5.740243	-3.901012	0.973120
C	7.107499	-3.995981	0.283366
C	3.780427	0.478719	2.510111
C	3.002295	-0.186199	3.652467
C	4.964930	-0.313649	-3.175942
C	5.090498	1.102575	3.011999
C	4.863114	-5.112298	0.628220
O	0.896491	-1.738859	-0.798701
C	-2.756908	-0.542430	-3.393034
C	-5.080424	-4.951904	-1.578335
C	-4.821270	-0.376221	3.382525
H	0.472069	4.373984	1.150470
H	-0.626252	6.242228	2.285755
H	-3.071332	6.176353	2.758071
H	-4.389794	4.180757	2.133022
H	-4.522217	1.942853	1.170831
H	4.424210	2.071634	-1.324013
H	-0.737682	4.107928	-1.449790
H	0.171046	5.831301	-2.927666
H	2.602425	5.882610	-3.469888
H	4.099643	4.137898	-2.562350
H	-5.017452	-2.095965	-2.466702
H	-5.022571	-3.067235	1.689425
H	-3.043886	1.036605	-1.992992
H	-2.825222	-0.206649	2.623738
H	5.013944	-1.901299	2.664359
H	4.923617	-2.989293	-1.459103
H	3.161176	1.295772	2.129890
H	2.945486	-0.034442	-2.507817
H	5.912451	-3.913699	2.057001
H	4.743993	-0.053862	-4.217145
H	5.381274	0.570255	-2.683517
H	5.742196	-1.086790	-3.176216
H	2.867565	-1.722904	-4.244323
H	3.854573	-2.844224	-3.310715
H	2.222869	-2.413139	-2.753810
H	5.353995	-6.043225	0.932299
H	3.894155	-5.054201	1.134389
H	4.677576	-5.171140	-0.450628
H	7.624962	-4.915179	0.579170
H	6.998800	-4.011052	-0.807299
H	7.741751	-3.143386	0.546130
H	2.742325	0.559205	4.411842
H	2.076942	-0.637577	3.284436
H	3.594741	-0.965093	4.146011
H	4.889061	1.831433	3.804776
H	5.762606	0.338225	3.419017
H	5.617358	1.614812	2.199797
H	-5.619390	-5.894711	-1.725180
H	-4.887423	-4.518276	-2.566440
H	-4.113832	-5.173960	-1.115576
H	-6.082003	-4.484731	0.254487
H	-7.824042	-4.611045	-1.501837
H	-7.853444	-3.021821	-0.708815
H	-7.138133	-3.198327	-2.318800
H	-2.710668	-1.888107	4.355520
H	-3.824158	-2.959336	3.503622
H	-2.217386	-2.610301	2.813764
H	-4.548697	-0.138529	4.417044
H	-5.193048	0.538179	2.908899
H	-5.646795	-1.097458	3.407073
H	-4.604056	1.475372	-3.838722
H	-5.520627	0.008140	-3.457689
H	-5.482402	1.347782	-2.301055
H	-2.446599	0.140429	-4.192061
H	-1.859203	-0.944393	-2.914822
H	-3.298426	-1.374780	-3.857366
H	1.682713	-2.210805	-0.480115

iminium_complex_Re
SCF Energy: -3138.00140483
Num. Imaginary Frequencies: 0

C	-4.525610	-0.697428	-1.781808
C	-4.116593	-0.579216	-0.442932
C	-4.396340	-1.609699	0.475025
C	-5.110981	-2.722871	0.040579
C	-5.535040	-2.859132	-1.278722
C	-5.228134	-1.838105	-2.170507
C	-3.395816	0.649345	0.009448
C	-2.049580	0.884928	-0.385623
C	-1.357703	2.030606	-0.051441
C	-1.957931	2.939189	0.879308
C	-3.306608	2.728731	1.277183
C	-4.007932	1.595864	0.790393
C	-3.906610	3.622745	2.201948
C	-3.193758	4.662728	2.739925
C	-1.842260	4.853008	2.371418
C	-1.243547	4.019279	1.461873
O	-1.469876	-0.033986	-1.217179
P	-0.247751	-0.977186	-0.667543
O	0.421079	-1.581621	-1.838984
C	-0.028626	2.292747	-0.665916
C	0.967101	1.339812	-0.582645
C	2.272310	1.542420	-1.103490
C	2.526458	2.731435	-1.739356
C	1.526664	3.715397	-1.928225
C	0.223559	3.493926	-1.405628
C	-0.779632	4.464743	-1.674760
C	-0.488602	5.602035	-2.382793
C	0.818586	5.836673	-2.866769
C	1.800516	4.907878	-2.647343
O	0.707024	0.168267	0.076384
C	3.363878	0.526029	-0.970119
C	3.695467	-0.283571	-2.073737
C	4.804339	-1.121541	-1.975229
C	5.592772	-1.186327	-0.829862
C	5.225525	-0.401534	0.257227
C	4.117118	0.446030	0.216031
C	2.906061	-0.239800	-3.375610
C	2.661974	-1.629965	-3.973134
C	6.810701	-2.097812	-0.819266
C	7.891865	-1.556486	-1.768006
C	3.758485	1.284018	1.440097
C	4.236805	2.738705	1.303182
C	-3.938606	-1.546786	1.924042
C	-3.181658	-2.808154	2.355989
C	-6.292621	-4.091574	-1.737312
C	-7.629724	-4.243756	-1.001008
C	-4.237810	0.376218	-2.821597
C	-3.345684	-0.161114	-3.948391
O	-0.683478	-1.799475	0.527335
C	3.609066	0.662827	-4.400677
C	4.315405	0.708941	2.749176
C	7.401582	-2.341584	0.570112
C	-5.109423	-1.252376	2.870192
C	-5.436540	-5.357408	-1.597223
C	-5.537238	0.979297	-3.372332
N	1.387496	-1.869941	2.168762
C	2.430391	-2.749638	1.748177
C	2.616868	-2.936883	0.380440
C	3.635837	-3.780317	-0.045131
C	4.453888	-4.426887	0.875896
C	4.252514	-4.235090	2.241005
C	3.234115	-3.400118	2.684353
C	1.489193	-1.075334	3.179929
C	0.510499	-0.118120	3.640595
C	0.914800	0.747197	4.671191
C	0.054169	1.729695	5.136277
C	-1.223665	1.837596	4.590910
C	-1.640200	0.961519	3.589872
C	-0.778954	-0.005315	3.096942
H	-1.790985	4.294461	-1.324091
H	-1.272401	6.327103	-2.580810
H	1.035408	6.744563	-3.421496
H	2.805069	5.062292	-3.033153
H	3.525888	2.921019	-2.122431
H	-5.047651	1.456667	1.075358
H	0.520335	-1.847989	1.535246
H	-0.203673	4.168653	1.192486
H	-1.273994	5.666271	2.812955
H	-3.661206	5.337731	3.450822
H	-4.942556	3.456065	2.486742

H	2.428366	-1.111970	3.726187
H	1.910181	0.650316	5.097206
H	0.376187	2.409221	5.918418
H	-1.902459	2.609965	4.938734
H	-2.637052	1.051839	3.175451
H	-1.090571	-0.659448	2.287116
H	2.002032	-2.422842	-0.352604
H	3.791405	-3.915618	-1.110029
H	5.247067	-5.083876	0.532741
H	4.876146	-4.751028	2.964168
H	3.043943	-3.289854	3.748065
H	5.814000	-0.455676	1.165406
H	5.067302	-1.749248	-2.824001
H	2.663994	1.294364	1.522974
H	1.921653	0.182173	-3.157769
H	-5.545325	-1.936760	-3.206711
H	-5.332087	-3.514205	0.753270
H	-3.691831	1.190735	-2.336752
H	-3.235295	-0.716152	2.002912
H	-6.514316	-3.957595	-2.804157
H	-4.756936	-1.167908	3.905181
H	-5.615489	-0.318227	2.603993
H	-5.854348	-2.055688	2.831250
H	-2.762470	-2.663898	3.359766
H	-3.839710	-3.683649	2.399672
H	-2.363293	-3.013174	1.661529
H	-5.963571	-6.229143	-2.001443
H	-4.486363	-5.248850	-2.129138
H	-5.208165	-5.561602	-0.544725
H	-8.189031	-5.102682	-1.388730
H	-7.471935	-4.405001	0.071731
H	-8.247341	-3.347543	-1.118160
H	-3.092277	0.643238	-4.648370
H	-2.417370	-0.572847	-3.543997
H	-3.854730	-0.948861	-4.516256
H	-5.313392	1.787596	-4.077610
H	-6.132858	0.228687	-3.904452
H	-6.155197	1.387654	-2.565452
H	8.195148	-3.094380	0.514007
H	7.847379	-1.427218	0.979520
H	6.642261	-2.696934	1.274213
H	6.480771	-3.070289	-1.212980
H	8.745454	-2.242252	-1.817094
H	7.503632	-1.420064	-2.782024
H	8.254260	-0.584040	-1.414812
H	1.974906	-1.545360	-4.821654
H	3.586391	-2.087177	-4.347056
H	2.195376	-2.287810	-3.237541
H	3.036105	0.700246	-5.333976
H	3.721519	1.686864	-4.031936
H	4.609676	0.277121	-4.631888
H	3.988867	3.308664	2.206451
H	5.324632	2.766983	1.170073
H	3.775535	3.240191	0.450198
H	3.821143	1.182911	3.604977
H	4.180313	-0.376198	2.812923
H	5.388804	0.905641	2.850051

iminium_complex_Si
SCF Energy: -3138.00305717
Num. Imaginary Frequencies: 0

C	-4.798943	-0.214524	-1.550884
C	-4.092213	-0.329400	-0.344248
C	-4.145961	-1.523411	0.403540
C	-4.945655	-2.563460	-0.061330
C	-5.668210	-2.469480	-1.249621
C	-5.574810	-1.291886	-1.980466
C	-3.300298	0.831531	0.163560
C	-2.044916	1.174062	-0.410487
C	-1.287527	2.240793	0.025570
C	-1.723072	2.966327	1.183398
C	-2.989243	2.656283	1.751084
C	-3.762970	1.607680	1.194146
C	-0.916202	3.940383	1.832211
C	-1.359115	4.588290	2.957208
C	-2.635678	4.307481	3.494979
C	-3.429883	3.360826	2.901515
C	0.025242	2.531598	-0.607491
C	0.972375	1.532384	-0.650358
C	2.332614	1.774225	-0.969186
C	2.676732	3.031736	-1.392645
C	1.712189	4.064238	-1.524734
C	0.370758	3.821648	-1.120277
C	2.063512	5.342640	-2.029230
C	1.125180	6.334497	-2.146873
C	-0.213115	6.087280	-1.765697
C	-0.580894	4.865286	-1.263636
O	0.629190	0.266280	-0.264299
P	-0.374146	-0.630763	-1.250524
O	-1.599105	0.438083	-1.476303
C	3.359018	0.716064	-0.721831
C	3.857424	0.550542	0.584161
C	4.906089	-0.346155	0.796171
C	5.454667	-1.091032	-0.244873
C	4.886028	-0.963984	-1.510205
C	3.849077	-0.071744	-1.776120
C	3.321483	1.386290	1.742840
C	3.319512	0.654086	3.088659
C	6.685127	-1.969664	-0.078771
C	7.014969	-2.336642	1.368924
C	3.316239	0.084361	-3.192803
C	3.080277	-1.254489	-3.896260
C	-3.357967	-1.698026	1.695530
C	-2.698157	-3.076947	1.810417
C	-6.519029	-3.626147	-1.741685
C	-5.657313	-4.850733	-2.077220
C	-4.747769	1.045237	-2.402359
C	-4.100199	0.771243	-3.765976
O	-0.800352	-1.716010	-0.281811
O	0.229476	-0.938453	-2.561569
C	-4.221414	-1.423413	2.933955
C	-7.623341	-3.985425	-0.739235
C	-6.137967	1.675834	-2.557708
C	4.098866	2.705449	1.864495
C	7.899735	-1.293008	-0.735413
C	4.254314	0.978125	-4.016701
N	0.738059	-1.961329	1.786337
C	0.244413	-1.291083	2.945263
C	-0.341828	-0.037880	2.779906
C	-0.821828	0.637397	3.895721
C	-0.722577	0.060502	5.159852
C	-0.146852	-1.198268	5.311535
C	0.336612	-1.884054	4.202340
C	1.866068	-2.586630	1.765425
C	2.455268	-3.304463	0.656660
C	3.704345	-3.898005	0.896306
C	4.355922	-4.593611	-0.109086
C	3.768120	-4.689876	-1.368838
C	2.524091	-4.110729	-1.612681
C	1.858848	-3.424153	-0.608621
H	-4.997489	-3.484910	0.512862
H	-6.122431	-1.209936	-2.917374
H	5.285769	-1.567025	-2.322667
H	5.316757	-0.445141	1.796151
H	-1.274099	1.616174	3.771401
H	-1.612808	4.679620	-0.984542
H	-0.957596	6.869883	-1.877364
H	1.403441	7.307062	-2.541462
H	3.093673	5.517916	-2.328823
H	3.716299	3.249319	-1.625116
H	-4.737811	1.392671	1.622570
H	0.116494	-1.870195	0.898368
H	0.068701	4.161071	1.436634
H	-0.720899	5.321586	3.441116
H	-2.978387	4.833419	4.380957
H	-4.405195	3.119011	3.316185
H	0.747304	-2.883889	4.309873
H	-0.085535	-1.657928	6.292745
H	-1.104780	0.588481	6.027762
H	-0.402589	0.398734	1.789918
H	4.160843	-3.810442	1.878298
H	5.320580	-5.051143	0.084930
H	4.279935	-5.223091	-2.164375
H	2.064533	-4.190274	-2.591637
H	0.883068	-2.994205	-0.806396
H	2.442170	-2.566105	2.690308
H	-2.549449	-0.963576	1.683615
H	-4.120852	1.780481	-1.889637
H	-7.007125	-3.299655	-2.669310
H	-3.616363	-1.506244	3.844855
H	-4.659737	-0.421661	2.910526
H	-5.043124	-2.146784	3.001414
H	-2.020067	-3.087285	2.672817
H	-3.434935	-3.872380	1.973148
H	-2.125578	-3.302396	0.908008
H	-6.273983	-5.658121	-2.488694
H	-4.884699	-4.596727	-2.809436
H	-5.155858	-5.234212	-1.181115
H	-8.272347	-4.771291	-1.142201
H	-7.197319	-4.354873	0.200815
H	-8.242181	-3.112814	-0.506468
H	-6.068770	2.622232	-3.105897
H	-6.815922	1.018228	-3.113853
H	-6.591195	1.876814	-1.581109
H	-4.004761	1.703088	-4.335108
H	-3.103756	0.339610	-3.639933
H	-4.705696	0.076865	-4.360489
H	2.278160	1.636632	1.523885
H	2.340021	0.573032	-3.131617
H	6.491222	-2.902447	-0.625156
H	2.754463	1.232609	3.826913
H	2.845291	-0.327910	3.009101
H	4.331438	0.513425	3.485716
H	3.699321	3.316666	2.681996
H	5.157507	2.507579	2.070378
H	4.035269	3.287944	0.941181
H	3.850850	1.130224	-5.023953
H	4.384593	1.960495	-3.551020
H	5.245554	0.517792	-4.112302
H	2.623594	-1.078152	-4.875626
H	4.013000	-1.808560	-4.060020
H	2.387295	-1.864844	-3.315346
H	7.836781	-3.059873	1.397582
H	7.333377	-1.457435	1.940913
H	6.156042	-2.778056	1.884339
H	8.788355	-1.931114	-0.665533
H	7.712642	-1.080319	-1.792293
H	8.120079	-0.342070	-0.236988

M1_Si_exo
SCF Energy: -3600.16489553
Num. Imaginary Frequencies: 0

C	-3.811359	4.198400	-1.386315
C	-3.295225	4.010933	-0.100090
C	-1.914576	3.868641	0.068294
C	-1.062817	3.897274	-1.030862
C	-1.586071	4.082101	-2.307368
C	-2.958732	4.241874	-2.481592
C	-4.203126	3.913727	1.048645
C	-5.464390	4.324148	1.209841

C	-5.979586	3.853567	2.544925
C	-4.669266	3.387960	3.204139
O	-3.708901	3.239358	2.145173
C	-2.678203	0.674718	1.216959
C	-3.437975	0.737360	-0.011619
C	-4.830324	0.838377	0.125359
C	-5.641138	0.917076	-0.994902
C	-5.063729	0.877457	-2.262805
C	-3.682151	0.774437	-2.405780
C	-2.863121	0.709629	-1.289294
N	-1.397994	0.759081	1.343921
C	-0.725804	0.696382	2.600974
C	0.485311	0.010264	2.663894
C	1.160882	-0.060187	3.876174
C	0.633808	0.557619	5.008453
C	-0.568932	1.255358	4.927499
C	-1.253854	1.335184	3.719531
O	0.396191	1.165798	-0.508523
P	0.727730	-0.067858	-1.315461
O	0.311600	-1.262499	-0.226923
C	0.786695	-2.530588	-0.407341
C	2.118669	-2.796732	-0.174360
C	2.610601	-4.109445	-0.462343
C	1.688755	-5.119476	-0.854013
C	0.306166	-4.810069	-0.932838
C	-0.160147	-3.539113	-0.719221
C	3.989854	-4.440491	-0.396521
C	4.423452	-5.709287	-0.683887
C	3.503956	-6.717346	-1.051738
C	2.168044	-6.424528	-1.136423
C	2.974414	-1.723597	0.398490
C	3.040224	-0.493559	-0.219824
C	3.827105	0.585411	0.272375
C	4.564325	0.365648	1.407176
C	4.465338	-0.841762	2.143476
C	3.637633	-1.891578	1.658173
C	5.118662	-0.992616	3.394545
C	4.933927	-2.118192	4.154775
C	4.081358	-3.145982	3.691874
C	3.454427	-3.038625	2.476627
C	3.759944	1.921404	-0.390015
C	3.159449	3.000649	0.292257
C	3.045954	4.225564	-0.360715
C	3.496520	4.416008	-1.664392
C	4.102206	3.343567	-2.307422
C	4.242981	2.096728	-1.698208
C	2.633926	2.889754	1.717964
C	1.198402	3.401640	1.856264
C	4.947942	0.985694	-2.462930
C	4.271096	0.689311	-3.806977
C	3.301388	5.743675	-2.372809
C	1.810422	6.011298	-2.622170
O	2.347903	-0.304159	-1.385864
C	-1.619611	-3.216619	-0.699103
C	-2.277743	-3.120270	0.542990
C	-3.657487	-2.914088	0.559004
C	-4.395295	-2.786109	-0.615651
C	-3.707862	-2.826684	-1.825069
C	-2.331518	-3.038429	-1.896188
C	-1.518919	-3.305864	1.854282
C	-2.139416	-2.571010	3.046993
C	-5.911570	-2.665208	-0.634732
C	-6.534370	-2.293726	0.711334
C	-1.648972	-3.141686	-3.252819
C	-2.036921	-2.011051	-4.210427
O	0.167645	-0.302802	-2.663314
C	-1.372965	-4.797891	2.192701
C	-6.534655	-3.970126	-1.157286
C	-1.927837	-4.516738	-3.876950
C	6.435219	1.319500	-2.647322
C	3.954893	6.906284	-1.615866
C	3.565330	3.607211	2.704284
H	2.578210	5.057006	0.161441
H	4.472510	3.482068	-3.321186
H	-4.269936	-2.700551	-2.747890
H	-4.167172	-2.865330	1.515463
H	2.102971	-0.598210	3.929129
H	4.705125	-3.671170	-0.125869
H	5.483464	-5.939776	-0.633904
H	3.860421	-7.718757	-1.273533
H	1.452133	-7.188135	-1.429707
H	-0.399162	-5.605982	-1.158893
H	5.191888	1.163299	1.795414
H	-0.743119	0.899560	0.503870
H	2.794841	-3.829769	2.138075
H	3.918177	-4.027344	4.304846
H	5.430806	-2.218944	5.115000
H	5.755879	-0.185567	3.747338
H	-2.155312	1.932389	3.626798
H	-0.968940	1.756840	5.803235
H	1.165852	0.503919	5.953140
H	0.881222	-0.462630	1.773340
H	-5.269708	0.882606	1.118386
H	-6.716730	1.004649	-0.880902
H	-5.695151	0.930243	-3.144985
H	-3.230917	0.747219	-3.390861
H	-1.791965	0.649566	-1.430168
H	-3.243585	0.539999	2.136035
H	-6.044050	4.875473	0.483264
H	-6.706557	3.036028	2.436133
H	-4.747508	2.427238	3.720553
H	-4.284098	4.136912	3.905639
H	-6.464509	4.640797	3.130759
H	2.607649	1.833728	1.994477
H	4.899192	0.069597	-1.867948
H	3.793121	5.667028	-3.351427
H	3.208680	3.474706	3.732428
H	4.589141	3.223044	2.644375
H	3.604781	4.682602	2.493717
H	0.833954	3.224660	2.874673
H	1.113296	4.475952	1.654747
H	0.558617	2.863550	1.154481
H	1.667358	6.946868	-3.174831
H	1.361830	5.195919	-3.198838
H	1.261384	6.090754	-1.676688
H	3.854956	7.840033	-2.180683
H	3.482522	7.058857	-0.638639
H	5.019889	6.717195	-1.447654
H	6.951784	0.499046	-3.158522
H	6.565851	2.226720	-3.248715
H	6.923737	1.484583	-1.680965
H	4.746848	-0.174602	-4.284845
H	3.210957	0.463764	-3.667378
H	4.358442	1.536588	-4.497378
H	-0.512735	-2.894184	1.721649
H	-0.570734	-3.050630	-3.093991
H	-6.160107	-1.868136	-1.348040
H	-1.441397	-2.578796	3.890532
H	-2.357475	-1.525824	2.811699
H	-3.068392	-3.045758	3.383443
H	-0.817524	-4.927835	3.128740
H	-2.360742	-5.257803	2.315497
H	-0.841935	-5.337261	1.404021
H	-1.404079	-4.619614	-4.833808
H	-1.598562	-5.328107	-3.219211
H	-3.000891	-4.651702	-4.060601
H	-1.517098	-2.144343	-5.165517
H	-3.113158	-1.993493	-4.421223
H	-1.724310	-1.051585	-3.793806
H	-7.607686	-2.111033	0.591634
H	-6.419864	-3.102829	1.442348
H	-6.079597	-1.391555	1.131927
H	-7.624798	-3.880606	-1.229803
H	-6.145806	-4.229036	-2.146819
H	-6.302307	-4.799702	-0.479535
H	-1.511887	3.720856	1.065033
H	0.002672	3.742217	-0.897317
H	-0.922382	4.085545	-3.166323
H	-3.370540	4.375291	-3.477669
H	-4.884907	4.271467	-1.531621

TS1_Si_exo
SCF Energy: -3600.12758267
Num. Imaginary Frequencies: 1

N	-0.763970	2.333888	0.197008
C	-0.561477	2.421444	1.578834
C	0.576750	1.797832	2.106716
C	0.833962	1.864839	3.466430
C	-0.030457	2.552787	4.318209
C	-1.167257	3.157257	3.795864
C	-1.442011	3.087808	2.433785
C	-1.914475	2.628607	-0.438039
C	-2.071686	2.042578	-1.798378
C	-3.196818	1.270484	-2.086884
C	-3.330698	0.690204	-3.344503
C	-2.349766	0.875244	-4.310136
C	-1.218983	1.632950	-4.018759
C	-1.082140	2.216578	-2.770032
C	-2.103720	4.553281	-0.890147
C	-1.830676	5.329480	0.240526
O	-2.922041	5.724989	0.885258
C	-4.094531	5.231491	0.183265
C	-3.580846	4.760646	-1.180921
H	1.711594	1.367572	3.866142
H	-2.347275	3.551081	2.058763
H	-1.857144	3.683320	4.449399
H	0.176794	2.601656	5.382575
H	1.225476	1.231921	1.445031
H	-3.945455	1.076266	-1.321548
H	-4.190737	0.065878	-3.552885
H	-2.452105	0.403161	-5.282128
H	-0.432646	1.748457	-4.757035
H	-0.180388	2.775082	-2.533838
H	-2.812204	2.590836	0.177635
H	-4.505914	4.417062	0.786549
H	-3.724229	5.524040	-1.952424
H	-4.813263	6.050121	0.148497
H	-4.078753	3.847490	-1.520186
H	-1.393373	4.561548	-1.706271
C	-0.547370	5.705000	0.794717
C	-0.474086	6.401407	2.011625
C	0.630776	5.324962	0.138177
C	0.759771	6.694116	2.565263
C	1.864459	5.625107	0.699027
C	1.929865	6.302235	1.912389
H	-1.388265	6.682165	2.522320
H	0.586764	4.787389	-0.802511
H	0.816092	7.219341	3.513034
H	2.773969	5.326217	0.189068
H	2.895949	6.526324	2.353776
H	-0.068938	1.751353	-0.336892
C	-4.226670	-1.402490	0.678531
C	-3.344657	-2.167887	-0.109722
C	-3.673740	-2.477175	-1.443719
C	-4.890519	-2.032182	-1.960578
C	-5.783033	-1.277169	-1.205092
C	-5.423431	-0.966739	0.102030
C	-2.136578	-2.791038	0.516223
C	-0.883659	-2.128289	0.637542
C	0.135685	-2.642606	1.417592

C	0.003076	-3.956031	1.972165
C	-1.217147	-4.659399	1.788527
C	-2.267701	-4.035802	1.077245
C	-1.366944	-5.959725	2.336332
C	-0.341063	-6.556221	3.019727
C	0.887455	-5.874026	3.174689
C	1.056761	-4.612186	2.665908
O	-0.716217	-0.914526	0.032042
P	0.354726	-0.749690	-1.250243
O	0.842442	0.669204	-1.100297
C	1.386246	-1.860963	1.601604
C	2.097847	-1.484411	0.484208
C	3.384357	-0.881571	0.559654
C	3.889092	-0.602301	1.803568
C	3.149254	-0.857345	2.986723
C	1.877921	-1.487452	2.891881
C	1.131585	-1.686805	4.083596
C	1.633004	-1.304921	5.301620
C	2.910997	-0.708552	5.398400
C	3.649034	-0.489819	4.263263
O	1.572474	-1.754988	-0.746703
C	4.192932	-0.642284	-0.674260
C	4.805703	-1.733356	-1.313424
C	5.610866	-1.494549	-2.427495
C	5.831921	-0.213870	-2.919474
C	5.206318	0.850133	-2.274054
C	4.379084	0.661070	-1.169936
C	4.620793	-3.166452	-0.834637
C	5.961408	-3.818816	-0.472436
C	6.726419	0.016305	-4.123853
C	5.956152	0.651724	-5.288550
C	3.698655	1.863179	-0.535739
C	3.015820	2.752401	-1.581163
C	-2.773144	-3.360459	-2.297348
C	-2.601218	-2.848021	-3.729765
C	-7.124309	-0.834075	-1.763553
C	-7.999458	-2.038264	-2.136222
C	-3.977969	-0.942684	2.116688
C	-3.453366	-1.966782	3.133404
O	-0.198453	-1.307194	-2.500309
C	3.849306	-3.998268	-1.867814
C	4.675297	2.672476	0.326309
C	7.957933	0.853994	-3.754713
C	-3.295723	-4.804732	-2.291569
C	-6.969901	0.116041	-2.957464
C	-3.094780	0.309589	2.122308
H	0.147747	-2.139003	4.017751
H	1.043153	-1.459816	6.200132
H	3.302110	-0.419834	6.369558
H	4.628168	-0.020926	4.322828
H	4.882960	-0.170390	1.889370
H	-3.224608	-4.546250	1.002888
H	2.010226	-4.109199	2.781543
H	1.708934	-6.357587	3.695217
H	-0.463086	-7.552559	3.434031
H	-2.313392	-6.475788	2.195233
H	5.358499	1.859399	-2.650120
H	6.083906	-2.337210	-2.928058
H	2.905334	1.485581	0.110582
H	4.020728	-3.150509	0.079610
H	-6.112747	-0.382810	0.711045
H	-5.153161	-2.298415	-2.981756
H	-4.964056	-0.637423	2.490837
H	-1.775236	-3.353843	-1.851669
H	-7.641147	-0.282640	-0.966632
H	-2.634189	-5.451445	-2.878695
H	-3.351511	-5.209878	-1.276057
H	-4.299459	-4.858008	-2.731520
H	-1.907269	-3.502532	-4.267655
H	-3.546104	-2.842872	-4.288217
H	-2.166064	-1.847923	-3.719631
H	-7.947287	0.481718	-3.292484
H	-6.349261	0.981556	-2.700656
H	-6.499969	-0.393828	-3.806879
H	-8.988774	-1.709805	-2.474965
H	-7.543116	-2.617443	-2.946974
H	-8.130897	-2.707566	-1.280352
H	-3.615998	-1.570079	4.142393
H	-3.975677	-2.924810	3.056133
H	-2.382563	-2.152179	3.021763
H	-2.913983	0.661755	3.143775
H	-2.127029	0.118041	1.650713
H	-3.585368	1.119830	1.568747
H	8.630126	0.957234	-4.614263
H	7.666163	1.861221	-3.434666
H	8.515064	0.390647	-2.934127
H	7.082647	-0.966703	-4.458924
H	6.600110	0.752542	-6.169795
H	5.087649	0.044263	-5.561950
H	5.593848	1.651545	-5.022537
H	5.797589	-4.820786	-0.059962
H	6.609714	-3.922963	-1.349985
H	6.499611	-3.224394	0.273722
H	3.676167	-5.011306	-1.486743
H	2.881279	-3.538713	-2.083680
H	4.409478	-4.083158	-2.806743
H	2.373553	3.479733	-1.072377
H	3.737911	3.312245	-2.188129
H	2.384332	2.145148	-2.232620
H	4.156305	3.499256	0.826952
H	5.133896	2.050048	1.101217
H	5.483066	3.093611	-0.284753

M2_Si_exo
SCF Energy: -3600.15287136

Num. Imaginary Frequencies: 0

N	-0.687910	2.914733	-0.094892
C	-0.960029	3.525149	1.118946
C	-0.634667	2.815109	2.287671
C	-0.842366	3.377830	3.534768
C	-1.375017	4.661410	3.660477
C	-1.701828	5.364290	2.508214
C	-1.503625	4.808687	1.245967
C	-0.913573	3.475260	-1.390984
C	-2.155148	2.905230	-2.055436
C	-3.318254	3.670927	-2.106328
C	-4.502274	3.117735	-2.590061
C	-4.526739	1.794465	-3.016481
C	-3.364374	1.027077	-2.972279
C	-2.181923	1.584045	-2.507533
C	0.382342	3.245524	-2.290329
C	1.406195	4.203518	-1.826180
O	1.546560	5.217707	-2.628699
C	0.648559	5.096855	-3.777262
C	0.220582	3.637457	-3.765539
H	-0.575125	2.808463	4.420083
H	-1.804529	5.377103	0.372013
H	-2.132087	6.359346	2.582644
H	-1.535938	5.100449	4.639768
H	-0.215408	1.816619	2.194764
H	-3.309310	4.696756	-1.743680
H	-5.406470	3.718861	-2.619533
H	-5.454296	1.353433	-3.369162
H	-3.373653	-0.018825	-3.262248
H	-1.289071	0.969261	-2.483915
H	-1.056058	4.554320	-1.277837
H	-0.170826	5.798193	-3.599289
H	0.885332	3.029323	-4.384840
H	1.222219	5.414293	-4.647121
H	-0.801525	3.500833	-4.120860
H	0.676696	2.198591	-2.139272
C	2.126515	4.195526	-0.599134
C	2.757084	5.374240	-0.137635
C	2.133815	3.026204	0.187866
C	3.349486	5.385995	1.106855
C	2.730140	3.059798	1.441157
C	3.323660	4.229153	1.898447
H	2.743784	6.267214	-0.753129
H	1.698916	2.102469	-0.187169
H	3.819729	6.289992	1.478746
H	2.727477	2.170638	2.058987
H	3.776798	4.242861	2.885251
H	-0.592894	1.902979	-0.076885
C	-4.653842	-0.485944	0.021270
C	-3.641805	-1.450220	0.159914
C	-3.545690	-2.516113	-0.765598
C	-4.467429	-2.588532	-1.806514
C	-5.494655	-1.659191	-1.950980
C	-5.567657	-0.626383	-1.027091
C	-2.716592	-1.489231	1.338138
C	-1.370797	-1.023121	1.278031
C	-0.450339	-1.290137	2.275249
C	-0.858612	-2.078771	3.405528
C	-2.227063	-2.436349	3.533210
C	-3.121252	-2.131026	2.478466
C	-2.660860	-3.171787	4.665828
C	-1.770504	-3.578629	5.623975
C	-0.398530	-3.281483	5.470169
C	0.045183	-2.556769	4.393445
O	-1.016083	-0.240593	0.215041
P	0.062047	-0.725758	-0.967394
O	0.877307	0.518892	-1.197902
C	0.975827	-0.897143	2.113465
C	1.643354	-1.267797	0.963734
C	3.055480	-1.174146	0.820967
C	3.768060	-0.615633	1.849554
C	3.125075	-0.076958	2.993563
C	1.714471	-0.202973	3.127113
C	1.087393	0.405201	4.247583
C	1.819053	1.094586	5.180383
C	3.223279	1.200596	5.056886
C	3.858599	0.620554	3.989520
O	0.940720	-1.807768	-0.076620
C	3.733659	-1.725806	-0.390964
C	3.794001	-3.117992	-0.579508
C	4.486946	-3.616579	-1.682420
C	5.123492	-2.784971	-2.596080
C	5.036829	-1.409890	-2.396179
C	4.339101	-0.861164	-1.322981
C	3.129310	-4.105874	0.369873
C	4.153930	-5.057300	1.001802
C	5.876822	-3.361724	-3.780660
C	5.280800	-2.890860	-5.113629
C	4.233473	0.652023	-1.206260
C	3.724100	1.288167	-2.505227
C	-2.526090	-3.640214	-0.598361
C	-2.015488	-4.215937	-1.923223
C	-6.503487	-1.772914	-3.079466
C	-7.322351	-3.066252	-2.970830
C	-4.864412	0.713307	0.941854
C	-5.594862	0.336323	2.239050
O	-0.613218	-1.444014	-2.067600
C	2.006024	-4.878870	-0.336303
C	5.556194	1.288333	-0.763365
C	7.375076	-3.039827	-3.703409
C	-3.115002	-4.766422	0.266599
C	-5.836063	-1.666338	-4.457375
C	-3.603904	1.529302	1.231237
H	0.009872	0.327331	4.350636
H	1.316497	1.562144	6.022015

H	3.793335	1.740035	5.807476
H	4.936803	0.702528	3.876088
H	4.850988	-0.556594	1.777179
H	-4.146766	-2.485524	2.546141
H	1.105002	-2.359232	4.287237
H	0.315572	-3.637796	6.206735
H	-2.110355	-4.145463	6.485492
H	-3.716007	-3.419951	4.749066
H	5.516976	-0.740635	-3.106738
H	4.532556	-4.692923	-1.835383
H	3.488193	0.864818	-0.438874
H	2.670723	-3.547153	1.190260
H	-6.357409	0.116310	-1.128122
H	-4.389981	-3.404739	-2.519071
H	-5.536001	1.380638	0.386042
H	-1.651948	-3.238275	-0.078400
H	-7.202008	-0.930406	-2.981406
H	-2.376030	-5.564411	0.403170
H	-3.413057	-4.410200	1.256638
H	-3.998309	-5.199229	-0.218803
H	-1.180848	-4.896720	-1.721314
H	-2.786581	-4.799669	-2.441389
H	-1.653566	-3.418759	-2.574220
H	-6.584705	-1.727270	-5.255614
H	-5.296473	-0.720080	-4.569139
H	-5.115384	-2.477504	-4.609806
H	-8.091247	-3.106449	-3.750785
H	-6.680410	-3.946891	-3.087003
H	-7.814457	-3.138038	-1.995719
H	-5.870651	1.241168	2.793336
H	-6.509037	-0.229694	2.029044
H	-4.956556	-0.269992	2.888753
H	-3.870727	2.494457	1.676415
H	-2.937852	1.023869	1.935127
H	-3.048571	1.718513	0.309961
H	7.914683	-3.504240	-4.536726
H	7.545954	-1.958169	-3.754777
H	7.808043	-3.403796	-2.766135
H	5.767769	-4.453129	-3.735448
H	5.784498	-3.378426	-5.956192
H	4.212111	-3.119793	-5.169488
H	5.398127	-1.807961	-5.237208
H	3.662973	-5.716865	1.726185
H	4.633608	-5.691429	0.247424
H	4.940776	-4.500536	1.522045
H	1.486608	-5.529449	0.376752
H	1.277614	-4.188553	-0.769778
H	2.404218	-5.511638	-1.138415
H	3.585656	2.367474	-2.359169
H	4.435214	1.163559	-3.329782
H	2.766152	0.844325	-2.787360
H	5.432344	2.369101	-0.622101
H	5.908891	0.861208	0.181185
H	6.340988	1.130722	-1.512978

TS2_Si_exo

SCF Energy: -3600.13606991

Num. Imaginary Frequencies: 1

N	-1.126998	2.633780	-0.208591
C	-0.838232	3.348318	0.892075
C	-0.286911	2.706386	2.031254
C	0.177603	3.463223	3.070000
C	0.070323	4.882651	3.063899
C	-0.520136	5.510259	2.003643
C	-0.930113	4.765227	0.866054
C	-1.224019	3.298463	-1.476670
C	-1.630922	2.299499	-2.549683
C	-2.806538	1.577563	-2.330018
C	-3.230483	0.627322	-3.247931
C	-2.495445	0.395670	-4.405084
C	-1.325422	1.108151	-4.629718
C	-0.891376	2.052062	-3.704244
C	0.117072	4.056127	-1.781918
C	0.685804	4.929704	-0.676226
O	0.570343	6.223365	-0.983654
C	-0.286797	6.382123	-2.127453
C	-0.086217	5.090942	-2.906717
H	0.651418	2.962929	3.909373
H	-1.601851	5.240825	0.159936
H	-0.640873	6.589001	1.991767
H	0.435435	5.450755	3.912666
H	-0.180610	1.625933	2.024217
H	-3.373420	1.725752	-1.414308
H	-4.120065	0.046824	-3.036860
H	-2.819149	-0.360676	-5.113245
H	-0.727428	0.912718	-5.514376
H	0.048920	2.562594	-3.886667
H	-2.017157	4.055527	-1.419155
H	-1.318434	6.511301	-1.778388
H	0.807439	5.158488	-3.533834
H	0.033820	7.289598	-2.638665
H	-0.937190	4.845923	-3.545433
H	0.847153	3.282636	-2.029510
C	1.857454	4.592805	0.139238
C	2.561799	5.617462	0.788315
C	2.262759	3.261348	0.297992
C	3.663561	5.316698	1.575683
C	3.356469	2.972176	1.103154
C	4.058088	3.991094	1.738914
H	2.242619	6.646418	0.666589
H	1.725507	2.441808	-0.178993
H	4.207210	6.116502	2.068787
H	3.654188	1.939014	1.233045
H	4.911745	3.749072	2.364876
H	-0.704472	1.699512	-0.279866
C	-4.738536	-0.285461	0.718522
C	-3.867251	-1.338293	0.386177
C	-4.083810	-2.090363	-0.786963
C	-5.198045	-1.808467	-1.574639
C	-6.085425	-0.781558	-1.261746
C	-5.822168	-0.025293	-0.126597
C	-2.774786	-1.756804	1.320474
C	-1.433819	-1.292362	1.185887
C	-0.448113	-1.630510	2.094618
C	-0.745030	-2.589800	3.121186
C	-2.075963	-3.067313	3.255346
C	-3.064182	-2.616735	2.346263
C	-2.389533	-4.002000	4.274705
C	-1.419956	-4.472814	5.120264
C	-0.086751	-4.032912	4.965305
C	0.242551	-3.120868	3.995232
O	-1.181721	-0.408438	0.183820
P	-0.054927	-0.648992	-1.044804
O	0.641157	0.686905	-1.069929
C	0.935595	-1.100754	1.956526
C	1.609827	-1.307596	0.774189
C	3.014874	-1.124159	0.641627
C	3.690505	-0.574683	1.699203
C	3.013164	-0.158068	2.877594
C	1.624074	-0.430498	3.018835
C	0.964925	0.006381	4.198551
C	1.649535	0.674070	5.183851
C	3.031709	0.935093	5.046292
C	3.693879	0.523803	3.918188
O	0.922693	-1.770774	-0.307144
C	3.703663	-1.645514	-0.579629
C	3.921037	-3.033645	-0.684767
C	4.551962	-3.530205	-1.821660
C	4.984080	-2.697109	-2.851380
C	4.760890	-1.332043	-2.721822
C	4.116709	-0.787484	-1.610320
C	3.468303	-4.011026	0.392397
C	4.622117	-4.891195	0.889944
C	5.666108	-3.262183	-4.083451
C	6.958619	-4.008077	-3.726924
C	3.914284	0.715122	-1.525763
C	3.267091	1.310826	-2.780338
C	-3.171826	-3.250482	-1.164177
C	-2.934341	-3.368978	-2.672638
C	-7.310632	-0.504616	-2.115508
C	-8.265602	-1.706115	-2.114499
C	-4.647430	0.588298	1.970049
C	-5.301856	-0.080432	3.188046
O	-0.660768	-1.303010	-2.218933
C	2.287130	-4.859705	-0.098394
C	5.240447	1.415740	-1.202731
C	4.714778	-4.160017	-4.885401
C	-3.726803	-4.565732	-0.596702
C	-6.941083	-0.100174	-3.548428
C	-3.251606	1.118478	2.315650
H	-0.096959	-0.188980	4.310024
H	1.125635	1.001319	6.077483
H	3.564386	1.458605	5.834653
H	4.757213	0.719397	3.800107
H	4.768724	-0.445249	1.635562
H	-4.082116	-2.982859	2.456241
H	1.274890	-2.810333	3.882781
H	0.688240	-4.426492	5.616524
H	-1.668087	-5.192505	5.894450
H	-3.416787	-4.346783	4.364184
H	5.093289	-0.668648	-3.517551
H	4.706104	-4.603374	-1.909462
H	3.213491	0.895767	-0.709715
H	3.117614	-3.436642	1.254690
H	-6.502067	0.785235	0.132825
H	-5.375511	-2.408064	-2.463346
H	-5.257024	1.471504	1.737787
H	-2.191989	-3.071494	-0.712535
H	-7.840451	0.341773	-1.658803
H	-3.060072	-5.399433	-0.843871
H	-3.829323	-4.523501	0.492338
H	-4.714528	-4.780677	-1.022854
H	-2.168796	-4.129286	-2.859004
H	-3.839995	-3.678076	-3.209589
H	-2.561970	-2.425329	-3.076405
H	-7.842856	0.118378	-4.131754
H	-6.303088	0.789461	-3.557783
H	-6.400758	-0.906185	-4.058964
H	-9.181013	-1.475831	-2.671474
H	-7.797953	-2.579215	-2.583694
H	-8.543350	-1.984204	-1.092788
H	-5.363436	0.629676	4.021247
H	-6.314852	-0.424463	2.954073
H	-4.715547	-0.940711	3.524673
H	-3.336326	2.003081	2.957381
H	-2.650482	0.380249	2.853670
H	-2.712284	1.398719	1.408094
H	5.196834	-4.513945	-5.803923
H	4.420448	-5.039455	-4.300869
H	3.802005	-3.620848	-5.157104
H	5.939716	-2.412698	-4.723358
H	7.471675	-4.347699	-4.633846
H	7.641721	-3.364568	-3.163203
H	6.748051	-4.891634	-3.113281
H	4.285220	-5.523003	1.719551
H	4.995398	-5.555265	0.102118
H	5.461314	-4.281246	1.241024
H	1.926541	-5.513516	0.704078
H	1.462193	-4.221383	-0.425821
H	2.585275	-5.493173	-0.942573

H	3.091777	2.383557	-2.620798
H	3.908291	1.213807	-3.664304
H	2.304278	0.832889	-2.975738
H	5.094788	2.496600	-1.095665
H	5.672392	1.036139	-0.269401
H	5.974819	1.245969	-1.999154

M3_Si_exo
SCF Energy: -3600.17360669
Num. Imaginary Frequencies: 0

C	3.756957	-1.776346	-0.450047
C	2.826283	-2.670791	0.116465
C	3.005714	-3.144322	1.429502
C	4.112386	-2.700080	2.155744
C	5.042270	-1.813664	1.622308
C	4.847279	-1.368525	0.317286
C	1.651329	-3.118677	-0.695576
C	0.492273	-2.299477	-0.789262
C	-0.570559	-2.607779	-1.614718
C	-0.575420	-3.865312	-2.297769
C	0.563740	-4.709111	-2.192199
C	1.664851	-4.293340	-1.402781
C	0.576540	-5.953285	-2.874232
C	-0.502020	-6.360597	-3.614110
C	-1.649230	-5.538741	-3.693334
C	-1.686491	-4.326443	-3.054121
O	0.470791	-1.129210	-0.085143
P	-0.550769	-0.981049	1.239055
O	-0.103222	-1.807944	2.376137
C	-1.699268	-1.647202	-1.734668
C	-2.351241	-1.232330	-0.592088
C	-3.501585	-0.393913	-0.617941
C	-3.937380	0.054764	-1.837698
C	-3.242999	-0.245601	-3.037106
C	-2.103651	-1.096213	-2.992830
C	-1.377214	-1.312928	-4.194544
C	-1.775609	-0.737335	-5.374667
C	-2.927876	0.080491	-5.423013
C	-3.643373	0.317849	-4.277196
O	-1.910680	-1.683724	0.618459
C	-4.231054	-0.061218	0.642224
C	-4.977452	-1.062983	1.286569
C	-5.687227	-0.735431	2.441463
C	-5.682440	0.548753	2.971681
C	-4.934633	1.523299	2.315895
C	-4.196790	1.245123	1.167708
C	-5.059376	-2.488695	0.758891
C	-4.486255	-3.496031	1.763748
C	-6.454876	0.873012	4.237164
C	-5.511576	1.292095	5.372660
C	-3.396314	2.367704	0.520977
C	-2.523386	3.118049	1.532984
C	2.076557	-4.191632	2.030349
C	2.665507	-5.592474	1.798531
C	6.232475	-1.316391	2.424939
C	6.986693	-2.450509	3.128775
C	3.614210	-1.300283	-1.893032
C	4.102385	-2.367167	-2.887008
O	-0.740637	0.514410	1.293500
C	-6.497229	-2.846914	0.358496
C	-4.314640	3.339068	-0.233322
C	-7.530463	1.939074	3.991604
C	1.777680	-3.983481	3.517576
C	5.810855	-0.234670	3.428977
C	4.361518	0.005009	-2.187603
N	1.189609	1.828631	0.080148
C	2.462645	2.235028	0.673226
C	2.714096	3.723111	0.368072
C	2.432758	4.095557	-1.123246
C	1.981928	2.821489	-1.935009
C	0.943715	2.066288	-1.174508
O	3.663119	4.526953	-1.674521
C	4.725746	4.038711	-0.872780
C	4.192038	4.105272	0.552981
C	1.624536	3.135540	-3.346031
C	0.469762	2.721936	-3.886961
C	-0.483141	1.962951	-3.100247
C	-0.273717	1.645584	-1.800710
C	2.490651	1.836062	2.136939
C	2.376469	0.476402	2.434810
C	2.329390	0.045251	3.753099
C	2.438203	0.966355	4.790253
C	2.585611	2.318853	4.501873
C	2.601608	2.755466	3.179558
H	-6.263476	-1.508183	2.946269
H	-4.915625	2.532053	2.721185
H	5.581303	-0.687796	-0.106296
H	4.249913	-3.062712	3.170084
C	1.394764	5.196940	-1.290943
H	-1.402926	1.640806	-3.578713
H	-2.579358	-3.713636	-3.111754
H	-2.512771	-5.874827	-4.259612
H	-0.484683	-7.316994	-4.127825
H	1.458744	-6.582910	-2.789215
H	2.543578	-4.931774	-1.356661
H	-4.829399	0.673501	-1.888156
H	0.464451	1.299819	0.655201
H	-0.488298	-1.933757	-4.167080
H	-1.202070	-0.911579	-6.280199
H	-3.239797	0.522073	-6.364755
H	-4.523580	0.955695	-4.297069
H	2.875879	2.179645	-1.957733
H	2.352386	3.709716	-3.909907
H	0.226375	2.944917	-4.920145
H	-0.981986	1.069054	-1.217639
H	2.305569	-0.256454	1.634828
H	2.201881	-1.011662	3.954580
H	2.404256	0.630739	5.822427
H	2.673618	3.043699	5.305649
H	2.702900	3.817731	2.980172
H	3.242480	1.645944	0.166491
H	4.982606	3.005753	-1.156086
H	4.276117	5.125041	0.938329
H	5.595516	4.671702	-1.058225
H	4.716439	3.433983	1.238478
H	2.060015	4.318559	1.006889
H	-2.718141	1.918322	-0.207414
H	-3.724310	4.115031	-0.736252
H	-4.911555	2.822906	-0.992435
H	-5.010217	3.833479	0.455119
H	-1.920174	3.872146	1.012940
H	-3.123482	3.652670	2.277833
H	-1.853536	2.422762	2.043384
H	-4.453780	-2.558741	-0.148942
H	-6.533056	-3.849837	-0.081863
H	-7.169225	-2.838449	1.224452
H	-6.888396	-2.135139	-0.376588
H	-4.502200	-4.505559	1.337253
H	-3.452988	-3.243307	2.015556
H	-5.074005	-3.515186	2.689096
H	-6.965244	-0.046548	4.552230
H	-6.069808	1.454738	6.301754
H	-4.752272	0.525163	5.554175
H	-4.990957	2.224820	5.126638
H	-8.108574	2.121465	4.904620
H	-7.079716	2.890700	3.686935
H	-8.221534	1.627076	3.201952
H	2.548572	-1.122120	-2.082449
H	6.928612	-0.853569	1.712019
H	1.117345	-4.127175	1.509705
H	6.684977	0.161995	3.958483
H	5.298386	0.595493	2.931477
H	5.117273	-0.642192	4.172299
H	7.892286	-2.064292	3.609462
H	6.373660	-2.914185	3.909468
H	7.278405	-3.231905	2.419933
H	1.986107	-6.361122	2.183500
H	2.835474	-5.791766	0.736042
H	3.627044	-5.696862	2.315873
H	1.068632	-4.747892	3.853623
H	2.674407	-4.079140	4.141746
H	1.309564	-3.010664	3.675283
H	4.024058	0.426540	-3.141226
H	4.204889	0.749141	-1.400584
H	5.442435	-0.156438	-2.268595
H	4.005510	-2.003402	-3.916671
H	5.158536	-2.595842	-2.703055
H	3.532003	-3.293725	-2.802220
C	1.663196	6.310022	-2.086046
C	0.689921	7.287195	-2.277161
C	-0.560773	7.161566	-1.681200
C	-0.832780	6.054264	-0.882615
C	0.139993	5.080964	-0.687253
H	2.638302	6.408727	-2.548606
H	0.913597	8.151509	-2.895644
H	-1.318204	7.924698	-1.832378
H	-1.800820	5.946202	-0.401920
H	-0.087617	4.231547	-0.050322

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SCF Energy: -3600.16416818
Num. Imaginary Frequencies: 0

C	2.502223	-5.134504	-0.461975
C	3.956566	-4.749413	-0.444850
C	4.189064	-3.915268	0.570229
O	3.077936	-3.650718	1.332460
C	1.980211	-4.422403	0.803860
C	2.295776	-1.058530	0.458909
C	2.744172	-1.332392	-0.890637
C	4.097843	-1.098659	-1.163951
C	4.622610	-1.387872	-2.414084
C	3.795793	-1.914246	-3.401775
C	2.447017	-2.152420	-3.138311
C	1.915053	-1.868189	-1.890342
N	1.072695	-1.099267	0.872030
C	0.686856	-0.905691	2.229706
C	-0.433748	-0.120439	2.494312
C	-0.817369	0.089227	3.813025
C	-0.092438	-0.490477	4.852919
C	1.011008	-1.292885	4.573392
C	1.404582	-1.513131	3.257166
O	-0.932445	-1.291334	-0.791422
P	-1.137709	0.028993	-1.506115
O	-0.398566	1.071314	-0.427734
C	-0.667961	2.408306	-0.496475
C	-1.910976	2.873725	-0.124362
C	-2.214048	4.255465	-0.333869
C	-1.187024	5.123233	-0.797322
C	0.120743	4.608091	-0.991315
C	0.400792	3.275119	-0.836774
C	-3.510926	4.793043	-0.121908
C	-3.766660	6.121198	-0.347546
C	-2.741350	6.985656	-0.793748
C	-1.481383	6.493625	-1.013778
C	-2.849140	1.930253	0.537697
C	-3.182611	0.745227	-0.083050
C	-4.036827	-0.223528	0.512381
C	-4.554510	0.058091	1.750013
C	-4.180709	1.215828	2.475707
C	-3.294761	2.155886	1.881843

C	-4.626504	1.420250	3.807262
C	-4.187136	2.492010	4.539838
C	-3.274968	3.406819	3.965958
C	-2.842607	3.246431	2.673811
C	-4.341480	-1.519413	-0.163473
C	-3.784723	-2.712492	0.341288
C	-4.140071	-3.918813	-0.255050
C	-5.005414	-3.980282	-1.345503
C	-5.518885	-2.787657	-1.839597
C	-5.204350	-1.553350	-1.269314
C	-2.806946	-2.722648	1.509684
C	-1.580590	-3.602391	1.239999
C	-5.822582	-0.291971	-1.853429
C	-5.399910	-0.082320	-3.312604
C	-5.354893	-5.307775	-1.992961
C	-4.123096	-5.940989	-2.654076
O	-2.702053	0.504276	-1.342797
C	1.807879	2.770290	-0.870716
C	2.505217	2.630410	0.346135
C	3.863838	2.310382	0.307456
C	4.538045	2.114699	-0.894788
C	3.804046	2.185828	-2.075897
C	2.446145	2.499999	-2.090945
C	1.818721	2.863684	1.689879
C	2.438113	2.072088	2.847233
C	6.034257	1.851696	-0.968433
C	6.660710	1.380238	0.345225
C	1.693371	2.578806	-3.410138
C	1.970933	1.376002	-4.316389
O	-0.718208	0.257095	-2.902361
C	1.796045	4.356719	2.054164
C	6.763513	3.104101	-1.480091
C	2.003450	3.899914	-4.126798
C	-7.349881	-0.305169	-1.703268
C	-6.004491	-6.277305	-0.997219
C	-3.484269	-3.149280	2.818540
H	-3.718387	-4.841486	0.136533
H	-6.189699	-2.819892	-2.695934
H	4.311875	1.989620	-3.017808
H	4.406297	2.225563	1.243242
H	-1.684119	0.709422	4.021866
H	-4.306116	4.133274	0.209420
H	-4.767043	6.512623	-0.188574
H	-2.956454	8.035708	-0.967084
H	-0.686501	7.147558	-1.363609
H	0.925042	5.295402	-1.242463
H	-5.238186	-0.649989	2.209835
H	0.261503	-1.209998	0.175448
H	-2.135606	3.951813	2.251730
H	-2.910002	4.243364	4.554393
H	-4.528407	2.635884	5.560618
H	-5.312663	0.696942	4.240632
H	2.228807	-2.178095	3.017904
H	1.560850	-1.764298	5.382040
H	-0.394727	-0.325355	5.882380
H	-0.976591	0.331597	1.673152
H	4.741123	-0.700540	-0.387540
H	5.674443	-1.207389	-2.611665
H	4.201271	-2.136844	-4.384293
H	1.798381	-2.546012	-3.913509
H	0.860951	-2.046752	-1.702492
H	3.057498	-0.807245	1.193846
H	4.686318	-5.087904	-1.166411
C	5.406399	-3.202943	0.976123
H	2.350703	-6.218282	-0.409441
H	1.660014	-5.119756	1.582752
H	1.160090	-3.730782	0.597714
H	2.000363	-4.776632	-1.368597
H	-2.434766	-1.704129	1.641167
H	-5.454435	0.567285	-1.285729
H	-6.088820	-5.103049	-2.783340
H	-2.762609	-3.129990	3.643694
H	-4.314798	-2.487204	3.080927
H	-3.883198	-4.167484	2.735532
H	-0.831542	-3.436195	2.024683
H	-1.827177	-4.671016	1.247606
H	-1.146194	-3.346671	0.270730
H	-4.391840	-6.870232	-3.169628
H	-3.675251	-5.256881	-3.381663
H	-3.359028	-6.180232	-1.905271
H	-6.306495	-7.203028	-1.500107
H	-5.307039	-6.546722	-0.195709
H	-6.890557	-5.831101	-0.534535
H	-7.780537	0.629897	-2.079070
H	-7.799694	-1.130650	-2.267036
H	-7.639368	-0.419919	-0.653148
H	-5.812639	0.857817	-3.696119
H	-4.310680	-0.038980	-3.395921
H	-5.765000	-0.892083	-3.955343
H	0.780064	2.527583	1.597375
H	0.622668	2.550185	-3.188554
H	6.182988	1.057361	-1.713958
H	1.767102	2.094912	3.712230
H	2.600549	1.022004	2.589266
H	3.398524	2.495943	3.163413
H	1.298651	4.505707	3.019600
H	2.818474	4.744720	2.134757
H	1.264773	4.947897	1.304350
H	1.449593	3.964619	-5.069851
H	1.726517	4.762091	-3.510608
H	3.073725	3.980012	-4.354274
H	1.345852	1.440184	-5.213032
H	3.018064	1.331377	-4.641185
H	1.714238	0.447988	-3.802069
H	7.705097	1.093970	0.182731
H	6.652760	2.177457	1.097657
H	6.144168	0.513725	0.771308
H	7.835326	2.910681	-1.603555
H	6.360308	3.433391	-2.442695
H	6.644064	3.928609	-0.767834
C	5.462152	-2.529693	2.200386
C	6.607195	-1.829318	2.570048
C	7.709664	-1.791598	1.722661
C	7.658915	-2.454574	0.497201
C	6.517675	-3.151236	0.125477
H	4.609044	-2.566713	2.869196
H	6.636102	-1.312929	3.524744
H	8.600507	-1.241066	2.008793
H	8.510982	-2.421887	-0.175189
H	6.475824	-3.640317	-0.842673

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SCF Energy: -3600.13949872

Num. Imaginary Frequencies: 1

C	2.141595	-3.497446	0.136173
C	0.943528	-3.564672	-0.605253
C	0.996271	-3.708931	-2.004082
C	2.241873	-3.828896	-2.625355
C	3.433988	-3.808618	-1.909053
C	3.358101	-3.631973	-0.530112
C	-0.369548	-3.588302	0.112383
C	-1.327775	-2.542912	-0.016009
C	-2.576126	-2.602157	0.578294
C	-2.837518	-3.660092	1.511398
C	-1.890841	-4.710241	1.651027
C	-0.690226	-4.662182	0.902930
C	-2.152083	-5.775174	2.552061
C	-3.290911	-5.788451	3.312811
C	-4.216378	-4.725450	3.206363
C	-3.998242	-3.692782	2.331160
O	-1.008825	-1.513938	-0.857130
P	-0.818111	0.033003	-0.318048
O	-0.999808	0.904182	-1.508128
C	-3.612396	-1.580941	0.261716
C	-3.303362	-0.243308	0.362609
C	-4.238456	0.802211	0.134791
C	-5.527196	0.444668	-0.163147
C	-5.899577	-0.911336	-0.351138
C	-4.928928	-1.938191	-0.183668
C	-5.305063	-3.272724	-0.493038
C	-6.580943	-3.572099	-0.896939
C	-7.555589	-2.556514	-1.016334
C	-7.216095	-1.255301	-0.754188
O	-2.045392	0.112300	0.763992
C	-3.778657	2.223396	0.146843
C	-3.333539	2.828534	1.337405
C	-2.854749	4.136272	1.295929
C	-2.808607	4.868465	0.113472
C	-3.282818	4.260192	-1.043047
C	-3.743964	2.943891	-1.062867
C	-3.371169	2.112824	2.680027
C	-4.376507	2.783254	3.626787
C	-2.275899	6.289407	0.074417
C	-3.300086	7.273602	0.656335
C	-4.176286	2.346324	-2.396434
C	-5.507140	2.954041	-2.860374
C	-0.254201	-3.764447	-2.869695
C	-0.366234	-5.107329	-3.604254
C	4.774452	-3.937229	-2.610084
C	5.590223	-5.117410	-2.067273
C	2.162058	-3.277322	1.643169
C	2.599714	-4.545997	2.387775
O	0.411661	0.159845	0.544097
C	-1.977528	2.021807	3.315760
C	-3.097315	2.490803	-3.476932
C	-0.919311	6.431202	0.775833
C	-0.308299	-2.580798	-3.844624
C	5.578027	-2.631204	-2.526210
C	3.051353	-2.092424	2.033400
N	2.242780	2.129660	0.903826
C	2.828275	1.744028	2.129380
C	2.025352	1.012269	3.012238
C	2.520957	0.640411	4.253316
C	3.819308	0.976050	4.629882
C	4.614219	1.703101	3.750576
C	4.124850	2.098242	2.510153
C	2.821556	2.901491	-0.024244
C	2.014634	3.762412	-0.918175
C	2.632123	4.908004	-1.438942
C	1.935838	5.765305	-2.278604
C	0.616820	5.473851	-2.624582
C	0.003339	4.334854	-2.115802
C	0.687765	3.486321	-1.252051
C	3.720447	1.758534	-1.563114
C	4.530088	0.896511	-0.835722
O	4.000624	-0.288195	-0.644779
C	2.750342	-0.404347	-1.403368
C	2.638210	0.903240	-2.195222
H	4.278562	-3.586758	0.046981
H	2.282512	-3.953642	-3.705790
H	-3.268952	4.826776	-1.972469
H	-2.503675	4.594369	2.217528
H	1.886195	0.070237	4.924706
H	-4.565752	-4.061828	-0.416631
H	-6.841915	-4.599694	-1.132257
H	-8.564706	-2.807210	-1.329550
H	-7.948687	-0.459865	-0.866029
H	-6.273995	1.219212	-0.318301
H	0.010971	-5.488590	0.982821
H	1.366604	1.619876	0.684876

H	-4.713826	-2.880828	2.268863
H	-5.106762	-4.723386	3.828239
H	-3.478719	-6.602283	4.006794
H	-1.419073	-6.573629	2.637010
H	4.776944	2.664899	1.856133
H	5.630796	1.970736	4.022762
H	4.207094	0.674792	5.597946
H	1.030813	0.714017	2.697804
H	3.664749	5.130136	-1.176085
H	2.419931	6.657188	-2.664434
H	0.069445	6.135790	-3.288960
H	-1.019432	4.090381	-2.374357
H	0.165346	2.606783	-0.889034
H	3.750147	3.365435	0.296096
H	4.136632	2.612592	-2.082245
C	5.813220	1.153691	-0.184975
H	2.843727	0.753618	-3.260815
H	2.841641	-1.300643	-2.013371
H	1.956564	-0.529487	-0.667815
H	1.631406	1.323947	-2.116434
H	1.146638	-3.030563	1.964430
H	-1.129129	-3.686905	-2.220472
H	4.572483	-4.134158	-3.671089
H	2.565047	-4.385894	3.471295
H	1.954821	-5.397581	2.149611
H	3.626979	-4.821706	2.120084
H	2.995596	-1.918795	3.112740
H	4.103968	-2.273187	1.784740
H	2.728715	-1.178386	1.530249
H	6.538432	-2.733014	-3.044188
H	5.030930	-1.799445	-2.983210
H	5.781010	-2.360863	-1.483796
H	6.525428	-5.231527	-2.626773
H	5.849667	-4.967023	-1.013092
H	5.026815	-6.052677	-2.142728
H	-1.309538	-5.157919	-4.159361
H	0.450074	-5.246116	-4.322635
H	-0.339529	-5.943501	-2.897568
H	-1.239591	-2.609077	-4.421280
H	-0.275581	-1.630633	-3.304572
H	0.525190	-2.612408	-4.557250
H	-3.721290	1.089942	2.517627
H	-4.329619	1.274291	-2.255576
H	-2.125721	6.546750	-0.982958
H	-2.017757	1.429087	4.236933
H	-1.277010	1.543757	2.626539
H	-1.587969	3.013060	3.576390
H	-4.437747	2.235781	4.574300
H	-4.083415	3.815132	3.853364
H	-5.375900	2.810450	3.179885
H	-5.839865	2.487024	-3.794304
H	-6.293872	2.818007	-2.110351
H	-5.403773	4.031189	-3.039417
H	-3.411904	1.970277	-4.388909
H	-2.927815	3.540990	-3.747442
H	-2.159979	2.048809	-3.128776
H	-0.517639	7.440189	0.628565
H	-1.010763	6.267796	1.855784
H	-0.194013	5.711343	0.384709
H	-2.940259	8.306002	0.575493
H	-4.258644	7.198968	0.132730
H	-3.480462	7.059488	1.716403
C	6.347714	0.205044	0.694279
C	7.529821	0.474496	1.369301
C	8.187306	1.687467	1.172787
C	7.666000	2.630406	0.288921
C	6.484551	2.364778	-0.390902
H	5.812248	-0.722581	0.862505
H	7.933920	-0.258793	2.059786
H	9.110014	1.897157	1.705118
H	8.181285	3.572103	0.128988
H	6.084936	3.100819	-1.082323

M2_Si_endo

SCF Energy: -3600.16061931

Num. Imaginary Frequencies: 0

C	6.400337	1.321848	-0.111133
C	5.486759	0.273917	0.074524
C	5.699271	-0.672530	1.088483
C	6.803662	-0.560409	1.915612
C	7.708618	0.484260	1.728573
C	7.511196	1.419486	0.714634
C	4.327548	0.137622	-0.779975
C	3.705996	1.167369	-1.674623
C	2.580024	0.376146	-2.382537
C	2.618321	-1.021713	-1.761573
O	3.770742	-1.002058	-0.844874
C	3.285236	2.330070	-0.742154
C	2.605333	3.465334	-1.483883
C	3.402030	4.519184	-1.939962
C	2.850950	5.573857	-2.657036
C	1.486094	5.576180	-2.930879
C	0.690454	4.528932	-2.479337
C	1.236680	3.476881	-1.748396
N	2.613125	1.722963	0.382266
C	2.417797	2.453848	1.562001
C	1.632714	1.877189	2.572708
C	1.457619	2.532894	3.780588
C	2.049191	3.775208	4.012990
C	2.815106	4.353048	3.008811
C	3.002840	3.705412	1.789515
O	0.586289	-0.257960	0.411062
P	-0.636774	-0.158672	-0.458487
O	-1.884966	0.125417	0.569562
C	-3.168750	-0.054012	0.122739
C	-3.664955	-1.333414	0.001484
C	-4.991668	-1.506483	-0.513323
C	-5.801667	-0.357741	-0.725645
C	-5.260447	0.930659	-0.486628
C	-3.953386	1.107253	-0.115807
C	-5.529136	-2.779011	-0.844284
C	-6.808463	-2.902804	-1.322209
C	-7.624674	-1.762254	-1.496121
C	-7.126419	-0.519016	-1.207821
C	-2.813079	-2.480042	0.408546
C	-1.529043	-2.597430	-0.088695
C	-0.687429	-3.694626	0.239749
C	-1.190314	-4.680551	1.049928
C	-2.466794	-4.575676	1.652045
C	-3.274565	-3.442546	1.366181
C	-2.929394	-5.555332	2.569131
C	-4.130588	-5.405481	3.209577
C	-4.914827	-4.255181	2.965726
C	-4.500452	-3.301749	2.072411
C	0.720152	-3.807056	-0.251338
C	1.779208	-3.567756	0.649178
C	3.080060	-3.864338	0.245672
C	3.367026	-4.366199	-1.023760
C	2.311415	-4.519773	-1.916105
C	0.989396	-4.243178	-1.557187
C	1.529319	-3.005055	2.043443
C	2.500080	-1.876624	2.407986
C	-0.110362	-4.403932	-2.594740
C	0.038396	-3.342937	-3.694380
C	4.783752	-4.737416	-1.429011
C	5.698160	-3.510496	-1.537235
O	-1.055503	-1.675612	-0.983721
C	-3.322877	2.452307	0.005315
C	-2.908380	2.927352	1.263307
C	-2.223121	4.136109	1.335330
C	-1.965962	4.906151	0.203625
C	-2.448898	4.447968	-1.017016
C	-3.095652	3.218814	-1.151142
C	-3.223919	2.181692	2.552301
C	-1.960491	1.834866	3.345920
C	-1.186996	6.204937	0.301133
C	0.200619	5.988491	0.920262
C	-3.536991	2.758844	-2.534795
C	-2.414926	2.835568	-3.575713
O	-0.638227	0.720602	-1.660117
C	-4.214148	2.987405	3.405441
C	-1.976589	7.271417	1.072019
C	-4.769790	3.547549	-2.997983
C	-0.154073	-5.821255	-3.178463
C	5.386118	-5.781507	-0.479816
C	1.583555	-4.107588	3.110023
H	3.894404	-3.708338	0.950170
H	2.521652	-4.883654	-2.920371
H	-2.300066	5.064386	-1.900914
H	-1.876661	4.486997	2.304764
H	0.843965	2.069224	4.547615
H	-4.909885	-3.660869	-0.721346
H	-7.196877	-3.885387	-1.573397
H	-8.637369	-1.874059	-1.871949
H	-7.734727	0.369429	-1.357865
H	-5.889313	1.801956	-0.649794
H	-0.576492	-5.550422	1.269307
H	1.838564	1.072952	0.191852
H	-5.108433	-2.419878	1.908277
H	-5.853116	-4.121596	3.495847
H	-4.473769	-6.155534	3.915788
H	-2.301010	-6.420690	2.765353
H	3.572074	4.206736	1.014488
H	3.267942	5.328797	3.161333
H	1.905965	4.285382	4.960484
H	1.157402	0.920310	2.380372
H	4.468824	4.520099	-1.717545
H	3.481777	6.391120	-2.994319
H	1.042524	6.395088	-3.489591
H	-0.371488	4.523571	-2.684099
H	0.584363	2.679645	-1.396464
H	4.226249	2.735763	-0.350835
H	4.443314	1.542875	-2.392928
H	2.766396	0.332014	-3.456882
H	2.821246	-1.841690	-2.448871
H	1.768709	-1.257263	-1.122378
H	1.591487	0.820203	-2.234652
H	0.528654	-2.565619	2.047308
H	-1.070917	-4.228228	-2.102638
H	4.725380	-5.193251	-2.425971
H	1.412533	-3.683493	4.105857
H	0.825601	-4.876535	2.937295
H	2.565757	-4.596376	3.113438
H	2.172238	-1.387205	3.331093
H	3.511569	-2.261093	2.593383
H	2.529613	-1.116603	1.623697
H	6.701399	-3.803589	-1.866913
H	5.303675	-2.783762	-2.255698
H	5.797882	-3.006698	-0.569190
H	6.371843	-6.103279	-0.834386
H	5.511889	-5.372918	0.529490
H	4.741301	-6.662568	-0.406494
H	-0.996687	-5.919984	-3.871483
H	0.760199	-6.059903	-3.734291
H	-0.271189	-6.568991	-2.387132
H	-0.765720	-3.437868	-4.432450
H	-0.014789	-2.337814	-3.265654
H	0.993253	-3.456049	-4.223543
H	-3.716298	1.239152	2.296111
H	-3.818479	1.705845	-2.465659

H	-1.037314	6.573863	-0.722680
H	-2.220517	1.255760	4.240200
H	-1.277376	1.242894	2.732261
H	-1.432994	2.737890	3.672872
H	-4.487285	2.428979	4.308413
H	-3.777922	3.942716	3.720116
H	-5.130080	3.205170	2.845818
H	-5.124812	3.177792	-3.967028
H	-5.591980	3.466473	-2.278999
H	-4.532953	4.612774	-3.108800
H	-2.746288	2.371836	-4.512068
H	-2.146895	3.873417	-3.809756
H	-1.530757	2.300682	-3.218113
H	0.765940	6.927963	0.929302
H	0.129676	5.630860	1.953764
H	0.774520	5.247522	0.356812
H	-1.430748	8.221857	1.092195
H	-2.955689	7.444900	0.613311
H	-2.143485	6.958348	2.109299
H	4.975713	-1.466444	1.228873
H	6.958985	-1.282990	2.709556
H	8.574168	0.570198	2.378139
H	8.224166	2.223823	0.568596
H	6.259790	2.041894	-0.910787

TS2_Si_endo
SCF Energy: -3600.13889324
Num. Imaginary Frequencies: 1

C	1.585833	-4.038140	0.145078
C	0.466891	-3.711047	-0.655983
C	0.635900	-3.512058	-2.038779
C	1.913951	-3.639526	-2.590243
C	3.024417	-3.972003	-1.824954
C	2.835465	-4.166005	-0.457434
C	-0.892675	-3.646617	-0.033265
C	-1.661376	-2.443889	-0.022164
C	-2.951202	-2.397863	0.484305
C	-3.422367	-3.527329	1.235751
C	-2.675153	-4.735008	1.219885
C	-1.441262	-4.771094	0.528136
C	-3.162119	-5.872286	1.915077
C	-4.325490	-5.810186	2.635196
C	-5.046727	-4.596168	2.695248
C	-4.611319	-3.489120	2.013462
O	-1.116282	-1.386628	-0.684274
P	-0.866479	0.128307	-0.075654
O	-0.935762	1.028080	-1.258046
C	-3.846103	-1.236907	0.220784
C	-3.403557	0.047826	0.439383
C	-4.201574	1.205881	0.228079
C	-5.510325	1.013522	-0.125797
C	-6.019472	-0.276133	-0.424262
C	-5.168755	-1.411328	-0.316867
C	-5.663879	-2.659965	-0.779695
C	-6.941594	-2.781430	-1.263386
C	-7.802576	-1.662931	-1.312450
C	-7.343619	-0.437285	-0.907992
O	-2.144774	0.236049	0.939823
C	-3.573428	2.560060	0.262999
C	-3.073335	3.107484	1.458094
C	-2.429346	4.342589	1.420275
C	-2.270763	5.056528	0.236238
C	-2.800006	4.508831	-0.926589
C	-3.428435	3.264552	-0.949392
C	-3.233305	2.410520	2.801431
C	-4.174130	3.208570	3.715274
C	-1.563586	6.399350	0.204637
C	-2.452830	7.498139	0.803074
C	-3.919095	2.722281	-2.287258
C	-5.164949	3.484994	-2.757976
C	-0.523419	-3.222632	-2.983118
C	-0.715480	-4.379366	-3.975185
C	4.399641	-4.103788	-2.454738
C	4.979069	-5.510731	-2.258708
C	1.485244	-4.167261	1.660624
C	2.386216	-5.257700	2.249378
O	0.320803	0.182003	0.846982
C	-1.880076	2.157579	3.479108
C	-2.827971	2.731338	-3.364233
C	-0.196112	6.360752	0.897129
C	-0.348474	-1.885120	-3.714614
C	5.367145	-3.035230	-1.926139
C	1.766763	-2.809769	2.313201
N	2.305574	2.163978	1.177263
C	2.997549	1.447212	2.090711
C	2.331600	0.558574	2.976213
C	3.068797	-0.220388	3.825391
C	4.488648	-0.177442	3.850238
C	5.143638	0.696906	3.033286
C	4.423019	1.502872	2.107244
C	3.058949	2.736315	0.092436
C	2.292888	3.680198	-0.806601
C	2.949804	4.847510	-1.210652
C	2.340013	5.749297	-2.073574
C	1.058572	5.486437	-2.550317
C	0.400595	4.329768	-2.149059
C	1.003989	3.430175	-1.273833
C	3.773041	1.585112	-0.718563
C	4.721127	0.707130	0.081590
O	4.314323	-0.542697	0.115129
C	2.950688	-0.656062	-0.390977
C	2.807402	0.540369	-1.317710
H	3.694584	-4.409284	0.161852
H	2.042560	-3.489713	-3.660222
H	-2.695765	5.063947	-1.856836
H	-2.038711	4.758658	2.346078
H	2.549703	-0.903966	4.489521
H	-5.014344	-3.527250	-0.761312
H	-7.291818	-3.745966	-1.619145
H	-8.814465	-1.773781	-1.690654
H	-7.981973	0.440587	-0.970544
H	-6.157690	1.875511	-0.264705
H	-0.892596	-5.709194	0.483101
H	1.365748	1.791534	0.982700
H	-5.171380	-2.562822	2.074705
H	-5.953749	-4.538312	3.289679
H	-4.687693	-6.682900	3.170243
H	-2.583209	-6.791853	1.876855
H	4.918502	2.401699	1.763148
H	6.225500	0.784373	3.060070
H	5.035261	-0.815292	4.536632
H	1.252337	0.478564	2.923610
H	3.950004	5.059908	-0.836437
H	2.861856	6.655007	-2.367892
H	0.574128	6.183456	-3.227925
H	-0.598144	4.110291	-2.504919
H	0.432597	2.549496	-0.988401
H	3.857637	3.342441	0.529265
H	4.350809	2.090343	-1.496579
C	6.193273	0.879988	0.063216
H	3.127881	0.281060	-2.330947
H	2.886353	-1.623635	-0.882630
H	2.256823	-0.623616	0.449186
H	1.771630	0.878627	-1.371810
H	0.458691	-4.432329	1.917089
H	-1.442471	-3.152639	-2.397847
H	4.281280	-3.939808	-3.533625
H	2.153623	-5.397718	3.310635
H	2.242466	-6.216045	1.739068
H	3.449028	-4.997223	2.185581
H	1.645910	-2.882056	3.400887
H	2.794121	-2.484775	2.106169
H	1.085406	-2.036400	1.941664
H	6.349210	-3.129961	-2.403209
H	4.990304	-2.025254	-2.118357
H	5.505185	-3.135696	-0.843252
H	5.937531	-5.612028	-2.780129
H	5.152545	-5.721130	-1.197051
H	4.294287	-6.273074	-2.642999
H	-1.597614	-4.198520	-4.599332
H	0.148320	-4.486482	-4.641678
H	-0.855965	-5.330586	-3.450787
H	-1.208197	-1.701531	-4.368669
H	-0.284398	-1.054701	-3.007150
H	0.549951	-1.887642	-4.344444
H	-3.700315	1.436374	2.631232
H	-4.199485	1.676472	-2.148701
H	-1.388255	6.645404	-0.851069
H	-2.021919	1.596287	4.409983
H	-1.225612	1.579262	2.821506
H	-1.377988	3.098520	3.733857
H	-4.326572	2.683745	4.665439
H	-3.761241	4.198735	3.941054
H	-5.150872	3.353176	3.241524
H	-5.545924	3.062788	-3.695062
H	-5.967136	3.442635	-2.013486
H	-4.933628	4.542702	-2.933215
H	-3.193873	2.228192	-4.266782
H	-2.550389	3.752180	-3.656516
H	-1.942660	2.201156	-3.002828
H	0.325744	7.314695	0.760202
H	-0.301543	6.193769	1.975397
H	0.431584	5.563197	0.489465
H	-1.965603	8.477632	0.731580
H	-3.415209	7.552270	0.283817
H	-2.654776	7.297121	1.861858
C	7.021538	-0.224906	0.279890
C	8.402603	-0.072779	0.259810
C	8.967733	1.178761	0.029258
C	8.145649	2.282442	-0.188223
C	6.764938	2.134411	-0.173113
H	6.574470	-1.196056	0.458157
H	9.039785	-0.936104	0.423744
H	10.046920	1.295103	0.014212
H	8.581199	3.259107	-0.373246
H	6.133220	3.001717	-0.347034

M3_Si_endo
SCF Energy: -3600.17224988
Num. Imaginary Frequencies: 0

C	2.197231	-4.234777	-0.764347
C	3.210627	-3.113172	-0.432597
C	3.433102	-3.261438	1.107531
O	2.865957	-4.499030	1.463381
C	1.765301	-4.754764	0.607923
C	2.688063	-2.100633	1.887974
C	1.426596	-1.666270	1.207385
N	1.472427	-1.467674	-0.076838
C	2.712887	-1.708897	-0.810765
C	2.534580	-2.407138	3.338136
C	1.374170	-2.219139	3.982315
C	0.206029	-1.729013	3.275819
C	0.214364	-1.465224	1.948605
C	2.519318	-1.425390	-2.287301
C	2.911982	-2.319457	-3.282992
C	2.735335	-1.996737	-4.625797
C	2.150647	-0.785912	-4.982985
C	1.762388	0.112036	-3.993536
C	1.964548	-0.197882	-2.655297
O	-0.869243	-0.904375	-1.145728

P	-1.143233	0.574743	-1.264347
O	-0.108014	1.180375	-0.093348
C	-0.375865	2.388964	0.483745
C	-1.399751	2.484081	1.403635
C	-1.703767	3.764871	1.967276
C	-0.874757	4.873513	1.641669
C	0.218535	4.690601	0.757598
C	0.477445	3.481966	0.166563
C	-2.817953	3.986869	2.820603
C	-3.067943	5.228990	3.345257
C	-2.223326	6.321539	3.045173
C	-1.154701	6.144251	2.206552
C	-2.172504	1.261545	1.751512
C	-2.761728	0.528717	0.741676
C	-3.584708	-0.607184	0.987265
C	-3.752543	-1.005490	2.287948
C	-3.082503	-0.362014	3.359635
C	-2.271097	0.776261	3.095584
C	-3.174885	-0.858723	4.686443
C	-2.465137	-0.279217	5.707161
C	-1.629828	0.829486	5.439901
C	-1.538621	1.345478	4.171892
C	-4.269823	-1.305957	-0.141381
C	-3.868690	-2.597816	-0.533908
C	-4.565232	-3.232046	-1.559790
C	-5.625203	-2.621356	-2.224810
C	-5.991925	-1.341085	-1.828623
C	-5.337252	-0.668460	-0.797102
C	-2.711515	-3.333482	0.128133
C	-1.727451	-3.912814	-0.895249
C	-5.821865	0.720849	-0.407117
C	-5.705029	1.709276	-1.573911
C	-6.350100	-3.326247	-3.356764
C	-5.404681	-3.621652	-4.528785
O	-2.591047	0.928894	-0.552718
C	1.649816	3.262290	-0.735367
C	2.829520	2.708873	-0.196544
C	3.904036	2.458973	-1.045383
C	3.843732	2.736963	-2.410215
C	2.681601	3.310893	-2.909870
C	1.573877	3.580908	-2.101437
C	2.949589	2.425541	1.296944
C	3.976018	1.338461	1.627297
C	5.021469	2.430913	-3.318056
C	5.402666	0.944244	-3.289915
C	0.350400	4.272564	-2.687157
C	-0.015314	3.809110	-4.099807
O	-1.064741	1.336817	-2.525143
C	3.302301	3.702498	2.075545
C	6.229086	3.313624	-2.973959
C	0.559000	5.795197	-2.663581
C	-7.251769	0.667278	0.148133
C	-7.045429	-4.605352	-2.872803
C	-3.223591	-4.431549	1.070587
H	-4.263348	-4.233272	-1.857740
H	-6.817538	-0.850789	-2.340731
H	2.630973	3.542123	-3.970580
H	4.817403	2.033670	-0.639136
H	-0.710874	-1.575387	3.836929
H	-3.483003	3.161135	3.049035
H	-3.927944	5.376361	3.991817
H	-2.430000	7.298533	3.471362
H	-0.506261	6.979013	1.952339
H	0.865422	5.537854	0.544480
H	-4.398231	-1.852051	2.505865
H	0.574886	-1.199504	-0.586131
H	-0.889218	2.191956	3.977170
H	-1.055405	1.276398	6.245865
H	-2.538967	-0.672365	6.716760
H	-3.810519	-1.720361	4.874879
H	3.363718	-1.234847	1.817175
H	3.418001	-2.772862	3.852197
H	1.286579	-2.426813	5.043377
H	-0.658900	-1.103192	1.418998
H	3.355982	-3.276410	-3.027675
H	3.045263	-2.702058	-5.390999
H	1.994794	-0.544981	-6.030163
H	1.298147	1.057776	-4.246096
H	1.685936	0.531796	-1.899789
H	3.444415	-0.974699	-0.441930
H	4.165532	-3.281850	-0.934149
C	4.898005	-3.262930	1.519316
H	2.686787	-5.029465	-1.332677
H	1.572523	-5.828687	0.636060
H	0.869185	-4.235034	0.976688
H	1.350500	-3.871752	-1.352833
H	-2.152740	-2.610804	0.726896
H	-5.185048	1.097844	0.397605
H	-7.127683	-2.642471	-3.721594
H	-2.386410	-4.927151	1.577294
H	-3.893953	-4.027266	1.836129
H	-3.780509	-5.194129	0.513246
H	-0.877286	-4.367076	-0.371627
H	-2.183666	-4.702130	-1.503387
H	-1.358083	-3.121644	-1.551553
H	-5.953029	-4.068497	-5.366026
H	-4.919015	-2.706665	-4.881450
H	-4.617770	-4.324213	-4.231352
H	-7.604451	-5.075048	-3.690200
H	-6.314178	-5.335158	-2.506142
H	-7.742621	-4.389642	-2.056806
H	-7.570766	1.661346	0.481698
H	-7.963620	0.325089	-0.611853
H	-7.315862	-0.018374	1.000025
H	-5.992755	2.715400	-1.247988
H	-4.677631	1.746728	-1.945508
H	-6.363621	1.427273	-2.403822
H	1.974890	2.071319	1.652165
H	-0.504896	4.031115	-2.049603
H	4.713582	2.671533	-4.343765
H	3.848756	0.992811	2.659296
H	3.865924	0.484186	0.953012
H	5.005414	1.701515	1.529236
H	3.409769	3.486167	3.144850
H	4.250640	4.115707	1.712643
H	2.531643	4.468160	1.961927
H	-0.329341	6.308412	-3.048459
H	0.751856	6.164439	-1.651599
H	1.413348	6.077135	-3.291208
H	-0.938548	4.307107	-4.415342
H	0.756448	4.065436	-4.835675
H	-0.201397	2.733741	-4.107801
H	6.232172	0.749702	-3.979275
H	5.727752	0.638780	-2.287443
H	4.558459	0.312447	-3.579496
H	7.054287	3.130947	-3.671685
H	5.967349	4.375612	-3.020677
H	6.593046	3.102786	-1.961318
C	5.418134	-4.298943	2.293458
C	6.755858	-4.283953	2.682050
C	7.588048	-3.237398	2.300242
C	7.075628	-2.201038	1.524046
C	5.740305	-2.213722	1.139267
H	4.769778	-5.117630	2.582628
H	7.146718	-5.098109	3.285076
H	8.630909	-3.228640	2.602032
H	7.716456	-1.381149	1.214337
H	5.363563	-1.396162	0.529841

M1_Re_exo

SCF Energy: -3600.16149037

Num. Imaginary Frequencies: 0

C	-6.999931	-0.249715	1.902893
O	-6.491111	-0.247418	0.562409
C	-5.286698	0.405336	0.583705
C	-4.833131	0.641708	1.824148
C	-5.808366	0.074140	2.823418
C	-2.403584	-1.472089	2.032244
C	-1.588371	-0.807121	3.034240
C	-2.159017	-0.597550	4.298331
C	-1.431348	0.037885	5.293913
C	-0.120106	0.441688	5.041537
C	0.461379	0.209561	3.797087
C	-0.264625	-0.413305	2.791898
N	-2.231029	-1.394573	0.758157
C	-2.990372	-2.090716	-0.225550
C	-2.426057	-2.192645	-1.493690
C	-3.118667	-2.877804	-2.485108
C	-4.360500	-3.443140	-2.217298
C	-4.924325	-3.312793	-0.948707
C	-4.244509	-2.635180	0.052624
O	-0.625405	0.507336	-0.089888
P	0.533485	0.064039	-0.950111
O	1.535889	1.307190	-1.292302
C	2.272482	1.894392	-0.298892
C	3.378940	1.242389	0.208781
C	4.119010	1.883092	1.257656
C	3.777802	3.213615	1.629379
C	2.665052	3.846483	1.021027
C	1.874183	3.196110	0.109972
C	4.523175	3.868386	2.644197
C	5.543551	3.226089	3.294560
C	5.853927	1.888373	2.961393
C	5.163550	1.235436	1.972345
C	3.715739	-0.129979	-0.265352
C	2.736826	-1.098483	-0.235197
C	2.966117	-2.471026	-0.523796
C	4.231340	-2.830984	-0.905030
C	5.263483	-1.867976	-1.060466
C	5.009726	-0.501024	-0.755923
C	6.546649	-2.246415	-1.533100
C	7.531278	-1.312869	-1.723980
C	7.269627	0.049237	-1.455282
C	6.044070	0.444756	-0.983753
O	1.471505	-0.745504	0.149424
C	1.808618	-3.409415	-0.378487
C	1.354141	-3.748883	0.911837
C	0.168895	-4.471847	1.041884
C	-0.573377	-4.869599	-0.066596
C	-0.073861	-4.568408	-1.329703
C	1.099844	-3.840519	-1.515947
C	0.604428	3.800019	-0.397874
C	-0.482948	3.963154	0.485921
C	-1.641781	4.580064	0.018937
C	-1.772601	5.018357	-1.296363
C	-0.700067	4.813603	-2.156551
C	0.487746	4.212708	-1.735889
C	-0.438280	3.503307	1.939089
C	-0.297989	4.694626	2.896007
C	-3.030817	5.723750	-1.770269
C	-4.282712	4.849987	-1.623205
C	1.620428	4.056278	-2.739687
C	2.142576	5.425656	-3.196631
C	2.160364	-3.364174	2.149269
C	1.370749	-3.423219	3.460605
C	-1.884324	-5.629973	0.048529
C	-2.575969	-5.476333	1.404473
C	1.609323	-3.574210	-2.926073
C	2.471886	-4.758728	-3.390303
O	0.320512	-0.691319	-2.206508

C	-1.655474	2.652210	2.311925
C	1.200180	3.190347	-3.934582
C	-3.209616	7.067533	-1.050060
C	3.408856	-4.253114	2.272568
C	-1.673907	-7.116676	-0.275880
C	0.505274	-3.293824	-3.950581
H	5.851360	1.494590	-0.791461
H	8.043689	0.790599	-1.629814
H	8.506931	-1.613816	-2.093669
H	6.729625	-3.295240	-1.752803
H	4.454564	-3.873571	-1.114992
H	2.407125	4.857691	1.324185
H	-1.513467	-0.689235	0.377922
H	5.409755	0.206715	1.735084
H	6.646001	1.371048	3.494839
H	6.104072	3.734612	4.073304
H	4.258063	4.890237	2.903983
H	-3.218044	-2.097838	2.390315
H	-3.180418	-0.916960	4.489694
H	-1.880383	0.212011	6.266207
H	0.452313	0.931978	5.823220
H	1.485931	0.509492	3.600732
H	0.205476	-0.603341	1.836325
H	-1.457983	-1.746380	-1.711349
H	-2.673335	-2.962458	-3.470992
H	-4.899408	-3.971481	-2.997790
H	-5.906727	-3.724132	-0.741424
H	-4.721404	-2.494223	1.016598
H	-0.191654	-4.716119	2.034850
H	-0.646353	-4.882447	-2.198635
H	2.498260	-2.328844	2.020395
H	2.236490	-2.679131	-2.891328
H	-0.789244	5.142928	-3.189855
H	-2.471956	4.726355	0.705951
H	2.452438	3.546344	-2.246666
H	0.438657	2.862625	2.068392
H	-2.899190	5.935969	-2.839407
H	-0.222186	4.347414	3.933219
H	0.592746	5.289397	2.670460
H	-1.167194	5.359193	2.823629
H	-1.574400	2.305895	3.348378
H	-2.595140	3.209982	2.222932
H	-1.694178	1.778823	1.656797
H	-5.165284	5.380558	-1.998459
H	-4.180646	3.912018	-2.175391
H	-4.468022	4.595241	-0.573056
H	-4.079437	7.604926	-1.444444
H	-3.367680	6.916610	0.024276
H	-2.325700	7.701692	-1.172968
H	2.048243	3.043276	-4.612731
H	0.855638	2.207648	-3.601058
H	0.395921	3.666290	-4.508153
H	2.990672	5.303413	-3.879826
H	1.367269	5.992838	-3.724746
H	2.473385	6.025196	-2.341755
H	-3.582056	-5.906968	1.363938
H	-2.027619	-5.992328	2.201436
H	-2.670573	-4.421854	1.685393
H	-2.559582	-5.212757	-0.710746
H	-2.624814	-7.661382	-0.249073
H	-1.232021	-7.245953	-1.268849
H	-0.995392	-7.574059	0.453768
H	0.961367	-3.036058	-4.912803
H	-0.133894	-4.168607	-4.122551
H	-0.102907	-2.446313	-3.628720
H	2.902119	-4.561110	-4.378669
H	3.292496	-4.961075	-2.695144
H	1.865689	-5.670405	-3.458690
H	3.999329	-3.967572	3.150979
H	3.115248	-5.303243	2.385831
H	4.050960	-4.171995	1.392188
H	1.957243	-2.969823	4.266705
H	0.421132	-2.885123	3.395807
H	1.158420	-4.458289	3.753887
H	-6.088847	0.777090	3.614465
H	-5.415614	-0.826866	3.322135
H	-7.457662	-1.224499	2.084932
H	-7.773886	0.523731	1.970970
C	-4.680222	0.667030	-0.727647
H	-3.905014	1.133308	2.078330
C	-5.268100	0.157921	-1.891102
C	-4.640526	0.327058	-3.118791
C	-3.423253	1.001524	-3.201339
C	-2.842466	1.523848	-2.049983
C	-3.473665	1.365063	-0.823186
H	-6.202761	-0.386840	-1.821077
H	-5.096876	-0.083668	-4.014764
H	-2.924530	1.114355	-4.159146
H	-1.893522	2.048327	-2.090390
H	-3.005705	1.782856	0.059173

TS1_Re_exo
SCF Energy: -3600.14542945
Num. Imaginary Frequencies: 1

C	3.334523	1.970427	-2.012267
C	2.859239	2.393663	-0.757216
C	3.612485	2.153551	0.404089
C	4.833352	1.485306	0.293064
C	5.341721	1.087497	-0.937245
C	4.575821	1.343549	-2.073301
C	1.580401	3.160291	-0.645407
C	0.367378	2.517005	-0.276433
C	-0.786706	3.217993	0.008559
C	-0.816480	4.628704	-0.243250
C	0.380211	5.281989	-0.645507
C	1.565848	4.521989	-0.802921
C	-2.002302	5.404862	-0.139043
C	-1.987503	6.753232	-0.387738
C	-0.788556	7.405375	-0.753524
C	0.366858	6.680870	-0.882760
C	-1.977475	2.502102	0.537818
C	-2.490085	1.427134	-0.156029
C	-3.703275	0.777069	0.205820
C	-4.364468	1.235260	1.316285
C	-3.822369	2.250387	2.144071
C	-2.603014	2.879898	1.770250
C	-4.444858	2.606727	3.368800
C	-3.870600	3.525095	4.208169
C	-2.643868	4.130695	3.852540
C	-2.030049	3.822364	2.665502
O	-1.857276	1.007342	-1.293127
P	-0.448381	0.172152	-1.164690
O	0.385856	1.158884	-0.114566
C	-4.213476	-0.377493	-0.589878
C	-4.286969	-1.655555	0.000134
C	-4.762372	-2.722881	-0.758362
C	-5.154861	-2.571237	-2.084711
C	-5.080295	-1.300657	-2.642743
C	-4.621458	-0.197192	-1.924046
C	-3.859353	-1.930506	1.435691
C	-5.062302	-2.276510	2.322106
C	-5.638995	-3.755273	-2.900840
C	-4.541189	-4.816813	-3.052456
C	-4.627451	1.164496	-2.605049
C	-6.067355	1.617133	-2.887663
C	3.127375	2.594847	1.779505
C	2.507210	1.414439	2.535493
C	6.705638	0.436986	-1.096784
C	7.243610	-0.207626	0.181280
C	2.552732	2.239278	-3.290476
C	3.065237	3.520600	-3.964031
O	-0.625953	-1.069034	-0.327179
O	0.166102	0.126855	-2.511414
C	4.224119	3.272515	2.609684
C	7.715071	1.456057	-1.648797
C	2.577613	1.063974	-4.272661
C	-2.788011	-3.022478	1.505822
C	-6.918840	-4.363337	-2.312814
C	-3.775602	1.173285	-3.880402
N	1.804286	-1.601782	1.023991
C	2.912012	-1.941669	0.224959
C	2.898093	-1.540224	-1.114421
C	3.927575	-1.927325	-1.956861
C	4.983467	-2.704259	-1.485100
C	5.012791	-3.070137	-0.144443
C	3.988682	-2.686982	0.714720
C	1.622670	-2.028119	2.278267
C	0.667651	-1.340308	3.179156
C	1.012773	-1.241350	4.531723
C	0.208488	-0.530335	5.416205
C	-0.947830	0.089653	4.953171
C	-1.297341	-0.009251	3.608305
C	-0.501957	-0.722322	2.721276
C	0.792476	-3.964385	2.241509
C	1.490542	-4.700094	1.286022
O	2.397542	-5.523366	1.815086
C	2.397192	-5.353467	3.250751
C	1.089794	-4.623526	3.572933
H	-2.933241	4.917087	0.127568
H	-2.908400	7.323543	-0.309584
H	-0.789799	8.474672	-0.942777
H	1.293396	7.165194	-1.180695
H	2.491134	5.035583	-1.051634
H	-5.306033	0.773094	1.602022
H	0.987029	-1.209885	0.526787
H	-1.084277	4.286266	2.407992
H	-2.181307	4.844238	4.527986
H	-4.349933	3.783503	5.147722
H	-5.380288	2.121161	3.635554
H	2.527169	-2.349359	2.783287
H	1.936627	-1.690350	4.889777
H	0.494731	-0.448287	6.460200
H	-1.572367	0.662754	5.631546
H	-2.189375	0.488127	3.241899
H	-0.776829	-0.771365	1.670352
H	2.080982	-0.939203	-1.503428
H	3.898205	-1.610107	-2.994431
H	5.781741	-3.010180	-2.154130
H	5.838281	-3.659206	0.243794
H	4.041521	-2.998998	1.752095
H	5.401604	1.286107	1.196226
H	4.965111	1.029486	-3.039429
H	2.336869	3.337532	1.634886
H	1.504361	2.388507	-3.017120
H	-5.392704	-1.163932	-3.675904
H	-4.819342	-3.707760	-0.299612
H	-4.194110	1.898907	-1.921264
H	-3.402494	-1.024362	1.838214
H	-5.879583	-3.381879	-3.904773
H	-4.745864	-2.426157	3.360958
H	-5.813154	-1.479567	2.304424
H	-5.550621	-3.196977	1.981299
H	-2.422907	-3.124745	2.535419
H	-3.168018	-3.998647	1.183695
H	-1.957427	-2.738563	0.854981
H	-4.876840	-5.630447	-3.705562
H	-3.632057	-4.382164	-3.479893
H	-4.278775	-5.253138	-2.081694
H	-7.287934	-5.177214	-2.947237
H	-6.736269	-4.775373	-1.313448

H	-7.707310	-3.609048	-2.225277
H	-3.747846	2.182027	-4.307573
H	-2.749739	0.863641	-3.665333
H	-4.189570	0.503162	-4.643276
H	-6.073029	2.618322	-3.333260
H	-6.569548	0.936904	-3.585436
H	-6.657348	1.647595	-1.965214
H	8.158333	-0.769902	-0.036911
H	7.498218	0.548121	0.933803
H	6.512065	-0.895477	0.616237
H	6.592096	-0.359355	-1.844811
H	8.689761	0.985773	-1.824128
H	7.367155	1.889330	-2.591942
H	7.854255	2.276520	-0.935094
H	1.917674	1.282223	-5.119057
H	3.580627	0.883075	-4.678629
H	2.201174	0.157557	-3.793478
H	2.497415	3.731036	-4.877505
H	2.972603	4.385991	-3.300071
H	4.122914	3.417063	-4.236101
H	3.794374	3.689648	3.527353
H	5.007002	2.566467	2.909091
H	4.699277	4.086755	2.052800
H	2.124205	1.726389	3.514379
H	1.680498	0.988966	1.963364
H	3.252495	0.623732	2.695024
H	0.293691	-5.324089	3.849916
H	1.202345	-3.913541	4.397151
H	3.281397	-4.758003	3.504629
H	2.495893	-6.343898	3.695344
H	-0.197139	-3.589355	2.017233
C	1.379138	-4.656194	-0.156879
C	0.401824	-3.843853	-0.744797
C	2.293421	-5.345990	-0.971295
C	0.356652	-3.685735	-2.122030
C	2.226900	-5.204363	-2.346517
C	1.266440	-4.367837	-2.922045
H	-0.291843	-3.273347	-0.144616
H	3.062393	-5.960096	-0.516272
H	-0.364454	-2.997839	-2.549594
H	2.939904	-5.726710	-2.976478
H	1.240243	-4.238890	-3.999924

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SCF Energy: -3600.16144222
Num. Imaginary Frequencies: 0

C	-3.095823	2.983772	-1.152319
C	-3.348378	2.197857	-0.011241
C	-3.056331	2.702209	1.269348
C	-2.519040	3.981777	1.386713
C	-2.263161	4.779688	0.275615
C	-2.575162	4.265325	-0.977579
C	-3.894242	0.817494	-0.176033
C	-3.066388	-0.307164	0.088575
C	-3.471352	-1.612360	-0.101121
C	-4.756329	-1.841253	-0.696441
C	-5.620171	-0.733015	-0.917038
C	-5.167949	0.577903	-0.620144
C	-5.197491	-3.126871	-1.110378
C	-6.439102	-3.304245	-1.664775
C	-7.313375	-2.207968	-1.838521
C	-6.905949	-0.951045	-1.476511
C	-2.559832	-2.722412	0.288742
C	-1.246507	-2.709718	-0.139657
C	-0.318510	-3.738544	0.174609
C	-0.776203	-4.821994	0.878472
C	-2.093284	-4.871515	1.396322
C	-2.983366	-3.789860	1.149138
C	-2.514650	-5.955173	2.210137
C	-3.754600	-5.957810	2.791111
C	-4.623014	-4.861060	2.590412
C	-4.249523	-3.808376	1.795084
O	-0.809192	-1.714033	-0.966751
P	-0.527958	-0.199520	-0.386621
O	-1.822635	-0.059954	0.611356
C	1.126739	-3.615293	-0.184454
C	2.075646	-3.470926	0.849100
C	3.433088	-3.479897	0.523880
C	3.878739	-3.598090	-0.791375
C	2.919863	-3.665249	-1.796850
C	1.552205	-3.686190	-1.522236
C	1.673890	-3.337942	2.314315
C	2.059363	-4.589052	3.114958
C	5.347897	-3.790639	-1.127956
C	6.277331	-2.761980	-0.478421
C	0.577501	-3.846655	-2.679786
C	0.788640	-5.188577	-3.394599
C	-3.326564	1.907897	2.540026
C	-2.039318	1.655202	3.336299
C	-1.677890	6.172070	0.419077
C	-0.418877	6.188054	1.292829
C	-3.376058	2.490355	-2.566661
C	-4.654654	3.134048	-3.122303
O	0.669707	-0.176002	0.524395
O	-0.573911	0.700680	-1.571301
C	-4.390443	2.600250	3.403043
C	-2.730909	7.154985	0.949233
C	-2.199784	2.720061	-3.523282
C	2.252361	-2.075783	2.961584
C	5.781093	-5.217965	-0.760299
C	0.660276	-2.666343	-3.655068
N	2.114412	2.347345	0.152911
C	1.944337	3.587733	-0.443798
C	0.893071	3.738278	-1.364496
C	0.719284	4.941419	-2.027850
C	1.571691	6.022953	-1.797670
C	2.596732	5.881226	-0.871612
C	2.785046	4.680128	-0.190873
C	3.206821	1.992850	0.993854
C	2.920921	2.110867	2.482720
C	3.800663	2.808591	3.308390
C	3.542799	2.935837	4.671721
C	2.398440	2.361652	5.214960
C	1.515385	1.664268	4.391753
C	1.770450	1.539294	3.031391
C	3.683359	0.511386	0.631270
C	4.429600	0.617921	-0.644492
O	5.716468	0.675464	-0.458589
C	6.039484	0.517905	0.960572
C	4.764714	-0.047949	1.561885
H	-4.533682	-3.976237	-0.993910
H	-6.750392	-4.296059	-1.979439
H	-8.295977	-2.362128	-2.274230
H	-7.557006	-0.093709	-1.628199
H	-5.836862	1.415347	-0.799547
H	-0.094895	-5.639388	1.100384
H	1.323149	1.709372	0.176296
H	-4.924521	-2.970916	1.662136
H	-5.593715	-4.847723	3.076983
H	-4.065748	-6.787650	3.418593
H	-1.822225	-6.776527	2.377580
H	4.042188	2.665117	0.763852
H	4.689971	3.271020	2.882269
H	4.228966	3.492239	5.303423
H	2.190957	2.463159	6.276018
H	0.615894	1.219509	4.806981
H	1.080354	0.996883	2.389470
H	0.224171	2.898730	-1.538589
H	-0.096012	5.031692	-2.740091
H	1.426632	6.962691	-2.321297
H	3.255142	6.717980	-0.654339
H	3.561027	4.622602	0.566015
H	-2.292485	4.366867	2.378296
H	-2.383714	4.881828	-1.852527
H	-3.730229	0.930825	2.259156
H	-3.532130	1.409639	-2.522256
H	3.252142	-3.750478	-2.829922
H	4.161369	-3.438040	1.332129
H	-0.437077	-3.858231	-2.274789
H	0.587836	-3.235559	2.359615
H	5.450969	-3.680979	-2.215349
H	1.725385	-4.496208	4.154429
H	1.607527	-5.491804	2.691505
H	3.146520	-4.734606	3.123030
H	1.854776	-1.954715	3.975515
H	3.344917	-2.122946	3.045433
H	1.969252	-1.194025	2.382473
H	7.317224	-2.946956	-0.769596
H	6.017104	-1.746405	-0.790249
H	6.230810	-2.815174	0.616266
H	6.822673	-5.399622	-1.049219
H	5.693132	-5.380396	0.320261
H	5.148230	-5.957128	-1.260759
H	-0.065699	-2.794483	-4.465909
H	0.430002	-1.730902	-3.139243
H	1.656533	-2.584060	-4.106810
H	0.032347	-5.326640	-4.175391
H	1.774219	-5.242450	-3.871541
H	0.710314	-6.023056	-2.689702
H	0.050421	7.177851	1.265174
H	-0.654385	5.962810	2.339801
H	0.311593	5.454869	0.941355
H	-1.380022	6.502324	-0.584465
H	-2.318320	8.168406	1.018005
H	-3.609951	7.182390	0.296581
H	-3.066578	6.858344	1.950216
H	-2.421982	2.267843	-4.497080
H	-2.012466	3.786774	-3.696473
H	-1.297753	2.253144	-3.122498
H	-4.882160	2.740978	-4.119960
H	-5.517384	2.943275	-2.475835
H	-4.536595	4.221290	-3.205184
H	-4.624484	1.993634	4.285680
H	-4.044051	3.579780	3.752835
H	-5.315580	2.754380	2.837811
H	-2.256501	1.053524	4.227366
H	-1.315096	1.115289	2.721283
H	-1.580848	2.593748	3.669216
H	4.763130	-1.138276	1.497975
H	4.619062	0.244258	2.602159
H	6.300710	1.512686	1.331570
H	6.909582	-0.136686	0.999954
H	2.785430	-0.110760	0.567622
C	3.914868	0.767230	-1.958358
C	2.537882	0.573321	-2.170114
C	4.750306	1.176061	-3.024504
C	1.987786	0.829443	-3.417771
C	4.194815	1.410921	-4.263344
C	2.813470	1.247938	-4.453681
H	1.902475	0.219397	-1.370012
H	5.810555	1.326450	-2.852752
H	0.917704	0.708566	-3.544079
H	4.820824	1.738077	-5.086762
H	2.384341	1.453940	-5.429813

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SCF Energy: -3600.15094874
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C	3.180705	2.312502	-2.013062
C	2.638994	2.564589	-0.740470

C	3.379170	2.256341	0.415990
C	4.672894	1.752621	0.277998
C	5.250970	1.544656	-0.969842
C	4.483156	1.823270	-2.097245
C	1.306217	3.229161	-0.604481
C	0.153451	2.497031	-0.213325
C	-1.055951	3.102664	0.061154
C	-1.206023	4.497778	-0.221589
C	-0.070391	5.240942	-0.645301
C	1.175392	4.581229	-0.794244
C	-2.453141	5.171031	-0.122437
C	-2.554921	6.510376	-0.397565
C	-1.417712	7.253710	-0.787369
C	-0.205335	6.628021	-0.911836
C	-2.161791	2.286457	0.628874
C	-2.563225	1.141667	-0.025162
C	-3.661331	0.347861	0.404527
C	-4.300277	0.712868	1.559437
C	-3.859619	1.808989	2.342144
C	-2.781061	2.611937	1.879637
C	-4.453692	2.094236	3.597969
C	-3.985759	3.114485	4.384590
C	-2.899922	3.901211	3.938146
C	-2.317596	3.661812	2.718667
O	-1.930100	0.779801	-1.183385
P	-0.447667	0.077656	-1.057241
O	0.291827	1.154596	-0.012338
C	-4.140272	-0.805705	-0.413697
C	-3.955705	-2.124981	0.033338
C	-4.501589	-3.167449	-0.718392
C	-5.190952	-2.946462	-1.904213
C	-5.330250	-1.632360	-2.342446
C	-4.822650	-0.556074	-1.619953
C	-3.193004	-2.458340	1.308922
C	-4.158544	-2.789841	2.454638
C	-5.766703	-4.104336	-2.698642
C	-7.290767	-3.993363	-2.836488
C	-5.043171	0.850949	-2.158537
C	-6.538786	1.188006	-2.229808
C	2.814141	2.522920	1.806178
C	3.303735	1.532291	2.868510
C	6.670383	1.029077	-1.149336
C	7.272046	0.402792	0.109209
C	2.394335	2.574516	-3.289937
C	2.888404	3.857355	-3.972614
O	-0.502484	-1.167329	-0.214714
O	0.185401	0.114492	-2.396887
C	3.116119	3.964127	2.243407
C	7.583644	2.146749	-1.676914
C	2.436290	1.385567	-4.257131
C	-2.204143	-3.610785	1.098183
C	-5.096505	-4.229291	-4.073335
C	-4.353141	1.045524	-3.514465
N	1.901047	-1.286270	1.164076
C	2.992880	-1.503111	0.402028
C	3.014920	-1.097965	-0.956673
C	4.031645	-1.522944	-1.764596
C	5.101840	-2.318198	-1.272104
C	5.139343	-2.644010	0.055415
C	4.061650	-2.289854	0.906129
C	1.732647	-2.018902	2.381325
C	0.476794	-1.555832	3.111030
C	0.092117	-0.216220	3.004181
C	-1.012636	0.263327	3.696347
C	-1.760092	-0.586244	4.504842
C	-1.383714	-1.918941	4.622331
C	-0.273879	-2.399412	3.931476
C	1.767493	-3.577263	2.118199
C	2.693484	-4.091696	1.030645
O	3.559737	-4.979633	1.512397
C	3.629087	-4.877400	2.940835
C	2.248110	-4.375342	3.351554
H	-3.336046	4.609599	0.163385
H	-3.519407	7.003530	-0.321051
H	-1.511966	8.314890	-0.997457
H	0.674314	7.183659	-1.227305
H	2.049518	5.164698	-1.073389
H	-5.160851	0.140869	1.895413
H	1.022778	-1.047216	0.672581
H	-1.477200	4.265807	2.394760
H	-2.519985	4.700062	4.568149
H	-4.441073	3.316537	5.349454
H	-5.281267	1.473205	3.932281
H	2.586504	-1.802518	3.040060
H	0.641894	0.453269	2.352837
H	-1.293820	1.305369	3.595511
H	-2.632940	-0.207743	5.027645
H	-1.958491	-2.596528	5.246858
H	-0.022936	-3.450183	4.035830
H	2.209915	-0.491329	-1.359378
H	4.017011	-1.234248	-2.811002
H	5.898644	-2.623277	-1.942345
H	5.970182	-3.208107	0.467887
H	4.215898	-2.353634	1.977945
H	5.240028	1.519463	1.172490
H	4.915874	1.640008	-3.079020
H	1.726073	2.418446	1.750196
H	1.344599	2.712579	-3.016421
H	-5.855324	-1.436626	-3.275031
H	-4.380235	-4.191189	-0.371887
H	-4.593252	1.564988	-1.463786
H	-2.599056	-1.584603	1.593833
H	-5.550606	-5.024457	-2.139515
H	-3.602425	-3.056630	3.359989
H	-4.805360	-1.940600	2.696152
H	-4.803230	-3.635828	2.186413
H	-1.574192	-3.712081	1.988918
H	-2.709555	-4.571378	0.943725
H	-1.568486	-3.403532	0.235269
H	-7.698870	-4.869983	-3.352462
H	-7.769152	-3.916846	-1.854791
H	-7.570639	-3.104943	-3.414383
H	-5.484539	-5.098405	-4.616852
H	-5.285575	-3.338626	-4.683404
H	-4.012325	-4.339845	-3.970837
H	-4.484649	2.076146	-3.863385
H	-3.282052	0.843043	-3.430776
H	-4.774158	0.378519	-4.276223
H	-6.682481	2.223312	-2.559421
H	-7.064911	0.536606	-2.937238
H	-7.013923	1.070627	-1.249891
H	8.240602	-0.053444	-0.122516
H	7.443107	1.156634	0.886908
H	6.617571	-0.372792	0.519298
H	6.627041	0.244141	-1.918009
H	8.594121	1.767484	-1.868344
H	7.195547	2.574421	-2.606620
H	7.655321	2.956331	-0.941378
H	1.814161	1.602092	-5.132621
H	3.451868	1.184486	-4.620193
H	2.028024	0.493237	-3.776863
H	2.307599	4.060941	-4.879227
H	2.798433	4.723917	-3.309372
H	3.943132	3.763966	-4.259484
H	2.679578	4.168110	3.228021
H	4.198806	4.124751	2.308715
H	2.706868	4.687717	1.532224
H	2.717278	1.648722	3.786348
H	3.194776	0.500662	2.520459
H	4.355158	1.699497	3.129408
H	1.578884	-5.217426	3.547909
H	2.291594	-3.760627	4.253684
H	4.430576	-4.176417	3.200623
H	3.886978	-5.867225	3.317027
H	0.749839	-3.854250	1.830279
C	2.314891	-4.282030	-0.367330
C	1.151420	-3.687565	-0.875577
C	3.138784	-5.033306	-1.218730
C	0.823960	-3.832727	-2.214527
C	2.790339	-5.194629	-2.552674
C	1.637539	-4.591910	-3.052576
H	0.513399	-3.058630	-0.264965
H	4.044600	-5.484653	-0.829894
H	-0.058536	-3.329333	-2.594324
H	3.426657	-5.782718	-3.206525
H	1.378955	-4.707773	-4.100788

M3_Re_exo

SCF Energy: -3600.17736929

Num. Imaginary Frequencies: 0

C	2.504235	2.253665	-2.145351
C	2.048854	2.728297	-0.901065
C	2.940266	2.840492	0.186718
C	4.271193	2.450259	0.009851
C	4.743480	1.974657	-1.211848
C	3.839330	1.871421	-2.265858
C	0.645501	3.227369	-0.744150
C	-0.426569	2.363590	-0.380333
C	-1.661040	2.853961	0.005554
C	-1.941835	4.246307	-0.180836
C	-0.901213	5.109336	-0.617386
C	0.387360	4.570542	-0.848179
C	-3.233907	4.802785	0.022028
C	-3.464115	6.139940	-0.173773
C	-2.418910	7.000037	-0.581111
C	-1.166547	6.490930	-0.800517
C	-2.670092	1.937092	0.600630
C	-3.050732	0.806168	-0.086272
C	-4.045864	-0.093883	0.383750
C	-4.667308	0.210726	1.566503
C	-4.267608	1.314842	2.361137
C	-3.231481	2.172523	1.898334
C	-4.837428	1.538091	3.641398
C	-4.380697	2.546563	4.449105
C	-3.326361	3.376978	4.006540
C	-2.769295	3.198308	2.765854
O	-2.489684	0.569798	-1.311684
P	-0.973058	-0.045921	-1.359396
O	-0.179042	1.017733	-0.319815
C	-4.395629	-1.331057	-0.377616
C	-3.981931	-2.587152	0.111811
C	-4.373888	-3.732300	-0.575177
C	-5.136165	-3.674049	-1.740217
C	-5.505079	-2.422244	-2.216939
C	-5.149015	-1.244489	-1.558020
C	-3.123792	-2.724419	1.361698
C	-3.966413	-3.122352	2.580564
C	-5.538485	-4.938650	-2.477147
C	-4.311260	-5.700604	-2.994583
C	-5.594282	0.089121	-2.140050
C	-7.124291	0.201824	-2.173898
C	2.486903	3.427459	1.522671
C	1.813574	2.375554	2.411949
C	6.215434	1.694620	-1.467797
C	6.995875	1.225926	-0.237818
C	1.610035	2.293402	-3.375456
C	1.751796	3.660478	-4.063544
O	-0.924691	-1.341851	-0.590641
O	-0.475890	0.069149	-2.747178
C	3.603147	4.135515	2.296958

C	6.874024	2.943059	-2.076828
C	1.874675	1.165543	-4.373925
C	-1.959288	-3.706193	1.183143
C	-6.422207	-5.841820	-1.607059
C	-4.981868	0.322268	-3.527191
N	1.479315	-1.637951	0.376466
C	2.318507	-1.667368	-0.621727
C	1.895110	-2.013164	-1.946485
C	2.823412	-2.081873	-2.929712
C	4.231241	-1.828838	-2.706484
C	4.668886	-1.479029	-1.488802
C	3.740075	-1.317014	-0.336996
C	1.921729	-1.221549	1.705265
C	0.789475	-1.339688	2.716888
C	-0.320144	-0.500294	2.578176
C	-1.357554	-0.537004	3.501523
C	-1.311660	-1.425071	4.571658
C	-0.220430	-2.274698	4.711602
C	0.825620	-2.228493	3.793276
C	3.201136	-1.980795	2.093609
C	4.257474	-2.052355	0.949184
O	5.401174	-1.357151	1.412500
C	5.013298	-0.481416	2.459774
C	3.955727	-1.264800	3.226378
H	-4.048549	4.152845	0.321470
H	-4.461234	6.542164	-0.021513
H	-2.614712	8.057554	-0.730146
H	-0.356154	7.137071	-1.128649
H	1.199749	5.245786	-1.107032
H	-5.461128	-0.436099	1.929575
H	0.445561	-1.657514	0.138968
H	-1.956050	3.838223	2.441456
H	-2.950639	4.160617	4.657731
H	-4.817715	2.702764	5.430748
H	-5.632669	0.877141	3.976897
H	2.174810	-0.155258	1.613014
H	-0.386578	0.171899	1.728745
H	-2.205017	0.128622	3.379674
H	-2.123966	-1.452561	5.291591
H	-0.174455	-2.976054	5.539338
H	1.669913	-2.893055	3.942027
H	0.842287	-2.188863	-2.131289
H	2.498155	-2.338310	-3.933579
H	4.919912	-1.929016	-3.538397
H	5.719170	-1.294068	-1.290508
H	3.724673	-0.239308	-0.081960
H	4.968833	2.567229	0.832744
H	4.204023	1.516050	-3.226331
H	1.727863	4.182889	1.298748
H	0.574744	2.173051	-3.049498
H	-6.088066	-2.360780	-3.133840
H	-4.061684	-4.701794	-0.194102
H	-5.230666	0.887710	-1.486723
H	-2.674616	-1.750544	1.561223
H	-6.131866	-4.634155	-3.349427
H	-3.330248	-3.207831	3.469191
H	-4.748331	-2.386357	2.792623
H	-4.454916	-4.090565	2.415943
H	-1.270078	-3.610592	2.031229
H	-2.300062	-4.748637	1.151801
H	-1.415909	-3.482274	0.262905
H	-4.616043	-6.578876	-3.575507
H	-3.693406	-5.060277	-3.631979
H	-3.685650	-6.048140	-2.164287
H	-6.749620	-6.723570	-2.169919
H	-5.876595	-6.193102	-0.723627
H	-7.310620	-5.304879	-1.259488
H	-5.258286	1.313888	-3.903708
H	-3.891305	0.261703	-3.481429
H	-5.340394	-0.420692	-4.249552
H	-7.426808	1.188600	-2.542687
H	-7.565815	-0.551078	-2.837118
H	-7.552210	0.061561	-1.175445
H	8.020250	0.960854	-0.521719
H	7.068336	2.018861	0.515870
H	6.534827	0.351169	0.231102
H	6.264202	0.897114	-2.221848
H	7.925572	2.750945	-2.318797
H	6.359311	3.255304	-2.990802
H	6.833634	3.777068	-1.366582
H	1.106152	1.185853	-5.152112
H	2.850398	1.265197	-4.866420
H	1.808771	0.195346	-3.879161
H	1.098229	3.712086	-4.941420
H	1.479069	4.479961	-3.391665
H	2.784794	3.822546	-4.395660
H	3.176645	4.670842	3.151721
H	4.338606	3.426701	2.696718
H	4.134528	4.858455	1.669791
H	1.380103	2.837489	3.305649
H	1.012121	1.857765	1.880502
H	2.545094	1.629302	2.748819
H	4.434581	-1.993406	3.886269
H	3.302290	-0.629702	3.830557
H	4.605333	0.453348	2.044948
H	5.909101	-0.243883	3.036702
H	2.929907	-3.000426	2.368399
C	4.658027	-3.479141	0.594041
C	3.686369	-4.426389	0.258701
C	6.002427	-3.846300	0.556994
C	4.054600	-5.714324	-0.113890
C	6.369163	-5.137324	0.187157
C	5.398861	-6.074038	-0.152326
H	2.630825	-4.170861	0.294851
H	6.757125	-3.116362	0.825165
H	3.287225	-6.438313	-0.369974
H	7.420406	-5.409267	0.165083
H	5.686064	-7.080875	-0.440002

M1_Re_endo

SCF Energy: -3600.16229721

Num. Imaginary Frequencies: 0

C	5.461743	-2.805764	2.674049
C	4.957827	-3.292110	1.460965
C	5.595761	-2.926215	0.270911
C	6.709493	-2.092824	0.293001
C	7.205399	-1.618791	1.503327
C	6.580264	-1.982999	2.694428
C	3.750452	-4.128772	1.440020
O	3.087223	-4.170370	0.236681
C	1.975340	-5.075984	0.384538
C	1.810999	-5.316704	1.895938
C	3.125034	-4.794280	2.414013
H	2.224950	-5.996970	-0.152673
C	1.915627	-1.618237	0.025764
C	1.135307	-1.820133	1.231396
C	1.795539	-1.731365	2.463793
C	1.097052	-1.925349	3.647563
C	-0.257665	-2.240165	3.606947
C	-0.915608	-2.355198	2.382042
C	-0.233024	-2.133474	1.197899
N	1.422710	-1.499091	-1.159764
C	2.217074	-1.374577	-2.338121
C	1.909978	-0.367043	-3.246430
C	2.670036	-0.266122	-4.405926
C	3.705727	-1.162774	-4.655782
C	3.986329	-2.177497	-3.743319
C	3.237378	-2.291801	-2.577717
O	-1.120406	-0.927717	-1.525086
P	-1.171733	0.580660	-1.413162
O	-2.550015	1.055932	-0.657796
C	-2.787848	0.640028	0.623704
C	-2.065429	1.196565	1.656297
C	-2.279840	0.705904	2.984293
C	-3.331250	-0.222655	3.215140
C	-4.124753	-0.660282	2.123542
C	-3.855761	-0.275976	0.835373
C	-1.458457	1.081122	4.080145
C	-1.683684	0.578059	5.336112
C	-2.746442	-0.324462	5.569229
C	-3.548828	-0.715122	4.528060
C	-1.084553	2.275943	1.367151
C	-0.069813	2.048638	0.459993
C	0.981068	2.982375	0.237512
C	0.888240	4.201976	0.858344
C	-0.197154	4.540512	1.703892
C	-1.197537	3.567968	1.972361
C	-0.298914	5.827737	2.292104
C	-1.359024	6.150765	3.097497
C	-2.371313	5.195097	3.341776
C	-2.294206	3.939921	2.795871
C	2.172699	2.620410	-0.596410
C	2.229899	2.994341	-1.952424
C	3.356752	2.642894	-2.694514
C	4.412984	1.922164	-2.149520
C	4.343582	1.579761	-0.803024
C	3.252065	1.928121	-0.005927
C	1.128945	3.821513	-2.602287
C	1.463852	5.317428	-2.494931
C	3.287431	1.610962	1.489783
C	4.335809	0.561298	1.876714
C	5.612113	1.579180	-3.016448
C	6.387600	0.348661	-2.540448
O	-0.042943	0.858048	-0.212095
C	-4.698552	-0.735143	-0.310364
C	-4.560261	-2.038335	-0.822300
C	-5.402064	-2.449253	-1.852097
C	-6.361119	-1.601646	-2.402703
C	-6.464146	-0.312466	-1.893213
C	-5.649177	0.142214	-0.856286
C	-3.524749	-3.002709	-0.266584
C	-4.166697	-4.024968	0.680451
C	-7.260237	-2.067335	-3.533405
C	-6.448318	-2.418992	-4.787116
C	-5.826231	1.564563	-0.345166
C	-7.214836	1.759183	0.277969
O	-0.960838	1.465767	-2.578424
C	-2.711911	-3.702932	-1.360677
C	-8.145584	-3.243800	-3.101717
C	-5.550038	2.596739	-1.445590
C	3.585290	2.871611	2.322434
C	6.547273	2.792234	-3.135424
C	0.859880	3.452613	-4.064696
H	-3.085516	3.221804	2.979831
H	-3.222522	5.460888	3.961666
H	-1.431668	7.139969	3.539255
H	0.478327	6.558146	2.081455
H	1.675051	4.935812	0.703449
H	-4.959935	-1.329334	2.315066
H	0.369985	-1.371865	-1.301572
H	-0.634999	1.766191	3.910130
H	-1.038517	0.874046	6.158163
H	-2.920811	-0.709634	6.569670
H	-4.362086	-1.418316	4.690781
H	2.997449	-1.563530	0.112431
H	2.856304	-1.511845	2.489608
H	1.609319	-1.833703	4.599793
H	-0.812654	-2.380359	4.528945
H	-1.974009	-2.590109	2.356281
H	-0.761133	-2.173752	0.251254

H	1.106581	0.336406	-3.046153
H	2.447592	0.526584	-5.113082
H	4.288781	-1.077325	-5.567708
H	4.779568	-2.890943	-3.944744
H	3.401920	-3.101044	-1.873589
H	5.166134	1.029911	-0.360190
H	3.407812	2.921938	-3.744244
H	2.298726	1.233016	1.783796
H	0.199311	3.630240	-2.060779
H	-7.203551	0.362178	-2.320487
H	-5.298776	-3.458033	-2.245072
H	-5.093923	1.739075	0.448021
H	-2.822221	-2.403071	0.314949
H	-7.922715	-1.230521	-3.790521
H	-3.406731	-4.697111	1.097825
H	-4.682369	-3.533302	1.512233
H	-4.903287	-4.638270	0.148187
H	-1.901831	-4.286077	-0.903125
H	-3.323467	-4.401727	-1.942764
H	-2.269262	-2.965290	-2.033863
H	-7.112801	-2.700658	-5.611953
H	-5.835948	-1.570813	-5.108530
H	-5.775099	-3.262464	-4.595431
H	-8.833584	-3.527512	-3.906203
H	-7.539481	-4.123442	-2.855209
H	-8.737053	-2.986517	-2.216946
H	-5.614342	3.611500	-1.036637
H	-4.549930	2.454817	-1.864343
H	-6.280610	2.518221	-2.259267
H	-7.308215	2.765531	0.701789
H	-8.007986	1.635984	-0.468637
H	-7.390771	1.031712	1.077798
H	7.131467	0.057003	-3.289959
H	6.926144	0.552992	-1.606968
H	5.717066	-0.499642	-2.370283
H	5.223989	1.355218	-4.018985
H	7.388916	2.573756	-3.803109
H	6.015963	3.665366	-3.527161
H	6.951251	3.059403	-2.151852
H	-0.029237	3.986972	-4.414069
H	1.690454	3.735254	-4.723647
H	0.654107	2.385655	-4.169114
H	0.667833	5.920305	-2.946163
H	1.579222	5.635039	-1.454553
H	2.400786	5.541501	-3.019751
H	3.680968	2.612223	3.383301
H	4.531169	3.319019	1.995621
H	2.801440	3.623629	2.232857
H	4.195569	0.265506	2.921845
H	4.306350	-0.342036	1.260013
H	5.350986	0.965559	1.796478
H	3.465175	-4.887083	3.435811
H	1.640549	-6.374672	2.118279
H	4.959625	-3.056643	3.603917
H	6.956065	-1.609041	3.641917
H	8.071223	-0.963962	1.519754
H	7.189850	-1.816611	-0.640283
H	5.221688	-3.303078	-0.673583
H	1.106538	-4.609780	-0.085820
H	0.970810	-4.747268	2.315762

TS1_Re_endo
SCF Energy: -3600.13817851
Num. Imaginary Frequencies: 1

C	-5.417613	-0.935851	-1.185969
C	-4.387158	-1.564187	-0.458999
C	-3.982188	-2.866312	-0.782541
C	-4.648630	-3.537726	-1.809486
C	-5.670763	-2.943608	-2.540154
C	-6.032858	-1.637552	-2.218400
C	-3.772954	-0.811014	0.675927
C	-2.818529	0.211509	0.416283
C	-2.470829	1.153486	1.359918
C	-2.885091	0.946010	2.714961
C	-3.756955	-0.136918	3.015245
C	-4.225675	-0.962135	1.960093
C	-4.129827	-0.374316	4.363542
C	-3.641379	0.409516	5.377388
C	-2.762008	1.475865	5.081703
C	-2.399656	1.741932	3.785946
O	-2.326969	0.310602	-0.855508
P	-0.729777	-0.001715	-1.123348
O	-0.407035	0.496016	-2.479408
C	-1.697979	2.354005	0.948971
C	-0.486839	2.200060	0.309136
C	0.341076	3.295302	-0.042921
C	-0.134388	4.558729	0.207640
C	-1.414216	4.785192	0.769891
C	-2.218441	3.673220	1.141167
C	-3.520064	3.924911	1.653528
C	-3.977727	5.207151	1.814545
C	-3.163870	6.311569	1.473446
C	-1.912179	6.100757	0.958964
O	-0.029057	0.938123	0.064217
C	1.703051	3.124562	-0.636983
C	1.904368	3.421449	-1.993788
C	3.209281	3.490896	-2.482180
C	4.321228	3.245299	-1.682177
C	4.084286	2.858835	-0.362014
C	2.801539	2.789853	0.179499
C	0.744483	3.695733	-2.942187
C	0.835446	2.859712	-4.224563
C	5.737182	3.458891	-2.216900
C	6.813687	2.738173	-1.397006
C	2.606495	2.389659	1.640736
C	2.355515	3.608937	2.542569
C	-2.862550	-3.561937	-0.022393
C	-1.891600	-4.291839	-0.955599
C	-6.362310	-3.693825	-3.663956
C	-6.147139	-3.002165	-5.016700
C	-5.851684	0.496785	-0.902719
C	-5.354540	1.439590	-2.007870
O	-0.327265	-1.373296	-0.642069
C	0.641924	5.191974	-3.268176
C	3.775470	1.581608	2.217073
C	5.881467	3.092439	-3.700411
C	-3.436200	-4.516779	1.033343
C	-7.856499	-3.890068	-3.376355
C	-7.367356	0.618906	-0.702839
N	2.365058	-0.951535	0.330550
C	3.281476	-0.743625	-0.718317
C	2.789785	-0.276640	-1.942853
C	3.657456	-0.116566	-3.012605
C	5.010779	-0.422722	-2.886649
C	5.502365	-0.843738	-1.656669
C	4.649463	-0.988058	-0.568836
C	2.657033	-1.567123	1.482670
C	1.758761	-1.456218	2.654337
C	2.350330	-1.579656	3.917956
C	1.580980	-1.500404	5.070691
C	0.204361	-1.314334	4.967447
C	-0.388934	-1.197328	3.714893
C	0.378073	-1.254835	2.555710
C	1.228001	-3.897401	0.533900
C	1.621860	-3.899701	-0.947001
O	3.077506	-4.040974	-0.955984
C	3.539312	-3.909946	0.271693
C	2.555736	-3.625243	1.212482
H	1.224692	-4.734395	-1.524442
H	-4.161680	3.088588	1.907975
H	-4.977867	5.376055	2.202621
H	-3.538992	7.321549	1.608985
H	-1.281434	6.939594	0.675268
H	0.490418	5.414357	-0.036041
H	-4.974833	-1.719985	2.174835
H	1.373141	-0.858834	0.076707
H	-1.711191	2.551334	3.568168
H	-2.366582	2.086686	5.887779
H	-3.925285	0.212833	6.406997
H	-4.802019	-1.201069	4.579256
H	3.709401	-1.563755	1.748014
H	3.425939	-1.726263	3.996050
H	2.053841	-1.583827	6.044333
H	-0.409668	-1.253935	5.860738
H	-1.459975	-1.056731	3.636327
H	-0.104229	-1.142364	1.588457
H	1.741229	-0.023855	-2.070406
H	3.261924	0.256184	-3.951982
H	5.680617	-0.317463	-3.734440
H	6.558731	-1.061634	-1.530682
H	5.073195	-1.303145	0.376912
H	4.925392	2.613097	0.274442
H	3.348059	3.760654	-3.523888
H	1.721544	1.743923	1.686107
H	-0.179021	3.390570	-2.442363
H	-6.819010	-1.149399	-2.790139
H	-4.360858	-4.557030	-2.055328
H	-5.384518	0.818950	0.032047
H	-2.280271	-2.791478	0.493736
H	-5.901524	-4.688693	-3.724067
H	-2.630120	-4.991535	1.605715
H	-4.084493	-3.984062	1.736740
H	-4.031260	-5.308529	0.562355
H	-1.112162	-4.782885	-0.363494
H	-2.385769	-5.074789	-1.541065
H	-1.415802	-3.581462	-1.637355
H	-8.329774	-4.481587	-4.168375
H	-8.009241	-4.404477	-2.422112
H	-8.375507	-2.926034	-3.323436
H	-6.588344	-3.592035	-5.828266
H	-6.615986	-2.011637	-5.030777
H	-5.080800	-2.869104	-5.223830
H	-5.603130	2.479504	-1.766350
H	-4.270507	1.361168	-2.127712
H	-5.822327	1.193396	-2.968719
H	-7.627223	1.644038	-0.416056
H	-7.919250	0.385565	-1.620418
H	-7.718612	-0.058473	0.082730
H	6.918473	3.234108	-4.024018
H	5.608757	2.046210	-3.868326
H	5.254360	3.713042	-4.346253
H	5.939813	4.537399	-2.133300
H	7.796280	2.881728	-1.859299
H	6.878094	3.121691	-0.373988
H	6.610660	1.662906	-1.347076
H	-0.049012	3.042034	-4.844806
H	1.717225	3.117180	-4.824249
H	0.853886	1.795340	-3.980573
H	-0.203083	5.382074	-3.939521
H	0.496900	5.790397	-2.362828
H	1.553526	5.548598	-3.763092
H	2.220240	3.290903	3.583071
H	3.212741	4.291721	2.503715
H	1.464829	4.164537	2.241077
H	3.470762	1.115372	3.160547
H	4.103969	0.797395	1.528746
H	4.641732	2.219346	2.430427
H	2.709346	-3.872964	2.255009
H	0.829811	-4.865599	0.856404
H	1.376214	-2.958173	-1.441528

H	0.463841	-3.138816	0.715449
C	4.981522	-4.044594	0.460013
C	5.546439	-3.899790	1.733551
C	5.812073	-4.280337	-0.642321
C	6.922745	-3.980481	1.899703
C	7.185998	-4.367225	-0.468983
C	7.744162	-4.214255	0.798987
H	4.912156	-3.722193	2.597115
H	5.370714	-4.373508	-1.627867
H	7.355598	-3.863151	2.887942
H	7.825913	-4.549115	-1.326540
H	8.819737	-4.279736	0.930441

M2_Re_endo
SCF Energy: -3600.15565252
Num. Imaginary Frequencies: 0

C	-1.120514	-3.627777	-1.917648
C	-1.404217	-3.625416	-0.537553
C	-0.576510	-4.344152	0.348033
C	0.507532	-5.057820	-0.166026
C	0.799789	-5.085222	-1.527238
C	-0.023227	-4.355965	-2.380159
C	-2.601027	-2.892037	-0.021734
C	-2.668182	-1.472993	-0.113607
C	-3.797815	-0.754556	0.234083
C	-4.850565	-1.445897	0.920337
C	-4.789223	-2.861390	1.042647
C	-3.671746	-3.556563	0.517086
C	-5.840278	-3.551893	1.700056
C	-6.897916	-2.871706	2.243316
C	-6.943796	-1.461838	2.155787
C	-5.950803	-0.769223	1.512261
O	-1.601757	-0.856977	-0.695355
P	-0.657642	0.256266	0.083233
O	-0.038534	1.019157	-1.040846
C	-3.906888	0.686720	-0.127029
C	-2.886170	1.554282	0.190780
C	-2.899027	2.941442	-0.120890
C	-4.026300	3.444307	-0.713943
C	-5.094925	2.602365	-1.116876
C	-5.021563	1.202401	-0.871880
C	-6.046128	0.376160	-1.406981
C	-7.104830	0.914966	-2.092460
C	-7.202126	2.310588	-2.286133
C	-6.212108	3.131360	-1.813614
O	-1.811035	1.080916	0.893669
C	-1.680807	3.767438	0.137329
C	-0.903983	4.207739	-0.952272
C	0.250285	4.945385	-0.693096
C	0.679552	5.231428	0.597618
C	-0.104931	4.784826	1.656621
C	-1.274598	4.055987	1.452675
C	-1.271837	3.910384	-2.400858
C	-0.086164	3.388853	-3.222195
C	1.956239	6.018076	0.829829
C	1.640730	7.455119	1.267500
C	-2.075901	3.609673	2.667295
C	-2.675427	4.818233	3.399180
C	-0.798541	-4.348788	1.854165
C	0.289124	-3.542250	2.570432
C	1.972133	-5.880863	-2.077455
C	1.937511	-7.345986	-1.625809
C	-1.996283	-2.916680	-2.941415
C	-1.223671	-1.833450	-3.705945
O	0.200231	-0.358130	1.148551
C	-1.884706	5.150272	-3.067607
C	-1.237446	2.739734	3.613156
C	2.894038	5.330841	1.828417
C	-0.913563	-5.771965	2.414650
C	3.320252	-5.235775	-1.724705
C	-2.641636	-3.926191	-3.901642
N	3.012216	0.589629	1.213123
C	3.545004	1.650145	0.464765
C	2.787666	2.268448	-0.539208
C	3.340239	3.301088	-1.289833
C	4.642780	3.737173	-1.063220
C	5.384877	3.147233	-0.040564
C	4.841286	2.126291	0.725054
C	3.791337	-0.604682	1.361777
C	3.440961	-1.395723	2.614277
C	4.197070	-2.519745	2.960162
C	3.937923	-3.221067	4.131463
C	2.916493	-2.800915	4.980103
C	2.161846	-1.683761	4.642773
C	2.418048	-0.984853	3.465758
C	2.311693	-2.059761	-0.268069
C	1.991608	-1.405948	-1.608146
O	3.277476	-0.819907	-2.059481
C	4.171692	-0.881411	-1.154546
C	3.721826	-1.558599	0.090190
H	1.695382	-2.098000	-2.396269
H	-5.982220	-0.697898	-1.277394
H	-7.872520	0.260227	-2.494368
H	-8.050457	2.726184	-2.821647
H	-6.258539	4.204843	-1.979216
H	-4.087121	4.507151	-0.932149
H	-3.650453	-4.642399	0.577961
H	2.009262	0.421272	1.087440
H	-5.993741	0.312997	1.458330
H	-7.770469	-0.922085	2.608065
H	-7.693697	-3.408640	2.750943
H	-5.780357	-4.634734	1.777458
H	4.841501	-0.311167	1.451554
H	5.015952	-2.848624	2.321775
H	4.538507	-4.089545	4.385972
H	2.711556	-3.343750	5.897948
H	1.357108	-1.352758	5.291978
H	1.813532	-0.124678	3.205729
H	1.765510	1.940425	-0.724221
H	2.733604	3.761840	-2.063777
H	5.067122	4.541353	-1.656989
H	6.391590	3.495272	0.173159
H	5.418778	1.705276	1.542901
H	0.204735	5.001762	2.676281
H	0.852741	5.295561	-1.528217
H	-2.913767	2.997344	2.322480
H	-2.022838	3.116712	-2.404391
H	0.181972	-4.377052	-3.449319
H	1.144960	-5.605057	0.525242
H	-2.812741	-2.418413	-2.413805
H	-1.745004	-3.846009	2.061247
H	1.882634	-5.871107	-3.171603
H	-1.163180	-5.736266	3.480795
H	-1.693804	-6.342116	1.898215
H	0.026982	-6.326392	2.316560
H	0.123928	-3.564439	3.653163
H	1.292041	-3.947352	2.382702
H	0.269710	-2.497182	2.247273
H	4.150338	-5.815547	-2.143918
H	3.386603	-4.216534	-2.123516
H	3.459089	-5.188699	-0.637293
H	2.734062	-7.918385	-2.114280
H	2.082315	-7.433610	-0.543124
H	0.977822	-7.809575	-1.873218
H	-1.884869	-1.335663	-4.423846
H	-0.839550	-1.073184	-3.020669
H	-0.387208	-2.263114	-4.271950
H	-3.327402	-3.413656	-4.585349
H	-1.890285	-4.444129	-4.509148
H	-3.209005	-4.683851	-3.350940
H	3.849574	5.864642	1.885184
H	2.461923	5.317554	2.835792
H	3.095161	4.297713	1.532222
H	2.483813	6.067288	-0.132064
H	2.562030	8.036733	1.390072
H	1.006819	7.961524	0.532168
H	1.108942	7.458459	2.226364
H	-0.431274	3.088943	-4.218760
H	0.683321	4.157944	-3.366329
H	0.354167	2.518578	-2.730555
H	-2.176867	4.930320	-4.101044
H	-2.771081	5.502099	-2.530031
H	-1.161120	5.974269	-3.088138
H	-3.287122	4.490289	4.247610
H	-1.889998	5.478065	3.786124
H	-3.307674	5.409508	2.728135
H	-1.860542	2.366456	4.434210
H	-0.819259	1.881906	3.079810
H	-0.412561	3.310105	4.056366
H	4.412352	-2.387946	0.281687
H	2.290447	-3.144323	-0.348927
H	1.300837	-0.559318	-1.558220
H	1.570208	-1.756904	0.473737
C	5.469403	-0.309158	-1.432990
C	6.579867	-0.667406	-0.652137
C	5.603746	0.641949	-2.455875
C	7.810126	-0.081483	-0.896379
C	6.837033	1.231972	-2.683653
C	7.936268	0.871375	-1.907939
H	6.482437	-1.409495	0.133837
H	4.731522	0.942081	-3.024977
H	8.671736	-0.361218	-0.299541
H	6.937381	1.986574	-3.456148
H	8.899173	1.339600	-2.087271

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SCF Energy: -3600.14633121
Num. Imaginary Frequencies: 1

C	-5.319158	-1.114108	-1.356098
C	-4.417082	-1.511401	-0.355082
C	-4.022191	-2.856911	-0.249807
C	-4.575561	-3.788845	-1.125035
C	-5.482229	-3.423200	-2.117095
C	-5.831988	-2.082111	-2.219445
C	-3.912108	-0.496715	0.617145
C	-2.954649	0.475299	0.214488
C	-2.600247	1.538277	1.016025
C	-3.030913	1.540041	2.382135
C	-3.958589	0.554346	2.815086
C	-4.418238	-0.416713	1.888835
C	-4.377055	0.540044	4.170890
C	-3.874979	1.443995	5.070928
C	-2.932054	2.407875	4.647714
C	-2.526807	2.460220	3.338773
O	-2.463496	0.397512	-1.059118
P	-0.874522	0.029258	-1.298236
O	-0.544103	0.391062	-2.696571
C	-1.785637	2.648261	0.459527
C	-0.559357	2.378876	-0.108138
C	0.341785	3.409755	-0.493377
C	-0.089236	4.708366	-0.405332
C	-1.394320	5.037613	0.037865
C	-2.258943	4.000154	0.480870
C	-3.571690	4.350023	0.896983
C	-3.986498	5.657069	0.895814
C	-3.114462	6.689307	0.482214
C	-1.847939	6.381695	0.060313
O	-0.150157	1.079897	-0.213206
C	1.759284	3.097530	-0.851251
C	2.147001	2.931484	-2.193739

C	3.490281	2.692175	-2.469627
C	4.453004	2.587566	-1.467015
C	4.041543	2.748542	-0.148677
C	2.712522	3.025799	0.179576
C	1.143057	3.094750	-3.326619
C	1.358419	2.124286	-4.490806
C	5.905691	2.366830	-1.858012
C	6.491607	3.654053	-2.460044
C	2.330822	3.256175	1.638466
C	3.353018	4.112060	2.395884
C	-3.015527	-3.313234	0.796149
C	-1.948397	-4.241918	0.210279
C	-6.048584	-4.450214	-3.080657
C	-6.800314	-5.570070	-2.350148
C	-5.751516	0.334159	-1.536827
C	-5.268734	0.889607	-2.883365
O	-0.502701	-1.300102	-0.697768
C	1.157947	4.546985	-3.827355
C	2.081374	1.931077	2.366488
C	6.794490	1.867578	-0.717930
C	-3.713279	-3.977780	1.990233
C	-4.949638	-5.022891	-3.986141
C	-7.268191	0.495131	-1.371120
N	2.161404	-0.736193	0.420984
C	3.054446	-0.753301	-0.592683
C	2.650770	-0.486210	-1.928406
C	3.541181	-0.683561	-2.949243
C	4.871822	-1.111268	-2.711963
C	5.298378	-1.292021	-1.424169
C	4.391996	-1.162057	-0.345001
C	2.438279	-1.497440	1.600109
C	1.387726	-1.366334	2.685067
C	1.818813	-1.389536	4.013548
C	0.909558	-1.284811	5.060595
C	-0.448946	-1.152229	4.787833
C	-0.885010	-1.132946	3.467604
C	0.022757	-1.239067	2.418204
C	1.445321	-3.613761	0.445447
C	1.933134	-3.742454	-0.990654
O	3.379646	-3.847215	-0.871053
C	3.790100	-3.310536	0.254883
C	2.651744	-3.015887	1.196264
H	1.607168	-4.643746	-1.508249
H	-4.255929	3.567551	1.205931
H	-4.997600	5.900152	1.208936
H	-3.454785	7.720539	0.489966
H	-1.170359	7.163213	-0.274333
H	0.595469	5.511221	-0.667497
H	-5.179652	-1.125695	2.202993
H	1.181127	-0.637559	0.150233
H	-1.794356	3.196448	3.026248
H	-2.522850	3.111102	5.366972
H	-4.193925	1.418040	6.108776
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H	-4.249525	-4.880505	1.673574
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H	-1.432244	-3.745912	-0.616971
H	-5.371753	-5.719831	-4.719462
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M3_Re_endo

SCF Energy: -3600.16146809

Num. Imaginary Frequencies: 0

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H	1.642937	0.557658	-1.368138
H	2.094078	-0.737178	0.590531
C	5.754209	1.548993	-0.964868
C	6.614065	1.985925	0.046922
C	6.281267	1.277902	-2.226474
C	7.972781	2.149411	-0.195630
C	7.642492	1.443726	-2.470516
C	8.491997	1.880044	-1.459482
H	6.229035	2.191080	1.043741
H	5.615984	0.931403	-3.008246
H	8.626985	2.484126	0.603802
H	8.039454	1.228725	-3.458186
H	9.552807	2.008201	-1.651625

SELECTED GEOMETRIC PARAMETERS AND CALCULATED ENERGIES FOR TERNARY COMPLEXES 6b/7d/5a (M_1 AND TS_1)

Selected geometric parameters,[a] bond distances (d) in Å [π-stacking interactions are described as parallel-displaced (PD) or T-shaped (T)] and dihedral angles (Dh) in degrees, for the ternary complexes **6b**/**7d**/**5a** (M_1) and transition structures of the first step (TS_1) corresponding to the four diastereomeric combinations in the Povarov reaction between benzylideneaniline **6b** and Ph-DHF **5a** catalyzed by (*R*)-TRIP **7d**.

	$M_{1Re\text{-}exo}$	$M_{1Re\text{-}endo}$	$M_{1Si\text{-}exo}$	$M_{1Si\text{-}endo}$	$TS_{1Re\text{-}exo}$	$TS_{1Re\text{-}endo}$	$TS_{1Si\text{-}exo}$	$TS_{1Si\text{-}endo}$
Dh_{abcd}	18.9	50.9	-40.2	-43.6	1.83	-9.9	-13.3	-1.9
Dh_{cdef}	-24.1	11.1	9.64	-9.5	32.1	28.6	-52.4	-26.3
$d_{N\text{-}H}$	1.08	1.07	1.07	1.08	1.03	1.03	1.05	1.03
$d_{H\text{-}OP^*}$	1.57	1.57	1.54	1.54	1.83	1.92	1.61	1.75
dππ Ar^2-TRIP[b]	5.62 (PD)	4.16 (PD)	--	--	4.06 (PD)	3.94 (PD)	--	--
dππAr^1-Naphth	6.93 (T)	4.13 (PD)	--	--	4.98 (T)	4.72 (T)	--	--
dππ Ar^2-Ar^3	4.19 (PD)	--	--	--	3.55 (PD)	--	4.00 (PD)	--
dππAr^1-TRIP[b]	--	--	3.94 (PD)	4.02 (PD)	--	--	4.62 (T)	5.10 (T)
dππAr^2-Naphth	--	--	4.92(T)	4.92 (T)	--	--	4.86 (T)	--
dππ Ar^1-Ar^3	--	--	3.72 (PD)	4.88 (PD)	--	4.85 (PD)	--	--
dC_{imine}-C_{DHF}	--	--	--	--	2.11	2.08	1.98	2.12

[a] Computed at the wB97XD-PCM(CH_2Cl_2)/6-31G*//wB97XD/6-31G* level. [b] TRIP refers to triisopropylphenyl group of **7d**.

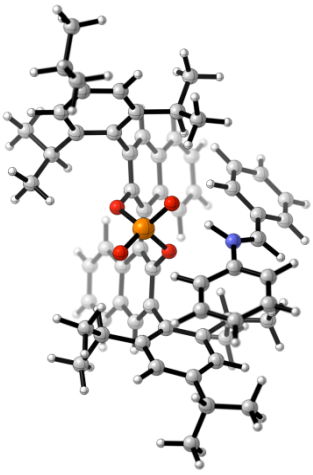
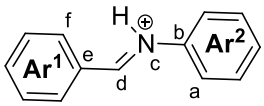
Calculated energies (ΔG_1; ΔG_2 are relative to the diastereomer minima, kcal/mol)[a] computed for the Povarov reaction between benzylideneaniline **6b** and Ph-DHF **5a** catalyzed by (R)-TRIP **7d**.

	ΔG_1	ΔG_2		ΔG_1	ΔG_2
M_1*Si-exo*	***0.0***	0.1	**M_1*Re-exo***	***0.0***	2.9
TS_1*Si-exo*	10.4	10.5	**TS_1*Re-exo***	6.5	9.5
M_2*Si-exo*	-3.4	-3.3	**M_2*Re-exo***	-9.8	-6.9
TS_2*Si-exo*	6.5	6.6	**TS_2*Re-exo***	-5.6	-2.7
M_3*Si-exo*	-21.3	-21.2	**M_3*Re-exo***	-24.6	-21.6
M_1*Si-endo*	***0.0***	***0.0***	**M_1*Re-endo***	***0.0***	1.9
TS_1*Si-endo*	15.2	15.2	**TS_1*Re-endo***	11.8	13.7
M_2*Si-endo*	-6.9	-6.9	**M_2*Re-endo***	-4.2	-2.3
TS_2*Si-endo*	8.5	8.5	**TS_2*Re-endo***	-0.4	1.5
M_3*Si-endo*	-19.5	-19.6	**M_3*Re-endo***	-12.7	-10.7

[a] Computed at the wB97XD-PCM(CH_2Cl_2)/6-31G*//wB97XD/6-31G* level.

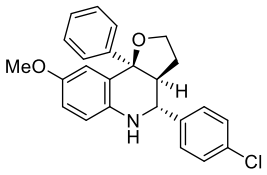
BINARY COMPLEXES 6b/7d

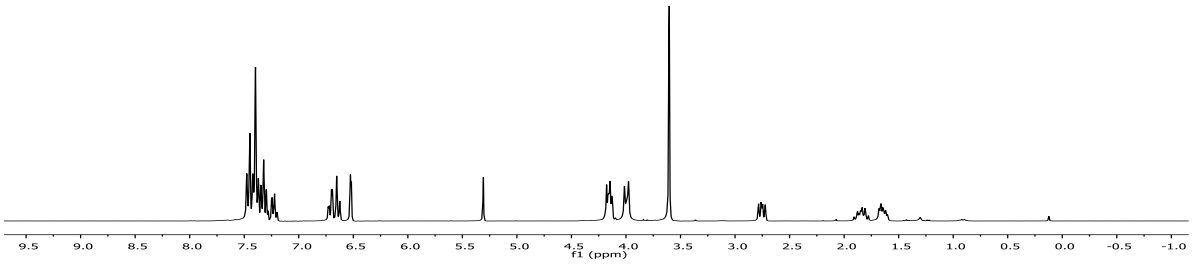
Representation of the binary complexes **6b**/**7d** and selected geometric data (distances in Å, dihedral angles in degrees) for the structures computed at the wB97XD-PCM(CH_2Cl_2)/6-31G* level.

Re 	 Dh_{abcd} 37.8 Dh_{cdef} 6.06 $d_{N\text{-}H}$ 1.07 Å $d_{H\text{-}OR^*}$ 1.57 Å d_{bc} 1.43 Å d_{cd} 1.29 Å d_{de} 1.44 Å d□□□ Ar^2-TRIP 4.06 Å
Si 	Dh_{abcd} -43.1 Dh_{cdef} 0.19 $d_{N\text{-}H}$ 1.09 Å $d_{H\text{-}OR^*}$ 1.50 Å d_{bc} 1.43 Å d_{cd} 1.29 Å d_{de} 1.45 Å d□□□ Ar^1-TRIP 4.01 Å d□□□ Ar^2-Napht 2.68 Å

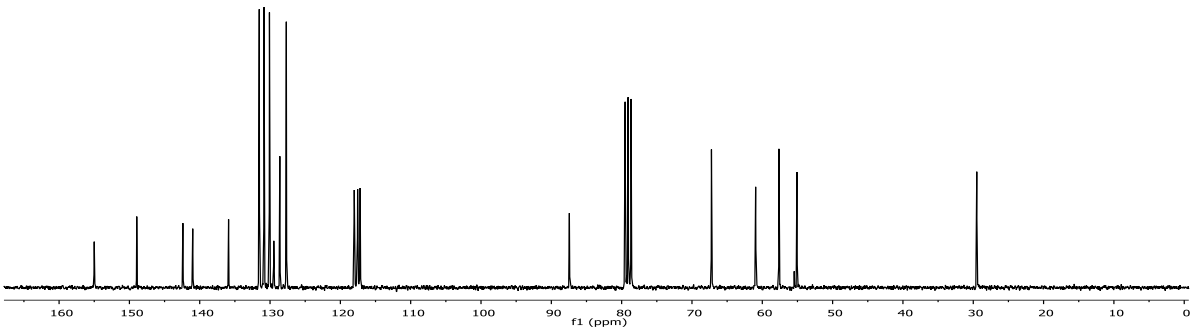
NMR SPECTRA

(3a*R*,4*S*,9b*S*)-4-(4-Chlorophenyl)-8-methoxy-9b-phenyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4a)



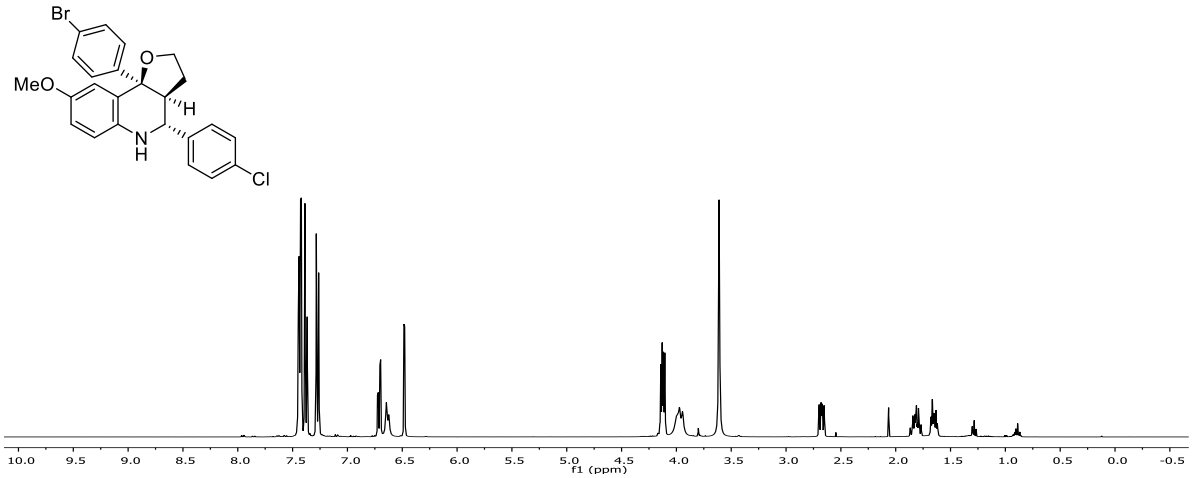


^{1}H-NMR

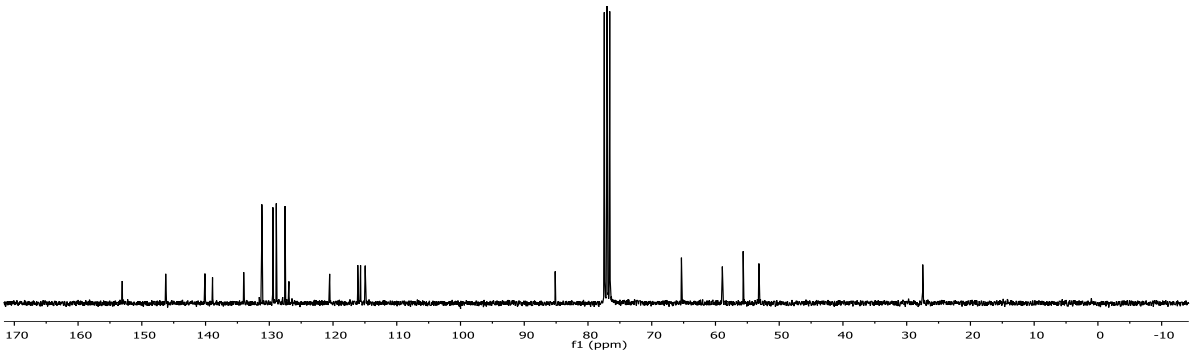


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-chlorophenyl)-8-methoxy-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4b)

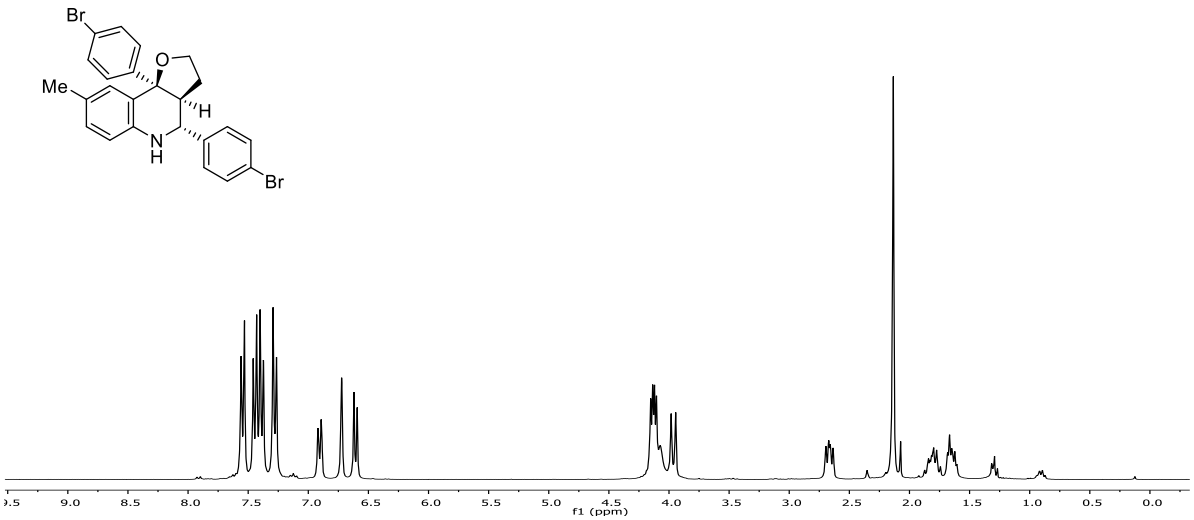


^{1}H-NMR

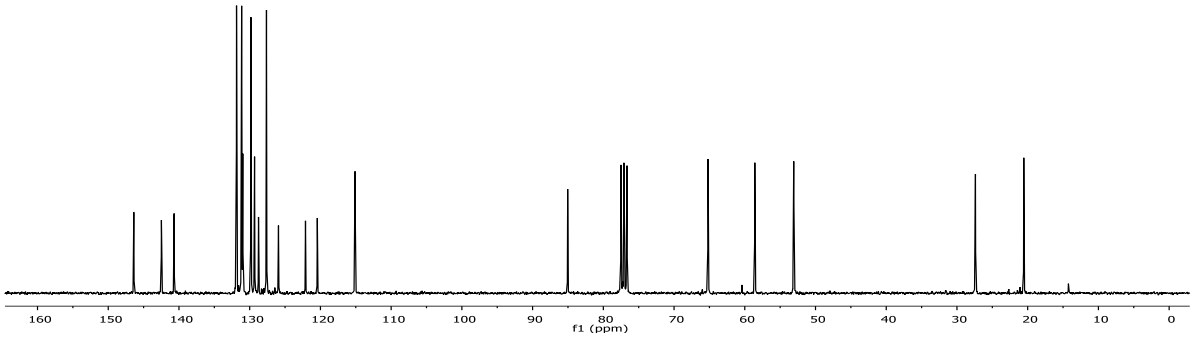


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-4,9b-Bis(4-bromophenyl)-8-methyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4c)

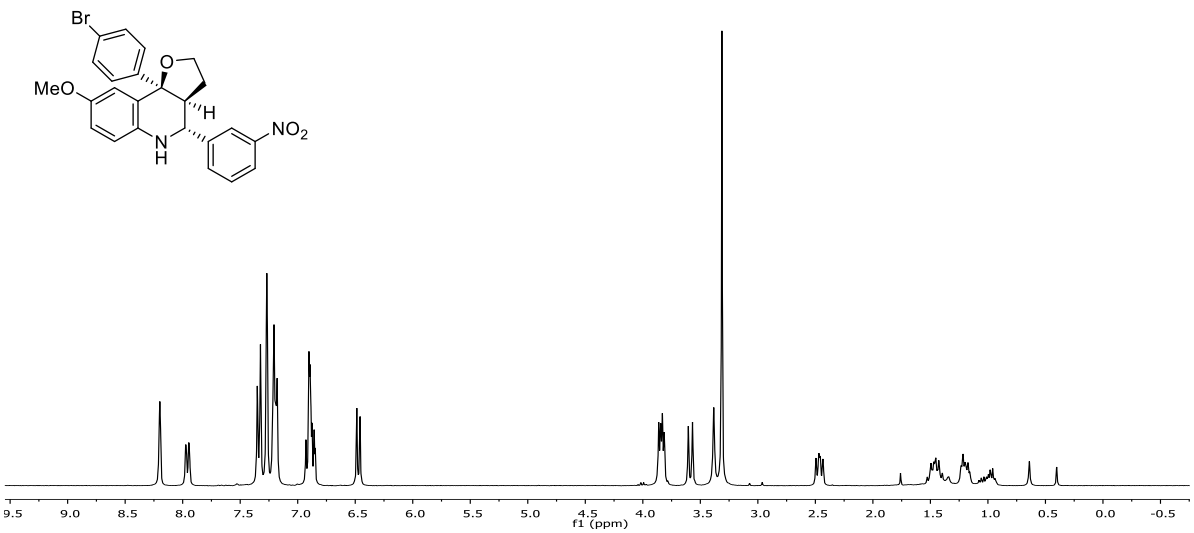


^{1}H-NMR

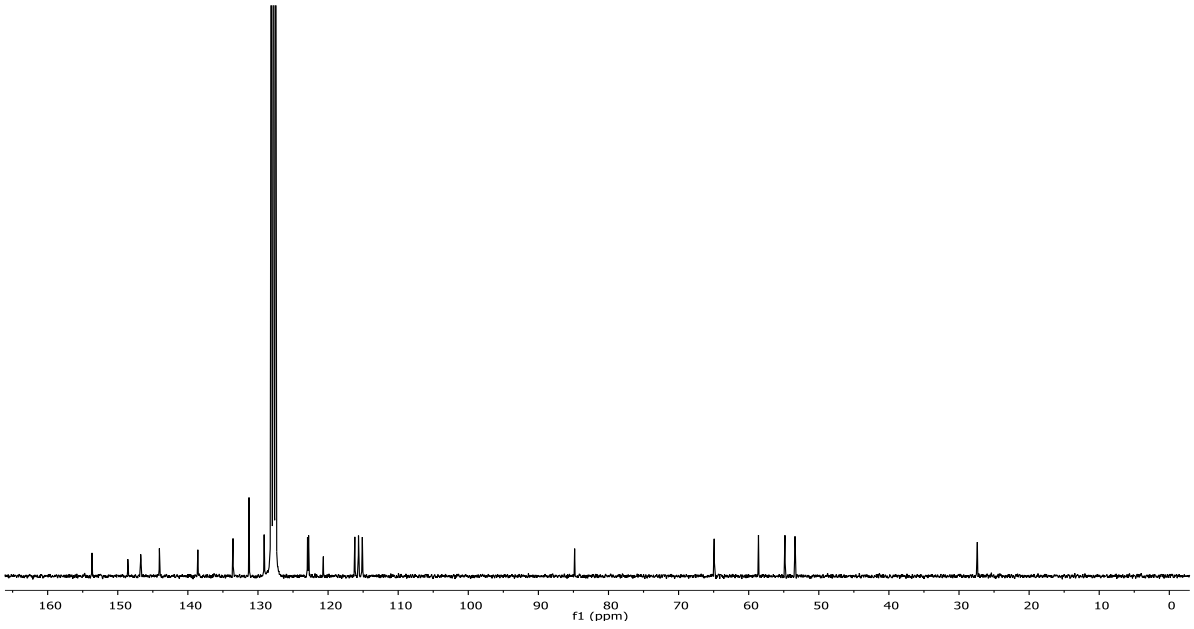


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-methoxy-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4d)

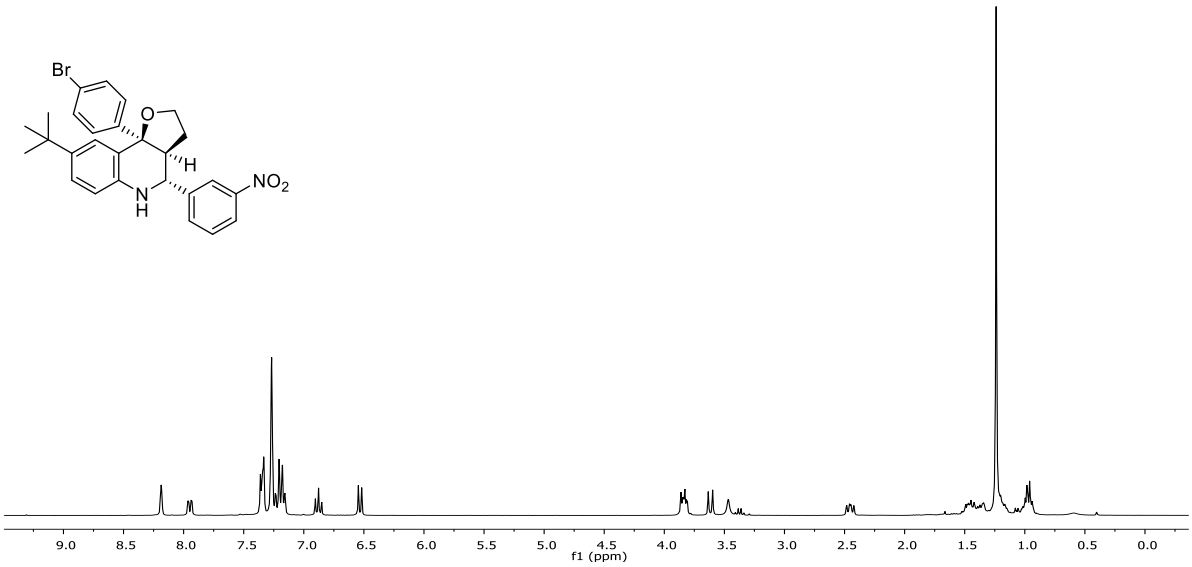


^{1}H-NMR

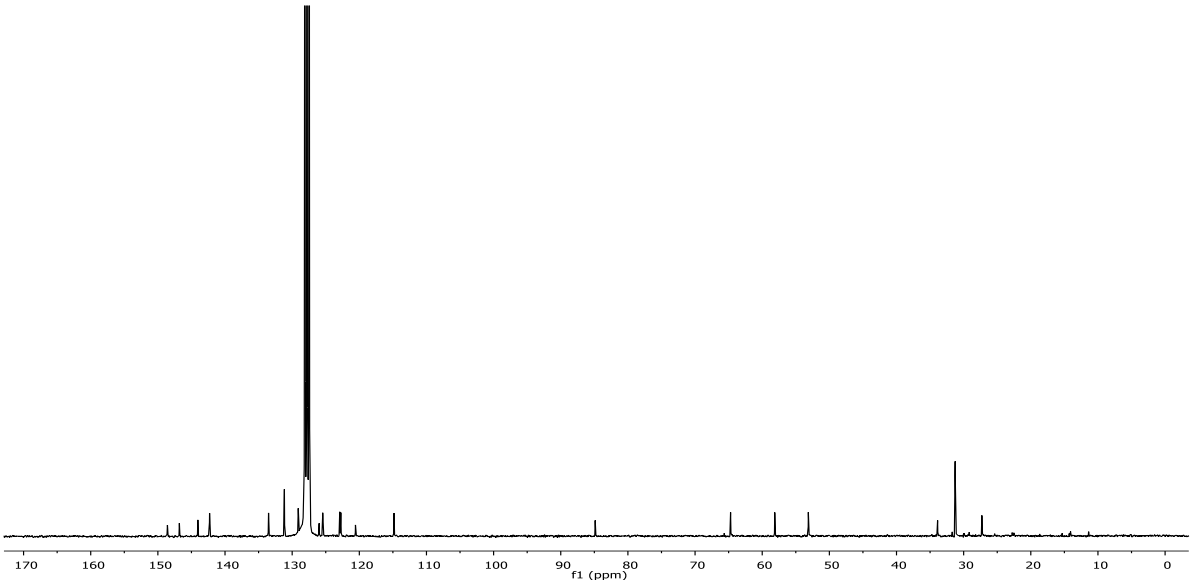


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-tert-butyl-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4e)

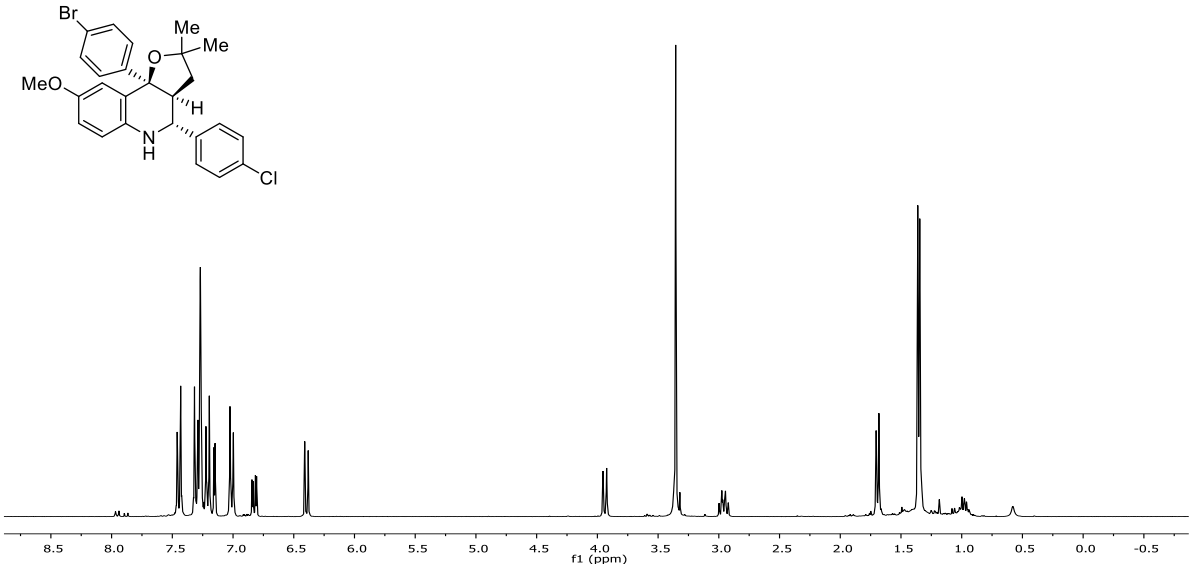


^{1}H-NMR

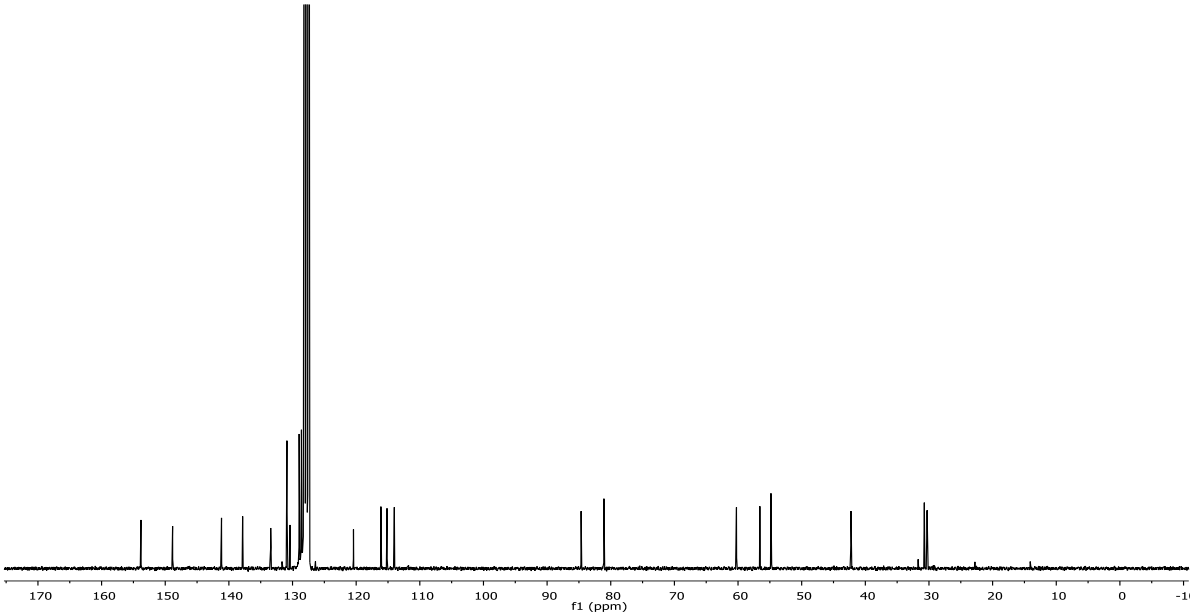


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-chlorophenyl)-8-methoxy-2,2-dimethyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4f)

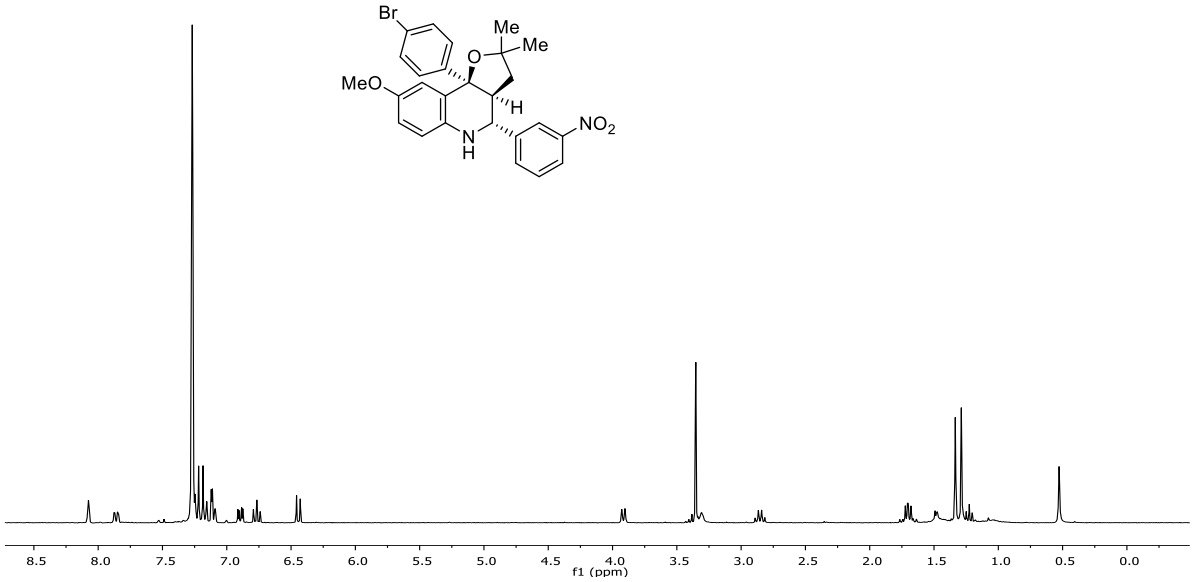


^{1}H-NMR

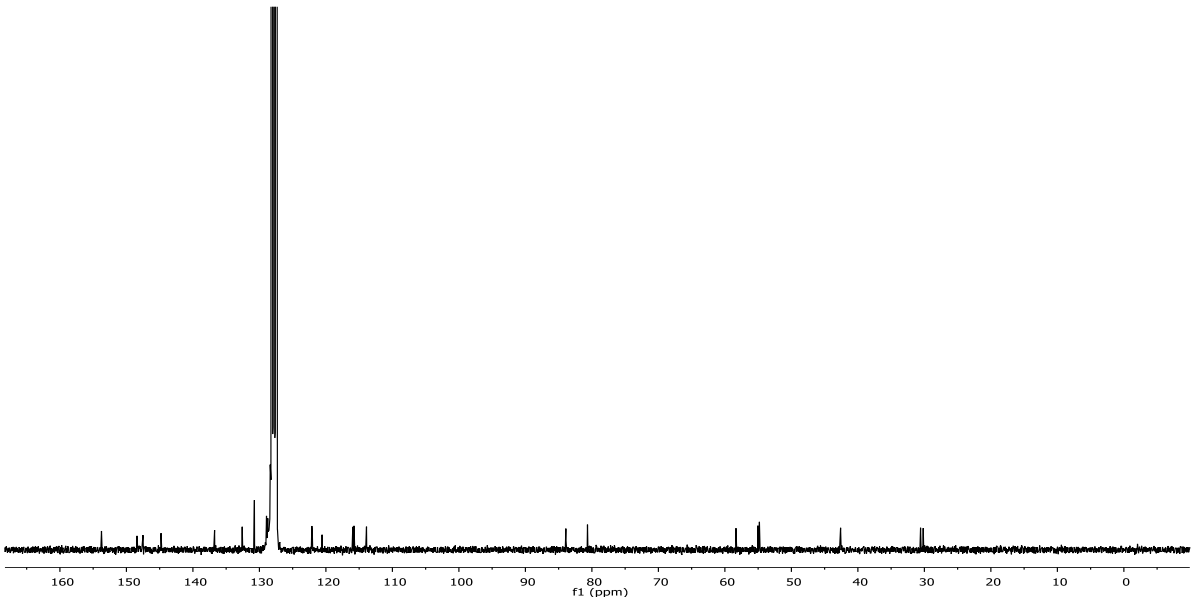


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-methoxy-2,2-dimethyl-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4g)

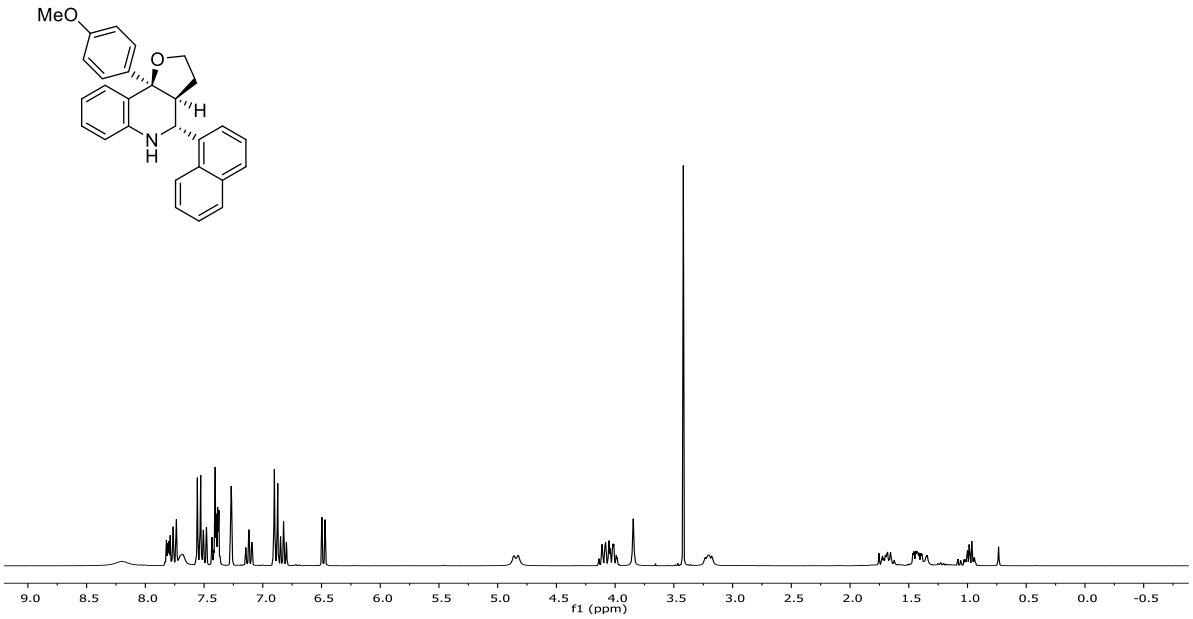


^{1}H-NMR

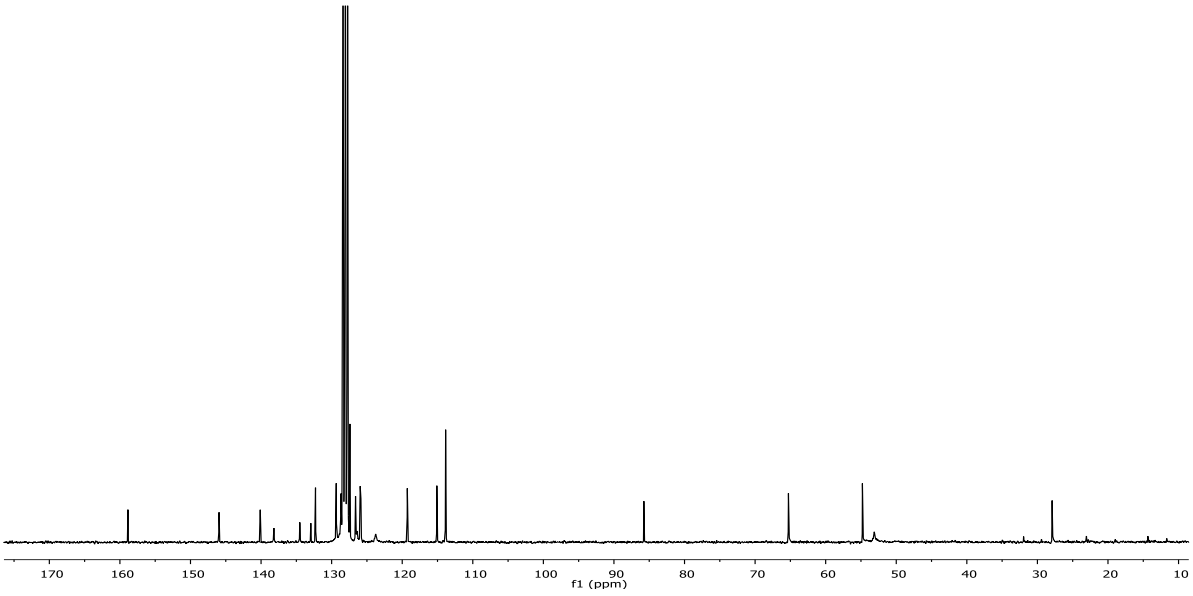


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-9b-(4-Methoxyphenyl)-4-(naphthalen-1-yl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4h)

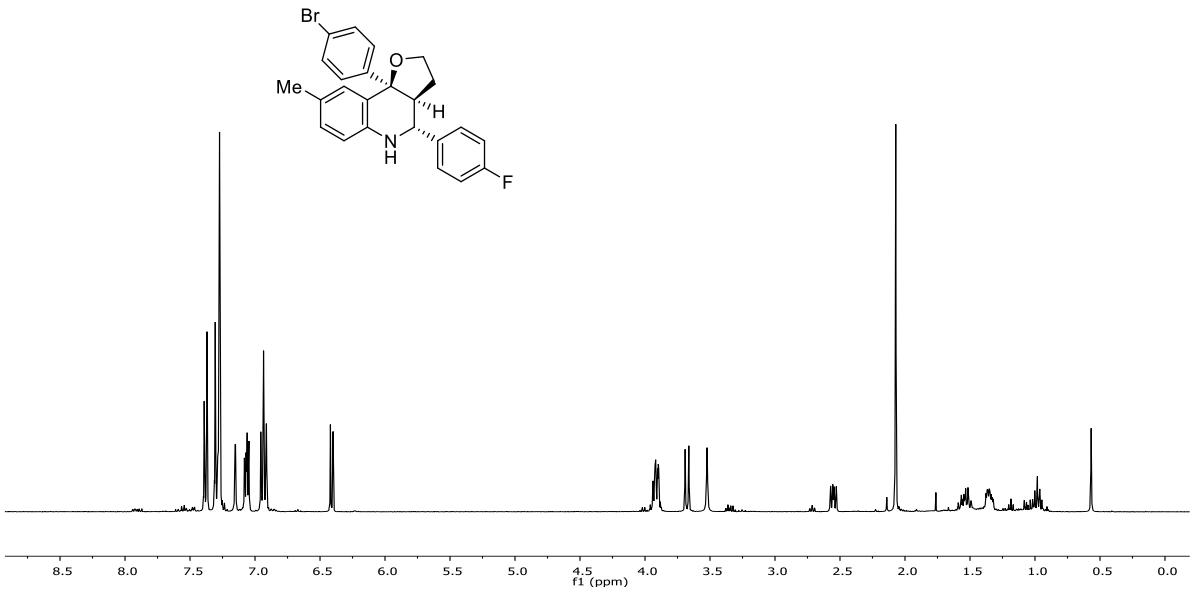


^{1}H-NMR

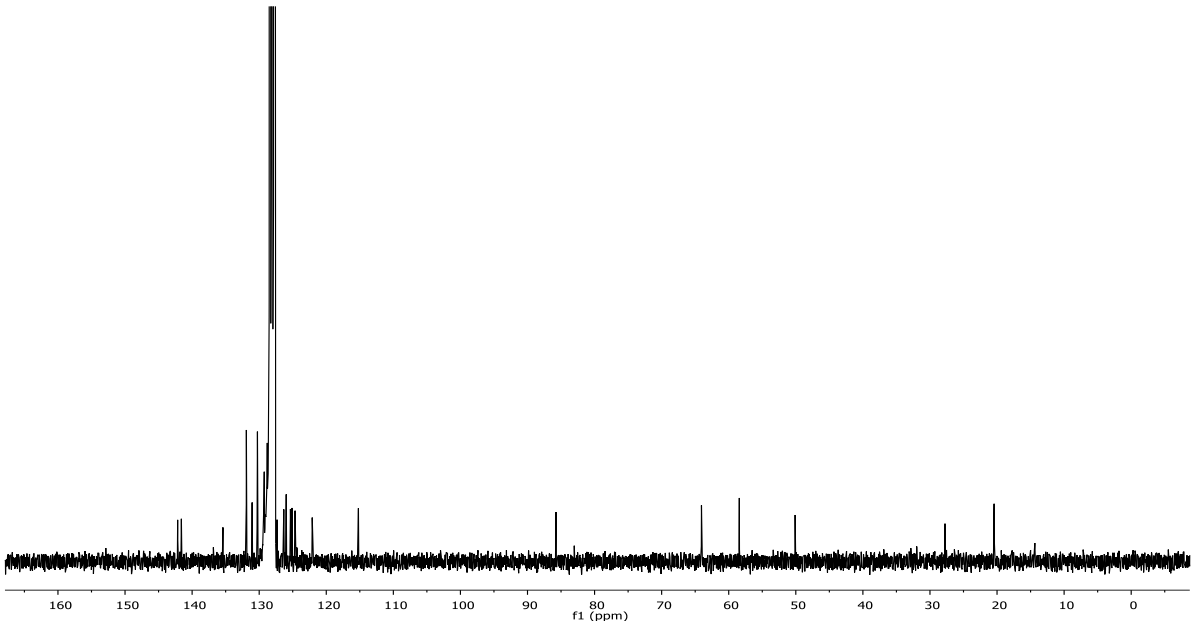


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-fluorophenyl)-8-methyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4i).

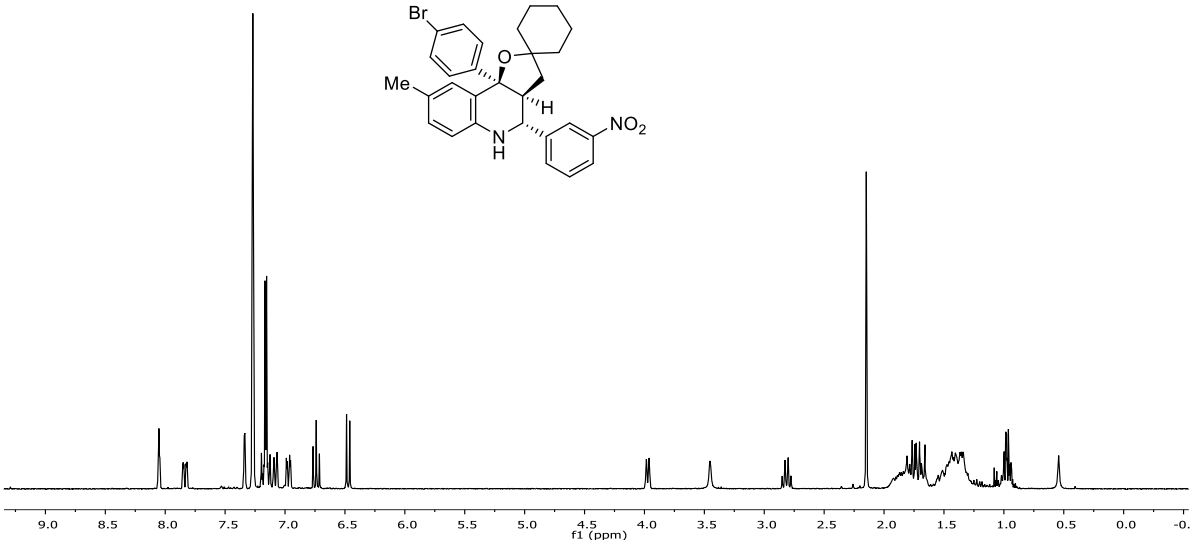


^{1}H-NMR

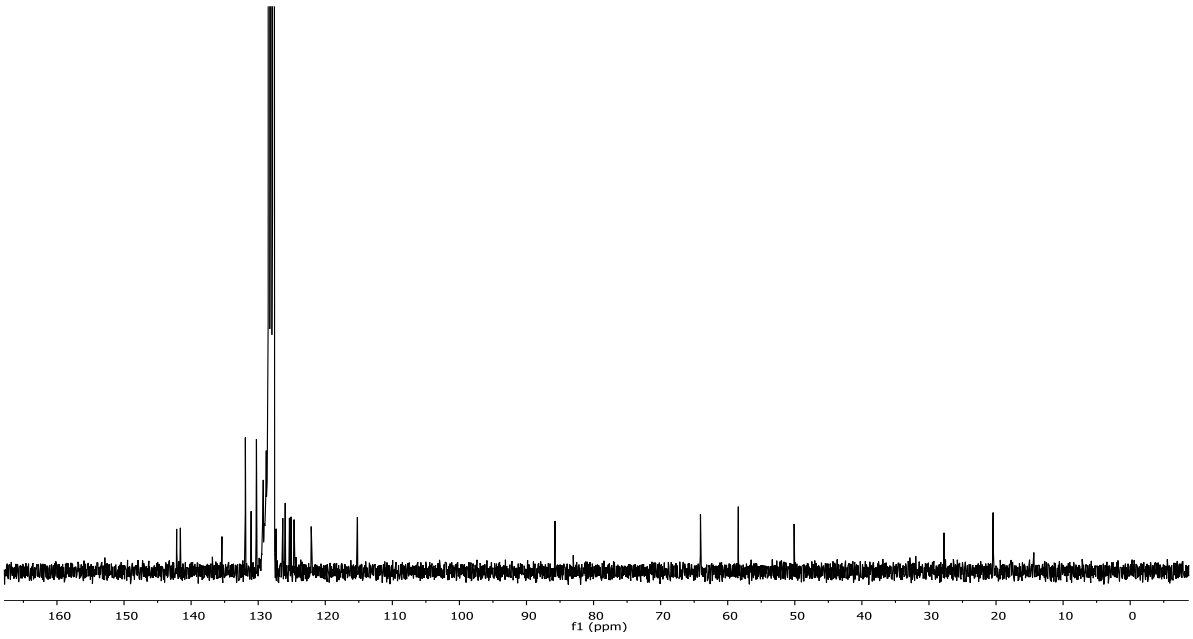


^{13}C-NMR

(3a'*R*,4'*S*,9b'*S*)-9b'-(4-Bromophenyl)-8'-methyl-4'-(3-nitrophenyl)-3a',4',5',9b'-tetrahydro-3'*H*-spiro[cyclohexane-1,2'-furo[3,2-*c*]quinoline] (4j)

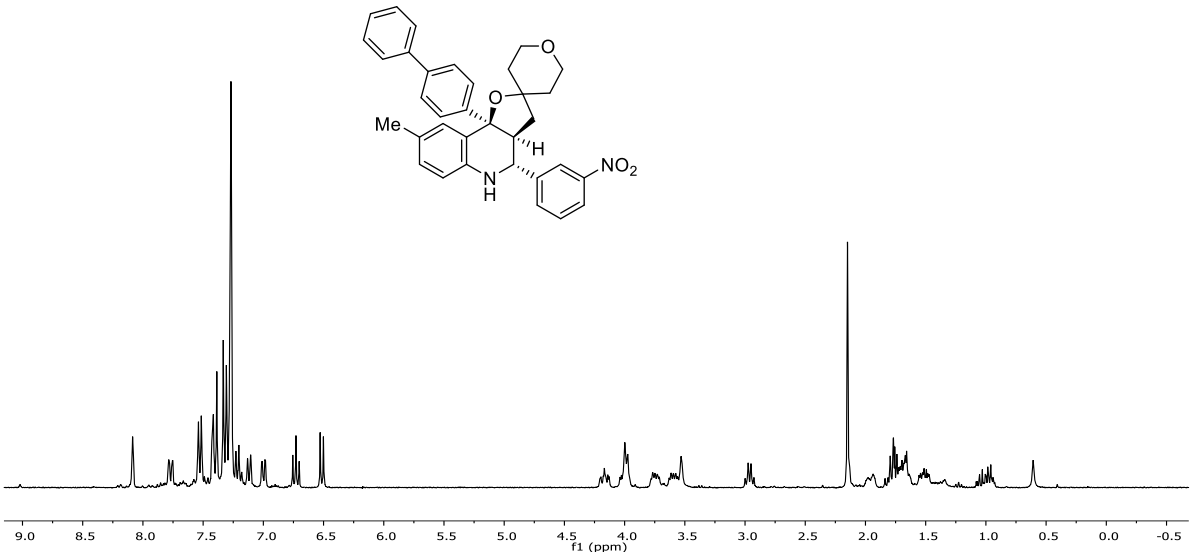


^{1}H-NMR

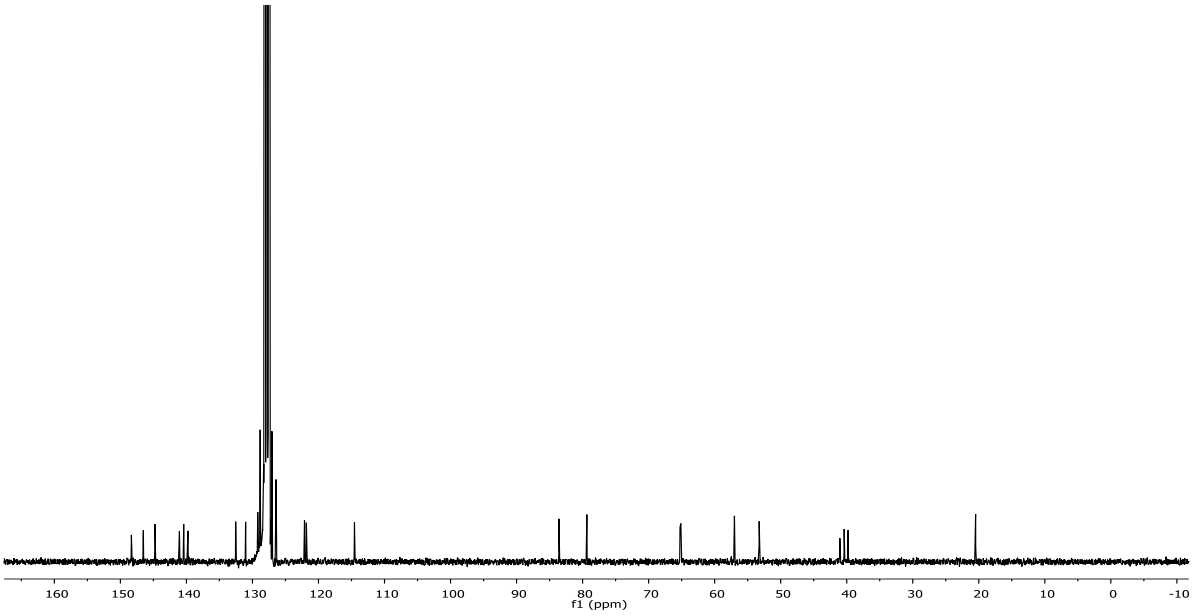


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-9b-(Biphenyl-4-yl)-8-methyl-4-(3-nitrophenyl)-2',3a,3',4,5,5',6',9b-octahydro-3*H*-spiro[furo[3,2-*c*]quinoline-2,4'-pyran] (4k)

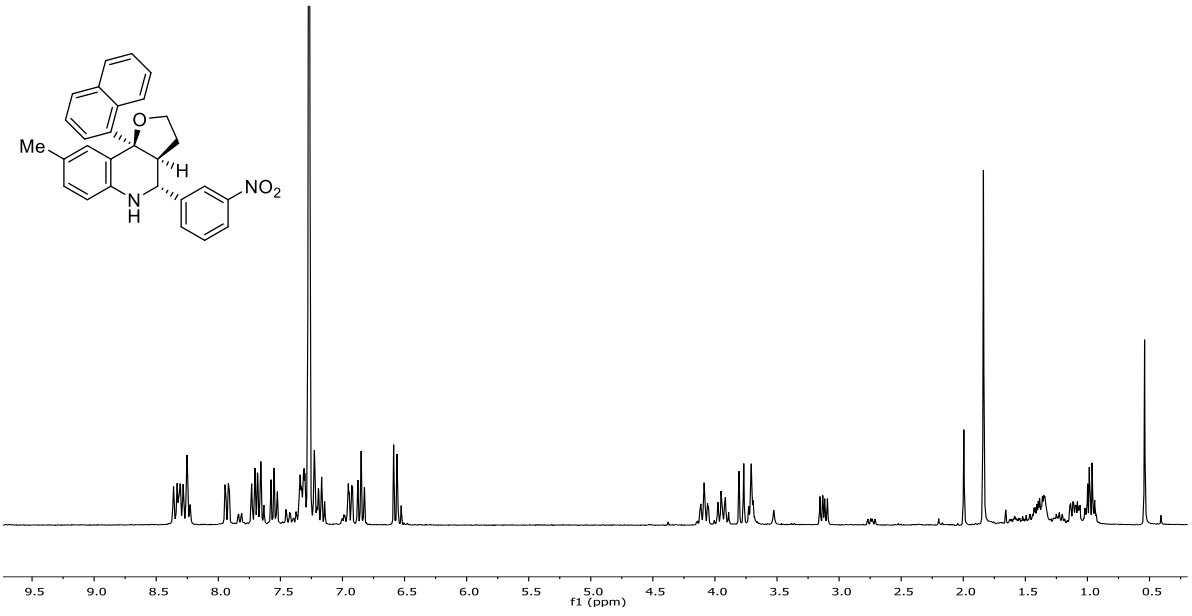


^{1}H-NMR

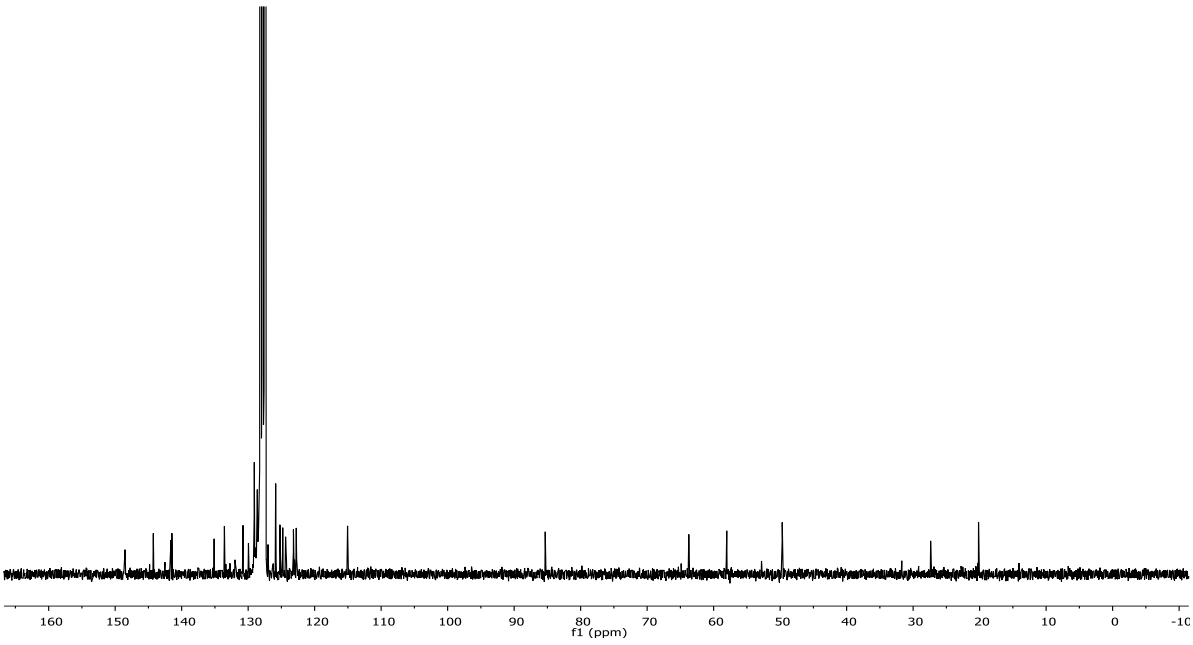


^{13}C-NMR

(3a*R*,4*S*,9b*S*)-8-Methyl-9b-(naphthalen-1-yl)-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4l)

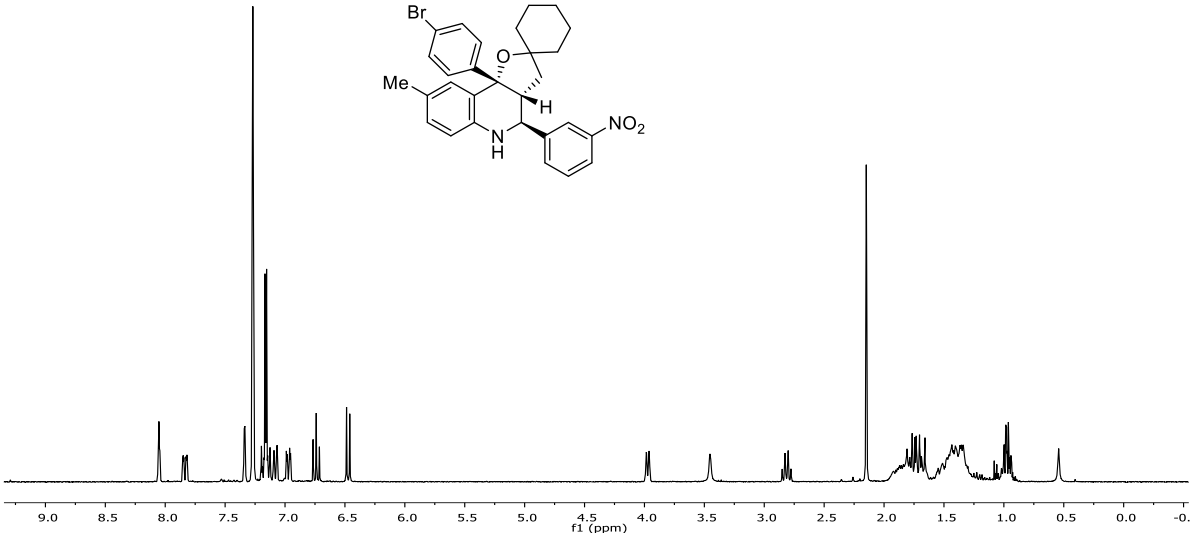


^{1}H-NMR

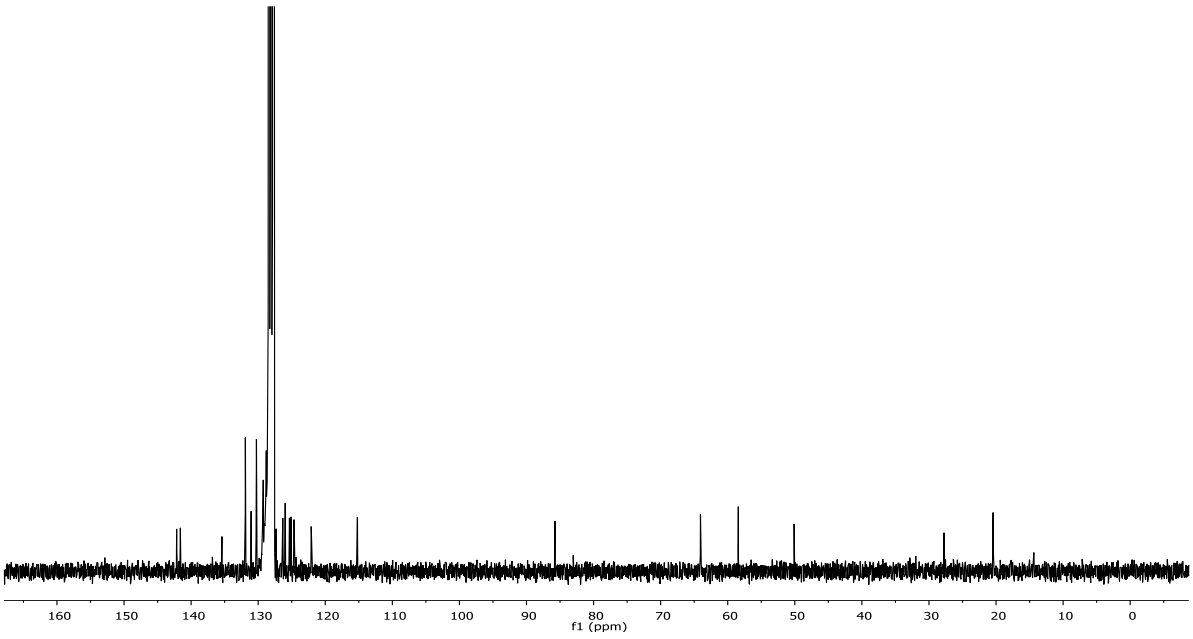


^{13}C-NMR

(3a'*S*,4'*R*,9b'*R*)-9b'-(4-Bromophenyl)-8'-methyl-4'-(3-nitrophenyl)-3a',4',5',9b'-tetrahydro-3'*H*-spiro[cyclohexane-1,2'-furo[3,2-*c*]quinoline] (*ent*-4j)



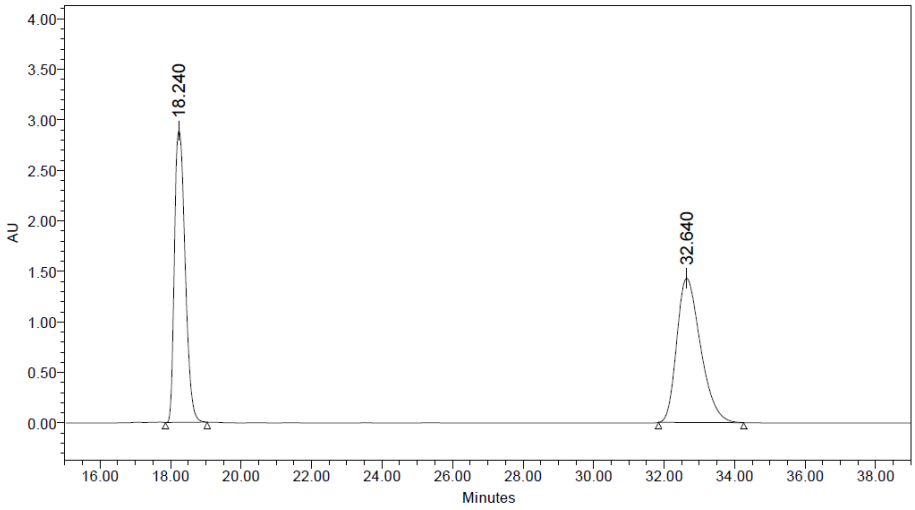
^{1}H-NMR



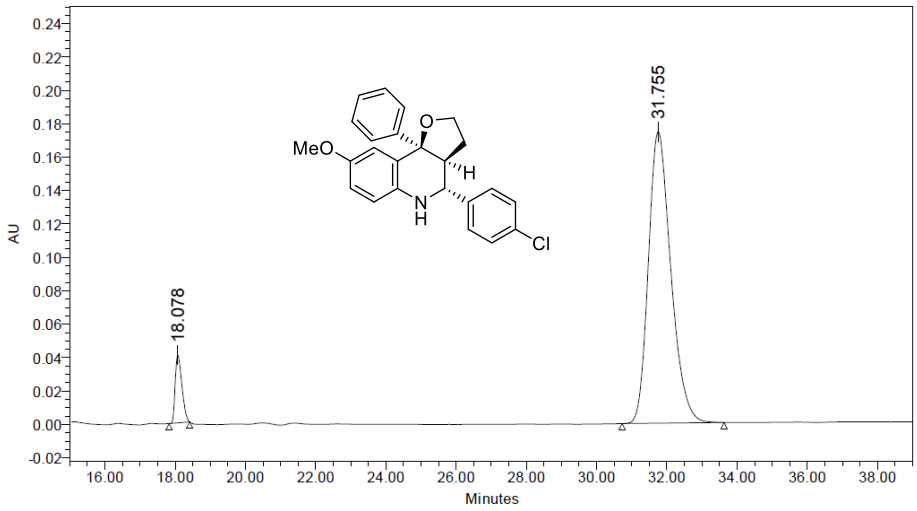
^{13}C-NMR

HPLC CHARTS

(3a*R*,4*S*,9b*S*)-4-(4-Chlorophenyl)-8-methoxy-9b-phenyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-c]quinoline (4a)

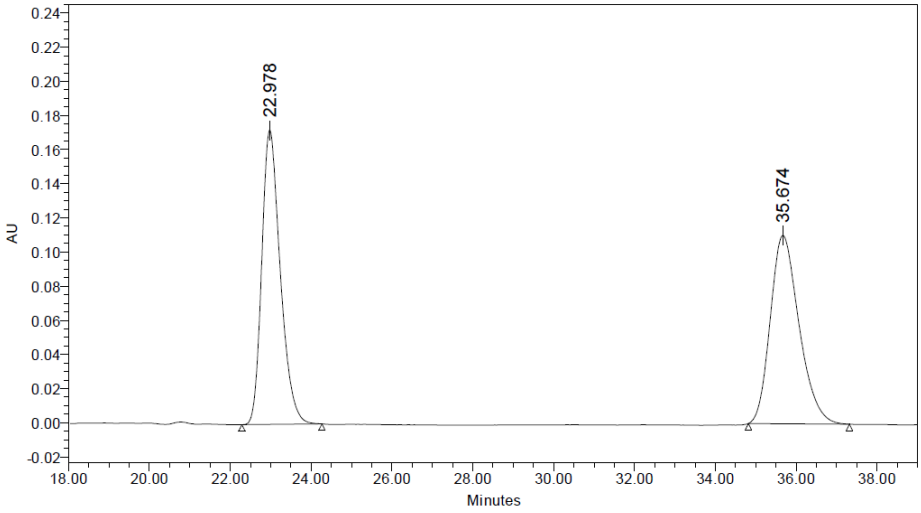


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 211.5 nm	18.240	60794723	47.64	2886665
2	PDA 211.5 nm	32.640	66827964	52.36	1427610

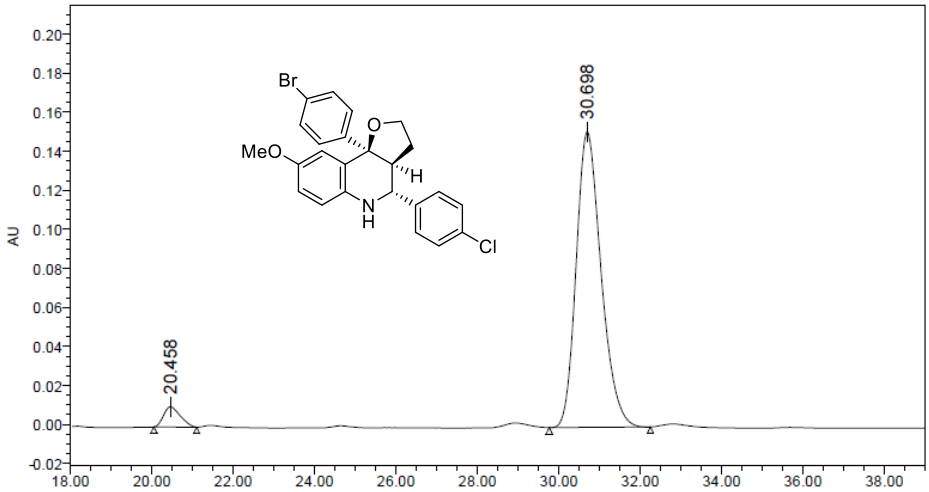


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 222.5 nm	18.078	538113	6.50	40624
2	PDA 222.5 nm	31.755	7744888	93.50	174519

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-chlorophenyl)-8-methoxy-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4b)

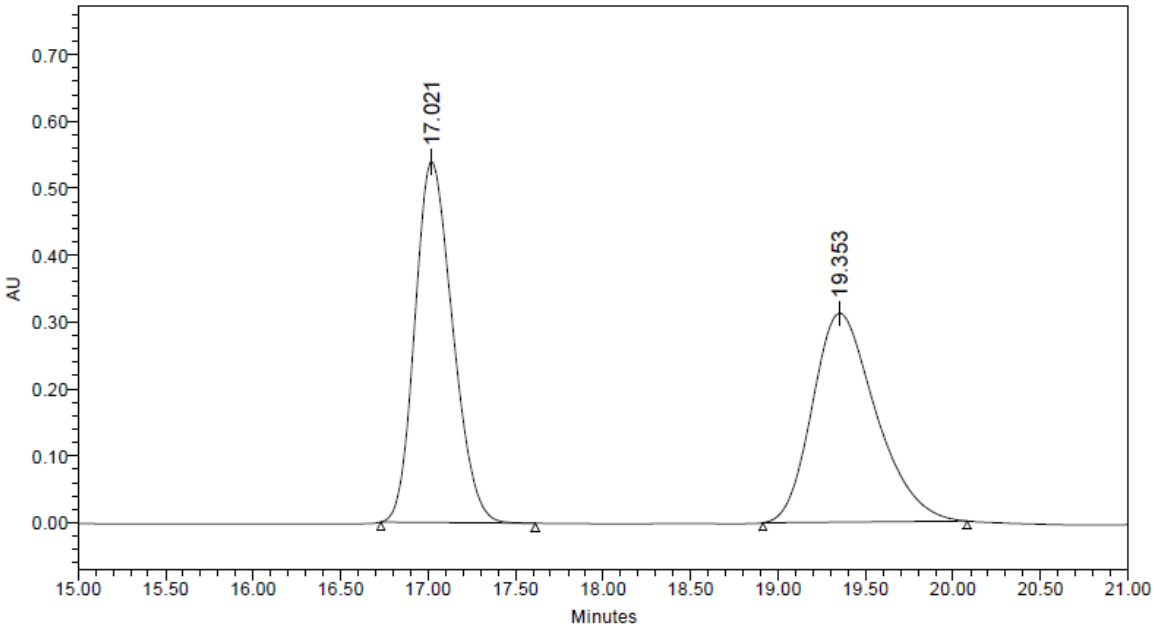


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 209.3 nm	22.978	5488591	50.20	172443
2	PDA 209.3 nm	35.674	5443904	49.80	110286

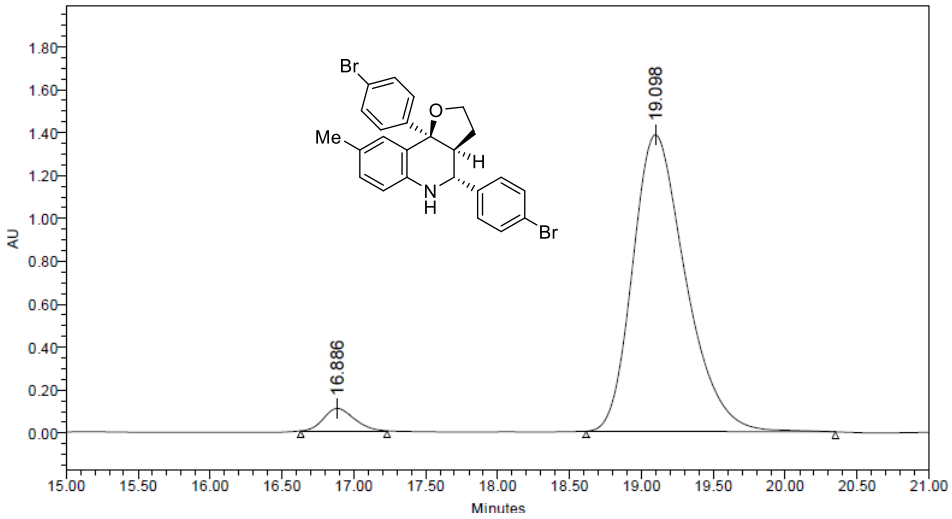


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 222.5 nm	20.458	295594	4.39	10393
2	PDA 222.5 nm	30.698	6444010	95.61	151401

(3a*R*,4*S*,9b*S*)-4,9b-Bis(4-bromophenyl)-8-methyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4c)

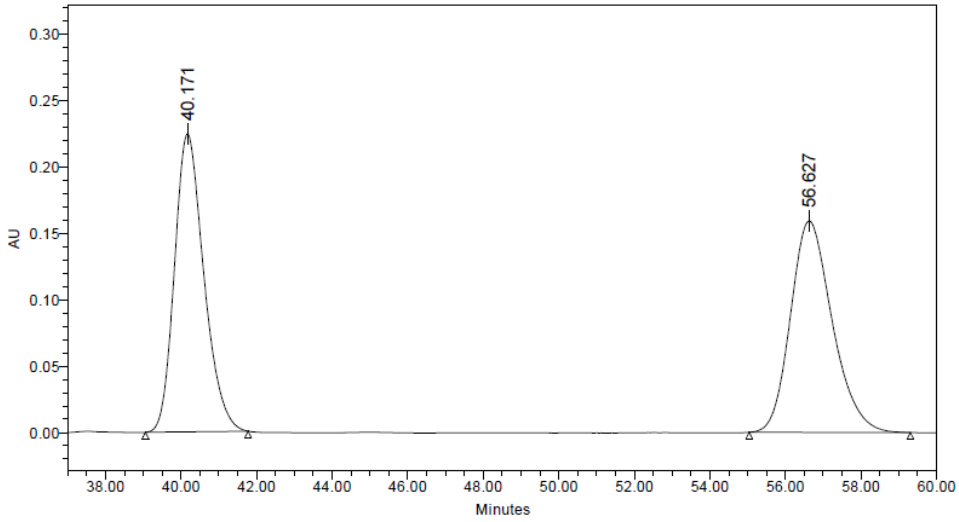


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 231.0 nm	17.021	8084256	50.66	541044
2	PDA 231.0 nm	19.353	7874691	49.34	312513

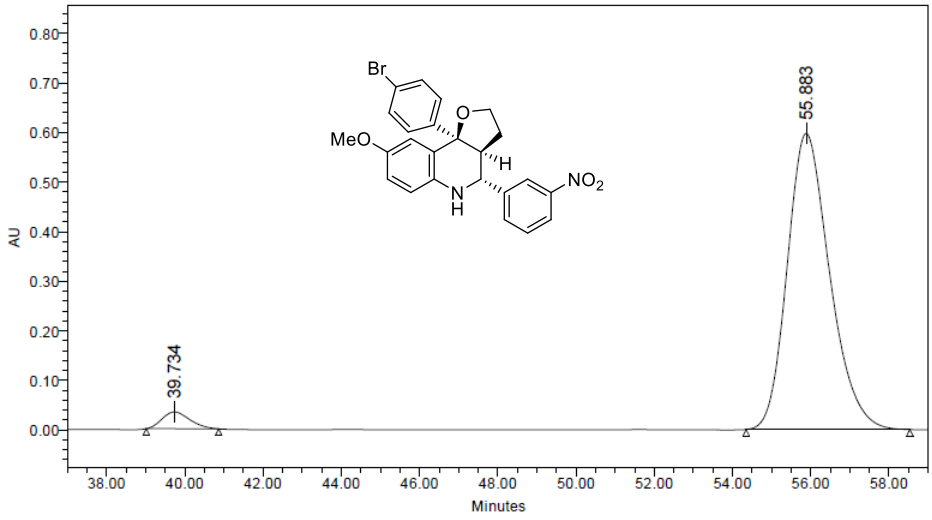


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 207.1 nm	16.886	1539034	4.16	104884
2	PDA 207.1 nm	19.098	35473867	95.84	1383770

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-methoxy-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4d)

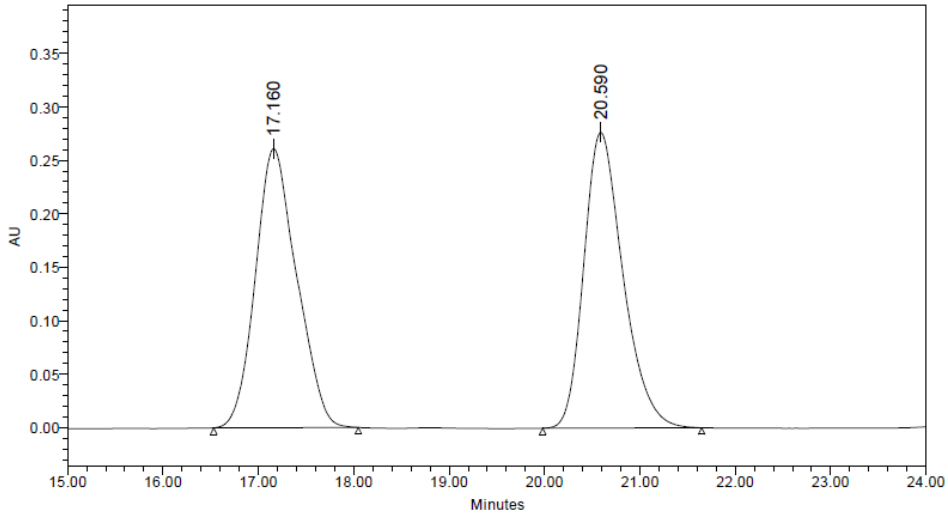


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 209.3 nm	40.171	12120008	49.79	224327
2	PDA 209.3 nm	56.627	12221988	50.21	159241

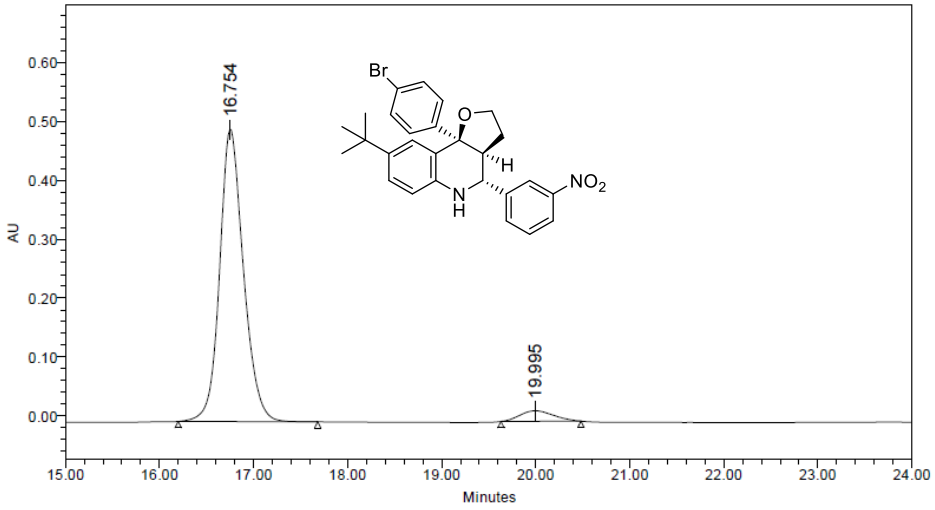


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 209.3 nm	39.734	1674184	3.59	33971
2	PDA 209.3 nm	55.883	45000276	96.41	597087

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-*tert*-butyl-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4e)

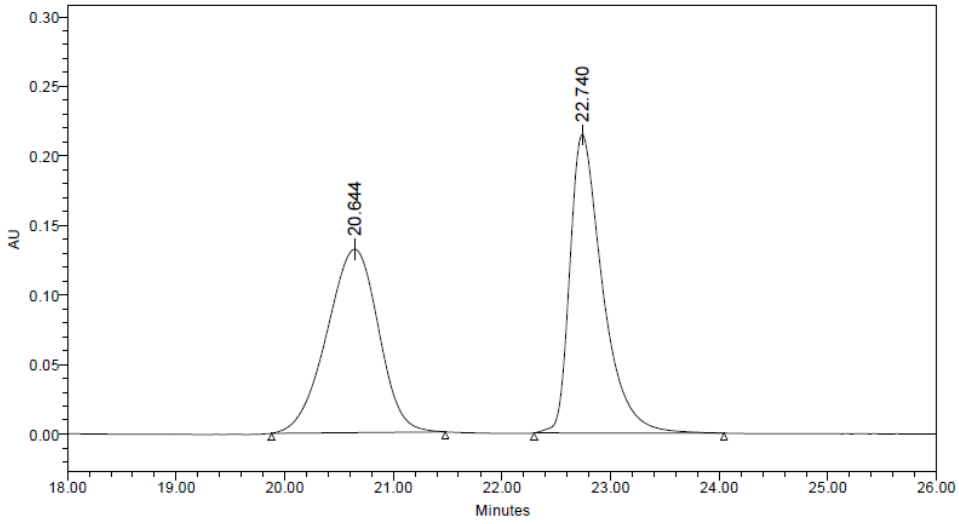


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 211.5 nm	17.160	7861713	49.92	261088
2	PDA 211.5 nm	20.590	7887994	50.08	276668

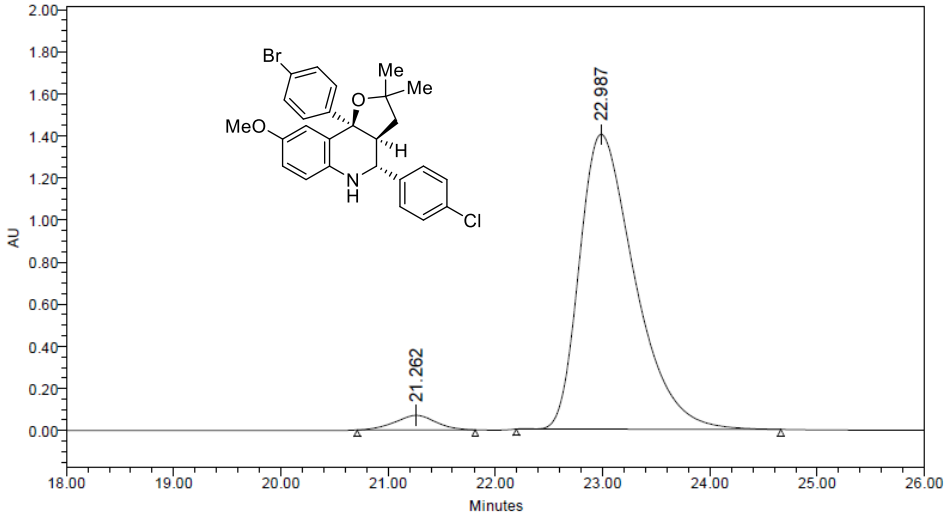


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 207.1 nm	16.754	8724461	95.18	496670
2	PDA 207.1 nm	19.995	441446	4.82	17921

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-chlorophenyl)-8-methoxy-2,2-dimethyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4f)

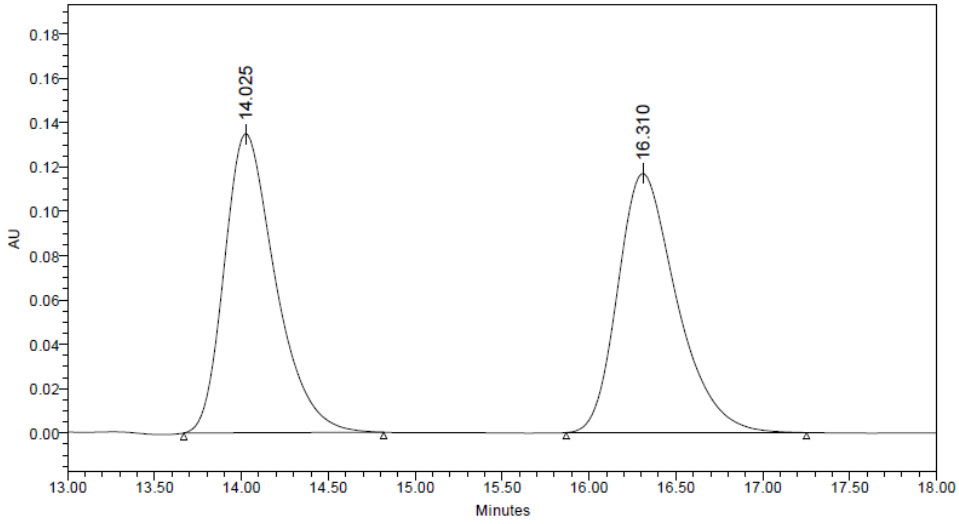


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 235.4 nm	20.644	4360116	49.21	131897
2	PDA 235.4 nm	22.740	4500809	50.79	214768

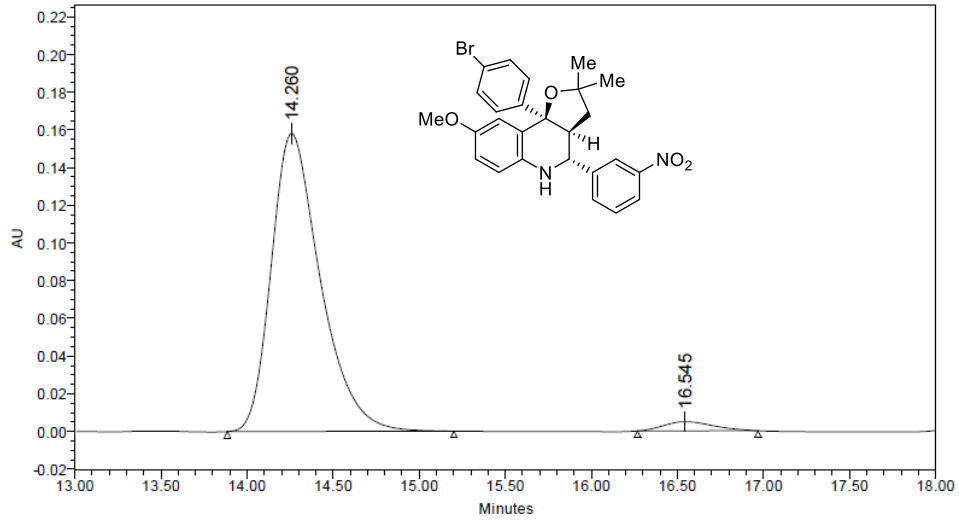


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 228.8 nm	21.262	1842834	3.54	69633
2	PDA 228.8 nm	22.987	50198947	96.46	1402040

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-8-methoxy-2,2-dimethyl-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4g)

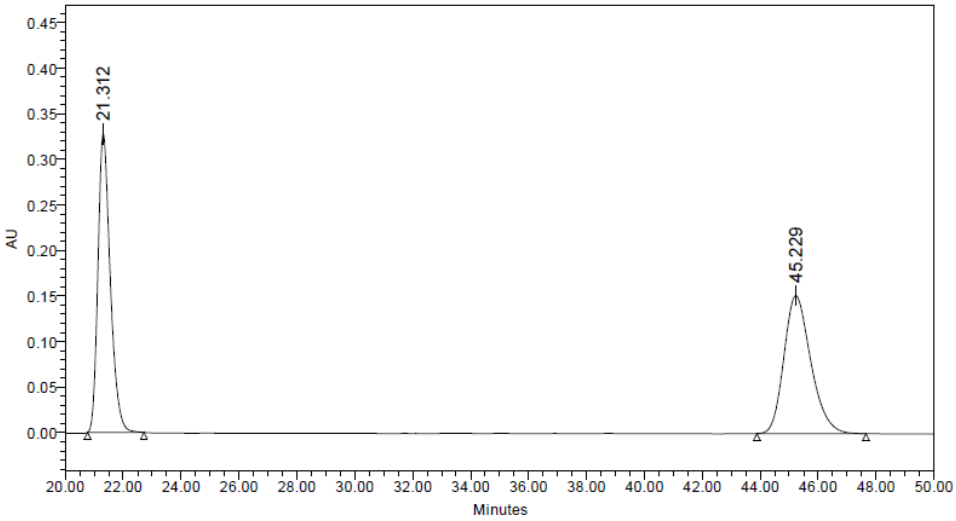


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 235.4 nm	14.025	2756388	50.04	134995
2	PDA 235.4 nm	16.310	2752190	49.96	116895

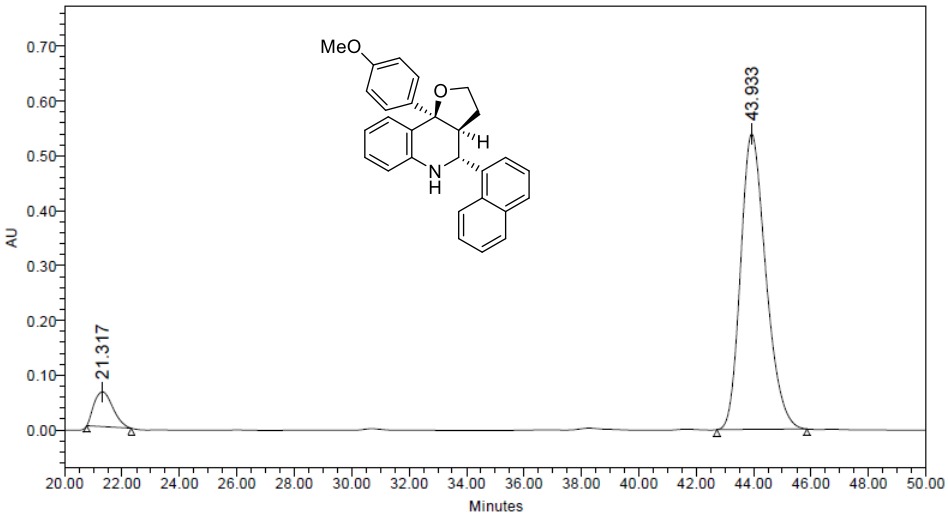


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 235.4 nm	14.260	3134434	96.95	158346
2	PDA 235.4 nm	16.545	98628	3.05	4914

(3a*R*,4*S*,9b*S*)-9b-(4-Methoxyphenyl)-4-(naphthalen-1-yl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4h)

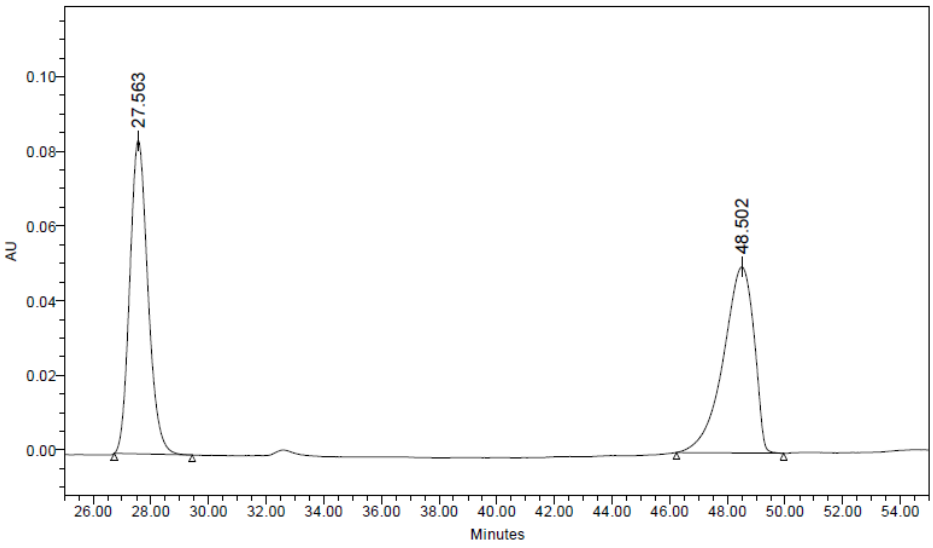


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 224.7 nm	21.312	9697284	49.84	327790
2	PDA 224.7 nm	45.229	9761103	50.16	151361

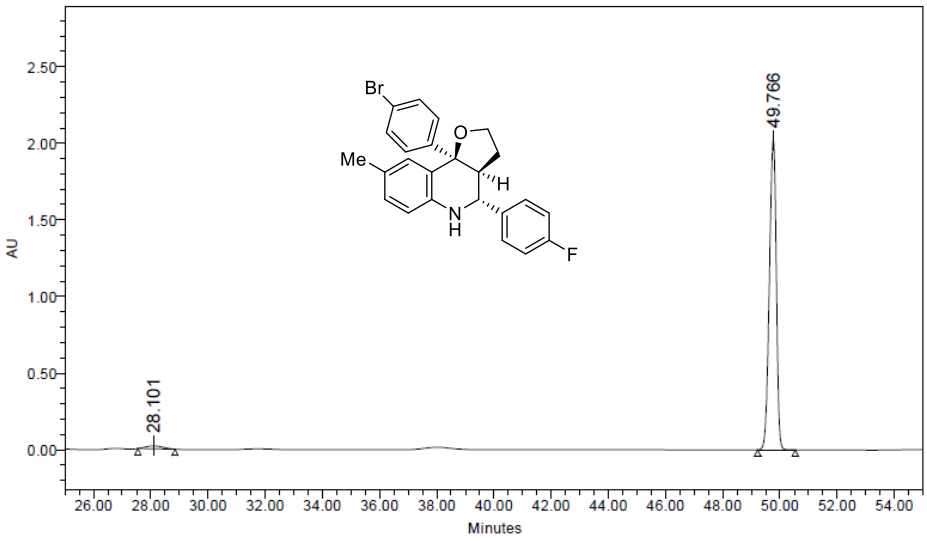


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 222.4 nm	21.317	2883475	8.04	63208
2	PDA 222.4 nm	43.933	32994559	91.96	538873

(3a*R*,4*S*,9b*S*)-9b-(4-Bromophenyl)-4-(4-fluorophenyl)-8-methyl-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4i)

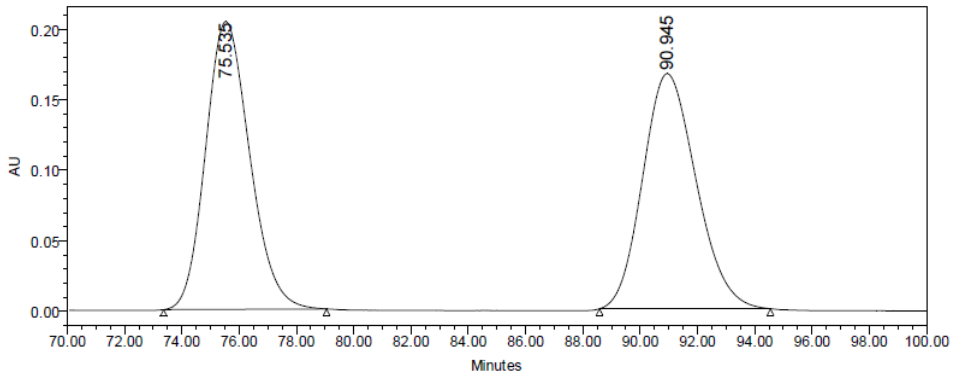


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 209.3 nm	27.563	3672711	49.97	83929
2	PDA 209.3 nm	48.502	3677549	50.03	49797

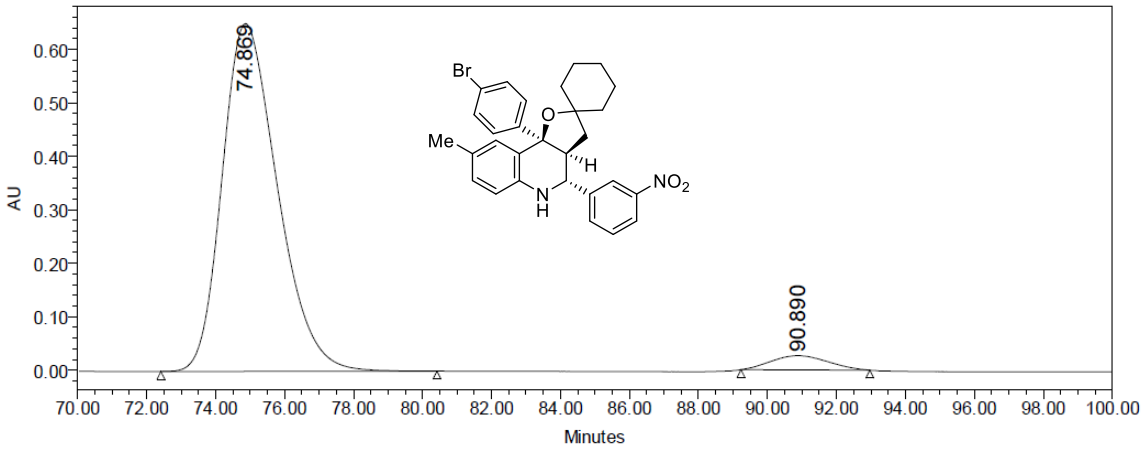


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 237.6 nm	28.101	791219	2.27	18353
2	PDA 237.6 nm	49.766	34048851	97.73	2020843

(3a'*R*,4'*S*,9b'*S*)-9b'-(4-Bromophenyl)-8'-methyl-4'-(3-nitrophenyl)-3a',4',5',9b'-tetrahydro-3'*H*-spiro[cyclohexane-1,2'-furo[3,2-*c*]quinoline] (4j)

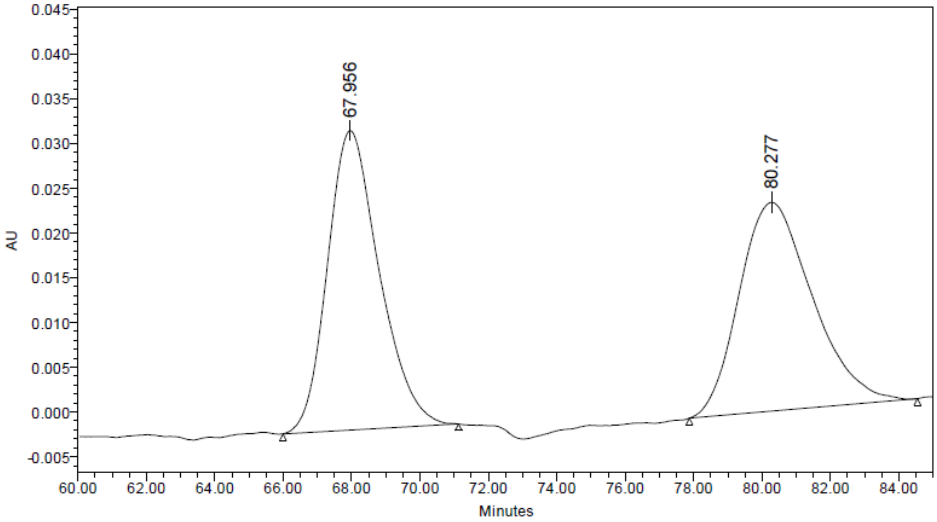


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 213.2 nm	75.535	21852066	50.30	204064
2	PDA 213.2 nm	90.945	21590694	49.70	166551

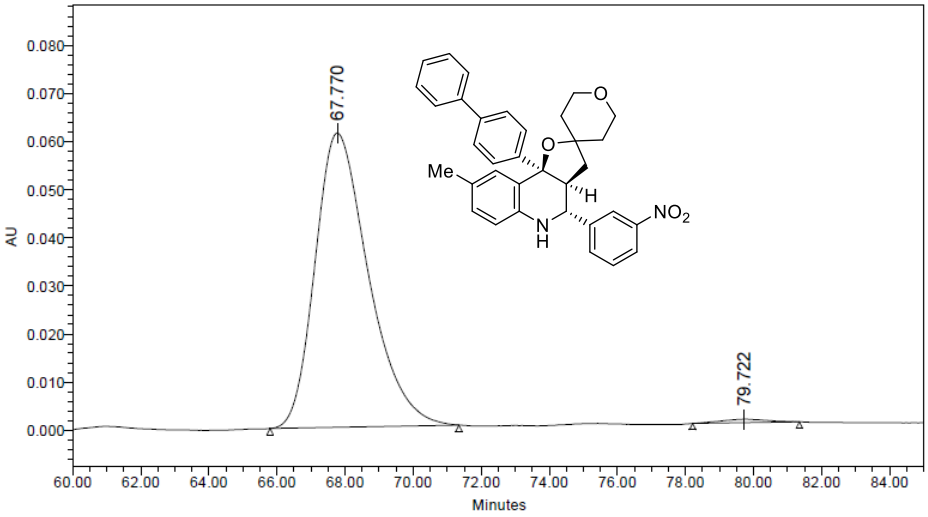


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 216.7 nm	74.869	72425195	95.98	650769
2	PDA 216.7 nm	90.890	3029921	4.02	26497

(3a*R*,4*S*,9b*S*)-9b-(Biphenyl-4-yl)-8-methyl-4-(3-nitrophenyl)-2',3a,3',4,5,5',6',9b-octahydro-3*H*-spiro[furo[3,2-*c*]quinoline-2,4'-pyran] (4k)

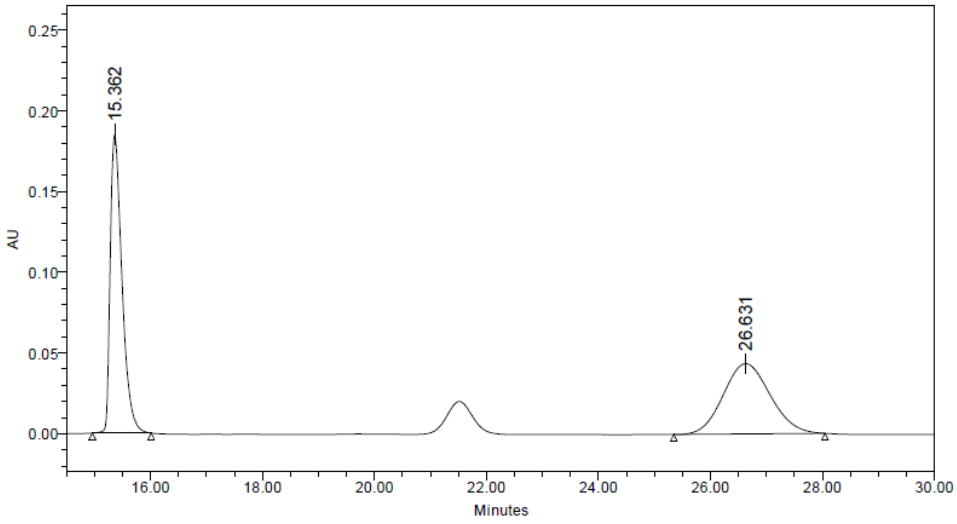


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 209.3 nm	67.956	3523575	50.39	33469
2	PDA 209.3 nm	80.277	3469418	49.61	23329

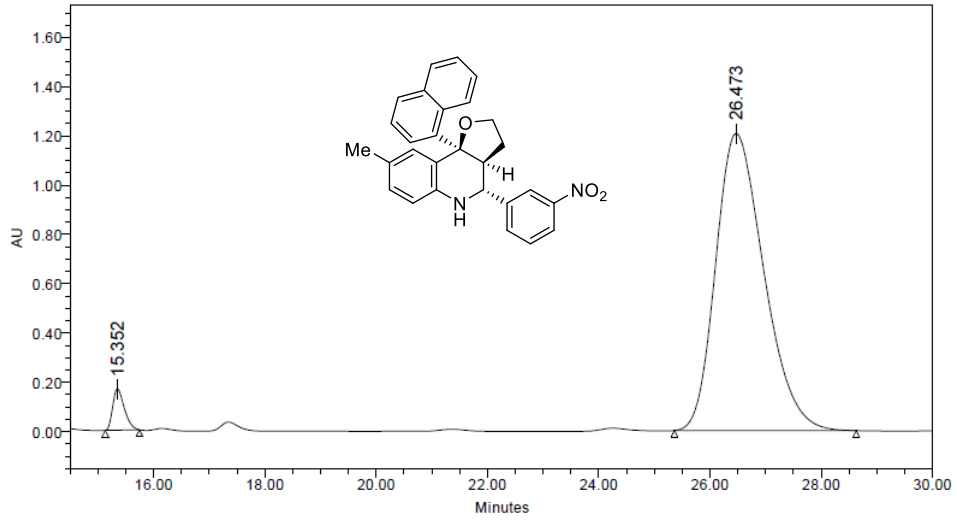


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 215.9 nm	67.770	6667152	99.00	61133
2	PDA 215.9 nm	79.722	67117	1.00	704

(3a*R*,4*S*,9b*S*)-8-Methyl-9b-(naphthalen-1-yl)-4-(3-nitrophenyl)-2,3,3a,4,5,9b-hexahydrofuro[3,2-*c*]quinoline (4l)

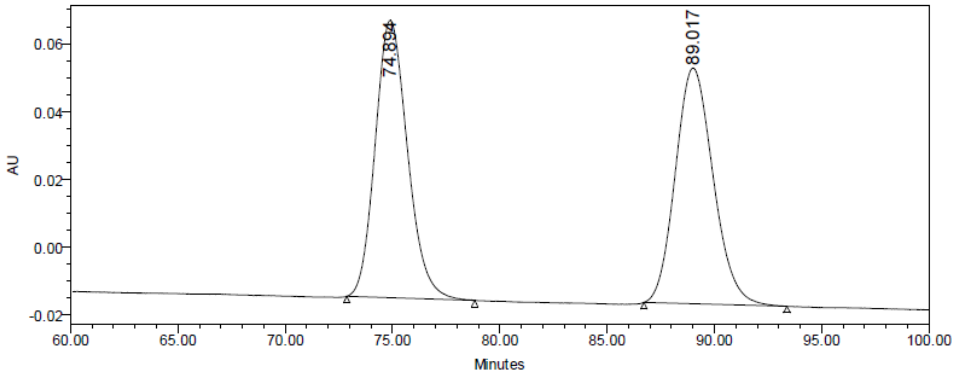


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 215.9 nm	15.362	2690558	51.49	184827
2	PDA 215.9 nm	26.631	2534632	48.51	43574

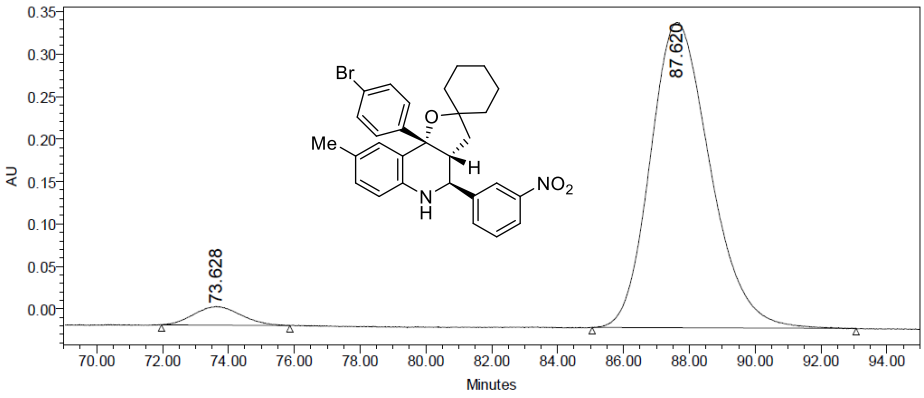


	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 209.3 nm	15.352	2429300	3.24	167472
2	PDA 209.3 nm	26.473	72580117	96.76	1205644

(3a'*S*,4'*R*,9b'*R*)-9b'-(4-Bromophenyl)-8'-methyl-4'-(3-nitrophenyl)-3a',4',5',9b'-tetrahydro-3'*H*-spiro[cyclohexane-1,2'-furo[3,2-*c*]quinoline] (*ent*-4j)



	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 221.2 nm	74.894	8566242	50.10	81778
2	PDA 221.2 nm	89.017	8531408	49.90	69521



	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 203.4 nm	73.628	2164507	4.56	21856
2	PDA 203.4 nm	87.620	45293466	95.44	359385