Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Effect of chiral *N*-substituents with methyl and trifluoromethyl groups on the catalytic performance of mono- and bifunctional thioureas.

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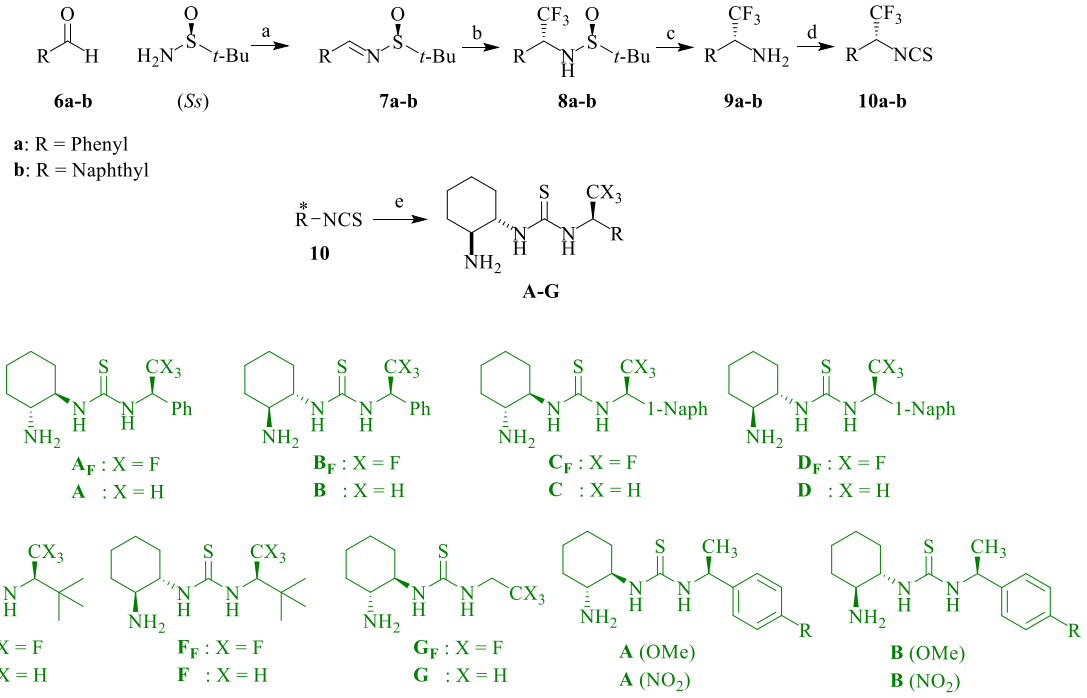
1 Synthesis of the catalysts.

General information.

Starting materials were purchased from Sigma-Aldrich and used as received. THF was freshly distilled from Na/benzophenone and dichloromethane was distilled from CaH_2. Inert atmosphere reactions were carried out under nitrogen atmosphere. Reactions were monitored by thin-layer chromatography (TLC) on silica gel plates F254 and the spots were detected either by UV absorption, Seebach's stain or $KMnO_4$. Flash column chromatography was performed using silica gel 60 (0.40/0.63 mm, 230–400 mesh). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded at ambient temperature using Bruker Fourier-300 MHz, Jeol Eclipse-300 MHz, and Bruker Avance III-400 MHz spectrometers. Chemical shifts (δ) are reported in ppm relative to residual solvent signals ($CDCl_3$ = δ 7.26 for ^{1}H NMR, δ 77.16 for ^{13}C NMR. DMSO-d_6 = δ 2.50 for ^{1}H NMR, δ 39.52 for ^{13}C NMR) or TMS as internal reference (δ 0.0) and coupling constants are in hertz (Hz). Mass spectra were obtained by EI or by direct analysis in real time (DART) in a JEOL AccuTOF JMS-T100LC spectrometer with TOF mass analyzer. CSP-HPLC analyses were performed using the indicated chiral column and UV detector. The FT-IR spectral data were recorded in a Bruker ATR in the 450-4000 cm^{-1} range. Uncorrected melting points were determined in a Fisher Johns melting point apparatus. β,γ-unsaturated α-keto esters,[1] *N*-phenylmaleimide,[2] catalysts **H**,[4] **I**,[3b] **J**,[3b] **O$_F$**,[9] **O**[9] and **P**[9] used in this work were synthesized according to the reported procedures.



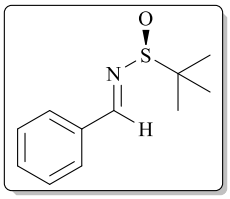
(a) $Ti(OEt)_4$, rt, 17 h. (b) TBAT, $TMSCF_3$, -50 °C 4 h, -20 °C 20 h. (c) HCl 4 M, rt, 0.5 h. (d) $CSCl_2$, $NaHCO_3$, rt. (e) (*R,R*) or (*S,S*) *trans*-1,2-diaminocyclohexane hydrochloride, KOH, CH_2Cl_2/i-PrOH

Scheme S1. Synthesis of bifunctional catalysts **A-G**.

General procedure for sulfinylimines **7**.[3b]

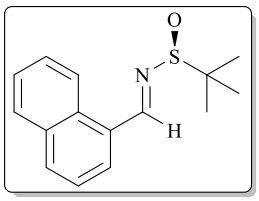
In a round-bottomed-flask was dissolved the aldehyde (7.5 mmol, 1.0 equiv) in anhydrous THF (20 mL) under nitrogen atmosphere. Then, titanium tetraethoxide (3.14 mL, 15 mmol, 2.0 equiv) and *(S)-tert*-butylsulfinamide (0.90 g, 7.5 mmol, 1.0 equiv) were added to the solution. This mixture was stirred at room temperature for 17 h. After that time, the reaction mixture was poured into brine (20 mL) with vigorous stirring, the suspension was filtered over celite and the cake was washed with ethyl acetate (2 x 10 mL). The organic layer was separated, and the aqueous phase was extracted with ethyl acetate (3 x 15 mL). The combined organic layers were dried over Na_2SO_4 and evaporated under reduced pressure. The resulting residue was purified by flash column with hexane/ethyl acetate as eluent (proportions indicated in each compound) to afford the sulfinylimine.

***(S)-N*-(Benzylidene)-*tert*-butanesulfinamide** (**7a**).



Purified by FC with Hex/EtOAc (97:3), light yellow liquid (1.45 g, 92% yield). $[\alpha]_D^{25}$ +98.3 (*c* 1.07, $CHCl_3$) (lit.,[3a] $[\alpha]_D^{20}$ +99.7 (*c* 1.15, $CHCl_3$)). **IR** $\tilde{\nu}_{max}$: 3565, 3500, 2978, 2960, 2868, 1715, 1606, 1573, 1450, 1363, 1216, 1172, 1086, 987, 855, 759, 730, 691, 584. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.55 (s, 1H), 7.80 (dd, *J* = 7.9 Hz, *J* = 1.7 Hz, 2H), 7.50-7.38 (m, 3H), 1.22 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 162.7, 134.0, 132.4, 129.3, 128.9, 57.7, 22.6. **HRMS** (DART+) calcd. for $C_{11}H_{16}N_1O_1S_1$ $[M + H]^+$ 210.09526, found 210.09588.

***(S)-N*-[(1-Naphthyl)methylidene]-*tert*-butanesulfinamide (7b)**.



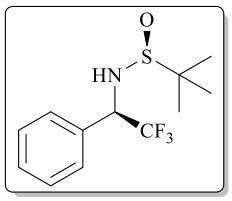
Purified by FC with Hex/EtOAc (95:5), colorless crystals (2.18 g, 90% yield), mp 54-56 °C (lit.,[5] 52-54 °C). $[\alpha]_D^{25}$ +1.45 (*c* 1.03, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3060, 2965, 2917, 1595, 1562, 1457, 1332, 1232, 1075, 976, 798, 771, 698, 580, 412. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 9.16 (s, 1H), 9.03 (d, *J* = 8.5 Hz, 1H), 8.02 (dd, *J* = 10.8 Hz, *J* = 7.8 Hz, 2H), 7.95-7.90 (m, 1H), 7.68-7.52 (m, 3H), 1.32 (s, 9H). (75 MHz, **^{13}C NMR** $CDCl_3$) δ: 162.6, 134.0, 133.4, 132.0, 131.3, 129.5, 128.9, 128.1, 126.6, 125.3, 124.4, 57.8, 22.7. **HRMS** (DART+) calcd. for $C_{15}H_{18}N_1O_1S_1$ $[M + H]^+$ 260.11091, found 260.11097.

General procedure for the synthesis of sulfinamides **8**.[3b]

In a round-botomed-flask a mixture of sulfinylimine **7** (7.16 mmol, 1.0 equiv), tetrabutylammonium difluorotriphenylsilicate (0.77 g, 1.43 mmol, 0.2 equiv) and anhydrous THF (22 mL) was cooled to -50 °C under nitrogen atmosphere. Then, trimethyl(trifluoromethyl)silane (1.26 mL, 8.59 mmol, 1.2 equiv) was added. The reaction mixture was stirred for 4 h at -50 °C and 20 h at -20 °C. The reaction was quenched

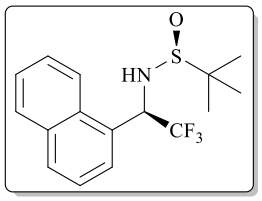
with 20 mL of a saturated solution of NH_4Cl and extracted with EtOAc (2 x 25 mL). The organic layer was dried over Na_2SO_4 and evaporated under reduced pressure. The resulting residue was purified by flash column with hexane/ethyl acetate as eluent (proportions indicated in each compound) to afford the sulfinamide.

***(S)*-*N*-[*(R)*-1-Phenyl-2,2,2-trifluoroethyl]-*tert*-butanesulfinamide (8a)**.



Purified by FC with Hex/EtOAc (85:15), colorless crystals (1.13 g, 57% yield after recrystallization), mp 104-105 °C, 99:1 dr. $[\alpha]_D^{25}$ +72.5 (*c* 0.95, $CHCl_3$) (lit.,[3b] $[\alpha]_D^{25}$ +75.2 (*c* 1.0, $CHCl_3$)). **IR** $\tilde{\nu}_{max}$: 3119, 2993, 2963, 2864, 1455, 1365, 1259, 1148, 1051, 909, 848, 759, 699, 589, 512, 452. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.42 (s, 5H), 4.89-4.78 (m, 1H), 3.62 (d, J = 5.5 Hz, 1H), 1.26 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 133.8, 129.6, 129.2, 128.0, 124.7 (J = 281.4 Hz), 61.3 (J = 30.7 Hz), 56.9, 22.3. **^{19}F NMR** (282 MHz, $CDCl_3$) δ: -73.9 (d, J_{F-H} = 7.4 Hz, 3F). **HRMS** (DART+) calcd. for $C_{12}H_{17}F_3N_1O_1S_1$ 280.09829, found 280.09723.

***(S)*-*N*-[*(R)*-1-(1-Naphthyl)-2,2,2-trifluoroethyl]-*tert*-butanesulfinamide (8b)**.

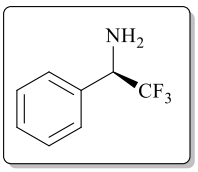


Purified by FC with Hex/EtOAc (8:2), colorless crystals (1.5 g, 60% yield after recrystallization), mp 133-134 °C, 99:1 dr. $[\alpha]_D^{25}$ +202.4 (*c* 0.97, $CHCl_3$) (lit.,[3b] $[\alpha]_D^{25}$ +203.0 (*c* 1.0, $CHCl_3$)). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.16 (d, J = 8.5 Hz, 1H), 7.95-7.87 (m, 2H), 7.71-7.60 (m, 2H), 7.59-7.47 (m, 2H), 5.79-5.66 (m, 1H), 3.79 (d, J = 5.2 Hz, 1H), 1.26 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 134.1, 131.0, 130.6, 129.9, 129.3, 127.5, 126.5, 125.6, 125.3, 125.2 (q, J = 282.0 Hz), 122.7, 57.2, 56.2 (q, J = 31.3 Hz), 22.5. **^{19}F NMR** (282 MHz, $CDCl_3$) δ: -72.6 (d, J_{F-H} = 7.1 Hz, 3F). **HRMS** (DART+) calcd. for $C_{16}H_{19}F_3N_1O_1S_1$ $[M + H]^+$ 330.11394, found 330.11408.

General procedure for the synthesis of trifluoromethyl amines **9**.[6]

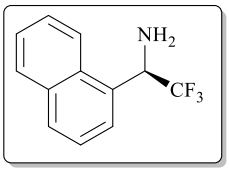
A solution of sulfinamide **8** (9.84 mmol, 1.0 equiv) in methanol (7 mL) was added HCl 4 M in dioxane (4.92 mL, 19.69 mmol, 2.0 equiv). The reaction mixture was stirred for 30 minutes at room temperature. The solvent was evaporated, and the residue dissolved in 20 mL of CH_2Cl_2. The organic layer was washed with 20 mL of NaOH (10% aqueous) and the aqueous phase was extracted with CH_2Cl_2 (3 x 15 mL). The combined organic layers were dried over Na_2SO_4 and evaporated under reduced pressure. The resulting residue was purified by flash column with hexane/ethyl acetate as eluent (proportions indicated in each compound) to afford the amine.

***(R)*-1-Phenyl-2,2,2-trifluoroethylamine (9a)**.



Purified by FC with Hex/EtOAc (9:1), yellow liquid (1.52 g, 96% yield). $[\alpha]_D^{25}$ -8.6 (*c* 0.82, $CHCl_3$) (lit.,[3b] $[\alpha]_D^{25}$ -12.2 (*c* 1.0, $CHCl_3$)). **IR** $\tilde{\nu}_{max}$: 3396, 3323, 3036, 2939, 1618, 1455, 1258, 1152, 1112, 986, 883, 757, 698, 509. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.48-7.35 (m, 5H), 4.39 (q, *J* = 7.5 Hz, 1H), 1.80 (br. s, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 135.5, 129.1, 128.8, 127.9, 125.8 (q, *J* = 281.6 Hz), 58.0 (*J* = 29.7 Hz). **HRMS** (DART+) calcd. for $C_8H_9F_3N_1$ $[M + H]^+$ 176.06871, found 176.06901.

***(R)*-1-(1-Naphthyl)-2,2,2-trifluoroethylamine (9b)**.



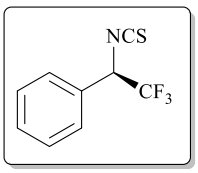
Purified by FC with Hex/EtOAc (85:15), colorless crystals (1.17 g, 93% yield), mp 57-58 °C. $[\alpha]_D^{25}$ -2.26 (*c* 0.75, $CHCl_3$) (lit.,[7] *S* enantiomer $[\alpha]_D^{20}$ +3.1 (*c* 2.5, $CHCl_3$)). **IR** $\tilde{\nu}_{max}$: 3373, 3280, 3057, 2909, 1599, 1369, 1259, 1153, 1115, 913, 800, 775, 689, 627, 457. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.11 (d, *J* = 8.3 Hz, 1H), 7.96-7.87 (m, 2H), 7.79 (d, *J* = 7.3 Hz, 1H), 7.64-7.48 (m, 3H), 5.34 (q, *J* = 7.2 Hz, 1H), 1.91 (s, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 133.9, 131.9, 131.6, 129.6, 129.2, 126.8, 126.2 (*J* = 282.1 Hz), 126.0, 125.4, 125.2, 122.8, 52.78 (*J* = 30.0 Hz). **HRMS** (DART+) calcd. for $C_{12}H_{11}F_3N_1$ $[M + H]^+$ 226.08436, found 226.08524.

General procedure for the synthesis of isothiocyanates **10**.[8]

A solution of amine **9** (5.19 mmol, 1.0 equiv) in chloroform (52 mL) and water (42 mL) was added $NaHCO_3$ (0.95 g, 11.42 mmol, 2.2 equiv) and thiophosgene (0.43 mL, 5.71 mmol, 1.1 equiv). The reaction mixture was stirred for 2 h at room temperature. Then, the organic layer was separated, dried over Na_2SO_4 and the solvent was removed by evaporation. The resulting residue was purified by flash column with hexane as eluent to afford the isothiocyanate.

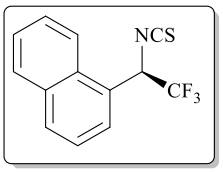
Note: Isothiocyanates **10c-f** were prepared using a methodology previously report.[9]

***(R)*-1-Phenyl-2,2,2-trifluoroethylisothiocyanate (10a)**.



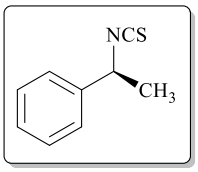
Purified by FC with Hexane (100%), yellow liquid (0.95 g, 85% yield). $[\alpha]_D^{25}$ -40.0 (*c* 1.54, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3069, 3038, 2917, 2847, 2022, 1456, 1337, 1254, 1180, 1130, 831, 755, 695, 630. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.46 (s, 5H), 5.18 (q, *J* = 6.4 Hz, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 141.2, 130.5, 130.4, 129.2, 128.0, 122.7 (*J* = 282.5 Hz), 62.4 (*J* = 33.4 Hz). **HRMS** (DART+) calcd. for $C_9H_7F_3N_1S_1$ $[M + H]^+$ 218.0251, found 218.0253.

***(R)*-1-(1-Naphthyl)-2,2,2-trifluoroethylisothiocyanate (10b)**.



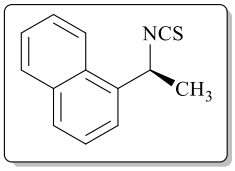
Purified by FC with Hexane (100%), yellow solid (1.28 g, 93% yield), mp 57-58 °C. $[\alpha]_D^{25}$ +78.0 (*c* 1.09, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3054, 2924, 2853, 2236, 2069, 1597, 1513, 1253, 1167, 837, 774, 692, 632, 533, 458. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.00-7.91 (m, 3H), 7.82 (d, *J* = 7.3 Hz, 1H), 7.66-7.53 (m, 3H), 6.12 (q, *J* = 6.1 Hz, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 141.1, 133.9, 131.1, 130.7, 129.4, 127.5, 127.0, 126.4, 126.4, 125.4, 123.2 (*J* = 283.3 Hz), 122.2, 58.5 (*J* = 33.8 Hz). **HRMS** (DART+) calcd. for $C_{13}H_9F_3N_1S_1$ $[M + H]^+$ 268.0408, found 268.0411.

***(S)*-1-Phenylethyl isothiocyanate (10c).**



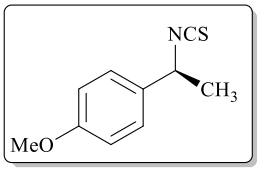
Purified by FC with Hexane (100%), yellow liquid (2.4 g, 95% yield). $[\alpha]_D^{25}$ +13.6 (*c* 1.07, $CHCl_3$) (lit.,[10] $[\alpha]_D^{20}$ +16.6 (*c* 1.02, $CHCl_3$)). **IR** $\tilde{\nu}_{max}$: 3062, 3030, 2982, 2077, 1602, 1492, 1449, 1306, 1201, 1019, 948, 756, 695, 531. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.44-7.30 (m, 5H), 4.92 (q, *J* = 6.8 Hz, 1H), 1.68 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 140.3, 129.0, 128.3, 125.5, 57.1, 25.1.

***(S)*-1-(1-Naphthyl)-ethylisothiocyanate (10d).**



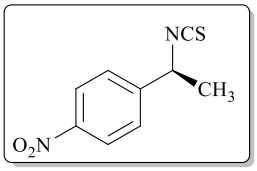
Purified by FC with Hexane (100%), yellow liquid (1.2 g, 99% yield). $[\alpha]_D^{25}$ +106.3 (*c* 0.69, $CHCl_3$) (lit.,[11] *R* enantiomer $[\alpha]_D^{21}$ -109.3 (*c* 1.0, $CHCl_3$)). **IR** $\tilde{\nu}_{max}$: 3046, 2982, 2079, 1596, 1509, 1444, 1321, 1117, 999, 797, 772, 603, 437. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.97-7.90 (m, 2H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.65 (d, *J* = 7.1 Hz, 1H), 7.63-7.48 (m, 3H), 5.69 (q, *J* = 6.7 Hz, 1H), 1.84 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 135.5, 133.9, 129.5, 129.2, 129.0, 126.8, 126.0, 125.5, 123.0, 122.2, 54.1, 24.0.

***(S)*-1-(4-methoxyphenyl)-ethylisothiocyanate (10e).**



Purified by FC with Hex/EtOAc (95:5), yellow liquid (0.35 g, 91% yield). $[\alpha]_D^{25}$ +5.9 (*c* 1.64, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 7.24 (d, *J* = 8.7 Hz, 1H), 6.90 (d, *J* = 8.7 Hz, 1H), 4.85 (q, *J* = 6.8 Hz, 1H), 3.80 (3H), 1.64 (d, *J* = 6.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 159.5, 132.4, 126.8, 114.3, 56.7, 55.4, 25.0.

***(S)*-1-(4-nitrophenyl)-ethylisothiocyanate (10f).**



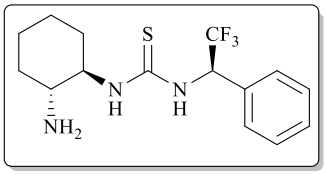
Purified by FC with Hex/EtOAc (95:5), yellow liquid (0.24 g, 99% yield). $[\alpha]_D^{25}$ +6.2 (*c* 1.13, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.25 (d, *J* = 8.8 Hz, 3H), 7.53 (d, *J* = 8.8 Hz, 5H), 5.09 (q, *J* = 6.8 Hz, 3H), 1.73 (d, *J* = 6.8 Hz, 5H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 147.7, 147.2, 134.9, 126.6, 124.3, 56.5, 25.0.

General procedure for the synthesis of bifunctional primary amine/thioureas catalysts (**A-G**).

A solution of KOH (0.24 g, 4.4 mmol) in isopropanol/CH_2Cl_2 (16 mL/8 mL) was added the corresponding enantiopure *trans*-1,2-diaminocyclohexane hydrochloride (0.40 g, 2.2 mmol), the reaction mixture was stirred for 30 minutes, then, a solution of isothiocyanate **10** (1.47 mmol) in CH_2Cl_2 (12 mL) was slowly added. The reaction was monitored by TLC and stopped when we observed bisthiourea such as minor product. The reaction mixture was concentrated, and the residue dissolved in CH_2Cl_2 (20 mL), washed with brine and water. The organic layer was dried over Na_2SO_4 and concentrated. The resulting residue was purified by flash column with CH_2Cl_2/MeOH (95:5 to 9:1) to afford the catalyst.

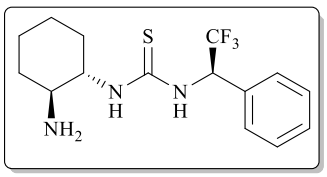
Note: Amine for catalysts **E-F** was prepared using a methodology previously report.[6] Isothiocyanates for thioureas **E-G** were used for the next step without further purification, the yield was calculated for the starting amine.

1-[(*1R*,*2R*)-2-Aminocyclohexyl]-3-[*(R)*-1-phenyl-2,2,2-trifluoroethyl]thiourea (A_F).



White solid (0.379 g, 78% yield), mp 88-90 °C, $[\alpha]_D^{25}$ +85.6 (*c* 0.83, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3256, 3036, 2928, 2856, 1538, 1450, 1336, 1231, 1169, 1114, 861, 756, 702, 638, 505. **^{1}H NMR** (300 MHz, DMSO-d_6) δ: 8.82 (br, 1H), 8.10 (br, 1H), 7.54-7.34 (m, 5H), 6.57-6.37 (m, 1H), 3.79 (br, 1H), 2.60 (br, 1H), 2.10 (br, 1H), 1.85 (br, 1H), 1.61 (br, 2H), 1.32-1.05 (m, 4H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ: 183.1, 133.5, 128.9, 128.7, 128.3, 125.0 (q, *J* = 282.3 Hz), 59.3, 58.0 (q, *J* = 29.0 Hz), 53.6, 33.5, 31.0, 24.2, 24.0. **HRMS** (DART+) calcd. for $C_{15}H_{21}F_3N_3S_1$ $[M + H]^+$ 332.14083, found 332.14088.

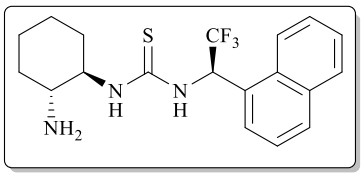
1-[(*1S*,*2S*)-2-Aminocyclohexyl]-3-[*(R)*-1-phenyl-2,2,2-trifluoroethyl]thiourea (B_F).



White solid (0.368 g, 76% yield), mp 85-87 °C, $[\alpha]_D^{25}$ -73.7 (*c* 0.82, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3245, 3057, 2929, 2857, 1540, 1450, 1231, 1169, 1114, 860, 756, 702, 576, 405. **^{1}H NMR** (300 MHz, DMSO-d_6) δ: 8.81 (br, 1H), 8.01 (br, 1H), 7.51-7.35 (m, 5H), 6.55-6.37 (m, 1H), 3.79 (br, 1H), 2.57 (br, 1H), 1.99 (br, 1H), 1.86 (br, 1H), 1.60 (br, 2H), 1.18 (br, 3H), 1.02 (br, 1H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ: 183.1,

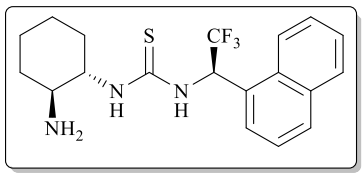
133.5, 128.9, 128.7, 128.2, 125.0 (q, *J* = 282.2 Hz), 59.4, 58.0 (q, *J* = 29.4 Hz), 53.9, 33.9, 31.0, 24.2, 24.1. **HRMS** (DART+) calcd. for $C_{15}H_{21}F_3N_3S_1$ $[M + H]^+$ 332.14083, found 332.14127.

1-[(*1R,2R*)-2-Aminocyclohexyl]-3-[*(R)*-1-(1-naphthyl)-2,2,2-trifluoroethyl]thiourea (C_F).



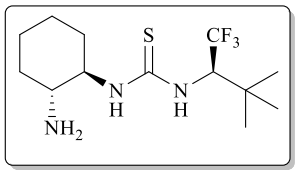
White solid (0.549 g, 77% yield), mp 89-92 °C, $[\alpha]_D^{25}$ +188.5 (*c* 0.83, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3241, 3053, 2927, 2855, 1540, 1319, 1230, 1164, 1115, 850, 796, 774, 700, 631, 533, 417. **^{1}H NMR** (300 MHz, DMSO-d_6) δ: 8.92 (br, 1H), 8.28 (d, *J* = 8.5 Hz, 1H), 8.08-7.93 (m, 3H), 7.80-7.54 (m, 4H), 7.52-7.36 (m, 1H), 3.79 (br, 1H), 2.57 (br, 1H), 2.12 (br, 1H), 1.84 (br, 1H), 1.61 (br, 2H), 1.31-1.05 (m, 4H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ: 183.2, 133.3, 131.0, 130.1, 129.5, 128.8, 127.1, 126.1, 125.9, 125.4, 125.3 (q, *J* = 282.9 Hz), 123.1, 59.4, 53.8, 53.4 (q, *J* = 30.6 Hz), 33.6, 31.0, 24.2, 24.0. **HRMS** (DART+) calcd. for $C_{19}H_{23}F_3N_3S_1$ $[M + H]^+$ 382.15648, found 382.15674.

1-[(*1S,2S*)-2-Aminocyclohexyl]-3-[*(R)*-1-(1-naphthyl)-2,2,2-trifluoroethyl]thiourea (D_F).



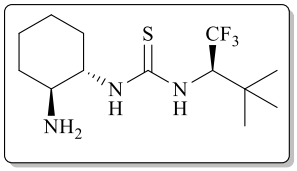
White solid (0.577 g, 81% yield), mp 101-104 °C, $[\alpha]_D^{25}$ +90.0 (*c* 1.01, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3242, 3050, 2928, 2856, 1540, 1319, 1230, 1164, 1114, 883, 848, 795, 774, 701, 631, 534, 434. **^{1}H NMR** (300 MHz, DMSO-d_6) δ: 8.95 (br, 1H), 8.28 (d, *J* = 8.6 Hz, 1H), 8.05-7.91 (m, 3H), 7.75-7.53 (m, 4H), 7.50-7.35 (m, 1H), 3.79 (br, 1H), 2.56 (br, 1H), 1.96 (m, 1H), 1.85 (br, 1H), 1.59 (br, 2H), 1.19 (m, 3H), 0.98 (br, 1H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ: 183.1, 133.3, 131.0, 130.2, 129.5, 128.8, 127.1, 126.1, 125.8, 125.4, 125.4 (q, *J* = 282.8 Hz), 123.1, 59.5, 53.9, 53.4 (d, *J* = 29.2 Hz), 34.0, 31.0, 24.2, 24.1. **HRMS** (DART+) calcd. for $C_{19}H_{23}F_3N_3S_1$ $[M + H]^+$ 382.15648, found 382.15652.

1-[(*1R,2R*)-2-Aminocyclohexyl]-3-[*(R)*-1-(*tert*-butyl)-2,2,2-trifluoroethyl]thiourea (E_F).



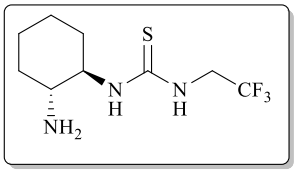
Light brown solid (0.052 g, 33% yield), mp 85-88 °C, $[\alpha]_D^{25}$ +113.9 (*c* 0.73, $CHCl_3$). **IR** (film) $\tilde{\nu}_{max}$: 3246, 3058, 2928, 2858, 1657, 1548, 1369, 1257, 1158, 1106, 925, 751, 705, 584. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 5.10 (q, *J* = 8.6 Hz, 1H), 4.17 (br, 2H), 2.73 (br, 1H), 1.99 (br, 2H), 1.74 (br, 2H), 1.25 (br, 5H), 1.07 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 185.4, 126.1 (q, *J* = 285.1 Hz), 63.2 (br), 55.8, 34.4, 33.9 (br), 32.1, 27.4, 24.7, 24.6. **HRMS** (DART+) calcd. for $C_{13}H_{25}F_3N_3S_1$ $[M + H]^+$ 312.17213, found 312.17225.

1-[(*1S,2S*)-2-Aminocyclohexyl]- 3-[*(R)*-1-(*tert*-butyl)-2,2,2-trifluoroethyl]thiourea (F_F).



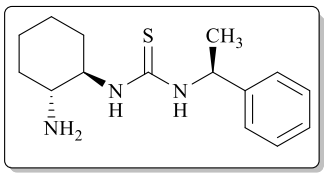
Light brown solid (0.063 g, 43% yield), mp 105-107 °C, $[\alpha]_D^{25}$ -189.0 (*c* 0.53, $CHCl_3$). **IR** (KBr) $\tilde{\nu}_{max}$: 3281, 3238, 3062, 2930, 2858, 1662, 1545, 1370, 1321, 1204, 1157, 1107, 925, 855, 751, 706, 485. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 5.14 (q, *J* = 8.4, 1H), 3.89 (br, 2H), 2.70 (br, 1H), 2.02 (br, 1H), 1.72 (br, 2H), 1.24 (5H), 1.07 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 185.5, 126.2 (q, *J* = 284.8 Hz), 62.9 (br), 59.3 (br), 55.4 (br), 34.6, 34.3, 32.1, 27.3, 24.7, 24.6. **HRMS** (DART+) calcd. for $C_{13}H_{25}F_3N_3S_1$ $[M + H]^+$ 312.17213, found 312.17315.

1-[(*1R,2R*)-2-Aminocyclohexyl]-3-[2,2,2-trifluoroethyl]thiourea (G_F).



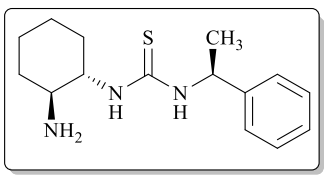
Yellow solid (0.174 g, 38% yield), mp 115-118 °C, $[\alpha]_D^{25}$ +80.0 (*c* 0.89, $CHCl_3$). **IR** (film) $\tilde{\nu}_{max}$: 3275, 2936, 2857, 1608, 1536, 1416, 1365, 1338, 1260, 1140, 1105, 976, 935, 825, 731, 660, 584, 526. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.89 (br, 1H), 6.68 (br, 1H), 4.47 (m, 1H), 4.21 (br, 1H), 3.20 (br, 1H), 2.63 (br, 1H), 2.02 (br, 1H), 1.91 (br, 1H), 1.75 (br, 2H), 1.27 (br, 4H). **^{13}C NMR** (75 MHz, CDCl3) δ: 185.0, 124.5 (q, *J* = 278.9 Hz), 62.7 (br), 56.0, 46.1 (br), 35.2, 32.2, 24.7. **HRMS** (DART+) calcd. for $C_9H_{17}F_3N_3S_1$ $[M + H]^+$ 256.10953, found 256.10947.

1-[(*1R,2R*)-2-Aminocyclohexyl]-3-[*(S)*-1-phenylethyl]thiourea (A).



White solid (0.580 g, 68% yield), mp 71-74 °C, $[\alpha]_D^{25}$ +70.5 (*c* 1.01, $CHCl_3$) (lit.,[11] $[\alpha]_D^{25}$ +63.2 (*c* 1.0, $CHCl_3$)). **IR** $\tilde{\nu}_{max}$: 3242, 3029, 2924, 2854, 1535, 1446, 1331, 1232, 1080, 943, 756, 697, 526. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.40-7.21 (m, 5H), 6.39 (br, 1H), 5.35 (br, 1H), 3.57 (br, 1H), 2.56-2.41 (m, 1H), 2.35 (s, 2H), 1.88-1.1.73 (m, 2H), 1.70-1.57 (m, 2H), 1.51 (d, *J* = 6.8 Hz, 3H), 1.30-0.80 (m, 4H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 181.7, 143.2, 128.8, 127.3, 126.1, 61.2, 55.8, 54.1, 34.5, 31.9, 24.7, 24.6, 22.9. **HRMS** (DART+) calcd. for $C_{15}H_{24}N_3S_1$ $[M + H]^+$ 278.16909, found 278.16944.

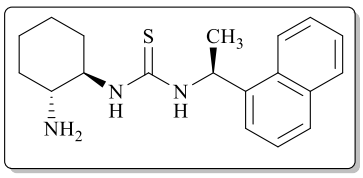
1-[(*1S,2S*)-2-Aminocyclohexyl]-3-[*(S)*-1-phenylethyl]thiourea (B).



White solid (0.450 g, 60% yield), mp 69-71, $[\alpha]_D^{25}$ -40.7 (*c* 1.0, $CHCl_3$) (lit.,[11] $[\alpha]_D^{29}$ -31.8 (*c* 1.0, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3252, 3031, 2925, 2853, 1532, 1446, 1330, 1232, 1080, 943, 755, 697, 526. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.44-7.19 (m, 5H), 6.50 (br, 1H), 5.27 (br, 1H), 3.75 (br, 1H), 2.65-2.23 (m, 3H), 2.10-1.93 (m, 1H), 1.83 (br, 1H), 1.75-1.60 (m, 2H), 1.51 (d, *J* = 6.4 Hz, 3H), 1.36-1.00 (m, 4H).

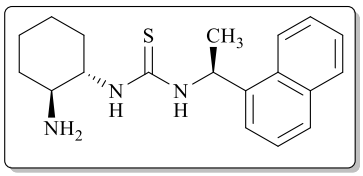
^{13}C NMR (75 MHz, $CDCl_3$) δ: 181.3, 143.0, 128.7, 127.4, 126.0, 61.0, 55.4, 53.9, 34.3, 32.1, 24.7, 24.6, 22.9. **HRMS** (DART+) calcd. for $C_{15}H_{24}N_3S_1$ $[M + H]^+$ 278.16909, found 278.16815.

1-[(*1R,2R*)-2-Aminocyclohexyl]-3-[*(S)*-1-(1-naphthyl)ethyl]thiourea (C).



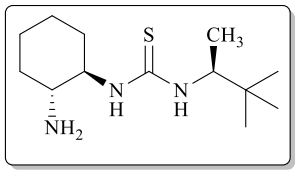
White solid (0.213 g, 52% yield), mp 81-83 °C, $[\alpha]_D^{25}$ +118.2 (*c* 1.04, $CHCl_3$) (lit.,[4] *S,S,R* enantiomer $[\alpha]_D^{20}$ -124.1 (*c* 0.61, $CHCl_3$)). **IR** $\tilde{\nu}_{max}$: 3237, 3041, 2924, 2853, 1532, 1332, 1234, 1072, 776, 540, 434. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.21 (d, *J* = 8.2 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.57-7.34 (m, 4H), 6.70-6.05 (m, 2H), 3.48 (br, 1H), 2.38 (br, 3H), 1.82-1.70 (m, 1H), 1.64 (d, *J* = 6.7 Hz, 3H), 1.58-1.40 (m, 2H), 1.17-0.8 (m, 4H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 181.6, 138.7, 133.8, 130.7, 128.7, 128.0, 126.4, 125.7, 125.4, 123.4, 122.8, 60.8, 55.7, 50.3, 34.3, 31.8, 24.5, 24.4, 21.5. **HRMS** (DART+) calcd. for $C_{19}H_{26}N_3S_1$ $[M + H]^+$ 328.18474, found 328.18418.

1-[(*1S,2S*)-2-Aminocyclohexyl]-3-[*(S)*-1-(1-naphthyl)ethyl]thiourea (D).



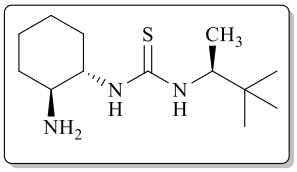
White solid (0.278 g, 51% yield), mp 76-79, $[\alpha]_D^{25}$ -19.1 (*c* 1.04, $CHCl_3$). **IR** $\tilde{\nu}_{max}$: 3226, 3044, 2924, 2852, 1529, 1445, 1330, 1235, 1072, 856, 776, 723, 434. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.18 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.59-7.37 (m, 4H), 6.14 (br, 1H), 3.57 (br, 1H), 2.22 (br, 1H), 2.08-1.82 (m, 4H), 1.74-1.50 (7H, m), 1.27-0.91 (4H, m). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 181.2, 138.2, 133.7, 130.8, 128.7, 128.1, 126.4, 125.7, 125.2, 123.2, 122.8, 61.1, 55.3, 50.2, 34.3, 32.0, 24.6, 24.5, 21.3. **HRMS** (DART+) calcd. for $C_{19}H_{26}N_3S_1$ $[M + H]^+$ 328.18474, found 328.18504.

1-[(*1R,2R*)-2-Aminocyclohexyl]-3-[*(R)*-3,3-dimethylbutan-2-yl]thiourea (E).



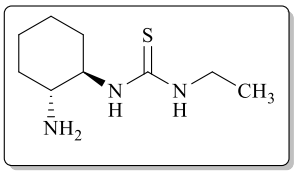
Yellowish solid (0.145 g, 45% yield), mp 76-78 °C, $[\alpha]_D^{25}$ +136.5 (*c* 1.1, $CHCl_3$) (lit.,[12] $[\alpha]_D^{20}$ +79.5 (*c* 0.0201, $CHCl_3$)). **IR** (KBr) $\tilde{\nu}_{max}$: 3243, 3059, 2929, 2857, 1536, 1447, 1334, 1239, 1199, 1085, 946, 849, 723, 571, 542. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.14 (br, 1H), 6.48 (br, 1H), 4.17 (br, 1H), 3.43 (br, 1H), 3.02 (br, 1H), 2.64 (br, 1H), 1.98 (br, 1H), 1.87 (br, 1H), 1.71 (br, 2H), 1.24 (br, 5H), 1.10 (d, *J* = 6.7 Hz, 1H), 0.92 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 182.6, 61.3, 59.3, 56.1, 34.7, 34.2, 32.3, 26.7, 24.9, 24.7, 15.6. **HRMS** (DART+) calcd. for $C_{13}H_{28}N_3S_1$ $[M + H]^+$ 258.20039, found 258.20070.

1-[(*1S,2S*)-2-Aminocyclohexyl]- 3-[*(R)*-3,3-dimethylbutan-2-yl]thiourea (F).



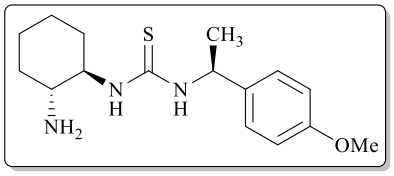
Yellowish solid (0.216 g, 67% yield), mp 82-85 °C, $[\alpha]_D^{25}$ -63.1 (*c* 0.83, $CHCl_3$) (lit.,[12] $[\alpha]_D^{20}$ -133.0 (*c* 0.02, $CHCl_3$)). **IR** (KBr) $\tilde{\nu}_{max}$: 3244, 3060, 2928, 2857, 1535, 1447, 1335, 1241, 1084, 946, 848, 723, 572. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.69 (br, 1H), 6.68 (br, 1H), 4.28 (br, 1H), 3.64 (br, 1H), 3.34 (br, 2H), 2.68 (br, 1H), 2.03 (br, 1H), 1.91 (br, 1H), 1.73 (br, 2H), 1.25 (br, 5H), 1.11 (d, *J* = 6.7 Hz, 1H), 0.93 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 182.5, 60.6, 59.1, 55.9, 34.8, 34.2, 32.4, 26.6, 24.9, 24.7, 16.2. **HRMS** (DART+) calcd. for $C_{13}H_{28}N_3S_1$ $[M + H]^+$ 258.20039, found 258.20131.

1-[(*1R,2R*)-2-Aminocyclohexyl]-3-ethylthiourea (G).



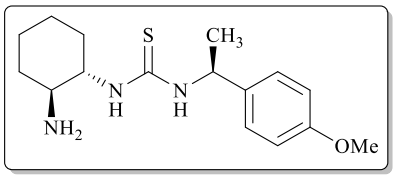
Hygroscopic yellow solid (0.174 g, 38% yield). $[\alpha]_D^{25}$ +80.7 (*c* 1.23, $CHCl_3$). **IR** (film) $\tilde{\nu}_{max}$: 3242, 3061, 2927, 2855, 1541, 1446, 1338, 1264, 1087, 937, 850, 731, 701, 571. **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 3.63-3.46 (m, 1H), 3.18 (br, 2H), 2.74-2.59 (m, 1H), 2.09-1.99 (m, 1H), 1.98-1.83 (m, 2H), 1.80-1.68 (m, 2H), 1.32-1.25 (m, 5H), 1.22 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 182.5, 60.6, 55.9, 39.8, 34.5, 32.3, 24.9, 24.7, 14.5. **HRMS** (DART+) calcd. for $C_9H_{20}N_3S_1$ $[M + H]^+$ 202.13779, found 202.13841.

1-[(*1R,2R*)-2-Aminocyclohexyl]- 3-[*(S)*-1-(4-methoxyphenyl)ethyl]thiourea (A (OMe)).



White solid (0.065 g, 58% yield), mp 115-117 °C, $[\alpha]_D^{25}$ +28.5 (*c* 0.8, $CHCl_3$). **IR** (KBr) $\tilde{\nu}_{max}$: 3243, 3041, 2931, 2860, 1608, 1543, 1509, 1448, 1337, 1241, 1176, 1028, 943, 831, 727, 544. **^{1}H NMR** (400 MHz, DMSO-d_6) δ: 8.11 (br, 1H), 7.82 (br, 1H), 7.29 (d, *J* = 8.7 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 5.37 (br, 1H), 4.10 (br, 1H), 3.72 (s, 3H), 2.89 (br, 1H), 2.08-1.87 (m, 2H), 1.64 (br, 2H), 1.37 (d, *J* = 6.8 Hz, 3H), 1.33-1.00 (4H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ: 181.6, 158.0, 136.1, 127.4, 113.5, 55.6, 55.1, 53.0, 51.9, 31.2, 30.1, 23.9, 23.4, 22.7. **HRMS** (DART+) calcd. for $C_{16}H_{26}N_3O_1S_1$ $[M + H]^+$ 308.17966, found 308.17954.

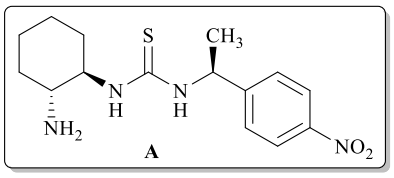
1-[(*1S,2S*)-2-Aminocyclohexyl]-3-[*(S)*-1-(4-methoxyphenyl)ethyl]thiourea (B (OMe)).



White solid (0.128 g, 54% yield), mp 66-69 °C, $[\alpha]_D^{25}$ -60.5 (*c* 1.0, $CHCl_3$). **IR** (KBr) $\tilde{\nu}_{max}$: 3246, 3047, 2925, 2854, 1607, 1538, 1509, 1447, 1240, 1175, 1029, 942, 830, 724, 545. **^{1}H NMR** (400 MHz, DMSO-d_6) δ: 7.81 (br, 1H), 7.32 (br, 1H), 7.24 (d, *J* = 8.7 Hz, 1H), 6.88 (d, *J* = 8.7 Hz, 1H), 5.36 (br, 1H), 3.76 (br, 1H), 3.72 (s, 3H), 2.00-1.90 (m, 1H), 1.86-1.75 (m, 1H), 1.60 (br, 2H), 1.37 (d, *J* = 6.9 Hz, 3H), 1.25-0.97 (m, 4H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ: 181.3, 158.0,

136.3, 127.2, 113.6, 58.8, 55.1, 54.0, 51.7, 33.6, 31.3, 24.4, 24.2, 22.5. **HRMS** (DART+) calcd. for $C_{16}H_{26}N_3O_1S_1$ $[M + H]^+$ 308.17966, found 308.17864.

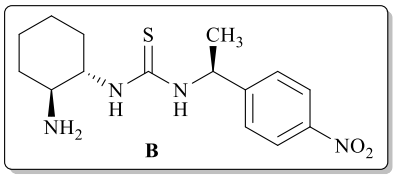
1-[(*1R,2R*)-2-Aminocyclohexyl]-3-[*(S)*-1-(4-nitrophenyl)ethyl]thiourea (A (NO_2)).



A

Yellow solid (0.146 g, 69% yield), mp 85-88 °C, $[\alpha]_D^{25}$ +117.7 (*c* 0.8, $CHCl_3$). **IR** (KBr) $\tilde{\nu}_{max}$: 3243, 3049, 2927, 2856, 1599, 1514, 1448, 1340, 1104, 1013, 852, 696, 519. **^{1}H NMR** (400 MHz, DMSO-d_6) δ: 8.17 (d, *J* = 8.8 Hz, 2H), 7.59 (d, *J* = 8.8 Hz, 2H), 5.50 (br, 1H), 3.75 (br, 3H), 2.59 (br, 1H), 1.97 (br, 1H), 1.89-1.78 (m, 1H), 1.61 (br, 2H), 1.42 (d, *J* = 7.0 Hz, 3H), 1.25-0.98 (m, 4H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ: 181.8, 153.1, 146.2, 127.3, 123.4, 58.7, 53.8, 52.3, 33.4, 31.4, 24.4, 24.2, 22.3. **HRMS** (DART+) calcd. for $C_{15}H_{23}N_4O_2S_1$ $[M + H]^+$ 323.15417, found 323.15344.

1-[(*1S,2S*)-2-Aminocyclohexyl]-3-[*(S)*-1-(4-nitrophenyl)ethyl]thiourea (B (NO_2)).



B

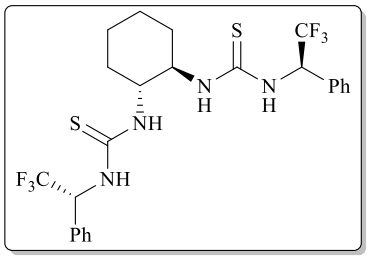
Yellow solid (0.174 g, 70% yield), mp 78-80 °C, $[\alpha]_D^{25}$ -43.7 (*c* 0.72, $CHCl_3$). **IR** (KBr) $\tilde{\nu}_{max}$: 3246, 3049, 2927, 2855, 1598, 1514, 1447, 1339, 1078, 1012, 851, 696, 519. **^{1}H NMR** (400 MHz, DMSO-d_6) δ: 8.18 (d, *J* = 8.8 Hz, 2H), 7.57 (d, *J* = 8.6 Hz, 2H), 5.52 (br, 1H), 3.71 (br, 1H), 3.31 (br, 3H), 2.00-1.88 (m, 1H), 1.86-1.77 (m, 1H), 1.59 (br, 2H), 1.42 (d, *J* = 7.0 Hz, 3H), 1.26-1.02 (m, 4H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ: 181.8, 153.0, 146.2, 127.3, 123.5, 59.1, 54.0, 52.3, 33.9, 31.3, 24.4, 24.3, 22.3. **HRMS** (DART+) calcd. for $C_{15}H_{23}N_4O_2S_1$ $[M + H]^+$ 323.15417, found 323.15349

General procedure for the synthesis of bisthioureas **K**-**N**.

The corresponding amine (0.3 mmol, 1 equiv) and isothiocyanate (0.6 mmol, 2 equiv) were dissolved in 1.2 mL of CH_2Cl_2 and stirred for 18 h at room temperature. After that time, solvent was evaporated and the resulting residue was purified by flash column with hexane/ethyl acetate as eluent (proportions indicated in each compound) to afford the resultant catalyst.

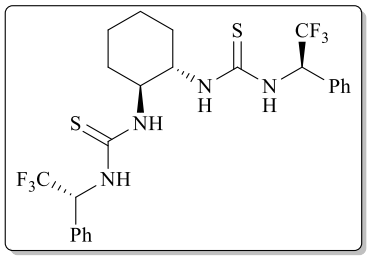
Note: Bis-thioureas **K**-**L** were obtained such as minor product in the reaction of bifunctional primary amine/thiourea catalyst in 12-15% yield.

1,1'-[(1*R*,2*R*)-Cyclohexane-1,2-diyl]bis{3-[(*R*)-2,2,2-trifluoro-1-phenylethyl]thiourea}, K_F.



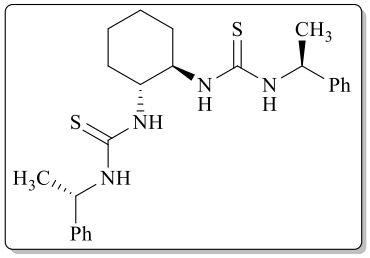
White solid, mp 242-243 °C. $[\alpha]_D^{25}$ +75.3 (*c* 1.0, DMSO). **^{1}H NMR** (300 MHz, $CDCl_3$, DMSO-d_6 drops) δ: 8.05 (br, 2H), 7.57 (br, 2H), 7.44-7.30 (m, 10H), 6.32 (br, 2H), 4.15 (br, 2H), 2.34 (br, 2H), 1.72 (br, 2H), 1.45-1.08 (br, 4H). **^{13}C NMR** (75 MHz, $CDCl_3$, DMSO-d_6 drops) δ: 182.9, 134.0, 128.7, 128.6, 128.2, 124.7 (q, *J*= 282.2 Hz), 58.6 (q, *J*= 30.2 Hz), 58.0, 32.5, 24.5. **MS** (DART+) *m/z* (%): 549 (40) $[M + H]^+$, 147 (100). **HRMS** (DART+) calcd. for $C_{24}H_{27}F_6N_4S_2$ $[M + H]^+$ 549.15813, found 549.15582.

1,1'-[(1*S*,2*S*)-Cyclohexane-1,2-diyl]bis{3-[(*R*)-2,2,2-trifluoro-1-phenylethyl]thiourea}, L_F.



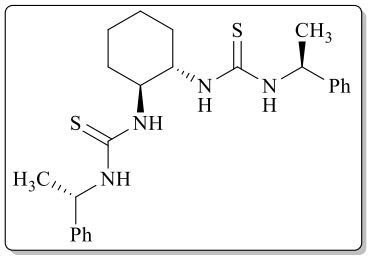
White solid, mp 230-231 °C. $[\alpha]_D^{25}$ +28.1 (*c* 1.0, DMSO). **^{1}H NMR** (300 MHz, $CDCl_3$, DMSO-d_6 drops) δ: 8.04 (br, 2H), 7.61 (br, 2H), 7.44-7.29 (m, 10H), 6.43 (p, *J* = 8.2 Hz, 2H), 4.26 (br, 2H), 2.18 (br, 2H), 1.65 (br, 2H), 1.36-1.08 (m, 4H). **^{13}C NMR** (75 MHz, $CDCl_3$, DMSO-d_6 drops) δ: 183.1, 133.5, 128.9, 128.8, 128.2, 125.0 (q, *J* = 282.1 Hz), 58.7 (q, *J* = 31.4 Hz), 58.4, 32.5, 24.7. **MS** (DART+) *m/z* (%): 549 (100) $[M + H]^+$, 374 (25), 147 (20). **HRMS** (DART+) calcd. for $C_{24}H_{27}F_6N_4S_2$ $[M + H]^+$ 549.15813, found 549.16014.

1,1'-[(1*R*,2*R*)-Cyclohexane-1,2-diyl]bis{3-[(*S*)-1-phenylethyl]thiourea}, K.



White solid, mp 99-100 °C. $[\alpha]_D^{25}$ +52.9 (*c* 1.0, DMSO). **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 7.41-7.21 (m, 10H), 6.46 (br, 4H), 4.92 (br, 2H), 4.07 (br, 2H), 1.76 (s, 2H), 1.54 (br, 2H), 1.41 (br, 6H), 1.13 (br, 2H), 0.78 (br, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 180.1, 141.9, 128.9, 127.8, 125.7, 59.2, 53.4, 31.6, 23.4, 25.1. **MS** (DART+) *m/z* (%): 441 (100) $[M + H]^+$. **HRMS** (DART+) calcd. for $C_{24}H_{33}N_4S_2$ $[M + H]^+$ 441.21466, found 441.21293.

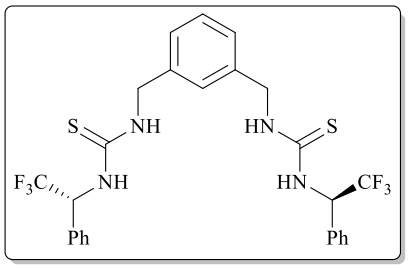
1,1'-[(1*S*,2*S*)-Cyclohexane-1,2-diyl]bis{3-[(*S*)-1-phenylethyl]thiourea}, L.



White solid, mp 185-186 °C (lit.,[9] *R,R,R* enantiomer mp 181-182 °C). $[\alpha]_D^{25}$ +11.9 (*c* 1.0, DMSO). **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 7.43-7.17 (m, 10H), 6.40 (br, 4H), 4.89 (br, 2H), 4.07 (s, 2H), 1.74 (s, 2H), 1.53 (br, 2H), 1.42 (br 6H), 1.13 (br, 2H), 0.77 (br, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 180.2, 142.5, 127.9, 125.9, 59.1, 53.5, 31.8, 23.5, 24.7. **MS** (DART+) *m/z* (%): 440 (19) $[M + H]^+$, 260 (17), 231 (25), 201 (14), 101

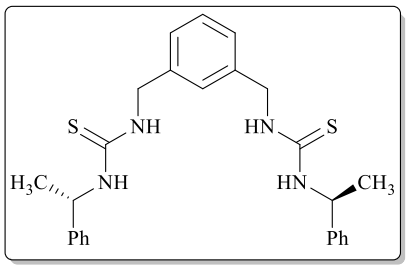
(11), 155 (60), 77 (25), 69 (18). **HRMS** (DART+) calcd. for $C_{24}H_{33}N_4S_2$ [M + H]$^+$ 441.21466, found 441.21259.

1,1'-(1,3-Phenylenebis(methylene))bis(3-((*R*)-2,2,2-trifluoro-1-phenylethyl)thiourea), M_F.



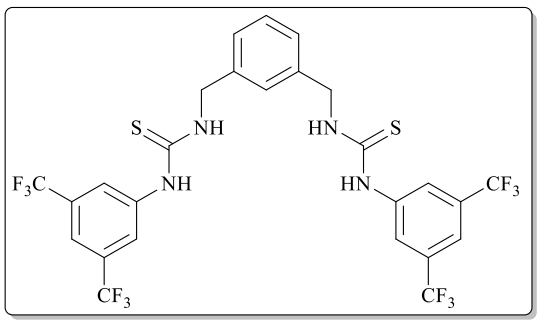
Purified by FC with Hex/EtOAc (8:2), white solid (0.040 g, 24% yield), mp 182-183 °C. $[\alpha]_D^{25}$ +28.4 (*c* 1.0, DMSO). **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.00 (br, 2H), 7.58 (br, 2H), 7.44-7.30 (m, 10H), 7.26-7.23 (m, 1H), 7.22-7.13 (m, 3H), 6.45 (p, *J* = 8.5 Hz, 2H), 4.75 (dd, *J* = 12.0, 4.6 Hz, 2H) 4.57 (dd, *J* = 12.0, 4.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 183.8, 138.5, 133.7, 129.2, 129.1, 128.9, 128.3, 127.4, 126.9, 124.9 (q, *J* = 280.0 Hz), 59.1 (q, *J* = 30.1 Hz), 48.8. **MS** (DART+) *m/z* (%): 570 (40) [M + H]$^+$, 354 (100). **HRMS** (DART+) calcd. for $C_{26}H_{25}F_6N_4S_2$ [M + H]$^+$ 571.14248, found 571.14047.

1,1'-(1,3-Phenylenebis(methylene))bis(3-((*S*)-1-phenylethyl)thiourea), M.



Purified by FC with Hex/EtOAc (7:3), white solid (0.245 g, 70% yield), mp 92-94 °C. $[\alpha]_D^{25}$ +24.4° (*c* 1.0, DMSO). **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 7.33-7.25 (m, 10H), 7.10 (t, *J* = 7.4 Hz, 1H), 6.88 (d, *J* = 7.4 Hz, 2H), 6.64 (s, 1H), 6.45 (br, 2H), 5.87 (br, 2H), 4.90 (br, 2H), 4.61-4.40 (m, 4H), 1.52-1.44 (m, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 181.3, 142.1, 137.8, 129.4, 129.2, 128.2, 126.7, 126.0, 54.1, 48.8, 23.7. **MS** (DART+) *m/z* (%): 463 (5) [M + H]$^+$, 342 (80), 300 (90), 105 (100). **HRMS** (DART+) calcd. for $C_{26}H_{31}N_4S_2$ [M + H]$^+$ 463.19901, found 463.20052.

1,1'-(1,3-Phenylenebis(methylene))bis(3-(3,5-bis(trifluoromethyl)phenyl)thiourea), N.



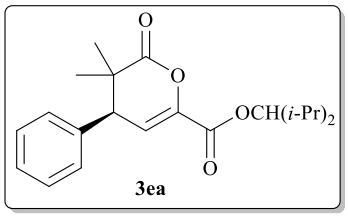
Purified by FC with Hex/EtOAc (7:3), white solid (0.343 g, 67% yield), mp 202-203 °C. **^{1}H NMR** (400 MHz, $CDCl_3$, DMSO-d_6 drops) δ: 9.49 (br, 2H), 8.14 (s, 4H), 7.81 (br, 2H), 7.56 (s, 2H), 7.37-7.28 (m, 4H), 4.84 (d, *J* = 5.1 Hz, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$, DMSO-d_6 drops) δ: 181.6, 141.2, 138.5, 131.5 (q, *J* = 33.3 Hz), 129.1, 127.2, 126.8, 123.2 (q, *J* = 274 Hz), 122.6, 117.4, 48.0. **MS** (EI) *m/z* (%): 678 (2) [M + H]$^+$, 390 (10), 271 (100), 252 (25), 213 (27), 119 (35).

2 General procedures for the stereoselective model reactions.

Addition of isobutyraldehyde to β,γ-unsaturated α-ketoesters.

A suspension of catalyst $\mathbf{A_F}$ (0.015 mmol, 0.2 equiv), DMAP (0.015 mmol, 0.2 equiv) in chloroform (0.7 M) was stirred for 5 min at 20 ºC. Then, isobutyraldehyde (0.42 mmol, 2.7 equiv) and β,γ-unsaturated α-ketoesters (0.15 mmol, 1 equiv) were added. The mixture was stirred at 20 ºC for 48 h. The solvent was removed and the crude was purified by flash chromatography with a hexane/ethyl acetate (85:15) mixture to give the cyclic hemiacetal. It was dissolved in dichloromethane (3 mL) and PCC (2.5 equiv) was added at 0 °C, after the mixture was stirred 1 h, it was warmed to room temperature and monitored by TLC. The mixture reaction was filtered over celite and the solid washed with ethyl acetate. The organic layer was washed with a saturated solution of NH_4Cl and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and the residue was purified by flash chromatography to give the product.

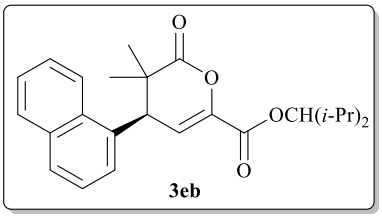
(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-phenyl-3,4-dihydro-2*H*-pyran-6-carboxylate



3ea

Data from Table 4, Entry 1. Purified by FC with Hex/EtOAc (85:15). White solid (16 mg, 45% yield), mp 105-108 °C, 76% ee. $[\alpha]_D^{25}$ -144.2 (*c* 1.1, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.38-7.30 (m, 3H), 7.16-7.09 (m, 2H), 6.60 (d, *J* = 5.3 Hz, 1H), 4.78 (t, *J* = 6.2 Hz, 1H), 3.51 (d, *J* = 5.3 Hz, 1H), 2.08-1.91 (m, 2H), 1.40 (s, 3H), 1.01 (s, 3H), 0.95-0.88 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 172.1, 160.6, 141.6, 137.2, 129.0, 128.7, 128.1, 117.1, 84.9, 50.1, 41.0, 29.6, 25.9, 21.6, 19.7, 19.6, 17.5, 17.4. **HRMS** (DART+) calcd. for $C_{21}H_{29}O_4$ $[M + H]^+$ 345.20658, found 345.20538. **CSP-HPLC**: Chiralpak IA, Hexane/EtOH (95:5), flow rate 0.5 mL/min, λ = 254 nm, retention times: 10.0 min (*R*), 10.9 min (*S*).

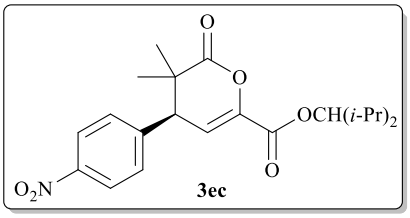
(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(1-naphthyl)-3,4-dihydro-2*H*-pyran-6-carboxylate



3eb

Data from Table 4, Entry 2. Purified by FC with Hex/EtOAc (85:15). White solid (10 mg, 58% yield), mp 128-130 °C, 82% ee. $[\alpha]_D^{25}$ -138.3 (*c* 0.36, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.07 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.61-7.49 (m, 2H), 7.45 (t, *J* = 7.7 Hz, 1H), 7.27 (d, *J* = 7.2 Hz, 1H), 6.65 (d, *J* = 5.7 Hz, 1H), 4.79 (t, *J* = 6.2 Hz, 1H), 4.52 (d, *J* = 5.7 Hz, 1H), 2.05-1.91 (m, 2H), 1.52 (s, 3H), 1.01 (s, 3H), 0.98-0.86 (m, 12H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 172.0, 160.6, 142.0, 134.1, 133.7, 132.1, 129.5, 128.7, 126.7, 126.0, 125.8, 125.6, 123.0, 117.6, 84.9, 43.3, 42.1, 29.6, 26.8, 21.5, 19.7, 19.6, 17.5, 17.4. **HRMS** (DART+) calcd. for $C_{25}H_{31}O_4$ $[M + H]^+$ 395.22223, found 395.22181. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (90:10), flow rate 1 mL/min, λ = 254 nm, retention times: 8.3 min (*S*), 9.2 min (*R*).

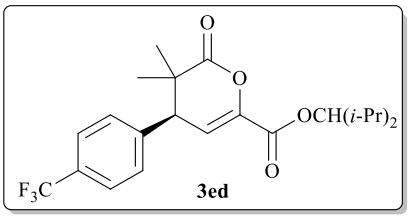
(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(4-nitrophenyl)-3,4-dihydro-2*H*-pyran-6-carboxylate



3ec

Data from Table 4, Entry 3. Purified by FC with Hex/EtOAc (85:15). White solid (15 mg, 41% yield), mp 98-100 °C, 68% ee. $[\alpha]_D^{25}$ -22.2 (*c* 0.9, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 8.22 (d, *J* = 8.8 Hz, 2H), 7.31 (d, *J* = 8.8 Hz, 2H), 6.55 (d, *J* = 5.3 Hz, 1H), 4.79 (t, *J* = 6.2 Hz, 1H), 3.65 (d, *J* = 5.3 Hz, 1H), 2.07-1.93 (m, 2H), 1.44 (s, 3H), 1.03 (s, 3H), 0.97-0.88 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 171.2, 160.3, 144.8, 142.5, 129.7, 124.3, 115.1, 85.4, 49.8, 40.8, 29.6, 25.9, 21.6, 19.7, 19.6, 17.4, 17.4. **HRMS** (DART+) calcd. for $C_{21}H_{28}N_1O_6$ $[M + H]^+$ 390.19166, found 390.19103. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (80:20), flow rate 1 mL/min, λ = 254 nm, retention times: 12.9 min (*R*), 19.4 min (*S*).

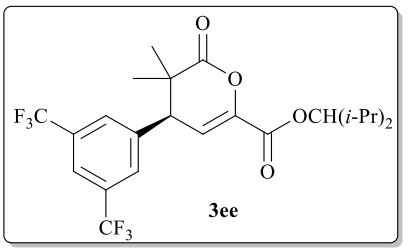
(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(4-(trifluoromethyl) phenyl)-3,4-dihydro-2*H*-pyran-6-carboxylate



3ed

Data from Table 4, Entry 4. Purified by FC with Hex/EtOAc (85:15). White solid (19 mg, 62% yield), mp 86-88 °C, 74% ee. $[\alpha]_D^{25}$ -106.0 (*c* 0.9, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.61 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 6.55 (d, *J* = 5.3 Hz, 1H), 4.78 (t, *J* = 6.2 Hz, 1H), 3.59 (d, *J* = 5.3 Hz, 1H), 2.05-1.91 (m, 2H), 1.42 (s, 3H), 1.02 (s, 3H), 0.95-0.87 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 171.6, 160.4, 142.2, 141.4, 130.3, 129.1, 126.0 (q, *J* = 4.0 Hz), 115.8, 85.2, 49.9, 40.8, 29.6, 25.91, 21.6, 19.7, 19.6, 17.5, 17.4. **HRMS** (DART+) calcd. for $C_{22}H_{28}F_3O_4$ $[M + H]^+$ 413.19397, found 413.19298. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (95:5), flow rate 1 mL/min, λ = 254 nm, retention times: 7.2 min (*S*), 8.1 min (*R*).

(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(4-(3,5-bistrifluoromethyl)phenyl)-3,4-dihydro-2*H*-pyran-6-carboxylate

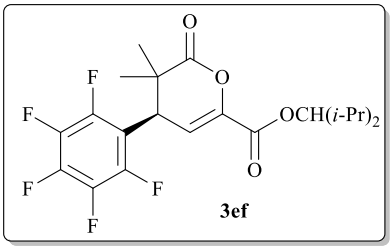


3ee

Data from Table 4, Entry 5. Purified by FC with Hex/EtOAc (85:15). White solid (14 mg, 51% yield), mp 107-110 °C, 87% ee. $[\alpha]_D^{25}$ -55.3 (*c* 0.76, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 7.85 (s, 1H), 7.56 (s, 2H), 6.53 (d, *J* = 5.0 Hz, 1H), 4.79 (t, *J* = 6.1 Hz, 1H), 3.72 (d, *J* = 5.0 Hz, 1H), 2.06-1.93 (m, 2H), 1.43 (s, 3H), 1.04 (s, 3H), 0.96-0.85 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 170.9, 160.2, 142.9, 140.1, 140.0, 132.7, 132.3, 128.9, 122.4, 114.6, 85.6, 49.5, 40.7, 29.6, 25.7, 21.4, 19.6, 17.4, 17.4.

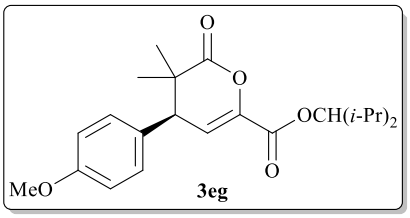
HRMS (DART+) calcd. for $C_{23}H_{27}F_6O_4$ $[M + H]^+$ 481.18135, found 481.18124. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (95:5), flow rate 1 mL/min, λ = 254 nm, retention times: 4.4 min (*R*), 5.0 min (*S*).

(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(2,3,4,5,6-pentafluorophenyl)-3,4-dihydro-2*H*-pyran-6-carboxylate



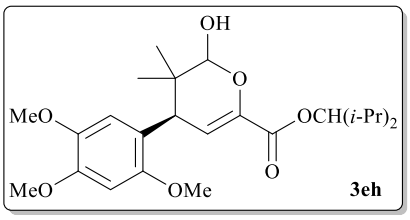
Data from Table 4, Entry 6. Purified by FC with Hex/EtOAc (85:15). Hygroscopic white solid (5 mg, 42% yield), 50% ee. $[\alpha]_D^{25}$ -84.3 (*c* 0.24, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) *δ*: 6.32 (d, *J* = 5.4 Hz, 1H), 4.76 (t, *J* = 6.1 Hz, 1H), 4.02 (d, *J* = 5.4 Hz, 1H), 2.04-1.91 (m, 2H), 1.46 (s, 3H), 1.13 (s, 3H), 0.95-0.85 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) *δ*: 170.6, 160.2, 147.8, 146.4, 144.6, 143.0, 142.8, 139.6, 136.3, 110.7, 85.4, 39.8, 39.4, 29.6, 26.8, 21.7, 19.6, 17.4, 17.4. **HRMS** (DART+) calcd. for $C_{21}H_{24}F_5O_4$ $[M + H]^+$ 435.15947, found 435.15970. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (95:5), flow rate 1 mL/min, λ = 254 nm, retention times: 5.9 min (*S*), 7.4 min (*R*).

(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(4-methoxyphenyl)-3,4-dihydro-2*H*-pyran-6-carboxylate



Data from Table 4, Entry 7. Purified by FC with Hex/EtOAc (85:15). White solid (17 mg, 65% yield), mp 128-130 °C, 80% ee. $[\alpha]_D^{25}$ -155.1 (*c* 0.74, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) *δ*: 7.02 (d, *J* = 8.7 Hz, 2H), 6.85 (d, *J* = 8.8 Hz, 2H), 6.57 (d, *J* = 5.3 Hz, 1H), 4.76 (t, *J* = 6.2 Hz, 1H), 3.79 (s, 3H), 3.45 (d, *J* = 5.3 Hz, 1H), 2.03-1.90 (m, 2H), 1.38 (s, 3H), 1.00 (s, 3H), 0.95-0.87 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) *δ*: 172.2, 160.6, 159.4, 141.4, 129.8, 129.1, 117.4, 114.4, 84.9, 55.4, 49.4, 41.2, 29.6, 25.9, 21.6, 19.7, 19.6, 17.5, 17.4. **HRMS** (DART+) calcd. for $C_{22}H_{31}O_5$ $[M + H]^+$ 375.21715, found 375.21661. **CSP-HPLC**: Chiralpak IA, Hexane/EtOH (95:5), flow rate 0.5 mL/min, λ = 254 nm, retention times: 14.3 min (*S*), 16.9 min (*R*).

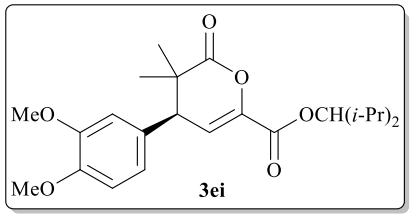
(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-hidroxy-4-(2,4,5-trimethoxyphenyl)-3,4-dihydro-2*H*-pyran-6-carboxylate



Data from Table 4, Entry 8. Purified by FC with Hex/EtOAc (95:5). Yellow solid (22 mg, 60% yield), mp 57-58 °C, 90% ee. $[\alpha]_D^{25}$ -62.8 (*c* 0.59, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) *δ*: 6.64 (s, 1H), 6.54 (s, 1H), 6.13 (d, *J* = 2.4 Hz, 1H), 5.13 (s, 1H), 4.72 (t, *J* = 6.1 Hz, 1H), 4.23 (s, 1H), 3.90 (s, 3H), 3.79 (s, 3H), 3.78 (s, 3H), 1.99-1.85

(m, 2H), 0.97 (s, 3H), 0.93-0.83 (m, 12H), 0.75 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 163.3, 152.4, 148.5, 142.6, 119.6, 116.3, 115.9, 115.1, 99.8, 97.4, 83.7, 56.5, 56.3, 56.2, 36.1, 29.6, 23.5, 20.8, 19.7, 19.6, 17.5, 17.2. **HRMS** (DART+) calcd. for $C_{24}H_{37}O_7$ $[M + H]^+$ 437.25393, found 437.25220. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (90:10), flow rate 0.5 mL/min, λ = 206 nm, retention times: 9.8 min (*R*), 17.6 min (*S*).

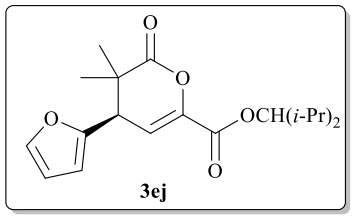
(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(3,4,-dimethoxyphenyl)-3,4-dihydro-2*H*-pyran-6-carboxylate



3ei

Data from Table 4, Entry 9. Purified by FC with Hex/EtOAc (85:15). White solid (20 mg, 65% yield), mp 138-140 °C, 89% ee. $[\alpha]_D^{25}$ -189.4 (*c* 0.81, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 6.81 (d, *J* = 8.2 Hz, 1H), 6.66 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.59 (d, *J* = 5.5 Hz, 1H), 6.56 (d, *J* = 2.1 Hz, 1H), 4.77 (t, *J* = 6.2 Hz, 1H), 3.86 (s, 3H), 3.83 (s, 3H), 3.41 (d, *J* = 5.5 Hz, 1H), 2.04-1.91 (m, 2H), 1.40 (s, 3H), 1.02 (s, 3H), 0.93-0.87 (m, 12H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 172.2, 160.6, 149.2, 148.9, 141.4, 129.6, 121.0, 117.2, 111.5, 111.4, 84.9, 56.0, 50.0, 41.2, 29.6, 26.1, 21.8, 19.7, 19.6, 17.4, 17.4. **HRMS** (DART+) calcd. for $C_{23}H_{33}O_6$ $[M + H]^+$ 405.22771, found 405.22843. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (90:10), flow rate 1.0 mL/min, λ = 254 nm, retention times: 19.7 min (*S*), 27.8 min (*R*).

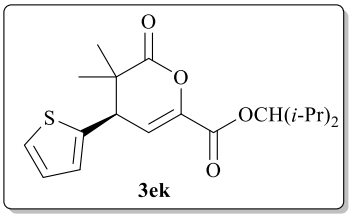
(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(furan-2-yl)-3,4-dihydro-2*H*-pyran-6-carboxylate



3ej

Data from Table 4, Entry 10. Purified by FC with Hex/EtOAc (85:15). White solid (8 mg, 28% yield), mp 63-65 °C, 84% ee. $[\alpha]_D^{25}$ -88.8 (*c* 0.62, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.35 (s, 1H), 6.48 (d, *J* = 5.4 Hz, 1H), 6.32 (dd, *J* = 3.2, 1.9 Hz, 2H), 6.16 (d, *J* = 3.2 Hz, 1H), 4.76 (t, *J* = 6.2 Hz, 1H), 3.61 (d, *J* = 5.4 Hz, 1H), 2.06-1.92 (m, 2H), 1.39 (s, 3H), 1.09 (s, 3H), 0.97-0.86 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 171.7, 160.5, 150.5, 142.8, 142.2, 113.8, 110.5, 108.5, 85.0, 43.3, 40.8, 29.6, 25.3, 21.6, 19.7, 17.4, 17.4. **HRMS** (DART+) calcd. for $C_{19}H_{27}O_5$ $[M + H]^+$ 335.18585, found 335.18569. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (90:10), flow rate 1.0 mL/min, λ = 254 nm, retention times: 6.5 min (*S*), 7.9 min (*R*).

(*S*)-2,4-dimethylpentan-3-yl 3,3-dimethyl-2-oxo-4-(thiophen-2-yl)-3,4-dihydro-2*H*-pyran-6-carboxylate



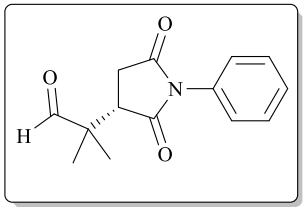
3ek

Data from Table 4, Entry 11. Purified by FC with Hex/EtOAc (85:15). Hygroscopic yellow solid (15 mg, 48% yield), 83% ee. $[\alpha]_D^{25}$ -121.0 (*c* 0.91, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 7.23 (d, *J* = 5.2 Hz, 1H), 6.98 (dd, *J* = 5.2, 3.0 Hz, 1H), 6.87 (d, *J* = 3.0 Hz, 1H), 6.61 (d, *J* = 5.3 Hz, 1H), 4.77 (t, *J* = 6.2 Hz, 1H), 3.81 (d, *J* = 5.3 Hz, 1H), 2.03-1.92 (m, 2H), 1.41 (s, 3H), 1.12 (s, 3H), 0.95-0.84 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 171.7, 160.5, 141.5, 139.3, 127.4, 126.9, 125.3, 116.6, 85.0, 44.8, 41.6, 29.6, 25.6, 21.7, 19.6, 17.4. **HRMS** (DART+) calcd. for $C_{19}H_{27}O_4S_1$ $[M + H]^+$ 351.16300, found 351.16155. **CSP-HPLC**: Chiralpak IC, Hexane/*i*-PrOH (95:5), flow rate 1.0 mL/min, λ = 254 nm, retention times: 11.4 min (*S*), 13.1 min (*R*).

Addition of isobutyraldehyde to *N*-phenylmaleimide.

A mixture of catalyst **B** (0.02 mmol, 0.1 equiv) and benzoic acid (0.02 mmol, 0.1 equiv) in dichloromethane (0.5 M) was stirred at 20 ºC for 5 min. After that time, isobutyraldehyde (0.40 mmol, 2 equiv) and *N*-phenylmaleimide (0.20 mmol, 1 equiv) were added and stirred for 40 min. The solvent was removed, and the crude was purified by flash chromatography with a hexane/ethyl acetate (60:40) mixture to give the product.

(*S*)-1-Phenyl-3-(formylmetylethyl)succinimide (4).

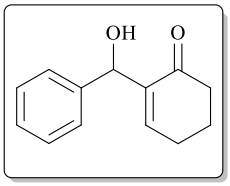


Data from Table 5, Entry 4. White solid (49 mg, 99% yield), mp 104-106 ºC, >99% ee. $[\alpha]_D^{25}$ -5.2 (*c* 0.99, $CHCl_3$). **^{1}H NMR** (300 MHz, $CDCl_3$) δ: 9.52, 7.51-7.36 (m, 3H), 7.31-7.25 (m, 2H), 3.16 (dd, *J* = 9.5, 5.5 Hz, 1H), 2.99 (dd, *J* = 18.3, 9.5 Hz, 1H), 2.63 (dd, *J* = 18.2, 5.5 Hz, 1H), 1.34 (s, 3H), 1.30 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 202.9, 177.0, 174.9, 131.9, 129.3, 128.8, 126.6, 48.6, 45.1, 31.9, 20.4, 19.6. **HRMS** (DART+) calcd. for $C_{14}H_{16}N_1O_3$ $[M + H]^+$ 246.11302, found 246.11419. **CSP-HPLC**: Chiralpak IA, Hexane/EtOH (1:1), flow rate 1 mL/min, λ = 210 nm, retention times: 13.4 min (*S*), 43.2 min (*R*).

Baylis-Hillman reaction.

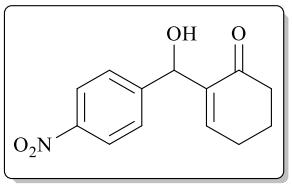
To a mixture of 2-cyclohexenone (0.34 mmol, 1.2 equiv,), bis/mono-thiourea catalyst (0.06 mmol, 0.2 equiv.) and DMAP (0.12 mmol, 0.4 equiv.) was added the corresponding aldehyde (0.28mmol, 1 equiv.). The resulting mixture was stirred for 72 h at 20 °C. The crude was purified by flash chromatography on silica gel (hexane/ethyl acetate, 85:15) to give the Baylis-Hillman product.

2-(Hydroxy(phenyl)methyl)cyclohex-2-en-1-one (5a)



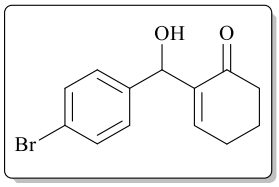
^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.37-7.22 (m, 5H), 6.74 (t, J = 4.1 Hz 1H), 5.55 (s, 1H), 3.49 (br, 1H), 2.47-2.32 (m, 4H), 2.04-1.93 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 200.6, 147.5, 141.8, 141.2, 128.4, 127.6, 126.6, 72.7, 38.7, 25.9, 22.6.

2-(Hydroxy(4-nitrophenyl)methyl)cyclohex-2-en-1-one (5b)



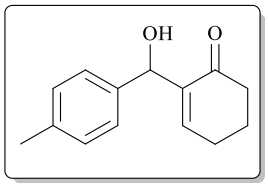
^{1}H NMR(300 MHz, $CDCl_3$) δ: 8.18 (d, J = 8.6 Hz, 2H), 7.55 (d, J = 8.2 Hz, 2H), 6.84 (t, J = 3.5 Hz, 1H), 5.61 (s, 1H), 3.47 (br, 1H), 2.50-2.36 (m, 4H), 2.07-1.95 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 200.1, 149.5, 148.2, 147.4, 140.4, 127.3, 123.6, 72.0, 38.5, 25.9, 22.5.

2-((4-Bromophenyl)(hydroxy)methyl)cyclohex-2-en-1-one (5c)



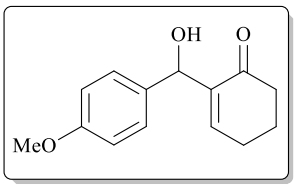
^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.46 (d, J = 8.6 Hz, 2H), 7.23 (d, J = 8.7 Hz, 2H), 6.75 (t, J = 4.2 Hz, 1H), 5.49 (s, 1H), 3.51 (br, 1H), 2.50-2.34 (m, 4H), 2.05-1.93 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 200.5, 147.7, 140.9, 131.5, 128.3, 121.5, 72.2, 38.6, 25.9, 22.6.

2-(Hydroxy(*p*-tolyl)methyl)cyclohex-2-en-1-one (5d)



^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.24 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 7.9 Hz, 2H), 6.74 (t, J = 3.9 Hz, 1H), 5.52 (s, 1H), 2.49-2.36 (m, 4H), 2.34 (s, 3H), 2.05-1.93 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 200.7, 147.4, 141.2, 138.8, 137.3, 129.2, 126.5, 72.7, 38.7, 25.9, 22.7.

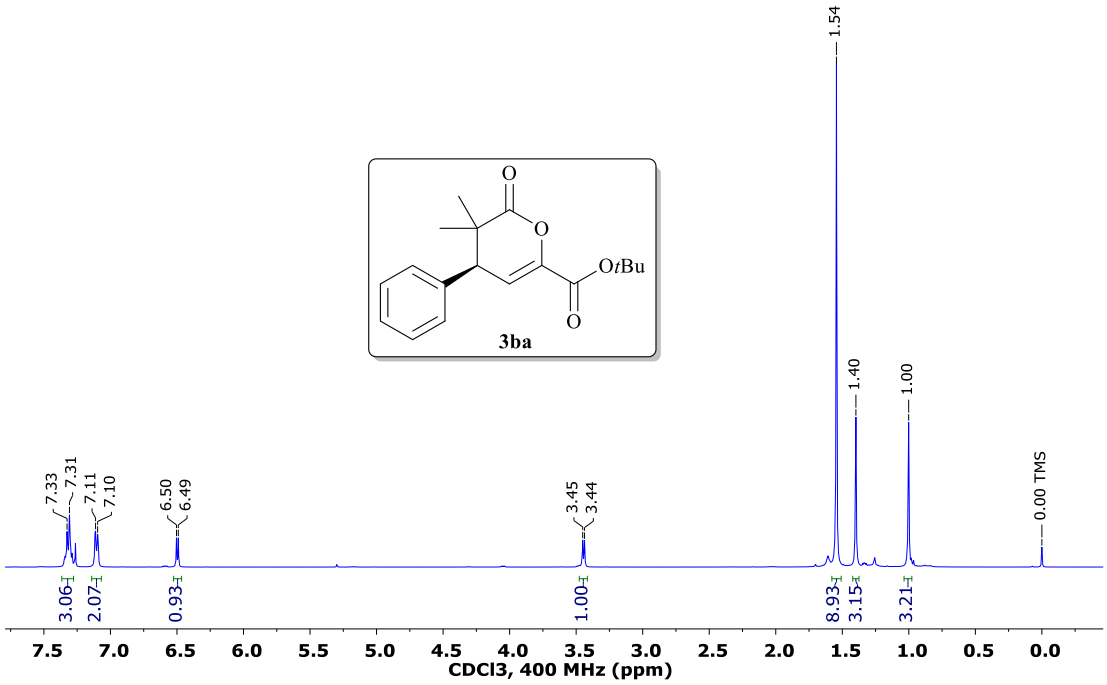
2-(Hydroxy(4-methoxyphenyl)methyl)cyclohex-2-en-1-one (5e).



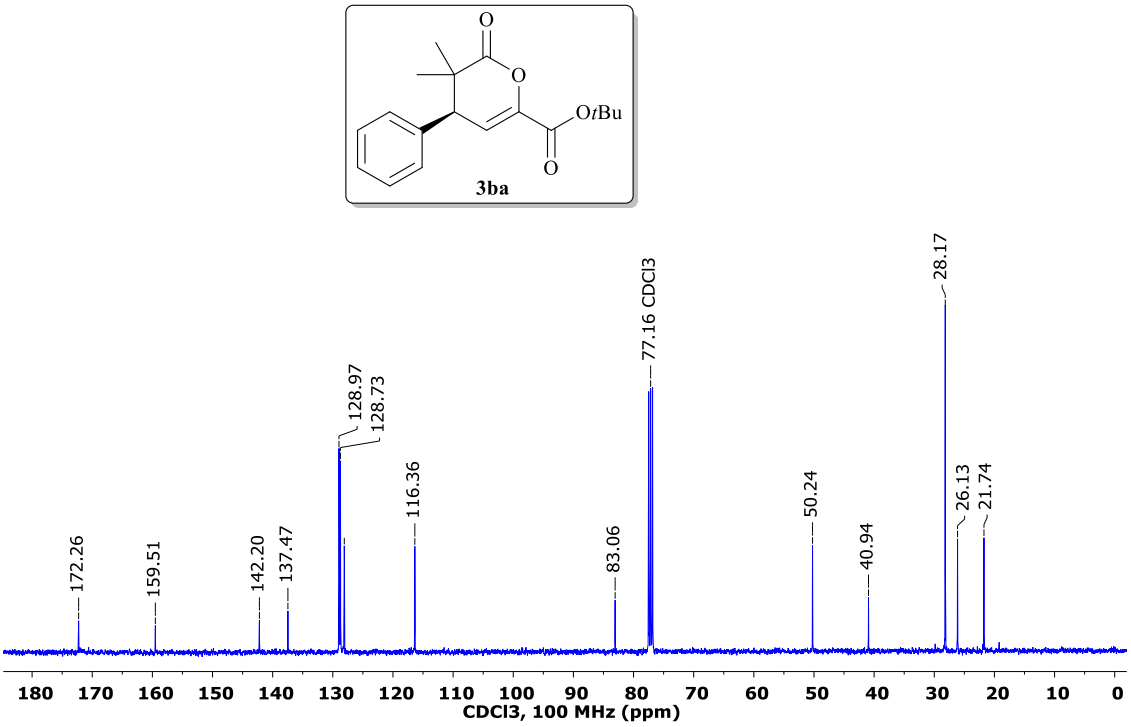
^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.27 (d, J = 8.4Hz, 2H), 6.87 (d, J = 8.6 Hz, 2H), 6.74 (t, J = 3.9 Hz, 1H), 3.80 (s, 3H), 5.52 (s, 1H), 3.36 (br, 1H), 2.51-2.33 (m, 4H), 2.05-1.93 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ: 200.7, 159.1, 147.2, 141.3, 133.9, 127.9, 113.8, 72.3, 55.4, 38.7, 25.9, 22.7.

3 X-Ray structure of (*S*)-*tert*-Butyl 3,3-dimethyl-2-oxo-4-phenyl-3,4-dihydro-2*H*-pyran-6-carboxylate (3ba).

After 3 recrystallizations by slow evaporation from a mixture of dichloromethane-hexane, compound **3ba** was obtained only as one enantiomer (98% ee). Single crystal was analyzed by X-ray crystallographic to determine the absolute configuration. CCDC 1859517 contains the supplementary crystallographic data. Colorless crystals. mp 139-141 °C, $[\alpha]_D^{25}$ -198.7 (*c* 0.24, $CHCl_3$). **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 7.37-7.28 (m, 3H), 7.14-7.07 (m, 2H), 6.50 (d, *J* = 5.4 Hz, 1H), 3.44 (d, *J* = 5.4 Hz, 1H), 1.54 (s, 9H), 1.40 (s, 3H), 1.00 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 172.3, 159.5, 142.2, 137.5, 129.0, 128.7, 128.1, 116.4, 83.1, 50.2, 40.9, 28.2, 26.1, 21.7. (DART+) *m/z* (%): 303 (30) $[M + H]^+$, 247 (100), 177 (20), 131 (40). **HRMS** (DART+) calcd. for $C_{18}H_{23}O_4$ $[M + H]^+$ 303.15963, found 303.16074. **CSP-HPLC**: Chiralcel OD-H, Hexane/EtOH (95:5), flow rate 0.4 mL/min, λ = 254 nm, retention times: 13.5 min (*R*), 14.6 min (*S*).



^{1}H NMR spectrum of compound **3ba**.

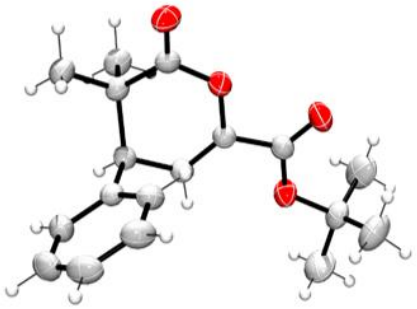


^{13}C NMR spectrum of compound **3ba**.

Table S1. Crystal data and structure refinement for **3ba**.

Identification code	170HRM18	
Empirical formula	C18 H22 O4	
Formula weight	302.35	
Temperature	298(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 6.2645(6) Å	a= 90°.
	b = 12.7734(12) Å	b= 95.177(8)°.
	c = 10.8124(15) Å	g = 90°.
Volume	861.67(17) Å^3	
Z	2	
Density (calculated)	1.165 Mg/m^3	
Absorption coefficient	0.661 mm^{-1}	
F(000)	324	

Crystal size	0.382 x 0.178 x 0.094 mm^3
Theta range for data collection	4.105 to 68.383°.
Index ranges	-5<=h<=7, -15<=k<=15, -12<=l<=13
Reflections collected	8238
Independent reflections	3135 [R(int) = 0.0219]
Completeness to theta = 67.679°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7531 and 0.6746
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3135 / 1 / 204
Goodness-of-fit on F^2	1.157
Final R indices [I>2sigma(I)]	R1 = 0.0477, wR2 = 0.1067
R indices (all data)	R1 = 0.0521, wR2 = 0.1108
Absolute structure parameter	0.09(14)
Extinction coefficient	n/a
Largest diff. peak and hole	0.136 and -0.162 $e.Å^{-3}$



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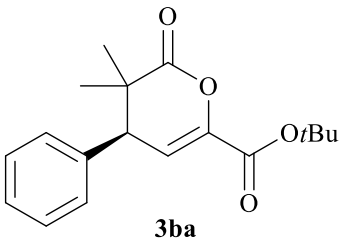


3ba

4 Confirmation of the enamine intermediate by DART-MS.

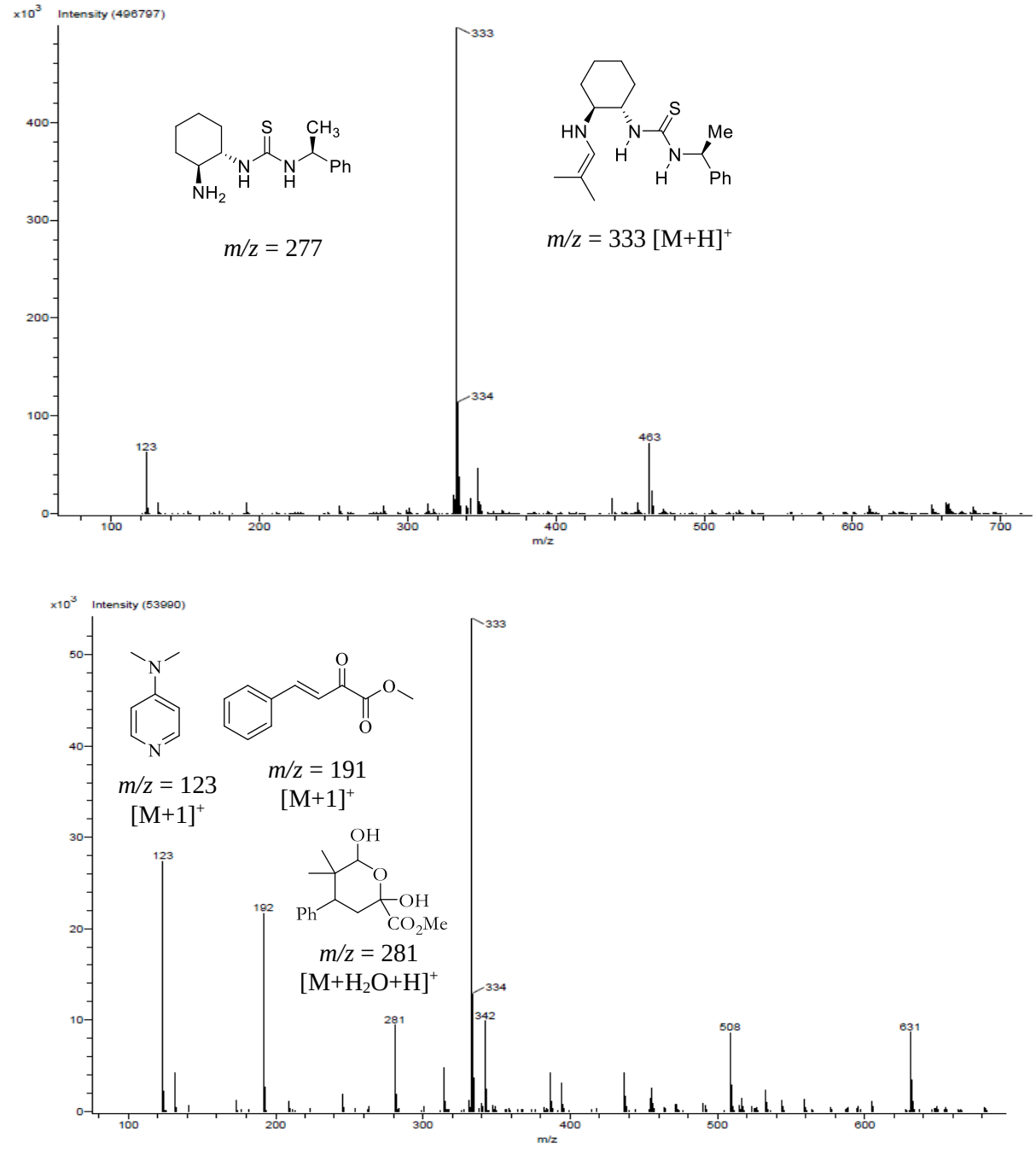


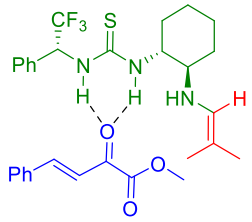
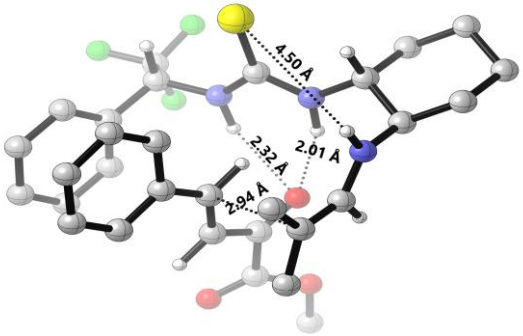
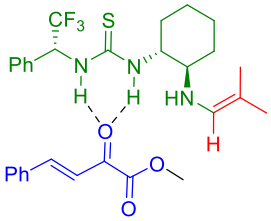
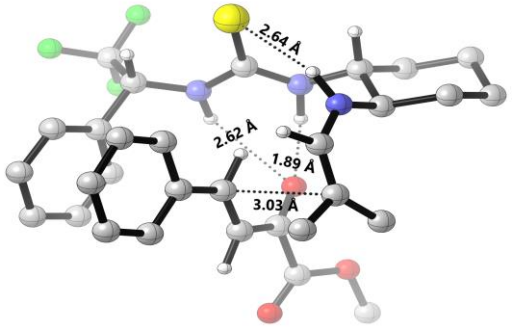
Figure S1. DART-MS spectrum of the Michael addition of isobutyraldehyde to methyl benzylidenepyruvate with catalysts **B**, after 30 minutes (top) and 1.5 h (bottom).

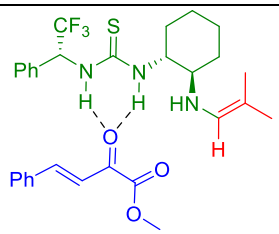
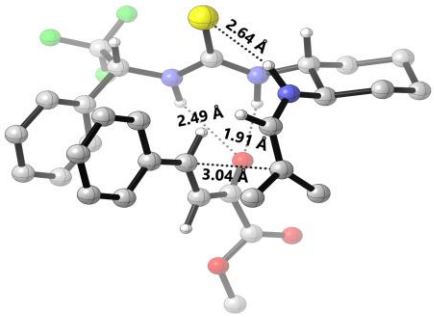
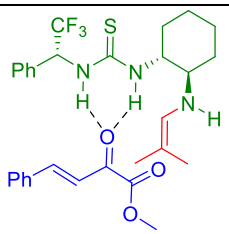
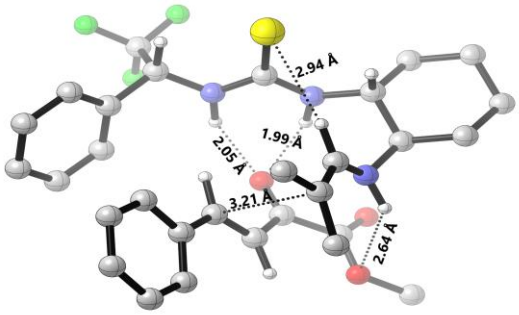
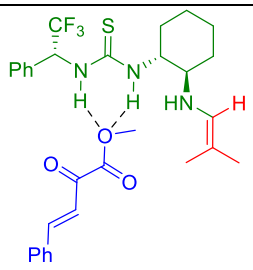
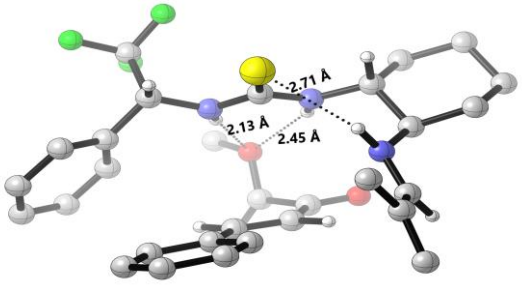
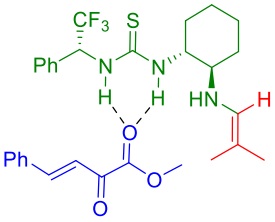
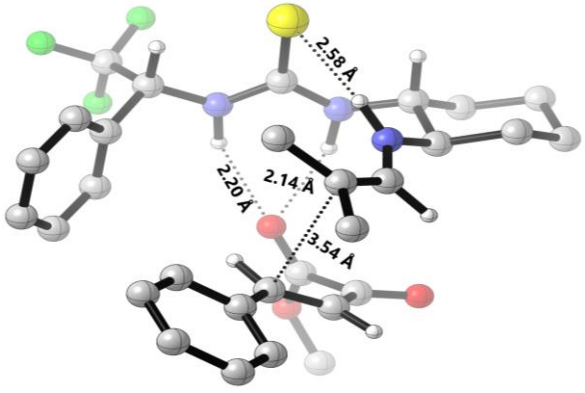
5 Computation details

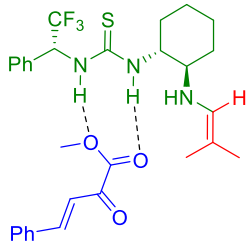
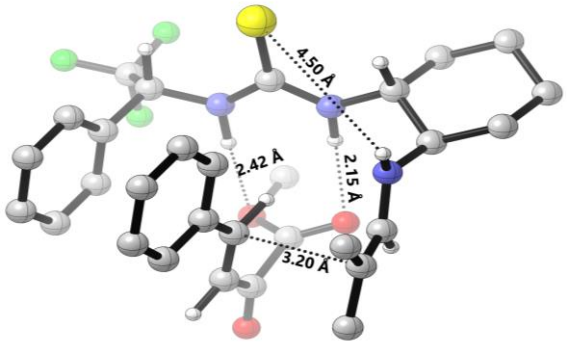
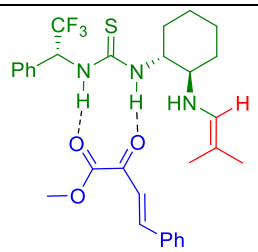
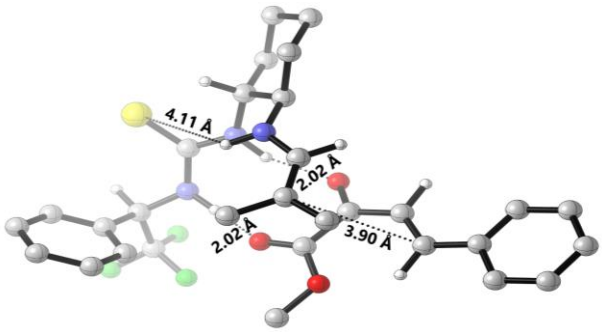
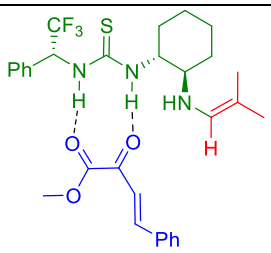
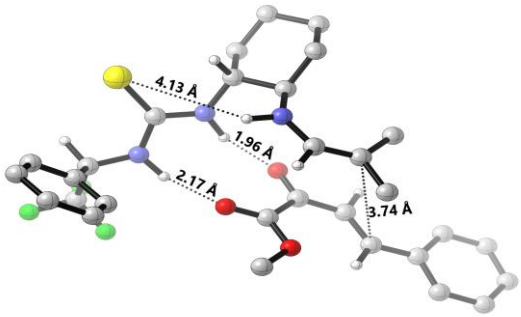
The geometry of all intermediates and transition states were completely optimized with PCM-($CHCl_3$)-B97D/TZVP for the ketoester substrate in the Gaussian 09 package.[13] The modeling of the isobutyraldehyde addition to *N*-phenylmaleimide using the B97D/TZVP approximation gives an endergonic product with a little activation barrier to the retro-Michael reaction, in opposition to the experimental results. This issue was solved using the M06-2X/TZVP level of theory. Each stationary point was characterized as a local minimum or a saddle point of first order via the computation of the corresponding harmonic frequencies. Intrinsic reaction coordinate calculations were carried out in all cases to verify that the localized transition state structures connect the two minima on the potential energy surface associated with reactants and products.

Conformational analysis of reactant complexes [Gas-phase (B97D/TZVP)].

Table S2. Different ways of association and conformations of the reactive cluster formed by the enamine of catalyst $\mathbf{A_F}$ and methyl benzylidenepyruvate (*Re* face addition, major enantiomer) modelled with B97D/TZVP.

Abbreviated structure **Label of the adduct** **Relative energy with respect to reactants**	**Structure showing HB and C-C distances**
 **KE-A_F-Maj-Cx1** **-21.3 kcal/mol**	
 **KE-A_F-Maj-Cx2** **-20.9 kcal/mol**	

 **KE-A$_F$-Maj-Cx3** **-19.7 kcal/mol**	
 **KE-A$_F$-Maj-Cx4** **-22.5 kcal/mol**	
 **KE-A$_F$-Maj-Cx5** **-18.4 kcal/mol**	
 **KE-A$_F$-Maj-Cx6** **-11.8 kcal/mol**	

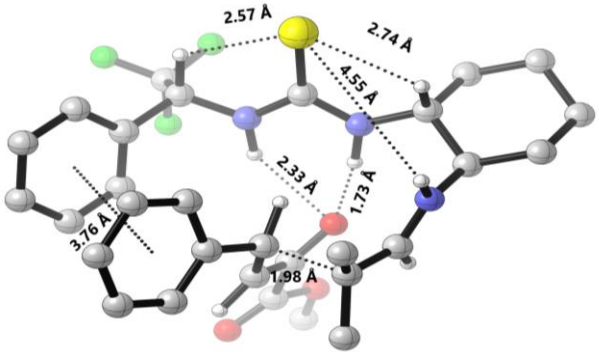
 **KE-A$_F$-Maj-Cx7** **-19.1 kcal/mol**	
 **KE-A$_F$-Maj-Cx8** **-15.8 kcal/mol**	
 **KE-A$_F$-Maj-Cx9** **-12.7 kcal/mol**	

The search for different conformations and arrangements of the TS was performed by studying different intermediates before the C-C bond formation; the most stable ones and with a short carbon-carbon distance were optimized via potential energy curves as a function of the C-C distance of interest until a TS was found. Only the TSs with lower energy were optimized with PCM and reported in the main body of the manuscript. Different arrangements and conformers arise due to single bond rotations, the most evident are of the C-N(enamine) and N-CH(CMe_2) and the single bonds in the ketoester. The conformer **Cx1** (Table S2) is the one reported in the manuscript, **Cx2** and **Cx3** are close in energy but this disposition with the hydrogens of the NH of enamine and vinylic CH in the same direction do not converge to a TS because of the clashing of the methyl groups with the cyclohexane moiety. Therefore, this conformation is not active in the formation of the C-C bond. The conformer **Cx4** was also optimized later with PCM and reported in

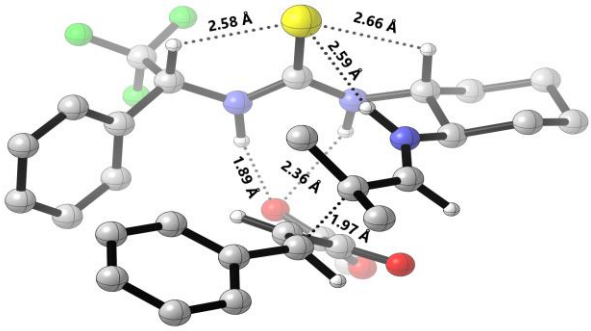
the ESI (**TS1** and **TS4** are both viable due to the low difference in energy but the most stable **TS1** is reported in the manuscript). The remaining complexes are too high in energy to be considered later or the TS was extremely high in energy (e.g. TS for **Cx6** was +6.1 kcal/mol whereas for C1 is -11.3 kcal/mol in gas phase). The finding that **Cx8** and **Cx9** with two hydrogen bonds towards both carbonyls are too high in energy is in line with previous report by Tsogoeva.[14]

Table S3. Relative energies with respect to reactants of the transition states and reactive complexes for the addition of isobutyraldehyde to methyl benzylidenepyruvate promoted by $\mathbf{A_F}$ and **B** (Maj and Min refers to the formation of the major and minor enantiomer of the product) [PCM($CHCl_3$)-B97D/TZVP].

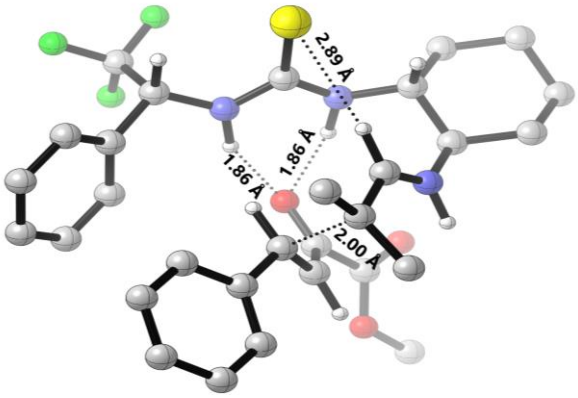
Cat.	TS	E_{rel} (kcal/mol)		Cat.	TS	E_{rel} (kcal/mol)	
		Maj	Min			Maj	Min
$\mathbf{A_F}$	TS1	-12.7	-12.2	**B**	TS1	-10.9	-9.8
	Cx1	-20.1	-20.4		Cx1	-18.4	-17.1
	TS4	-12.1	-8.3		TS4	-8.8	-6.0
	Cx4	-21.6	-16.2		Cx4	18.0	-14.2



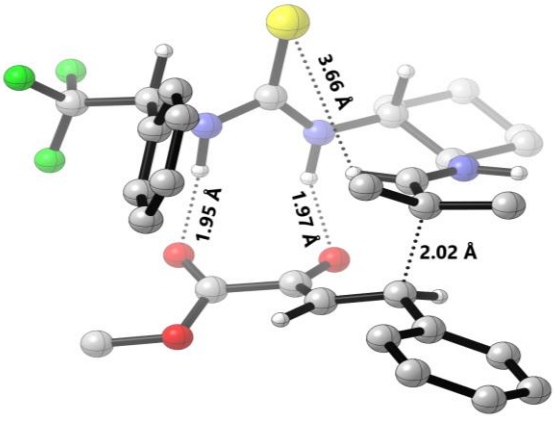
KE-A_F-Maj-TS1 (-12.7 kcal/mol)



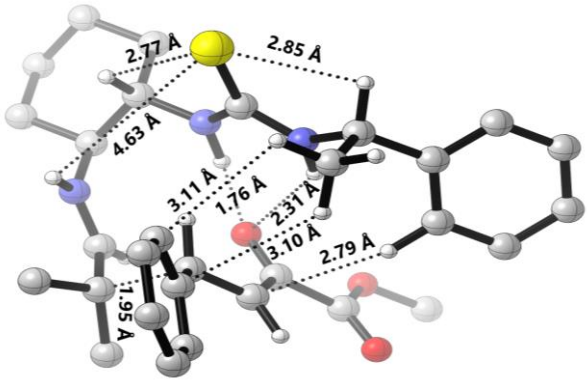
KE-A_F-Min-TS1 (-12.2 kcal/mol)



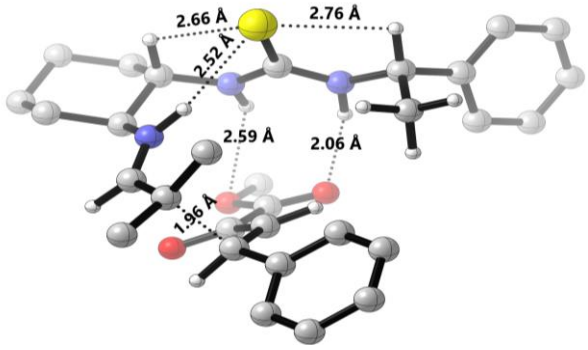
KE-A_F-Maj-TS4 (-12.1 kcal/mol)



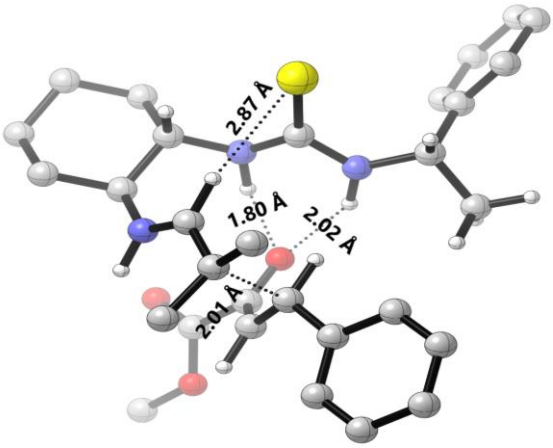
KE-A_F-Min-TS4 (-8.3 kcal/mol)



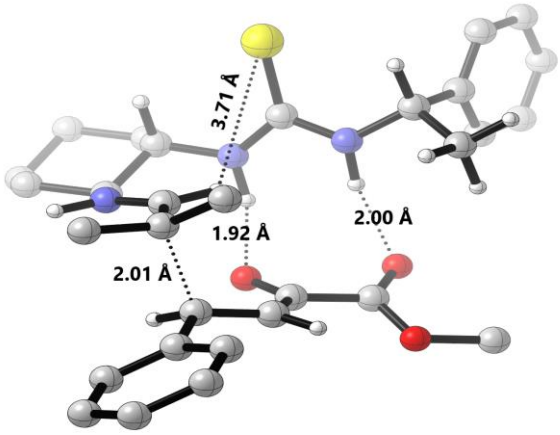
KE-B-Maj-TS1 (-10.9 kcal/mol)



KE-B-Min-TS1 (-9.8 kcal/mol)



KE-B-Maj-TS4 (-8.8 kcal/mol)



KE-B-Min-TS4 (-6.0 kcal/mol)

Figure S2. Structures of the transition states. Labels represent the ketoester electrophile (KE), catalyst (**A**$_{\mathbf{F}}$ or **B**), enantiomer produced (Maj or Min) and the number assigned in Table S3. Calculated at PCM($CHCl_3$)-B97D/TZVP level of theory.

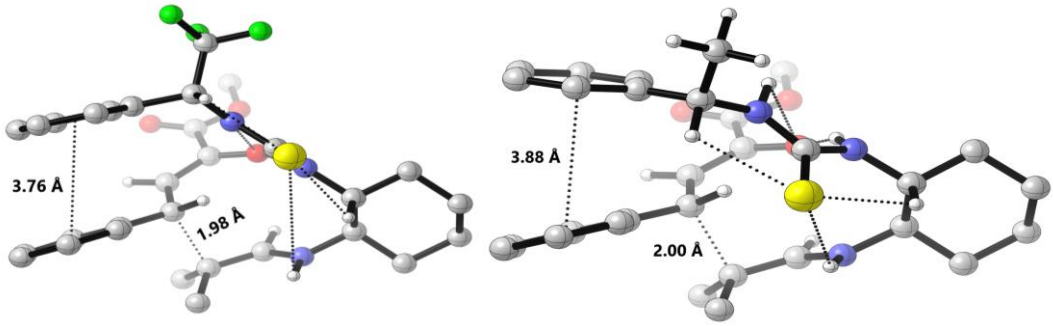
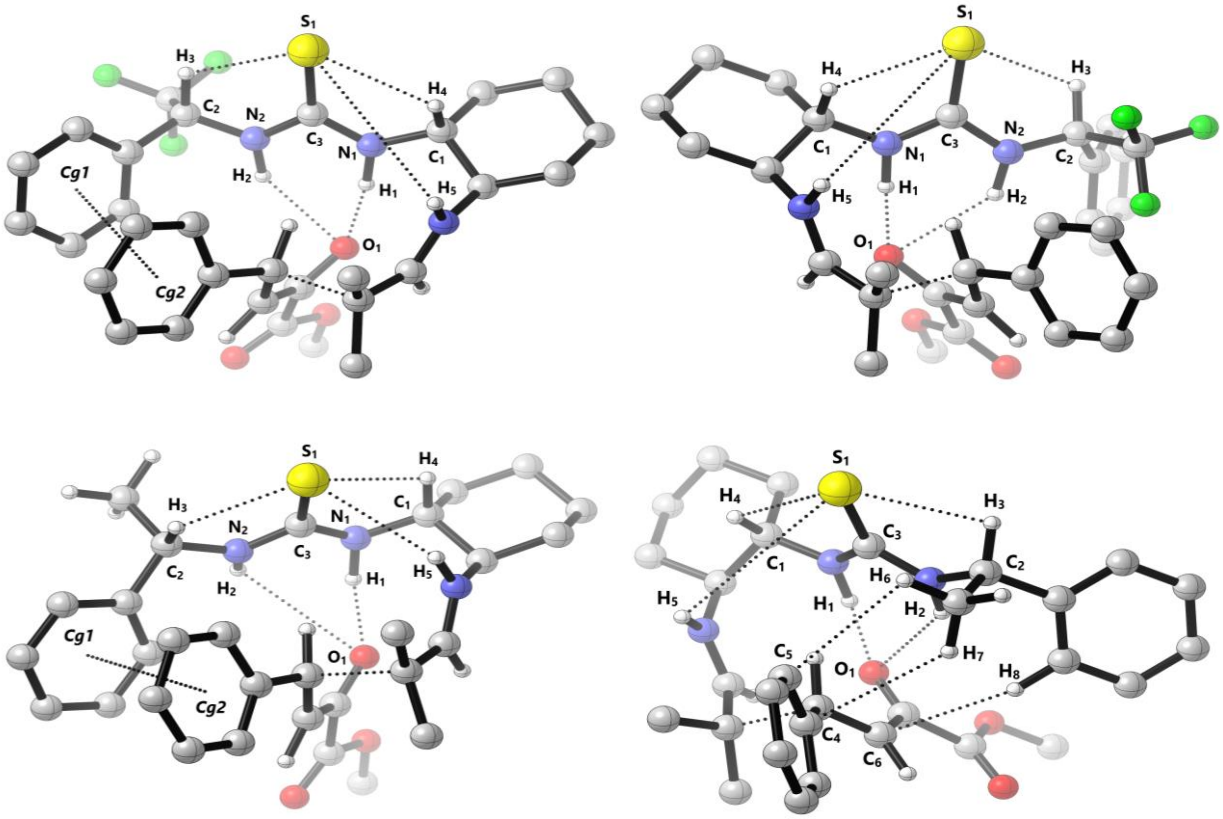


Figure S3. Comparison of π-π stacking with catalysts **A**$_{\mathbf{F}}$ (left) and **A** (right) in the transition state by a lateral view of the aryl groups. Calculated at PCM($CHCl_3$)-B97D/TZVP level of theory. Labels for these structures are KE-A$_F$-Maj-TS1 (left) and KE-A-Maj-TS1 (right).

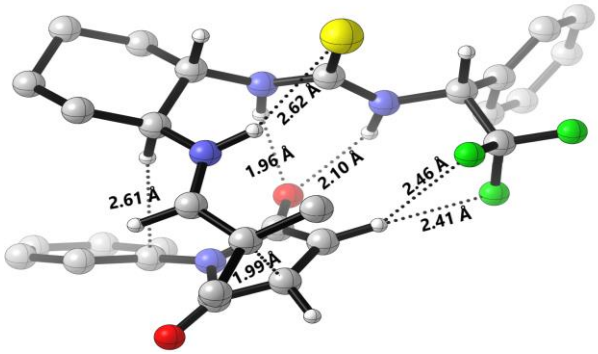
Table S4. Relevant distances and angles within transition states KE-A_F-Maj-TS1, KE-B_F-Maj-TS1, KE-A-Maj-TS1 and KE-B-Maj-TS1. Calculated at PCM($CHCl_3$)-B97D/TZVP level of theory.



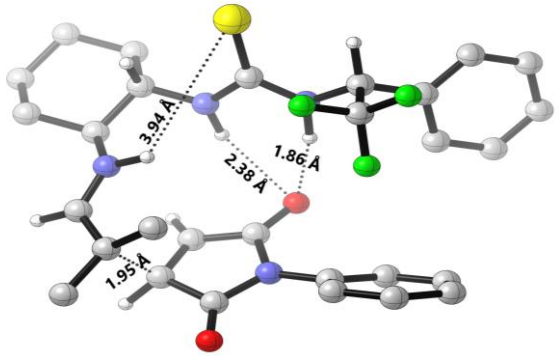
TS	KE-A_F-Maj-TS1	KE-B_F-Maj-TS1	KE-A-Maj-TS1	KE-B-Maj-TS1
d (H_1⋯O_1)	1.73 Å	1.70 Å	1.83 Å	1.76 Å
d (H_2⋯O_1)	2.33 Å	2.47 Å	3.13 Å	2.31 Å
d (H_6⋯C_5)	-	-	-	3.11 Å
d (H_7⋯C_4)	-	-	-	3.10 Å
d (H_8⋯C_6)	-	-	-	2.79 Å
d (S_1⋯H_3)	2.57 Å	2.66 Å	2.64 Å	2.85 Å
d (S_1⋯H_4)	2.74 Å	2.83 Å	2.61 Å	2.77 Å
d (S_1⋯H_5)	4.55 Å	4.73 Å	2.94 Å	4.63 Å
d (*Cg1*⋯*Cg2*)	3.76 Å	-	3.88 Å	-
Dihedral H_3-C_2-N_2-C_3(S_1)	-1.8°	-2.8°	-20.9°	-39.1°
Dihedral H_4-C_1-N_1-C_3(S_1)	31.3°	-34.8°	-10.9°	-34.2°

Table S5. Relative energies with respect to reactants of the transition states and reactive complexes for the addition of isobutyraldehyde to *N*-phenylmaleimide promoted by $\mathbf{B_F}$ and **B** (Maj and Min refers to the formation of the major and minor enantiomer of the product) [M06-2X/TZVP].

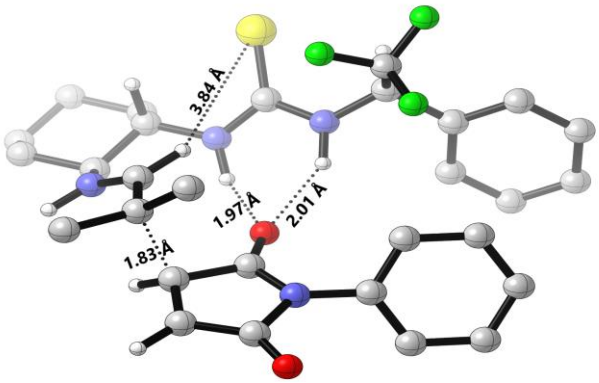
Cat.	TS	E_{rel} (kcal/mol)		Cat.	TS	E_{rel} (kcal/mol)	
		Maj	Min			Maj	Min
$\mathbf{B_F}$	TS1	-10.9	0.6	**B**	TS1	-12.2	-2.7
	Cx1	-19.0	-12.7		Cx1	-19.7	-15.0
	TS2	7.7	-		TS2	-	-4.5
	Cx2	-10.0	-		Cx2	-	-15.4
	TS3	-	-1.2		TS3	3.1	5.1
	Cx3	-	-10.0		Cx3	-13.7	-15.0



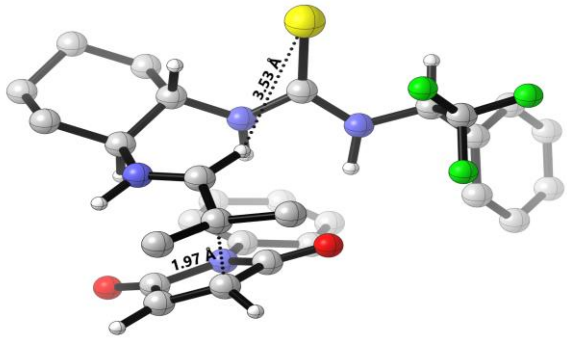
M-B_F-Maj-TS1 (-10.9 kcal/mol)



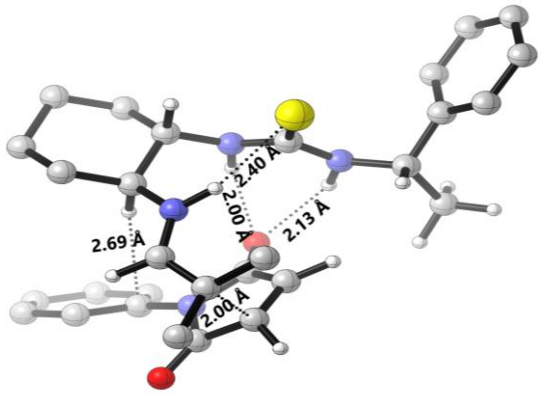
M-B_F-Min-TS1 (0.6 kcal/mol)



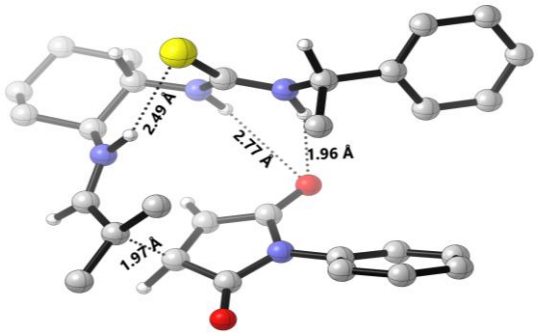
M-B_F-Maj-TS2 (7.7 kcal/mol)



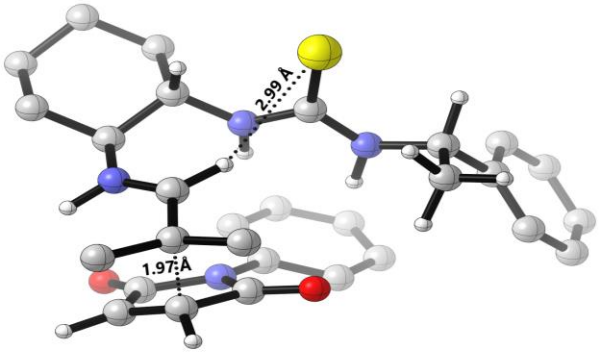
M-B_F-Min-TS3 (-1.2 kcal/mol)



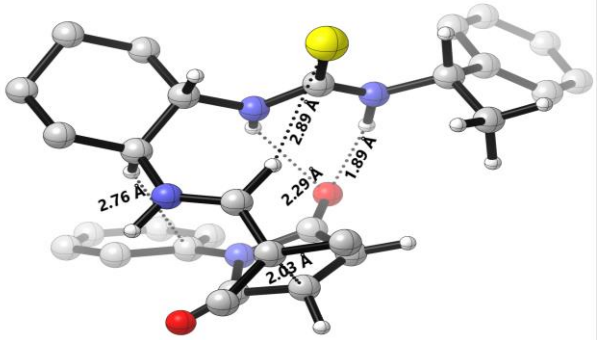
M-B-Maj-TS1(-12.2 kcal/mol)



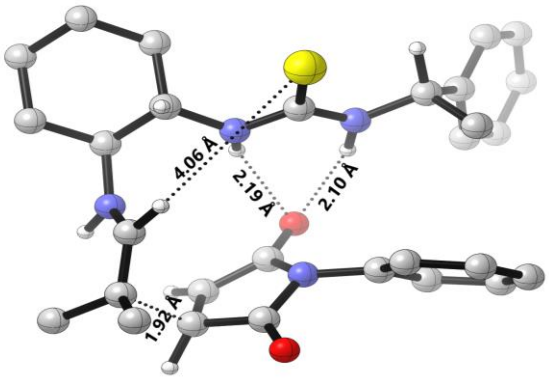
M-B-Min-TS1(-2.7 kcal/mol)



M-B-Min-TS2 (-4.5 kcal/mol)



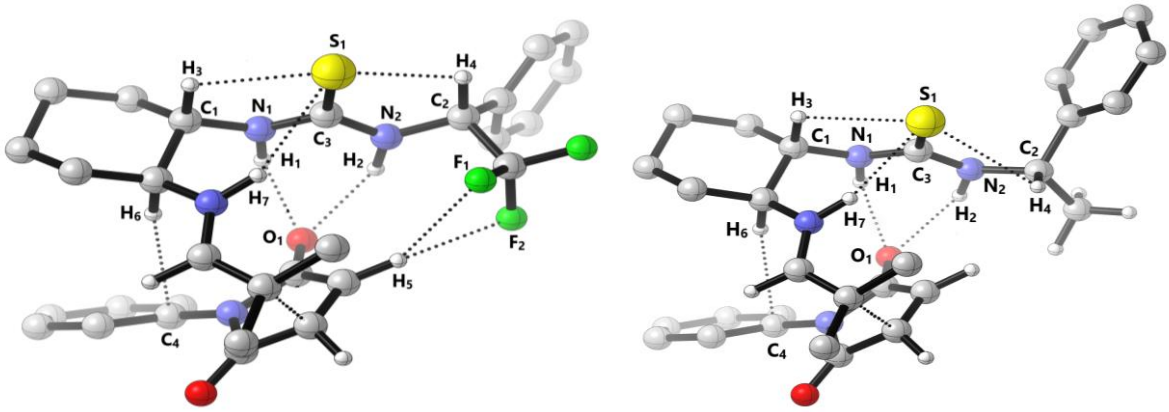
M-B-Maj-TS3(3.1 kcal/mol)



M-B-Min-TS3 (5.1 kcal/mol)

Figure S4. Structures of the transition states. Labels represent the maleimide electrophile (M), catalyst (**B_F** or **B**), enantiomer produced (Maj or Min) and the number assigned in Table S5. Calculated at M06-2X/TZVP level of theory.

Table S6. Relevant distances and angles within transition states M-B_F-Maj-TS1 and M-B-Maj-TS1. Calculated at M06-2X/TZVP level of theory.



TS	M-B_F-Maj-TS1	M-B-Maj-TS1
d (H_1···O_1)	1.96 Å	2.00 Å
d (H_2···O_1)	2.10 Å	2.13 Å
d (H_5···F_1)	2.46 Å	-
d (H_5···F_2)	2.41 Å	-
d (H_6···C_4)	2.61 Å	2.69 Å
d (S_1···H_3)	2.60 Å	2.65 Å
d (S_1···H_4)	2.59 Å	2.82 Å
d (S_1···H_7)	2.62 Å	2.40 Å
Dihedral H_3-C_1-N_1-C_3(S_1)	20.75°	26.93°
Dihedral H_4-C_1-N_1-C_3(S_1)	-7.50°	44.19°

Table S7. Mulliken charges of the aryl ring for catalysts $\mathbf{A_F}$ and **A**. Calculated at B97-D/TZVP level of theory.

	$\mathbf{A_F}$	**A**
$\mathbf{C}_i$	0.243657	0.229442
$\mathbf{C}_o$	-0.139317	-0.114334
$\mathbf{C}_m$	-0.067283	-0.072604
$\mathbf{C}_p$	-0.087839	-0.095195
$\mathbf{C}_m'$	-0.070932	-0.072919
$\mathbf{C}_o'$	-0.131516	-0.179928
TOTAL	-0.253230	-0.305538

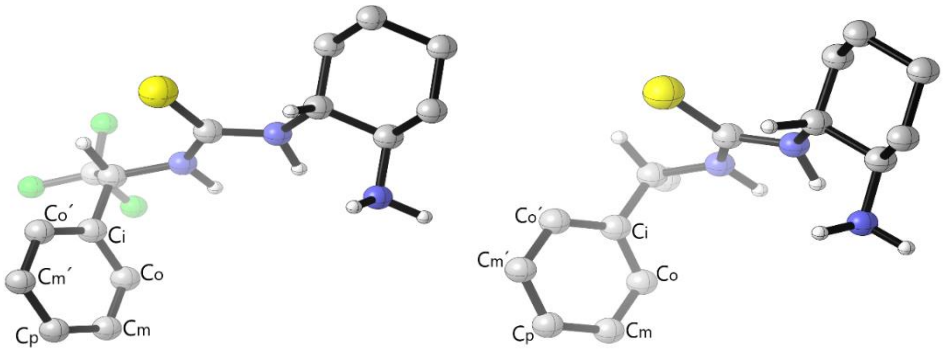
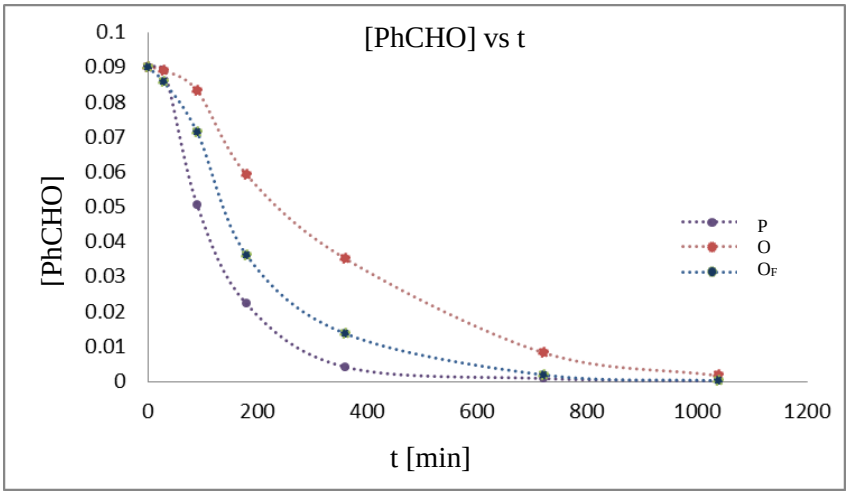


Figure S5. Geometry for catalysts $\mathbf{A_F}$ (left) and **A** (rigth). Calculated at B97-D/TZVP level of theory

6 Kinetics of the Baylis-Hillman reaction between 2-cyclohexenone and benzaldehyde

a)



b)

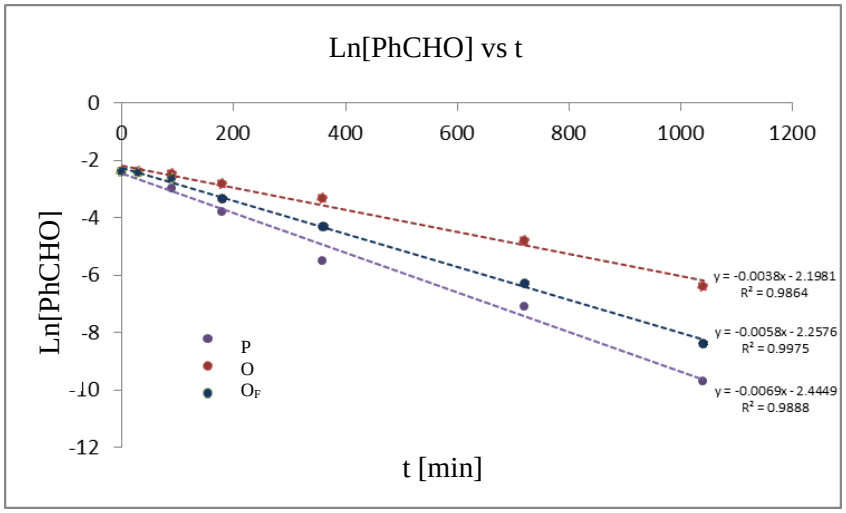


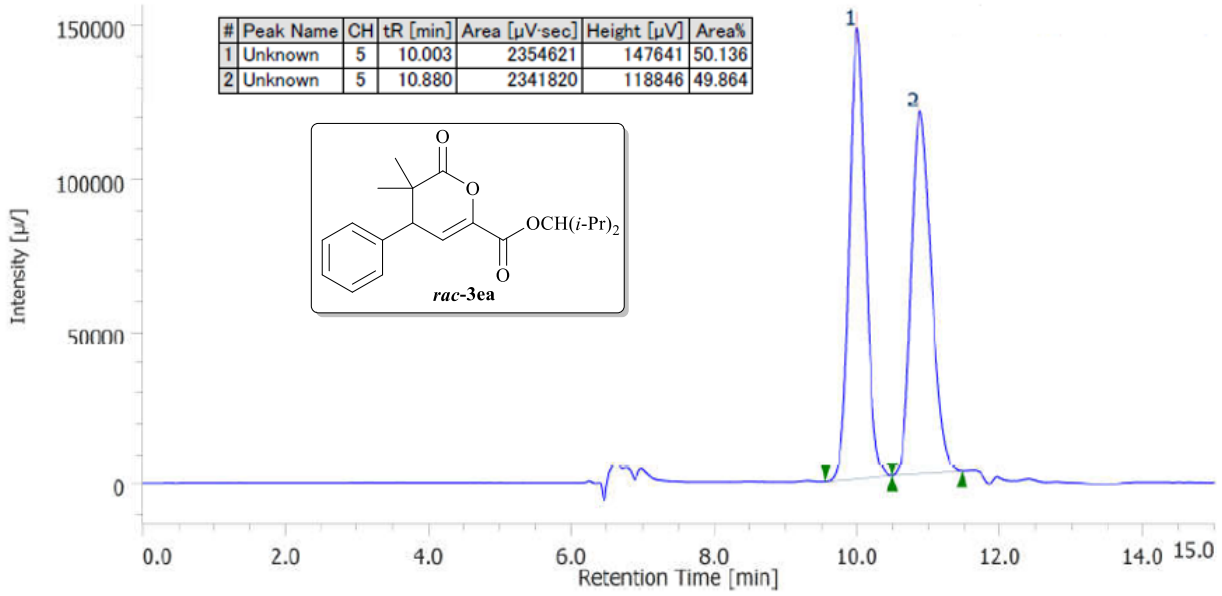
Figure S6. Kinetics of the Baylis-Hillman reaction between 2-cyclohexenone and benzaldehyde with catalysts **P**, **O** and **O_F** under pseudo first order conditions. (a) mmol of benzaldehyde as a function of time. (b) Plot in a logarithmic scale for the mmol of benzaldehyde.

Table S8. Rate constants observed for the Baylis-Hillman reaction between 2-cyclohexenone and benzaldehyde in $CDCl_3$.

Cat.	**$k_{obs.}$**	**$k_{ref.}$**
O	0.0038	1.0
O_F	0.0058	1.5
P	0.0069	1.8

7 CSP-HPLC

Figure S7. HPLC chromatogram of *rac*-**3ea** (above) and enantioenriched **3ea** with catalyst $\mathbf{A_F}$, Table 4, Entry 1 (below).



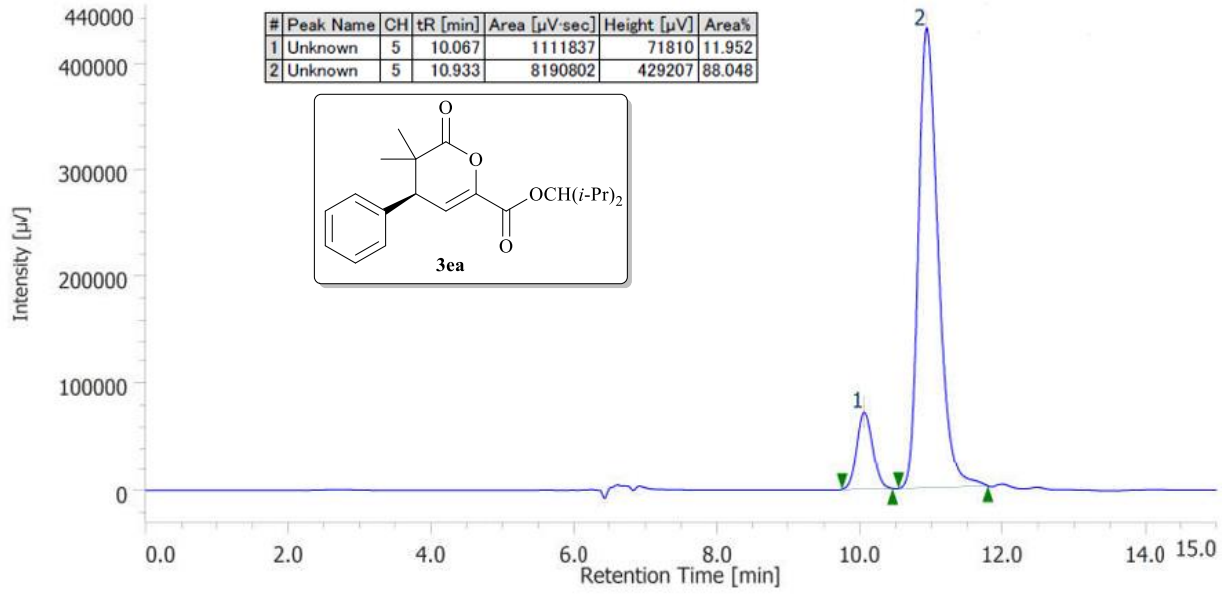
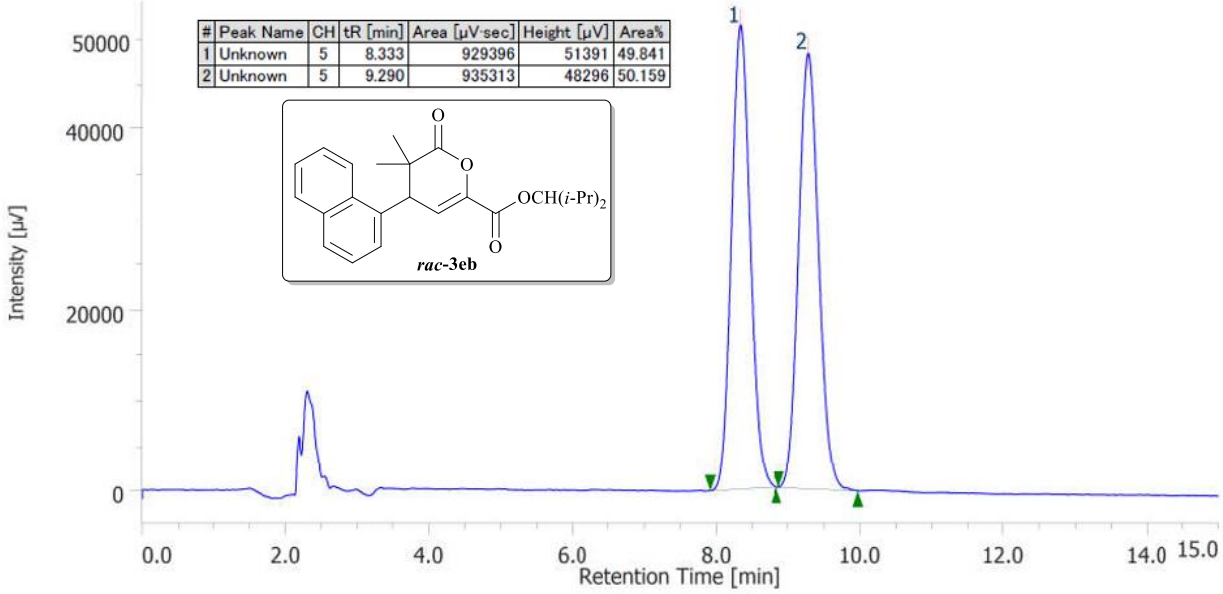
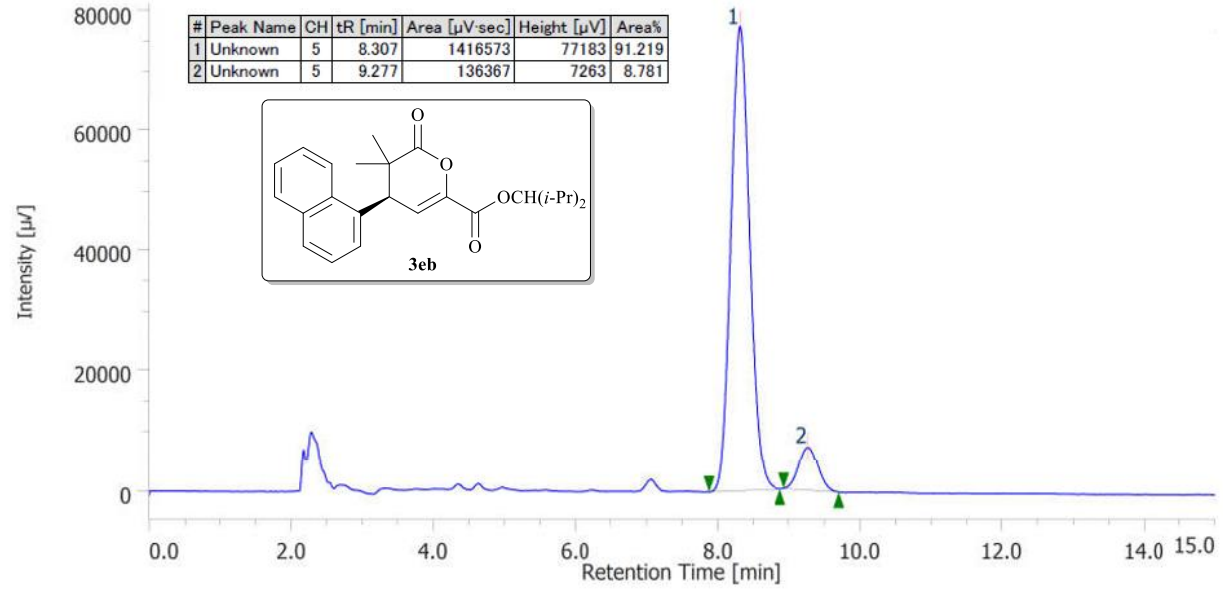


Figure S8. HPLC chromatogram of *rac*-**3eb** (above) and enantioenriched **3eb** with catalyst $\mathbf{A_F}$, Table 4, Entry 2 (below).

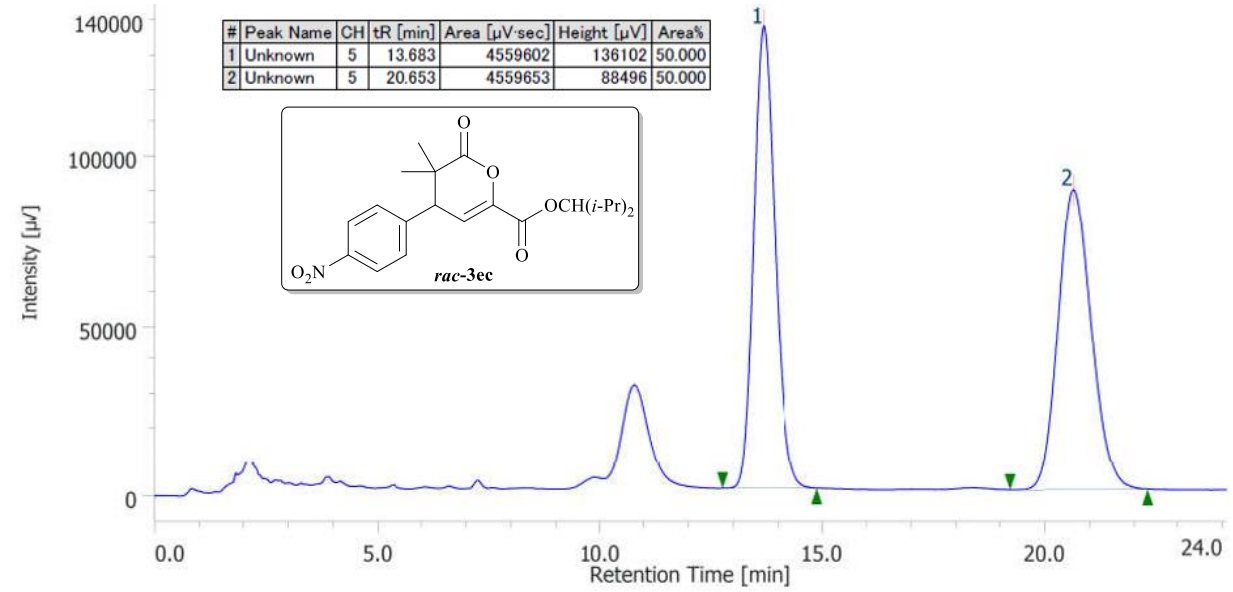


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	8.333	929396	51391	49.841
2	Unknown	5	9.290	935313	48296	50.159

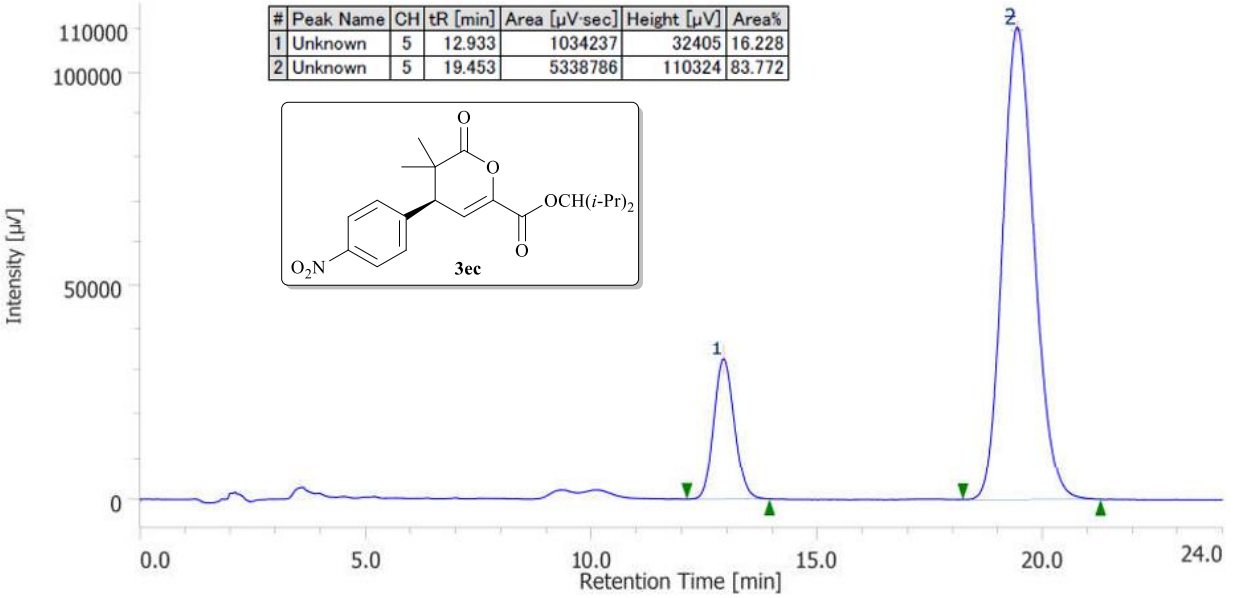


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	8.307	1416573	77183	91.219
2	Unknown	5	9.277	136367	7263	8.781

Figure S9. HPLC chromatogram of *rac*-**3ec** (above) and enantioenriched **3ec** with catalyst $\mathbf{A_F}$, Table 4, Entry 3 (below).

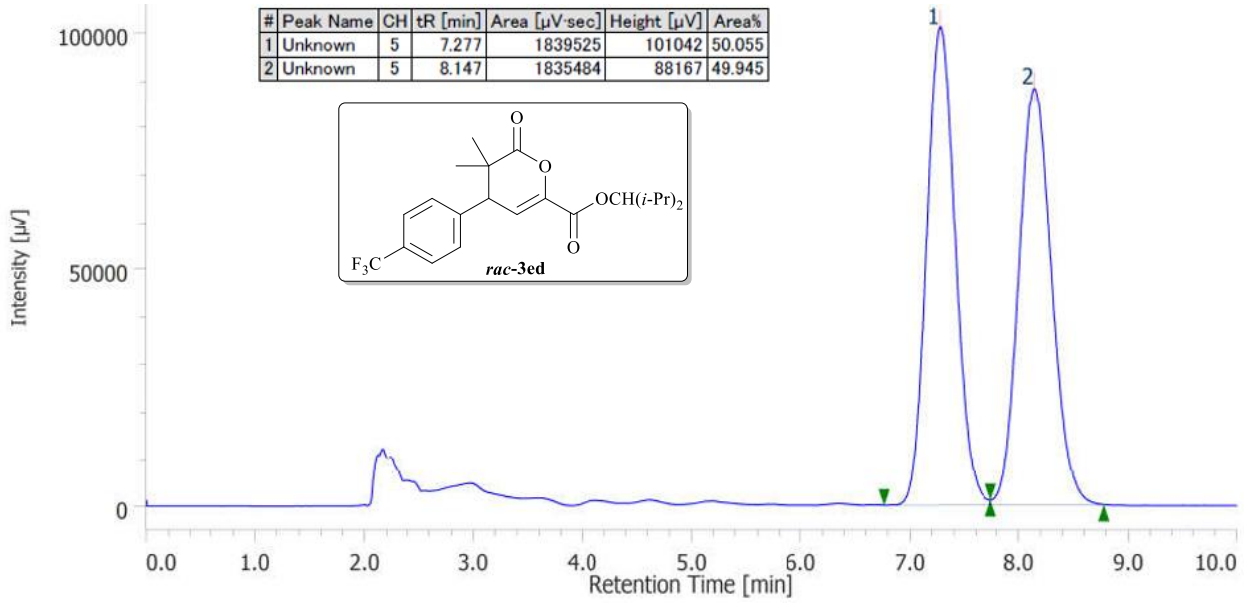


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	13.683	4559602	136102	50.000
2	Unknown	5	20.653	4559653	88496	50.000

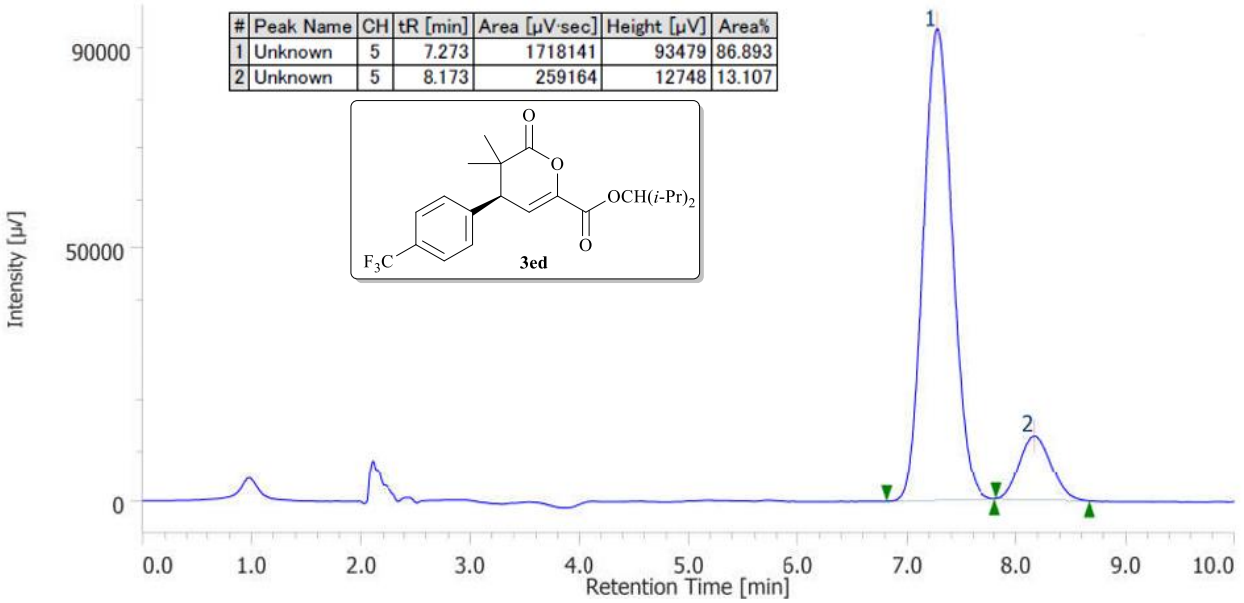


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	12.933	1034237	32405	16.228
2	Unknown	5	19.453	5338786	110324	83.772

Figure S10. HPLC chromatogram of *rac*-**3ed** (above) and enantioenriched **3ed** with catalyst $\mathbf{A_F}$, Table 4, Entry 4 (below).

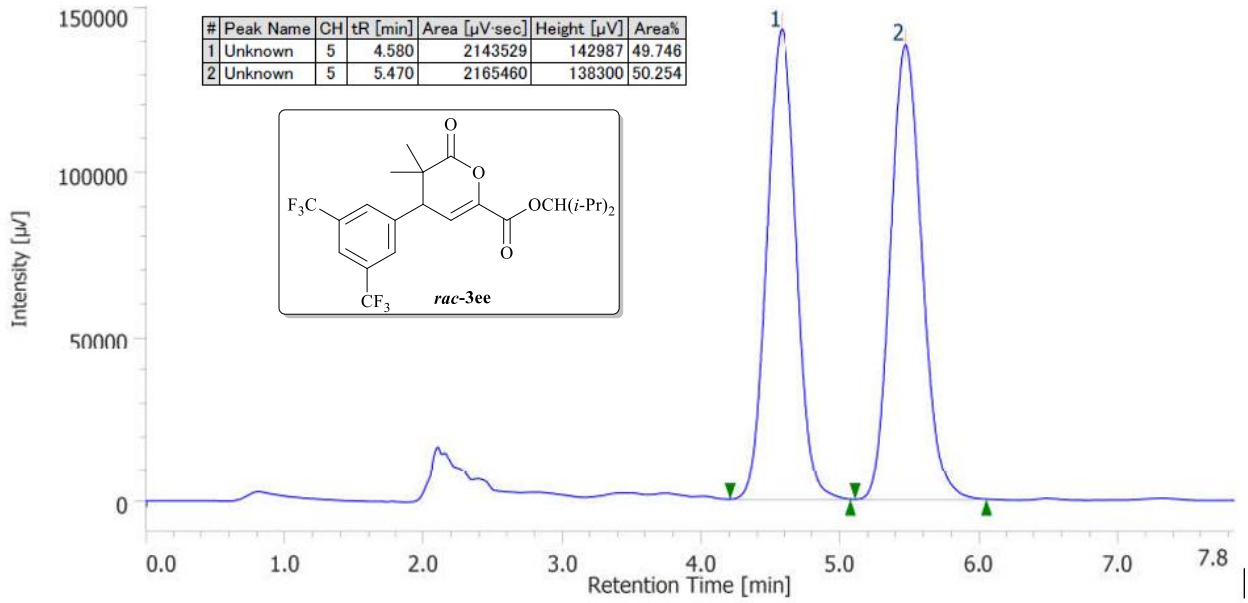


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	7.277	1839525	101042	50.055
2	Unknown	5	8.147	1835484	88167	49.945

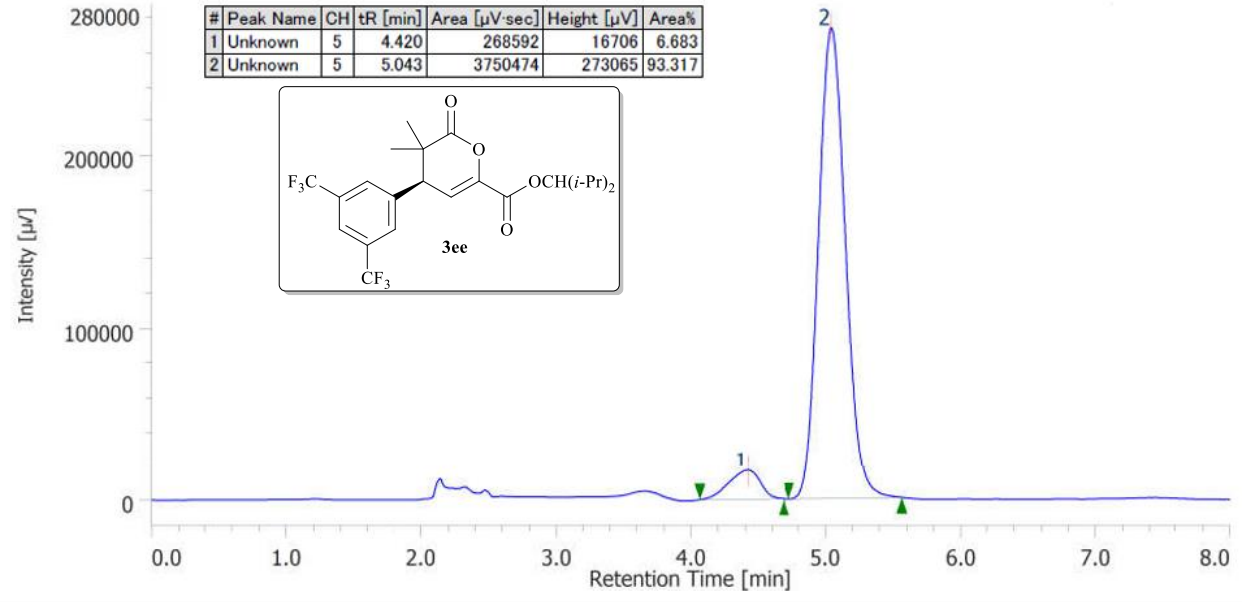


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	7.273	1718141	93479	86.893
2	Unknown	5	8.173	259164	12748	13.107

Figure S11. HPLC chromatogram of *rac*-**3ee** (above) and enantioenriched **3ee** with catalyst $\mathbf{A_F}$, Table 4, Entry 5 (below).

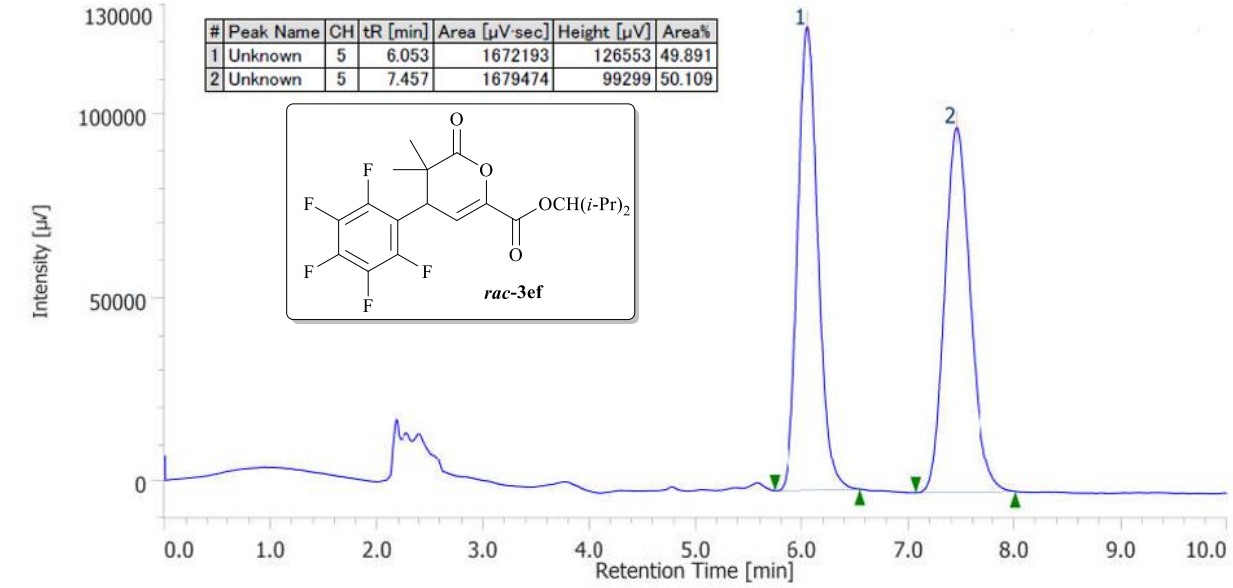


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	4.580	2143529	142987	49.746
2	Unknown	5	5.470	2165460	138300	50.254

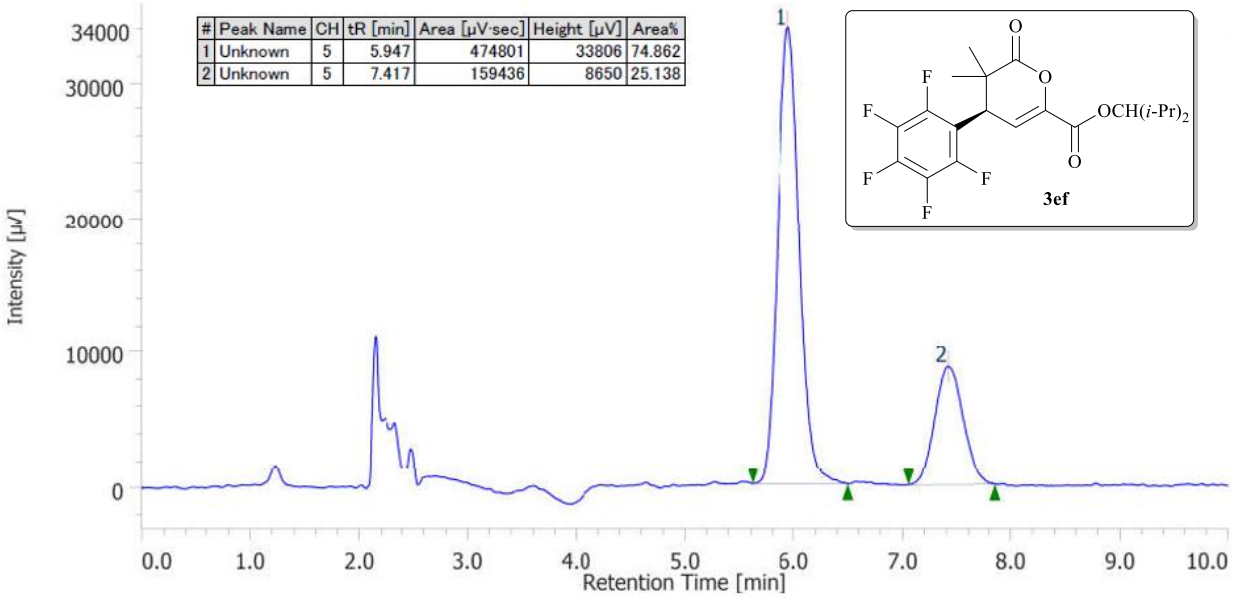


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	4.420	268592	16706	6.683
2	Unknown	5	5.043	3750474	273065	93.317

Figure S12. HPLC chromatogram of *rac*-**3ef** (above) and enantioenriched **3ef** with catalyst $\mathbf{A_F}$, Table 4, Entry 6 (below).

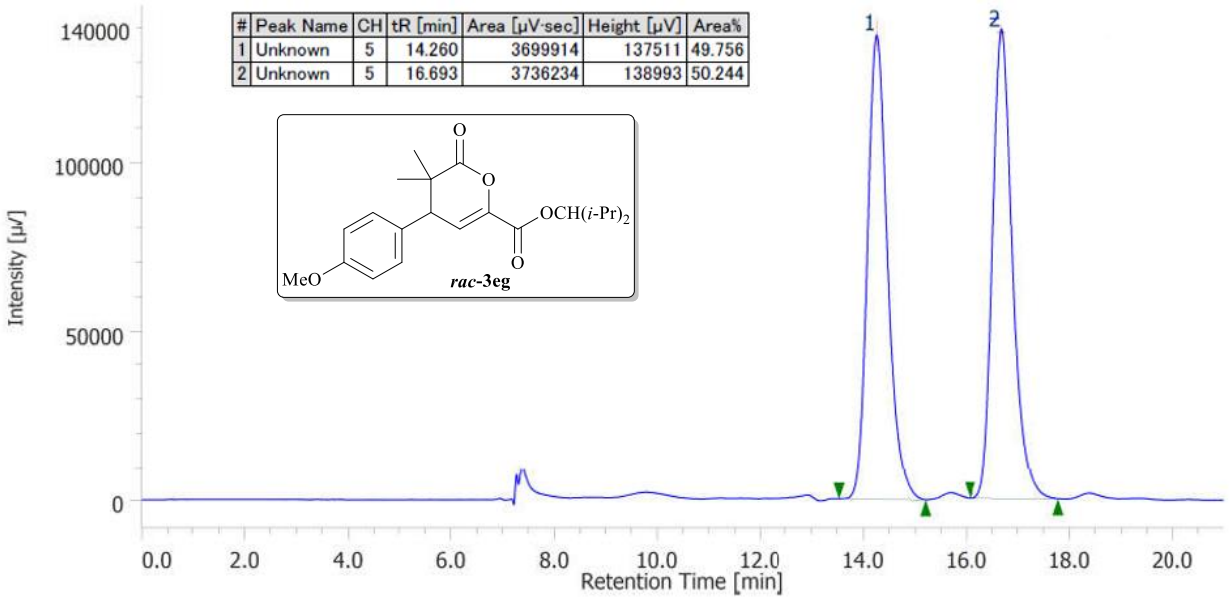


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	6.053	1672193	126553	49.891
2	Unknown	5	7.457	1679474	99299	50.109

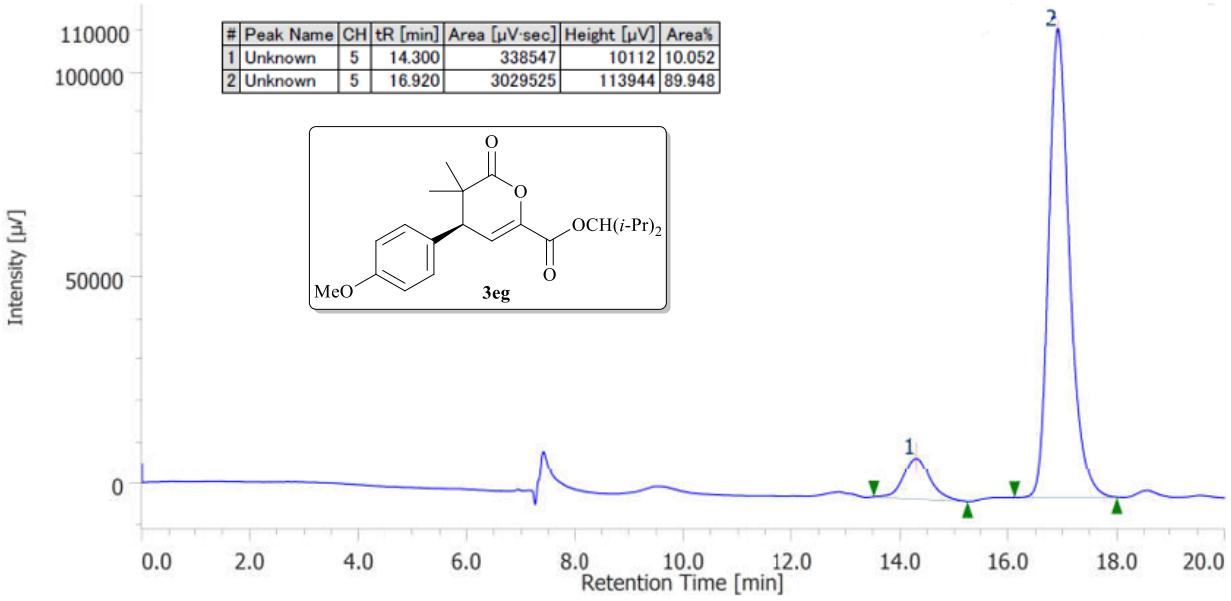


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	5.947	474801	33806	74.862
2	Unknown	5	7.417	159436	8650	25.138

Figure S13. HPLC chromatogram of *rac*-**3eg** (above) and enantioenriched **3eg** with catalyst $\mathbf{A_F}$, Table 4, Entry 7 (below).

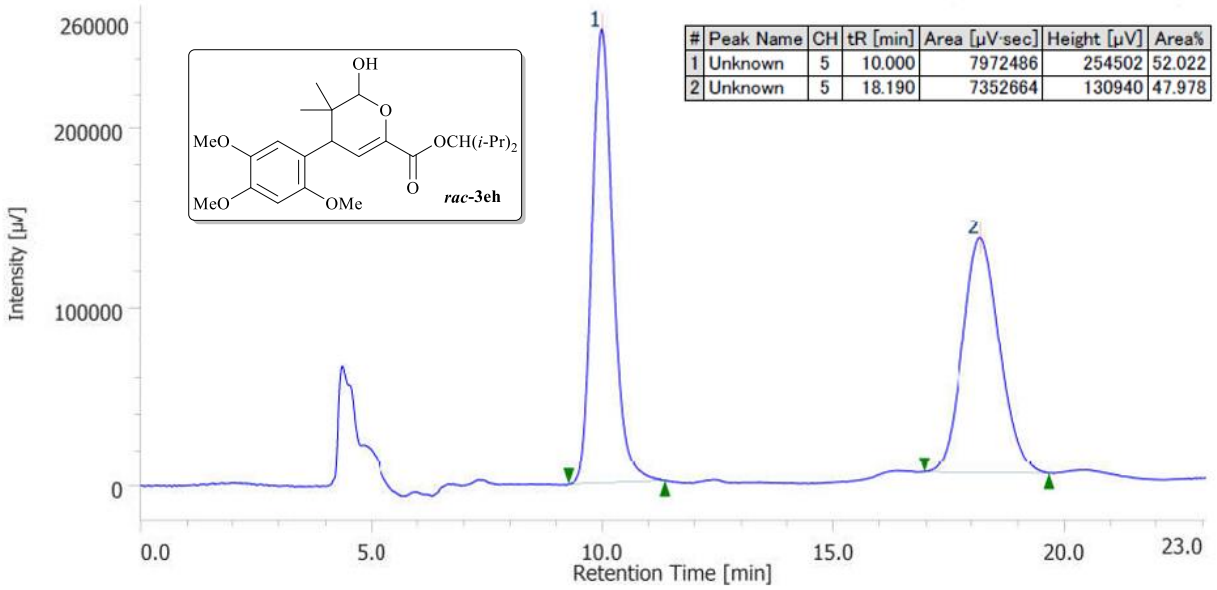


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	14.260	3699914	137511	49.756
2	Unknown	5	16.693	3736234	138993	50.244

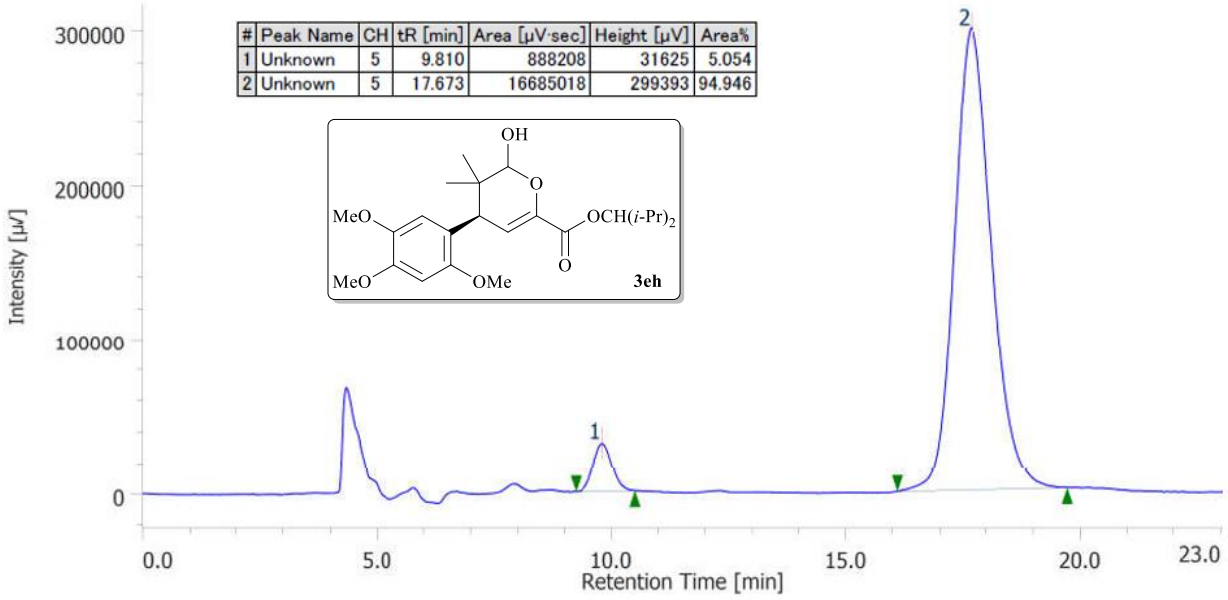


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	14.300	338547	10112	10.052
2	Unknown	5	16.920	3029525	113944	89.948

Figure S14. HPLC chromatogram of *rac*-**3eh** (above) and enantioenriched **3eh** with catalyst $\mathbf{A_F}$, Table 4, Entry 8 (below).

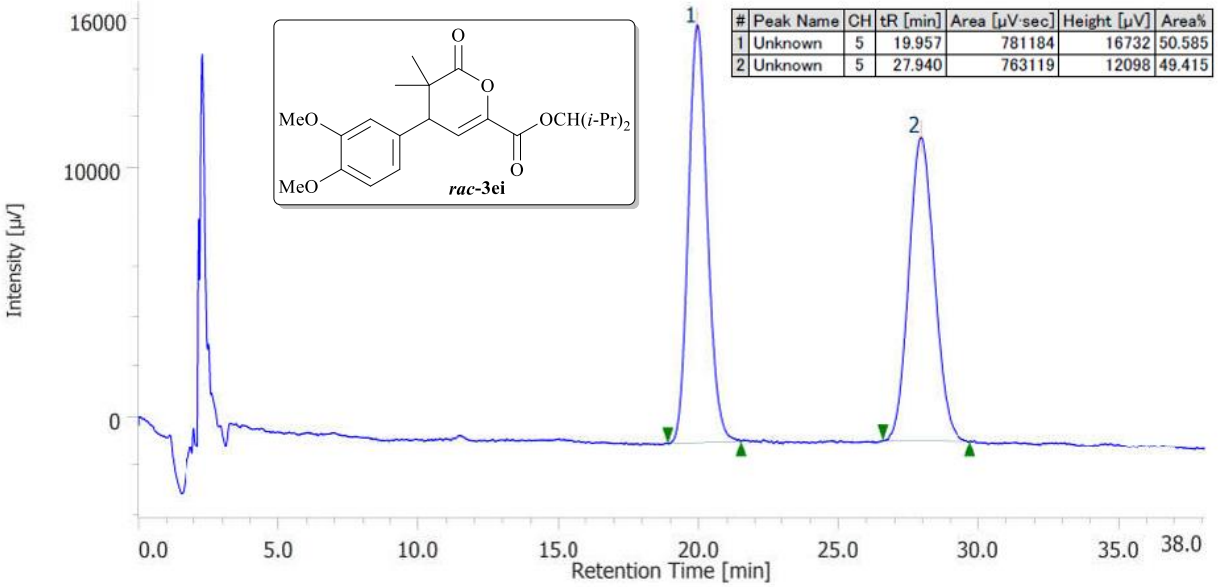


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	10.000	7972486	254502	52.022
2	Unknown	5	18.190	7352664	130940	47.978



#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	9.810	888208	31625	5.054
2	Unknown	5	17.673	16685018	299393	94.946

Figure S15. HPLC chromatogram of *rac*-**3ei** (above) and enantioenriched **3ei** with catalyst $\mathbf{A_F}$, Table 4, Entry 9 (below).



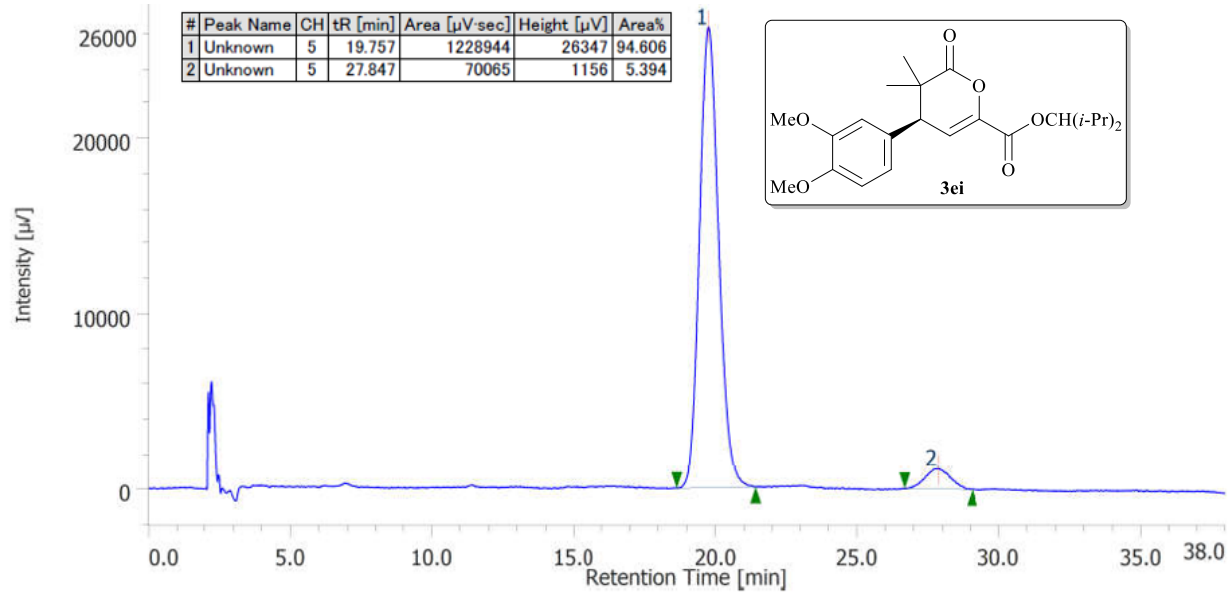
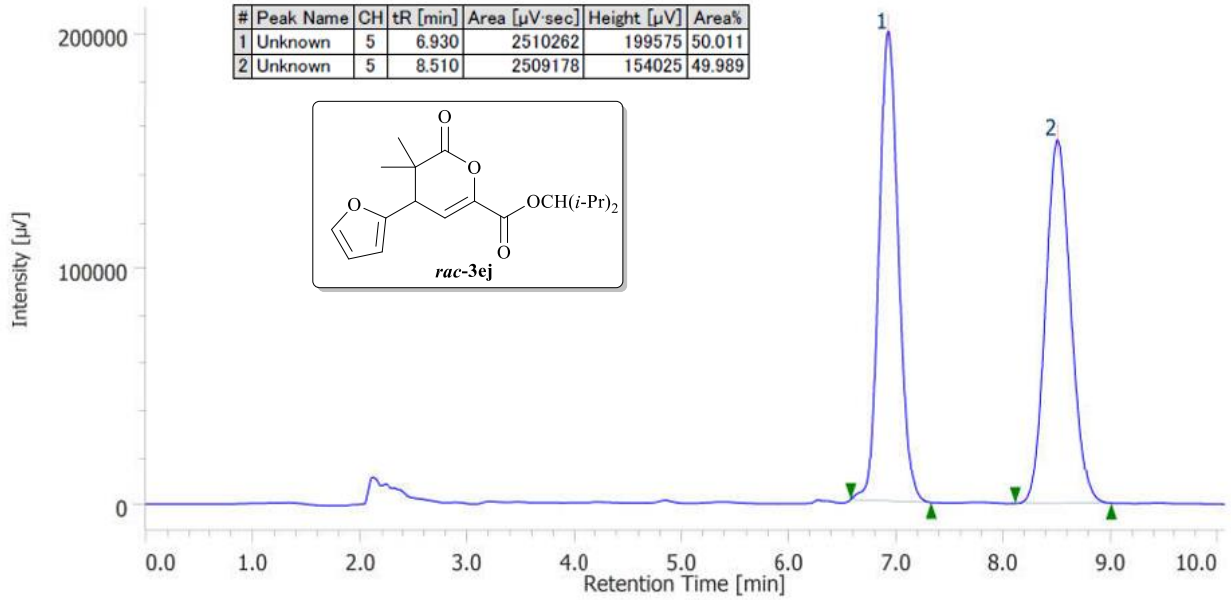


Figure S16. HPLC chromatogram of *rac*-**3ej** (above) and enantioenriched **3ej** with catalyst $\mathbf{A_F}$, Table 4, Entry 10 (below).



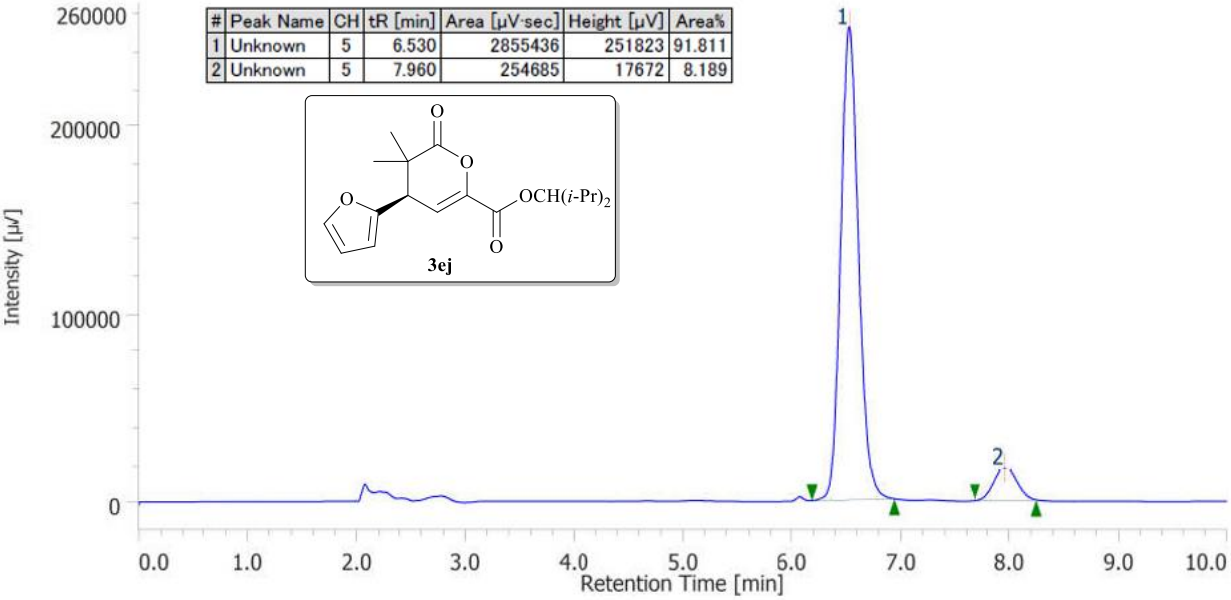
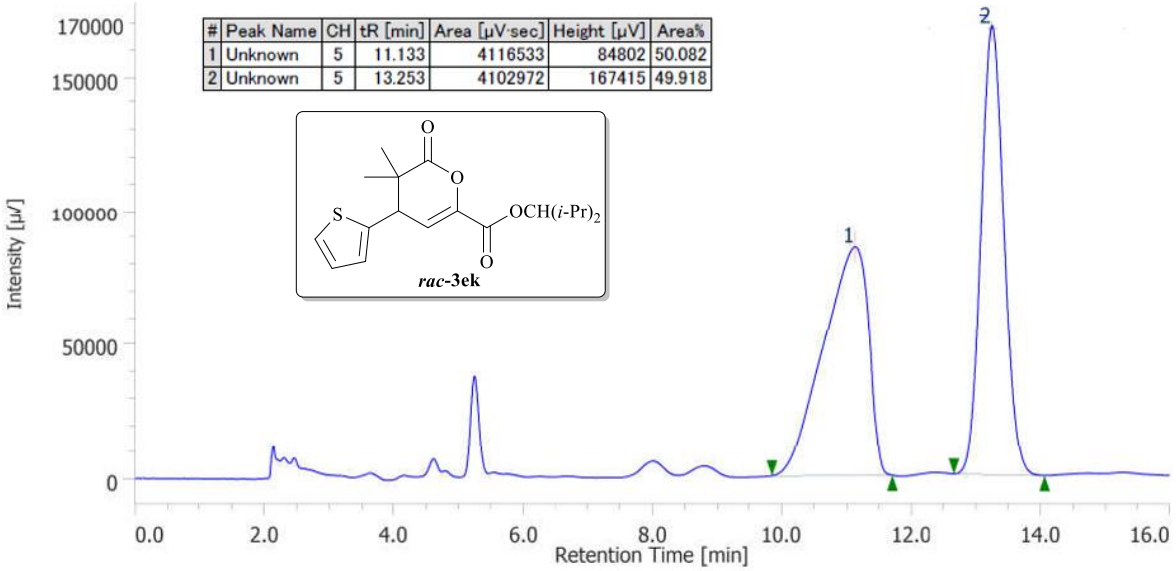
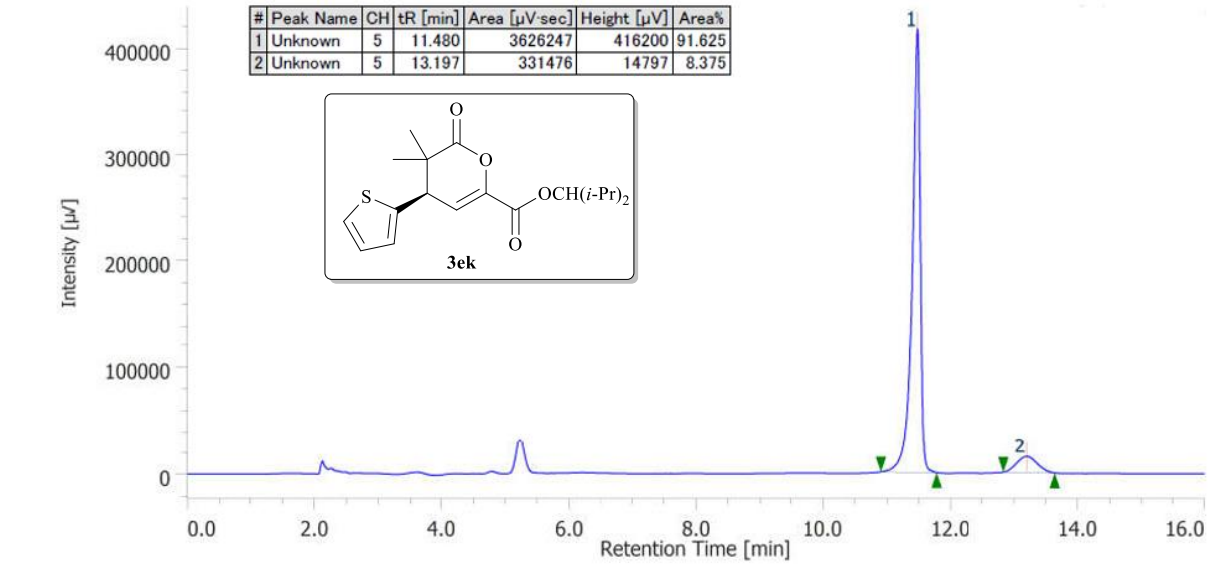


Figure S17. HPLC chromatogram of *rac*-**3ek** (above) and enantioenriched **3ek** with catalyst $\mathbf{A_F}$, Table 4, Entry 11 (below).

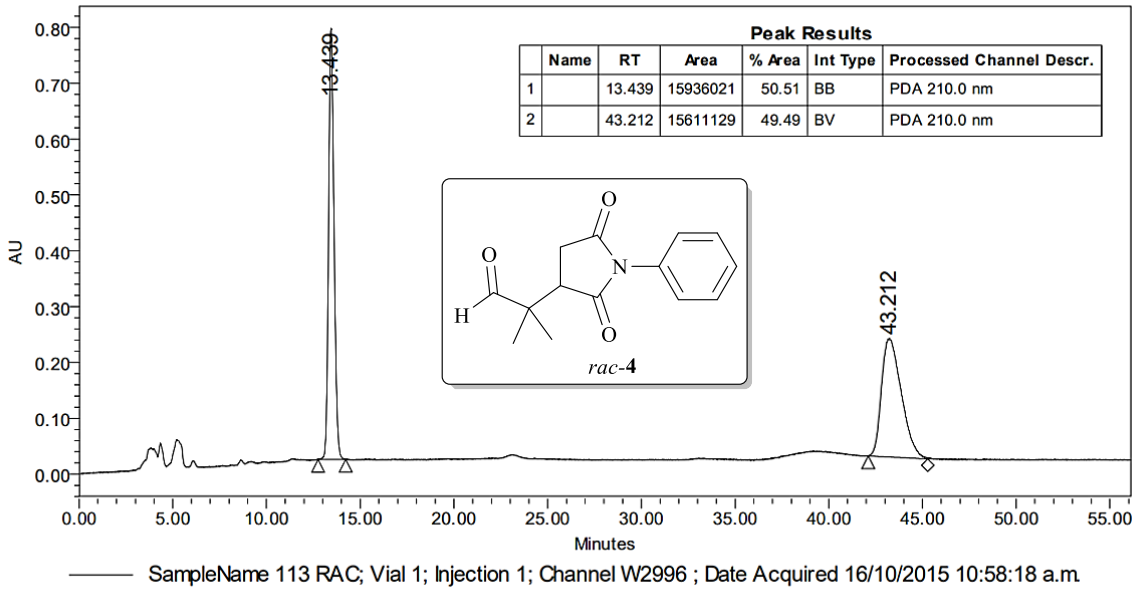


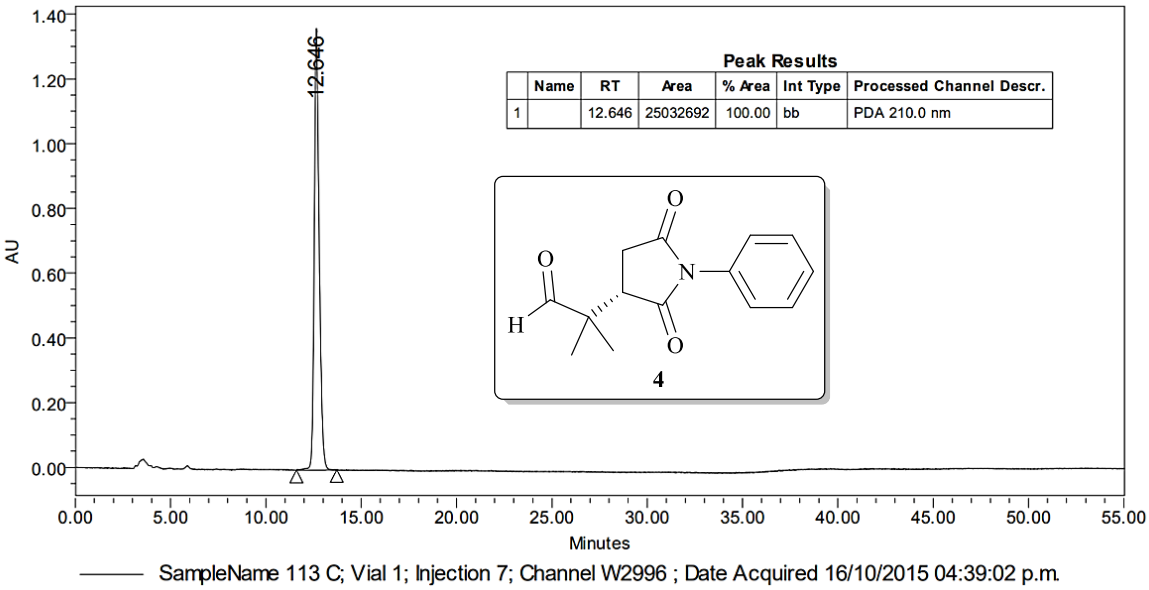
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	11.133	4116533	84802	50.082
2	Unknown	5	13.253	4102972	167415	49.918



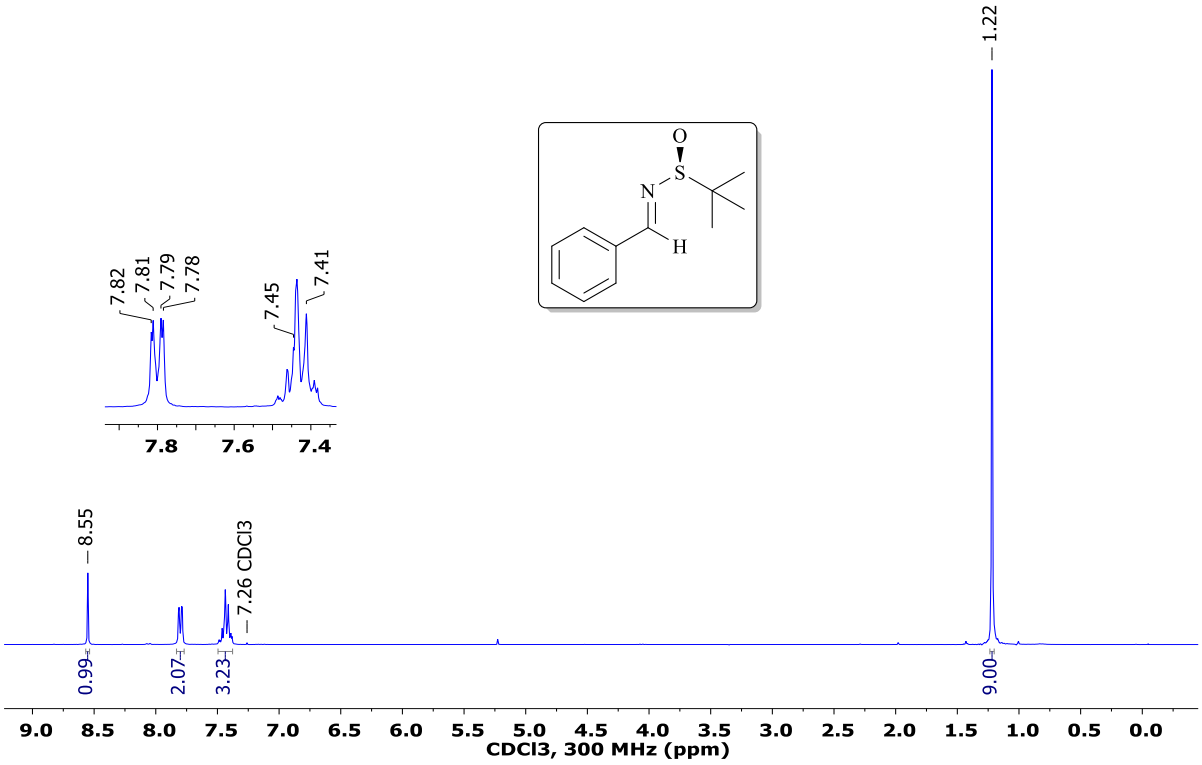
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%
1	Unknown	5	11.480	3626247	416200	91.625
2	Unknown	5	13.197	331476	14797	8.375

Figure S18. HPLC chromatogram of *rac*-**4** (above) and enantioenriched **4** with catalyst **B**, Table 5, Entry 4 (below).

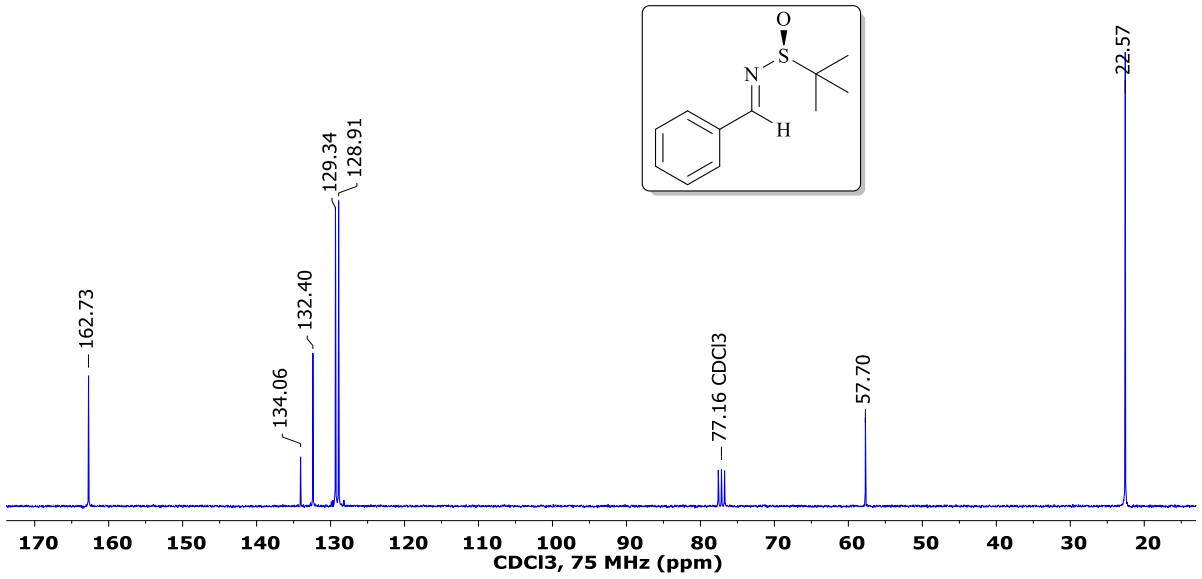




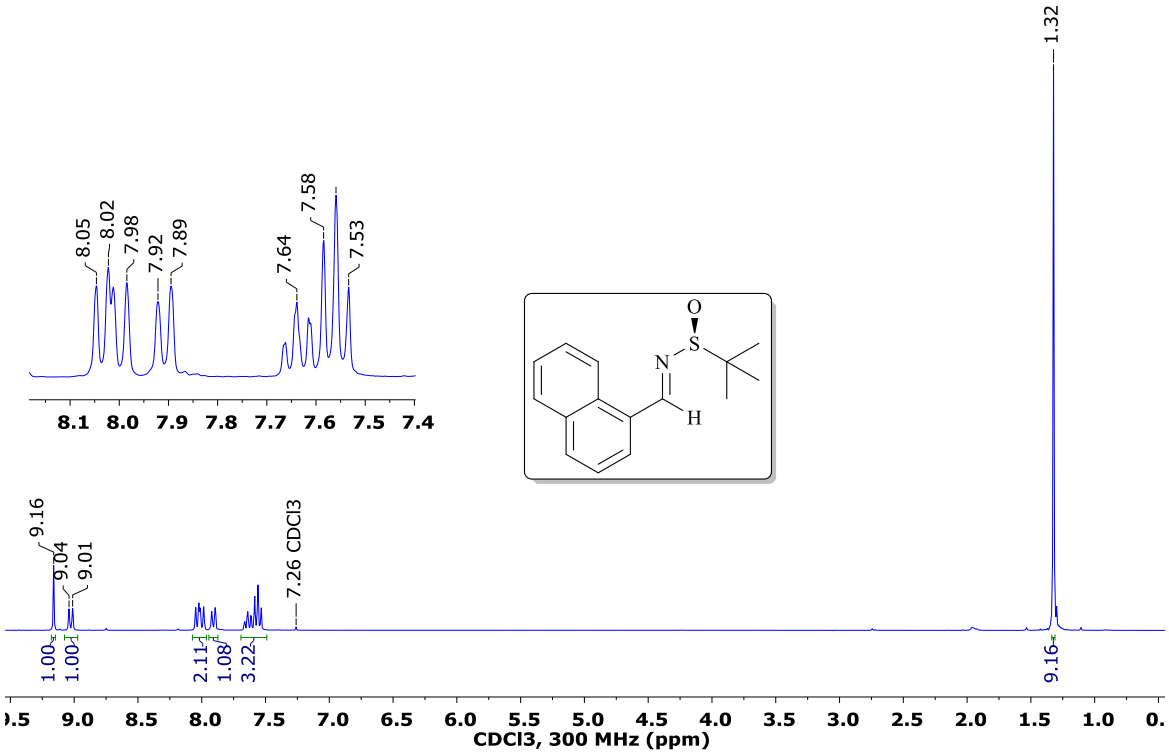
8 NMR spectra



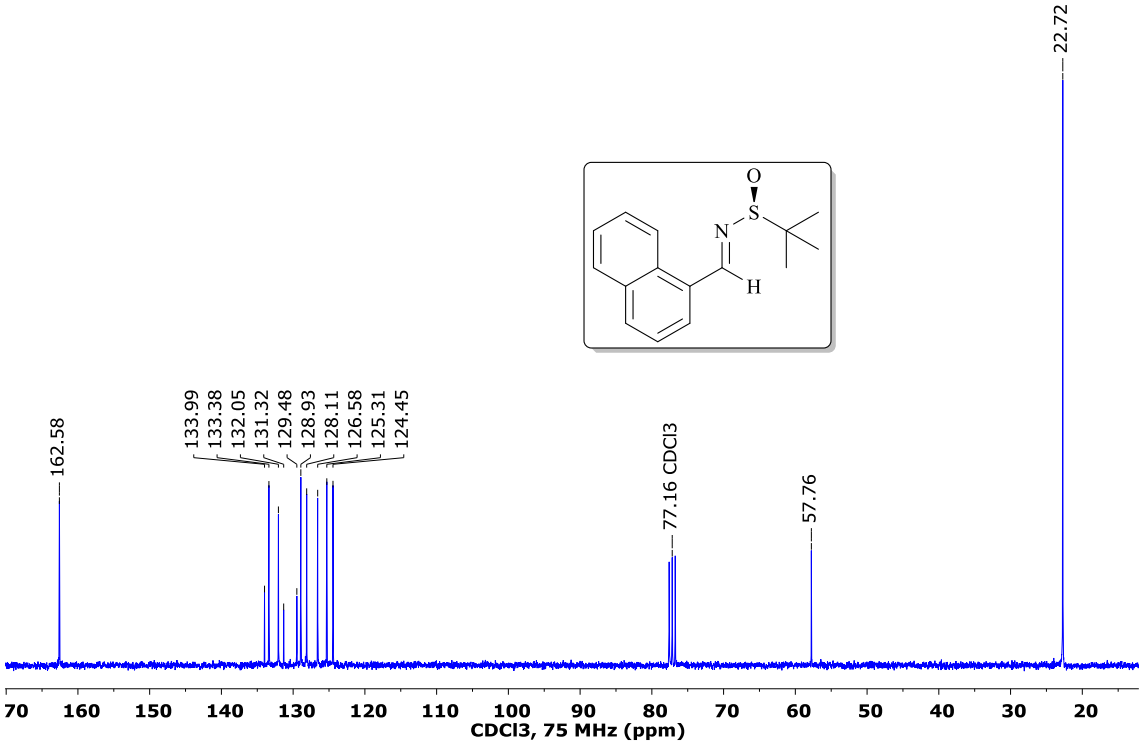
^{1}H NMR spectrum of compound **7a**.



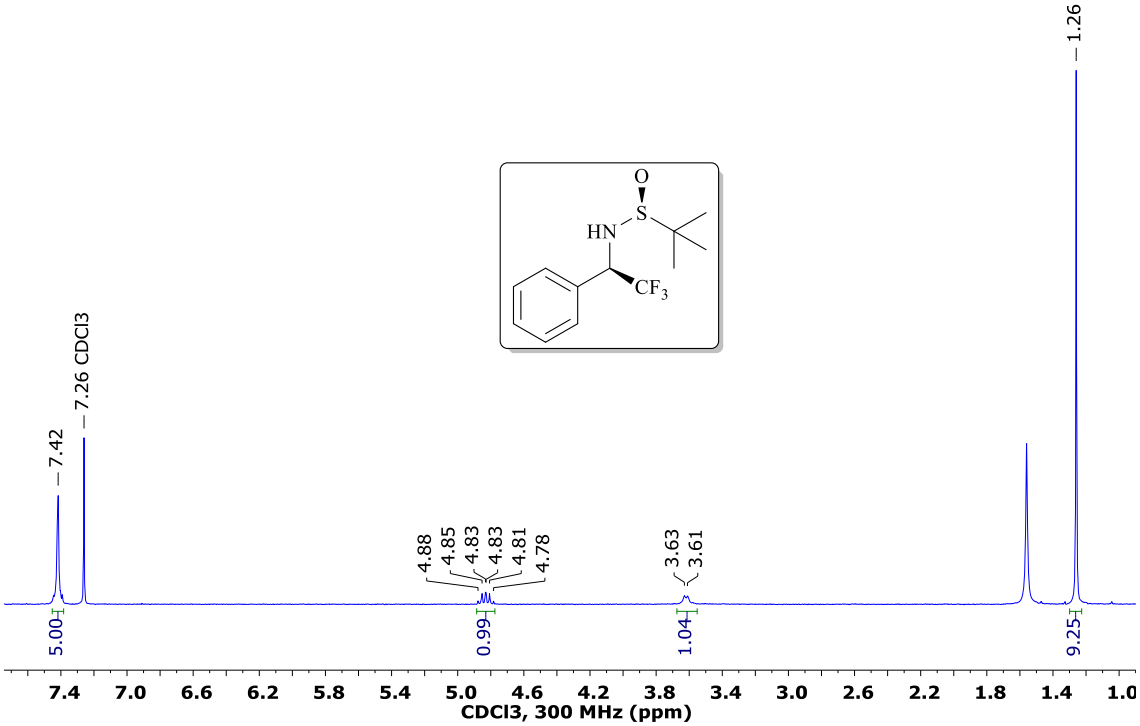
^{13}C NMR spectrum of compound **7a**.



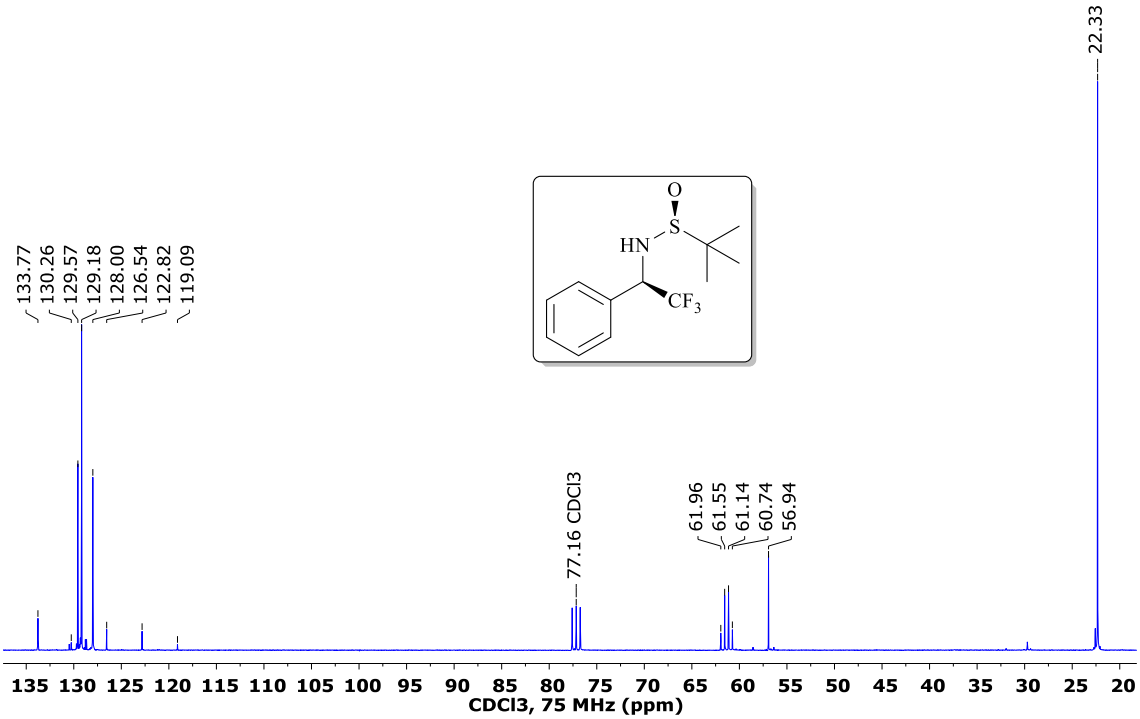
^{1}H NMR spectrum of compound **7b**.



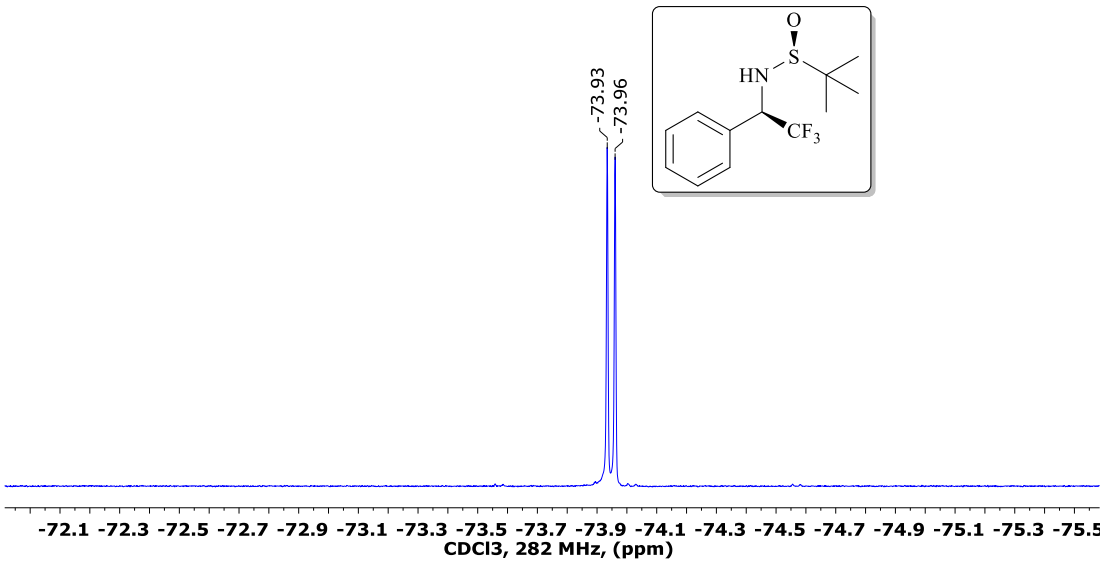
^{13}C NMR spectrum of compound **7b**.



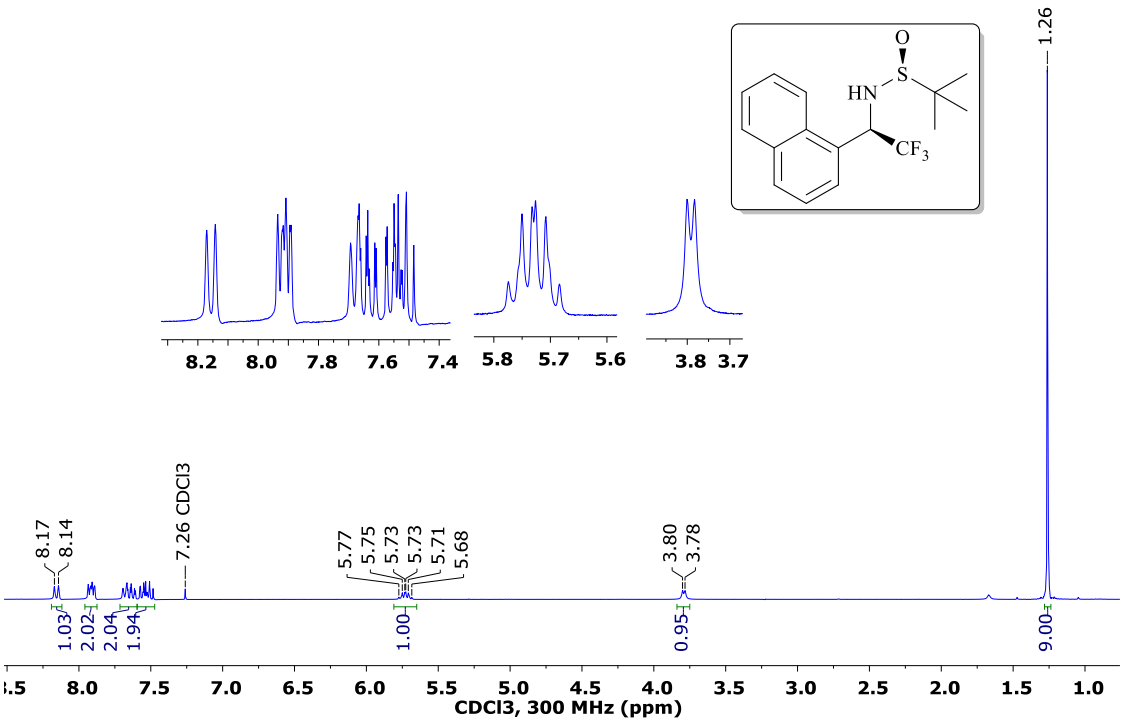
^{1}H NMR spectrum of compound **8a**.



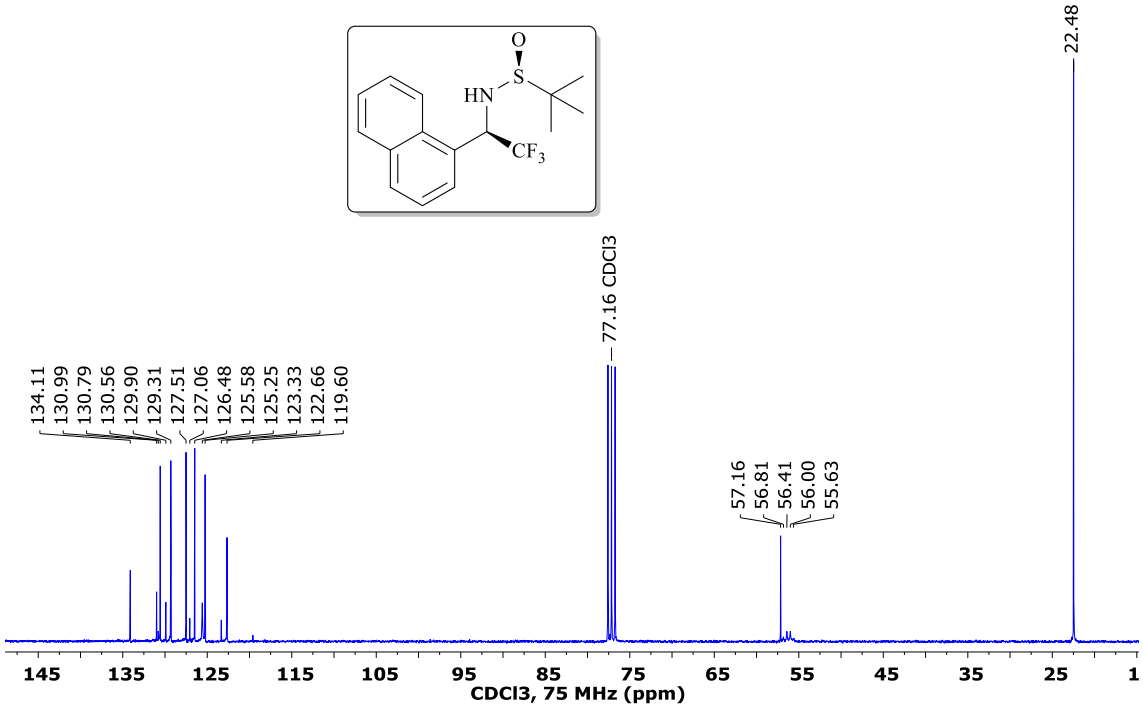
^{13}C NMR spectrum of compound **8a**.



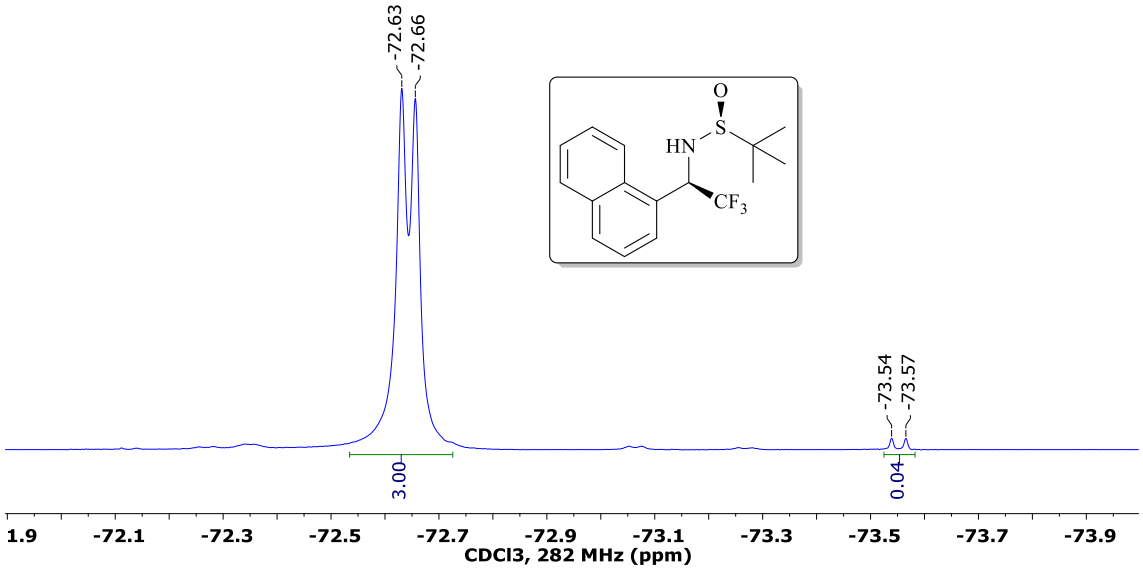
^{19}F NMR spectrum of compound **8a**.



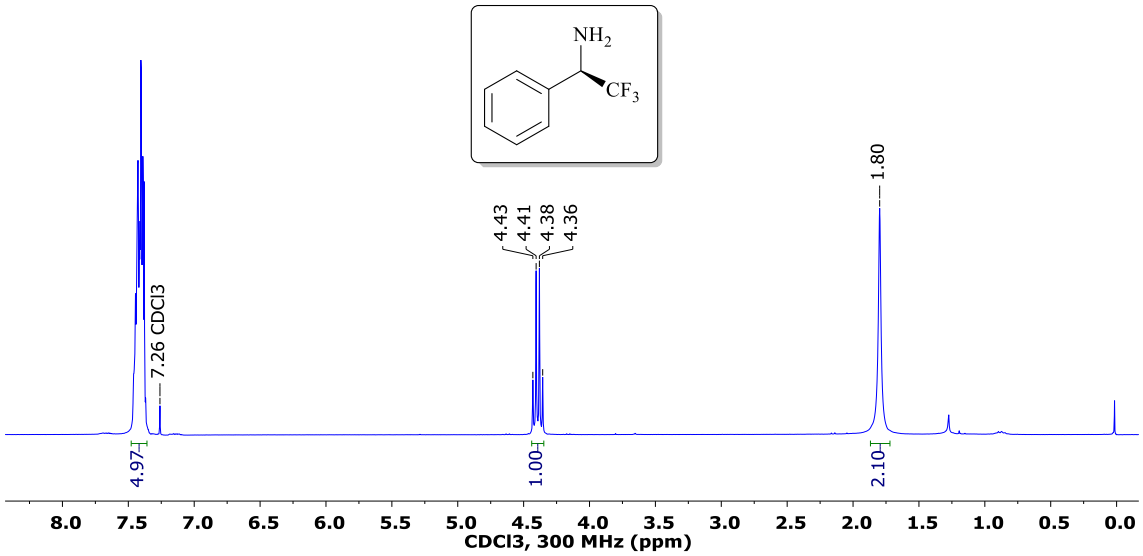
^{1}H NMR spectrum of compound **8b**.



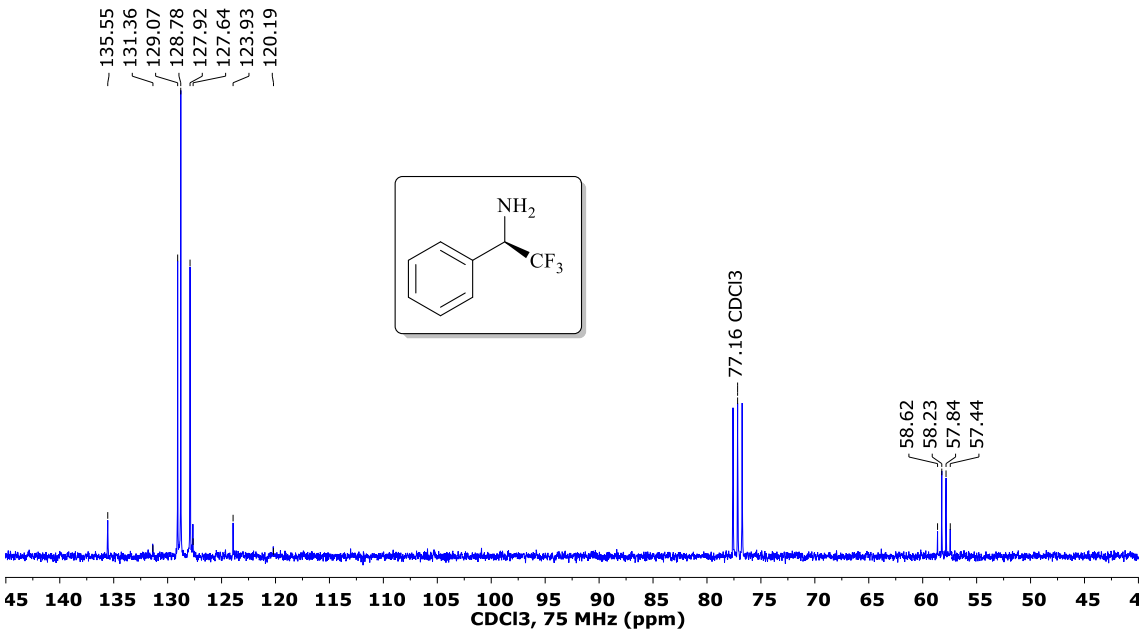
^{13}C NMR spectrum of compound **8b**.



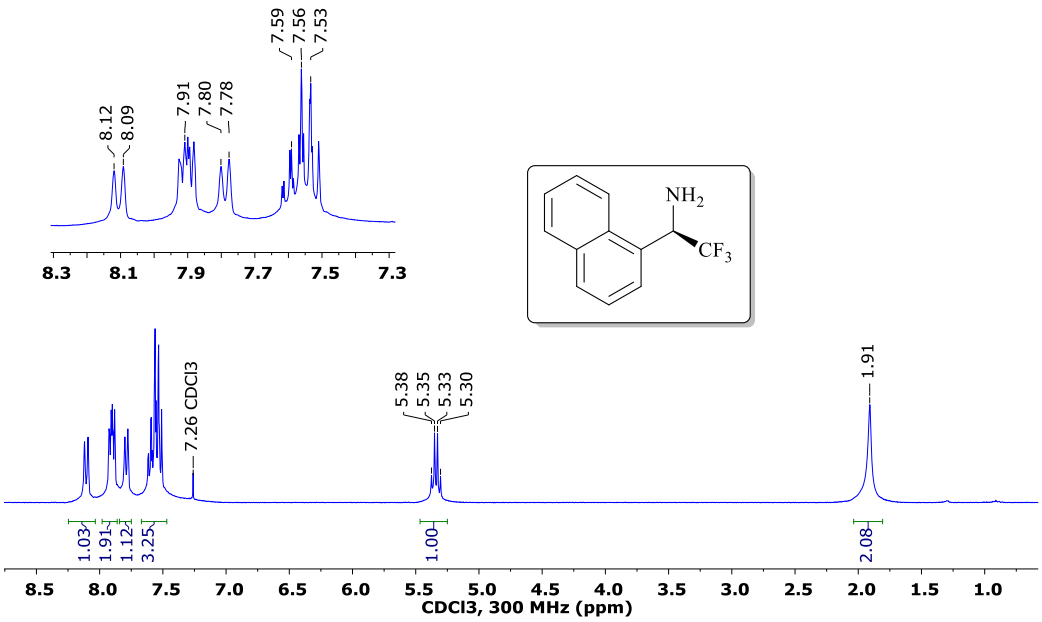
^{19}F NMR spectrum of compound **8b**.



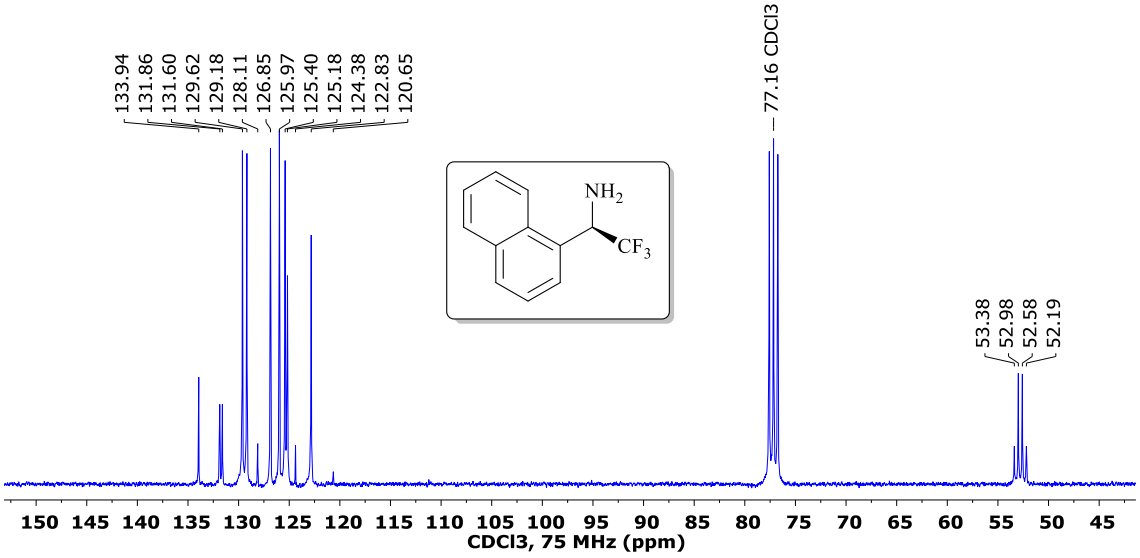
^{1}H NMR spectrum of compound **9a**.



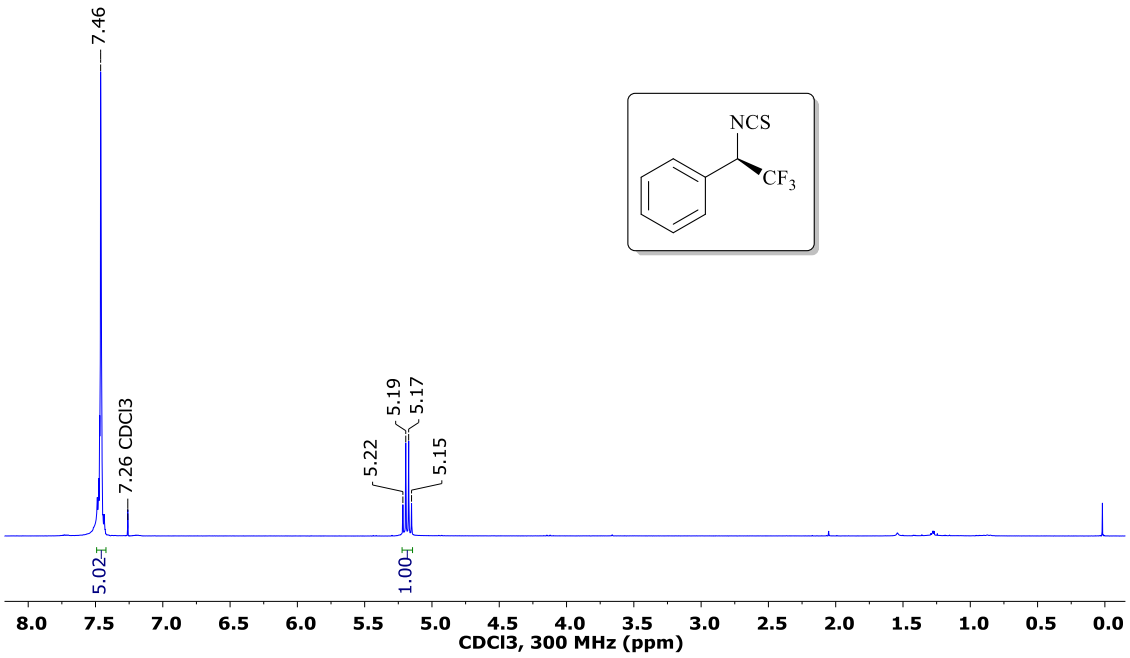
^{13}C NMR spectrum of compound **9a**.



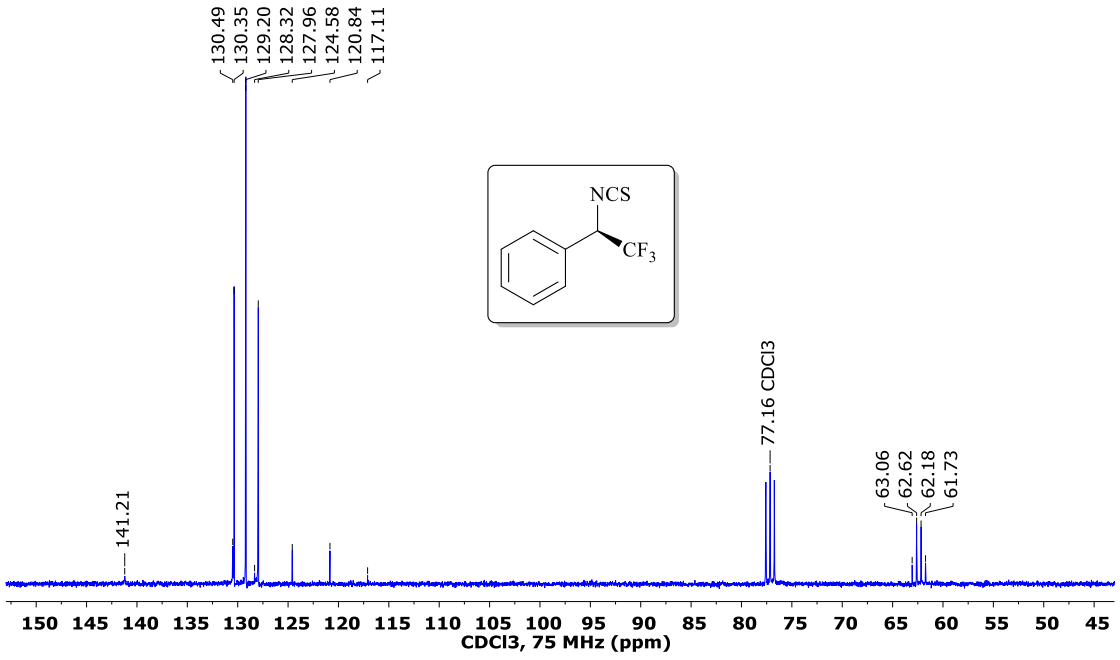
^{1}H NMR spectrum of compound **9b**.



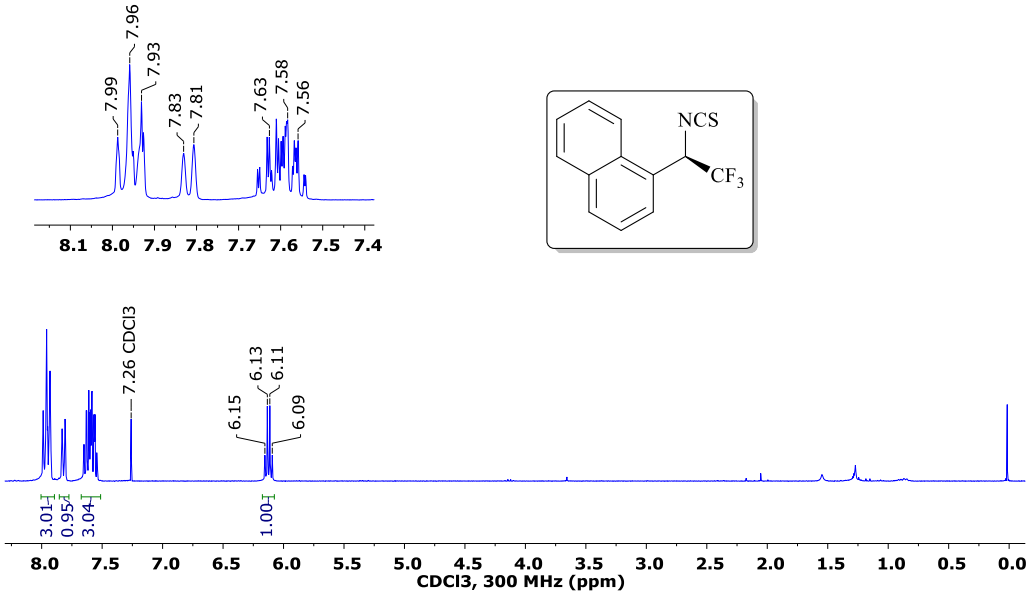
^{13}C NMR spectrum of compound **9b**.



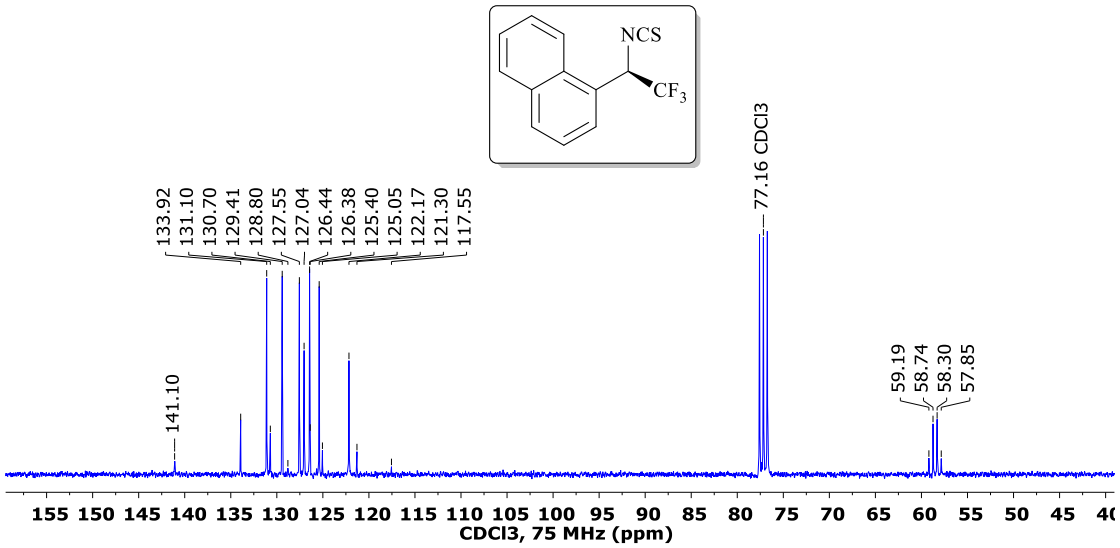
^{1}H NMR spectrum of compound **10a**.



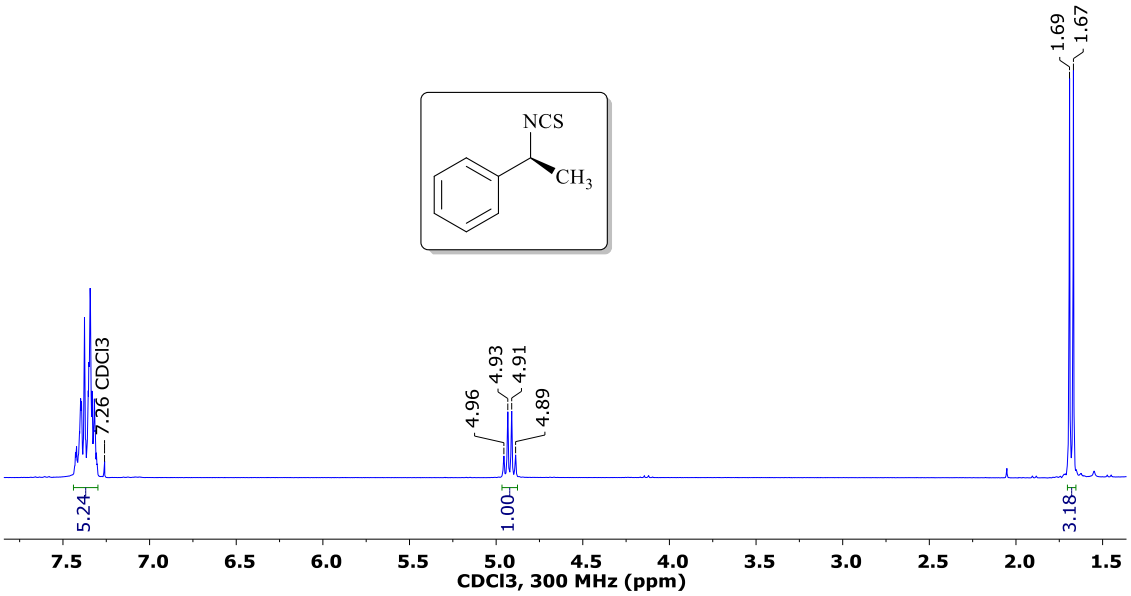
^{13}C NMR spectrum of compound **10a**.



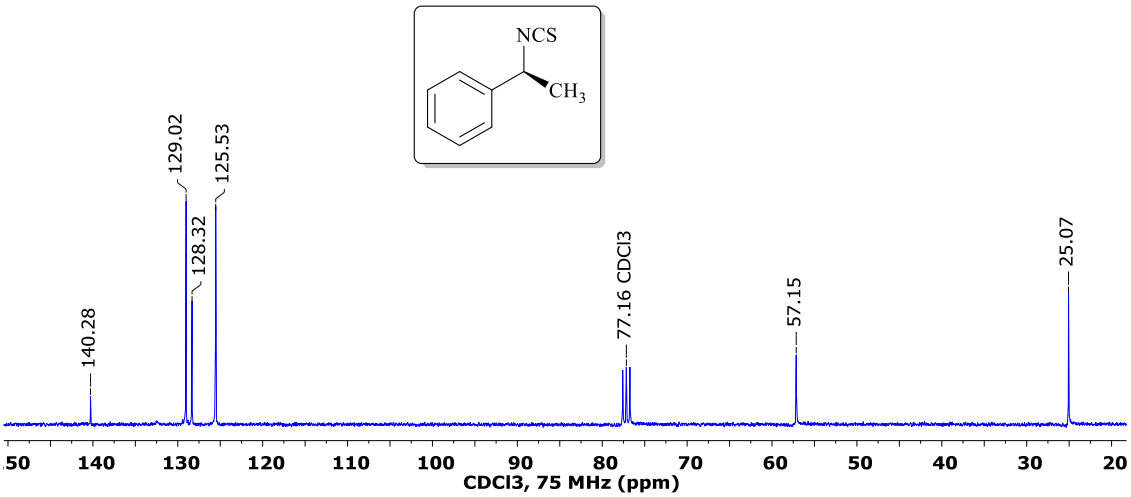
^{1}H NMR spectrum of compound **10b**.



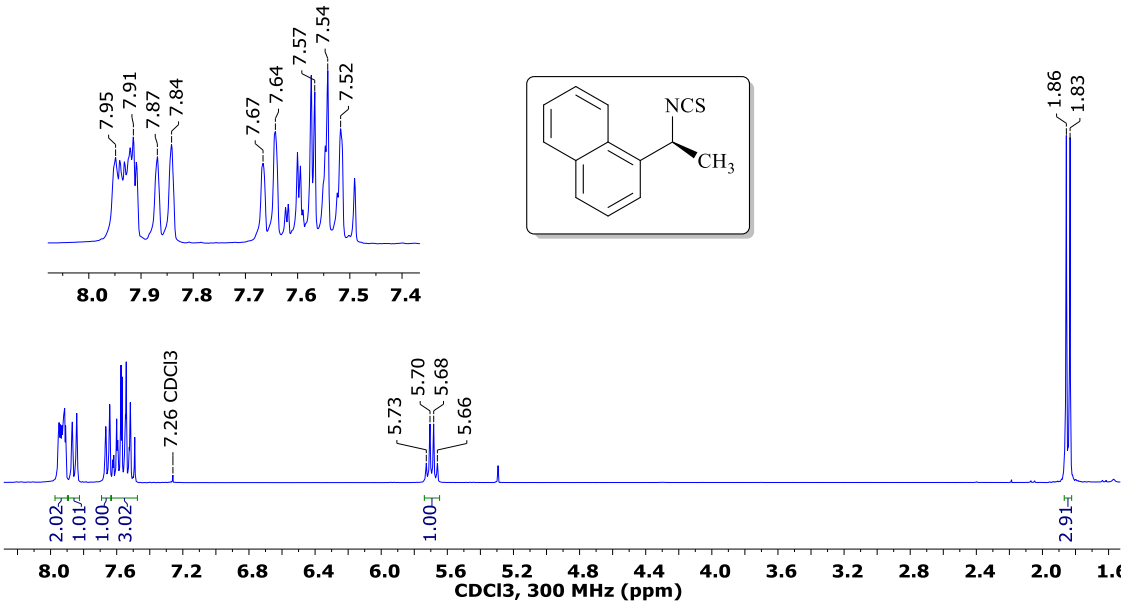
^{13}C NMR spectrum of compound **10b**.



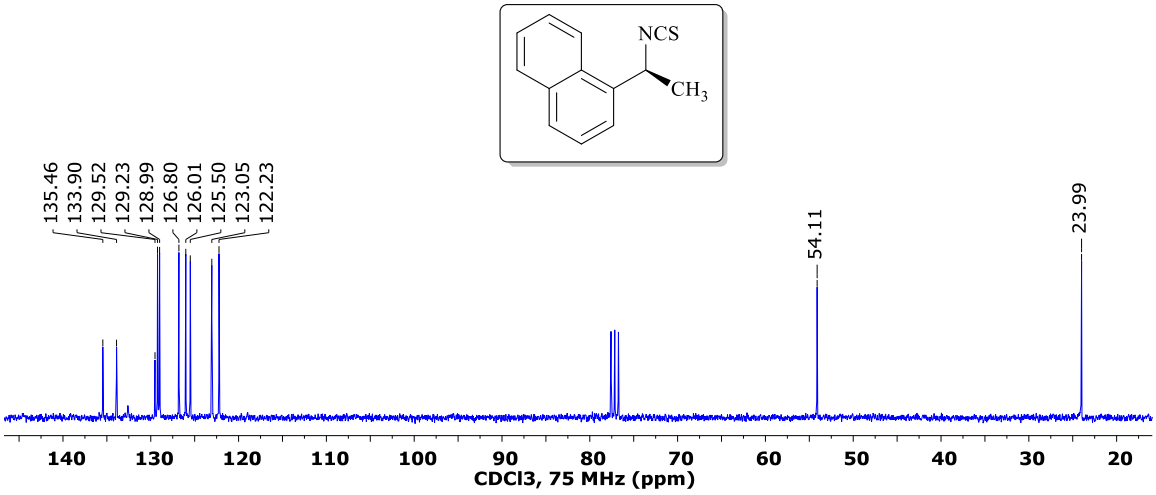
^{1}H NMR spectrum of compound **10c**.



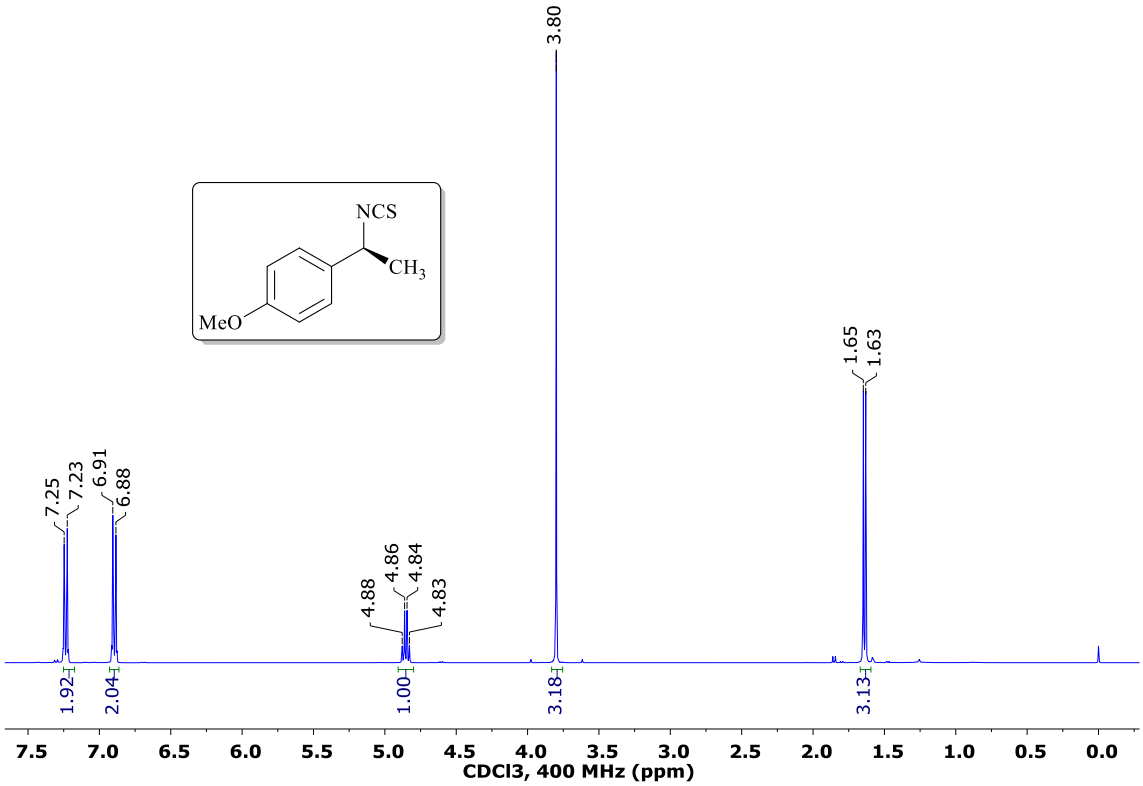
^{13}C NMR spectrum of compound **10c**.



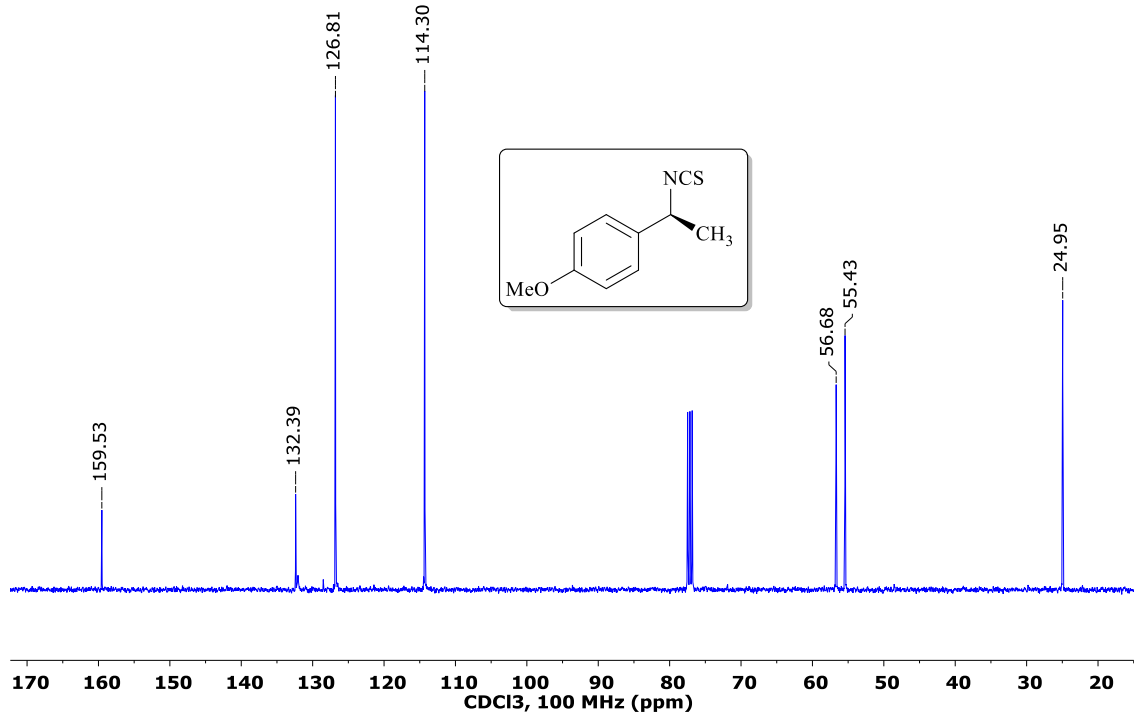
^{1}H NMR spectrum of compound **10d**.



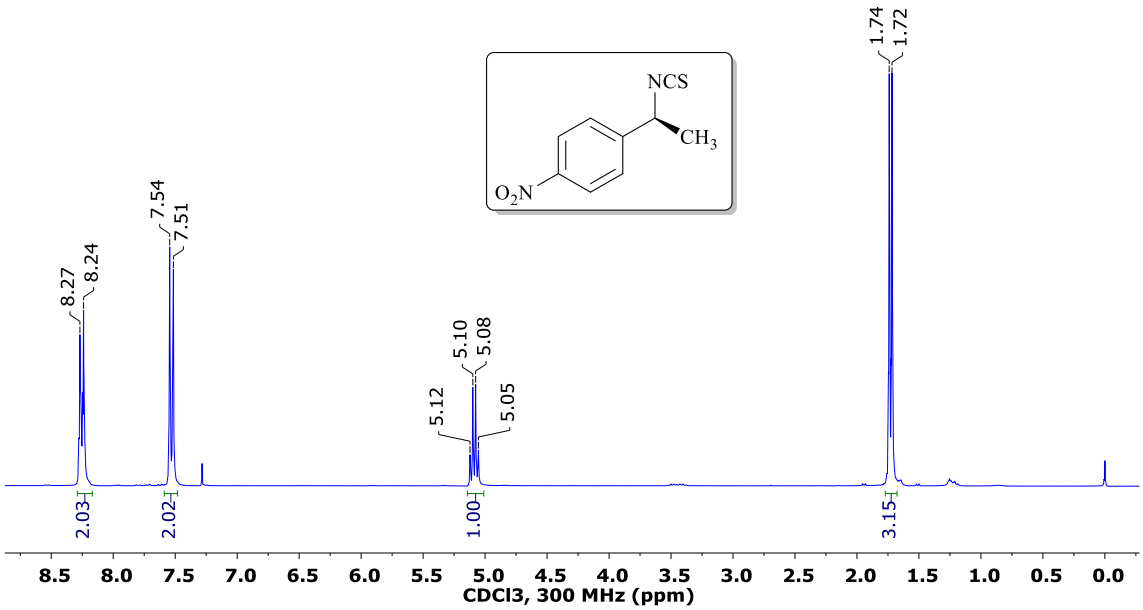
^{13}C NMR spectrum of compound **10d**.



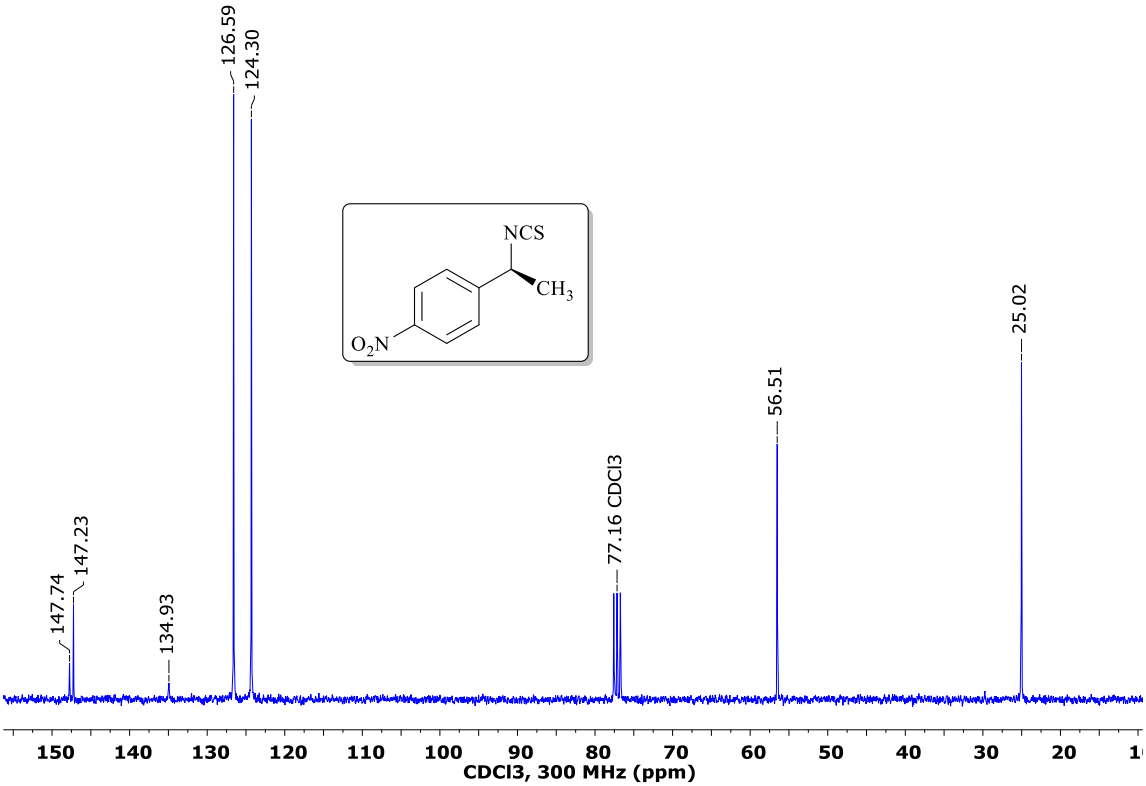
^{1}H NMR spectrum of compound **10e**.



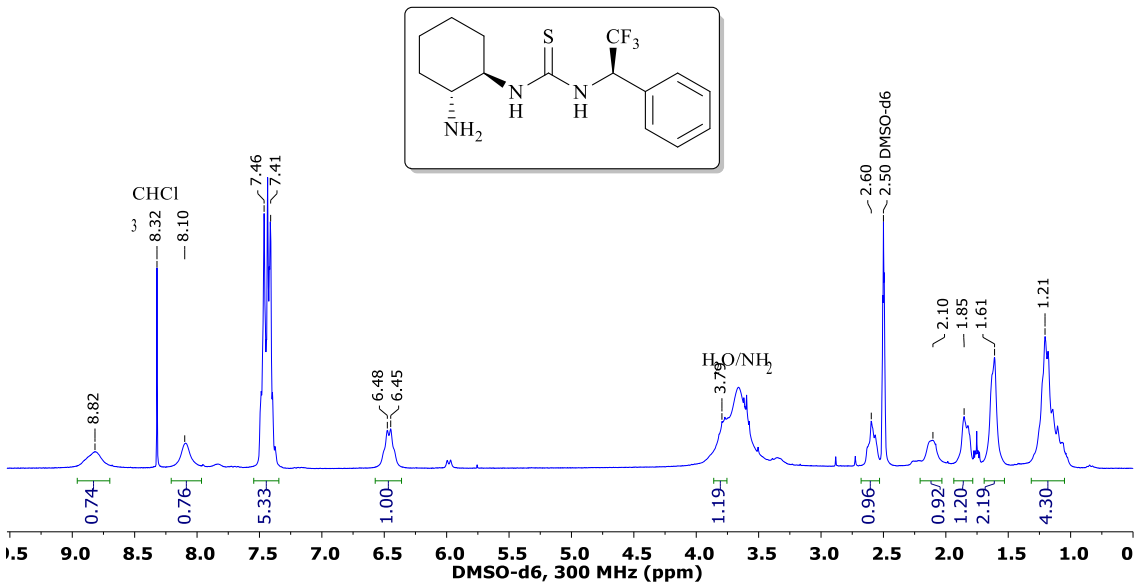
^{13}C NMR spectrum of compound **10e**.



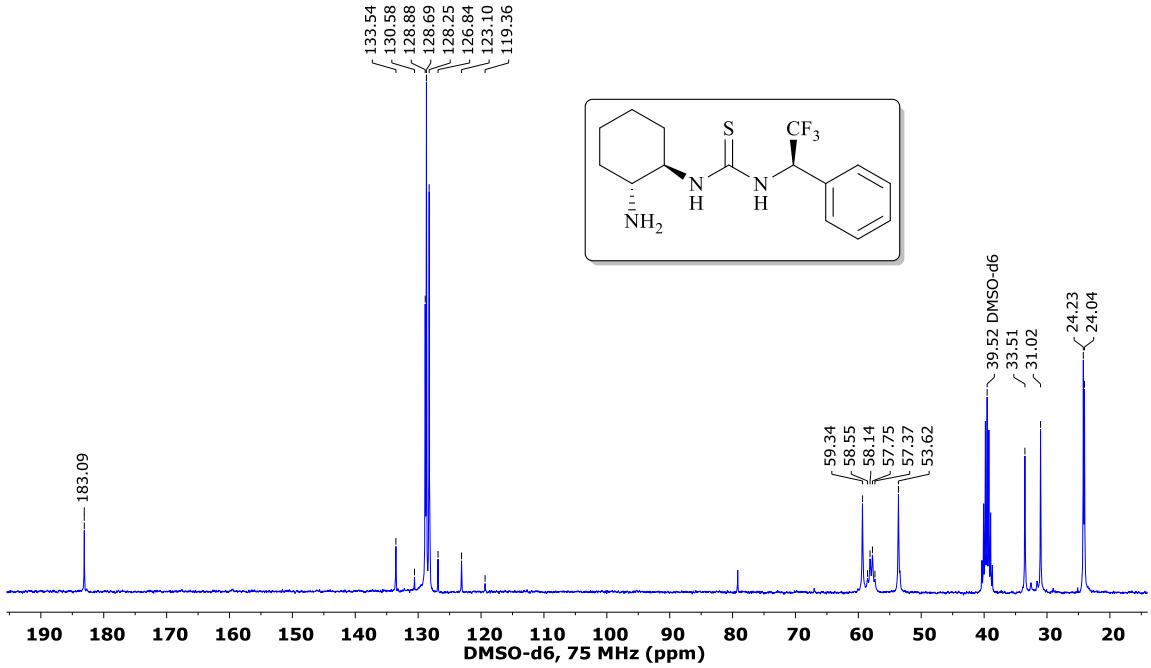
^{1}H NMR spectrum of compound **10f**.



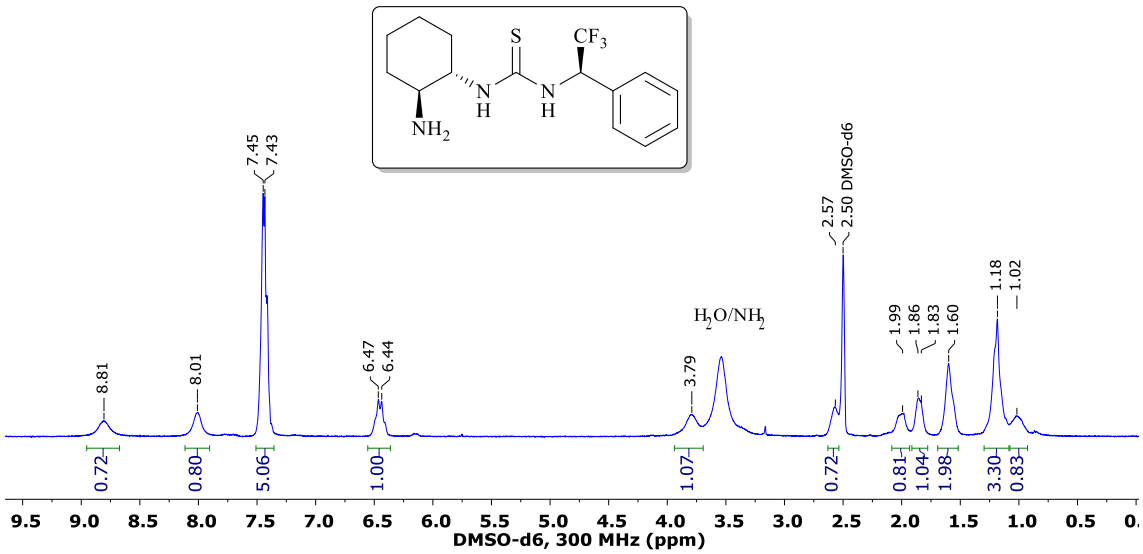
^{13}C NMR spectrum of compound **10f**.



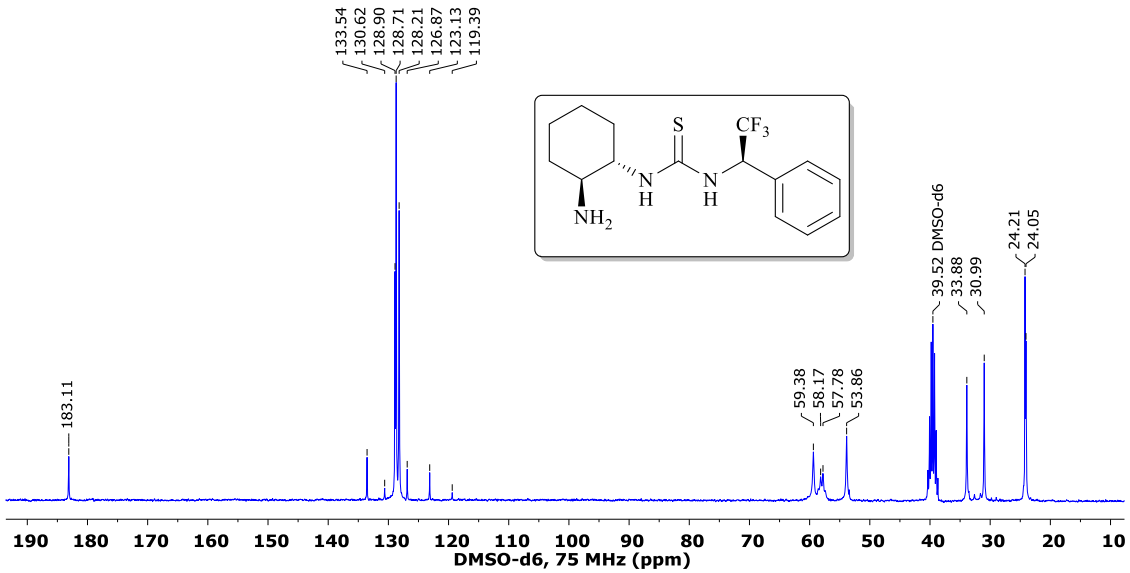
^{1}H NMR spectrum of compound **A_F**.



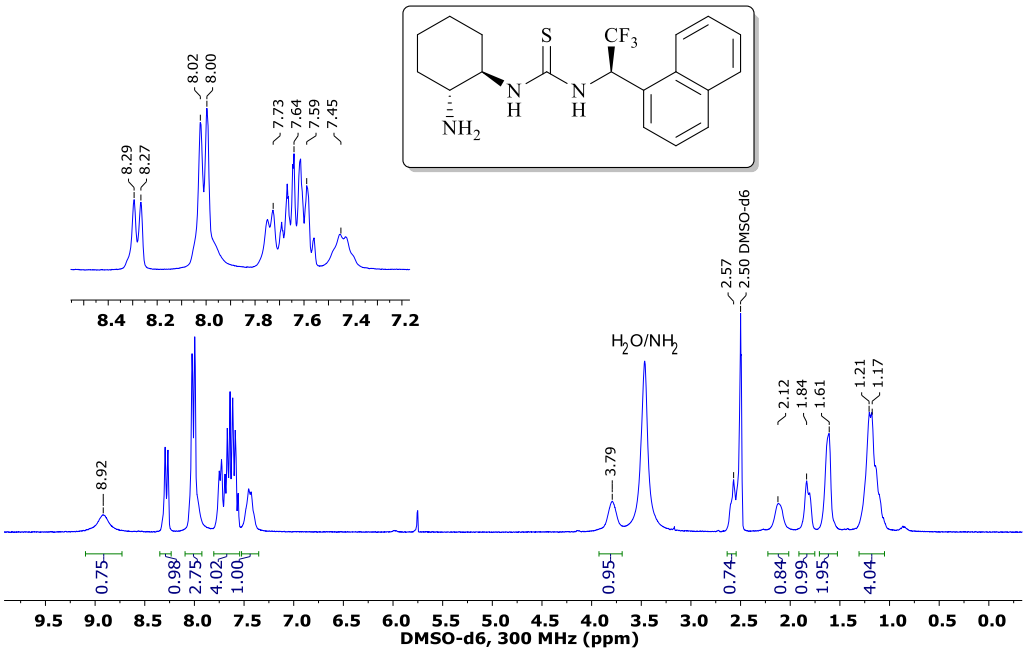
^{13}C NMR spectrum of compound **A_F**.



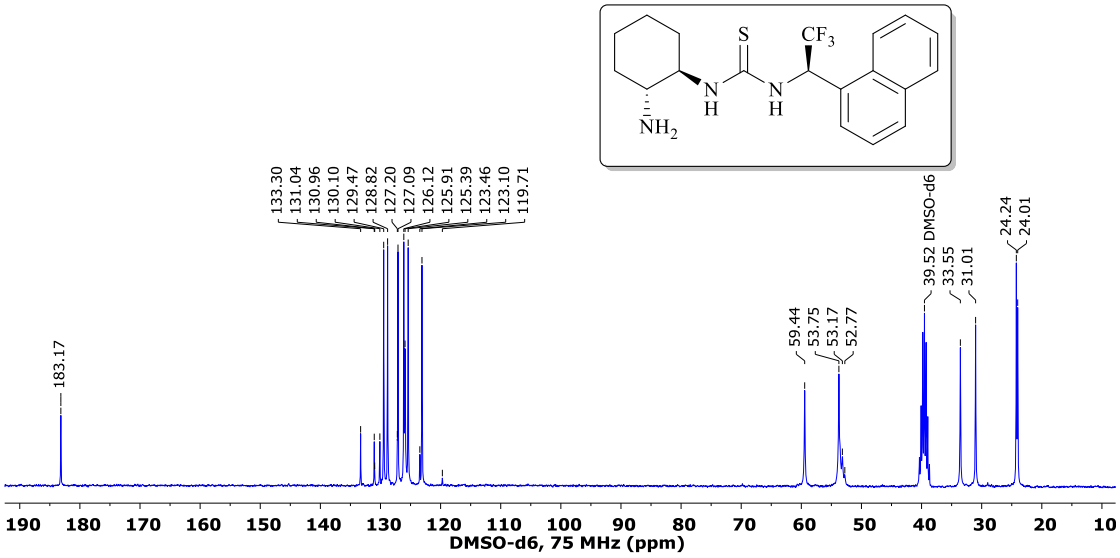
^{1}H NMR spectrum of compound **B$_F$**.



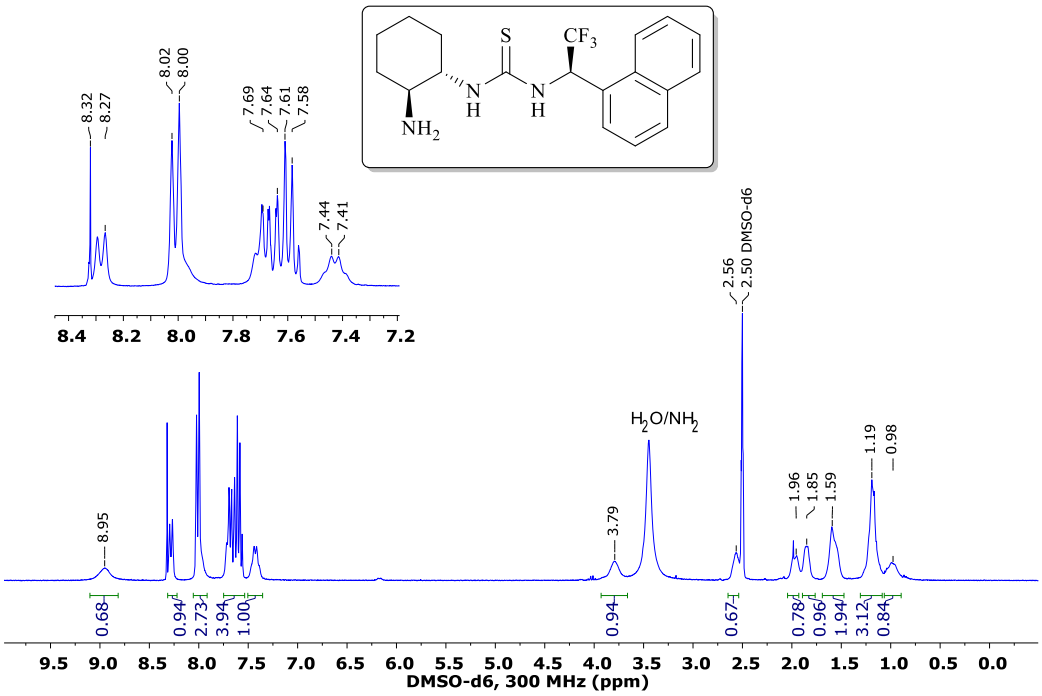
^{13}C NMR spectrum of compound **B$_F$**.



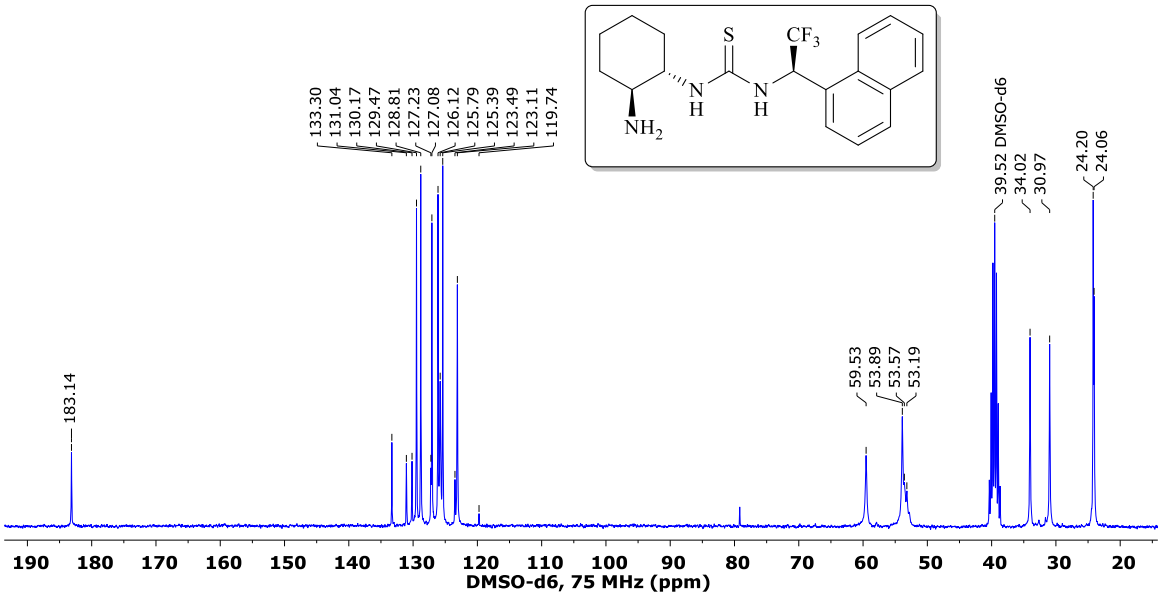
^{1}H NMR spectrum of compound **C_F**.



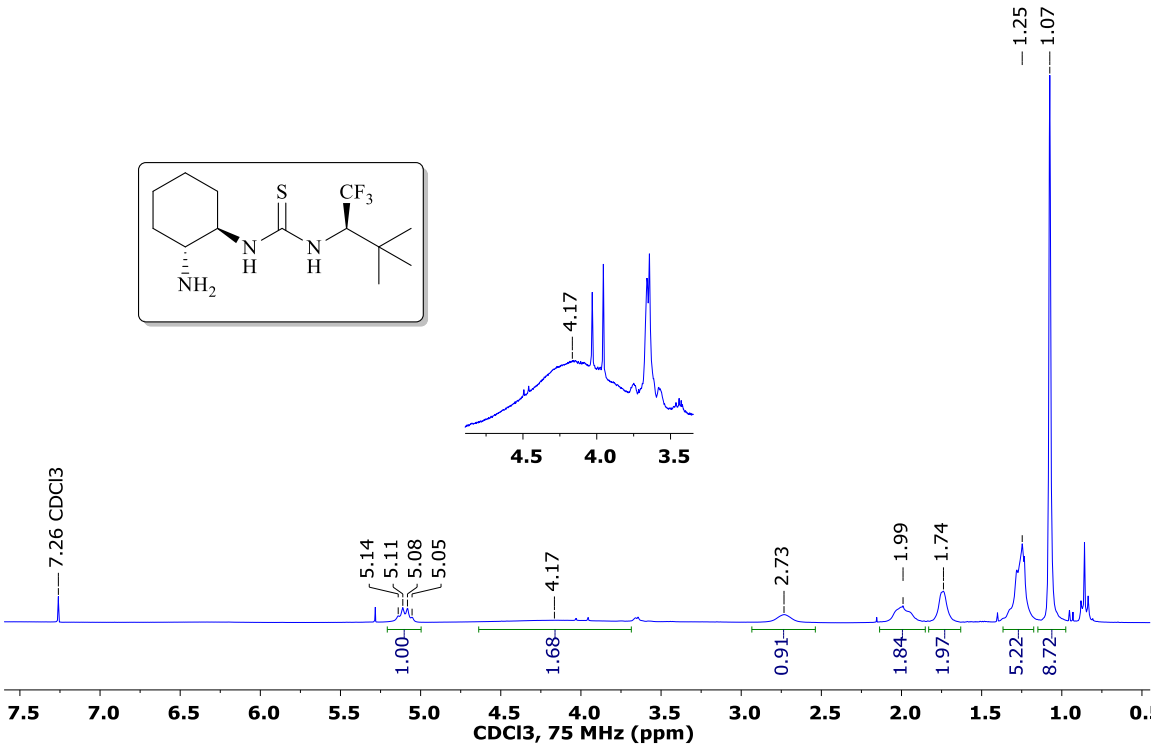
^{13}C NMR spectrum of compound **C_F**.



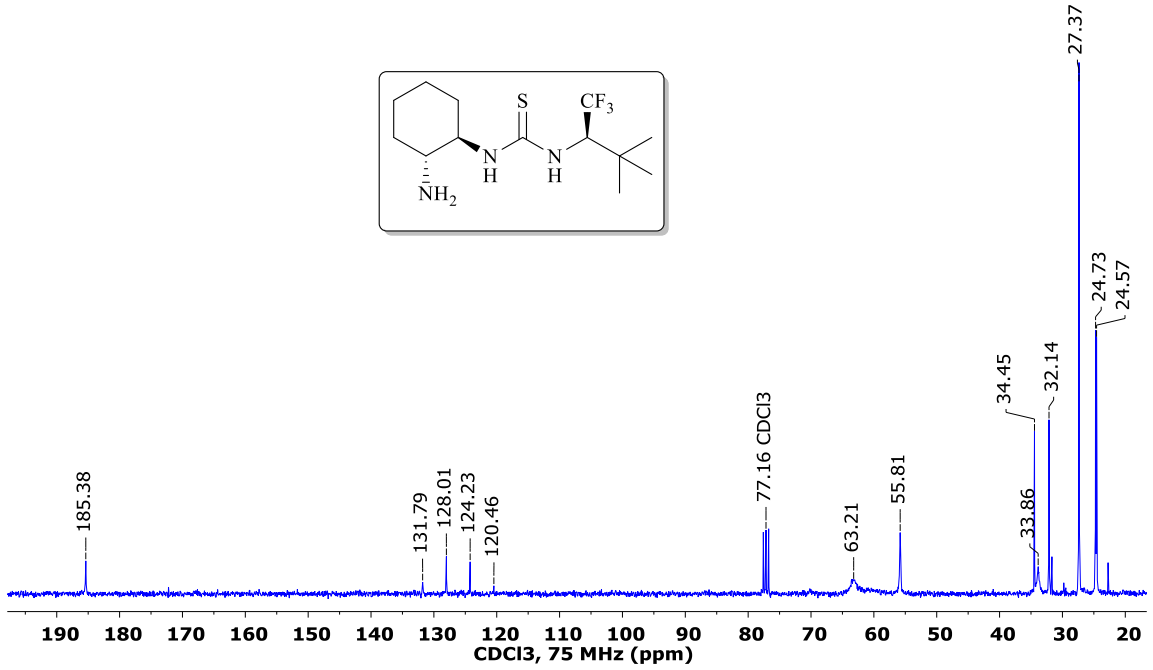
^{1}H NMR spectrum of compound **D_F**.



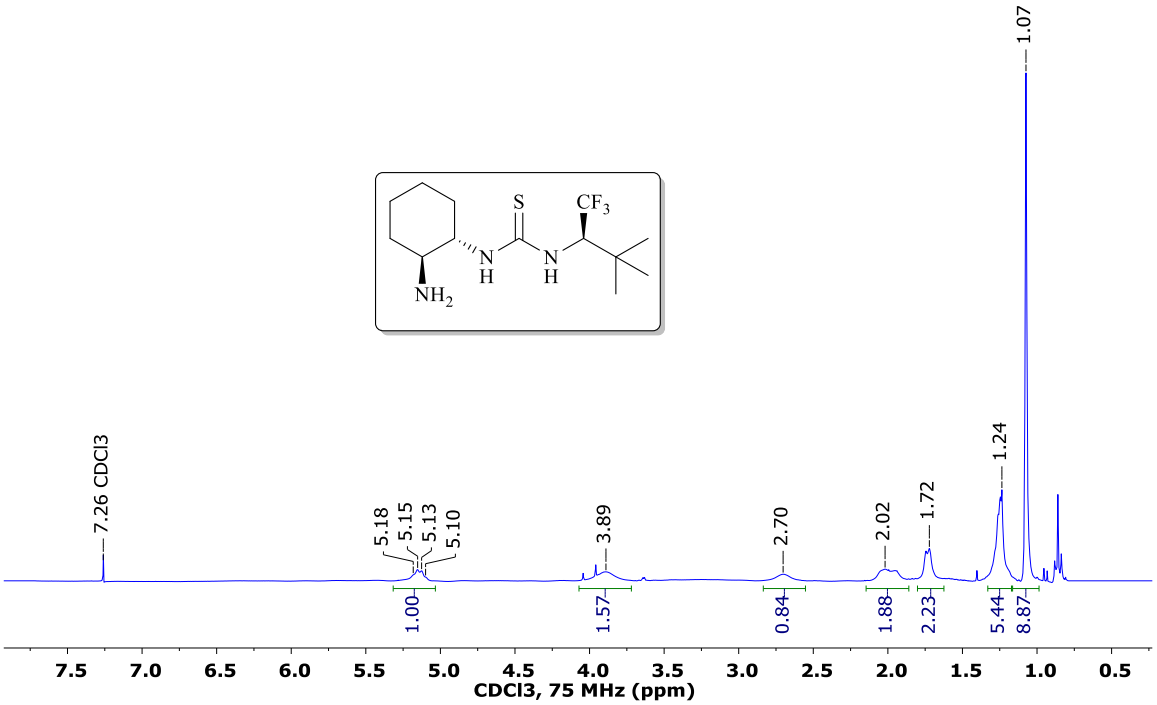
^{13}C NMR spectrum of compound **D_F**.



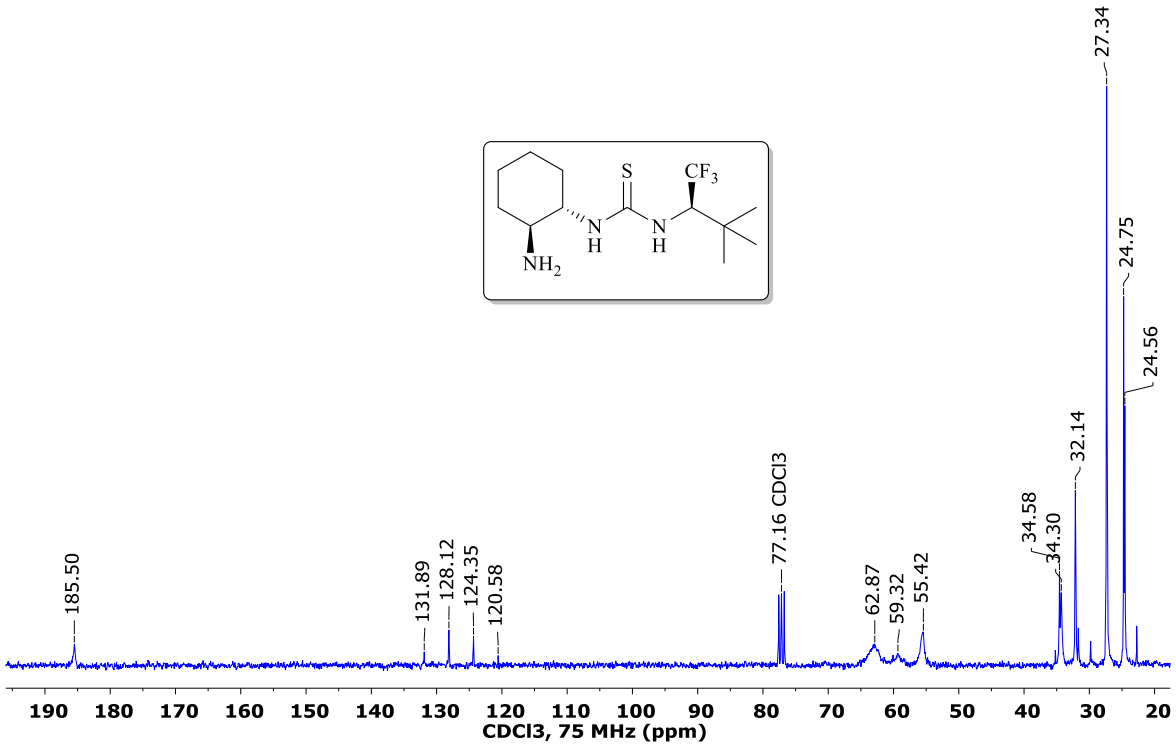
^{1}H NMR spectrum of compound **E_F**.



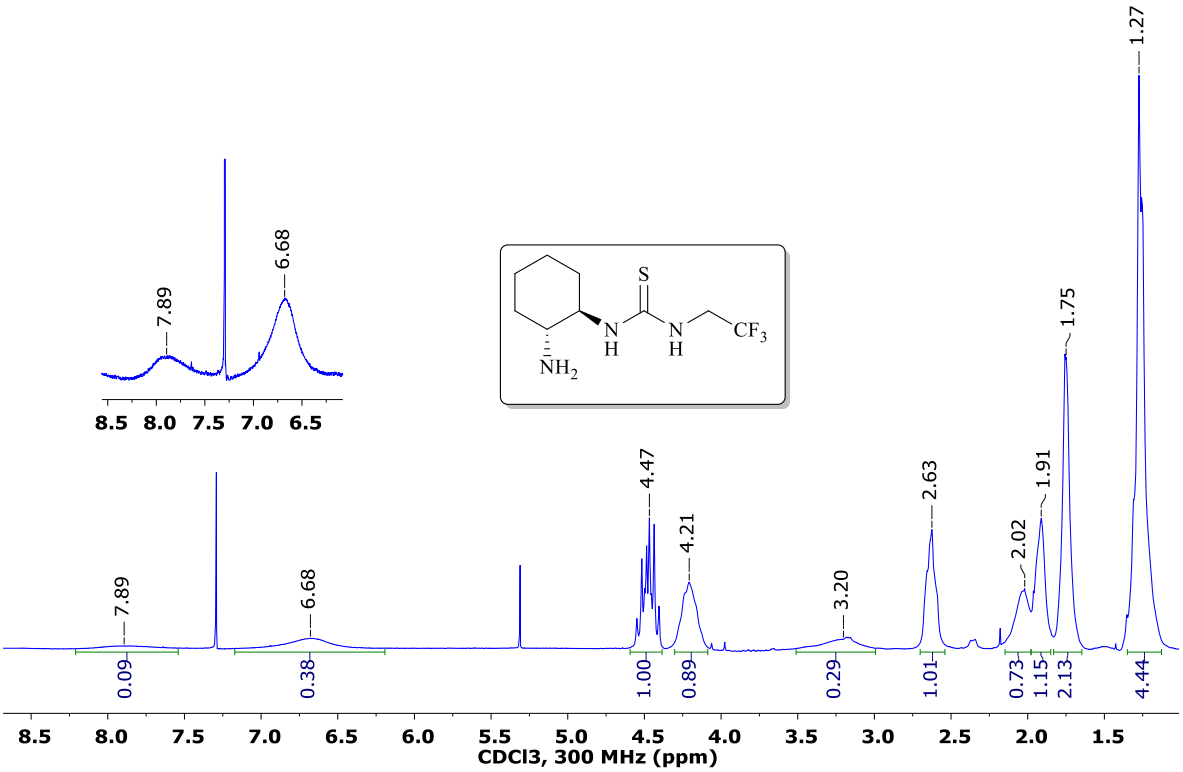
^{13}C NMR spectrum of compound **E_F**.



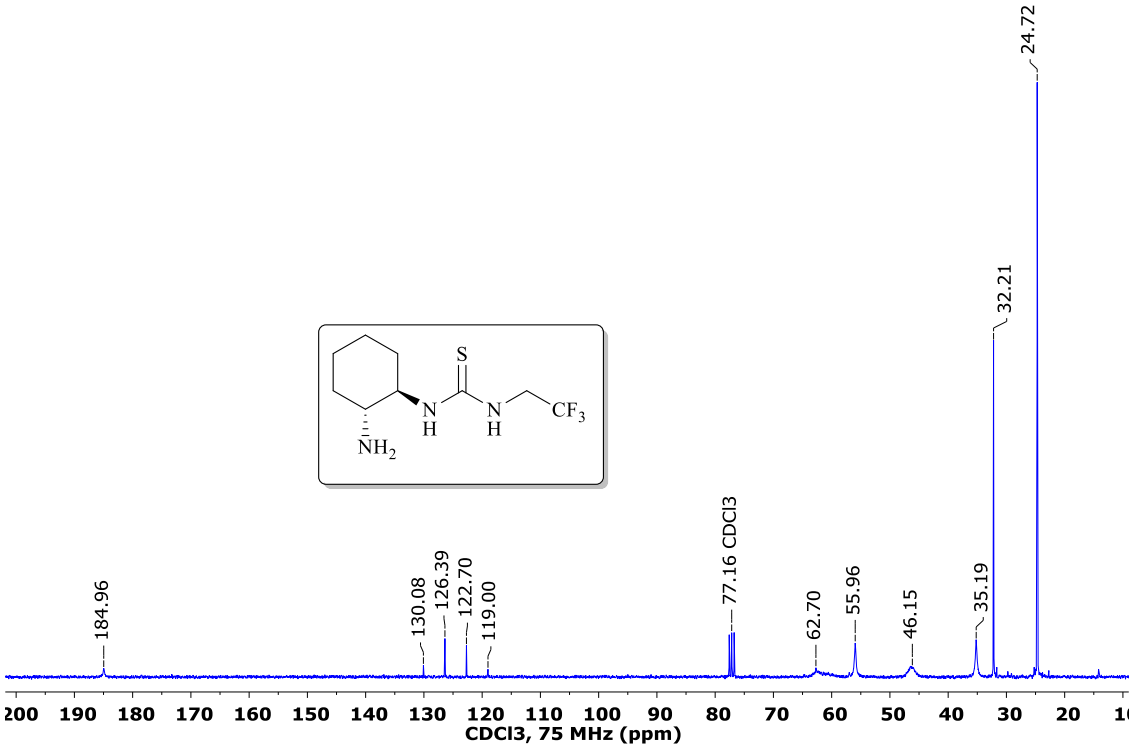
^{1}H NMR spectrum of compound **F_F**.



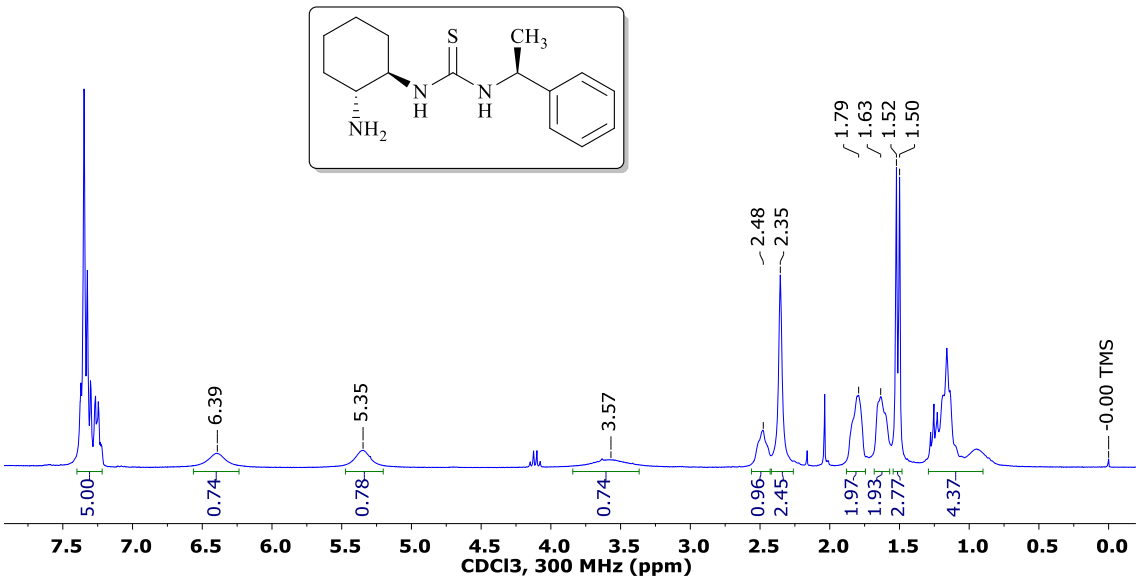
^{13}C NMR spectrum of compound **F_F**.



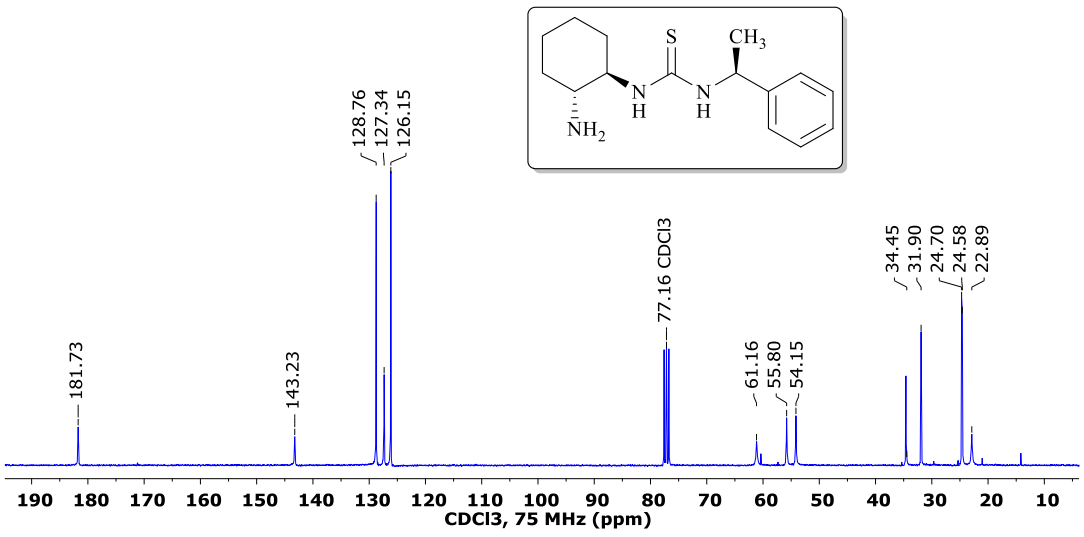
^{1}H NMR spectrum of compound **G_F**.



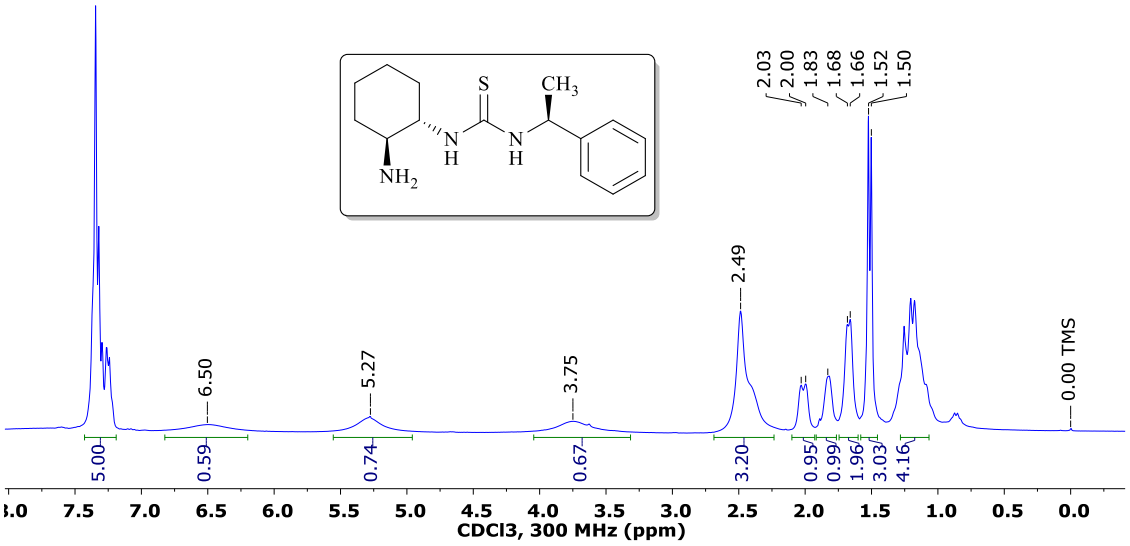
^{13}C NMR spectrum of compound **G_F**.



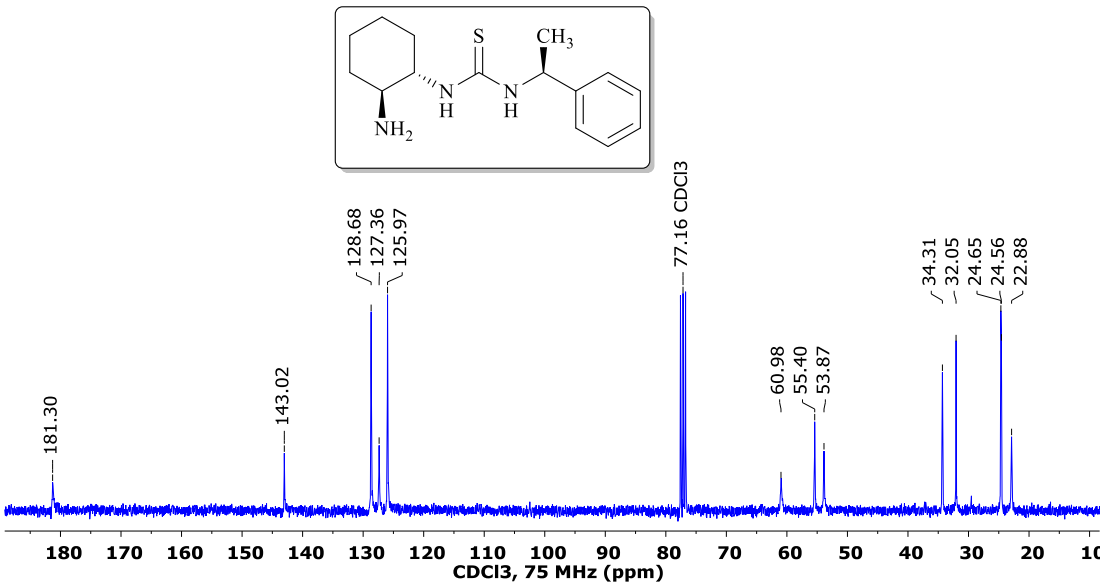
^{1}H NMR spectrum of compound **A**.



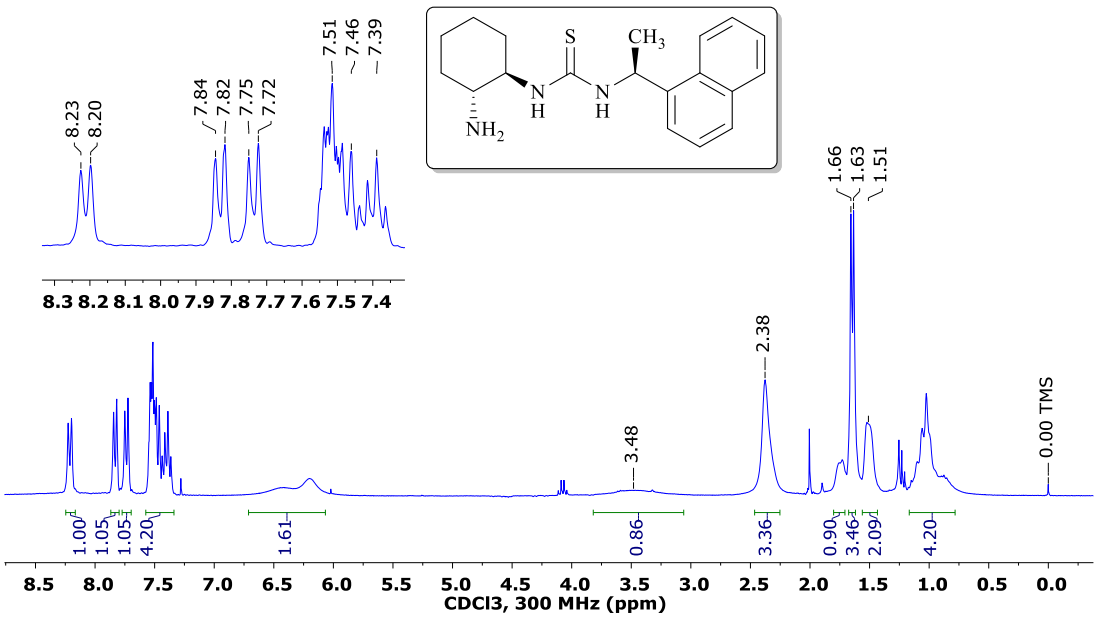
^{13}C NMR spectrum of compound **A**.



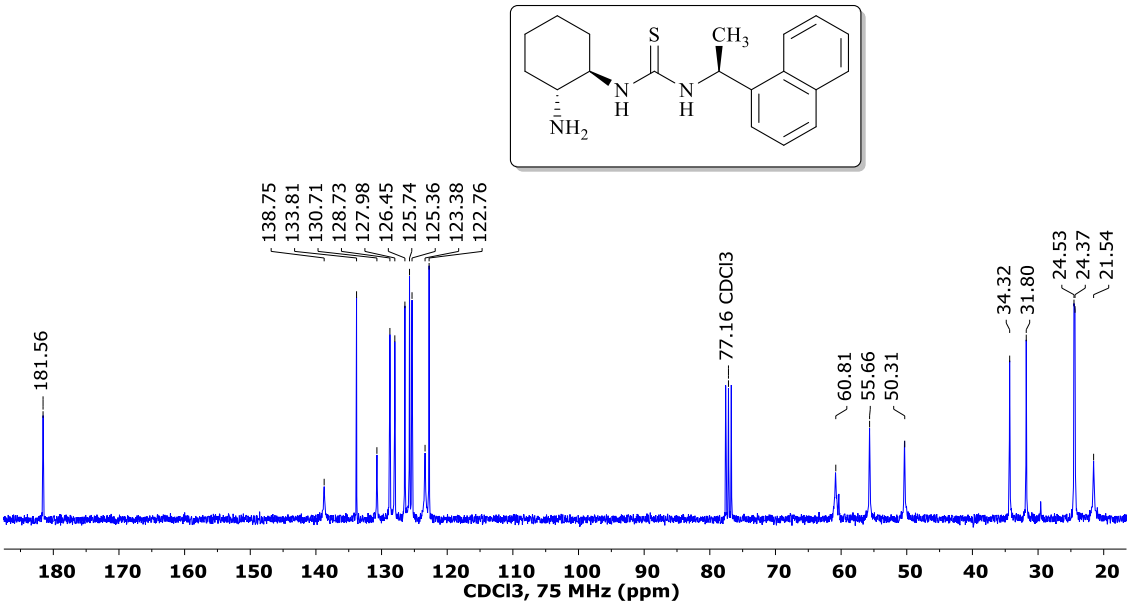
^{1}H NMR spectrum of compound **B**.



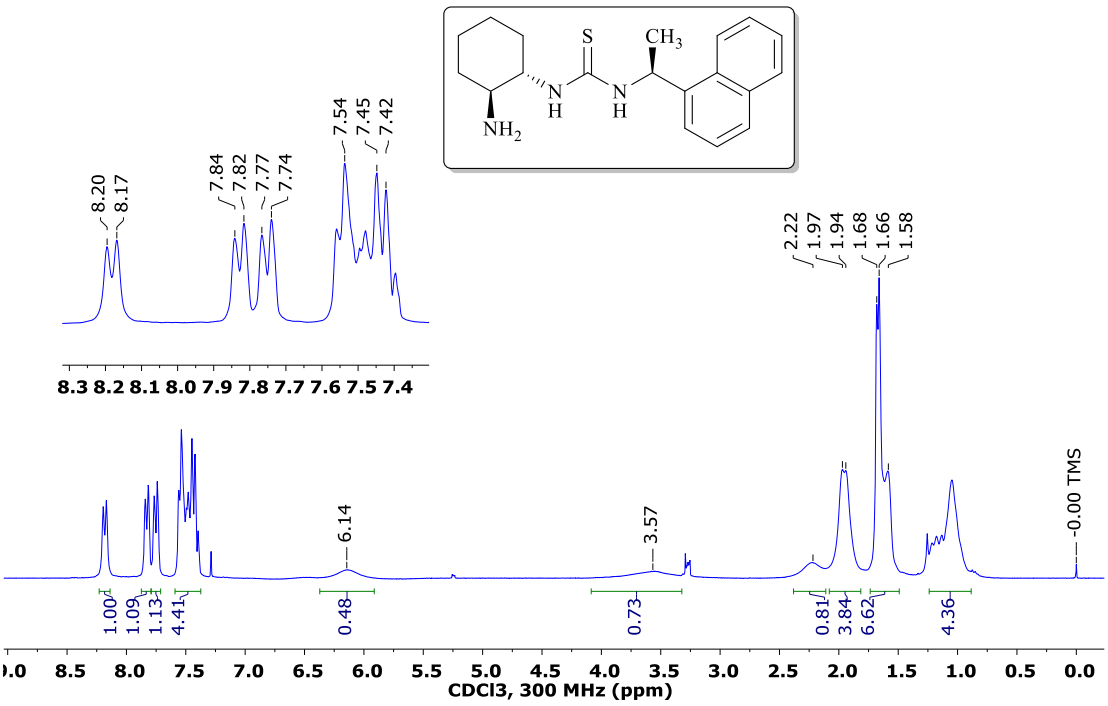
^{13}C NMR spectrum of compound **B**.



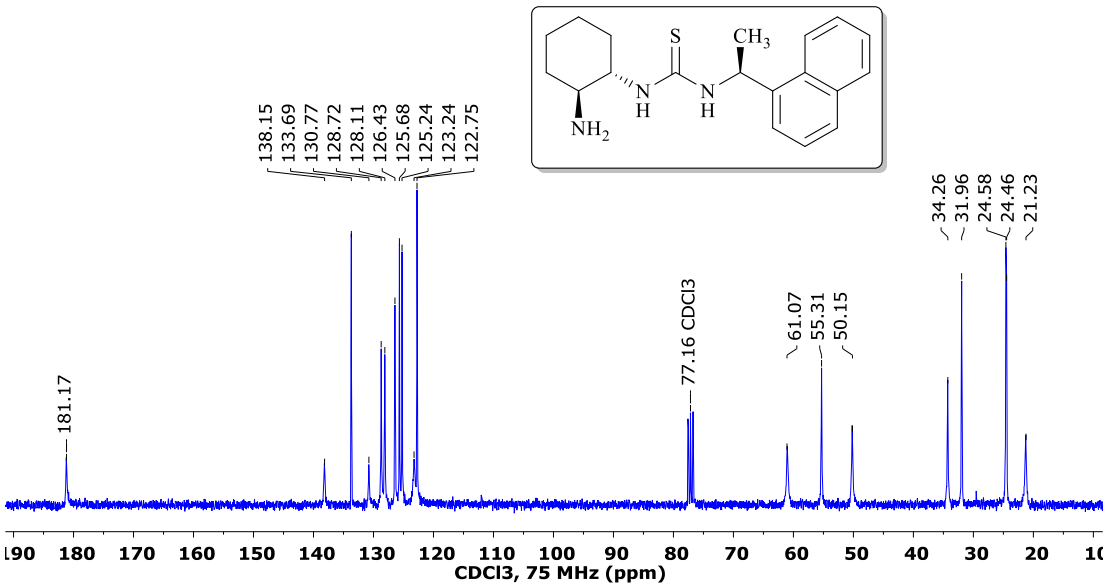
^{1}H NMR spectrum of compound **C**.



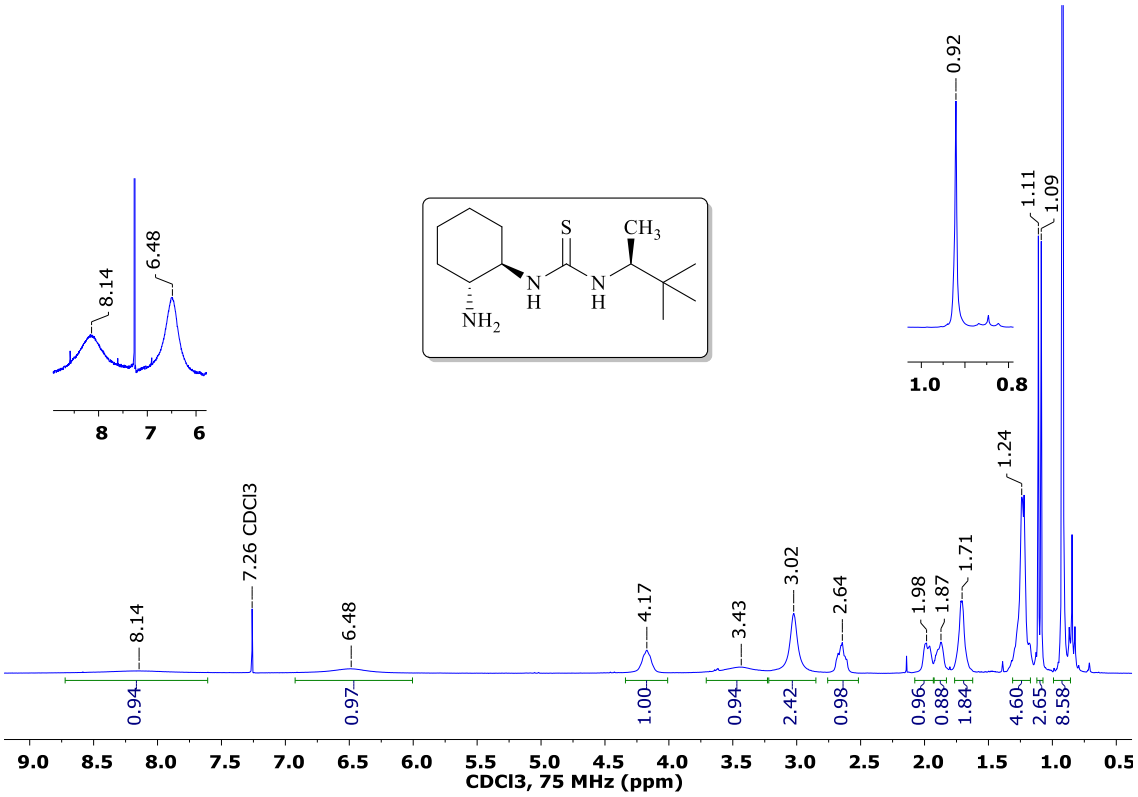
^{13}C NMR spectrum of compound **C**.



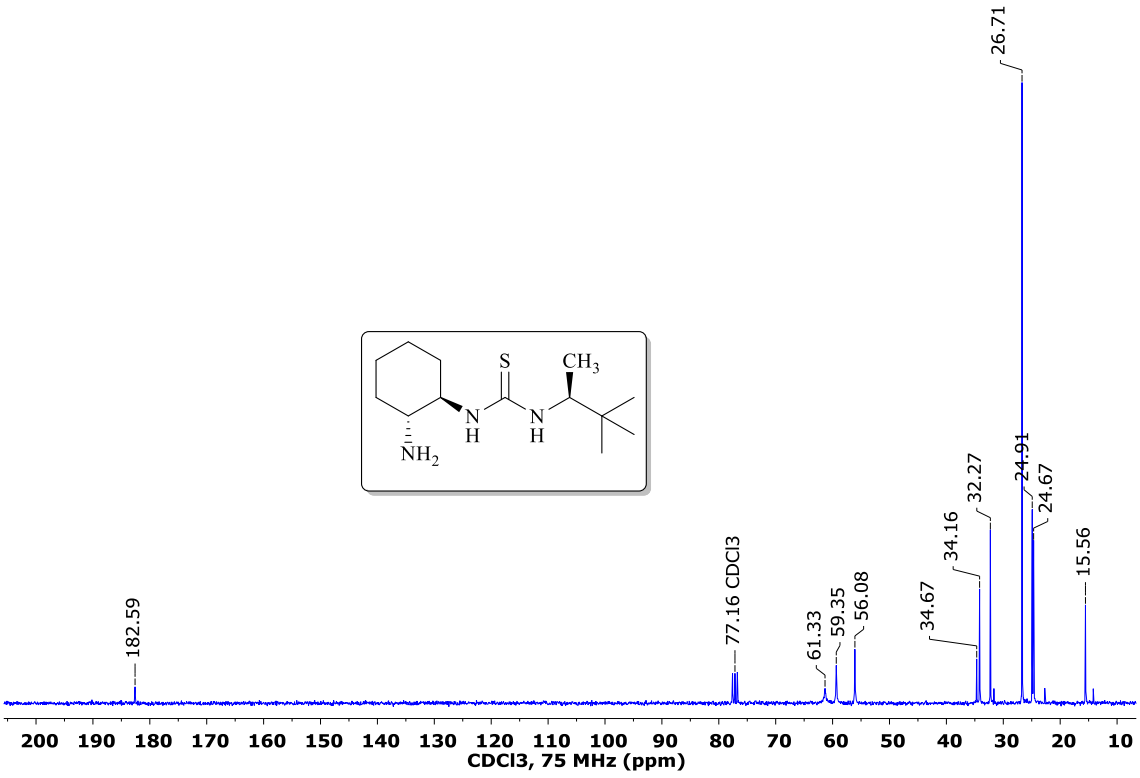
^{1}H NMR spectrum of compound **D**.



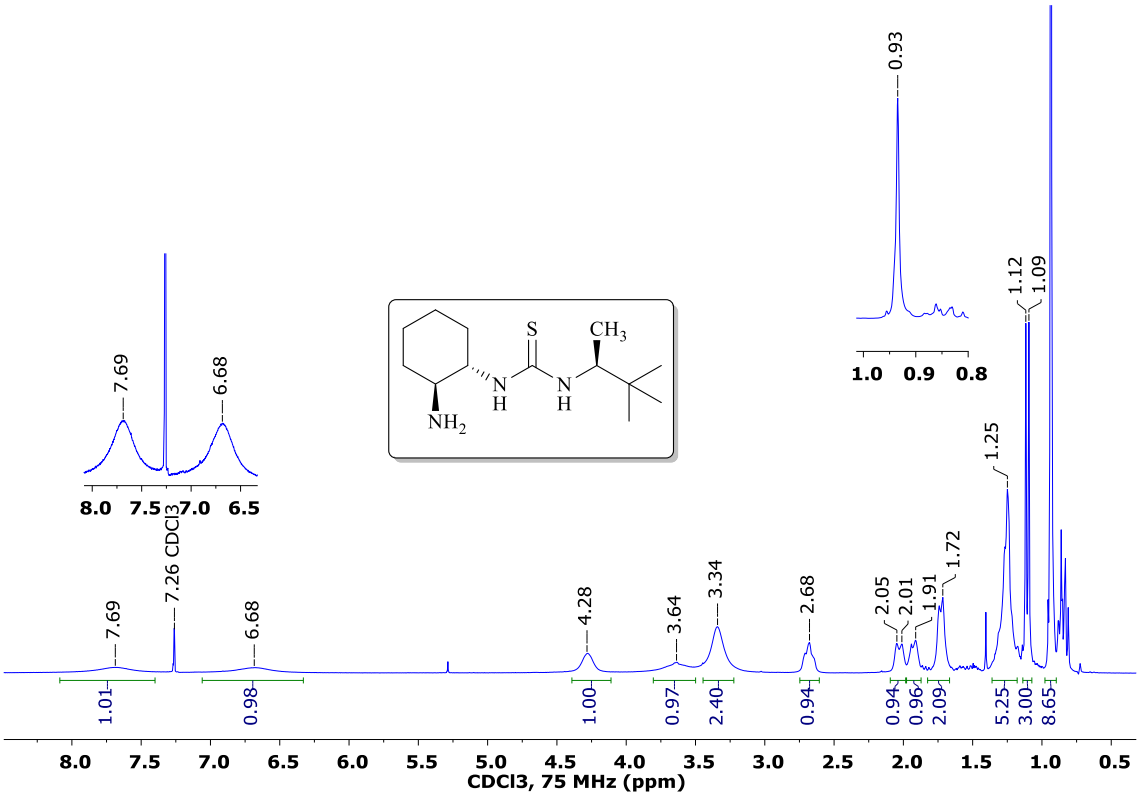
^{13}C NMR spectrum of compound **D**.



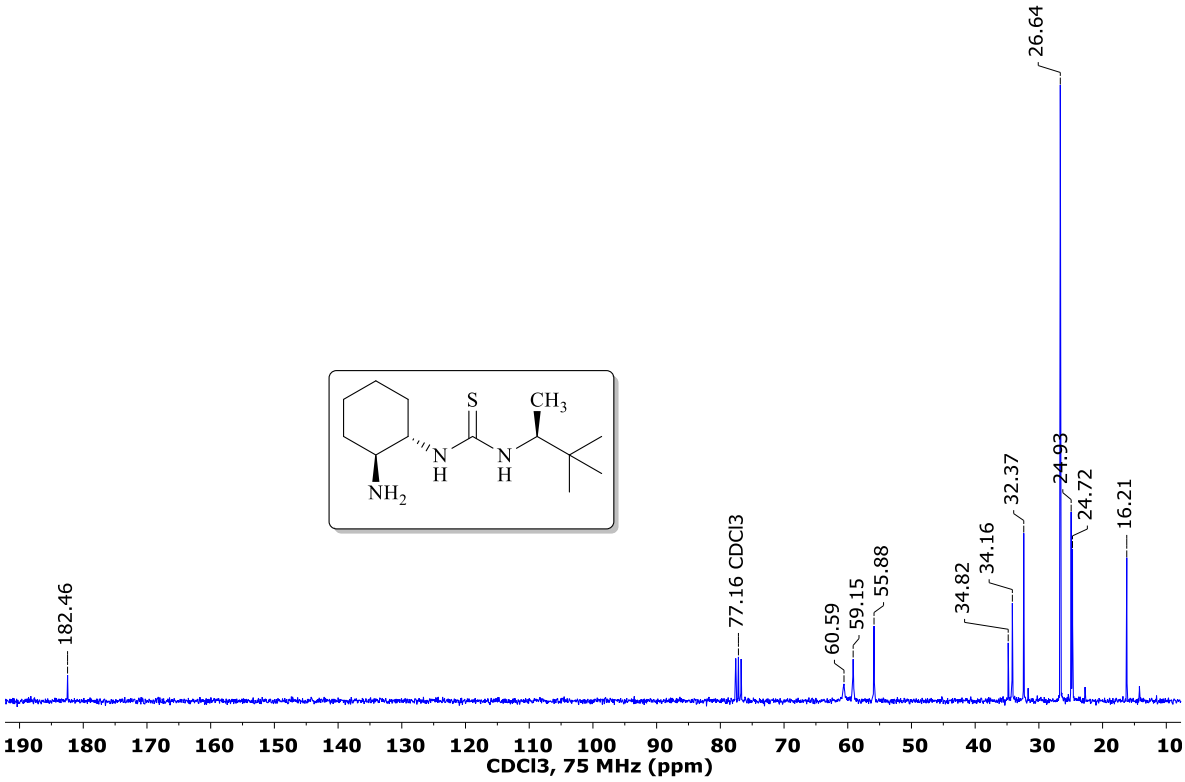
^{1}H NMR spectrum of compound **E**.



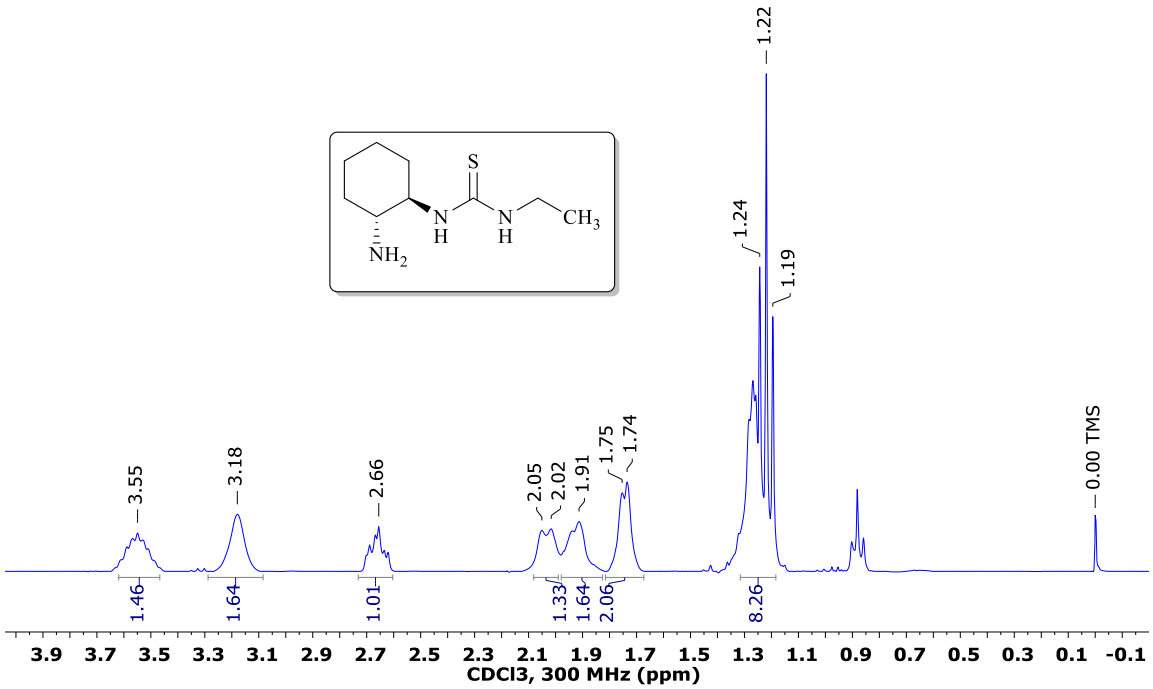
^{13}C NMR spectrum of compound **E**.



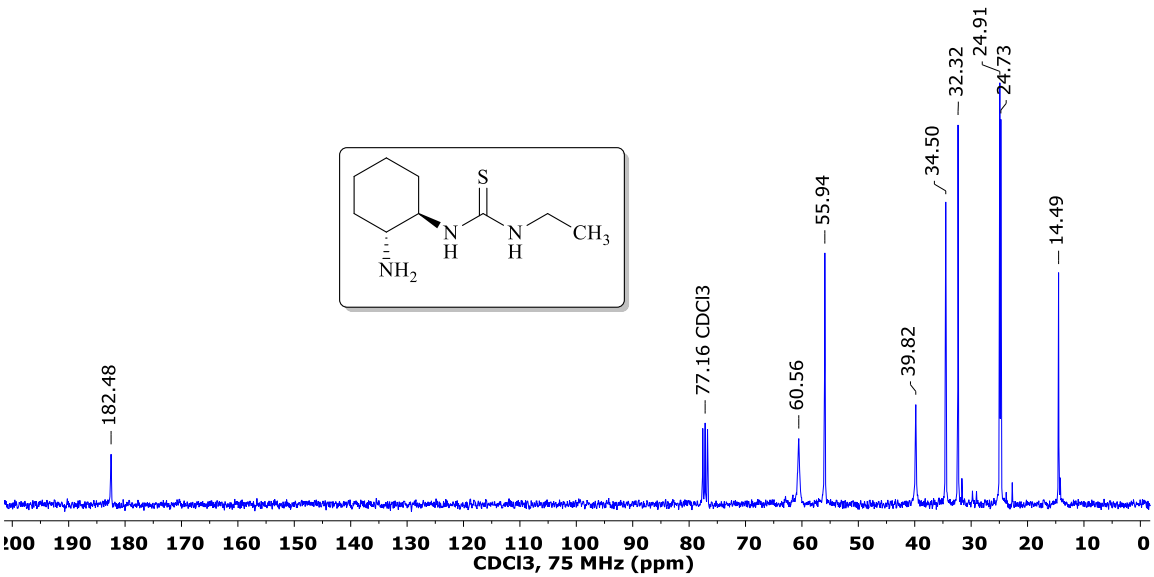
^{1}H NMR spectrum of compound **F**.



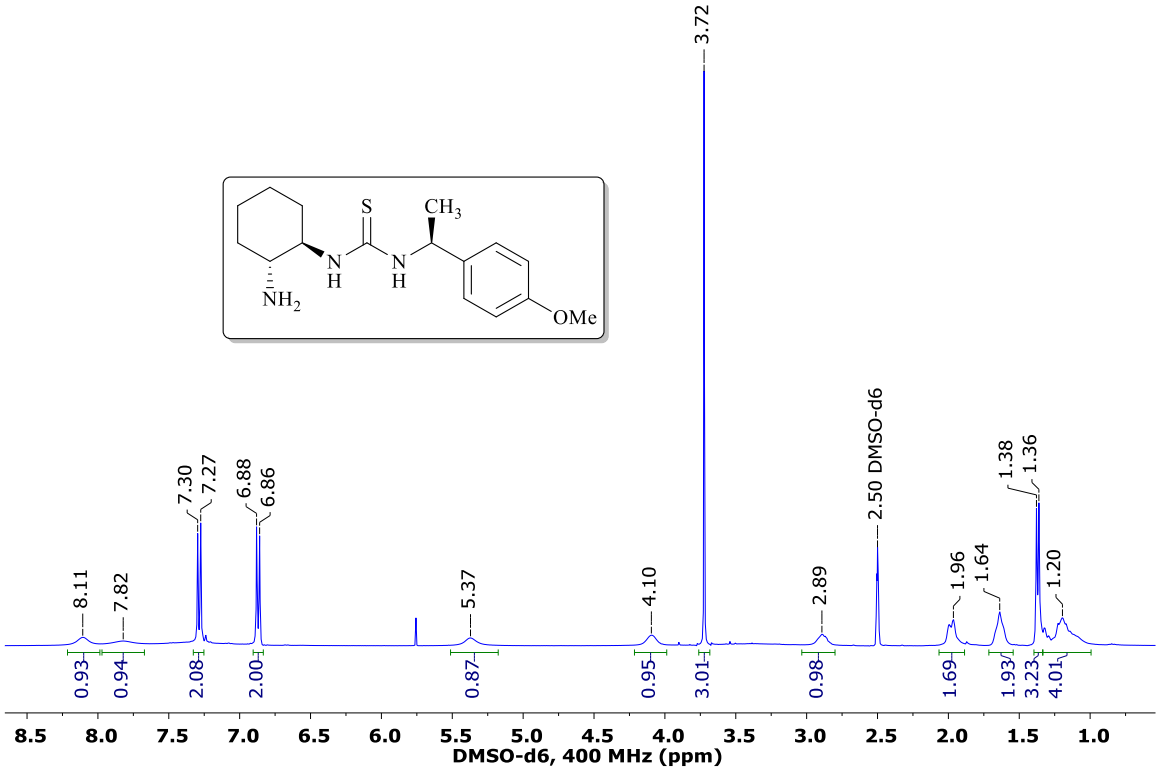
^{13}C NMR spectrum of compound **F**.



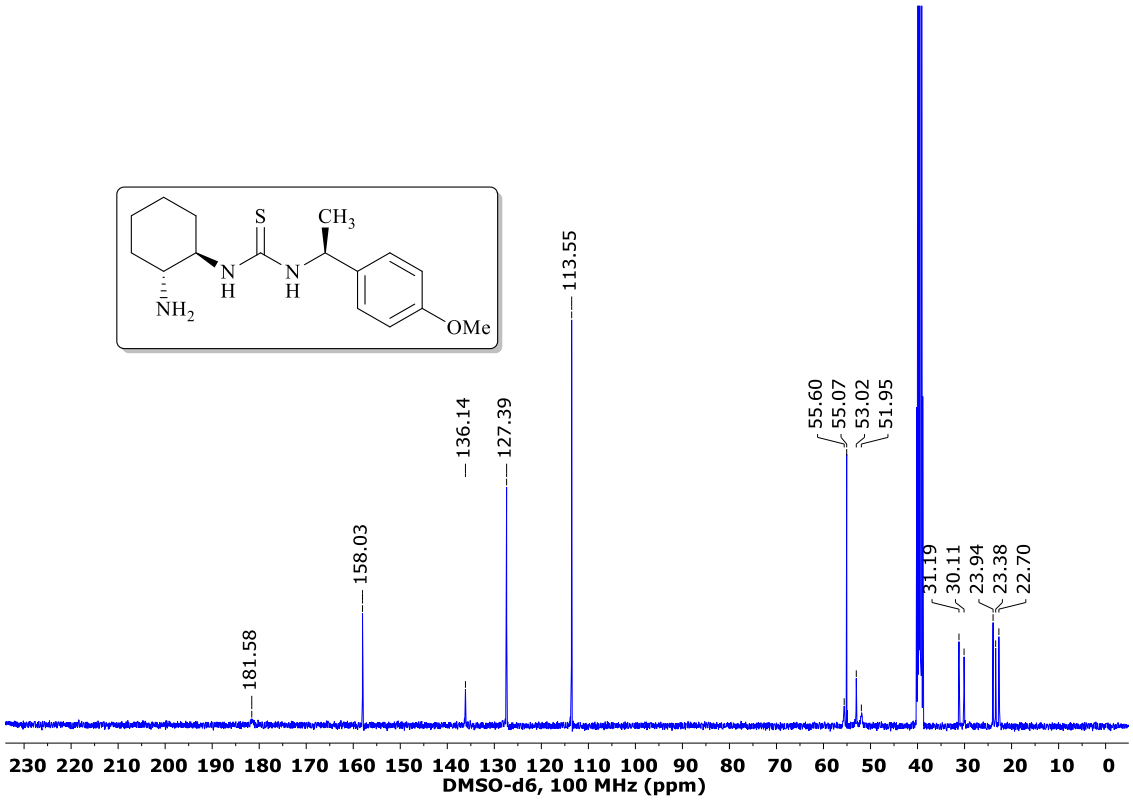
^{1}H NMR spectrum of compound **G**.



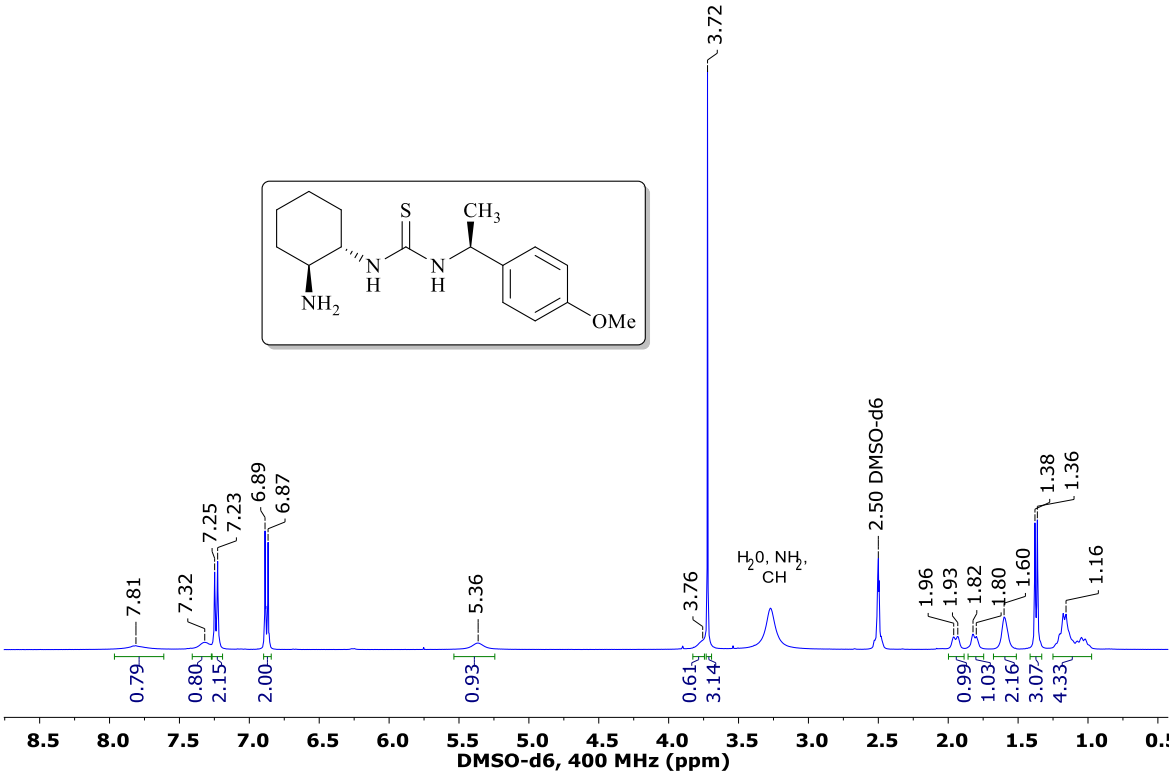
^{13}C NMR spectrum of compound **G**.



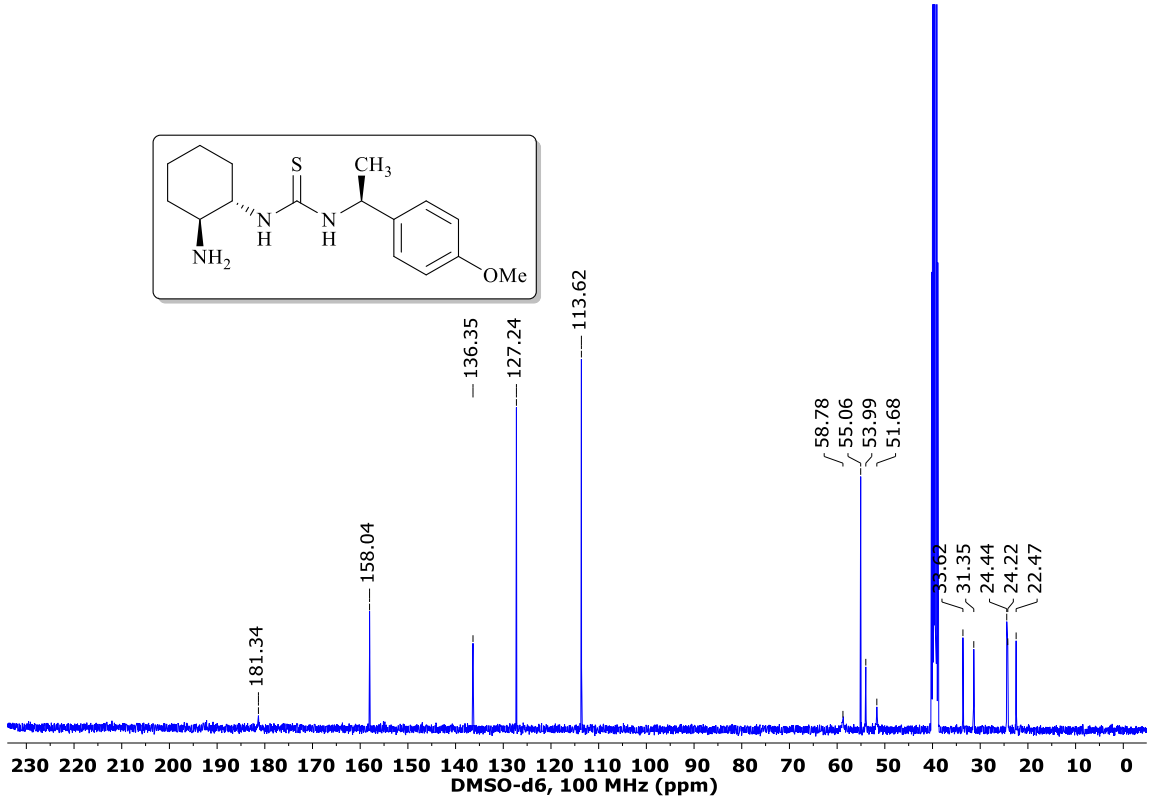
^{1}H NMR spectrum of compound **A(OMe)**.



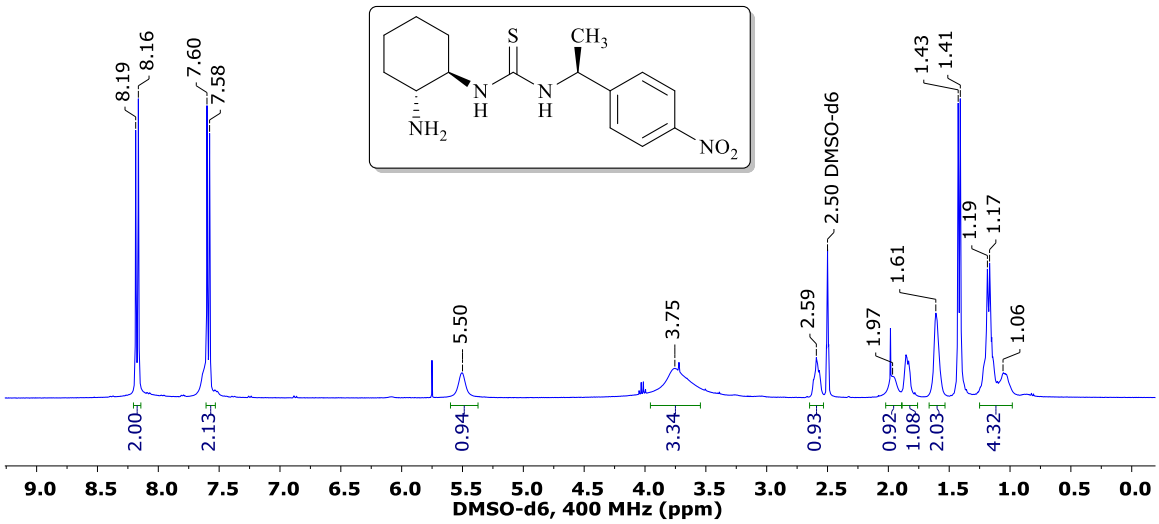
^{13}C NMR spectrum of compound **A(OMe)**.



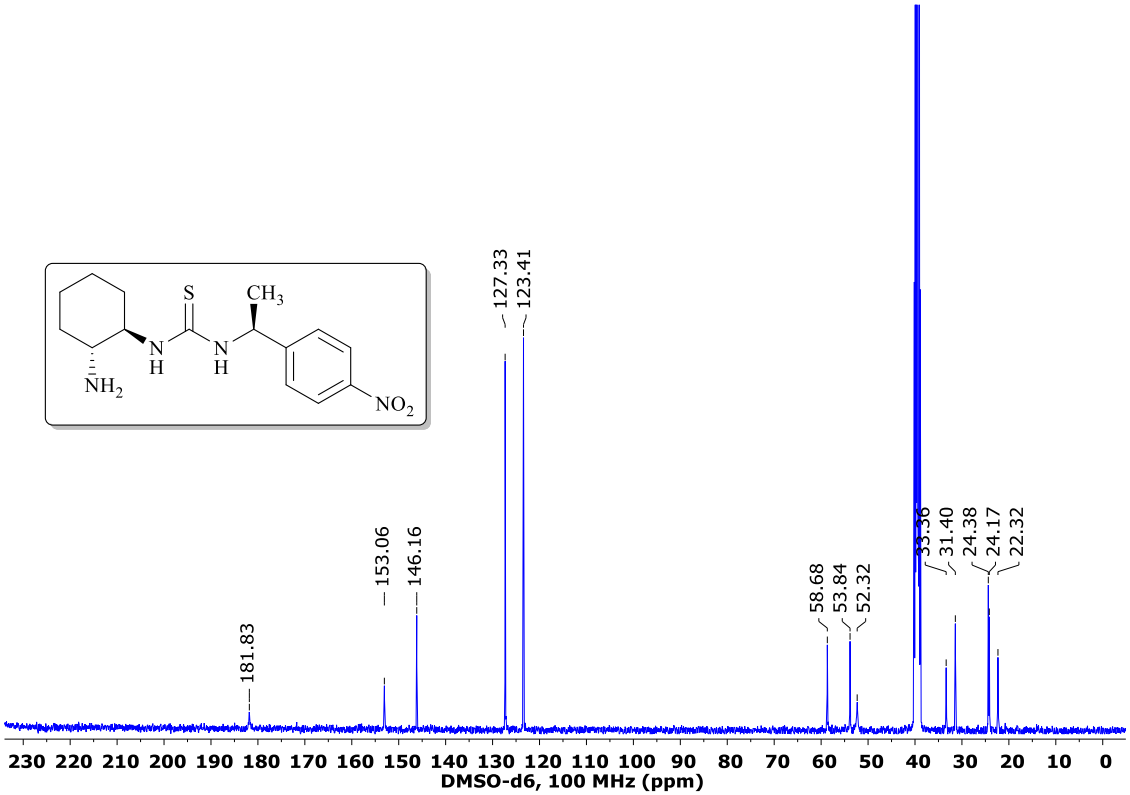
^{1}H NMR spectrum of compound **B(OMe)**.



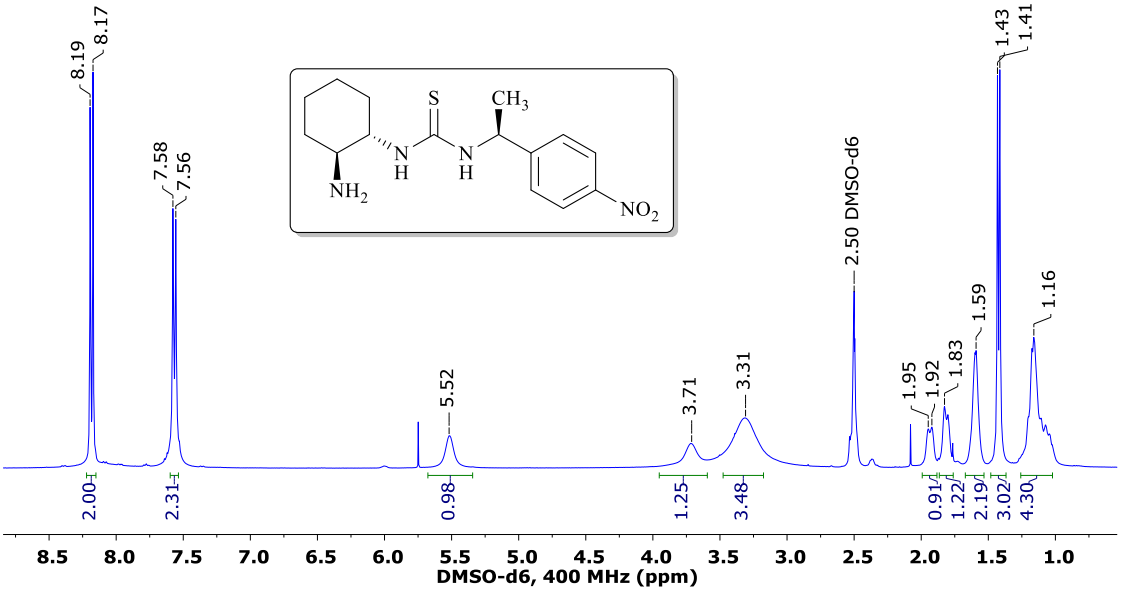
^{13}C NMR spectrum of compound **B(OMe)**.



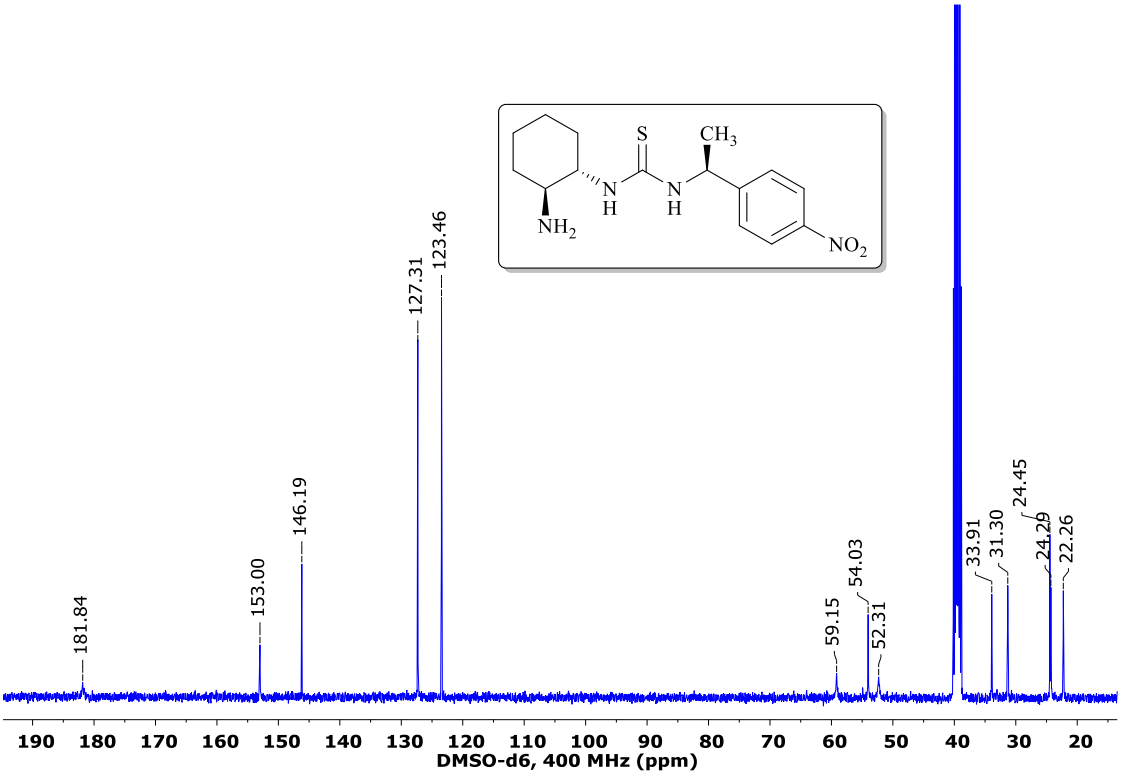
^{1}H NMR spectrum of compound **A(NO$_2$)**.



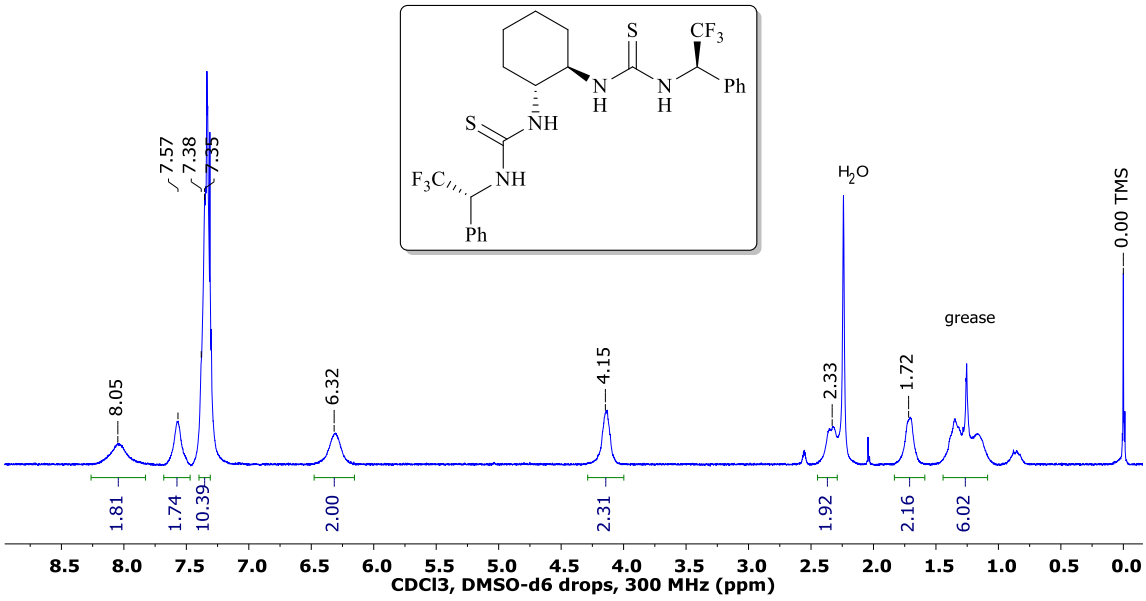
^{13}C NMR spectrum of compound **A(NO$_2$)**.



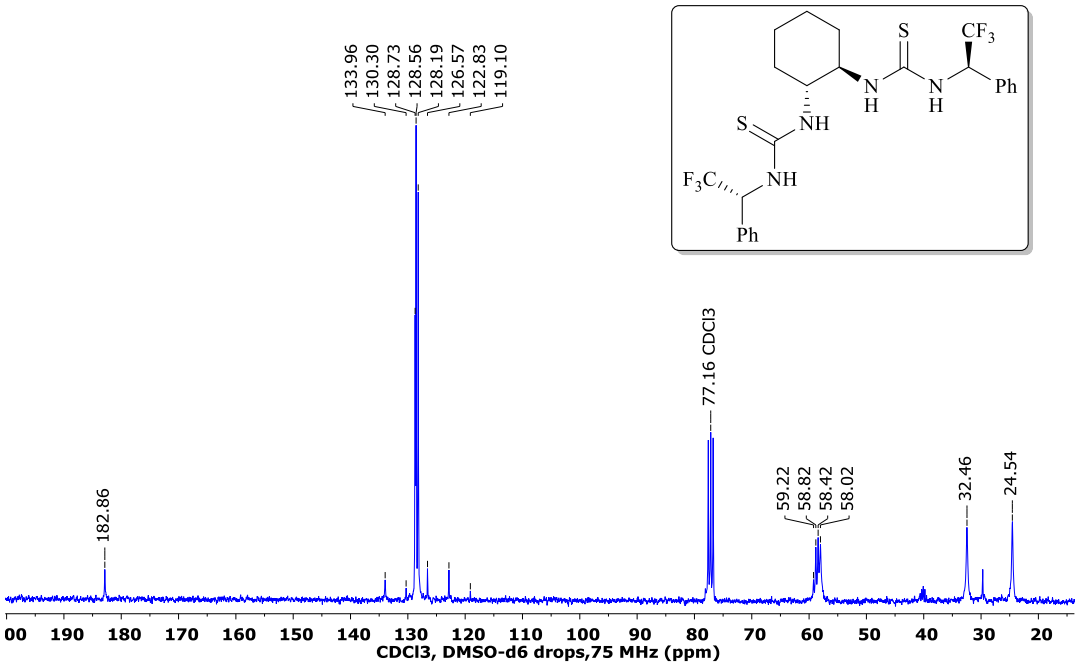
^{1}H NMR spectrum of compound **B(NO$_2$)**.



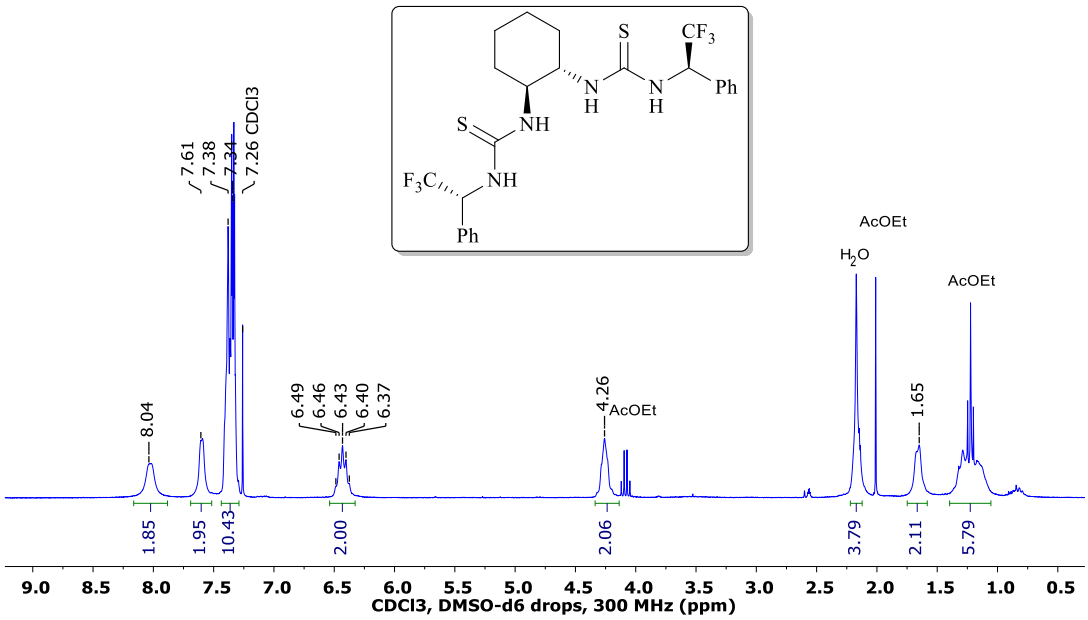
^{13}C NMR spectrum of compound **B(NO$_2$)**.



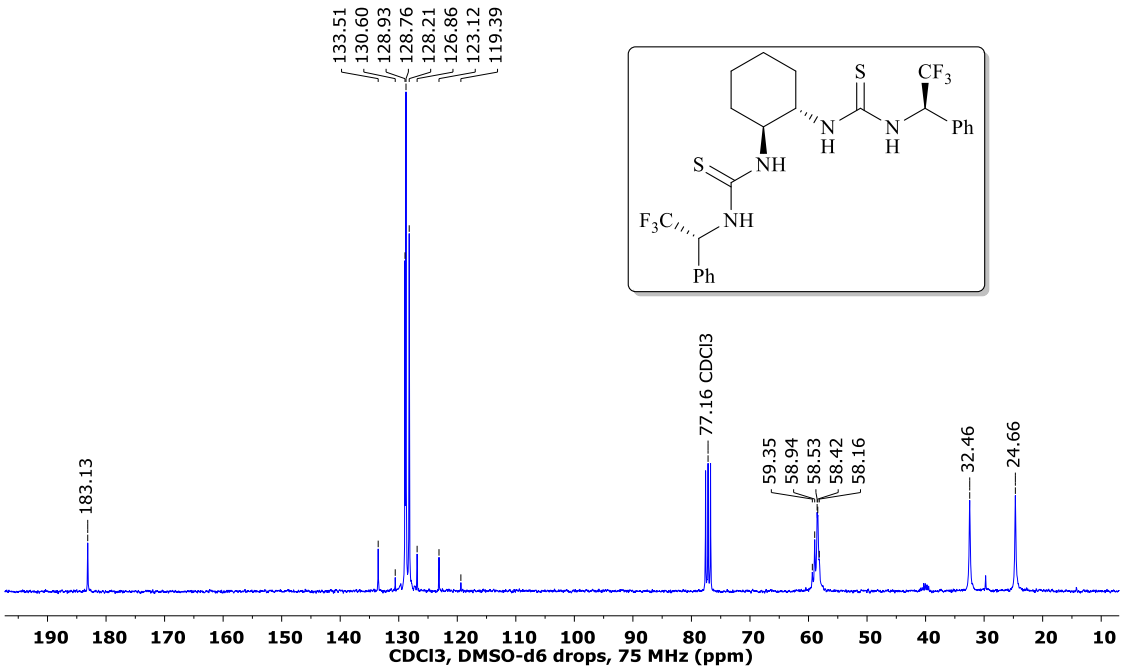
^{1}H NMR spectrum of compound **K_F**.



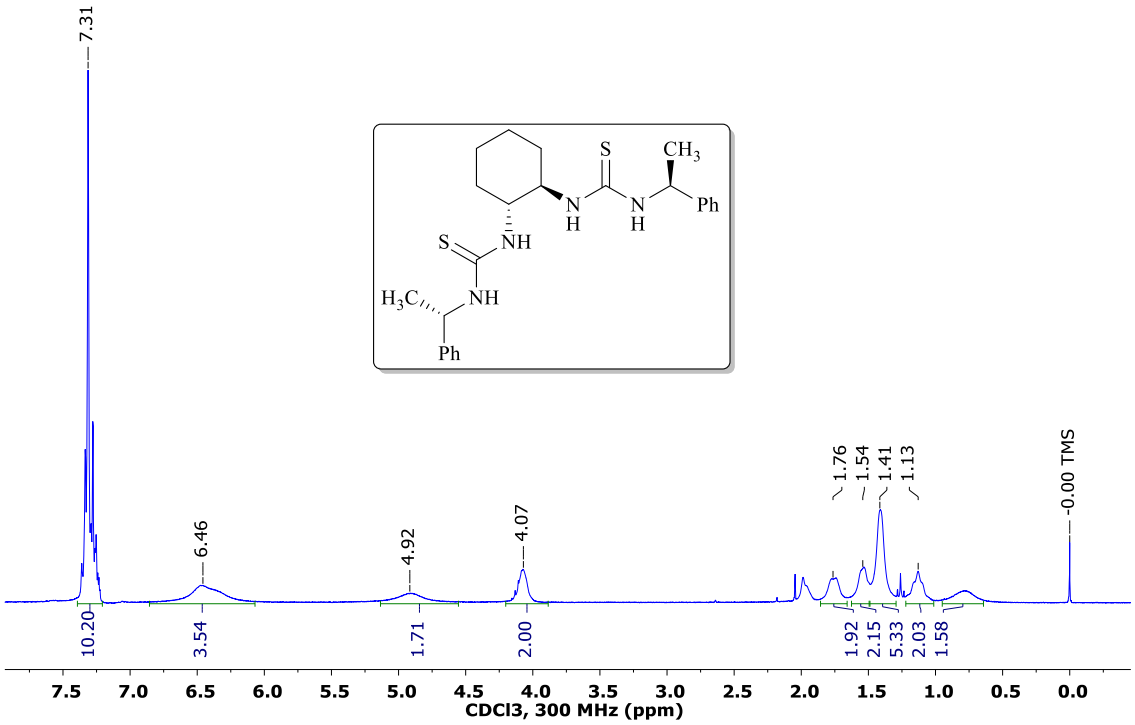
^{13}C NMR spectrum of compound **K_F**.



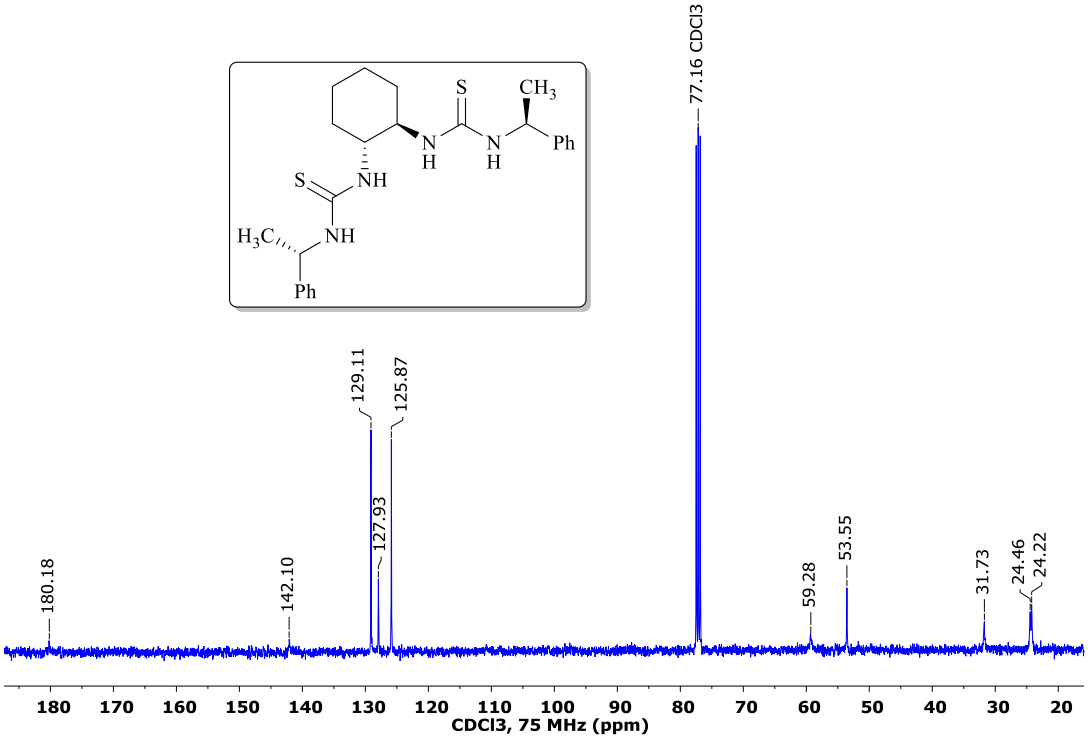
^{1}H NMR spectrum of compound **L_F**.



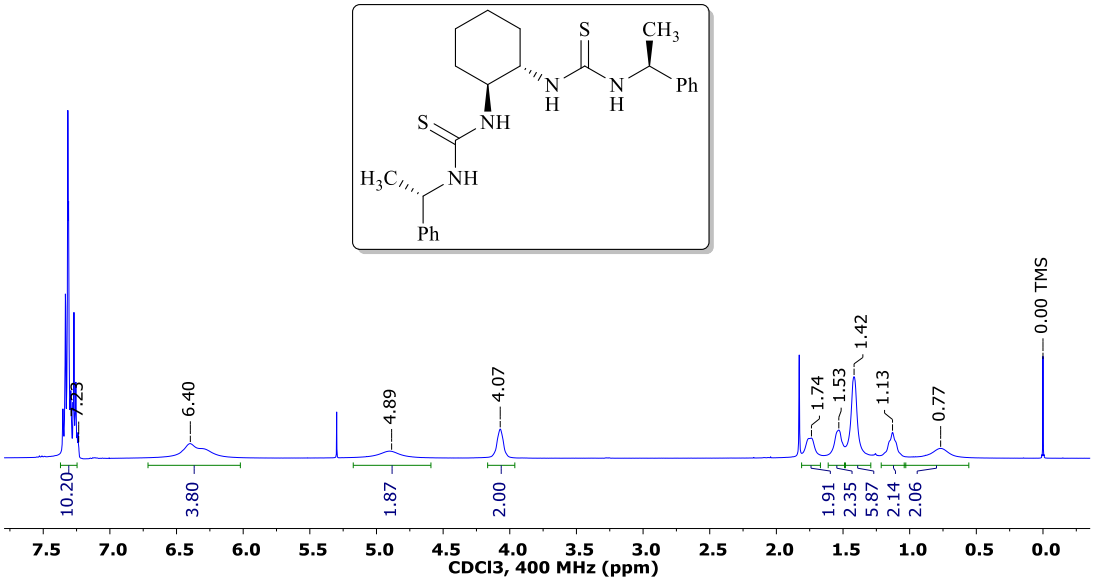
^{13}C NMR spectrum of compound **L_F**.



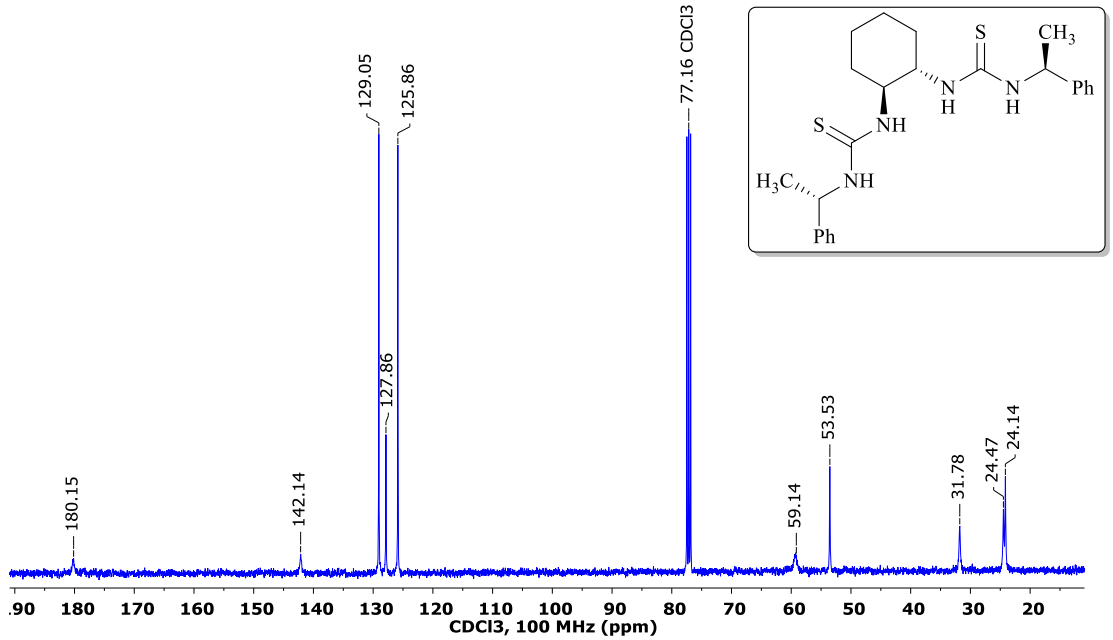
^{1}H NMR spectrum of compound **K**.



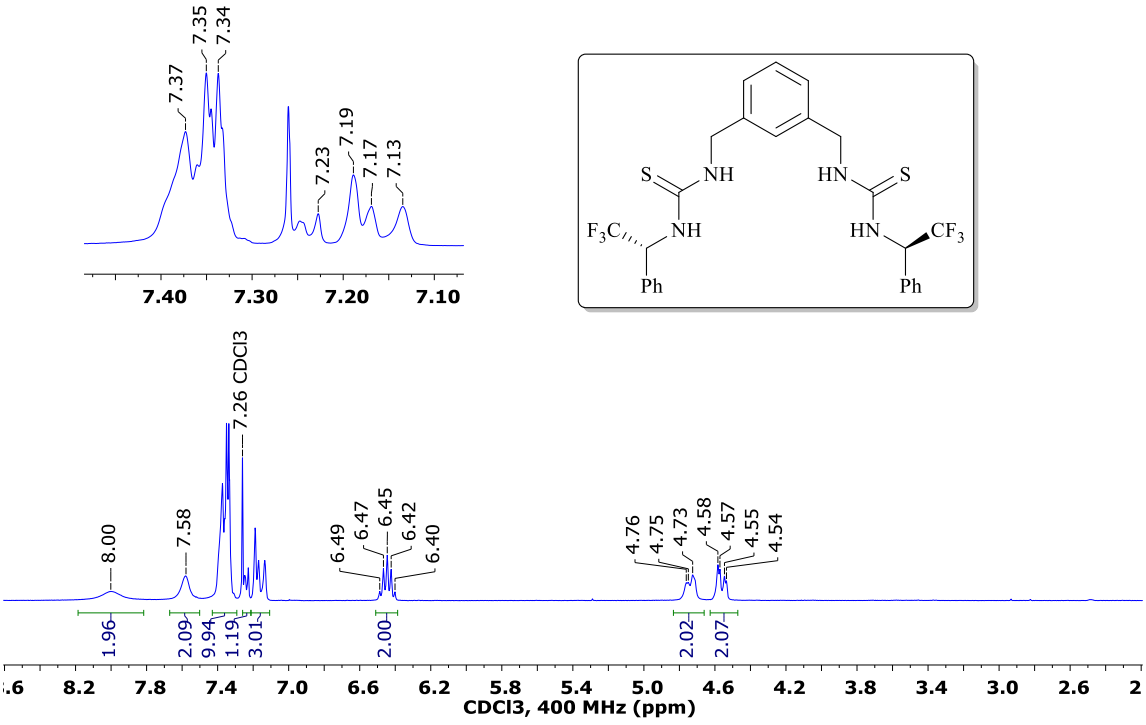
^{13}C NMR spectrum of compound **K**.



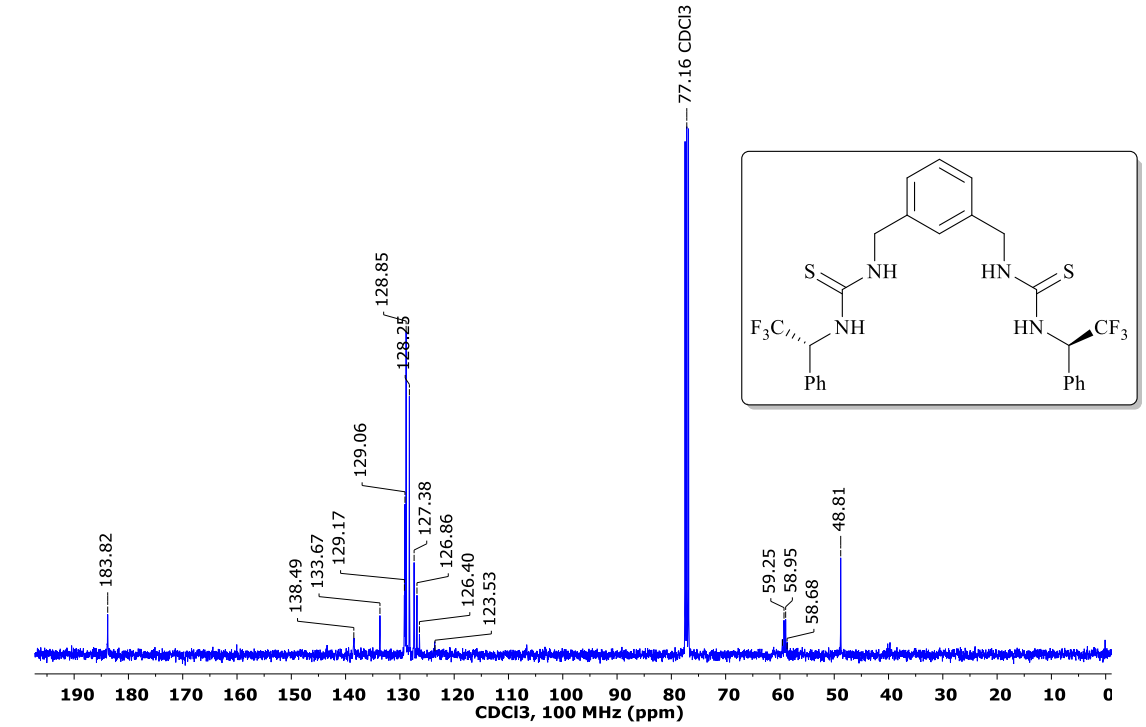
^{1}H NMR spectrum of compound **L**.



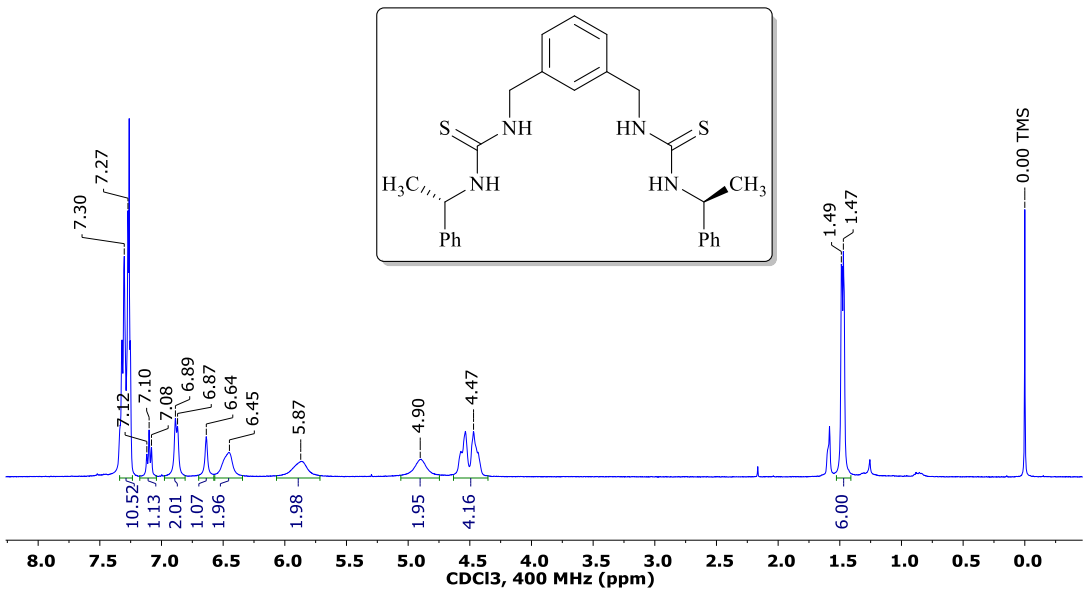
^{13}C NMR spectrum of compound **L**.



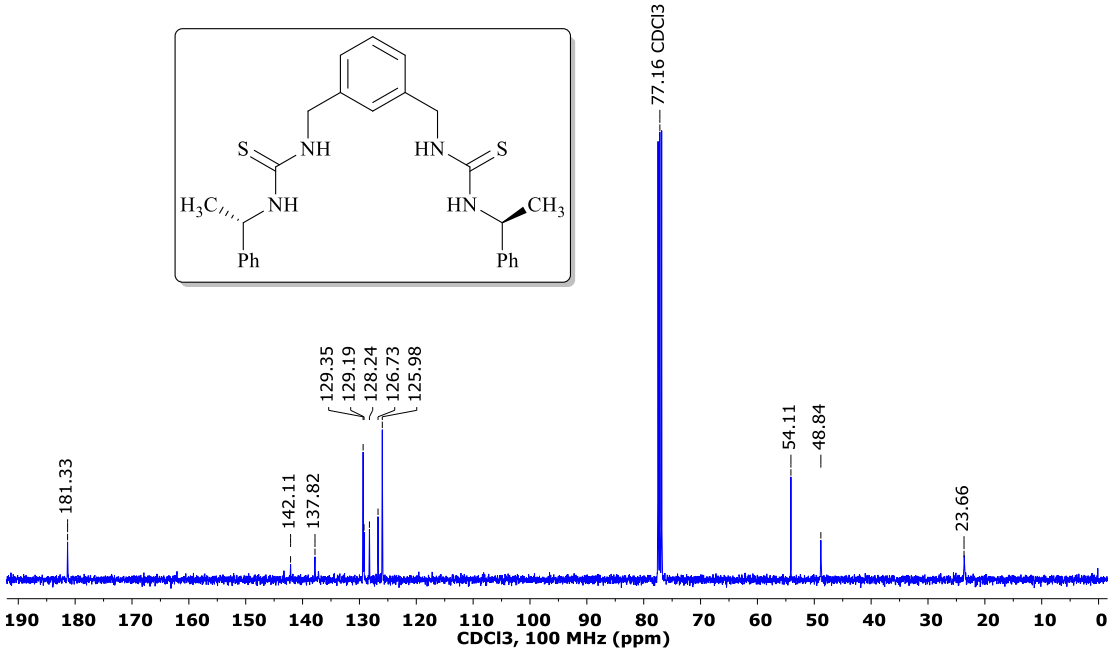
^{1}H NMR spectrum of compound **M_F**.



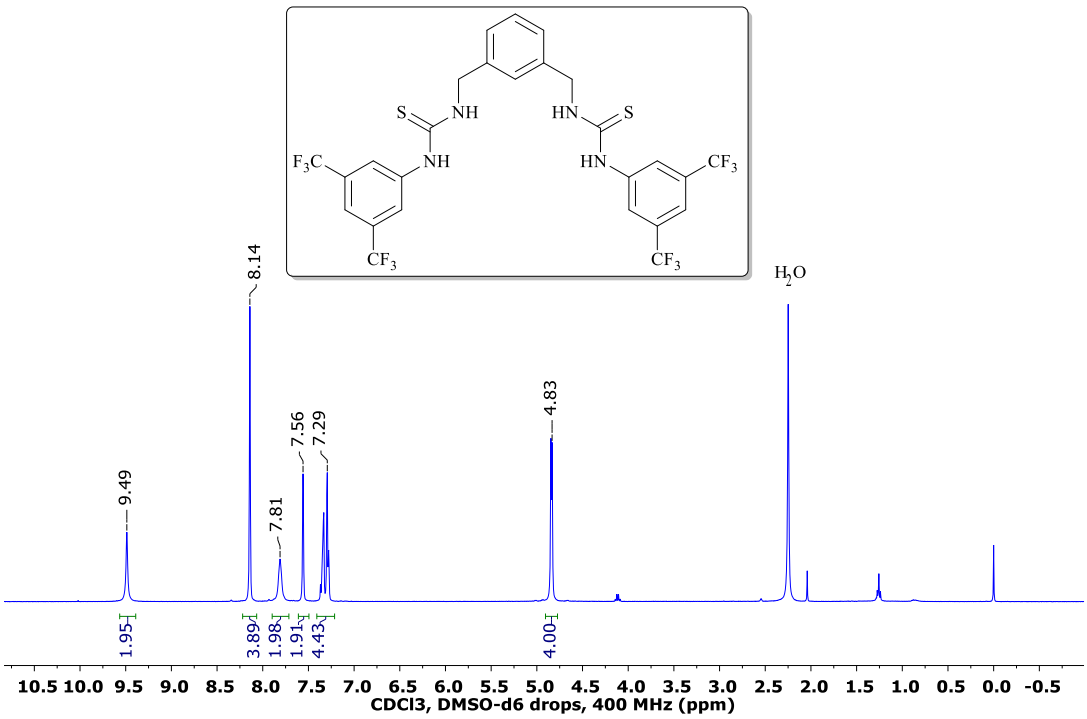
^{13}C NMR spectrum of compound **M_F**.



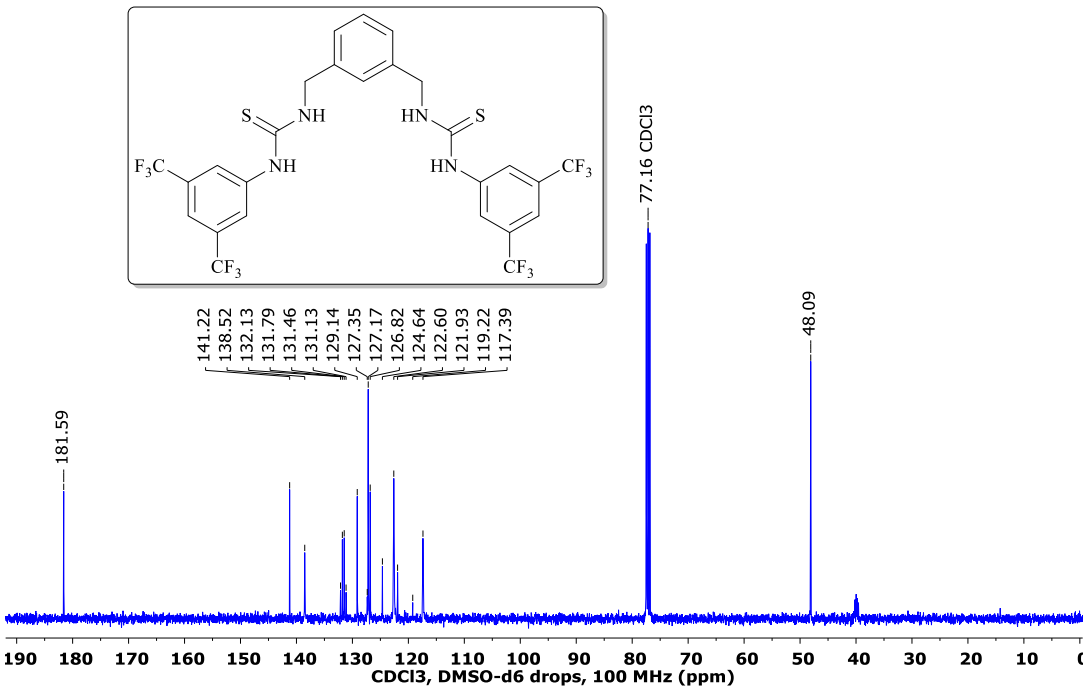
^{1}H NMR spectrum of compound **M**.



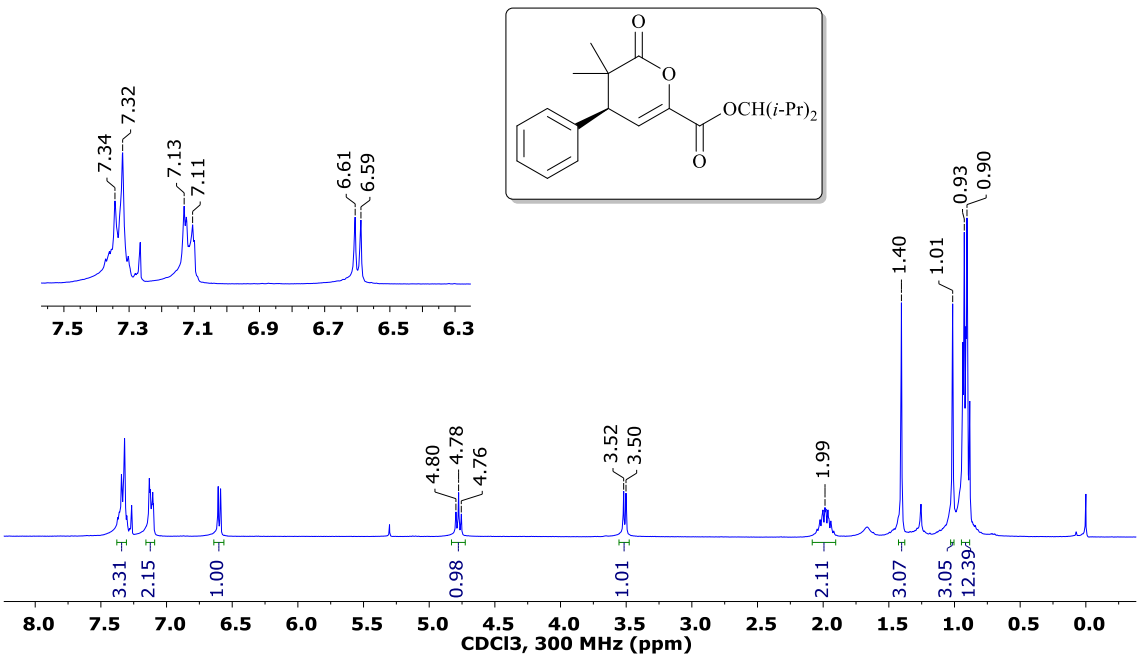
^{13}C NMR spectrum of compound **M**.



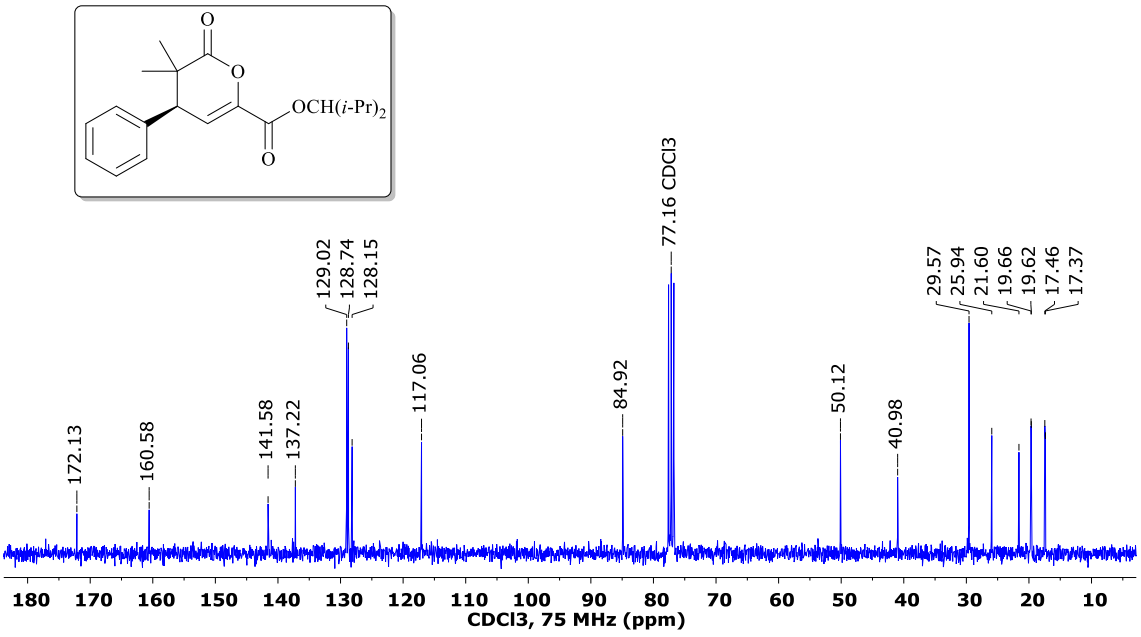
^{1}H NMR spectrum of compound **N**.



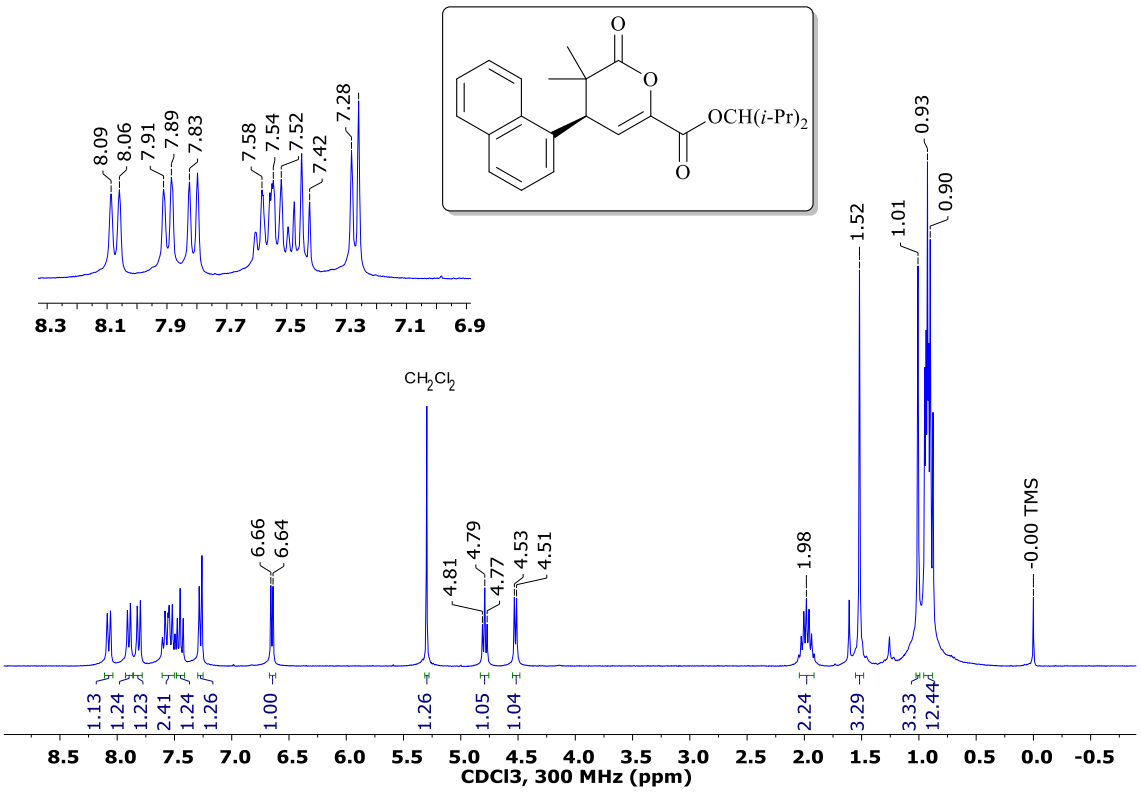
^{13}C NMR spectrum of compound **N**.



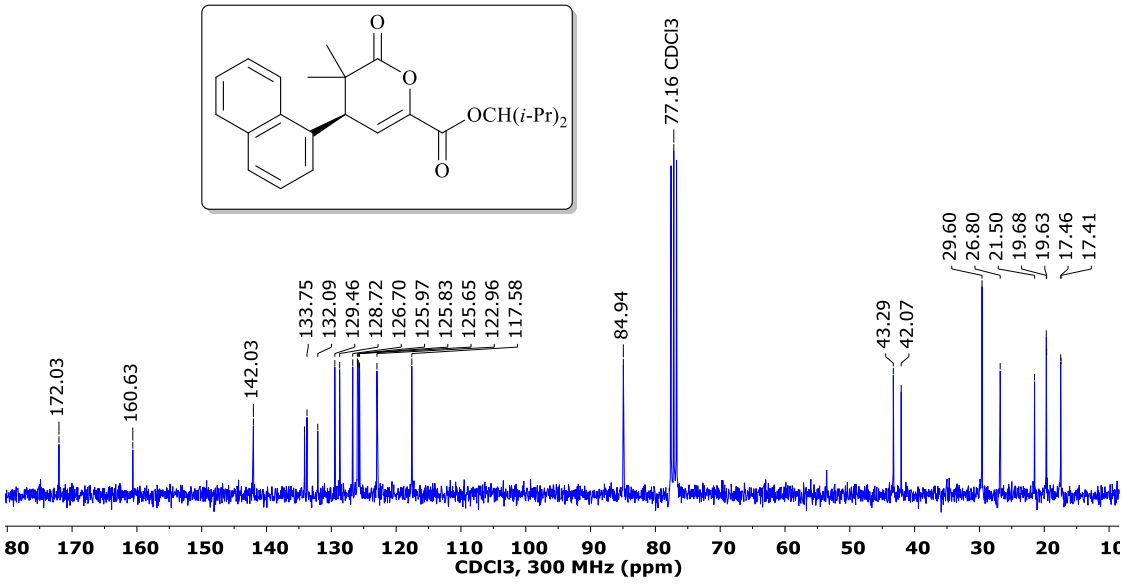
^{1}H NMR spectrum of compound **3ea**.



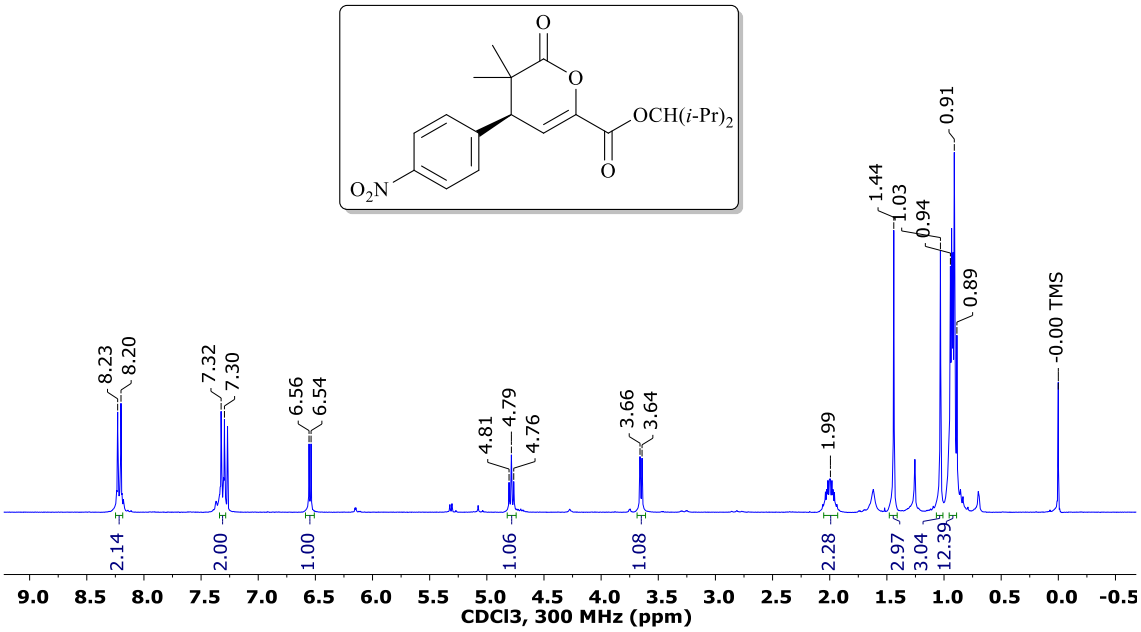
^{13}C NMR spectrum of compound **3ea**.



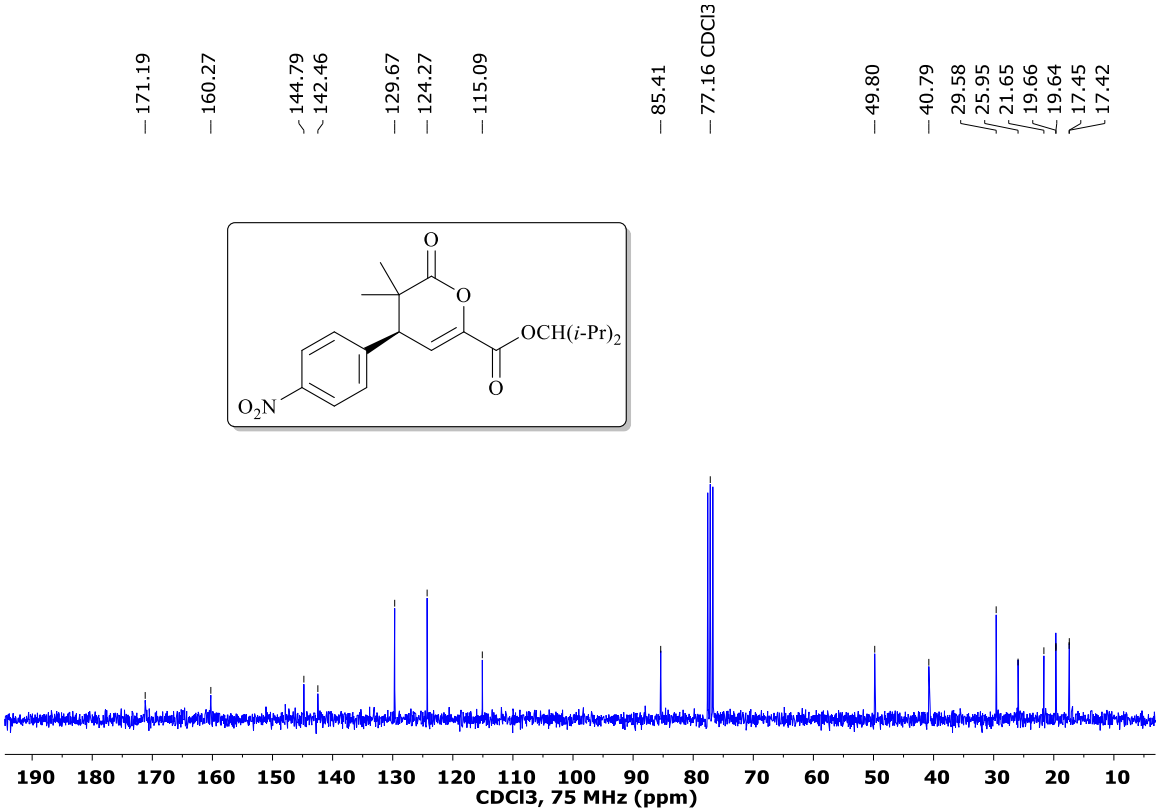
^{1}H NMR spectrum of compound **3eb**.



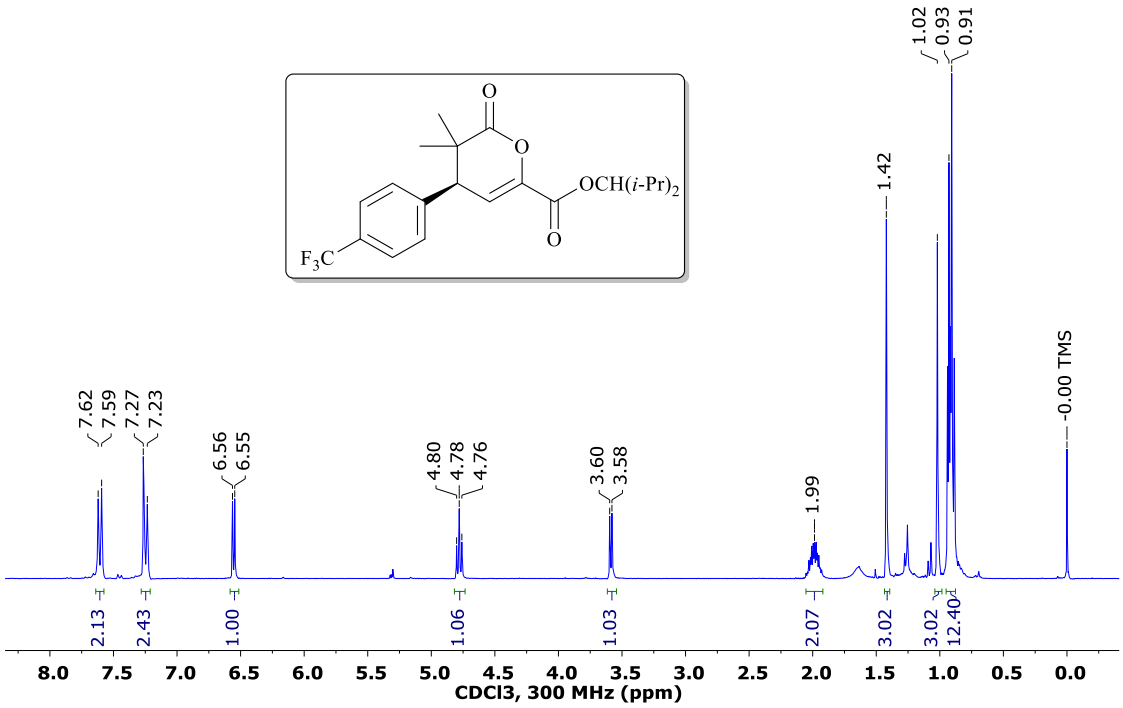
^{13}C NMR spectrum of compound **3eb**.



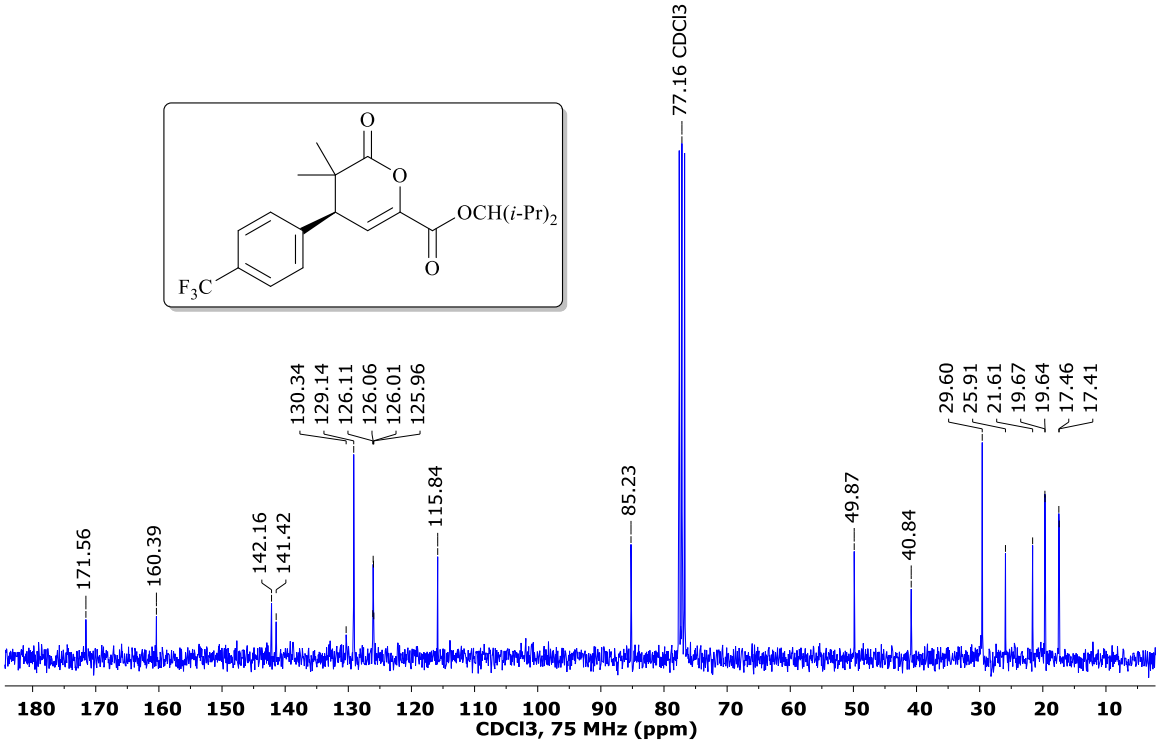
^{1}H NMR spectrum of compound **3ec**.



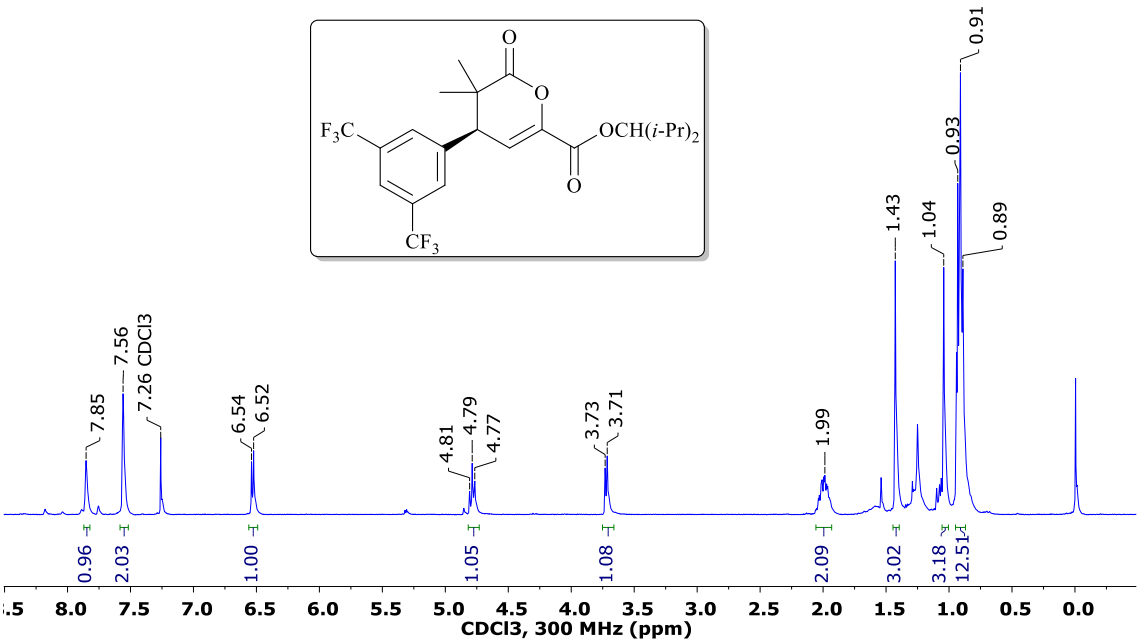
^{13}C NMR spectrum of compound **3ec**.



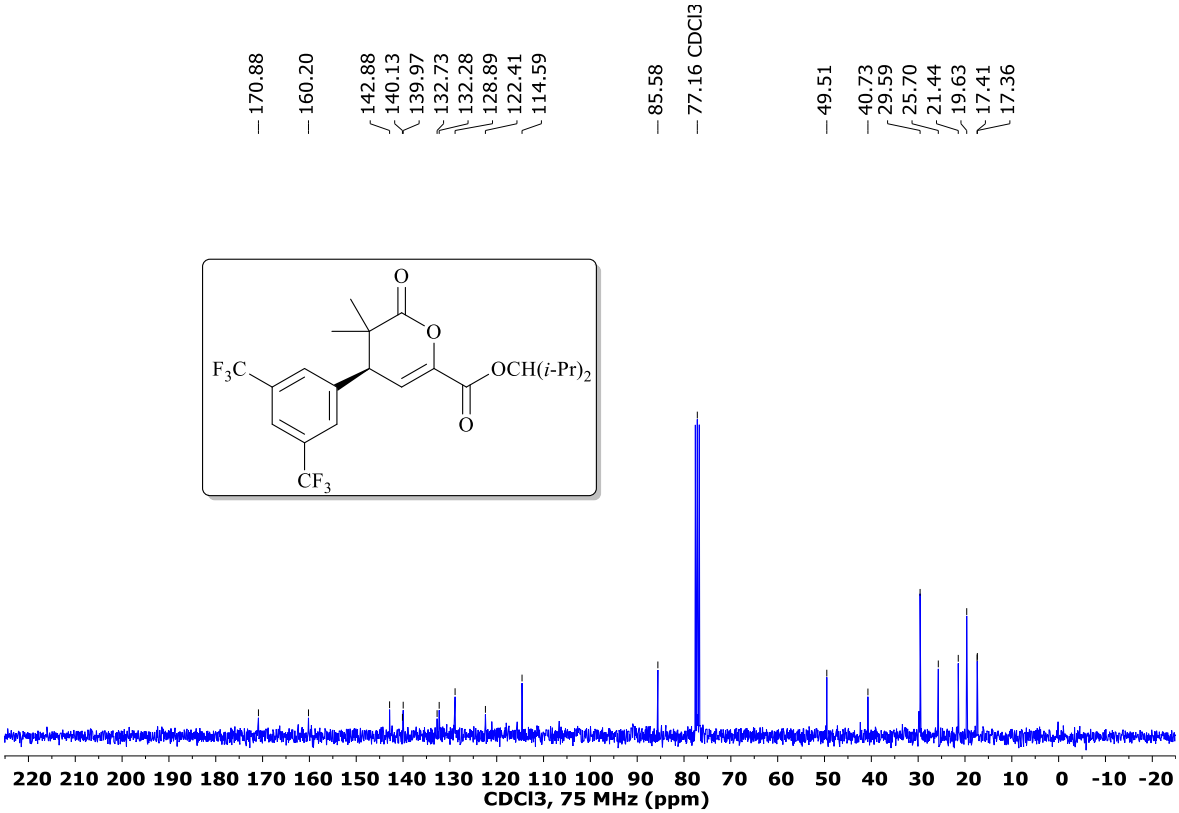
^{1}H NMR spectrum of compound **3ed**.



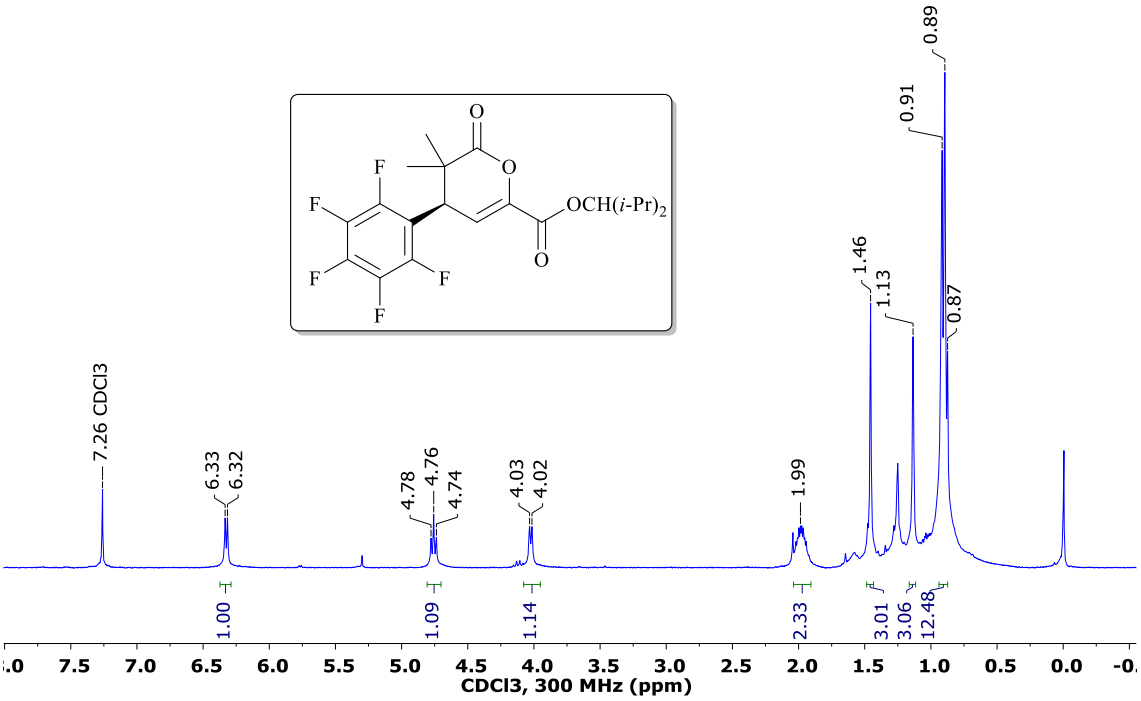
^{13}C NMR spectrum of compound **3ed**.



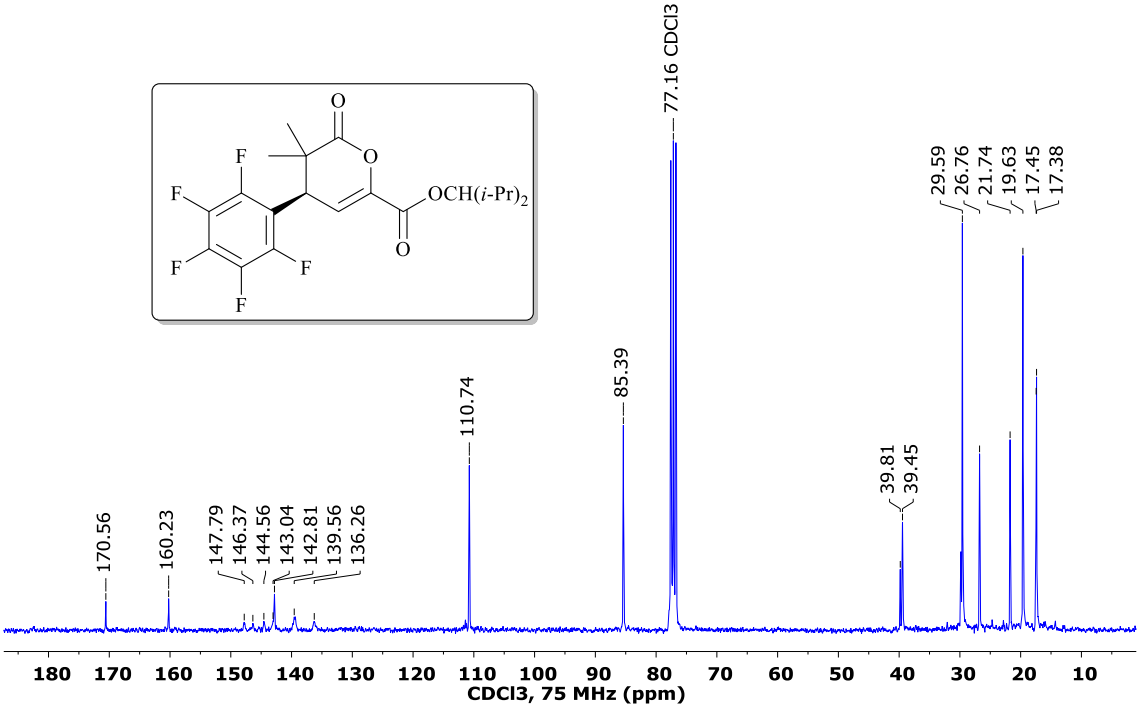
^{1}H NMR spectrum of compound **3ee**.



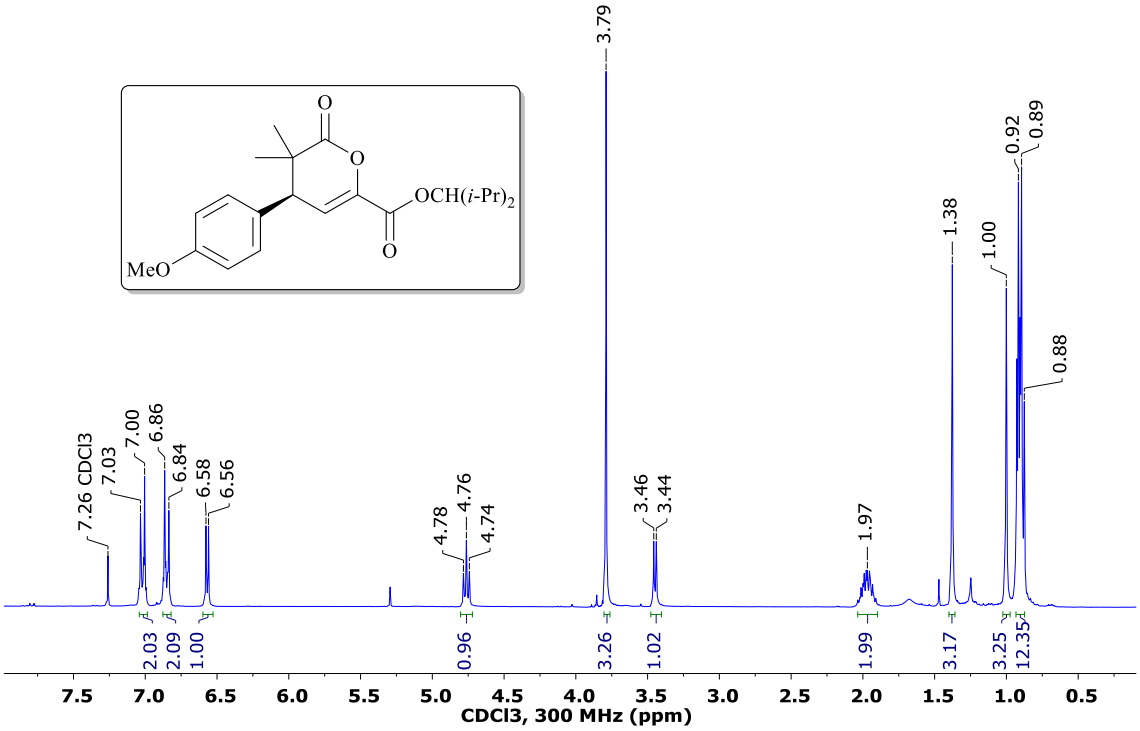
^{13}C NMR spectrum of compound **3ee**.



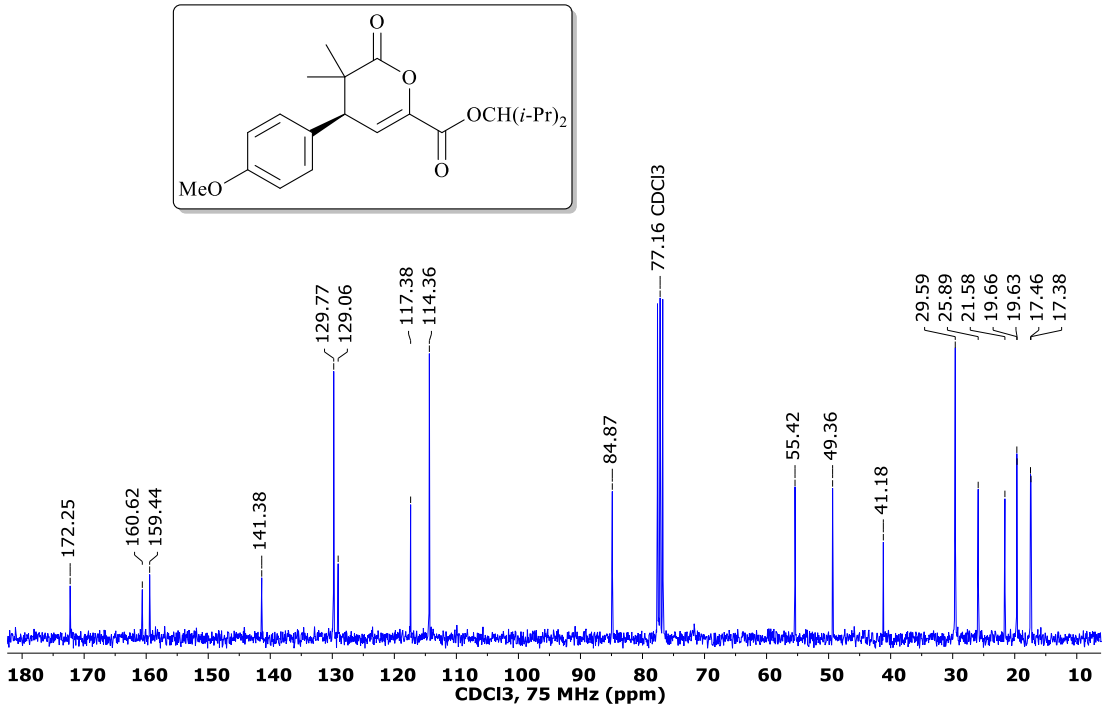
^{1}H NMR spectrum of compound **3ef**.



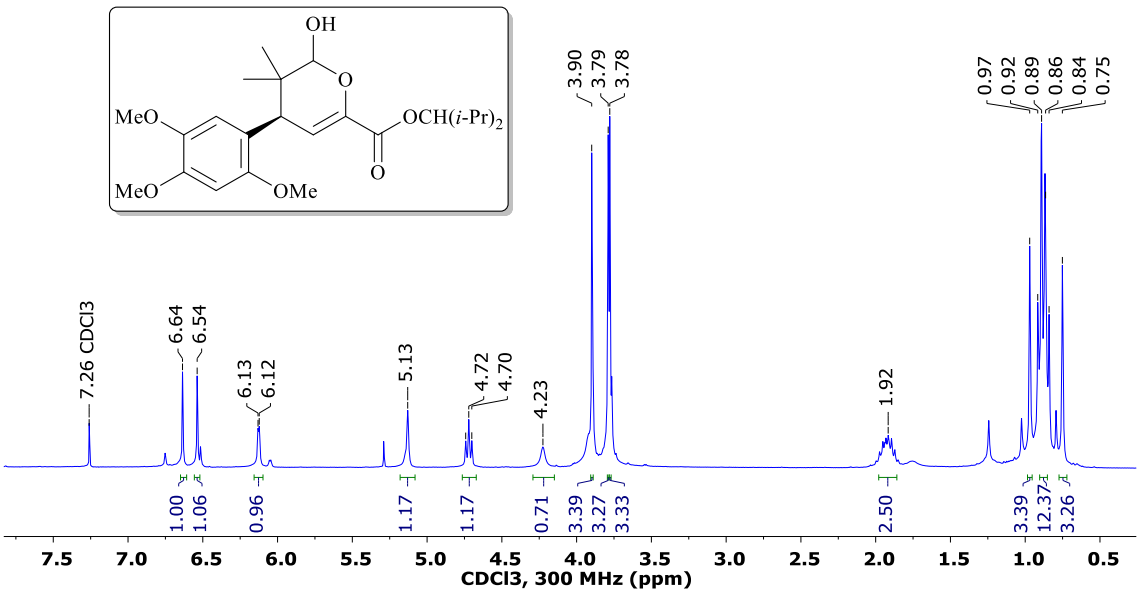
^{13}C NMR spectrum of compound **3ef**.



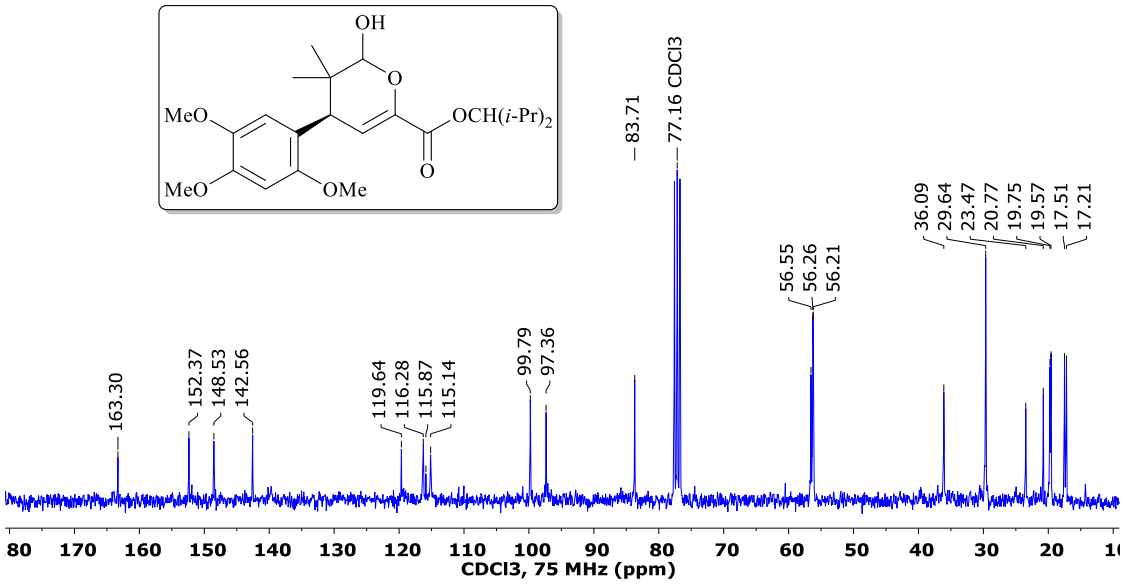
^{1}H NMR spectrum of compound **3eg**.



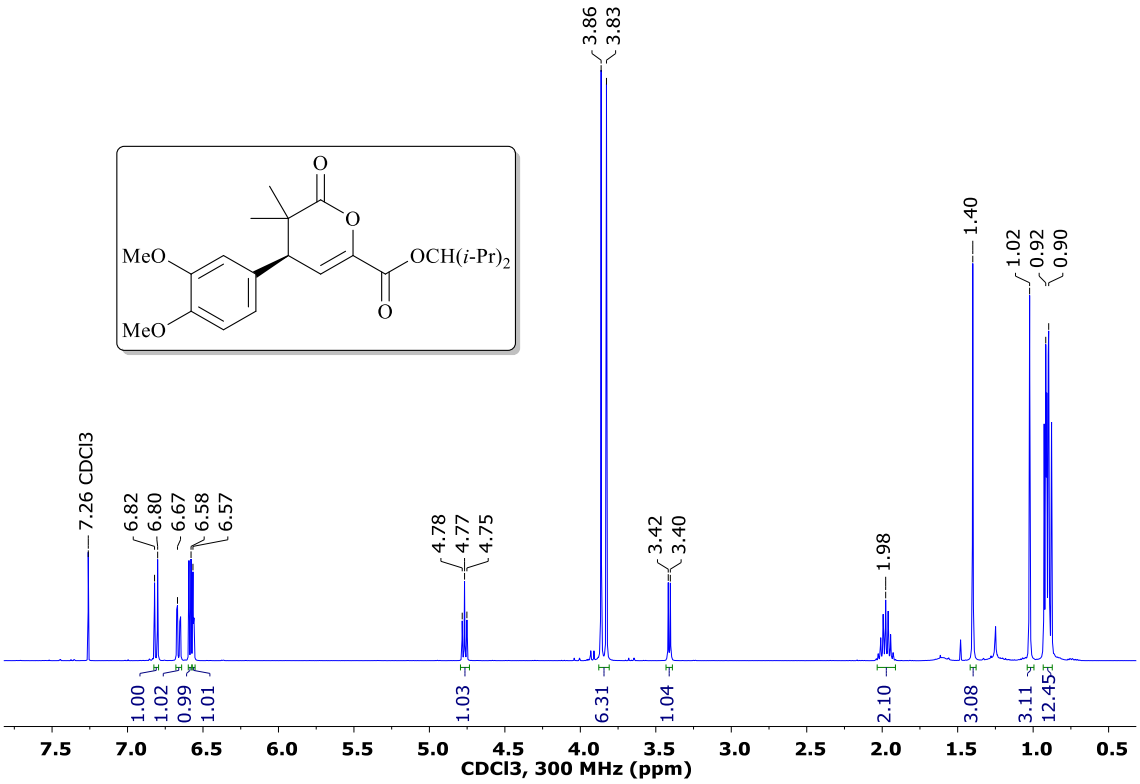
^{13}C NMR spectrum of compound **3eg**.



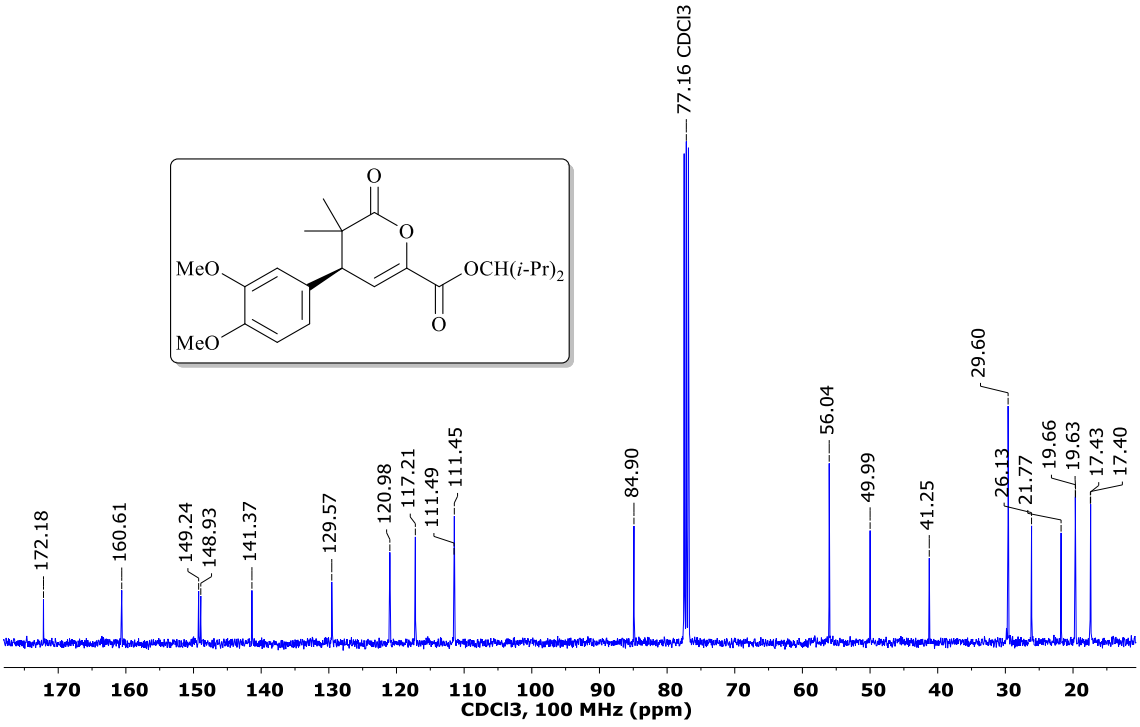
^{1}H NMR spectrum of compound **3eh**.



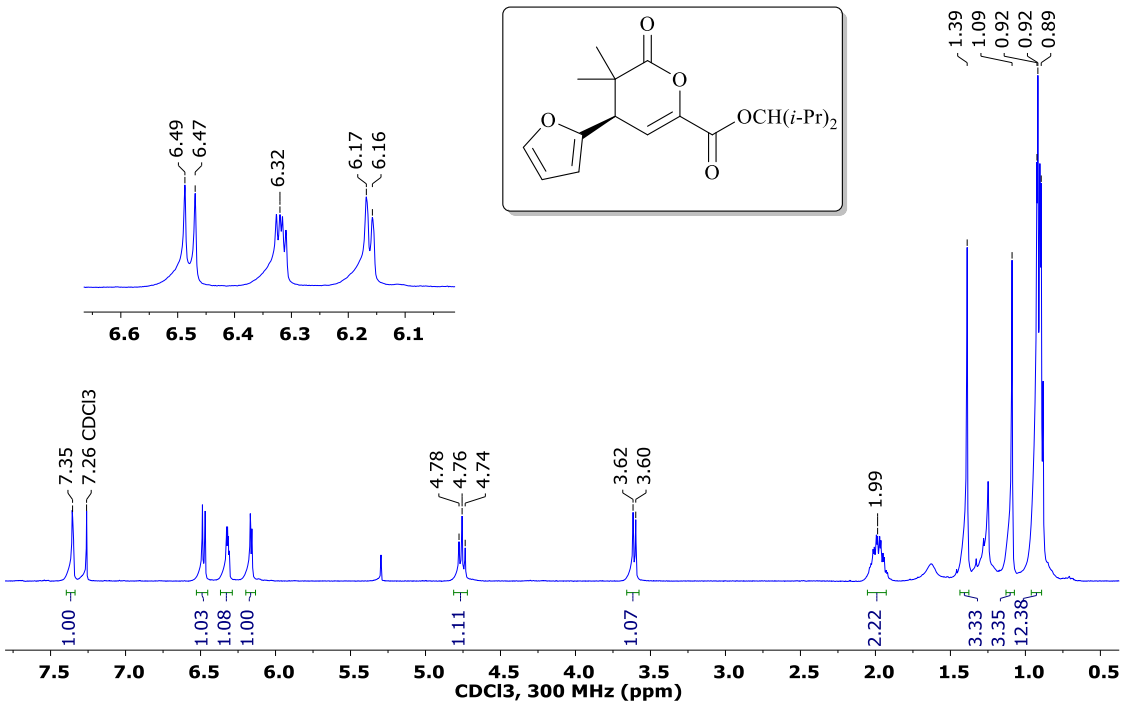
^{13}C NMR spectrum of compound **3eh**.



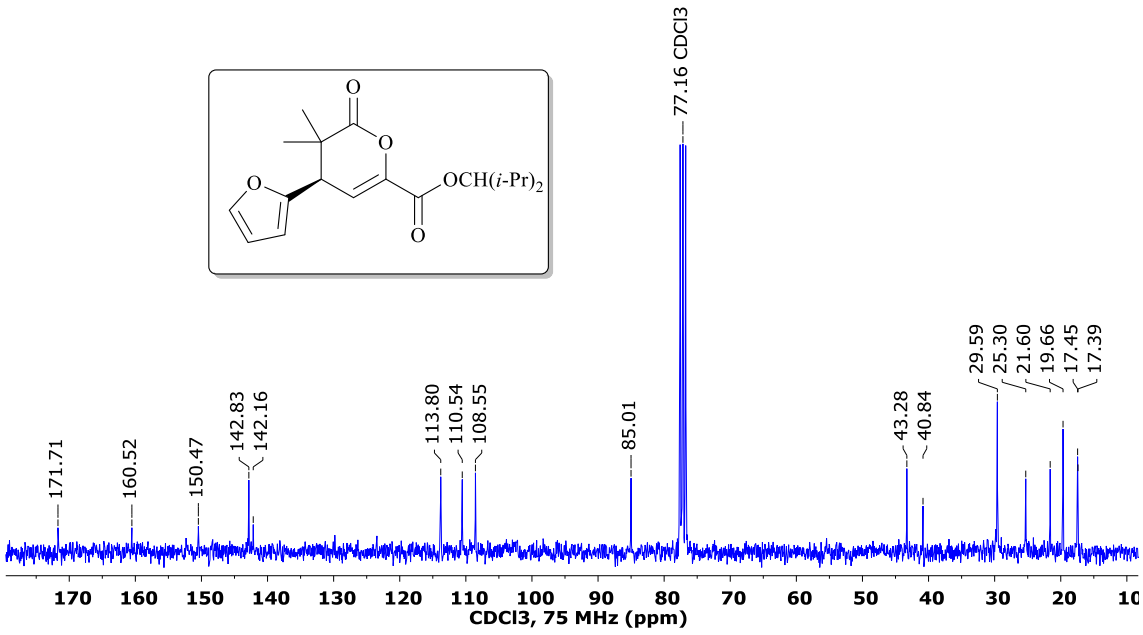
^{1}H NMR spectrum of compound **3ei**.



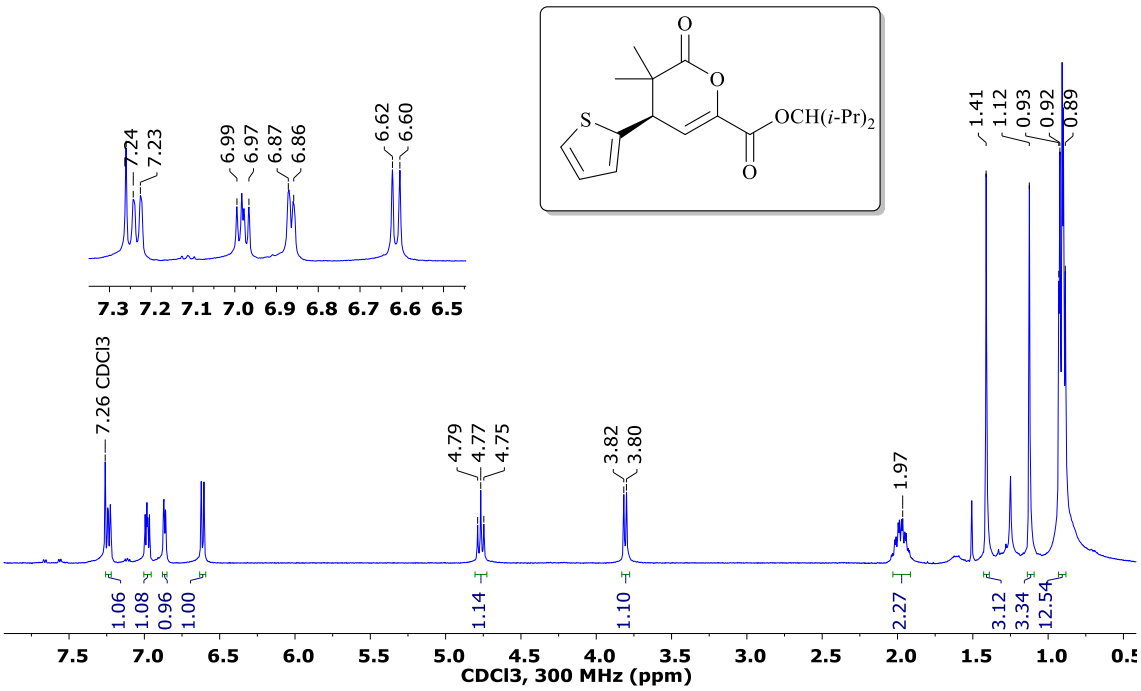
^{13}C NMR spectrum of compound **3ei**.



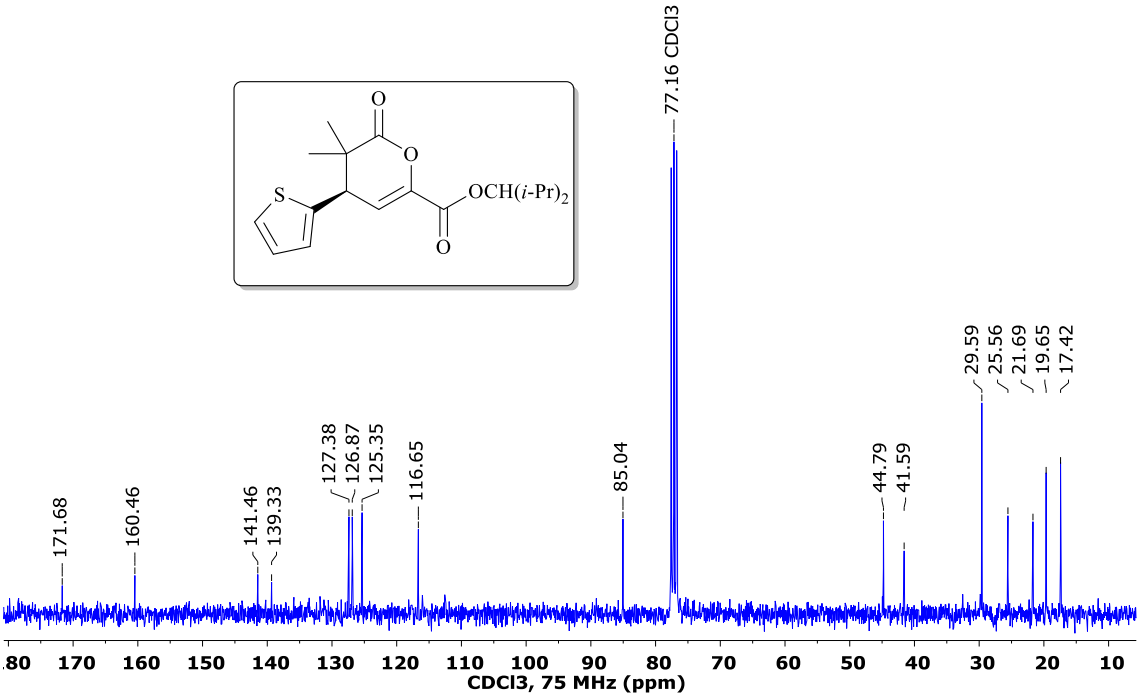
^{1}H NMR spectrum of compound **3ej**.



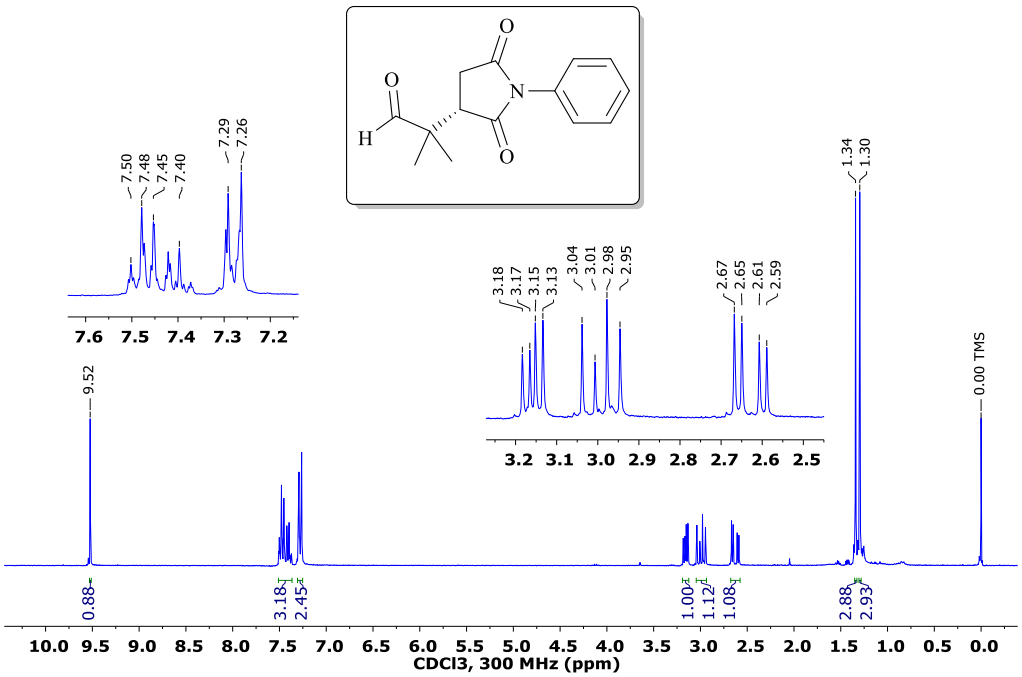
^{13}C NMR spectrum of compound **3ej**.



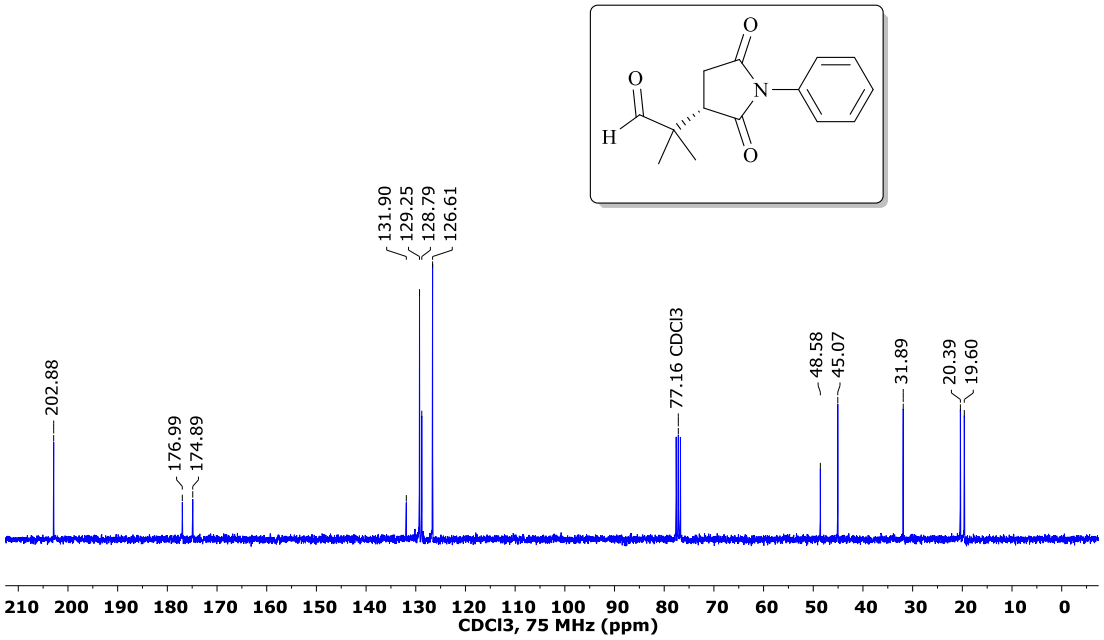
^{1}H NMR spectrum of compound **3ek**.



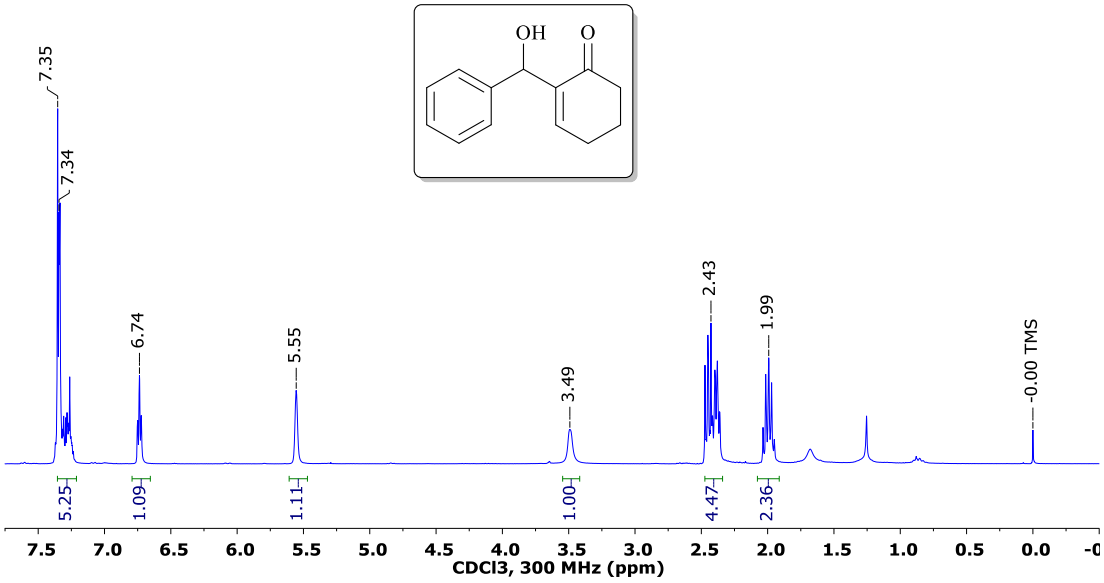
^{13}C NMR spectrum of compound **3ek**.



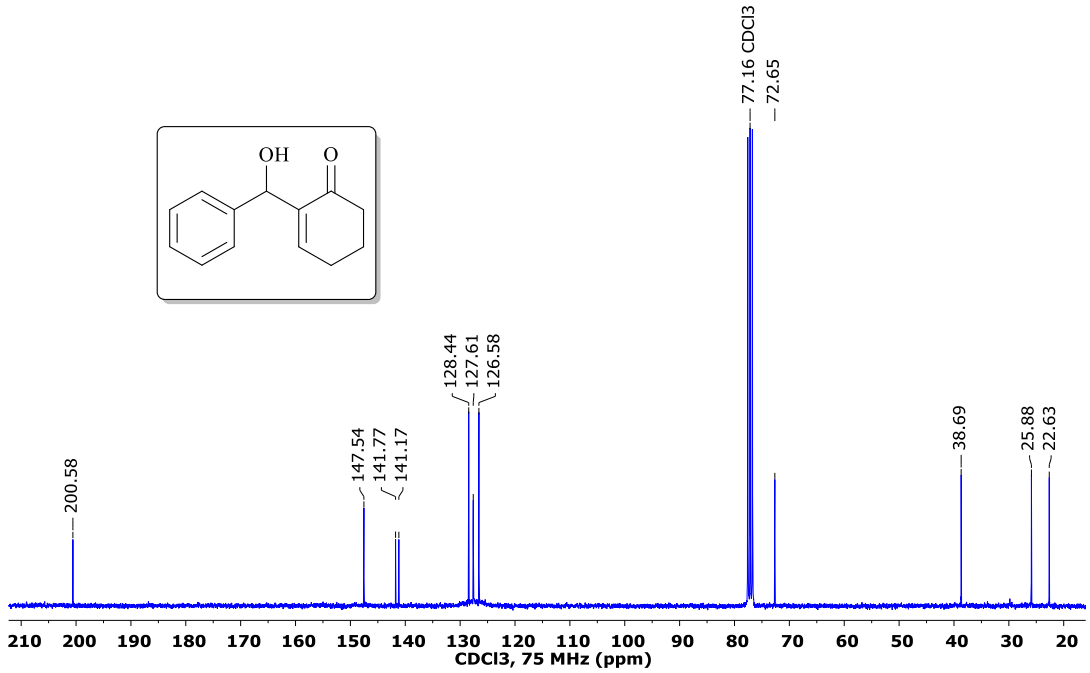
^{1}H NMR spectrum of compound **4**.



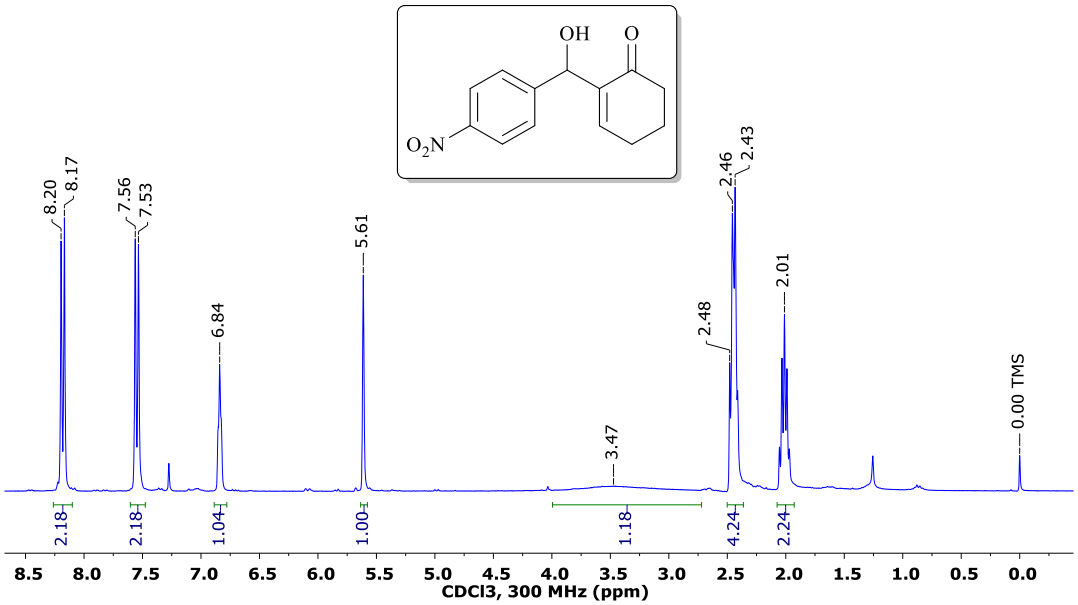
^{13}C NMR spectrum of compound **4**.



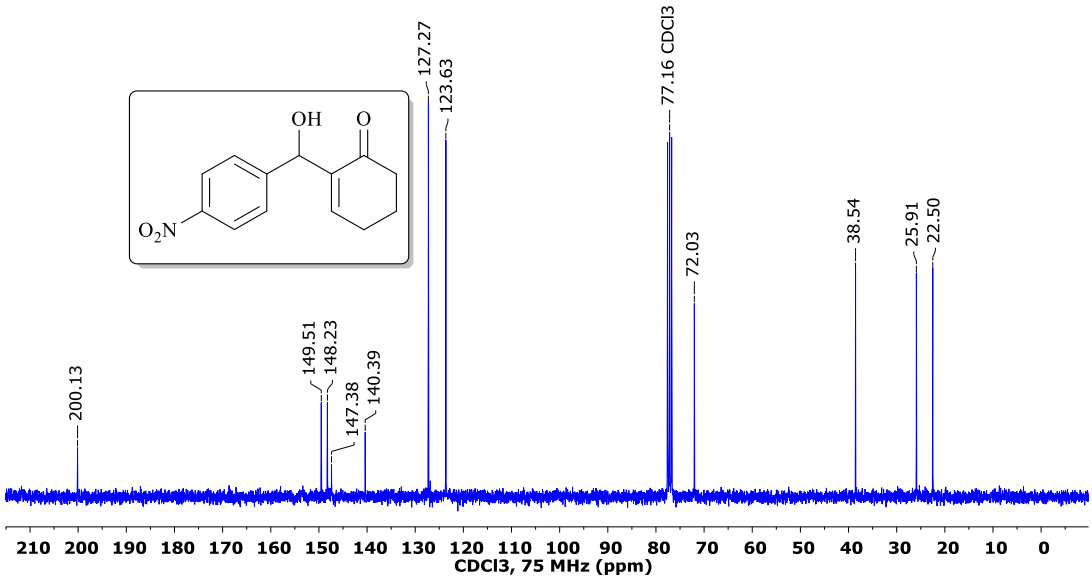
^{1}H NMR spectrum of compound **5a**.



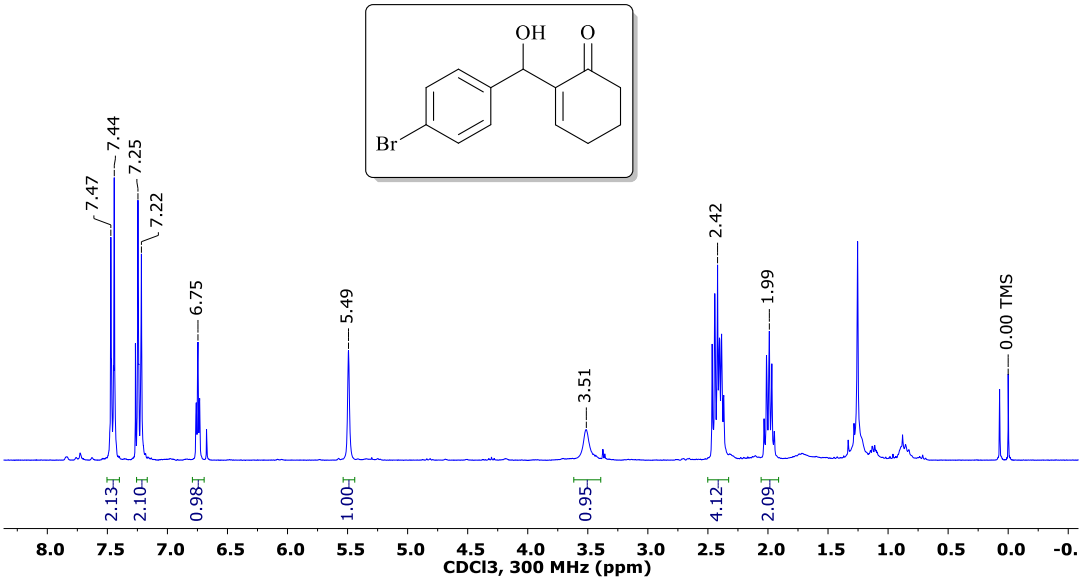
^{13}C NMR spectrum of compound **5a**.



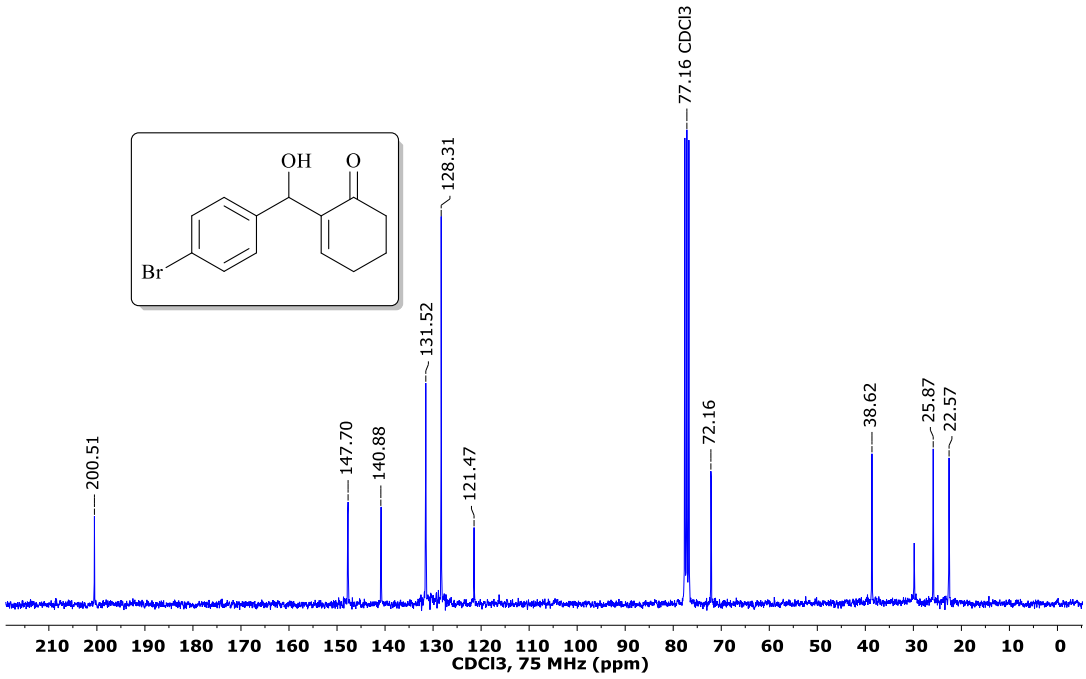
^{1}H NMR spectrum of compound **5b**.



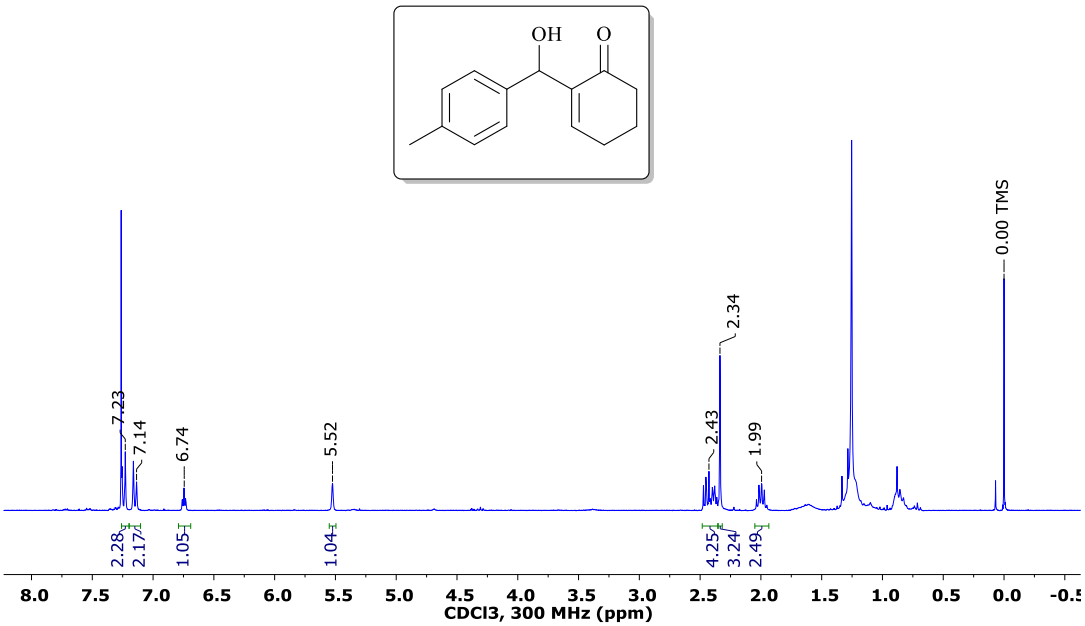
^{13}C NMR spectrum of compound 5**b**.



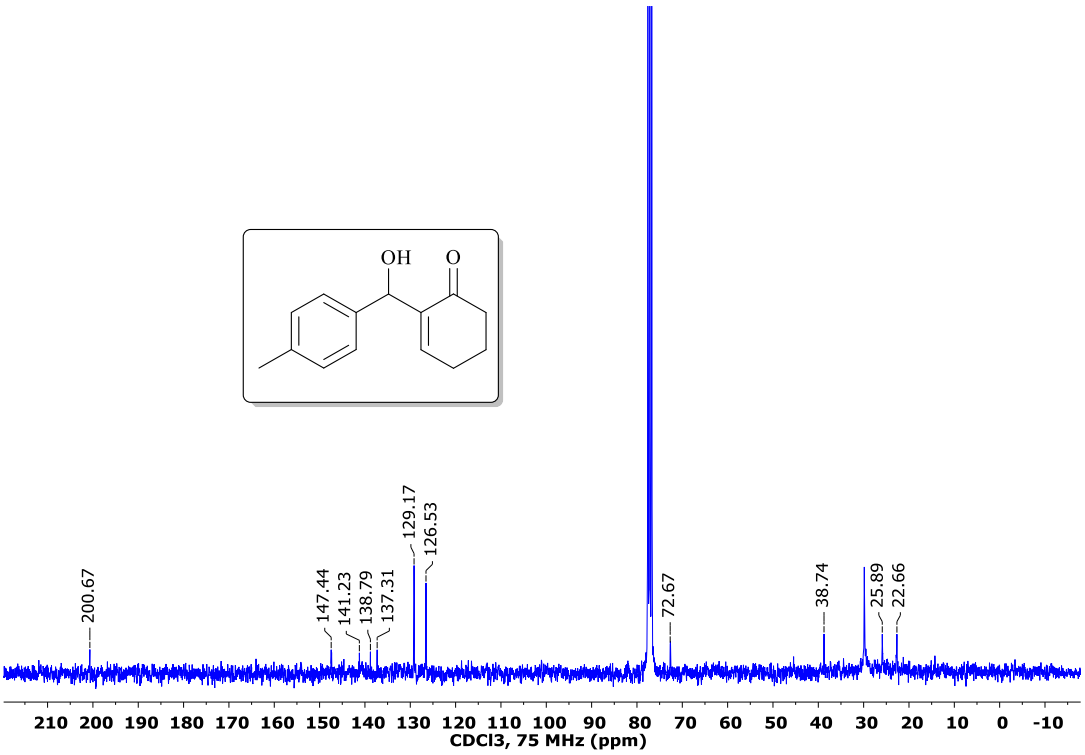
^{1}H NMR spectrum of compound **5c**.



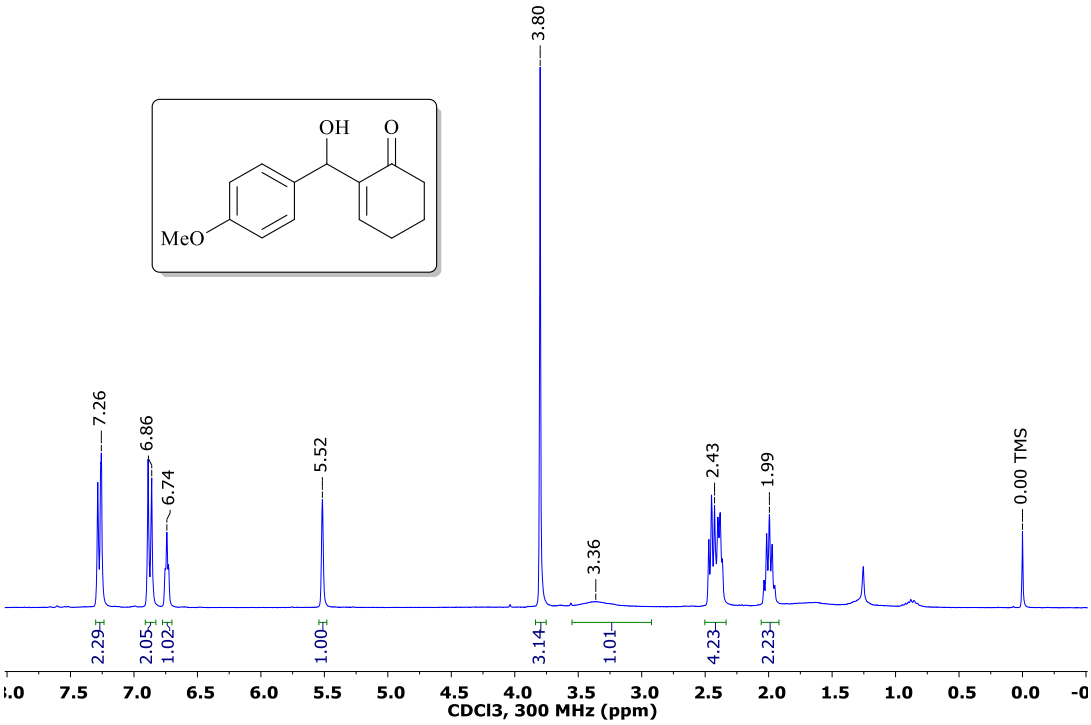
^{13}C NMR spectrum of compound **5c**.



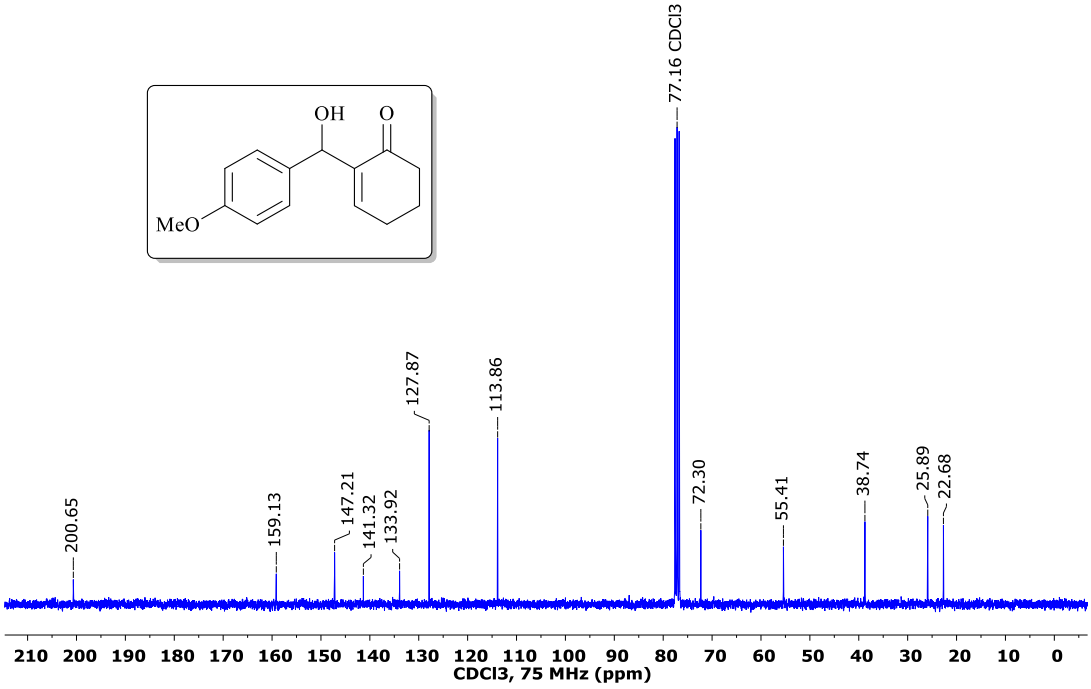
^{1}H NMR spectrum of compound **5d**.



^{13}C NMR spectrum of compound **5d**.



^{1}H NMR spectrum of compound **5e**.



^{13}C NMR spectrum of compound **5e**.

9 XYZ Coordinates and energies

Conformational analysis of reactant complexes [Gas-phase (B97D/TZVP)]

Methyl benzylidenepyruvate
Total Energy= -650.621988
Imaginary frequency= 0

XYZ coordinates

C	2.10783900	0.25671400	0.00051500
C	3.16697400	1.19083900	-0.00616500
C	2.42772900	-1.12035700	-0.01260800
C	4.49676400	0.76945400	-0.02550200
H	2.93091400	2.25385300	0.00435700
C	3.75483300	-1.53921300	-0.03195300
H	1.63012400	-1.85928200	-0.00686400
C	4.79484000	-0.59732100	-0.03852100
H	5.29944400	1.50408800	-0.03024400
H	3.98557200	-2.60264700	-0.04171200
H	5.83076100	-0.93040300	-0.05346300
C	0.74077700	0.75522100	0.02144200
H	0.62887300	1.84193200	0.03343000
C	-0.39972400	0.02359200	0.02746200
H	-0.39040700	-1.06259300	0.01875300
C	-1.71611800	0.68125900	0.04466500
O	-1.90412800	1.88850400	0.07144800
C	-2.92010300	-0.31973700	0.04050600
O	-2.79705100	-1.52236300	0.17413900
O	-4.08950400	0.32232300	-0.11883300
C	-5.27175500	-0.51982500	-0.11721500
H	-6.10997200	0.16489700	-0.26417000
H	-5.21489100	-1.25376300	-0.92984700
H	-5.35728900	-1.04754600	0.83996400

Isobutyraldehyde
Total Energy= -232.388583
Imaginary frequency= 0

XYZ coordinates

C	0.94891000	-0.60049900	0.20928200
H	1.02112600	-1.66909900	0.54187500
C	-0.42746400	0.01060200	0.41953300
C	-0.51451300	1.46720700	-0.04293800
H	-0.34668600	1.53271100	-1.12537600
H	-1.50717500	1.87725200	0.18188400
H	0.24613000	2.08405300	0.44932800
C	-1.48050000	-0.89303100	-0.26061400
H	-1.38856500	-1.93690700	0.06882700
H	-2.49044100	-0.54268900	-0.01547000
H	-1.36078200	-0.86206900	-1.35182000
O	1.90863600	-0.04249000	-0.27625000

H	-0.60129100	-0.04900800	1.50917300

H_2O

Total Energy= -76.419564

Imaginary frequency= 0

XYZ coordinates

O	0.00000000	0.00000000	0.11840800
H	0.00000000	0.76282900	-0.47363200
H	0.00000000	-0.76282900	-0.47363200

Catalyst A_F

Total Energy= -1445.357189

Imaginary frequency= 0

XYZ coordinates

H	-4.86844000	1.95815300	0.43842800
H	-5.65140200	-1.70564000	1.19926000
H	-2.77932300	0.67331700	0.93473400
H	-4.92319800	-0.25351300	1.89699400
H	0.64610500	-0.45040600	-1.43873800
H	-3.84283900	-1.78331200	-0.54280700
H	-1.37061800	0.26606600	-1.36997500
H	-6.11179300	-0.50217200	-0.92387700
H	-6.82111800	0.40141200	0.42115400
H	-3.84344400	0.27987100	-1.90437300
H	-5.58521000	1.91546100	-1.18244500
C	1.98555500	-0.77241700	0.14392000
N	-1.57365400	-0.24299300	-0.51182600
N	0.66561400	-0.69946800	-0.45721600
S	-0.57897800	-0.81107100	1.93827400
C	-0.50088800	-0.56668400	0.26779700
C	-5.86843900	0.08406000	-0.02418200
C	-3.67288800	0.91587000	-1.02116700
C	-5.04213300	1.31457000	-0.43876600
C	-5.07895400	-0.80116100	0.95490000
C	-2.90428100	0.07365200	0.01798800
C	-3.71023500	-1.18757200	0.37285000
H	1.84501200	-1.17220100	1.15488400
C	2.81323600	-1.82848300	-0.61355300
C	2.68386000	0.57679200	0.23465300
C	2.88029800	1.37622800	-0.90054900
C	3.10913800	1.04242300	1.48430200
C	3.50121700	2.62215100	-0.78612400
H	2.55898800	1.02411000	-1.87859200
C	3.72921400	2.29036600	1.60089100
H	2.93861600	0.42842900	2.36638000
C	3.92733200	3.08188400	0.46563900
H	3.65426600	3.23383200	-1.67324000
H	4.05181800	2.64506100	2.57784200
H	4.40947600	4.05358500	0.55434800

H	-3.13527500	-1.78434900	1.08749500
F	4.07477300	-1.90010400	-0.12534100
F	2.26102500	-3.06107400	-0.51216400
F	2.90772700	-1.54323000	-1.95212500
N	-2.83628000	2.04350700	-1.47196600
H	-2.67739000	2.68292600	-0.69380500
H	-3.32426800	2.56876800	-2.19390400

KE-A_F-Maj-Cx1

Total Energy= -2251.982193

Imaginary frequency= 0

XYZ coordinates

H	-5.45249500	-0.36902400	-1.52747300
H	-6.15746500	2.90358300	0.26181100
H	-3.31409000	1.12001000	-1.51508300
H	-5.67979300	2.21588000	-1.29680800
H	0.26825300	1.43724600	0.97722500
H	-4.02760200	2.10694900	1.29249600
H	-1.66553400	0.68427000	0.89782300
H	-6.16705900	0.62942800	1.28743600
H	-7.23568700	0.64966700	-0.12221800
H	-3.78254600	-0.50535200	1.03306000
H	-5.77273900	-1.40020300	-0.12439000
C	1.45613800	2.52120000	-0.38860100
N	-1.90252000	1.10282500	-0.00347100
N	0.22185500	1.92293700	0.08731800
S	-1.13091900	2.48557700	-2.19070800
C	-0.93921500	1.82125400	-0.63911500
C	-6.18563200	0.72511600	0.19060600
C	-3.88099800	-0.36537600	-0.05340200
C	-5.37565000	-0.42391200	-0.42979900
C	-5.59412700	2.08602200	-0.20706200
C	-3.29536200	1.01727800	-0.42267600
C	-4.11610200	2.16580200	0.19652500
H	1.24286800	2.92013400	-1.38719200
C	1.78857100	3.75378600	0.47928400
C	2.59680500	1.52054100	-0.47457500
C	3.08493200	0.86017500	0.66085100
C	3.13444600	1.21113000	-1.73064000
C	4.09471600	-0.09658600	0.54116500
H	2.67700000	1.08555700	1.64224800
C	4.14580400	0.25588200	-1.85292700
H	2.74360400	1.71123700	-2.61455500
C	4.62465700	-0.40277200	-0.71654900
H	4.45297000	-0.61101600	1.43027600
H	4.54628300	0.01464400	-2.83503900
H	5.40647100	-1.15404500	-0.81055100
H	-3.66625600	3.11321200	-0.12380400
F	2.95375400	4.32554800	0.08341400
F	0.81699300	4.69389000	0.39018400

F	1.91616000	3.43938700	1.80510500
N	-3.16072900	-1.45990700	-0.68834300
H	-3.18279500	-1.48542700	-1.69822500
C	-2.35189700	-2.34327400	-0.02410700
H	-2.35630400	-2.20888800	1.05652600
C	-1.58710300	-3.32831700	-0.56971400
C	-1.52032900	-3.59213400	-2.04865600
H	-0.50181000	-3.88947800	-2.33360100
H	-2.19684200	-4.41274600	-2.34204700
H	-1.77621100	-2.71368200	-2.65540200
C	-0.84924200	-4.29154500	0.31631100
H	-0.90083200	-3.99573400	1.37138900
H	-1.26078100	-5.31102900	0.22904000
H	0.21209500	-4.35274300	0.02597700
C	1.12714900	-1.77351800	-1.39103100
C	0.70785800	-1.12729300	-2.57497600
C	2.10539900	-2.78681900	-1.48118000
C	1.25433300	-1.47843600	-3.80683400
H	-0.02896200	-0.32717500	-2.51051400
C	2.64026800	-3.14457400	-2.71631100
H	2.44213400	-3.28995600	-0.57855500
C	2.22054000	-2.48959700	-3.88244700
H	0.93088000	-0.96181700	-4.70831600
H	3.39163500	-3.92982200	-2.77430500
H	2.64528300	-2.76803300	-4.84518500
C	0.54335000	-1.35249500	-0.13792700
H	-0.28674200	-0.66309700	-0.22704700
C	0.99648700	-1.64978300	1.11793300
H	1.85698200	-2.29143300	1.27562300
C	0.37012400	-1.08935700	2.28311400
O	-0.58057000	-0.28210200	2.29047900
C	1.01176500	-1.51786000	3.62431200
O	2.17718300	-1.85105400	3.73464500
O	0.13199100	-1.44883800	4.64204200
C	0.66350900	-1.78131600	5.95140600
H	-0.18403100	-1.69280400	6.63486600
H	1.06532900	-2.80157600	5.95140600
H	1.46109100	-1.07974800	6.22238900

KE-A_F-Maj-Cx2

Total Energy= -2251.981446

Imaginary frequency= 0

XYZ coordinates

H	-4.38740800	1.85032500	-2.61868300
H	-5.61067100	3.41860500	0.60254000
H	-2.32332000	3.01194800	-1.36417200
H	-4.88186800	3.77497800	-0.96999000
H	0.63444500	1.41522100	1.42153500
H	-3.58622500	2.15820200	1.29800900
H	-1.34932200	1.36480400	0.89851400

H	-5.54383400	0.97160700	0.09342500
H	-6.43491400	1.82680200	-1.17521400
H	-3.08129000	0.24249300	-0.36590400
H	-4.79855500	0.18956500	-2.17803300
C	2.39085000	1.88412900	0.36750600
N	-1.25658700	2.02947000	0.12419200
N	0.95631300	1.84887900	0.56384300
S	0.37043100	2.93766700	-1.84826700
C	-0.00176300	2.25473800	-0.33341600
C	-5.44038500	1.69800200	-0.72793600
C	-3.04433700	0.96894900	-1.18707300
C	-4.45832100	1.15102700	-1.77244100
C	-4.92409400	3.02962600	-0.16101900
C	-2.51541200	2.28322800	-0.56808700
C	-3.52433800	2.85356000	0.44666700
H	2.56837900	2.21865800	-0.66073200
C	3.00416000	2.98141600	1.27145000
C	3.04999500	0.53356800	0.59860800
C	2.72102200	-0.26167500	1.70369600
C	3.99897700	0.06966400	-0.31936500
C	3.31955700	-1.51095700	1.87762000
H	1.99201500	0.08169100	2.43428700
C	4.60315000	-1.17705600	-0.14592700
H	4.25073900	0.68338100	-1.18167600
C	4.25912700	-1.97265800	0.95087300
H	3.04312000	-2.12653300	2.73102100
H	5.32498400	-1.53451400	-0.87673500
H	4.71837900	-2.95054500	1.08106300
H	-3.13476900	3.80519600	0.82885500
F	4.34803000	3.05905200	1.09308600
F	2.48145600	4.19957000	0.99995700
F	2.77816400	2.73027200	2.59483100
N	-2.11063300	0.49201300	-2.19755600
H	-1.48268300	1.19780200	-2.57000200
C	-1.77137200	-0.80189700	-2.47647500
H	-0.98305800	-0.84758000	-3.22562400
C	-2.20995600	-2.00156900	-1.99178600
C	-3.25744700	-2.23541000	-0.93860400
H	-3.74977700	-3.20308000	-1.11040800
H	-2.79997900	-2.29224500	0.06735200
H	-4.03704300	-1.46835200	-0.90918600
C	-1.57520500	-3.25962800	-2.52827100
H	-0.79175700	-3.05101400	-3.26564100
H	-1.11565300	-3.84046700	-1.71048200
H	-2.32950700	-3.91400300	-2.99478000
C	1.11695300	-1.83685500	-1.26045800
C	1.54084700	-0.93330200	-2.26013200
C	1.62829100	-3.15125100	-1.28206000
C	2.42393600	-1.33478000	-3.25790300
H	1.16771400	0.09031600	-2.24043400
C	2.51324500	-3.55167000	-2.28117800

H	1.33032500	-3.85899000	-0.51299700
C	2.91190000	-2.64856300	-3.27476100
H	2.73830100	-0.62399200	-4.01980700
H	2.89638700	-4.57031800	-2.28687100
H	3.60197000	-2.96572200	-4.05445800
C	0.18717300	-1.36573800	-0.25384800
H	-0.12031900	-0.33014500	-0.35374900
C	-0.26110200	-2.05299100	0.83926100
H	-0.01164300	-3.09792700	0.99706300
C	-1.08362600	-1.42626000	1.84405000
O	-1.34792800	-0.21243600	1.93090300
C	-1.61633800	-2.39665000	2.92739500
O	-1.08929500	-3.45797300	3.20397600
O	-2.72003700	-1.90832800	3.52840100
C	-3.27398200	-2.73906200	4.58136700
H	-4.15616900	-2.20114100	4.93604700
H	-3.54640400	-3.72437900	4.18453100
H	-2.54094700	-2.86561700	5.38664700

KE-A_F-Maj-Cx3

Total Energy= -2251.979577

Imaginary frequency= 0

XYZ coordinates

H	4.62050900	-1.81742300	-2.29579000
H	5.74691200	-3.25419700	1.02145100
H	2.54399000	-3.02040600	-1.10237000
H	5.10362800	-3.67818200	-0.57176300
H	-0.61303600	-1.39192400	1.45147600
H	3.64934000	-2.05185000	1.59069300
H	1.40148000	-1.37257000	1.07814900
H	5.61770900	-0.82552100	0.44105200
H	6.59557700	-1.68146100	-0.76128200
H	3.15817500	-0.19844500	-0.15037500
H	4.95044100	-0.13160600	-1.88211800
C	-2.28696300	-2.04231700	0.35589900
N	1.37168800	-2.04176400	0.30542300
N	-0.86893900	-1.90461000	0.61472400
S	-0.11759500	-3.06594500	-1.71646200
C	0.14985500	-2.31617700	-0.21016500
C	5.57760200	-1.57673100	-0.36315600
C	3.18161100	-0.94888200	-0.95010900
C	4.62663900	-1.09444800	-1.46647700
C	5.08296100	-2.91077400	0.21728700
C	2.67205200	-2.26451300	-0.31874200
C	3.65128700	-2.77035200	0.75646100
H	-2.38978600	-2.48445500	-0.64173200
C	-2.88673600	-3.08252800	1.33235100
C	-3.03007800	-0.71753900	0.41743300
C	-2.83324700	0.18351900	1.47240000
C	-3.91780900	-0.38288800	-0.61097300

C	-3.50292000	1.40818200	1.48749700
H	-2.15323400	-0.06131500	2.28480100
C	-4.59147200	0.84031600	-0.59696100
H	-4.06670500	-1.07794300	-1.43465500
C	-4.37997500	1.74124200	0.45019000
H	-3.33056700	2.10562200	2.30469700
H	-5.26356200	1.09731400	-1.41252900
H	-4.89335700	2.70066100	0.45646800
H	3.27850600	-3.72557900	1.14627000
F	-4.21369100	-3.25347000	1.10005400
F	-2.28716700	-4.28901200	1.20294000
F	-2.74349400	-2.69749700	2.63493700
N	2.27785400	-0.53566800	-2.01448100
H	1.70096700	-1.27600200	-2.40161700
C	1.91619100	0.73502700	-2.36017000
H	1.17629300	0.72830100	-3.15832100
C	2.28863400	1.96443000	-1.89457000
C	3.25720600	2.26393500	-0.78424200
H	3.70781600	3.25451700	-0.93756500
H	2.74124400	2.30341900	0.19352200
H	4.07417700	1.54070800	-0.69835900
C	1.65728500	3.18222100	-2.51953600
H	0.93413000	2.92404500	-3.30160000
H	1.12299600	3.77667400	-1.75839900
H	2.42341000	3.84342800	-2.95611200
C	-1.06532800	1.75521000	-1.36559700
C	-1.40810600	0.81450000	-2.36168600
C	-1.58764700	3.06185300	-1.46648000
C	-2.21696100	1.17434300	-3.43545500
H	-1.02844400	-0.20332900	-2.27824500
C	-2.39991000	3.42006200	-2.54054000
H	-1.35418000	3.79670500	-0.70019300
C	-2.71332400	2.48142700	-3.53166600
H	-2.46841700	0.43631100	-4.19474400
H	-2.79173800	4.43321300	-2.60782600
H	-3.34582900	2.76564500	-4.37062800
C	-0.20346500	1.32702800	-0.28247000
H	0.10860400	0.28839500	-0.32027300
C	0.18054100	2.05897000	0.80702000
H	-0.06503100	3.11292000	0.89241800
C	0.93666300	1.46804800	1.88523100
O	1.15662000	0.25401600	2.04386100
C	1.56293700	2.41969000	2.93399700
O	2.61153600	2.20142100	3.49594100
O	0.78291200	3.51446800	3.15293400
C	1.29632900	4.45804400	4.13095100
H	0.53886000	5.24237200	4.20104300
H	1.43844400	3.96001600	5.09695100
H	2.25550300	4.86654800	3.79163800

KE-A_F-Maj-Cx4

Total Energy= -2251.984038

Imaginary frequency= 0

XYZ coordinates

H	-4.45496300	0.02402700	-2.27065700
H	-5.61909400	3.53287200	-1.31066400
H	-2.48256200	1.56898100	-1.92098300
H	-4.71769600	2.63388600	-2.53953100
H	0.58358600	1.51707900	1.08699500
H	-3.88119400	2.97032300	0.40048800
H	-1.48003700	1.52415800	0.84335300
H	-5.98817500	1.44325500	-0.01060100
H	-6.57456400	1.21987500	-1.66584700
H	-3.71711000	0.49075800	0.65936100
H	-5.23129600	-0.76082500	-0.88315000
C	2.13269600	2.39143300	-0.06351700
N	-1.47016700	1.81011100	-0.13541700
N	0.78490300	1.92762700	0.17772100
S	-0.06054100	2.49725000	-2.33324700
C	-0.26329500	2.07060900	-0.70084400
C	-5.66958200	1.36933600	-1.06176600
C	-3.43829700	0.35564500	-0.39520900
C	-4.73124600	0.16094800	-1.21468400
C	-4.95759500	2.67051200	-1.46597600
C	-2.72528900	1.64145000	-0.85535300
C	-3.65529600	2.85423100	-0.67011100
H	2.17796900	2.70966700	-1.11160900
C	2.39934300	3.66700500	0.77269200
C	3.18854800	1.32962300	0.19379000
C	3.18425000	0.56137900	1.36662800
C	4.19872500	1.12693600	-0.75481200
C	4.17441800	-0.39963400	1.58184700
H	2.40812400	0.70868300	2.11366300
C	5.19358100	0.16901800	-0.53713400
H	4.20123800	1.72345700	-1.66522900
C	5.18254800	-0.59616100	0.63263900
H	4.15578000	-0.99777200	2.49041700
H	5.97287100	0.01899500	-1.28195400
H	5.94984400	-1.34910700	0.80055900
H	-3.11413900	3.74873200	-0.99959500
F	3.64837700	4.15004500	0.53809800
F	1.51627800	4.64861500	0.47050000
F	2.29656600	3.43074200	2.11316800
N	-2.56677400	-0.83090300	-0.44197000
H	-3.03562100	-1.66088400	-0.10039100
C	-1.67548900	-1.05200300	-1.47879300
H	-1.28623200	-0.15214800	-1.94769600
C	-1.20008000	-2.25223000	-1.89528700
C	-1.63286400	-3.57950400	-1.34086900
H	-2.10284500	-4.19146100	-2.12732800

H	-0.75399200	-4.14216200	-0.99043800
H	-2.33309200	-3.50864600	-0.50011100
C	-0.19882900	-2.31034600	-3.01550700
H	0.08465600	-1.30730000	-3.35704800
H	0.71394300	-2.83596000	-2.69612300
H	-0.60478500	-2.87071500	-3.87382100
C	1.59178000	-2.71627500	-0.01155800
C	2.57091900	-2.26582500	-0.92277100
C	1.51072100	-4.10183600	0.25652600
C	3.43130300	-3.16486500	-1.55078500
H	2.65308500	-1.20019500	-1.12213600
C	2.37061600	-4.99849100	-0.37324400
H	0.78160300	-4.46955100	0.97461000
C	3.33328500	-4.53440800	-1.28164600
H	4.18197800	-2.79560700	-2.24633100
H	2.29845500	-6.06209300	-0.15373700
H	4.00520200	-5.23781400	-1.76969700
C	0.72712100	-1.73410900	0.61317000
H	0.96499300	-0.69491000	0.39313800
C	-0.32479400	-1.97337700	1.44304700
H	-0.68035000	-2.98324600	1.62065400
C	-1.07785600	-0.87864500	2.02225700
O	-0.65242100	0.27931600	2.16411700
C	-2.51579100	-1.14767700	2.52424500
O	-3.25179700	-0.28355200	2.94693200
O	-2.88169400	-2.46075700	2.40647500
C	-4.22048000	-2.77576400	2.86948300
H	-4.33300700	-3.85217600	2.71837300
H	-4.32602700	-2.51452000	3.92865300
H	-4.96575400	-2.21802000	2.28920500

KE-A_F-Maj-Cx5

Total Energy= -2251.977533

Imaginary frequency= 0

XYZ coordinates

H	-5.13548300	0.89872000	-1.45247200
H	-4.82752200	4.47391800	-0.21439300
H	-2.76808500	1.67242500	-1.76773300
H	-4.70167600	3.45273000	-1.65482300
H	1.09393400	1.60212600	0.20315700
H	-2.90140100	3.30128300	0.82752900
H	-0.91770700	2.04116100	0.47106900
H	-5.37558800	2.47787900	1.17710700
H	-6.50613400	2.58128400	-0.18121800
H	-3.42745300	0.82333400	1.09126900
H	-5.64797300	0.22674800	0.10228600
C	2.18722900	0.84628200	-1.41709800
N	-1.22911100	1.61142300	-0.39281700
N	0.97575900	1.09250200	-0.66545800
S	-0.64721000	0.28880200	-2.67684500

C	-0.29867100	1.03394300	-1.19405400
C	-5.45442900	2.40430700	0.08152900
C	-3.54500600	0.72087800	0.00165200
C	-5.02191100	0.99954700	-0.36165400
C	-4.55452900	3.46930900	-0.56410100
C	-2.65296800	1.77992300	-0.68202400
C	-3.07349000	3.19825400	-0.25535800
H	1.89779300	0.30381300	-2.32467500
C	2.77177100	2.20002600	-1.89897800
C	3.23491500	0.05796200	-0.64797600
C	3.53819700	0.35009000	0.68829800
C	3.95098400	-0.94977500	-1.30354500
C	4.54003900	-0.35303400	1.36096400
H	2.99518900	1.13192800	1.20983500
C	4.95944800	-1.65139300	-0.63698900
H	3.71446500	-1.18542000	-2.33908800
C	5.25838900	-1.35343300	0.69591200
H	4.75897600	-0.11925400	2.40085200
H	5.50742700	-2.43398600	-1.15775200
H	6.04197600	-1.90011800	1.21664600
H	-2.43082400	3.92596600	-0.76776800
N	-3.10407600	-0.61890900	-0.36659200
H	-2.76342200	-0.71020200	-1.31870300
C	-3.70732700	-1.72800800	0.20437000
H	-4.05487400	-1.56227000	1.22611900
C	-3.81918000	-2.95283700	-0.35637300
C	-3.38074500	-3.20574800	-1.77935400
H	-3.87193700	-4.10014000	-2.18585500
H	-3.62747400	-2.35736500	-2.43578200
H	-2.29222300	-3.35762000	-1.86268700
C	-4.32635200	-4.12729400	0.43926800
H	-5.18428200	-4.60748700	-0.05932500
H	-3.55331100	-4.90687500	0.55142600
H	-4.64027700	-3.82455400	1.44740400
C	0.55309800	-1.32194700	1.64427800
C	-0.62477700	-0.72722400	1.97177500
H	-1.57992500	-1.15003600	1.67352700
C	-0.70127000	0.55408600	2.63665700
O	-1.74674100	1.14164600	2.91968300
C	0.60702700	1.29012400	3.02543400
O	1.30083600	1.03560700	3.97989400
O	0.80836500	2.34751800	2.17635900
C	1.86682200	3.28436700	2.54201400
H	2.80163100	2.74699100	2.73334200
H	1.96777400	3.95325400	1.68506300
H	1.56704100	3.83204300	3.44171300
C	0.72692600	-2.55467200	0.90048800
C	2.03339700	-3.06934100	0.75274700
C	-0.35072900	-3.25237400	0.30881200
C	2.25857300	-4.25584400	0.05798800
H	2.86905300	-2.52209800	1.18136200

C	-0.11998600	-4.43957300	-0.37979800
H	-1.36252200	-2.86243400	0.38053600
C	1.18129400	-4.94745600	-0.50715200
H	3.27226900	-4.63645200	-0.04887300
H	-0.95670100	-4.96842800	-0.83019600
H	1.35238200	-5.87413900	-1.05195600
H	1.48227900	-0.84814200	1.96204600
F	3.90672800	2.02597000	-2.61949800
F	1.89311000	2.88094400	-2.66732500
F	3.08259100	3.01224600	-0.83531900

KE-A_F-Maj-Cx6

Total Energy= -2251.966987

Imaginary frequency= 0

XYZ coordinates

H	3.05797400	3.27936200	-2.63038900
H	5.62994700	3.68235800	0.14793400
H	3.61502700	1.01949100	-1.66630700
H	5.36596800	2.95528400	-1.44319500
H	1.39900500	-1.59194000	1.05873100
H	3.89693300	2.20581200	1.14788700
H	2.33606800	0.26139900	0.88371700
H	3.30602500	4.58799400	0.14472700
H	4.15701400	5.12266700	-1.31329200
H	1.68596200	2.67181200	0.03128100
H	1.83632700	4.29983600	-1.85451700
C	1.00904500	-3.12910800	-0.31748600
N	2.70460300	0.11198600	-0.05275000
N	1.61983100	-1.89195500	0.11820400
S	2.54169400	-1.31124600	-2.35498600
C	2.27619800	-1.00827800	-0.70005400
C	3.74821200	4.24083300	-0.80200900
C	2.07118000	2.34626200	-0.94815600
C	2.65034000	3.59055400	-1.65691400
C	4.86771000	3.23098200	-0.50101800
C	3.20435200	1.32408700	-0.69756100
C	4.31281800	1.95641500	0.15844200
H	1.20993400	-3.21940700	-1.39160500
C	1.73619200	-4.32691800	0.33686600
C	-0.49090900	-3.17048300	-0.06696500
C	-1.02669500	-2.91247700	1.20436500
C	-1.35429600	-3.49179800	-1.12073300
C	-2.40347900	-3.00118600	1.41991000
H	-0.37251200	-2.65750800	2.03360800
C	-2.73404800	-3.57900000	-0.90638600
H	-0.94100100	-3.67834500	-2.11012100
C	-3.26025700	-3.34347000	0.36691700
H	-2.80880900	-2.80615500	2.41085900
H	-3.39445100	-3.83330700	-1.73316300
H	-4.33276900	-3.41125300	0.53798200

H	5.10813400	1.21612600	0.30995200
N	0.98750600	1.71550700	-1.68114800
H	1.22687700	0.90689900	-2.24427000
C	-0.23823900	2.30857800	-1.84628800
H	-0.31773600	3.29681200	-1.39200300
C	-1.31896000	1.78954300	-2.48144300
C	-1.34698700	0.40938900	-3.07938600
H	-1.37538800	0.44924400	-4.18143500
H	-0.48948100	-0.20933400	-2.78758900
H	-2.26069000	-0.11868500	-2.76061000
C	-2.55411400	2.62036400	-2.68292300
H	-2.69848600	2.87008600	-3.74871300
H	-3.45344900	2.07662000	-2.36220500
H	-2.50533000	3.56300600	-2.12169900
C	-2.04585200	1.30447100	0.95144600
C	-1.41594500	2.41432800	1.43426400
H	-1.79442600	3.41241800	1.21464300
C	-0.18295700	2.40365200	2.18710900
O	0.54667600	3.38989100	2.34686600
C	0.26683200	1.08585400	2.86050800
O	0.67053800	0.13101600	2.21803700
O	0.27408800	1.02465000	4.20290500
C	-0.22621100	2.14716600	4.98813300
H	-0.27247700	1.77314300	6.01332100
H	0.46196400	2.99339600	4.90610100
H	-1.22649900	2.43927700	4.64546300
C	-3.32917200	1.26490600	0.27551900
C	-3.73331500	0.05726000	-0.33416200
C	-4.21829900	2.36301900	0.24906500
C	-4.97729500	-0.04857600	-0.95318600
H	-3.06528900	-0.79855800	-0.30567600
C	-5.46434500	2.25082500	-0.36153800
H	-3.93263000	3.29889900	0.72333700
C	-5.85066400	1.04572400	-0.96518600
H	-5.26802300	-0.98702100	-1.42102700
H	-6.14092800	3.10296900	-0.36785600
H	-6.82557600	0.96293600	-1.44131900
H	-1.55635700	0.33800500	1.07645300
F	1.18392200	-5.50378700	-0.05804300
F	3.04552000	-4.35268400	-0.00248000
F	1.67422500	-4.28409700	1.70177600

KE-A_F-Maj-Cx7

Total Energy= -2251.978611

Imaginary frequency= 0

XYZ coordinates

H	5.02985500	-0.47475200	-1.63830100
H	5.08873000	-4.21533600	-1.01046800
H	2.61060300	-1.47459300	-1.90993000
H	4.73051100	-2.98760500	-2.23249900

H	-0.93550000	-1.36082200	0.63084200
H	3.18439200	-3.41213500	0.38845000
H	1.21063300	-1.56570700	0.67435800
H	5.57454800	-2.42997000	0.66769400
H	6.59355200	-2.20397200	-0.76078800
H	3.46103900	-0.85769600	0.95958300
H	5.57010200	-0.01947700	-0.01366700
C	-2.34671900	-1.62735800	-0.88026400
N	1.28279500	-1.66161300	-0.33483100
N	-1.00386200	-1.69288500	-0.32292900
S	0.14702200	-1.97384900	-2.75734900
C	0.15138600	-1.76870500	-1.07523100
C	5.55560500	-2.17363400	-0.40299500
C	3.51258200	-0.65861500	-0.12003900
C	4.98224200	-0.75779300	-0.57425600
C	4.69341100	-3.20092700	-1.15310700
C	2.65258500	-1.71936400	-0.84205200
C	3.23489000	-3.13528500	-0.67647500
H	-2.24809500	-1.83560400	-1.95197700
C	-3.18324600	-2.79295000	-0.31479100
C	-2.98336500	-0.26214000	-0.68543800
C	-3.26847000	0.24227100	0.59139100
C	-3.22155400	0.53831600	-1.81006400
C	-3.79092500	1.52904000	0.73691500
H	-3.07617900	-0.36111200	1.47428100
C	-3.74036500	1.82640500	-1.66383800
H	-2.97850200	0.15332900	-2.79823800
C	-4.02510100	2.32430600	-0.38893200
H	-4.00315200	1.91261400	1.73276400
H	-3.90777100	2.44527400	-2.54246300
H	-4.42308200	3.33041400	-0.27303900
H	2.60195900	-3.83585500	-1.23470900
F	-4.45281400	-2.75191500	-0.78474200
F	-2.65136700	-3.99136000	-0.66084900
F	-3.25223100	-2.77503400	1.05438700
N	2.96331100	0.67594000	-0.33193500
H	3.11562300	1.05209300	-1.25904600
C	2.87156500	1.59225400	0.70259600
H	2.78093100	1.12421000	1.68097000
C	2.78609000	2.93848400	0.59778300
C	2.88586100	3.67733700	-0.70916000
H	1.88975800	3.93986100	-1.09738100
H	3.44039500	4.61789600	-0.57498500
H	3.40226700	3.09990500	-1.48894100
C	2.49544200	3.77085000	1.81575200
H	2.43138400	3.15665200	2.72242800
H	3.26718000	4.54208800	1.97043000
H	1.53572900	4.30574000	1.70349700
C	-0.29864200	2.44389500	-0.32588000
C	-0.00515600	1.87860300	-1.58454600
C	-0.77003900	3.77280000	-0.27502800

C	-0.18383600	2.61333200	-2.75529700
H	0.35270400	0.85375800	-1.63607000
C	-0.94274600	4.50663700	-1.44573200
H	-0.99614200	4.22961500	0.68507000
C	-0.65695500	3.92825700	-2.69087700
H	0.03682900	2.15404000	-3.71668700
H	-1.30434500	5.53172400	-1.39263700
H	-0.79914900	4.50420000	-3.60338600
C	-0.12355100	1.61968900	0.85394300
H	0.33607400	0.65491200	0.65061800
C	-0.50029400	1.91309100	2.12736800
H	-0.94339400	2.87282200	2.38593300
C	-0.38783600	0.98474600	3.23101900
O	-0.65504800	1.24082600	4.40296800
C	0.09845300	-0.45770500	2.93059800
O	1.24943600	-0.76459600	2.66899800
O	-0.91483700	-1.33891900	3.05328100
C	-0.56213200	-2.75735500	3.01318600
H	-1.50190000	-3.28399800	3.18210400
H	-0.14906400	-3.02127000	2.03320300
H	0.16964300	-2.97437600	3.79801400

KE-A_F-Maj-Cx8

Total Energy= -2251.973411
Imaginary frequency= 0

XYZ coordinates

H	-0.10531800	-4.41070000	2.16045500
H	0.57318200	-6.45012700	-0.99522200
H	1.65983400	-3.33334500	0.78080300
H	1.33614600	-5.84174600	0.47978200
H	1.87295100	0.44575700	-1.08129700
H	0.28051000	-4.10829400	-1.83152700
H	0.61083400	-1.27960000	-1.01504500
H	-1.56831500	-5.34162900	-0.38279800
H	-1.04892700	-6.39257700	0.94271600
H	-1.17758600	-2.82670700	-0.22659200
H	-1.81910800	-4.14750200	1.79598200
C	3.95841200	0.67164800	-0.95612300
N	1.36028700	-1.86792500	-0.64512500
N	2.73330700	-0.09822200	-1.09106800
S	3.96982900	-2.31050600	-0.12687400
C	2.63507300	-1.39501000	-0.63628100
C	-0.79700100	-5.47641800	0.39181900
C	-0.45793600	-2.97507600	0.58896800
C	-0.82581700	-4.26668600	1.34197000
C	0.57819500	-5.61280100	-0.28472000
C	0.94638300	-3.12450400	-0.02902300
C	0.97608200	-4.31314400	-1.00392600
H	4.79548600	-0.01113200	-1.13877100
C	4.01119000	1.70942300	-2.09292300

C	4.13934700	1.30477900	0.41929400
C	3.13828500	2.10439100	0.98804600
C	5.31275400	1.05575000	1.13965400
C	3.31538800	2.65124900	2.26168400
H	2.21972400	2.28892500	0.44001500
C	5.49127700	1.60397300	2.41327500
H	6.07504000	0.41195900	0.70641400
C	4.49266900	2.40425400	2.97718900
H	2.53351500	3.27133100	2.69785900
H	6.40464200	1.39788600	2.96815100
H	4.62837600	2.82847900	3.97051200
H	1.98806800	-4.38552900	-1.41767700
F	5.13300200	2.46868300	-2.00131200
F	4.01975700	1.11675900	-3.31279700
F	2.94045900	2.56159200	-2.07147900
N	-0.49753300	-1.79346600	1.45950500
H	0.39057900	-1.34506500	1.64384000
C	-1.62787300	-1.05797700	1.65284100
H	-2.54522200	-1.55086500	1.33402000
C	-1.69208000	0.19061300	2.19948400
C	-0.44819100	0.89110100	2.68576400
H	0.37449200	0.83581500	1.95832500
H	-0.64979700	1.95184200	2.88109200
H	-0.07931200	0.45214000	3.62789200
C	-3.01873000	0.83638300	2.47332300
H	-3.85353500	0.22447300	2.11280800
H	-3.16225600	1.00829400	3.55304000
H	-3.08613600	1.82179700	1.98316300
C	-5.69671600	1.03069700	-0.57732200
C	-6.46286100	2.10071100	-0.06424400
C	-6.38147700	-0.11507700	-1.04262800
C	-7.85500700	2.03156600	-0.01126500
H	-5.94727800	2.98952500	0.29704800
C	-7.77115600	-0.18252600	-0.99122700
H	-5.82303000	-0.95222000	-1.45432600
C	-8.51507100	0.88846900	-0.47470700
H	-8.42521100	2.86731300	0.38937200
H	-8.28161000	-1.07125800	-1.35715700
H	-9.60099400	0.83036600	-0.43724700
C	-4.24510300	1.16617400	-0.58750600
H	-3.86840000	2.12320500	-0.24180700
C	-3.35793800	0.21110100	-0.96529400
H	-3.72483900	-0.75221900	-1.31902400
C	-1.89850600	0.25610300	-0.99798400
O	-1.26239500	-0.69238200	-1.47487500
C	-1.03605800	1.44451000	-0.51239600
O	0.17888900	1.37637400	-0.48323900
O	-1.71665100	2.56910500	-0.20081200
C	-0.89981800	3.70671900	0.19588500
H	-1.60900300	4.51819100	0.37472200
H	-0.34143900	3.46472300	1.10584900

H	-0.19973600	3.96341300	-0.60662000

KE-A_F-Maj-Cx9

Total Energy= -2251.968350

Imaginary frequency= 0

XYZ coordinates

H	0.00954400	4.60687200	1.89024000
H	-0.42788800	6.15354300	-1.55956300
H	-1.75491800	3.36867300	0.61164800
H	-1.27225900	5.81818600	-0.04228600
H	-1.93959000	-0.62113500	-0.83040000
H	-0.21794200	3.69984100	-2.00802100
H	-0.64578400	1.07427600	-0.83066100
H	1.63173800	5.05525700	-0.68591800
H	1.11901500	6.32691600	0.43284500
H	1.09270200	2.61824500	-0.16928800
H	1.72273400	4.22024800	1.67432700
C	-4.02742800	-0.78679700	-1.02340700
N	-1.40756600	1.70982500	-0.58011600
N	-2.77187700	-0.06311500	-0.99934200
S	-4.04358900	2.25689300	-0.39997400
C	-2.68872700	1.27178800	-0.66540500
C	0.83915800	5.34788900	0.02113000
C	0.36597900	2.92751200	0.58883800
C	0.76386700	4.30512400	1.14903900
C	-0.50058900	5.43860100	-0.72921200
C	-1.00321200	3.03098200	-0.11611500
C	-0.93534800	4.06194100	-1.25639900
H	-4.79979500	-0.08710600	-1.36186800
C	-3.93464300	-1.87379700	-2.11311600
C	-4.45102700	-1.36706300	0.32095600
C	-3.53986100	-2.05487800	1.13314200
C	-5.77430000	-1.21297200	0.74913700
C	-3.95391000	-2.58682200	2.35737100
H	-2.50680400	-2.16437200	0.81649900
C	-6.18931000	-1.74436900	1.97339100
H	-6.47491300	-0.66140100	0.12528600
C	-5.27946700	-2.43545500	2.78020000
H	-3.24118500	-3.12233700	2.98299700
H	-7.21907900	-1.61205400	2.30001200
H	-5.59969400	-2.84827900	3.73520800
H	-1.92443600	4.11109200	-1.72516600
F	-5.07860100	-2.60183800	-2.17336700
F	-3.72909600	-1.33773000	-3.34185000
F	-2.90718000	-2.74820100	-1.88117800
N	0.30250200	1.89762700	1.62902100
H	-0.62816300	1.55440300	1.82090400
C	1.30532200	1.09074100	2.08979900
H	0.90898600	0.31504500	2.74565000
C	2.66011600	1.08754400	1.91307500

C	3.50418500	2.08503900	1.16139500
H	4.09475800	2.68418700	1.87530100
H	4.23002400	1.55545300	0.52746900
H	2.94397700	2.77406000	0.53007500
C	3.47475000	0.06948600	2.66659800
H	2.84985200	-0.62338400	3.24307800
H	4.09153100	-0.52375800	1.97149600
H	4.17434200	0.56511500	3.36008800
C	5.54250500	-1.52678100	-0.64780100
C	6.29758100	-2.59672400	-0.11895600
C	6.21947300	-0.54532100	-1.40693700
C	7.67186200	-2.68898100	-0.34000600
H	5.78826800	-3.35846700	0.46990300
C	7.59094700	-0.63796300	-1.62698100
H	5.66922300	0.29398600	-1.82491200
C	8.32429800	-1.70910200	-1.09574200
H	8.23387200	-3.52276700	0.07593800
H	8.09554300	0.12696300	-2.21392800
H	9.39622100	-1.77607000	-1.27034200
C	4.11091500	-1.48855600	-0.37006400
H	3.74149500	-2.29057400	0.26175800
C	3.23533500	-0.55860500	-0.83060700
H	3.59128600	0.23048300	-1.49139500
C	1.79878000	-0.44064700	-0.61273200
O	1.14595700	0.39251000	-1.25438300
C	0.96400500	-1.35319100	0.32354400
O	-0.24979500	-1.28304900	0.36151500
O	1.67766900	-2.22899400	1.06332900
C	0.90268100	-3.08275000	1.94764200
H	1.63816600	-3.70833500	2.45856700
H	0.34309600	-2.47074900	2.66455000
H	0.20173400	-3.69173600	1.36575400

Addition of isobutyraldehyde to methyl benzylidenepyruvate [PCM($CHCl_3$)-B97D/TZVP].

Methyl benzylidenepyruvate
Total Energy= -650.630085
Imaginary frequency= 0

XYZ coordinates

C	-2.10426200	0.25629200	-0.00050800
C	-3.16661200	1.18850500	0.01522200
C	-2.41688300	-1.12322000	0.03147200
C	-4.49400200	0.76149700	0.06129000
H	-2.93551300	2.25215700	-0.00996500
C	-3.74198200	-1.54655900	0.07745100
H	-1.61793100	-1.86034100	0.01911900
C	-4.78535300	-0.60725600	0.09248300
H	-5.29974800	1.49232600	0.07253400

H	-3.96883800	-2.61033600	0.10128500
H	-5.81930500	-0.94430100	0.12803500
C	-0.74217800	0.76029000	-0.05093200
H	-0.63957900	1.84727400	-0.07605900
C	0.40365700	0.03231600	-0.06908200
H	0.39407800	-1.05353600	-0.04810800
C	1.71441100	0.68557400	-0.10794800
O	1.91052500	1.89552900	-0.16465200
C	2.91910000	-0.30924300	-0.10490400
O	2.82340300	-1.47574600	-0.44092200
O	4.05036700	0.29200100	0.28913300
C	5.24778900	-0.53871400	0.29573000
H	6.04383700	0.11287200	0.66073200
H	5.10465900	-1.39686500	0.96174000
H	5.46185500	-0.89041200	-0.71942600

Isobutyraldehyde

Total Energy= -232.392423

Imaginary frequency= 0

XYZ coordinates

C	0.94843900	-0.59618600	0.21030700
H	1.02453700	-1.66073500	0.54450900
C	-0.42497500	0.01051200	0.41702300
C	-0.52477000	1.46670400	-0.04350400
H	-0.36309900	1.53626500	-1.12691000
H	-1.52148200	1.86407500	0.18446900
H	0.22728400	2.09182200	0.45231500
C	-1.47461800	-0.90067100	-0.26045500
H	-1.37787700	-1.94220900	0.07358600
H	-2.48362500	-0.55070600	-0.01231000
H	-1.35650000	-0.87185500	-1.35174400
O	1.91284400	-0.03715500	-0.27631500
H	-0.59644100	-0.05157600	1.50638200

H_2O

Total Energy= -76.425025

Imaginary frequency= 0

XYZ coordinates

O	0.00000000	0.00000000	0.11886000
H	0.00000000	0.76199000	-0.47543900
H	0.00000000	-0.76199000	-0.47543900

Catalyst A_F

Total Energy= -1445.366035

Imaginary frequency= 0

XYZ coordinates

H	-4.86349500	1.43948600	1.18930300
H	-6.17217500	-1.55225000	-0.76142600

H	-3.06443700	-0.34990000	1.05157300
H	-5.57027900	-1.04804400	0.82485700
H	0.59501900	-0.41103400	-1.33492700
H	-3.95236400	-1.09764300	-1.78467900
H	-1.51709000	-0.49000100	-1.45503200
H	-5.82160200	0.74866500	-1.65119700
H	-6.84874600	0.81923000	-0.21105900
H	-3.33367700	1.36543900	-1.45757200
H	-5.05560800	2.59027500	-0.14500400
C	1.93111600	-0.67166500	0.25920100
N	-1.66886300	-0.55699300	-0.45394400
N	0.61252900	-0.62619200	-0.34564000
S	-0.64842500	-0.65334100	2.04762100
C	-0.57441700	-0.59533400	0.34522900
C	-5.83280700	0.59264800	-0.56120700
C	-3.37278600	1.24843000	-0.36119000
C	-4.81833900	1.54392600	0.09384000
C	-5.47487600	-0.87037800	-0.25702100
C	-3.03199500	-0.22203600	-0.03591300
C	-4.03373500	-1.18748800	-0.68984000
H	1.77937100	-0.82790900	1.33299000
C	2.67089000	-1.92966200	-0.24201900
C	2.73438500	0.60143800	0.04307100
C	2.94327700	1.12411000	-1.24169300
C	3.26273500	1.27234000	1.15300000
C	3.66979700	2.30537000	-1.41191000
H	2.54920100	0.60773300	-2.11437900
C	3.99068700	2.45464800	0.98393500
H	3.09684000	0.86982600	2.15041800
C	4.19487900	2.97343700	-0.29890100
H	3.82745100	2.70325400	-2.41231100
H	4.39353200	2.97068500	1.85304800
H	4.75946700	3.89409500	-0.43222000
H	-3.76195000	-2.21570500	-0.42048300
F	3.91406300	-2.01333200	0.29729300
F	2.00387600	-3.06437500	0.09194000
F	2.81580500	-1.94092500	-1.60229500
N	-2.35666100	2.14389300	0.21471200
H	-2.24630100	1.93503900	1.20647300
H	-2.68396000	3.10622600	0.14986700

Catalyst B_F

Total Energy= -1445.367837

Imaginary frequency= 0

XYZ coordinates

H	-4.87185500	2.21727200	0.91157100
H	-5.99452000	-1.22629100	-0.26635900
H	-2.92586300	0.48564500	1.08606900
H	-5.35597500	-0.34796000	1.13306600
H	0.63793300	-0.23436700	-1.35430600

H	-3.87476200	-0.84386100	-1.49378300
H	-1.43677800	0.14791100	-1.44094600
H	-3.49115000	-1.98336300	1.17810500
H	-5.84224600	0.84427000	-1.65699000
H	-6.82072300	1.15429000	-0.21544900
H	-3.35939500	1.68299800	-1.70634900
H	-2.71603000	2.54374400	-0.29413300
H	-5.16993000	3.01564400	-0.63979700
C	1.94628200	-0.64807300	0.22390800
N	-1.57435700	0.12362800	-0.43590400
N	-3.50618800	-2.05657600	0.16076800
N	0.63000600	-0.47838200	-0.37067500
S	-0.59000400	-0.33277700	2.04041500
C	-0.51864000	-0.21725400	0.34368200
C	-5.80242700	0.93053000	-0.56005000
C	-3.40651400	1.75003700	-0.60728300
C	-4.84705100	2.07268000	-0.17912800
C	-5.32990600	-0.40620500	0.03300900
C	-2.94539100	0.41169200	-0.00624700
C	-3.89548300	-0.75303600	-0.39561500
H	1.78808100	-0.87021500	1.28478400
C	2.59598600	-1.91304800	-0.37203400
C	2.82744700	0.58468300	0.09351500
C	3.37036200	1.16256900	1.24786500
C	3.08572000	1.16676500	-1.15645700
C	4.16388300	2.31092500	1.15692300
H	3.16322900	0.71506100	2.21792400
C	3.87850100	2.31348800	-1.24849400
H	2.67806700	0.72196700	-2.06171600
C	4.41894800	2.88822100	-0.09133700
H	4.57808400	2.75494300	2.05978100
H	4.07625100	2.75720100	-2.22214000
H	5.03516600	3.78213700	-0.16384400
F	1.86565000	-3.02411800	-0.09667700
F	2.71577500	-1.84470900	-1.73371600
F	3.83975800	-2.10637200	0.13408000
H	-2.54470700	-2.26035800	-0.10817000

Catalyst A

Total Energy= -1147.659103
Imaginary frequency= 0

XYZ coordinates

H	4.69094300	-1.37312000	1.41616500
H	5.46266100	1.71868500	-0.68486100
H	2.64078400	0.06958500	1.16562300
H	4.91036300	1.20712400	0.91622100
H	-1.11230800	-0.42363600	-0.96115800
H	3.40013000	0.73652200	-1.72168700
H	0.90269800	-1.09003300	-0.61794000
H	5.60160700	-0.64861900	-1.42975400

H	6.56077200	-0.44320600	0.04408200
H	3.24054200	-1.69317800	-1.25681900
H	5.12899700	-2.52305800	0.13973200
C	-2.24292500	1.13478500	-0.08557900
N	1.21234900	-0.15723200	-0.35449300
N	-1.01668800	0.34894800	-0.31153900
S	0.55673300	2.05607500	1.06607400
C	0.24008800	0.69167700	0.08880200
C	5.53618500	-0.43379100	-0.35183100
C	3.23713800	-1.52590500	-0.16828800
C	4.69642500	-1.52999900	0.32583200
C	4.89042500	0.94683500	-0.15322600
C	2.61441300	-0.13633400	0.08375000
C	3.43314600	0.94663400	-0.64183900
H	-2.12178600	1.61534700	0.89000900
C	-2.40338900	2.22783900	-1.15537900
C	-3.42670700	0.18275200	-0.02105600
C	-3.87280600	-0.49363400	-1.16774500
C	-4.08325500	-0.04375800	1.19634100
C	-4.94971600	-1.38300000	-1.09709500
H	-3.38176900	-0.32074100	-2.12426300
C	-5.16722000	-0.92572500	1.27003300
H	-3.74013600	0.47611700	2.08960500
C	-5.60165200	-1.59950300	0.12304900
H	-5.28412600	-1.90125200	-1.99399600
H	-5.66963900	-1.08812900	2.22184100
H	-6.44358700	-2.28694400	0.17808400
H	2.96152500	1.91943100	-0.46990000
N	2.38792400	-2.57937700	0.41860300
H	2.39511900	-2.48886600	1.43445700
H	-1.52728700	2.88593000	-1.13271000
H	-3.30435800	2.82103900	-0.95351600
H	-2.49374200	1.78477600	-2.15500600
H	2.78887300	-3.49057200	0.20598000

Catalyst B

Total Energy= -1147.657829
Imaginary frequency= 0

XYZ coordinates

H	5.00319200	0.01652200	1.10381000
H	3.63681400	-3.31419900	-0.09438100
H	2.41786300	0.07675300	1.17180800
H	3.71046900	-2.22559200	1.29981700
H	-0.76406400	1.50688300	-1.50076800
H	2.32136400	-1.63060800	-1.37395800
H	1.20423500	0.71192400	-1.44155900
H	4.92735000	-1.67592900	-1.46512700
H	5.83478400	-2.06828600	0.00356700
H	3.64687900	0.56878800	-1.57536700
H	5.83279900	0.40975100	-0.41092800

C	-2.33876300	1.51474200	-0.09339200
N	1.23051800	0.63273700	-0.42990400
N	-0.94444600	1.34717700	-0.51636100
S	-0.14056600	0.45835300	1.89638100
C	0.05665900	0.81425500	0.24315000
C	4.92671200	-1.57555000	-0.36857900
C	3.68710300	0.65195600	-0.46878000
C	4.94714600	-0.08684800	0.01042600
C	3.67178600	-2.25685500	0.20044400
C	2.42881900	-0.04124900	0.08373600
C	2.40196300	-1.53745200	-0.27929100
H	-2.31863300	1.88590600	0.93651700
H	1.50224600	-1.98532800	0.16056500
N	3.73311700	2.04972400	-0.00836200
H	4.50724500	2.52850800	-0.46483000
C	-3.12547800	0.20910900	-0.11323000
C	-4.02510600	-0.07585500	0.92158600
C	-3.01204100	-0.69113800	-1.18152400
C	-4.80169700	-1.23888000	0.89201900
H	-4.10504000	0.61343300	1.76112900
C	-3.78292400	-1.85730500	-1.21436500
H	-2.30820200	-0.48532200	-1.98657100
C	-4.68260500	-2.13383000	-0.17754100
H	-5.49074900	-1.45141400	1.70751800
H	-3.68139300	-2.55081000	-2.04751100
H	-5.28054500	-3.04296800	-0.20025200
C	-2.99635900	2.56729900	-1.00087600
H	-2.46454700	3.52448200	-0.92891600
H	-2.98993100	2.22951400	-2.04664100
H	-4.03920400	2.71286100	-0.69906100
H	2.88050500	2.52962200	-0.29126900

KE-A_F-Maj-Cx1

Total Energy= -2251.995559

Imaginary frequency= 0

XYZ coordinates

H	-5.40336300	-0.41941000	-1.66319300
H	-6.19343900	2.81987300	0.15882800
H	-3.30218000	1.10761700	-1.60278100
H	-5.68089600	2.16226000	-1.40288600
H	0.25153500	1.40610900	0.94555200
H	-4.06708500	2.04067400	1.20999800
H	-1.67338500	0.65630400	0.82173400
H	-6.18241600	0.53290800	1.15116600
H	-7.22582500	0.55382700	-0.27850100
H	-3.77856400	-0.54246100	0.92605300
H	-5.72714800	-1.46950100	-0.27345500
C	1.45130700	2.53976000	-0.36732700
N	-1.90374600	1.09756200	-0.07168400
N	0.20926600	1.93493700	0.07917000

S	-1.12828800	2.59246900	-2.18525000
C	-0.94430300	1.84986300	-0.65938700
C	-6.18374500	0.64284700	0.05580200
C	-3.85807200	-0.40069300	-0.16108100
C	-5.34356800	-0.48396400	-0.56554600
C	-5.60988200	2.01905900	-0.31386200
C	-3.29221000	0.99551100	-0.51215200
C	-4.14012800	2.11927400	0.11464600
H	1.26617500	2.93941700	-1.37066700
C	1.75645700	3.77507800	0.50637500
C	2.59987100	1.54618400	-0.42055500
C	3.05083900	0.88056300	0.72754400
C	3.18522800	1.25257600	-1.65912000
C	4.07394800	-0.06562900	0.63605700
H	2.60170300	1.09029400	1.69444500
C	4.20810000	0.30584300	-1.75231500
H	2.82475200	1.75722900	-2.55319900
C	4.65231200	-0.35696400	-0.60399200
H	4.40713000	-0.58494200	1.53196400
H	4.64503800	0.07504800	-2.72116100
H	5.44221000	-1.10189200	-0.67524000
H	-3.70496200	3.08148500	-0.18130700
F	2.92552000	4.35963500	0.13368600
F	0.77950500	4.71202000	0.39470300
F	1.85987600	3.47055600	1.83463700
N	-3.10054900	-1.47572400	-0.78699900
H	-3.13457800	-1.52461300	-1.79604100
C	-2.30406600	-2.35408200	-0.10683000
H	-2.33338800	-2.22405300	0.97384200
C	-1.51850700	-3.33421900	-0.63793400
C	-1.41785300	-3.59296400	-2.11525300
H	-0.39289900	-3.89079600	-2.37544000
H	-2.08596600	-4.41457900	-2.42434000
H	-1.66356600	-2.71370700	-2.72426000
C	-0.80537600	-4.30313400	0.26174700
H	-0.87844700	-4.01119000	1.31652400
H	-1.22048700	-5.31981400	0.16020100
H	0.26101600	-4.36917700	-0.00788300
C	1.20596300	-1.79648900	-1.34874300
C	0.83308800	-1.16140400	-2.55466100
C	2.18940700	-2.80881600	-1.39204000
C	1.42894300	-1.51861800	-3.76137900
H	0.08535700	-0.37017500	-2.52483100
C	2.77572500	-3.17204700	-2.60235600
H	2.49019600	-3.30811800	-0.47488600
C	2.40259300	-2.52585000	-3.78944500
H	1.13955400	-1.01221800	-4.67991500
H	3.53122100	-3.95489600	-2.62419000
H	2.86823400	-2.80828700	-4.73165700
C	0.57163400	-1.36541500	-0.12493000
H	-0.24071200	-0.66073100	-0.25345500

C	0.96677500	-1.66431800	1.15321200
H	1.79807200	-2.33371100	1.34536400
C	0.31132900	-1.08530600	2.28749600
O	-0.60908500	-0.23860700	2.25237100
C	0.85109300	-1.55928000	3.65893200
O	1.94622600	-2.07150600	3.81739900
O	-0.03139100	-1.32176200	4.64559800
C	0.39062000	-1.71017200	5.98340800
H	-0.44938900	-1.45547300	6.63266900
H	0.59932400	-2.78550500	6.01497200
H	1.28974700	-1.15278500	6.26852500

KE-A_F-Maj-TS1

Total Energy= -2251.983711

Imaginary frequency= 1

XYZ coordinates

H	-5.09610000	-1.19701400	-2.19373800
H	-6.53190700	2.07961200	-0.89814700
H	-3.24800700	0.61818100	-2.07299700
H	-5.72894700	1.34350700	-2.29276700
H	0.01310300	1.29722700	0.72674600
H	-4.48282000	1.73416000	0.49330400
H	-1.82400000	0.44854600	0.49878600
H	-6.37689900	-0.06440200	0.35886000
H	-7.19998100	-0.33956800	-1.18357200
H	-3.85663300	-0.78778200	0.58183300
H	-5.48224200	-2.12262400	-0.73018700
C	1.18975300	2.59754400	-0.44871800
N	-2.06155600	0.92571800	-0.39168500
N	0.02116200	1.79268700	-0.16003400
S	-1.24291200	2.44659500	-2.47355000
C	-1.10168200	1.69652000	-0.94434400
C	-6.23651200	-0.07052500	-0.73239800
C	-3.81214800	-0.77326400	-0.51410600
C	-5.18667400	-1.13242800	-1.09875700
C	-5.79142300	1.32563700	-1.19414600
C	-3.35896800	0.62889400	-0.98003100
C	-4.41871600	1.68213100	-0.60335100
H	1.01716100	3.08083500	-1.41644400
C	1.27232700	3.74802700	0.57963800
C	2.47740500	1.79202300	-0.50418400
C	2.80755600	0.88249800	0.50828200
C	3.34285700	1.95506500	-1.59326700
C	3.98362300	0.13505500	0.42564900
H	2.14032900	0.72819100	1.35108700
C	4.52449200	1.21283900	-1.67258600
H	3.08283700	2.65740800	-2.38353100
C	4.84573000	0.29973900	-0.66284000
H	4.21817700	-0.58381100	1.20721700
H	5.18572900	1.33798000	-2.52775700

H	5.75577800	-0.29243600	-0.73176700
H	-4.06952800	2.65540800	-0.96636700
F	2.34326100	4.54925800	0.33693900
F	0.16263000	4.53187600	0.54116100
F	1.38937500	3.28830100	1.86059400
N	-2.80650000	-1.76833100	-0.90870400
H	-2.63328300	-1.84466300	-1.90657900
C	-2.00585800	-2.40747100	-0.07752800
H	-2.23165200	-2.28403300	0.97796800
C	-0.83929000	-3.13078900	-0.47053800
C	-0.71028700	-3.43563000	-1.95506800
H	0.23375500	-3.95163600	-2.15057900
H	-1.53576800	-4.08630100	-2.28083200
H	-0.71573400	-2.52513700	-2.56846800
C	-0.48843400	-4.30144100	0.43332400
H	-0.52092100	-4.00668900	1.48830800
H	-1.19279100	-5.13019500	0.27428100
H	0.51837400	-4.66375700	0.19673500
C	1.66017600	-2.09084800	-0.88745800
C	1.84476100	-1.41973200	-2.10848900
C	2.58441200	-3.08522800	-0.52005500
C	2.92062100	-1.73093000	-2.94056600
H	1.14817700	-0.63245100	-2.38996600
C	3.65503200	-3.40590800	-1.35643700
H	2.47204100	-3.60216200	0.42901700
C	3.82529900	-2.73277200	-2.57244200
H	3.05798100	-1.18566700	-3.87205600
H	4.36160000	-4.17779100	-1.05680500
H	4.66437600	-2.97808100	-3.22069600
C	0.49614600	-1.73256800	-0.03447100
H	-0.04547400	-0.87888400	-0.44190400
C	0.71215000	-1.66899100	1.39042700
H	1.55348200	-2.19995100	1.81994900
C	-0.12858300	-0.97263600	2.24752600
O	-1.18138000	-0.31847800	1.91132600
C	0.27027400	-1.01944100	3.73201300
O	1.32879200	-1.45259600	4.16239600
O	-0.70004500	-0.50960700	4.52650600
C	-0.40594900	-0.49158300	5.94742700
H	-1.28838000	-0.05152900	6.41776000
H	-0.23584800	-1.51045500	6.31504600
H	0.48399200	0.11773600	6.14291400

KE-A_F-Min-Cx1

Total Energy= -2251.996095
Imaginary frequency= 0

XYZ coordinates

H	-4.44733900	-0.69382100	-2.32049100
H	-5.97850400	2.64826700	-1.35016100
H	-2.66283800	1.06911600	-2.29286000

H	-5.14127800	1.79801300	-2.65757800
H	0.49540400	2.05470500	0.58148100
H	-3.97289300	2.45997600	0.10250400
H	-1.56610100	2.08808200	0.24347100
H	-5.85493100	0.61291200	0.08318100
H	-6.62708200	0.20661600	-1.45689400
H	-3.41368700	-0.00196400	0.47316200
H	-4.90195000	-1.51768900	-0.81919300
C	2.11108000	2.03158900	-0.77732200
N	-1.52352800	1.66841100	-0.67842600
N	0.72818300	1.85144500	-0.38718100
S	-0.03548900	0.86391000	-2.79019700
C	-0.29596600	1.48975100	-1.22337400
C	-5.67858500	0.51661300	-0.99924600
C	-3.25435100	-0.13507800	-0.60835500
C	-4.60067100	-0.55026600	-1.24012800
C	-5.23055500	1.87364500	-1.56360400
C	-2.80372000	1.21264700	-1.21581400
C	-3.87124500	2.29438700	-0.98166100
H	2.18148700	1.79061200	-1.84350900
C	2.46494700	3.53322800	-0.66373300
C	3.08947100	1.16648300	0.00266300
C	2.89506600	0.87848200	1.35990900
C	4.20911700	0.64717900	-0.65861500
C	3.80141800	0.06082900	2.04002000
H	2.03173300	1.27147000	1.89057500
C	5.12054800	-0.16276100	0.02336400
H	4.35649200	0.86611700	-1.71450800
C	4.91556000	-0.46125400	1.37429800
H	3.63373400	-0.17046200	3.08977700
H	5.97950100	-0.57291100	-0.50350400
H	5.61615700	-1.10331200	1.90420700
H	-3.52781700	3.23396000	-1.43156100
N	-2.20407900	-1.13452900	-0.78495600
H	-1.65209900	-1.02941300	-1.62994200
C	-2.33527900	-2.39501800	-0.25780300
H	-2.94766800	-2.43121300	0.64294100
C	-1.72498800	-3.53098300	-0.68652200
C	-0.89148500	-3.62068800	-1.93369700
H	-1.26091200	-4.43538600	-2.57680200
H	-0.88402900	-2.69899300	-2.52741500
H	0.15269000	-3.86007700	-1.68347600
C	-1.88072100	-4.81128700	0.08650200
H	-2.34316600	-5.59499400	-0.53573700
H	-0.89616000	-5.20049900	0.39459700
H	-2.49310200	-4.67271600	0.98644600
C	0.19644600	-2.34499200	1.38606600
C	-0.12801100	-1.03213900	1.58281500
H	0.43162600	-0.24308800	1.09647800
C	-1.24299700	-0.66246400	2.42121200
O	-2.04860200	-1.44281000	2.94147900

C	-1.40782600	0.86868500	2.65386200
O	-0.59463300	1.72045200	2.30775300
O	-2.54948200	1.15366600	3.28745600
C	-2.78856100	2.55696900	3.59834200
H	-3.75198100	2.57315800	4.11073700
H	-1.99006300	2.93499400	4.24534200
H	-2.82534200	3.14700900	2.67625900
C	1.24658900	-2.83444200	0.51722800
C	1.68463200	-4.17191000	0.64666600
C	1.82558900	-2.03208500	-0.49116300
C	2.68341300	-4.68079900	-0.18405700
H	1.23870200	-4.80140400	1.41449700
C	2.81873000	-2.54346900	-1.32051500
H	1.47720700	-1.01462100	-0.63763200
C	3.25694000	-3.86672900	-1.16921200
H	3.01353500	-5.71113400	-0.06673700
H	3.25008500	-1.90967900	-2.09136300
H	4.03329100	-4.26310900	-1.82069000
H	-0.34010000	-3.09113000	1.97042900
F	2.33661800	3.99182800	0.61527000
F	1.65240600	4.29514600	-1.44308900
F	3.74268800	3.77164300	-1.05564700

KE-A_F-Min-TS1

Total Energy= -2251.982991

Imaginary frequency= 1

XYZ coordinates

H	-4.41609600	-1.74862800	-2.22928600
H	-6.84041300	0.34225700	-0.14787100
H	-3.48217800	0.55985500	-1.87360200
H	-6.05690100	0.25647700	-1.73218000
H	-0.21781200	1.80133600	0.75312000
H	-4.64480600	0.69614700	0.95992800
H	-2.25827100	1.30578500	0.70591800
H	-5.66773200	-1.72589600	0.58109900
H	-6.53612300	-2.04234500	-0.92824400
H	-3.15964100	-1.32059600	0.53042000
H	-4.20803400	-2.99415800	-0.98175600
C	0.97687900	2.74056200	-0.73248800
N	-2.29900500	1.18247500	-0.29970200
N	-0.18834300	2.03491300	-0.24298400
S	-1.14177600	1.49361700	-2.72377600
C	-1.21432500	1.58321600	-1.01629000
C	-5.70042700	-1.48145700	-0.49103100
C	-3.20768800	-1.12420700	-0.54948100
C	-4.38082400	-1.92316600	-1.14404300
C	-5.92366500	0.03014200	-0.66390500
C	-3.42032500	0.38601500	-0.79411500
C	-4.72905700	0.83800100	-0.12895400
H	0.96978600	2.67516300	-1.82601300

C	0.82337300	4.24879600	-0.41065800
C	2.29015900	2.19818100	-0.19562200
C	2.45673600	1.88193400	1.16035400
C	3.37365400	2.05899800	-1.07336700
C	3.69425500	1.43323400	1.62932600
H	1.62757000	1.97885500	1.85523500
C	4.61428800	1.62186300	-0.60092500
H	3.24466600	2.30031300	-2.12670200
C	4.77686300	1.31010900	0.75250100
H	3.81105700	1.18062400	2.68087300
H	5.44913100	1.51861300	-1.29106000
H	5.73851500	0.95906400	1.12031300
H	-4.86726200	1.90955600	-0.31646000
N	-1.90978300	-1.53984700	-1.10379500
H	-1.41122900	-0.85811600	-1.67684600
C	-1.36043900	-2.71668700	-0.89257000
H	-1.95154800	-3.43076200	-0.32756000
C	-0.00277400	-3.01643700	-1.22105300
C	0.66865600	-2.10276800	-2.23525900
H	0.13950900	-2.14534400	-3.19826500
H	0.68821300	-1.05755300	-1.90098300
H	1.70264300	-2.42148900	-2.39575000
C	0.24892400	-4.49867100	-1.46445700
H	-0.16459000	-4.79751300	-2.43822100
H	1.32435700	-4.70404300	-1.47865700
H	-0.21800200	-5.11613700	-0.68627800
C	0.84734200	-2.64072800	0.51534600
C	0.40285900	-1.41018200	1.12330700
H	1.00552100	-0.51031800	1.06891800
C	-0.78991500	-1.41775100	1.85767400
O	-1.59432300	-2.39633600	1.94522500
C	-1.10495600	-0.13286600	2.63613800
O	-0.64942300	0.99029500	2.40490500
O	-1.98044400	-0.35011300	3.63263500
C	-2.35456200	0.80836000	4.42716900
H	-3.05699100	0.42780000	5.17154300
H	-1.46934800	1.23937900	4.90769100
H	-2.82979700	1.56506300	3.79245700
C	2.30207400	-2.80747100	0.24247700
C	2.89801300	-4.06668400	0.44659600
C	3.11424900	-1.75244200	-0.21362000
C	4.25775100	-4.27256400	0.19811200
H	2.28381700	-4.88675000	0.81338900
C	4.47081200	-1.95833400	-0.46984100
H	2.68821600	-0.76447300	-0.36455900
C	5.04920800	-3.21809100	-0.27009800
H	4.69701300	-5.25356800	0.37030500
H	5.07748000	-1.12746500	-0.82009800
H	6.10785000	-3.37301000	-0.47016700
H	0.42211800	-3.51587700	1.01135600
F	0.75684300	4.48756500	0.92985800

F	-0.30955200	4.75889900	-0.96199500
F	1.87030000	4.96385700	-0.90071700

KE-A_F-Maj-Cx4

Total Energy= -2251.997919

Imaginary frequency= 0

XYZ coordinates

H	-4.45552400	-0.04177600	-2.25702200
H	-5.68875400	3.43592700	-1.26409200
H	-2.52239600	1.53401500	-1.91501900
H	-4.77933900	2.56526200	-2.50854700
H	0.58134000	1.44502400	1.02741000
H	-3.92636300	2.89632300	0.42727700
H	-1.47970700	1.46057200	0.83007000
H	-6.00776600	1.32952700	0.01921600
H	-6.59549500	1.10391000	-1.63555700
H	-3.71547900	0.42823200	0.67113400
H	-5.20493400	-0.85155400	-0.86809400
C	2.10344600	2.41421800	-0.08667800
N	-1.49422000	1.79008900	-0.13575500
N	0.76242700	1.92361200	0.14526800
S	-0.14196500	2.64987100	-2.30917700
C	-0.30472300	2.10654600	-0.69791000
C	-5.69231500	1.26950100	-1.03357600
C	-3.43758400	0.30093300	-0.38460200
C	-4.72937000	0.08209000	-1.19895400
C	-5.01136200	2.58886300	-1.43302700
C	-2.75501300	1.60236200	-0.84715600
C	-3.70724900	2.79454400	-0.64580000
H	2.15748700	2.73499700	-1.13261000
C	2.33930900	3.69631700	0.74923300
C	3.17551100	1.37168300	0.18217900
C	3.18804300	0.62290200	1.36784000
C	4.18316900	1.16898200	-0.76973600
C	4.19441000	-0.31927600	1.59368200
H	2.41393000	0.76907500	2.11712300
C	5.19351800	0.22956300	-0.54153900
H	4.17250800	1.74824500	-1.69104400
C	5.20053300	-0.51562900	0.64162700
H	4.18973800	-0.90222200	2.51204400
H	5.96866300	0.07653700	-1.28959700
H	5.98039400	-1.25349400	0.81744900
H	-3.18968700	3.70422300	-0.97228200
F	3.57626300	4.21279600	0.51511700
F	1.43275000	4.66022900	0.44494500
F	2.24141500	3.46708700	2.09044900
N	-2.54094200	-0.86733900	-0.43464500
H	-2.98958500	-1.70588900	-0.08559700
C	-1.64713500	-1.07165000	-1.47080200
H	-1.25610200	-0.16390400	-1.92206200

C	-1.17143300	-2.26671500	-1.90489500
C	-1.61939300	-3.60042400	-1.37998800
H	-1.86873400	-4.27198800	-2.21524900
H	-0.80182000	-4.08538800	-0.82350000
H	-2.49107900	-3.55176200	-0.71632900
C	-0.13976600	-2.31012500	-2.99766600
H	0.15647100	-1.30375900	-3.31835600
H	0.76323600	-2.84043700	-2.65858400
H	-0.52192000	-2.86032900	-3.87277600
C	1.63846600	-2.74469700	-0.00340700
C	2.63257100	-2.29745200	-0.90142900
C	1.53949400	-4.13165400	0.25503800
C	3.49064000	-3.20068700	-1.52670400
H	2.72660200	-1.23153400	-1.09402600
C	2.39647100	-5.03256600	-0.37335600
H	0.80121800	-4.49794800	0.96425600
C	3.37393200	-4.57160100	-1.26822100
H	4.25268800	-2.83579300	-2.21201100
H	2.31098900	-6.09669900	-0.16263400
H	4.04351300	-5.27851500	-1.75405500
C	0.77649400	-1.75866800	0.61596100
H	1.03127300	-0.72127200	0.40710200
C	-0.29184600	-1.99256200	1.42841100
H	-0.65868700	-3.00046300	1.59278300
C	-1.04028400	-0.89946900	2.00794200
O	-0.61318400	0.26406000	2.14427200
C	-2.46721600	-1.17003900	2.53832900
O	-3.16789600	-0.30864000	3.03093500
O	-2.86211900	-2.45734200	2.35856800
C	-4.20447400	-2.78141300	2.81949600
H	-4.33181000	-3.84469300	2.60630600
H	-4.29077100	-2.58295300	3.89320800
H	-4.94285500	-2.18085100	2.27586700

KE-A_F-Maj-TS4

Total Energy= -2251.982761

Imaginary frequency= 1

XYZ coordinates

H	-4.63986400	-0.52339200	-2.36212900
H	-6.44529200	2.37886900	-0.70559400
H	-2.96226700	1.41775400	-1.85572000
H	-5.51100700	1.92087100	-2.13772200
H	0.20359000	1.25635900	0.94073400
H	-4.45044700	2.00534600	0.74746100
H	-1.78222700	1.03235200	0.80860700
H	-6.14943800	0.09133200	0.24585700
H	-6.87149800	-0.02391400	-1.36699900
H	-3.60755600	-0.41309900	0.51909000
H	-5.01682100	-1.69238900	-1.08125900
C	1.54026600	2.67839300	0.07347800

N	-1.92675700	1.56713100	-0.05760100
N	0.29130400	1.96375300	0.19872300
S	-0.80554300	2.98819600	-2.06836200
C	-0.81870700	2.15614000	-0.57588500
C	-5.96026200	0.25900800	-0.82478200
C	-3.48954800	-0.24756800	-0.56160100
C	-4.79674400	-0.63484200	-1.27954400
C	-5.62561100	1.74005600	-1.05818400
C	-3.14488000	1.23599800	-0.78958900
C	-4.32341600	2.12042800	-0.33862000
H	1.58528900	3.11546400	-0.93027300
C	1.55065900	3.88798300	1.04666800
C	2.75312200	1.79324700	0.30962400
C	2.80179600	0.88682000	1.37969100
C	3.86635300	1.92588400	-0.53061000
C	3.95266500	0.12807300	1.60447900
H	1.94572100	0.76422500	2.03866400
C	5.02072300	1.17053900	-0.30065000
H	3.82846400	2.62701900	-1.36223400
C	5.06660700	0.27390700	0.77109400
H	3.97619000	-0.58096400	2.42892600
H	5.87900400	1.28028100	-0.96040300
H	5.95982800	-0.32167000	0.94685800
H	-4.05087500	3.16393700	-0.53408500
F	2.69059800	4.61978500	0.90462600
F	0.50476400	4.72259500	0.81565100
F	1.47295700	3.50427000	2.35098700
N	-2.41681500	-1.17288100	-0.98678000
H	-2.54963400	-2.13190700	-0.68373800
C	-1.34750200	-0.90656800	-1.70750000
H	-1.20393400	0.12583600	-2.01483000
C	-0.32373100	-1.85505600	-1.99252000
C	-0.72769500	-3.31805900	-2.08560500
H	-1.41225600	-3.46335400	-2.93327000
H	0.15908800	-3.93767800	-2.25161800
H	-1.21962400	-3.67916300	-1.17377600
C	0.59989600	-1.40832800	-3.11724400
H	0.91788100	-0.36685400	-2.98617900
H	1.49025200	-2.04318900	-3.15629500
H	0.08071500	-1.49319000	-4.08290400
C	1.93616300	-2.46902500	-0.59834800
C	3.04837200	-1.75562300	-1.07896000
C	2.05252200	-3.86429900	-0.44593800
C	4.23712400	-2.41151100	-1.40468100
H	2.98244700	-0.67527900	-1.17754500
C	3.23867100	-4.52250100	-0.77521600
H	1.21506300	-4.43795200	-0.05917000
C	4.33631300	-3.79931600	-1.26056400
H	5.08765600	-1.83510800	-1.76236900
H	3.30984500	-5.60113200	-0.64737800
H	5.26175500	-4.31323300	-1.51354300

C	0.68815900	-1.72714800	-0.27036600
H	0.85635500	-0.65074500	-0.23807600
C	-0.16209600	-2.20814600	0.78800200
H	-0.31428000	-3.27648400	0.90079000
C	-0.83650900	-1.36817400	1.67467000
O	-0.70539800	-0.10550600	1.81460100
C	-1.93161300	-2.00992100	2.53668300
O	-3.01170100	-1.48062400	2.74103900
O	-1.58357100	-3.22256200	3.03422500
C	-2.60101600	-3.90763200	3.81766100
H	-2.13263400	-4.83844700	4.14497600
H	-2.89289000	-3.29366200	4.67672100
H	-3.48203400	-4.11086100	3.19768100

KE-A_F-Min-Cx4

Total Energy= -2251.989391

Imaginary frequency= 0

XYZ coordinates

H	-2.15438500	4.58081500	-1.35581200
H	-0.73859600	6.43449600	1.64501000
H	0.32482700	3.88250500	-0.97718900
H	-0.53955300	6.20337500	-0.09919700
H	2.14576200	0.33214800	0.86653100
H	-0.10941200	4.05659600	2.05634100
H	0.72861400	1.87766800	1.16107100
H	-2.58894900	4.76778400	1.67918300
H	-2.95312600	6.03570900	0.49767600
H	-1.69565000	2.47834900	0.82367000
H	-3.42410100	3.75057900	-0.43482400
C	3.32216500	-0.19172600	-0.80653400
N	0.93130300	2.35581900	0.28311300
N	2.42622900	0.66702500	-0.05532000
S	2.19656400	2.41772600	-2.10886700
C	1.82737000	1.79293200	-0.56298600
C	-2.27483700	5.20076200	0.71738900
C	-1.44192200	2.95107800	-0.13610200
C	-2.39531900	4.13299800	-0.37883300
C	-0.82643800	5.69804300	0.83549800
C	0.02071600	3.45953400	-0.01529300
C	0.13141400	4.52517600	1.08969900
H	3.52805800	0.32386900	-1.75179200
C	4.68497100	-0.27155500	-0.09101900
C	2.72421200	-1.55858900	-1.10757400
C	2.35276000	-2.44397800	-0.08496400
C	2.51336100	-1.92660000	-2.44252500
C	1.77869400	-3.67916700	-0.39598600
H	2.51189500	-2.16510000	0.95142200
C	1.94090200	-3.16387700	-2.75462400
H	2.79126900	-1.23662900	-3.23671200
C	1.57371700	-4.04368400	-1.73191200

H	1.49214700	-4.35895700	0.40433100
H	1.77834700	-3.43689900	-3.79532100
H	1.12478300	-5.00519900	-1.97294200
H	1.17179200	4.86949900	1.13974200
N	-1.61974100	1.96815200	-1.20718300
H	-2.28108700	2.21918900	-1.92895000
C	-1.32327200	0.63889900	-1.05784300
H	-0.55168200	0.43421300	-0.32525400
C	-1.86962900	-0.40812900	-1.73740400
C	-2.99864200	-0.25647900	-2.71599000
H	-3.72149300	-1.07411600	-2.58107300
H	-3.54495000	0.68841200	-2.59566900
H	-2.64091600	-0.30856900	-3.75761000
C	-1.29811000	-1.78474000	-1.57899800
H	-2.09430800	-2.50752200	-1.33539300
H	-0.82658400	-2.13335700	-2.51074400
H	-0.53376800	-1.82261700	-0.79528900
C	-2.91028800	-0.63378100	1.11264800
C	-1.83859500	-1.19475600	1.75839900
H	-1.71774600	-2.27145400	1.81958000
C	-0.77904700	-0.37293200	2.28054600
O	-0.77277300	0.87075600	2.32598700
C	0.51773800	-1.07418400	2.73956600
O	1.61856000	-0.55959300	2.62079400
O	0.29927300	-2.27806800	3.29291400
C	1.47500400	-2.99081700	3.78625500
H	1.08724800	-3.91893100	4.20961600
H	2.16313400	-3.19333800	2.95925400
H	1.98004300	-2.38849700	4.54833100
C	-4.01969300	-1.33371200	0.49886600
C	-5.08971700	-0.57716500	-0.03151400
C	-4.08048200	-2.74331800	0.39820100
C	-6.18297300	-1.20110900	-0.62881200
H	-5.04573100	0.50883900	0.03072100
C	-5.17426400	-3.36511600	-0.20121900
H	-3.27007200	-3.34941800	0.79427300
C	-6.22988600	-2.59906700	-0.71552900
H	-6.99761400	-0.60181400	-1.03007200
H	-5.20699900	-4.45057600	-0.26974000
H	-7.08222700	-3.08894800	-1.18173500
H	-2.97205800	0.45287500	1.10157000
F	4.59367000	-0.76998100	1.17652800
F	5.26140500	0.95439200	0.00928900
F	5.54643600	-1.07107400	-0.77708300

KE-A_F-Min-TS4

Total Energy= -2251.976763

Imaginary frequency= 1

XYZ coordinates

H	-0.25014600	5.28617400	-1.18764400

H	2.60326400	6.38366100	1.03996800
H	1.58660000	3.43470000	-1.16826000
H	2.18085400	5.96144000	-0.62720500
H	2.10890200	-0.37678900	0.92552700
H	2.12587900	4.05596900	1.78354400
H	1.23352300	1.56146900	1.08474500
H	0.27454800	5.87628900	1.77988600
H	0.23374500	7.07104400	0.47332100
H	-0.32659700	3.37319300	1.21139400
H	-1.47316300	5.28193600	0.09978900
C	2.95898600	-1.35884800	-0.75148000
N	1.71548400	1.92363300	0.25080100
N	2.51576400	-0.19889800	0.00261700
S	3.02284500	1.46658400	-2.07448100
C	2.39087700	1.05355000	-0.53910900
C	0.47976400	6.02803900	0.70966700
C	-0.10822000	3.61077700	0.16314400
C	-0.41214200	5.09303000	-0.11650500
C	1.96076800	5.73804200	0.42760900
C	1.38528900	3.30511200	-0.09974400
C	2.27700400	4.26519800	0.71405000
H	3.42920100	-0.97553600	-1.66447800
C	4.09387000	-2.07401700	0.00450800
C	1.81524800	-2.28627900	-1.13959300
C	1.02924000	-2.93128600	-0.17402600
C	1.51604500	-2.46519600	-2.49666600
C	-0.03993300	-3.74283200	-0.55948900
H	1.25684200	-2.80012500	0.87754100
C	0.44552700	-3.27756900	-2.88443200
H	2.11920000	-1.95883600	-3.24759000
C	-0.33444700	-3.91865900	-1.91661800
H	-0.64352200	-4.23445100	0.20074900
H	0.21903100	-3.40483900	-3.94108000
H	-1.17034500	-4.54719900	-2.21729500
H	3.32072900	4.02862800	0.47528400
N	-1.04814200	2.80778300	-0.65758500
H	-1.85211500	3.32228500	-1.00414500
C	-1.08344900	1.49052500	-0.76149000
H	-0.20809200	0.95827500	-0.43000800
C	-2.19333400	0.72674100	-1.22096300
C	-3.31899900	1.48130000	-1.90401600
H	-4.14281300	0.80105400	-2.13838700
H	-3.72527700	2.28367800	-1.27292900
H	-2.96020700	1.92595600	-2.84458800
C	-1.80894700	-0.58192600	-1.88859500
H	-2.69362700	-1.21677200	-2.00982900
H	-1.38921800	-0.39275200	-2.88621800
H	-1.06199600	-1.12432900	-1.29918900
C	-2.88426000	0.18268000	0.59349900
C	-1.95431400	-0.66741000	1.29191000
H	-2.11670200	-1.73882200	1.30540600

C	-0.82636000	-0.15314400	1.92428600
O	-0.46894200	1.07372300	1.94560100
C	0.14587300	-1.13478800	2.57541100
O	1.35424400	-0.93657800	2.63529600
O	-0.44326700	-2.23555200	3.08951200
C	0.44332000	-3.21710300	3.69957900
H	-0.21509000	-4.00884200	4.06290300
H	1.14771400	-3.60680100	2.95622900
H	0.99958300	-2.75898200	4.52419000
C	-4.22349900	-0.37578600	0.27471800
C	-5.35728600	0.45301400	0.36488900
C	-4.40535300	-1.71383200	-0.12547400
C	-6.63284900	-0.03639300	0.07500800
H	-5.22994200	1.48905500	0.67344000
C	-5.67856500	-2.20346200	-0.42415600
H	-3.54509700	-2.37345900	-0.20163000
C	-6.79806700	-1.36745200	-0.32589100
H	-7.49700600	0.61969400	0.16123400
H	-5.79881500	-3.24059700	-0.73178900
H	-7.79000100	-1.75177200	-0.55521200
H	-2.93822800	1.19862900	0.98998500
F	3.72154100	-2.52561600	1.23589800
F	5.15769700	-1.25008000	0.19155500
F	4.53344200	-3.15098200	-0.70303600

KE-B-Maj-Cx1

Total Energy= -1954.284608

Imaginary frequency= 0

XYZ coordinates

H	2.51315400	3.96222400	-0.07973000
H	0.65755800	2.57479600	-3.02338000
H	3.53389100	2.55067400	0.19905300
H	3.92046500	3.67881100	-1.12055400
H	4.77390000	-3.82564000	0.15753100
H	1.68598400	0.58598900	-2.46664900
H	5.11322700	-1.06987400	-2.45177700
H	3.18390400	-1.85492600	0.69710300
H	5.30038100	-1.41369000	-0.72302900
H	0.60347300	3.82323900	-1.75719100
H	1.82382600	3.92002600	-3.03527100
H	-1.09197200	-1.17457600	0.13014900
H	2.67040700	-1.40522200	-2.28487900
H	0.72112600	-1.38956000	-0.84007400
H	3.82082800	0.57075700	-0.40467300
H	4.30419100	-3.39549400	-2.84673500
H	5.88164600	-3.43490000	-2.04543300
H	2.14989800	-3.78237100	-1.44305100
H	2.29664600	-4.12495400	0.29342600
H	4.25403300	-5.06195200	-0.99752400
C	-1.74154200	-1.40252400	2.14118100

N	1.24767400	-1.66749500	-0.01486300
N	3.19726500	0.21026600	-1.11366800
N	-0.76259700	-1.48098800	1.04229400
S	1.28154700	-2.27219900	2.62364200
C	2.33614900	1.06844100	-1.73824500
C	3.09530500	3.17957600	-0.58550600
C	0.55339800	-1.79221800	1.15166900
C	1.27614200	3.21738800	-2.38523700
C	2.21969300	2.41254900	-1.53657100
C	4.82627000	-3.16597800	-1.90518900
C	2.74306200	-3.57056400	-0.54019200
C	4.20182300	-3.98934900	-0.76861800
C	4.71038900	-1.66066700	-1.61959100
C	2.63437600	-2.06522500	-0.22879500
C	3.25365100	-1.22236500	-1.37074300
H	-1.53473200	-2.24730900	2.80755400
C	-1.59511500	-0.09760000	2.94187900
C	-3.12713700	-1.57180100	1.53652900
C	-3.83843600	-2.76538800	1.71579400
C	-3.69819600	-0.55117500	0.75979300
C	-5.09916000	-2.93826500	1.13282700
H	-3.39847300	-3.56204300	2.31394700
C	-4.95154800	-0.72373100	0.16539700
H	-3.16145100	0.38462500	0.61918600
C	-5.65677300	-1.91879800	0.35278200
H	-5.64273100	-3.86918300	1.28385900
H	-5.37632000	0.07590500	-0.43836300
H	-6.63512800	-2.05386500	-0.10466800
H	-0.58526400	-0.03742800	3.35978000
H	-1.76420400	0.77367800	2.29968400
H	-2.32621000	-0.08182000	3.76026400
C	0.52440700	2.46772800	1.22051900
C	0.10710000	3.80966100	1.36591200
C	1.48188100	1.95362300	2.12364500
C	0.62902700	4.60544200	2.38373400
H	-0.62072300	4.22556000	0.67343200
C	1.99542000	2.74954700	3.14566900
H	1.79732200	0.91657700	2.02233600
C	1.57221000	4.07860400	3.27854200
H	0.30349500	5.63895700	2.48346700
H	2.72303300	2.33623400	3.84112500
H	1.97428500	4.70223600	4.07449300
C	0.02012700	1.59417400	0.18398200
C	-1.08282100	1.80799200	-0.60219700
H	-1.67213600	2.71564100	-0.52069600
H	0.52558300	0.63999800	0.09834900
C	-1.49294900	0.83122100	-1.57178000
O	-0.92585000	-0.25919300	-1.78794800
C	-2.77656900	1.19721300	-2.36035900
O	-3.53179700	2.10122500	-2.04506700
O	-2.96167000	0.37984200	-3.41061600

C	-4.16883000	0.61077500	-4.18915300
H	-4.13808300	-0.13038200	-4.99022800
H	-5.05298800	0.46852700	-3.55764500
H	-4.16660500	1.62872300	-4.59481700

KE-B-Maj-TS1

Total Energy= -1954.272626

Imaginary frequency= 1

XYZ coordinates

H	-3.50891200	3.45962800	1.00482500
H	-0.60653100	2.28329800	3.29199400
H	-1.99904000	4.20383400	0.42402100
H	-2.69317800	2.85235500	-0.46477500
H	-5.31055800	-2.90071500	-1.26498600
H	-1.91802700	0.39107400	2.44640900
H	-5.42189700	-0.69373200	1.84351300
H	-3.39188500	-1.16254800	-1.30783200
H	-5.51479400	-0.64993700	0.07233500
H	-0.56494500	3.83482200	2.42130000
H	-2.03247400	3.35905800	3.30302200
H	0.85021300	-1.17296400	-0.32914200
H	-3.04754200	-1.41102400	1.72961000
H	-1.03348700	-1.26211000	0.44141700
H	-3.53900000	0.99303300	0.06261000
H	-5.02063800	-3.15308800	1.78245100
H	-6.51291700	-2.76211000	0.91582600
H	-2.83796500	-3.62688000	0.41668200
H	-2.90796900	-3.57432700	-1.35651100
H	-5.08329200	-4.40731000	-0.36556900
C	1.67999300	-1.11183600	-2.28144800
N	-1.51245700	-1.43844800	-0.45924800
N	-3.18324700	0.45659700	0.84869200
N	0.58026100	-1.21298500	-1.30686900
S	-1.36354000	-1.51584400	-3.16619600
C	-2.29545600	1.01969500	1.64493700
C	-2.53210300	3.25615500	0.54284800
C	-0.73980800	-1.38768400	-1.57492000
C	-1.19910000	2.98324600	2.69281300
C	-1.72443400	2.31626000	1.43112800
C	-5.42079400	-2.65806900	0.88488900
C	-3.32310800	-3.13800300	-0.44102400
C	-4.84431500	-3.33607700	-0.36813900
C	-5.05015900	-1.16642700	0.92581800
C	-2.94959000	-1.64357500	-0.42366500
C	-3.52758400	-0.97224300	0.84599300
H	1.47142600	-1.83386100	-3.07956200
C	1.76450000	0.29533500	-2.89595400
C	2.96619500	-1.50583700	-1.57137200
C	3.65586500	-2.67097000	-1.93036700
C	3.46679200	-0.71354300	-0.52538000

C	4.82813700	-3.03964400	-1.25927700
H	3.26860900	-3.29282100	-2.73639900
C	4.62990300	-1.08430700	0.15460600
H	2.93606100	0.18993700	-0.23064300
C	5.31599700	-2.24845200	-0.21300200
H	5.35524100	-3.94684200	-1.54940400
H	4.99499100	-0.46445200	0.97087800
H	6.22387500	-2.53781300	0.31328600
H	0.82162600	0.53160400	-3.39939800
H	1.94981200	1.04463300	-2.11845800
H	2.58307400	0.33204500	-3.62637300
C	0.16223700	2.94479700	-0.44377000
C	0.87111100	4.06669400	0.02354200
C	-0.28900300	2.94304500	-1.77511500
C	1.12152200	5.15237800	-0.81856600
H	1.23232400	4.08780500	1.04875200
C	-0.03224600	4.02307200	-2.62207900
H	-0.82933400	2.07521600	-2.14829700
C	0.67069800	5.13537200	-2.14476500
H	1.67322400	6.01156600	-0.44161400
H	-0.37728600	3.99516800	-3.65390200
H	0.87148900	5.97967100	-2.80140200
C	-0.14108600	1.77440900	0.42745000
C	0.91407900	1.33484200	1.31474600
H	1.72397900	2.01529800	1.55223600
H	-0.59288100	0.96557600	-0.14746400
C	0.91517200	0.08192900	1.91112800
O	0.00134700	-0.81162700	1.78928200
C	2.16007400	-0.24149300	2.75305100
O	3.02855400	0.55875500	3.06746000
O	2.20212700	-1.55188000	3.08791400
C	3.37780200	-1.97830700	3.82167000
H	3.22324400	-3.04159100	4.01943300
H	4.27603700	-1.82463100	3.21228700
H	3.47009100	-1.41605800	4.75806800

KE-B-Min-Cx1

Total Energy= -1954.282645

Imaginary frequency= 0

XYZ coordinates

H	3.09852700	-2.28144900	-1.81842800
H	5.40457100	-0.20315900	0.26527800
H	1.83374300	-1.05801500	-2.01275700
H	3.31727200	-0.96742300	-2.98634300
H	0.75095200	5.52649800	-1.99947300
H	3.62739200	1.29292400	0.35484900
H	3.52322700	3.42248400	-0.47296300
H	0.19542300	2.99329000	-2.02265400
H	2.56435400	3.63919300	-1.94784000
H	5.00640800	-1.87608900	-0.21578200

H	5.67492100	-0.75900500	-1.40649000
H	-2.32107600	0.28577600	0.32803500
H	1.45783100	2.71945600	0.75123500
H	-1.32445700	2.15647800	0.34741600
H	1.35574300	0.89540300	-1.50623400
H	2.14987800	5.13999300	0.70581900
H	2.87663200	5.83027400	-0.75349500
H	-0.39642400	4.42094400	0.62266300
H	-1.28803100	4.64866400	-0.89639800
H	0.43486900	6.45712400	-0.52714100
C	-2.85740400	-1.03432400	-1.23443500
N	-0.92452900	2.04602500	-0.57522500
N	1.84643200	1.27029800	-0.69859100
N	-2.23982300	0.18309900	-0.68010200
S	-0.83096000	0.70533800	-2.92633400
C	3.07500800	0.74602000	-0.40549700
C	2.92002100	-1.21117900	-1.98678600
C	-1.35186200	0.98446900	-1.31753700
C	4.99415900	-0.82465300	-0.54110400
C	3.60396400	-0.39997900	-0.92057800
C	2.13817800	5.10169700	-0.39415900
C	-0.30238400	4.41736500	-0.47382900
C	0.73456900	5.46926200	-0.90087000
C	2.52797600	3.68741300	-0.84901300
C	0.11435500	3.00988100	-0.93007100
C	1.50074800	2.64932600	-0.34548400
H	-3.02184400	-0.84578900	-2.29944100
C	-1.92099500	-2.24517600	-1.08428500
C	-4.19771000	-1.26027500	-0.55468700
C	-5.37910600	-1.27698500	-1.30705800
C	-4.27018400	-1.47056700	0.83212600
C	-6.61472900	-1.50091500	-0.68851400
H	-5.32858900	-1.11258300	-2.38242100
C	-5.50325700	-1.68441400	1.45464100
H	-3.35979600	-1.46313500	1.42977300
C	-6.67955700	-1.70308300	0.69444500
H	-7.52479500	-1.51357200	-1.28547100
H	-5.54608500	-1.84097200	2.53091200
H	-7.63956900	-1.87420900	1.17772800
C	2.28327400	-1.64294300	1.39868300
C	1.12009500	-0.93820600	1.54351600
H	0.17119100	-1.32864900	1.18963600
C	1.12369500	0.35868000	2.17757900
O	2.12519200	0.96740300	2.58050400
C	-0.27946400	0.98207400	2.38198300
O	-1.33993100	0.39070900	2.22214200
O	-0.20064100	2.26586800	2.78014400
C	-1.45818500	2.91951100	3.10712400
H	-1.18332700	3.93110600	3.41100200
H	-2.12364800	2.94679300	2.23560400
H	-1.95586900	2.38296200	3.92182900

C	2.42514300	-2.96000100	0.80524900
C	3.62738300	-3.67605700	1.00079800
C	1.41330800	-3.55659800	0.01945600
C	3.80962300	-4.94114200	0.43962200
H	4.41204400	-3.23065300	1.60906500
C	1.59654300	-4.81788700	-0.54120600
H	0.49029400	-3.01630900	-0.16418100
C	2.79554500	-5.51679000	-0.33493400
H	4.74175700	-5.47796100	0.60478700
H	0.80826100	-5.25717700	-1.14957100
H	2.93707400	-6.50110200	-0.77672300
H	3.17916100	-1.22174800	1.85160300
H	-2.38065300	-3.13464200	-1.53298200
H	-0.97291300	-2.03548000	-1.59175300
H	-1.73309600	-2.45058600	-0.02327700

KE-B-Min-TS1

Total Energy= -1954.270927

Imaginary frequency= 1

XYZ coordinates

H	2.79698400	-2.16041600	-2.11130600
H	5.21338000	-0.51117600	0.20405400
H	1.43885400	-1.05238000	-1.85605800
H	2.81438500	-0.54751700	-2.86261700
H	0.69552900	5.73384300	-1.69000600
H	3.63613500	1.34063400	0.27131500
H	3.51800600	3.57177900	-0.34352000
H	0.13341900	3.19667200	-1.90182400
H	2.56121500	3.89994400	-1.80183100
H	4.85891000	-2.00312000	-0.70328400
H	5.25342800	-0.51082500	-1.57817000
H	-2.24833600	0.28886500	0.36340800
H	1.48794400	2.69884200	0.80496200
H	-1.27254000	2.18702200	0.47087000
H	1.26838500	1.00515200	-1.47402500
H	2.12651900	5.16708400	0.96732500
H	2.82781900	5.98405000	-0.43848200
H	-0.39920700	4.41785200	0.85828100
H	-1.32087400	4.74820400	-0.62312000
H	0.38118400	6.54850900	-0.15032400
C	-2.80124000	-0.94395700	-1.26069800
N	-0.89922900	2.12549900	-0.46783500
N	1.89413600	1.44119300	-0.79279100
N	-2.20845100	0.26238100	-0.65424300
S	-0.82336600	0.91382400	-2.88397000
C	2.98716300	0.81033700	-0.41842200
C	2.52925900	-1.11036600	-1.96224700
C	-1.33742600	1.10235600	-1.25824000
C	4.73465800	-0.91508100	-0.69728900
C	3.25533400	-0.55627600	-0.74475100

C	2.10540000	5.21715500	-0.13147600
C	-0.32478500	4.50050000	-0.23666900
C	0.69122100	5.59597000	-0.59862500
C	2.52098200	3.85351100	-0.70358100
C	0.09864100	3.13768600	-0.80856300
C	1.50693800	2.77044300	-0.29093700
H	-2.98640600	-0.70790700	-2.31252000
C	-1.83132600	-2.13513900	-1.17990300
C	-4.12524100	-1.23877000	-0.57467900
C	-5.31699900	-1.24951000	-1.31064800
C	-4.16988100	-1.52109000	0.80040300
C	-6.53654100	-1.53922600	-0.68720700
H	-5.28756200	-1.02864100	-2.37674000
C	-5.38720800	-1.80125700	1.42760000
H	-3.25127400	-1.51445800	1.38438000
C	-6.57429200	-1.81394300	0.68420400
H	-7.45517100	-1.54626400	-1.27104900
H	-5.40894900	-2.01381700	2.49489300
H	-7.52178700	-2.03619200	1.17147400
C	2.48246700	-1.45215400	0.81967900
C	1.19696200	-0.91943200	1.19237200
H	0.28061600	-1.42783900	0.91658400
C	1.14262900	0.26058100	1.94497800
O	2.14580900	0.95589000	2.29306900
C	-0.26608000	0.72629300	2.32974800
O	-1.30450000	0.08625600	2.18591800
O	-0.26072800	1.97947900	2.84883700
C	-1.54386500	2.49145800	3.29427100
H	-1.33406900	3.48800400	3.68845400
H	-2.25444000	2.55048400	2.45934600
H	-1.96206100	1.84129800	4.07035900
C	2.56623600	-2.90537400	0.49910700
C	3.69111100	-3.64273700	0.91137800
C	1.54843500	-3.58088600	-0.20011200
C	3.79719900	-5.01025500	0.63923800
H	4.48088100	-3.13515500	1.46170700
C	1.65174700	-4.94512200	-0.47583500
H	0.67131900	-3.03274800	-0.52913100
C	2.77840600	-5.66688400	-0.05956900
H	4.67361800	-5.56183700	0.97480100
H	0.85169500	-5.44736600	-1.01691800
H	2.85752100	-6.73104500	-0.27353100
H	3.27198100	-1.13585600	1.50413200
H	-2.27902000	-3.01610800	-1.65637700
H	-0.90030800	-1.88078600	-1.69847100
H	-1.61313700	-2.37745900	-0.13320900

KE-B-Maj-Cx4

Total Energy= -1954.283922

Imaginary frequency= 0

XYZ coordinates

H	-1.28638700	-3.86082500	-2.64549300
H	1.38653200	-6.08791600	-1.11649000
H	0.81783100	-2.44731300	-2.00127000
H	1.05168600	-5.00293400	-2.47479400
H	1.14534700	0.46370500	1.10724600
H	1.20237100	-4.17945400	0.48426500
H	0.53096800	-1.42832300	0.74321000
H	-0.86814000	-5.61966600	-0.15770400
H	-1.03916200	-6.20169600	-1.82151300
H	-1.10605000	-3.06422900	0.30663100
H	-2.50428400	-4.20844800	-1.40232500
C	2.68582800	1.68891600	0.26384300
N	1.05810600	-1.57265500	-0.13011300
N	1.78467500	0.53828300	0.31252100
S	2.60052200	-0.46715100	-2.06261600
C	1.78944900	-0.50755700	-0.55648500
C	-0.66726000	-5.36960800	-1.21003400
C	-0.91332400	-2.88467000	-0.76107200
C	-1.42724000	-4.08553700	-1.57834500
C	0.84419200	-5.17951000	-1.40847600
C	0.60221100	-2.68547300	-0.95243800
C	1.34824300	-3.98386300	-0.58801500
H	2.68182000	2.08129700	-0.76059700
H	2.41763500	-3.80792800	-0.75311300
N	-1.70762300	-1.68416500	-1.10434900
H	-2.66846000	-1.70594200	-0.77946900
C	-1.30435700	-0.60153400	-1.73617500
H	-0.26628600	-0.57607800	-2.05831500
C	-2.09175700	0.57544600	-1.88820400
C	-3.60202300	0.42600200	-1.95457700
H	-3.88524300	-0.08379100	-2.88633000
H	-4.07211400	1.41525300	-1.95084300
H	-4.01071500	-0.14024500	-1.10894800
C	-1.53353800	1.53246200	-2.93172900
H	-0.45036900	1.66208500	-2.81840000
H	-2.01395900	2.51248600	-2.85117500
H	-1.73121600	1.14047500	-3.93995400
C	-2.19693400	2.75563900	-0.24153900
C	-1.25805100	3.72673300	-0.63699900
C	-3.52673700	3.16370800	-0.02462900
C	-1.62822100	5.06273900	-0.80606000
H	-0.22931200	3.42183900	-0.81660400
C	-3.90149700	4.49726400	-0.20118700
H	-4.26843900	2.43860400	0.29872400
C	-2.95507600	5.45297700	-0.59276600
H	-0.88270500	5.79705600	-1.10526300
H	-4.93374100	4.79431400	-0.02508400
H	-3.24884200	6.49259100	-0.72347600
C	-1.74969800	1.34736800	-0.06592300
H	-0.66227800	1.27576600	-0.03690100

C	-2.40192600	0.50457300	0.90234400
H	-3.48267600	0.53887000	0.99267700
C	-1.71444900	-0.38232300	1.73439800
O	-0.45500000	-0.48027800	1.90751100
C	-2.56473700	-1.42558700	2.47427200
O	-2.24758900	-2.60040400	2.56257400
O	-3.70297800	-0.91273800	3.00467000
C	-4.58119300	-1.86086700	3.67395300
H	-5.42099800	-1.26570400	4.03936900
H	-4.05377600	-2.34296500	4.50441600
H	-4.92287600	-2.62437800	2.96530900
C	2.14305900	2.76038400	1.22537200
H	1.12249100	3.05278600	0.95010400
H	2.13534200	2.37526600	2.25350900
H	2.78874400	3.64450700	1.19373900
C	4.12340800	1.32980100	0.62470400
C	5.18459300	1.96708000	-0.03057100
C	4.40575700	0.41682200	1.64990100
C	6.50924100	1.69933400	0.33042000
H	4.96832700	2.66498500	-0.83875700
C	5.72848600	0.14381700	2.01256000
H	3.58559000	-0.09188000	2.15323400
C	6.78492100	0.78636200	1.35521500
H	7.32505600	2.19465300	-0.19340800
H	5.93529100	-0.57183400	2.80657700
H	7.81485900	0.57114700	1.63409700

KE-B-Maj-TS4

Total Energy= -1954,269289

Imaginary frequency= 1

XYZ coordinates

H	-1.28638700	-3.86082500	-2.64549300
H	1.38653200	-6.08791600	-1.11649000
H	0.81783100	-2.44731300	-2.00127000
H	1.05168600	-5.00293400	-2.47479400
H	1.14534700	0.46370500	1.10724600
H	1.20237100	-4.17945400	0.48426500
H	0.53096800	-1.42832300	0.74321000
H	-0.86814000	-5.61966600	-0.15770400
H	-1.03916200	-6.20169600	-1.82151300
H	-1.10605000	-3.06422900	0.30663100
H	-2.50428400	-4.20844800	-1.40232500
C	2.68582800	1.68891600	0.26384300
N	1.05810600	-1.57265500	-0.13011300
N	1.78467500	0.53828300	0.31252100
S	2.60052200	-0.46715100	-2.06261600
C	1.78944900	-0.50755700	-0.55648500
C	-0.66726000	-5.36960800	-1.21003400
C	-0.91332400	-2.88467000	-0.76107200
C	-1.42724000	-4.08553700	-1.57834500

C	0.84419200	-5.17951000	-1.40847600
C	0.60221100	-2.68547300	-0.95243800
C	1.34824300	-3.98386300	-0.58801500
H	2.68182000	2.08129700	-0.76059700
H	2.41763500	-3.80792800	-0.75311300
N	-1.70762300	-1.68416500	-1.10434900
H	-2.66846000	-1.70594200	-0.77946900
C	-1.30435700	-0.60153400	-1.73617500
H	-0.26628600	-0.57607800	-2.05831500
C	-2.09175700	0.57544600	-1.88820400
C	-3.60202300	0.42600200	-1.95457700
H	-3.88524300	-0.08379100	-2.88633000
H	-4.07211400	1.41525300	-1.95084300
H	-4.01071500	-0.14024500	-1.10894800
C	-1.53353800	1.53246200	-2.93172900
H	-0.45036900	1.66208500	-2.81840000
H	-2.01395900	2.51248600	-2.85117500
H	-1.73121600	1.14047500	-3.93995400
C	-2.19693400	2.75563900	-0.24153900
C	-1.25805100	3.72673300	-0.63699900
C	-3.52673700	3.16370800	-0.02462900
C	-1.62822100	5.06273900	-0.80606000
H	-0.22931200	3.42183900	-0.81660400
C	-3.90149700	4.49726400	-0.20118700
H	-4.26843900	2.43860400	0.29872400
C	-2.95507600	5.45297700	-0.59276600
H	-0.88270500	5.79705600	-1.10526300
H	-4.93374100	4.79431400	-0.02508400
H	-3.24884200	6.49259100	-0.72347600
C	-1.74969800	1.34736800	-0.06592300
H	-0.66227800	1.27576600	-0.03690100
C	-2.40192600	0.50457300	0.90234400
H	-3.48267600	0.53887000	0.99267700
C	-1.71444900	-0.38232300	1.73439800
O	-0.45500000	-0.48027800	1.90751100
C	-2.56473700	-1.42558700	2.47427200
O	-2.24758900	-2.60040400	2.56257400
O	-3.70297800	-0.91273800	3.00467000
C	-4.58119300	-1.86086700	3.67395300
H	-5.42099800	-1.26570400	4.03936900
H	-4.05377600	-2.34296500	4.50441600
H	-4.92287600	-2.62437800	2.96530900
C	2.14305900	2.76038400	1.22537200
H	1.12249100	3.05278600	0.95010400
H	2.13534200	2.37526600	2.25350900
H	2.78874400	3.64450700	1.19373900
C	4.12340800	1.32980100	0.62470400
C	5.18459300	1.96708000	-0.03057100
C	4.40575700	0.41682200	1.64990100
C	6.50924100	1.69933400	0.33042000
H	4.96832700	2.66498500	-0.83875700

C	5.72848600	0.14381700	2.01256000
H	3.58559000	-0.09188000	2.15323400
C	6.78492100	0.78636200	1.35521500
H	7.32505600	2.19465300	-0.19340800
H	5.93529100	-0.57183400	2.80657700
H	7.81485900	0.57114700	1.63409700

KE-B-Min-Cx4

Total Energy= -1954.277924

Imaginary frequency= 0

XYZ coordinates

H	-0.93901600	5.01272800	0.31331700
H	2.03552000	5.84136900	-1.86390500
H	1.00523300	3.31859300	0.82514000
H	1.48468500	5.73657300	-0.18437000
H	1.75759700	-0.79828000	-0.36423400
H	1.75972000	3.38287500	-2.14214100
H	0.85808600	1.00147100	-0.97729000
H	-0.18097400	5.01380500	-2.66207900
H	-0.41295800	6.44623900	-1.64636400
H	-0.70184500	2.63963200	-1.61732400
H	-2.03927500	4.65265800	-1.03256000
C	2.90811200	-1.35013000	1.31566700
N	1.32365600	1.57211700	-0.25889500
N	2.07888500	-0.42652000	0.53206400
S	2.68681400	1.71549600	2.07615600
C	2.01230200	0.92009700	0.71772200
C	-0.08493900	5.39901100	-1.63586100
C	-0.58210700	3.10864900	-0.63156900
C	-0.99273100	4.59033700	-0.70135500
C	1.37712100	5.28661300	-1.18300100
C	0.89862100	2.96828400	-0.20789200
C	1.80126500	3.81421000	-1.13079500
H	2.95797100	-0.94478900	2.33046600
H	2.83025600	3.70689800	-0.76800800
N	-1.54239100	2.43687500	0.27938300
H	-2.41323100	2.94223100	0.41043000
C	-1.49809300	1.19424600	0.72687200
H	-0.56250600	0.67004500	0.61592600
C	-2.60270000	0.49212000	1.29332000
C	-3.80175300	1.32021500	1.72154900
H	-4.60029100	0.66882300	2.08803700
H	-4.21847200	1.91051700	0.89426700
H	-3.51580700	2.00798400	2.53144100
C	-2.20544000	-0.59564400	2.27618400
H	-3.06865500	-1.23217600	2.50109000
H	-1.85587300	-0.15167600	3.21908000
H	-1.40047600	-1.21686600	1.86519200
C	-3.16440100	-0.49623700	-0.36689300
C	-2.18423800	-1.47401200	-0.76420700

H	-2.35099700	-2.52007800	-0.53390500
C	-1.01167300	-1.10504900	-1.41860700
O	-0.66506200	0.09001500	-1.70919800
C	0.00453000	-2.19807600	-1.76031700
O	1.20548000	-1.98241300	-1.87309000
O	-0.54256300	-3.41908300	-1.94583600
C	0.38526300	-4.50124300	-2.24017800
H	-0.23998600	-5.38797500	-2.36429600
H	1.08787800	-4.63220600	-1.40953100
H	0.94025800	-4.28134900	-3.15867400
C	-4.52430700	-0.98452600	-0.01873600
C	-5.64892300	-0.23448000	-0.41045800
C	-4.73484200	-2.17475300	0.70315500
C	-6.94251600	-0.65888600	-0.09849600
H	-5.49987000	0.68594600	-0.97248800
C	-6.02661400	-2.59681900	1.02456500
H	-3.88168000	-2.77248700	1.01208900
C	-7.13626800	-1.84054600	0.62642000
H	-7.79834400	-0.06814500	-0.41978000
H	-6.16886100	-3.51956700	1.58400000
H	-8.14248600	-2.17277000	0.87423600
H	-3.19171100	0.38745800	-1.00799300
C	2.22233000	-2.72546700	1.34567400
H	1.21460100	-2.63875300	1.77190100
H	2.14622600	-3.13414400	0.33127900
H	2.81361800	-3.41856700	1.95542200
C	4.32582800	-1.44607600	0.76597600
C	5.42585300	-1.25652100	1.61157400
C	4.54875300	-1.74983600	-0.58633500
C	6.73181700	-1.37067600	1.11955600
H	5.25457300	-1.00556200	2.65738800
C	5.85109800	-1.86155700	-1.08151100
H	3.69993800	-1.89425700	-1.25203400
C	6.94739800	-1.67368200	-0.22917000
H	7.57808000	-1.21451700	1.78650300
H	6.01221600	-2.09438100	-2.13288500
H	7.96147800	-1.75809000	-0.61585300

KE-B-Min-TS4

Total Energy= -1954.264841
Imaginary frequency= 1

XYZ coordinates

H	-0.93901600	5.01272800	0.31331700
H	2.03552000	5.84136900	-1.86390500
H	1.00523300	3.31859300	0.82514000
H	1.48468500	5.73657300	-0.18437000
H	1.75759700	-0.79828000	-0.36423400
H	1.75972000	3.38287500	-2.14214100
H	0.85808600	1.00147100	-0.97729000
H	-0.18097400	5.01380500	-2.66207900

H	-0.41295800	6.44623900	-1.64636400
H	-0.70184500	2.63963200	-1.61732400
H	-2.03927500	4.65265800	-1.03256000
C	2.90811200	-1.35013000	1.31566700
N	1.32365600	1.57211700	-0.25889500
N	2.07888500	-0.42652000	0.53206400
S	2.68681400	1.71549600	2.07615600
C	2.01230200	0.92009700	0.71772200
C	-0.08493900	5.39901100	-1.63586100
C	-0.58210700	3.10864900	-0.63156900
C	-0.99273100	4.59033700	-0.70135500
C	1.37712100	5.28661300	-1.18300100
C	0.89862100	2.96828400	-0.20789200
C	1.80126500	3.81421000	-1.13079500
H	2.95797100	-0.94478900	2.33046600
H	2.83025600	3.70689800	-0.76800800
N	-1.54239100	2.43687500	0.27938300
H	-2.41323100	2.94223100	0.41043000
C	-1.49809300	1.19424600	0.72687200
H	-0.56250600	0.67004500	0.61592600
C	-2.60270000	0.49212000	1.29332000
C	-3.80175300	1.32021500	1.72154900
H	-4.60029100	0.66882300	2.08803700
H	-4.21847200	1.91051700	0.89426700
H	-3.51580700	2.00798400	2.53144100
C	-2.20544000	-0.59564400	2.27618400
H	-3.06865500	-1.23217600	2.50109000
H	-1.85587300	-0.15167600	3.21908000
H	-1.40047600	-1.21686600	1.86519200
C	-3.16440100	-0.49623700	-0.36689300
C	-2.18423800	-1.47401200	-0.76420700
H	-2.35099700	-2.52007800	-0.53390500
C	-1.01167300	-1.10504900	-1.41860700
O	-0.66506200	0.09001500	-1.70919800
C	0.00453000	-2.19807600	-1.76031700
O	1.20548000	-1.98241300	-1.87309000
O	-0.54256300	-3.41908300	-1.94583600
C	0.38526300	-4.50124300	-2.24017800
H	-0.23998600	-5.38797500	-2.36429600
H	1.08787800	-4.63220600	-1.40953100
H	0.94025800	-4.28134900	-3.15867400
C	-4.52430700	-0.98452600	-0.01873600
C	-5.64892300	-0.23448000	-0.41045800
C	-4.73484200	-2.17475300	0.70315500
C	-6.94251600	-0.65888600	-0.09849600
H	-5.49987000	0.68594600	-0.97248800
C	-6.02661400	-2.59681900	1.02456500
H	-3.88168000	-2.77248700	1.01208900
C	-7.13626800	-1.84054600	0.62642000
H	-7.79834400	-0.06814500	-0.41978000
H	-6.16886100	-3.51956700	1.58400000

H	-8.14248600	-2.17277000	0.87423600
H	-3.19171100	0.38745800	-1.00799300
C	2.22233000	-2.72546700	1.34567400
H	1.21460100	-2.63875300	1.77190100
H	2.14622600	-3.13414400	0.33127900
H	2.81361800	-3.41856700	1.95542200
C	4.32582800	-1.44607600	0.76597600
C	5.42585300	-1.25652100	1.61157400
C	4.54875300	-1.74983600	-0.58633500
C	6.73181700	-1.37067600	1.11955600
H	5.25457300	-1.00556200	2.65738800
C	5.85109800	-1.86155700	-1.08151100
H	3.69993800	-1.89425700	-1.25203400
C	6.94739800	-1.67368200	-0.22917000
H	7.57808000	-1.21451700	1.78650300
H	6.01221600	-2.09438100	-2.13288500
H	7.96147800	-1.75809000	-0.61585300

KE-B_F-Maj-Cx1

Total Energy= -2251.992098

Imaginary frequency= 0

XYZ coordinates

H	5.55928400	-1.86619700	0.64857800
H	2.37082700	-2.31527800	2.95150000
H	4.31541700	-2.80850600	-0.19416500
H	4.52498800	-1.10028700	-0.58118000
H	3.14726500	5.26465500	-0.25641600
H	2.37765200	-0.06911100	2.36339100
H	4.87184400	2.78279600	2.06494400
H	2.36072400	2.84106500	-0.76088800
H	4.66990600	3.21972700	0.35917900
H	2.68356300	-3.45627100	1.62316500
H	3.98102100	-3.05178400	2.75494900
H	-1.20564100	0.55719800	0.32747700
H	2.48678300	2.15111200	2.21566600
H	0.52047000	1.41895800	1.03545100
H	4.09319800	0.83599000	0.11478800
H	3.30599300	4.60182600	2.73800200
H	4.61958300	5.27062400	1.75889500
H	0.99348900	4.16064000	1.63924700
H	0.74791000	4.58207600	-0.06824200
H	2.36344600	6.16813900	1.04824600
C	-2.31559700	0.78099200	-1.45772600
N	0.76383500	1.90371500	0.17507300
N	3.41655300	0.89727800	0.86297100
N	-1.17716800	0.99695500	-0.59246300
S	0.11448300	2.60918500	-2.34999400
C	3.08632600	-0.23765000	1.55347300
C	4.53468700	-1.82490900	0.24227800
C	-0.11162100	1.81286700	-0.85931300

C	3.11697800	-2.63265500	2.21330700
C	3.53492800	-1.50206000	1.31788600
C	3.73694800	4.61834300	1.72524200
C	1.48645500	4.22133000	0.65677500
C	2.69280100	5.16681400	0.74137700
C	4.16212600	3.19405400	1.33620000
C	1.91564600	2.80114200	0.24050900
C	2.96282400	2.23157600	1.22725000
H	-2.19036200	1.42961800	-2.33185000
C	-2.29000000	-0.66044100	-2.01894700
C	-3.64054600	1.08095100	-0.77179500
C	-4.61547300	1.81303600	-1.46126000
C	-3.90875900	0.62888900	0.52917600
C	-5.84658800	2.09446800	-0.85978600
H	-4.40686700	2.16483300	-2.46996100
C	-5.13801400	0.91211800	1.13066800
H	-3.16937600	0.05761400	1.08486600
C	-6.11017900	1.64410100	0.43825900
H	-6.59531700	2.66772500	-1.40284700
H	-5.33480100	0.55963000	2.14127400
H	-7.06636800	1.86440000	0.90892500
C	1.67212800	-2.23310700	-1.16294300
C	1.85625500	-3.62776500	-1.29870000
C	2.23045100	-1.37777000	-2.13996000
C	2.57436100	-4.14361100	-2.37514100
H	1.43911600	-4.30266100	-0.55565000
C	2.94255800	-1.89758000	-3.21876100
H	2.08541200	-0.30354900	-2.04181200
C	3.11801000	-3.28234600	-3.33978100
H	2.71187100	-5.21902100	-2.46786400
H	3.35871600	-1.22707700	-3.96781400
H	3.67402700	-3.69031700	-4.18147700
C	0.94142200	-1.63736000	-0.06759300
C	0.15161000	-2.28639800	0.84604800
H	0.04933000	-3.36686200	0.84441300
H	0.95806900	-0.55309400	-0.03969900
C	-0.61522700	-1.55351200	1.80891700
O	-0.60774700	-0.31179200	1.96587000
C	-1.53508600	-2.41789500	2.70082800
O	-1.30323500	-3.57687600	2.99502100
O	-2.61421400	-1.72183500	3.10415900
C	-3.55897200	-2.43911100	3.94746300
H	-4.36835000	-1.73076400	4.13507700
H	-3.92875100	-3.32843700	3.42505600
H	-3.07273100	-2.73635000	4.88311800
F	-1.12721900	-0.92854800	-2.66227000
F	-2.43402000	-1.60085800	-1.04150800
F	-3.30173400	-0.84845000	-2.91062300

KE-B_F-Maj-TS1

Total Energy= -2251.980624

Imaginary frequency= 1

XYZ coordinates

H	-3.96532400	3.37316300	0.42324500
H	-1.60102400	2.26307400	3.32057700
H	-2.39422100	4.18974300	0.23642500
H	-2.79052000	2.82506400	-0.80399800
H	-4.94287600	-3.16225900	-2.08239700
H	-2.67852300	0.36728400	2.21010900
H	-5.79408800	-0.86301500	0.85042500
H	-3.18396500	-1.31577200	-1.82008000
H	-5.52845500	-0.86818200	-0.90400400
H	-1.43884600	3.83550900	2.50092900
H	-3.03796600	3.28461900	3.04171800
H	0.71322200	-0.63106700	-0.13195100
H	-3.41583000	-1.48439900	1.23229800
H	-1.19868500	-1.19317200	0.34473400
H	-3.59553300	0.88447400	-0.54153400
H	-5.27375400	-3.29147800	0.96833100
H	-6.57325100	-3.01626300	-0.20136500
H	-2.83030100	-3.67296700	0.09580000
H	-2.54173500	-3.69298800	-1.65726000
H	-4.82742200	-4.61879900	-1.08466100
C	1.96321800	-1.03602100	-1.75522900
N	-1.47800300	-1.42123100	-0.63175400
N	-3.44893100	0.37067700	0.32217800
N	0.66933000	-0.85889300	-1.11961200
S	-0.77368700	-1.80833400	-3.21341100
C	-2.83825600	0.97669100	1.32608000
C	-2.89672700	3.21846800	0.21492100
C	-0.52669200	-1.36016100	-1.58659400
C	-2.07936400	2.95383900	2.61691300
C	-2.29467200	2.29532900	1.26534300
C	-5.50501100	-2.85005000	-0.01265200
C	-3.15632600	-3.25040400	-0.86597200
C	-4.64894900	-3.53591200	-1.08981200
C	-5.22343700	-1.33864400	0.04301100
C	-2.88252700	-1.73426500	-0.84935600
C	-3.72734900	-1.07069900	0.26566400
H	1.82202000	-1.67513200	-2.63359400
C	2.47666400	0.31042200	-2.32012900
C	2.96976800	-1.66291000	-0.80205600
C	3.65453500	-2.82285100	-1.18433100
C	3.20773200	-1.10668700	0.46490000
C	4.56506100	-3.42579200	-0.30978200
H	3.47022800	-3.25550400	-2.16590900
C	4.11467800	-1.70987900	1.33912300
H	2.68892200	-0.20158500	0.77366400
C	4.79615100	-2.87065800	0.95345800
H	5.08999100	-4.32888400	-0.61472400
H	4.28903200	-1.26788700	2.31759300

H	5.50335800	-3.34010700	1.63450100
C	-0.00704400	3.05782000	-0.08365700
C	0.54009200	4.15417700	0.60794800
C	-0.13377200	3.13968800	-1.48130500
C	0.94654200	5.29859900	-0.08081100
H	0.65167300	4.10782100	1.68831600
C	0.28269900	4.27807300	-2.17360000
H	-0.53920900	2.28994200	-2.02655900
C	0.81857000	5.36572700	-1.47430700
H	1.36871400	6.13793400	0.46863100
H	0.19301400	4.31501400	-3.25750100
H	1.14210400	6.25576400	-2.01046900
C	-0.46428200	1.82902300	0.61502000
C	0.36268900	1.34369100	1.69263700
H	1.11285300	2.00157800	2.11686200
H	-0.78806300	1.06678100	-0.09337300
C	0.21240000	0.08091000	2.25331200
O	-0.66430600	-0.78997500	1.91141100
C	1.20996400	-0.27026600	3.36963900
O	2.12909700	0.44405700	3.74029500
O	0.96679000	-1.49621200	3.88562400
C	1.88840100	-1.94008100	4.91442100
H	1.53158500	-2.92850700	5.21270500
H	2.90497500	-2.00043400	4.50904700
H	1.87603800	-1.24683900	5.76345700
F	1.62310500	0.82922700	-3.23721200
F	2.64975800	1.25368900	-1.35533400
F	3.67856900	0.13829900	-2.94039700

KE-A-Maj-Cx1

Total Energy= -1954.287887

Imaginary frequency= 0

XYZ coordinates

H	-5.47521500	-0.73688800	0.64505300
H	-6.27942200	2.79575200	-0.50420700
H	-3.71413900	0.06162100	-1.08578400
H	-6.09348200	1.13021200	-1.07429500
H	0.29223200	1.77978000	-0.84921900
H	-3.85324200	2.88668800	0.08466500
H	-1.44692300	1.43083000	0.20438900
H	-5.64084000	2.10288400	1.80288300
H	-7.00844800	1.12568500	1.24834100
H	-3.23696300	1.01113800	1.78079300
H	-5.25099100	-0.30277100	2.34863200
C	0.98762300	1.21574500	-2.77601200
N	-1.97725000	1.07140400	-0.58775700
N	-0.04052900	1.41287300	-1.73788600
S	-2.02648200	0.27189800	-3.17443900
C	-1.31976700	0.95767600	-1.77364800
C	-5.94398300	1.33330900	1.07634500

C	-3.61710800	0.27038900	1.06254700
C	-5.12197700	0.05806300	1.32045000
C	-5.71758900	1.86559500	-0.34669300
C	-3.39714100	0.82530700	-0.36558100
C	-4.22252500	2.10609500	-0.59814000
H	0.67743000	0.34544800	-3.36325800
C	1.06423000	2.43463600	-3.70843600
C	2.30589300	0.90146000	-2.08667000
C	2.96324500	1.87400300	-1.31742000
C	2.85610400	-0.38305000	-2.16838600
C	4.13930900	1.56221100	-0.63086100
H	2.54552300	2.87601600	-1.23885500
C	4.03973700	-0.69649900	-1.49250200
H	2.34092100	-1.14711600	-2.74689500
C	4.68077500	0.27356700	-0.71639500
H	4.63261000	2.32240600	-0.02862600
H	4.44916900	-1.70239500	-1.55869900
H	5.59415300	0.02888200	-0.17772200
H	-4.04280700	2.44754200	-1.62488200
N	-2.88530100	-0.96515300	1.29985200
H	-3.21553400	-1.78749300	0.81406900
C	-1.79911300	-1.07247900	2.12468500
H	-1.51775800	-0.13556100	2.60339900
C	-1.07277400	-2.19592000	2.38336900
C	-1.39830300	-3.53297200	1.77628500
H	-0.47570400	-4.10254800	1.60211700
H	-2.03562900	-4.13517500	2.44592100
H	-1.91072800	-3.44847800	0.80948600
C	0.03554100	-2.16507500	3.39702300
H	0.24398900	-1.14527800	3.74234800
H	-0.21039500	-2.78222800	4.27746900
H	0.96307600	-2.57917500	2.97024500
C	0.91808300	-2.27292900	-0.10777000
C	0.05483400	-2.69448900	-1.14304900
C	1.93116400	-3.15327500	0.33067400
C	0.20779000	-3.94936100	-1.73046800
H	-0.72060700	-2.01454500	-1.49406200
C	2.07431000	-4.41135500	-0.25046300
H	2.60420400	-2.84643300	1.12723100
C	1.21687000	-4.81352000	-1.28544500
H	-0.45759500	-4.25512400	-2.53539300
H	2.85593200	-5.08307700	0.09922100
H	1.33574800	-5.79488700	-1.74041300
C	0.73669600	-0.94623700	0.43910400
H	-0.15703900	-0.43011300	0.11034300
C	1.62725300	-0.25502400	1.21448600
H	2.56627300	-0.69588400	1.52972900
C	1.38360000	1.11098700	1.57795400
O	0.36308500	1.77551300	1.30065800
C	2.52736600	1.77549100	2.38154700
O	3.33149200	1.15739700	3.05694000

O	2.51208400	3.11471600	2.24617500
C	3.54694900	3.83782000	2.96818100
H	3.38168300	4.88997800	2.72762500
H	3.44719300	3.66137200	4.04486200
H	4.53795800	3.51023600	2.63361600
H	0.08720700	2.59364500	-4.17902700
H	1.81585100	2.26263600	-4.48966300
H	1.34173900	3.33618900	-3.14834300

KE-A-Maj-TS1

Total Energy= -1954.271147
Imaginary frequency= 1

XYZ coordinates

H	-4.91107800	-1.67102800	1.72292800
H	-6.68541900	-1.06514400	-1.60388100
H	-3.39562900	-2.26688100	-0.21017700
H	-5.93465600	-2.32920700	-0.61799700
H	-0.10934900	-0.60524800	-2.42085700
H	-4.47289600	0.06045100	-1.88679100
H	-1.81584400	0.01741800	-1.22148000
H	-6.11695400	0.64886400	0.10571100
H	-7.02833000	-0.66334800	0.86711000
H	-3.56086100	0.72708600	0.36799000
H	-5.03575700	0.01753000	2.25617100
C	1.33582200	-2.07796600	-1.99929900
N	-2.07206700	-0.98114900	-1.15233800
N	0.06270000	-1.38815400	-1.80051900
S	-0.99364000	-3.29753500	-0.19944600
C	-1.01081600	-1.83497600	-1.09563600
C	-6.07502800	-0.41526100	0.38307500
C	-3.57582100	-0.31871700	0.69806300
C	-4.91934700	-0.62729900	1.37577900
C	-5.87940900	-1.26323200	-0.88566000
C	-3.37107000	-1.22188800	-0.53910800
C	-4.51554100	-0.98262600	-1.53941000
H	1.40926800	-2.81424200	-1.19226300
C	1.31836700	-2.83343100	-3.34402600
C	2.52644900	-1.13137200	-1.89821000
C	2.41020800	0.26303300	-1.88325900
C	3.80744100	-1.69973800	-1.80402500
C	3.54619800	1.07309200	-1.76923900
H	1.43655600	0.74214600	-1.89919800
C	4.94254400	-0.89629900	-1.69034200
H	3.91128100	-2.78395400	-1.79459000
C	4.81530000	0.49882400	-1.67248800
H	3.42703600	2.15400500	-1.73211500
H	5.92462600	-1.35716900	-1.60061500
H	5.69721700	1.12865700	-1.57206500
H	-4.35923700	-1.63002600	-2.41089100
N	-2.44370200	-0.47920600	1.61602500

H	-2.12274200	-1.43387400	1.77098000
C	-1.68780500	0.52861100	2.01074400
H	-2.04096600	1.51379300	1.71979100
C	-0.44165700	0.40491900	2.68748100
C	-0.16354800	-0.94188800	3.33584700
H	0.83201400	-0.94361000	3.78893200
H	-0.90666000	-1.13824400	4.12332300
H	-0.19624900	-1.76555700	2.61076400
C	-0.05774200	1.60180200	3.53993200
H	-0.22762300	2.54003200	2.99863500
H	-0.64384300	1.61831100	4.47021100
H	1.00323200	1.53800700	3.80932100
C	2.03887500	-0.00450500	1.59157800
C	2.29558600	-1.37835200	1.43425900
C	3.00934400	0.78922600	2.23017700
C	3.48660300	-1.94385700	1.88934600
H	1.54519700	-1.99956300	0.94885900
C	4.20022400	0.22435400	2.69209600
H	2.83727600	1.85464900	2.35751000
C	4.44447200	-1.14427900	2.52322900
H	3.67013800	-3.00692600	1.74452900
H	4.94218100	0.85412700	3.17982100
H	5.37578200	-1.58148700	2.87858500
C	0.75505200	0.54539000	1.08681900
H	0.21781400	-0.17872900	0.47788600
C	0.74710700	1.87891900	0.54685600
H	1.55314200	2.56155500	0.78911900
C	-0.26629100	2.33151100	-0.29243900
O	-1.30580500	1.67320300	-0.64488700
C	-0.08818000	3.77105900	-0.80546600
O	0.92745300	4.44265400	-0.69528000
O	-1.20899700	4.22534800	-1.42093900
C	-1.13098600	5.57056800	-1.95666300
H	-2.10995300	5.75997400	-2.40366500
H	-0.92350700	6.29029500	-1.15583700
H	-0.33976500	5.63412800	-2.71300700
H	0.49324400	-3.55579500	-3.35016300
H	2.26383100	-3.36824500	-3.49124100
H	1.18788500	-2.12599300	-4.17360000

Addition of isobutyraldehyde to *N*-phenylmaleimide in gas phase (M06-2X/TZVP).

_N_-Phenyl maleimide

Total Energy= -590.440143

Imaginary frequency= 0

XYZ coordinates

H	-3.81161900	-1.31982100	0.29929200
H	-3.81133000	1.32016400	-0.30072900

O	-1.18019100	2.22722000	-0.50586000
O	-1.18080800	-2.22716600	0.50614000
N	-0.75814100	0.00005900	0.00057600
C	-1.56222400	1.12049900	-0.25342600
C	-1.56244500	-1.12028500	0.25364200
C	-2.98334000	-0.64593900	0.14434700
C	-2.98319600	0.64624300	-0.14517600
C	0.66405300	-0.00006800	0.00029500
C	3.43542900	-0.00014200	-0.00034500
C	1.35220600	1.03538600	0.62191000
C	1.35185400	-1.03555300	-0.62161500
C	2.73870500	-1.03440000	-0.61106300
C	2.73902200	1.03416600	0.61072300
H	0.80510100	1.83754000	1.09709600
H	0.80454600	-1.83773900	-1.09651500
H	3.27481500	-1.84416600	-1.08907600
H	3.27541300	1.84388100	1.08850900
H	4.51767400	-0.00014600	-0.00060700

Isobutyraldehyde

Total Energy= -232.428472
Imaginary frequency= 0

XYZ coordinates

C	-0.92312100	-0.62264000	0.20845500
O	-1.87188900	-0.07008700	-0.27653900
H	-0.99685600	-1.68473000	0.52132900
C	0.42877600	0.01317400	0.42673900
H	0.60616200	-0.03555700	1.50890800
C	0.45311700	1.45901500	-0.04157800
H	1.42584300	1.90919300	0.15986200
H	0.26281000	1.51163900	-1.11470800
H	-0.31742700	2.04709200	0.45585000
C	1.49204100	-0.84948500	-0.26115800
H	2.48863200	-0.46215500	-0.04879200
H	1.45271900	-1.88618200	0.07860200
H	1.34835500	-0.83898900	-1.34348700

H_2O

Total Energy= -76.423341
Imaginary frequency= 0

XYZ coordinates

O	0.00000000	0.00000000	0.11651100
H	0.00000000	0.76307500	-0.46604400
H	0.00000000	-0.76307500	-0.46604400

Catalyst B_F

Total Energy= -1445.598325
Imaginary frequency= 0

XYZ coordinates

H	4.96052400	-2.25670300	0.61185900
H	5.80339000	1.37831500	-0.06764400
H	2.89547900	-0.73244900	0.97392100
H	5.23254600	0.28330200	1.18363000
H	-0.72227300	-0.06662500	-1.32747000
H	3.76465500	0.98280200	-1.38474500
H	1.38182600	-0.23660500	-1.49830900
H	3.20908200	1.75281800	1.37711800
H	5.85676600	-0.48656300	-1.70946100
H	6.82172900	-0.90892200	-0.30493000
H	3.45772600	-1.49086600	-1.93322000
H	2.86755100	-2.57812500	-0.67595600
H	5.34156600	-2.80620300	-1.01271900
C	-1.92446900	0.56842500	0.26133100
N	1.53928100	-0.28078300	-0.49998900
N	3.28671600	1.94314100	0.38219200
N	-0.66637500	0.22336000	-0.36055400
S	0.62528300	0.13317700	1.98610300
C	0.50674400	0.02335300	0.31052500
C	5.80027100	-0.72012700	-0.64062600
C	3.49302000	-1.70140600	-0.85633900
C	4.93949200	-1.96592500	-0.44355900
C	5.21456500	0.47640500	0.10394900
C	2.92158000	-0.50763900	-0.09430100
C	3.77229700	0.75914500	-0.30912500
H	-1.71376400	0.70602400	1.32501000
C	-2.34282100	1.93666100	-0.25767200
C	-2.95201600	-0.53639900	0.09060800
C	-2.64234300	-1.75428600	0.69822100
C	-4.13591400	-0.41478300	-0.62823300
C	-3.50365900	-2.83277400	0.59056300
H	-1.71887300	-1.84087100	1.26219900
C	-4.99921700	-1.50098200	-0.73389800
H	-4.40348200	0.51653500	-1.10807100
C	-4.68807600	-2.70767800	-0.12798300
H	-3.25549000	-3.77008500	1.07199900
H	-5.91988200	-1.39613000	-1.29367600
H	-5.36512600	-3.54828400	-0.21162300
F	-3.49115000	2.34441800	0.28941000
F	-1.41546100	2.85436000	0.02020200
F	-2.50698800	1.94054800	-1.59429700
H	2.34983900	2.18187600	0.07430000

Catalyst B

Total Energy= -1147.828457

Imaginary frequency= 0

XYZ coordinates

H	-4.09195400	2.37238100	0.78728500
H	-5.41217200	-1.17342900	0.71744100

H	-2.18152100	0.64468300	0.86840300
H	-4.43898600	-0.06103800	1.67365500
H	0.70681500	-1.10962800	-1.84362500
H	-3.71028900	-1.10296300	-1.09023200
H	-1.28755800	-0.43759900	-1.70469900
H	-2.27790300	-1.71510100	1.38184300
H	-5.65623600	0.52518000	-1.07402500
H	-6.23050000	1.17675700	0.45256200
H	-3.26733700	1.23161600	-1.92359300
H	-2.31484900	2.33109500	-0.92848200
H	-4.77632500	2.81923600	-0.76772400
C	2.19643700	-1.39918300	-0.37449200
N	-1.18880200	-0.06244100	-0.77031800
N	-2.78312200	-1.98182400	0.54136200
N	0.88808200	-0.98527400	-0.85831400
S	0.14201400	-0.18827200	1.56610900
C	-0.07357300	-0.42761300	-0.08798600
C	-5.33526200	0.84307200	-0.07587400
C	-3.04918500	1.52486100	-0.88900100
C	-4.33600700	1.99073400	-0.20952900
C	-4.70314200	-0.34370700	0.64793400
C	-2.43948400	0.33849100	-0.14771700
C	-3.43295900	-0.82633800	-0.06198400
H	2.03909800	-1.92889900	0.56669300
C	2.80638000	-2.34804400	-1.40312900
H	3.77972900	-2.69179700	-1.05596300
H	2.16107900	-3.21368800	-1.56157200
H	2.95831800	-1.83324900	-2.35564100
C	3.12488000	-0.22972400	-0.10744100
C	3.97037700	-0.26027400	0.99519600
C	3.19331700	0.84902800	-0.98192200
C	4.87782000	0.76591500	1.21827900
H	3.89862000	-1.08456300	1.69616400
C	4.09697800	1.87944500	-0.76057900
H	2.52302500	0.89292800	-1.83332100
C	4.94487700	1.83849200	0.33870800
H	5.52400200	0.73533600	2.08664300
H	4.13681200	2.71826500	-1.44434100
H	5.64739400	2.64330200	0.51417500
H	-3.46331000	-2.69063200	0.78871900

M-B_F-Maj-Cx1
Total Enegy= -2192.07386764
Imaginary frequency= 0

XYZ coordinates

H	0.67743000	3.35597600	2.89685000
H	4.14254500	3.52786000	0.77367200
H	0.62228900	4.43813700	1.50887700
H	0.00109900	2.78557200	1.37631300
H	2.08813500	-3.30751300	3.68133100

H	3.41001500	1.31040400	0.92679500
H	3.96822700	-0.42692000	2.12636400
H	0.45992400	-1.43363000	2.87073600
H	2.83313700	-0.82089200	3.41165800
H	2.89039700	4.71085200	0.39872700
H	3.44237700	4.52896300	2.05779600
H	-1.89274900	-0.64567600	-0.69020400
H	2.24151000	-1.04936100	0.43378900
H	-0.23446200	-1.61223000	0.01668400
H	0.73213100	0.82381300	2.05905900
H	3.86916300	-2.74259200	1.26218500
H	4.38002600	-2.73671600	2.94494900
H	1.38564200	-3.37952000	0.70801300
H	0.29125800	-3.75308600	2.03938600
H	2.64486700	-4.49989100	2.51704500
C	-3.50731100	0.28990100	0.29812600
N	-0.39177200	-1.41362200	0.99897800
N	1.50997600	0.61663900	1.44111800
N	-2.18502600	-0.28048100	0.20853900
S	-1.70699000	0.04369600	2.83009800
C	2.42685900	1.63168700	1.25443100
C	0.79532800	3.40296000	1.80908300
C	-1.40592500	-0.58115500	1.28764300
C	3.21849300	3.97555300	1.14085600
C	2.15888400	2.94108400	1.37772700
C	3.53341900	-2.53688100	2.28542300
C	1.15010100	-3.14394400	1.75321500
C	2.36101700	-3.45209600	2.63079200
C	3.12433100	-1.06904600	2.38485900
C	0.75928300	-1.67075800	1.84769400
C	1.94191500	-0.77519000	1.45547600
H	1.20312000	3.75815700	-1.23453000
H	-0.77568200	1.92026800	-1.14527200
O	0.27528000	-0.61556100	-1.65200500
O	3.63076800	2.48120200	-1.81302900
N	2.23666700	0.62028800	-1.73607500
C	0.86281100	0.44330600	-1.57048900
C	2.54565600	1.99947400	-1.64834300
C	1.25260800	2.68802100	-1.35966300
C	0.27753400	1.78541900	-1.32731900
C	3.18429900	-0.41968400	-1.92710800
C	5.01723800	-2.49032200	-2.22158100
C	2.85497900	-1.53331200	-2.69466700
C	4.43509000	-0.33302600	-1.31895600
C	5.34625900	-1.36674900	-1.47395800
C	3.77213500	-2.56652600	-2.83001600
H	1.88596600	-1.59344000	-3.16740200
H	4.69986900	0.54707200	-0.75091000
H	6.31910400	-1.29026900	-1.00521800
H	3.50923600	-3.43309200	-3.42329500
H	5.73051500	-3.29617600	-2.33578300

H	-3.71314900	0.45177400	1.35734200
C	-3.50433300	1.67786100	-0.33492800
C	-4.57651300	-0.59331700	-0.31013600
C	-5.70907800	-0.90431900	0.43345700
C	-4.44500800	-1.10312800	-1.60010700
C	-6.69843000	-1.71922500	-0.10089800
H	-5.81320300	-0.51095300	1.43780300
C	-5.43192200	-1.91867900	-2.13327500
H	-3.57653000	-0.85869600	-2.20149800
C	-6.56048300	-2.22847300	-1.38429100
H	-7.57435900	-1.95945400	0.48805300
H	-5.32138400	-2.31113400	-3.13603000
H	-7.32921000	-2.86642300	-1.80130200
F	-4.71059800	2.24152200	-0.28110000
F	-2.64360900	2.49692100	0.27927700
F	-3.13447400	1.63579900	-1.63034100

M-B_F-Maj-TS1
Total Enegy= -2192.06089955
Imaginary frequency= 1

XYZ coordinates

H	0.73492946	4.10035314	1.76738336
H	3.84345246	3.76207214	-0.55151464
H	0.24466346	4.46794114	0.11107936
H	-0.16263754	2.90765214	0.81703736
H	2.43787946	-2.26688786	4.36880536
H	3.45737746	1.67447814	0.59549536
H	4.18066246	0.24642914	2.15286636
H	0.69504946	-0.69381286	3.20998836
H	3.10324346	0.11450514	3.54213936
H	2.52783246	4.90420514	-0.83162464
H	3.23649146	4.77937314	0.77467636
H	-1.67282554	-0.74290086	-0.41834964
H	2.42386346	-0.76903886	0.70567136
H	0.00397346	-1.50510686	0.45205136
H	0.73799946	1.28384714	1.68448936
H	4.14608046	-2.20517986	1.83383236
H	4.69644146	-1.80898386	3.45704836
H	1.68376446	-3.02664386	1.50397636
H	0.63117746	-3.13965486	2.91336436
H	3.01832346	-3.67202886	3.48826736
C	-3.38598554	0.20235714	0.41435936
N	-0.14775154	-1.10467486	1.37657736
N	1.68543646	1.04812214	1.39218336
N	-2.04006054	-0.31393786	0.42850136
S	-1.50564354	0.65927014	2.87737736
C	2.42851346	1.95756614	0.80097936
C	0.61102346	3.67610114	0.76712836
C	-1.21935254	-0.29806886	1.50687136
C	2.95010346	4.20303714	-0.10869964

C	1.93006546	3.15020014	0.25471636
C	3.82838446	-1.78832886	2.79623836
C	1.45814746	-2.57676786	2.47838736
C	2.69594146	-2.63622486	3.37084736
C	3.37154546	-0.34634886	2.58571736
C	1.00186646	-1.13549286	2.25969236
C	2.15154046	-0.31552986	1.66666636
H	1.30855446	3.34523214	-1.93091964
H	-0.74179054	1.72560814	-1.26699864
O	0.16148746	-0.93340586	-1.41790064
O	3.67474346	1.91208514	-2.19157664
N	2.18167946	0.20173514	-1.71997664
C	0.76068146	0.14561614	-1.48347364
C	2.57848046	1.52772514	-1.86438764
C	1.37622846	2.35895714	-1.48721864
C	0.29754546	1.47510414	-1.37660764
C	3.04258246	-0.91759986	-1.82420264
C	4.73553146	-3.12699786	-1.93749464
C	2.60709746	-2.09685586	-2.42359164
C	4.33017146	-0.84277986	-1.29174264
C	5.17161746	-1.94254386	-1.35667064
C	3.45498046	-3.19566786	-2.46839164
H	1.60924546	-2.14956886	-2.83191164
H	4.67672446	0.08458614	-0.85533464
H	6.17268746	-1.87089486	-0.95031564
H	3.10856446	-4.11130786	-2.93093264
H	5.39214246	-3.98623786	-1.98270364
H	-3.64769554	0.46890014	1.43912236
C	-3.44702254	1.50756214	-0.37795064
C	-4.37845154	-0.80041586	-0.13835564
C	-5.56687654	-1.03794086	0.54173836
C	-4.12064154	-1.48317486	-1.32483264
C	-6.48834754	-1.95191986	0.04709336
H	-5.77112054	-0.50746186	1.46437636
C	-5.04025654	-2.39682286	-1.81804564
H	-3.20482254	-1.30059186	-1.87624164
C	-6.22549254	-2.63318286	-1.13284964
H	-7.40972554	-2.13272086	0.58568236
H	-4.83167354	-2.92280986	-2.74079264
H	-6.94196454	-3.34690786	-1.51938864
F	-4.68347154	2.01129714	-0.37445464
F	-2.63108254	2.43749014	0.13016536
F	-3.08482954	1.33120814	-1.65939464

M-B_F-Min-Cx1

Total Energy= -2192.063805

Imaginary frequency= 0

XYZ coordinates

H	-1.34955100	4.61018400	-0.50539400
H	-2.18154000	3.81279500	-1.84487500

H	-5.63349000	4.18517100	-0.29555500
H	-4.79880600	3.57743300	-1.71592700
H	-2.43852700	0.42800000	1.04426500
H	-0.76471200	1.25363900	-1.00632200
H	-3.23440900	1.58746300	-1.49463700
H	1.16699800	0.62857900	-0.58660900
H	-4.79195300	-3.61761200	0.44229400
H	-5.89859300	-2.30776700	-0.02319200
H	-4.48525400	2.49340300	1.13094900
H	-2.07717400	2.83015600	1.03248800
H	-5.35868400	1.71632500	-0.18066000
H	-4.72023800	-0.39724700	-0.61737600
H	-3.48048100	4.88972900	0.70724400
H	-2.11153500	-1.49550900	1.84892900
H	-2.89899100	-3.06563700	2.01581600
H	-3.63846800	5.59729600	-0.89187500
H	-5.74052600	-2.78730600	1.67039300
H	-3.44985000	-1.70476100	2.98740700
N	-0.77470300	2.00448400	-0.32674100
N	-2.96333800	0.38542500	0.17974800
N	1.36706000	1.38328600	0.06098200
S	0.49613800	3.47970800	1.50190700
C	-3.98133700	-0.56116100	0.16141300
C	-3.07568800	-1.98690900	1.99845800
C	0.35773700	2.24110900	0.36830600
C	-5.18954000	-2.64033700	0.73703400
C	-4.07054600	-1.65773500	0.92225800
C	-4.70192700	3.72825500	-0.63488600
C	-2.20429500	3.98509600	-0.76312000
C	-3.51681100	4.65158400	-0.36096600
C	-4.51448100	2.37110300	0.04276500
C	-2.04678500	2.64394300	-0.04740900
C	-3.20473600	1.70727800	-0.40167400
H	-3.90268100	-2.70983900	-2.18666600
H	-2.50806400	-0.54705100	-3.04327100
O	-0.00873300	-0.50328500	-1.82006700
O	-2.31668500	-4.17671200	-0.40174200
N	-0.84318400	-2.44115200	-0.86783900
C	-2.05800200	-3.15421800	-0.96749900
C	-0.89340000	-1.32115100	-1.68278400
C	-2.90451100	-2.38514700	-1.93729400
C	-2.21935200	-1.33043400	-2.36000300
C	0.33589900	-2.93386100	-0.23513400
C	2.62178000	-3.95042600	0.95234200
C	1.52410900	-2.98235600	-0.95668700
C	0.28116600	-3.39625800	1.07170600
C	1.42836200	-3.91124100	1.65872600
C	2.66810400	-3.48233000	-0.35432100
H	1.54685800	-2.62951100	-1.97982300
H	-0.65282100	-3.36525700	1.61364300
H	1.38745700	-4.27460000	2.67722100

H	3.59777200	-3.50582700	-0.90846200
H	3.51674100	-4.33973000	1.41973500
C	2.68872200	1.44395300	0.62724500
H	2.80547600	2.42530700	1.08956300
C	3.76963300	1.21412700	-0.40704800
C	4.87764200	2.05245300	-0.44296600
C	3.67413200	0.16930000	-1.32360000
C	5.87807800	1.85609700	-1.38615700
H	4.95582500	2.86537300	0.26927600
C	4.67229100	-0.02586400	-2.26684500
H	2.82285100	-0.50277800	-1.30195900
C	5.77585500	0.81772800	-2.30096900
H	6.73477700	2.51746100	-1.40760200
H	4.58763300	-0.83742800	-2.97888300
H	6.55252700	0.66621300	-3.03988600
C	2.80693500	0.43253100	1.76962000
F	4.00879300	0.51342700	2.35385100
F	1.88398000	0.63469600	2.70940900
F	2.65517300	-0.82891100	1.33647300

M-B_F-Min-TS1

Total Energy= -2192.042634

Imaginary frequency= 1

XYZ coordinates

H	2.85129600	-4.01355500	-0.82138900
H	3.34089900	-2.91000700	-2.11141300
H	6.85483500	-2.41664300	-0.69854800
H	5.80879900	-1.92538000	-2.01959300
H	2.37039700	0.17779300	0.69179000
H	1.30734900	-1.08992800	-1.17105600
H	3.78607900	-0.48392400	-1.53950300
H	-0.68950400	-0.99810700	-0.64193000
H	2.78691800	4.80129700	0.86182700
H	4.36379500	4.17859900	0.34765800
H	5.37611700	-1.25633000	0.93894700
H	3.11389800	-2.24605500	0.85085700
H	5.92269900	-0.14008700	-0.31220900
H	4.65728500	1.82057600	-0.15556700
H	5.03871600	-3.78389000	0.28129900
H	1.03172000	1.58390200	1.24968100
H	1.17823900	3.18641400	1.96156000
H	5.30157000	-4.26089400	-1.38762800
H	3.87231700	4.05804800	2.04430700
H	2.14086800	1.85335600	2.60335500
N	1.58709200	-1.66217500	-0.37841000
N	3.28457200	0.37319900	0.29508800
N	-0.63258400	-1.74006800	0.05788500
S	0.88647200	-3.36544700	1.56584900
C	3.70777200	1.61167500	0.33021000
C	1.74104500	2.29505800	1.68690000

C	0.59034800	-2.21637700	0.37271900
C	3.51581900	4.00344000	1.01313800
C	2.86734400	2.66690800	0.74017900
C	5.81711000	-2.20443600	-0.96043900
C	3.47766000	-3.15080000	-1.05129300
C	4.94795300	-3.44487900	-0.75570900
C	5.30949500	-1.02554000	-0.12846800
C	2.99356900	-1.97862300	-0.20322200
C	3.85105000	-0.73845600	-0.47459600
H	2.78331600	3.54658400	-1.42964200
H	2.28387900	0.99242200	-2.21925500
O	-0.40015000	0.45695900	-1.76025900
O	0.59591000	4.65140500	-0.18419700
N	-0.26737800	2.60799100	-0.84485100
C	0.73174800	3.53704800	-0.62423200
C	0.28781700	1.43753300	-1.46853300
C	2.04415300	2.86792400	-1.01951700
C	1.66754100	1.65791600	-1.63923900
C	-1.63244900	2.77367000	-0.49923400
C	-4.30751200	3.05383400	0.19512300
C	-2.62430900	2.34609400	-1.37655300
C	-1.97604800	3.35550000	0.71652200
C	-3.31244600	3.49899500	1.05511700
C	-3.95821100	2.47832600	-1.01886800
H	-2.34388600	1.90387100	-2.32246700
H	-1.20036700	3.70036600	1.38578300
H	-3.57599400	3.95282600	2.00186200
H	-4.72818800	2.13213900	-1.69683000
H	-5.34952500	3.15600700	0.46901400
C	-1.84903100	-2.08197700	0.75294600
H	-1.67725700	-3.00810000	1.30279700
C	-3.02468900	-2.22868100	-0.18904200
C	-3.89512800	-3.30384500	-0.05180600
C	-3.25303300	-1.28277300	-1.18619200
C	-4.98142400	-3.43972500	-0.90671100
H	-3.72148200	-4.03954900	0.72500700
C	-4.33616900	-1.42245900	-2.04074600
H	-2.59204300	-0.43043300	-1.29915400
C	-5.20220800	-2.49991300	-1.90418400
H	-5.65239000	-4.28188800	-0.79498100
H	-4.50265100	-0.68489600	-2.81615100
H	-6.04617000	-2.60717600	-2.57390500
C	-2.13381700	-1.00693200	1.80638900
F	-3.21097900	-1.32079200	2.53338300
F	-1.10572600	-0.85809000	2.64859700
F	-2.35293700	0.19101700	1.24753200

M-B_F-Maj-Cx2

Total Energy= -2192.05949

Imaginary frequency= 0

XYZ coordinates

H	3.63439500	3.24950900	1.65797100
H	-0.01017400	1.09138100	2.36049400
H	2.21281800	4.05129600	2.32480200
H	3.24379100	3.08747200	3.37290000
H	5.90579700	-2.43901200	-1.34104500
H	1.69038600	0.03801000	1.26715600
H	5.89413400	1.18153500	-0.31102400
H	3.76261900	-1.92061800	0.11350000
H	5.92556800	-0.46449400	0.31254800
H	0.54970400	2.07579300	3.71274700
H	0.01257600	2.86610900	2.24082700
H	-0.32601300	-0.78790300	-0.34172400
H	3.59362500	0.84488400	-1.13531200
H	1.57794300	-0.32916100	-0.99434800
H	4.33928800	1.32264800	1.28932400
H	5.69245600	0.32049400	-2.63609900
H	7.12358900	-0.33057800	-1.85139600
H	3.57783700	-1.12704700	-2.82733300
H	3.57706200	-2.76361900	-2.17346700
H	5.84107900	-2.11970500	-3.06778600
C	-1.15286500	-2.55650000	0.45347000
N	2.00607600	-1.20319700	-0.70595400
N	3.68446700	0.61711100	0.98154600
N	-0.10254300	-1.74675700	-0.09392200
S	1.73835100	-3.67184600	0.27714900
C	2.38032800	0.85824000	1.41808700
C	2.81162700	3.13747100	2.36878700
C	1.20206800	-2.15048300	-0.19384200
C	0.55242600	1.98991200	2.62220200
C	1.95053900	1.94213200	2.07695400
C	6.03224500	-0.34665000	-1.83653300
C	3.98291700	-1.76089700	-2.02995700
C	5.50475700	-1.75467700	-2.09574600
C	5.53097000	0.16505400	-0.49170800
C	3.46083300	-1.24202400	-0.68818100
C	4.00532300	0.15761300	-0.37359900
H	2.31054200	2.93204300	-0.71781300
H	1.31614800	5.36753600	-0.08442600
O	-1.48391200	5.20454100	0.04883100
O	0.20687700	1.11596000	-1.04852200
N	-1.01073900	3.00022000	-0.50422400
C	-0.69457300	4.34340700	-0.20167400
C	0.14625700	2.28590600	-0.74274300
C	1.28776500	3.24556800	-0.58105000
C	0.79945400	4.43962000	-0.27284200
C	-2.32996300	2.46432100	-0.55150700
C	-4.87929900	1.40412800	-0.64771400
C	-3.30006800	3.09367900	-1.31964200
C	-2.62250200	1.31740400	0.17256300
C	-3.90004800	0.78156600	0.11467000

C	-4.58064400	2.56118300	-1.35674000
H	-3.05441500	3.99228200	-1.86948100
H	-1.85637500	0.85448900	0.77969600
H	-4.12368300	-0.12500500	0.66279800
H	-5.34520900	3.05010800	-1.94658600
H	-5.87614400	0.98420600	-0.69030400
H	-0.79944400	-3.59182100	0.43781100
C	-1.33052700	-2.21200000	1.94226700
C	-2.45392400	-2.42128000	-0.32889400
C	-3.65560800	-2.91970700	0.17846300
C	-2.45817100	-1.81824400	-1.58315800
C	-4.83259200	-2.79093500	-0.54476900
H	-3.68215800	-3.41320400	1.14019600
C	-3.63728900	-1.69364500	-2.30693600
H	-1.53721700	-1.44274500	-2.00846300
C	-4.83019300	-2.17154400	-1.78814500
H	-5.75496300	-3.18181600	-0.13355000
H	-3.61811500	-1.21215800	-3.27635700
H	-5.75072800	-2.07104800	-2.34915200
F	-1.99128600	-3.17365000	2.60059200
F	-0.16281600	-2.04245600	2.55480400
F	-2.02593600	-1.06919300	2.11476300

M-B_F-Maj-TS2

Total Energy= -2192.03138

Imaginary frequency= 1

XYZ coordinates

H	3.71658400	3.79302300	0.91205600
H	0.28189500	1.47224600	2.18292300
H	2.54136100	4.41585000	2.05346400
H	3.68847700	3.17048000	2.57779600
H	5.79220200	-2.76625500	-0.53900800
H	1.91052900	0.33780400	0.94232600
H	5.98400600	0.98853900	-0.91353000
H	3.67001700	-1.64967200	0.42855700
H	5.84028600	-0.30028400	0.27979000
H	1.35295400	2.17097100	3.40695900
H	0.33887400	3.23101600	2.41512600
H	-0.38057800	-0.76372800	-0.34842900
H	3.74291200	0.41561900	-1.81081100
H	1.53962800	-0.40892900	-1.08246000
H	4.18544900	1.96396100	0.07980500
H	5.92062100	-0.66594200	-2.75650100
H	7.21741600	-1.05049400	-1.63433100
H	3.68511200	-1.95016600	-2.60365200
H	3.51622700	-3.25159000	-1.42623900
H	5.87525500	-3.09162900	-2.26259900
C	-1.21715800	-2.49692500	0.54501500
N	1.96327100	-1.23840600	-0.67381000
N	3.61004100	1.13044900	0.13112200

N	-0.15843000	-1.69785700	-0.00695300
S	1.69962900	-3.48781600	0.74388000
C	2.52099000	1.22624900	0.86049500
C	3.06724600	3.51120900	1.74638200
C	1.14505500	-2.08993000	-0.01122500
C	0.93875300	2.31643900	2.40768800
C	2.03588300	2.46120300	1.37502800
C	6.13217400	-1.00780400	-1.73808200
C	3.98626400	-2.28577700	-1.60529700
C	5.50459000	-2.38090400	-1.52267300
C	5.56416900	-0.00653900	-0.73793000
C	3.41335800	-1.30083000	-0.57801900
C	4.03736700	0.07472600	-0.80900900
H	2.16447600	3.08361300	-0.79603900
H	1.21636600	5.38597800	0.23211700
O	-1.60256800	5.15152300	0.11594900
O	0.27050600	1.07469600	-0.85440400
N	-0.99149000	2.93989700	-0.36657700
C	-0.69865400	4.35984700	0.00274200
C	0.14929600	2.25275800	-0.50841100
C	1.29901500	3.17951900	-0.13607400
C	0.70866300	4.44763400	0.09101700
C	-2.29834000	2.42566200	-0.55379600
C	-4.85673800	1.41724300	-0.89299700
C	-3.20263200	3.10839300	-1.35889100
C	-2.67060100	1.25174000	0.08842900
C	-3.94845900	0.74329000	-0.08747800
C	-4.48363700	2.59948400	-1.52060100
H	-2.90299000	4.03452900	-1.82890700
H	-1.96303800	0.75343700	0.73726800
H	-4.22917900	-0.18062000	0.40350100
H	-5.19318700	3.13221400	-2.14090900
H	-5.85505300	1.02034300	-1.02798300
H	-0.84525500	-3.52355900	0.59819000
C	-1.47977500	-2.10399200	2.01458400
C	-2.48515800	-2.44154200	-0.29663300
C	-3.68249100	-2.96435600	0.19492100
C	-2.46752600	-1.89524800	-1.57527600
C	-4.83794200	-2.91531100	-0.57059600
H	-3.72202000	-3.40892600	1.18073000
C	-3.62617700	-1.84793100	-2.34067600
H	-1.55122400	-1.49455500	-1.98740800
C	-4.81607800	-2.35100900	-1.84015900
H	-5.75926300	-3.32005000	-0.17092300
H	-3.59357200	-1.40309600	-3.32692900
H	-5.72039300	-2.30889600	-2.43385100
F	-1.99979200	-3.13176000	2.69930100
F	-0.36382700	-1.73168900	2.63984200
F	-2.34248500	-1.08080300	2.13020300

M-B_F-Min-Cx3

Total Energy= -2192.05955
Imaginary frequency= 0

XYZ coordinates

H	-4.15894300	-2.58512000	-1.79633200
H	-0.24483600	-3.68535300	-0.47959300
H	-3.40487900	-4.06489000	-2.38496600
H	-4.22497800	-4.06168500	-0.83028900
H	-3.45225900	0.78440400	4.24637100
H	-1.20425300	-1.79888700	0.40088300
H	-5.21683600	0.28475700	0.96140900
H	-1.93349900	-0.65898000	2.60387800
H	-4.53247400	-0.56651600	2.34538700
H	-1.38460100	-5.03650400	-0.55412300
H	-0.89857200	-4.22057800	-2.03130900
H	1.17936800	-0.30014500	-0.21807200
H	-2.96476400	1.02625300	0.29042300
H	-0.59695500	0.73258000	0.38603200
H	-4.07405400	-1.31237200	-0.12471300
H	-4.41823500	2.45490700	1.87487100
H	-5.45207000	1.63499200	3.03569800
H	-1.86333800	2.35579900	2.15695300
H	-1.16889100	1.47414700	3.51710000
H	-3.36614900	2.53470500	4.12572200
C	2.84133000	-0.77199900	0.97933000
N	-0.64061900	0.20766000	1.24974100
N	-3.14183900	-1.06294500	0.16498300
N	1.45761400	-0.44952200	0.74759300
S	0.72327300	-0.82684600	3.30496300
C	-2.15706900	-1.99804100	-0.06621600
C	-3.58550800	-3.46489700	-1.48941100
C	0.50949200	-0.32923100	1.71554500
C	-1.14277200	-4.05580100	-0.97570700
C	-2.28912900	-3.09829000	-0.82611600
C	-4.48503000	1.58098300	2.53233800
C	-2.00566100	1.49250600	2.81799600
C	-3.34096300	1.61392300	3.54018400
C	-4.40821300	0.30839900	1.69809300
C	-1.91047600	0.22546800	1.96060600
C	-3.07353700	0.15961900	0.96048500
H	-3.88208400	-0.72160400	-3.62756900
H	-1.63917700	-2.22423700	-3.34495400
O	0.30668600	-0.75264600	-2.01270900
O	-3.45644500	1.79393800	-2.50861700
N	-1.34976300	0.87504200	-2.13291200
C	-0.79809000	-0.39728700	-2.34109800
C	-2.69128100	0.87444400	-2.58772300
C	-2.93438300	-0.47170700	-3.17747000
C	-1.83848700	-1.20944900	-3.04041700
C	-0.66792400	1.98019600	-1.54640400
C	0.71007900	4.02715300	-0.24739800

C	0.72080100	2.06941400	-1.65074500
C	-1.37071800	2.94663200	-0.82420500
C	-0.67550500	3.96673700	-0.19031800
C	1.40313300	3.07656900	-0.98286800
H	1.27238700	1.34593800	-2.23074400
H	-2.44791900	2.91103200	-0.77241500
H	-1.22933500	4.71293500	0.36518400
H	2.48488500	3.10339600	-1.04278200
H	1.24399200	4.81144000	0.27292400
H	3.02878400	-0.68321700	2.05066400
C	3.10724800	-2.24027500	0.63871100
C	3.74762500	0.16023900	0.20097900
C	3.65898300	0.25030400	-1.18808500
C	4.64581300	0.97414100	0.88053700
C	4.45975300	1.14639900	-1.88181100
H	2.96613200	-0.38406500	-1.72958700
C	5.44506100	1.87381700	0.18586100
H	4.71542200	0.90808500	1.95990000
C	5.35346900	1.96142900	-1.19612700
H	4.38837500	1.20667600	-2.96089100
H	6.14028500	2.50363800	0.72618900
H	5.97808300	2.65904300	-1.73967000
F	4.38913300	-2.55005900	0.86692200
F	2.35312800	-3.06115900	1.36644000
F	2.85119100	-2.51560300	-0.65085900

M-B_F-Min-TS3

Total Energy= -2192.04552

Imaginary frequency= 1

XYZ coordinates

H	4.14809600	-2.87069300	1.56261400
H	-0.11298000	-3.17959400	0.86807200
H	3.17538600	-4.04363600	2.43723200
H	3.54074400	-4.31034800	0.72958900
H	3.52469400	0.86205600	-4.19558400
H	1.11397000	-1.66089800	-0.45739800
H	5.23186000	0.14758300	-0.91327100
H	1.92190700	-0.52541600	-2.61754900
H	4.51179300	-0.61918500	-2.33057300
H	0.90261200	-4.55631800	0.39450700
H	0.66502700	-4.17759100	2.09835500
H	-1.19676100	-0.17538500	0.17310700
H	3.03744000	0.99883800	-0.21852500
H	0.58421800	0.91468200	-0.41597900
H	3.88501000	-1.22705600	0.39742300
H	4.57894600	2.38612900	-1.76326400
H	5.56707000	1.54281400	-2.94727800
H	2.01679700	2.46965900	-2.07177700
H	1.28592100	1.66937200	-3.46359800
H	3.55429500	2.60946000	-4.01626700

C	-2.83074300	-0.66785900	-1.05954700
N	0.65194200	0.34698300	-1.25250200
N	3.05379400	-1.07442100	-0.16319900
N	-1.46039300	-0.30356100	-0.80209300
S	-0.66318200	-0.68443700	-3.34190000
C	2.03332300	-1.87579200	0.06774700
C	3.29765500	-3.54645300	1.47260100
C	-0.49472100	-0.18582600	-1.74753600
C	0.79375300	-3.73553700	1.10778900
C	2.01608200	-2.84512300	1.08626500
C	4.59543000	1.53405100	-2.45093200
C	2.11419000	1.61843400	-2.75592200
C	3.46254200	1.67346700	-3.46292700
C	4.43637900	0.24151000	-1.65775200
C	1.93215400	0.33383500	-1.94022200
C	3.08531000	0.17591000	-0.94308800
H	3.91223500	-1.17762800	3.29062600
H	1.48457300	-2.39299000	3.23564200
O	-0.38863400	-0.85214700	1.91830100
O	3.56460400	1.45141700	2.37571000
N	1.39559900	0.62259700	2.03012900
C	0.77942600	-0.60186300	2.15753200
C	2.80943300	0.50310200	2.42796100
C	2.99702400	-0.84581500	2.83013600
C	1.83528500	-1.59028200	2.59540100
C	0.74841400	1.83058300	1.65777800
C	-0.56996200	4.13149800	0.76337600
C	-0.62343500	1.99160300	1.87337200
C	1.46300400	2.85449900	1.02535200
C	0.80072100	3.99366900	0.59176300
C	-1.27415700	3.12734300	1.41111300
H	-1.18150700	1.22707200	2.39030000
H	2.53216200	2.77043100	0.90863900
H	1.36857000	4.77867400	0.10805800
H	-2.34328900	3.21457200	1.56206700
H	-1.08162100	5.01423200	0.40290000
H	-3.00713100	-0.56841400	-2.13155100
C	-3.05180500	-2.14985900	-0.74341900
C	-3.78237000	0.21316600	-0.27677900
C	-3.67299600	0.32437700	1.10902900
C	-4.75208900	0.94874300	-0.94696800
C	-4.52270400	1.16892200	1.80853000
H	-2.92693800	-0.25275700	1.64407300
C	-5.60150500	1.79534700	-0.24564300
H	-4.83910500	0.86391900	-2.02388100
C	-5.48665300	1.90817900	1.13256000
H	-4.43374200	1.24778000	2.88519000
H	-6.35230500	2.36554300	-0.77761300
H	-6.14862900	2.56614100	1.68138300
F	-4.30452000	-2.51055100	-1.04187500
F	-2.22555800	-2.93381800	-1.43685200

F	-2.85044000	-2.42656400	0.55438100

M-B-Maj-Cx1
Total Enegy= -1894.30505841
Imaginary frequency= 0

XYZ coordinates

H	-0.39748500	1.51549200	-4.22764000
H	-4.09342500	1.89587100	-2.73795600
H	-0.66475300	3.10073100	-3.51323600
H	0.18812100	1.85013800	-2.60027600
H	-0.33107500	-4.70124100	-1.98603300
H	-3.02541300	0.15896500	-1.59961000
H	-2.98760800	-2.03231700	-2.13320700
H	0.70365500	-2.32414500	-1.64259600
H	-1.48773700	-2.55963600	-2.88274700
H	-3.13758300	3.37109600	-2.79897100
H	-3.28267900	2.36747800	-4.24139400
H	1.80503300	0.15065200	1.75529300
H	-1.75250800	-1.52408000	-0.02452500
H	0.55253600	-1.36133300	1.13283500
H	-0.10750300	-0.13993200	-1.97766600
H	-2.79704300	-3.81763600	-0.41558400
H	-2.79993100	-4.51032800	-2.03005900
H	-0.52382800	-3.58545800	0.85211800
H	0.95441200	-4.10093900	0.04368800
H	-1.01076300	-5.53123800	-0.59427300
C	3.38722900	1.18723200	0.79792300
N	0.95153600	-1.46822200	0.20763300
N	-0.99136800	-0.25826900	-1.49190000
N	2.34626700	0.17581800	0.90000400
S	2.46134900	-0.33886900	-1.71687100
C	-2.05495900	0.48128600	-1.96504500
C	-0.63890000	2.03142300	-3.29251700
C	1.88803200	-0.56003900	-0.13909400
C	-3.18553700	2.33585100	-3.15204200
C	-1.96216200	1.57125600	-2.74331800
C	-2.21784000	-3.89380200	-1.34258300
C	-0.03196000	-3.66600000	-0.12503900
C	-0.87109900	-4.54739600	-1.04602700
C	-2.02214000	-2.49800700	-1.92792900
C	0.14914200	-2.26313500	-0.70300100
C	-1.21052100	-1.60629600	-0.98077700
H	-1.07763200	3.73262900	-0.94075200
H	0.77403600	2.11896900	0.18960900
O	-0.50158200	0.30219800	1.90785500
O	-3.62870800	2.98114100	-0.06030600
N	-2.36330000	1.35158300	1.01579500
C	-0.99613400	1.12456500	1.16645300
C	-2.56842800	2.47592800	0.18115200
C	-1.21039400	2.90305900	-0.26417400

C	-0.29912900	2.11845800	0.30348800
C	-3.39696800	0.57267900	1.59945400
C	-5.41074800	-0.99162100	2.70648800
C	-3.24317500	0.04917900	2.88035300
C	-4.56224000	0.32718500	0.87692400
C	-5.56512900	-0.44988900	1.43713600
C	-4.24906900	-0.73783300	3.42234200
H	-2.34049300	0.24942400	3.43753200
H	-4.69143600	0.76633800	-0.10231000
H	-6.47256800	-0.63181000	0.87566900
H	-4.12342000	-1.14786000	4.41637000
H	-6.19403900	-1.60166000	3.13734700
H	3.19452900	1.78243600	-0.09984700
C	3.30849200	2.07599200	2.03740400
H	4.05719000	2.86428500	1.97280700
H	2.32109000	2.53392100	2.13204200
H	3.51451900	1.49105300	2.93671500
C	4.77157000	0.58187400	0.66295000
C	5.71190300	1.17995000	-0.16702400
C	5.13644000	-0.53470900	1.40729400
C	7.00259400	0.67531800	-0.24899100
H	5.42334500	2.03416500	-0.76989300
C	6.42523200	-1.04362900	1.32567800
H	4.40023600	-1.01720600	2.04020100
C	7.36275800	-0.43812600	0.49882700
H	7.72409400	1.14304100	-0.90717100
H	6.69734200	-1.91744000	1.90474700
H	8.36641100	-0.83814400	0.42976200

M-B-Maj-TS1
Total Energy=-1894.29311907
Imaginary frequency= 1

XYZ coordinates

H	0.32349476	2.74731302	-3.22694832
H	-3.29271124	3.41569102	-1.95724632
H	0.38635876	3.97272502	-1.95725032
H	0.86980276	2.30959102	-1.60683532
H	-0.98812024	-4.08848898	-2.82572832
H	-2.77393824	1.08406702	-1.74880232
H	-3.11483624	-0.97301698	-2.63070832
H	0.44560276	-2.03083998	-2.05978432
H	-1.68778024	-1.64845498	-3.41427732
H	-2.03669024	4.64429902	-1.83304232
H	-2.24096124	3.76633202	-3.34603032
H	1.62692776	-0.28608298	1.72882568
H	-1.94437524	-1.06608598	-0.43223232
H	0.25210576	-1.49880898	0.83629268
H	0.10422176	0.39450902	-1.75882532
H	-3.36004624	-3.00160798	-1.23338732
H	-3.37323624	-3.42977998	-2.93898532

H	-1.17247424	-3.39197098	0.14530868
H	0.23882376	-4.05939198	-0.67129532
H	-1.90210524	-4.97225298	-1.61304032
C	3.32989076	0.74897902	1.01519068
N	0.69120276	-1.51767798	-0.08097932
N	-0.90460324	0.26920502	-1.64219232
N	2.25330376	-0.22831798	0.92999068
S	2.41213976	-0.27915298	-1.74167632
C	-1.70890824	1.29694302	-1.79080832
C	0.15809976	2.92456202	-2.16037332
C	1.75570176	-0.69666298	-0.23164632
C	-2.27610724	3.66680002	-2.25786432
C	-1.27777724	2.63298102	-1.79465332
C	-2.74124124	-3.04634598	-2.13633432
C	-0.63552724	-3.42221598	-0.81058632
C	-1.55462124	-3.97712698	-1.89537532
C	-2.26165724	-1.63864598	-2.48176932
C	-0.15586824	-2.01151998	-1.14822832
C	-1.36856324	-1.09501498	-1.36698332
H	-1.07365124	3.90623602	0.09976668
H	0.82321076	2.13516802	0.85297568
O	-0.47383824	-0.06998198	2.03939968
O	-3.61620124	2.84062302	0.42193368
N	-2.31800424	1.08090002	1.19316768
C	-0.90686624	0.89712602	1.40995568
C	-2.54217224	2.32007902	0.59901268
C	-1.18451724	2.83289502	0.19756768
C	-0.24360724	1.99570102	0.80563368
C	-3.33304324	0.14834402	1.51970068
C	-5.31598424	-1.73234398	2.06510768
C	-3.23677424	-0.65355698	2.65449168
C	-4.42884124	0.01387102	0.66567868
C	-5.41595724	-0.91766598	0.94441968
C	-4.22632124	-1.59369698	2.91334668
H	-2.38852824	-0.54664798	3.31308768
H	-4.52131024	0.66337202	-0.19380032
H	-6.26751424	-1.00445198	0.28143068
H	-4.14465324	-2.21638598	3.79539768
H	-6.08611724	-2.46210898	2.27935068
H	3.13610476	1.54066002	0.28331768
C	3.31755576	1.33441502	2.42571968
H	4.09525076	2.09133702	2.51824268
H	2.35090076	1.78976302	2.65269568
H	3.51873676	0.55111002	3.15948968
C	4.68627876	0.15104502	0.69870768
C	5.63740976	0.92034102	0.03877568
C	5.02127176	-1.13258898	1.11367468
C	6.90842376	0.41824502	-0.20158632
H	5.37073576	1.91284802	-0.30826232
C	6.29079076	-1.63962498	0.87095468
H	4.27524776	-1.74082398	1.61195168

C	7.23863276	-0.86514198	0.21474468
H	7.63790276	1.02376402	-0.72481532
H	6.54003176	-2.64388998	1.19057068
H	8.22698276	-1.26293198	0.02168568

M-B-Min-Cx1

Total Energy= -1894.297628

Imaginary frequency= 0

XYZ coordinates

H	1.83837100	-4.44399100	-0.96261700
H	2.50915100	-3.30432700	-2.12856300
H	5.99082200	-3.37474600	-0.55646800
H	5.08154000	-2.64420400	-1.86839800
H	2.17302300	-0.43033700	1.26001100
H	0.54783300	-1.76918100	-1.25731500
H	3.22773200	-1.05333700	-1.37610500
H	-1.41064900	-1.23120800	-0.68457400
H	3.51462200	4.12385900	0.98316700
H	4.93809100	3.12353000	0.63278600
H	4.56388900	-2.17388500	1.11572000
H	2.26970900	-2.84610000	0.87738100
H	5.32099700	-1.04061600	0.00486400
H	4.36365100	0.97817800	-0.11944300
H	3.98874000	-4.58448100	0.21911900
H	1.14591200	1.50334500	1.70065200
H	1.66999900	3.06802200	2.35576100
H	4.25632500	-4.93902200	-1.48045300
H	4.46160600	3.44229000	2.30330000
H	2.17027000	1.56720000	3.13226500
N	0.82412100	-2.08237100	-0.33432600
N	2.72681800	-0.19030200	0.44325100
N	-1.28439400	-1.50155300	0.28318600
S	0.34206000	-2.11037200	2.31304000
C	3.49397400	0.95664100	0.53109900
C	1.98278200	2.03962400	2.16247300
C	-0.05899500	-1.88408900	0.67543400
C	4.08015400	3.24052900	1.29776500
C	3.20250900	2.02528000	1.28406200
C	5.00158300	-3.00912200	-0.83810300
C	2.56931100	-3.64364200	-1.08711000
C	3.98119100	-4.14514500	-0.78352800
C	4.59104700	-1.84968700	0.06987900
C	2.20183300	-2.49301300	-0.15343000
C	3.19737100	-1.33715300	-0.31374400
H	3.31304100	2.84578900	-1.93937700
H	2.30436000	0.50431800	-2.86039100
O	-0.31877000	0.20227800	-1.98457000
O	1.34958400	4.17284200	-0.45514000
N	0.16453700	2.24710400	-0.99480300
C	1.29189600	3.09818000	-0.98052700

C	0.44445500	1.11148500	-1.75192700
C	2.33927100	2.40487900	-1.79440100
C	1.84208600	1.26112900	-2.24679900
C	-1.11667500	2.62037800	-0.50444200
C	-3.60999200	3.39832600	0.43187300
C	-2.24790100	2.39432000	-1.28250000
C	-1.22403200	3.24760300	0.73118900
C	-2.47274000	3.63921000	1.19080600
C	-3.49346100	2.77520500	-0.80386200
H	-2.15029800	1.91790700	-2.24866400
H	-0.33564400	3.43318400	1.31595300
H	-2.55547500	4.12766200	2.15312500
H	-4.37576600	2.58510700	-1.40204700
H	-4.58314500	3.69593500	0.79993700
C	-2.43332200	-1.33349000	1.17352900
H	-2.30813300	-2.06310200	1.97267400
C	-3.69658500	-1.65596500	0.40474800
C	-4.54417800	-2.67265400	0.82979800
C	-4.03584800	-0.92995300	-0.73644500
C	-5.71096900	-2.96085600	0.13181500
H	-4.28562600	-3.24572100	1.71276900
C	-5.19526400	-1.22103100	-1.44080300
H	-3.38968700	-0.12536700	-1.07402000
C	-6.03781700	-2.23752700	-1.00650400
H	-6.36153600	-3.75545300	0.47511000
H	-5.44442700	-0.65349800	-2.32913900
H	-6.94383500	-2.46445300	-1.55396400
C	-2.47323000	0.06839400	1.77438400
H	-1.54069800	0.26702500	2.30382000
H	-2.60560700	0.81329000	0.98939500
H	-3.30694000	0.15409500	2.47322900

M-B-Min-TS1

Total Energy= -1894.278061

Imaginary frequency= 1

XYZ coordinates

H	3.38849500	-3.65915200	-1.32690900
H	3.65117200	-2.26020700	-2.36722600
H	7.04850700	-1.44668900	-0.80193800
H	5.92858500	-0.88978400	-2.03410900
H	2.35114100	0.08191100	1.10590000
H	1.33878200	-1.57818400	-1.37370100
H	3.70685400	0.00562900	-1.39325400
H	-0.66977600	-1.49389600	-0.68994500
H	1.62228400	4.75755800	1.10536500
H	3.29119700	4.46345400	0.58699900
H	5.38676500	-0.88300700	0.98282400
H	3.36940600	-2.19606700	0.67167600
H	5.72919300	0.52870300	-0.01531600
H	3.97292400	2.24307200	-0.08818600

H	5.51526600	-3.26501100	-0.16114000
H	0.55862400	1.22751900	1.30372300
H	0.31102800	2.79940300	2.08100300
H	5.82504600	-3.34854000	-1.88762700
H	2.83112200	4.20295900	2.27371900
H	1.49240600	1.65925800	2.73796800
N	1.72990400	-1.76839700	-0.45820600
N	3.04748900	0.52179300	0.50091000
N	-0.43325500	-1.82173000	0.24571700
S	1.38811800	-1.93835400	2.20348000
C	3.14603200	1.82703100	0.48446600
C	1.06251700	2.05607200	1.81373200
C	0.85555600	-1.84318600	0.58551500
C	2.48969800	4.11039200	1.23996900
C	2.12035400	2.67931900	0.93401200
C	5.98886200	-1.36226000	-1.04770300
C	3.84091900	-2.66748100	-1.36663500
C	5.34744500	-2.74854200	-1.11134000
C	5.28494700	-0.46954700	-0.02524100
C	3.17237800	-1.78154800	-0.31874800
C	3.80042500	-0.37942700	-0.37141200
H	1.98882000	3.51547600	-1.25567800
H	1.84206300	0.90952000	-2.02538900
O	-0.81167100	0.11551800	-1.80410600
O	-0.35494800	4.34995600	-0.09167600
N	-0.95012100	2.23278800	-0.80785600
C	-0.07145200	3.26045200	-0.52717700
C	-0.23687900	1.13527300	-1.42613000
C	1.32215300	2.75168700	-0.87065300
C	1.12015100	1.50482600	-1.49460100
C	-2.34477700	2.27276900	-0.57290200
C	-5.08105400	2.28466000	-0.07013300
C	-3.22349500	1.71161200	-1.49654800
C	-2.83638200	2.85581000	0.59312100
C	-4.20119200	2.86476900	0.83521900
C	-4.58630500	1.71145700	-1.23329000
H	-2.83264500	1.26561700	-2.39968600
H	-2.14948500	3.30141800	1.29883100
H	-4.57738700	3.31937700	1.74289900
H	-5.26537600	1.26452600	-1.94863000
H	-6.14498400	2.28386400	0.12830300
C	-1.54941000	-1.90124600	1.19169600
H	-1.21990500	-2.54772200	2.00408400
C	-2.73812300	-2.53835800	0.50492000
C	-3.30026800	-3.70141100	1.01894200
C	-3.30571400	-1.95175300	-0.62580600
C	-4.41500400	-4.27412100	0.41902800
H	-2.86114000	-4.16252200	1.89622500
C	-4.41419100	-2.52793800	-1.23011600
H	-2.88063300	-1.03979800	-1.03556500
C	-4.97353500	-3.68860800	-0.70822900

H	-4.84364400	-5.17937100	0.83059600
H	-4.84591000	-2.06625700	-2.10963200
H	-5.84076900	-4.13396100	-1.17933100
C	-1.89250100	-0.52172500	1.74839200
H	-1.03885800	-0.12147900	2.29669700
H	-2.15468900	0.15752900	0.93536800
H	-2.74647100	-0.59030700	2.42362100

M-B-Min-Cx2

Total Energy= -1894.29830

Imaginary frequency= 0

XYZ coordinates

H	5.83413200	-0.98916500	-2.05227700
H	2.72358700	0.20031800	-3.72856400
H	5.13965100	-1.21569000	-0.45106900
H	4.82340600	-2.38895400	-1.73408700
H	3.18853200	4.29646700	0.74235300
H	1.99489600	0.53864700	-1.58773400
H	4.70460400	0.94256400	1.68144900
H	2.01400900	2.40073900	-0.43235500
H	4.37488700	1.98156100	0.29730700
H	4.48403600	0.08526600	-3.90170100
H	3.50416300	-1.37072500	-3.95228800
H	-1.55982000	0.05481000	-0.28885300
H	2.26829300	0.66156200	2.05341600
H	0.17346700	0.52506600	0.79617400
H	3.44901100	-0.82185900	0.58210500
H	3.59624100	2.53828700	3.20689400
H	4.86477100	3.35999600	2.31263300
H	1.10908700	2.82399600	2.43782800
H	0.77029900	3.88423400	1.06473900
H	2.74431300	4.70886900	2.39117300
C	-2.69792100	1.09336200	-1.70773600
N	0.37694000	1.35699500	0.25589700
N	2.72536200	-0.20694300	0.22931600
N	-1.60828400	0.95591100	-0.74951300
S	-0.28850600	3.10812100	-1.65435400
C	2.82276800	-0.02099000	-1.16160700
C	4.93988400	-1.32047500	-1.51848600
C	-0.51837400	1.74563900	-0.67898800
C	3.60070500	-0.39204800	-3.46842400
C	3.74497200	-0.53711100	-1.98005100
C	3.88958200	2.88034400	2.20817300
C	1.50170900	3.19158800	1.48271500
C	2.85000300	3.87508500	1.69466800
C	3.99670000	1.67269000	1.27821900
C	1.64244200	2.01149800	0.51968600
C	2.63954700	0.99425300	1.07497100
H	3.44789900	-4.04584400	-0.03391700
H	2.30007400	-3.02043500	-2.26165100

O	-0.08674400	-1.73361100	-1.55996100
O	1.87094700	-3.42673900	2.18901200
N	0.50798600	-2.56685500	0.51882700
C	0.67029900	-2.34178900	-0.85528100
C	1.65038100	-3.19575200	1.03305400
C	2.51912300	-3.50804300	-0.14677800
C	1.95636900	-3.01101000	-1.23893800
C	-0.52960300	-1.98320200	1.28721500
C	-2.56743900	-0.73809000	2.70076100
C	-1.84607400	-2.08934400	0.84379700
C	-0.23116200	-1.28098300	2.45146100
C	-1.25766200	-0.66525100	3.15679600
C	-2.86012400	-1.45233800	1.54533300
H	-2.06544600	-2.64301000	-0.05952000
H	0.79215600	-1.22847800	2.79779300
H	-1.02622700	-0.11744600	4.06128900
H	-3.87887800	-1.50160300	1.17930800
H	-3.36214100	-0.23730800	3.23845900
H	-2.77359200	2.16090400	-1.92442500
C	-2.38580900	0.35258400	-3.00014500
H	-3.19358100	0.47249700	-3.72407000
H	-1.47136900	0.76778600	-3.42341800
H	-2.22117700	-0.70947600	-2.81117100
C	-3.96940900	0.65577000	-0.99830200
C	-4.34903100	1.35599700	0.14846200
C	-4.74699200	-0.41923100	-1.41210000
C	-5.47626300	0.99215600	0.86517900
H	-3.73688200	2.18895000	0.47680200
C	-5.88121000	-0.79064900	-0.69154400
H	-4.47596400	-0.97682800	-2.29969200
C	-6.24752300	-0.08964300	0.44718200
H	-5.75949000	1.55161500	1.74838900
H	-6.47752000	-1.63073500	-1.02573100
H	-7.13027800	-0.37757200	1.00423300

M-B-Min-TS2

Total Energy= -1894.28094
Imaginary frequency= 1

XYZ coordinates

H	4.42297400	-2.77260000	-2.04600400
H	0.60493700	-2.58191300	-2.31879400
H	4.41836500	-2.73227000	-0.27549700
H	3.78441500	-4.13496000	-1.12152800
H	3.75734500	3.89363100	-1.37802700
H	1.45856100	-0.55965100	-1.49511300
H	5.00399300	1.08749200	0.78826100
H	2.21243800	1.74378700	-1.72131900
H	4.72304400	1.57783300	-0.88264900
H	2.04928900	-3.02243400	-3.25255800
H	1.40190100	-4.12805000	-2.03961700

H	-1.52730900	0.31063900	-0.12517500
H	2.59539800	1.02803900	1.22488200
H	0.27715300	1.23337200	0.45087800
H	3.81734400	-0.85825700	0.22800300
H	4.00930900	3.22334600	1.59488600
H	5.34972000	3.53537900	0.50183000
H	1.59332500	3.43805800	0.73352400
H	1.30297000	3.85625100	-0.95389900
H	3.36642000	4.97727100	-0.05117800
C	-2.55276900	0.18946700	-1.95623800
N	0.60698700	1.33527900	-0.50195300
N	3.07918700	-0.35172900	-0.24779100
N	-1.46584400	0.63835300	-1.08364500
S	0.04691300	1.51377900	-3.11439700
C	2.31273200	-1.05666600	-1.05436100
C	3.85300400	-3.04558300	-1.15412100
C	-0.29617900	1.15427800	-1.50018300
C	1.57608700	-3.07404200	-2.26830600
C	2.46504800	-2.44544200	-1.21955000
C	4.33560800	3.13602900	0.55335000
C	1.98929400	3.33516000	-0.28396500
C	3.39169800	3.92699600	-0.34649400
C	4.34241800	1.66881900	0.14015700
C	1.95302100	1.85114600	-0.66457700
C	2.94345500	1.04750700	0.18180300
H	3.50114600	-2.91894300	1.96931800
H	1.76128000	-4.04755600	0.22065200
O	-0.53818000	-2.57027200	-0.01470300
O	2.23321300	-0.71866400	3.15468800
N	0.56914900	-1.35957400	1.62990300
C	0.44723200	-2.33042100	0.64689800
C	1.88805400	-1.46449100	2.25936700
C	2.55690300	-2.54183500	1.61278000
C	1.78860100	-3.01218800	0.54255900
C	-0.47609600	-0.51646600	2.07405500
C	-2.53926800	1.22868800	2.80867500
C	-1.81379600	-0.89878300	1.92685600
C	-0.18331400	0.73248800	2.63420500
C	-1.21250400	1.58995300	2.99905800
C	-2.83043600	-0.02059400	2.27972000
H	-2.05712400	-1.86229300	1.50686600
H	0.84583700	1.00962000	2.80926100
H	-0.96668800	2.55177400	3.43173000
H	-3.86035500	-0.31781500	2.12244200
H	-3.33888100	1.90878000	3.07159800
H	-2.66241300	0.95252000	-2.73034600
C	-2.21151400	-1.14006500	-2.61810300
H	-3.03904500	-1.47992900	-3.24310300
H	-1.33580100	-1.00166900	-3.25127100
H	-1.98427700	-1.89725100	-1.86592300
C	-3.81750100	0.17066000	-1.11325500

C	-4.30910000	1.37902100	-0.61805300
C	-4.48478900	-1.00528900	-0.79048200
C	-5.44740100	1.41378200	0.17179000
H	-3.78255400	2.29676600	-0.85661700
C	-5.62962000	-0.97436500	0.00155700
H	-4.11682100	-1.95558600	-1.15463300
C	-6.11466100	0.23270800	0.48268700
H	-5.81967800	2.36124800	0.54172800
H	-6.14130500	-1.89847200	0.24011900
H	-7.00738400	0.25575100	1.09516200

M-B-Maj-Cx3

Total Energy= -1894.29564

Imaginary frequency= 0

XYZ coordinates

H	-3.42149400	-1.48952600	2.02296900
H	0.10797300	-0.09149500	4.10041600
H	-2.50673600	-2.62612400	3.00868600
H	-3.44904900	-1.36421500	3.77832600
H	-1.96918300	4.91831800	0.66807200
H	-0.44972100	0.85480100	2.08785700
H	-4.19408000	1.84845700	0.39598800
H	-0.69745500	2.80729700	1.15835100
H	-3.15937400	2.72196400	1.52487900
H	-1.28173300	-0.61991600	5.05998600
H	-0.30108800	-1.80904700	4.21638400
H	2.04034800	-0.05790400	-0.27763400
H	-2.23446600	1.34492200	-1.02782400
H	0.13202500	0.73491000	-0.60704600
H	-2.82451500	-0.18371500	0.67256900
H	-3.63736700	3.43107300	-1.41603600
H	-4.27100800	4.31883700	-0.03776400
H	-1.04667300	3.36832100	-1.80491000
H	-0.00674600	4.26048500	-0.68779200
H	-2.22272300	5.41690400	-0.99659900
C	3.73639500	0.66675200	0.74437800
N	0.33736100	1.64276000	-0.20292700
N	-1.97511700	0.35546500	0.75254000
N	2.41484900	0.78683200	0.13852900
S	1.93440400	3.13097400	1.34507200
C	-1.32156800	0.21804500	1.96978000
C	-2.80462800	-1.57580900	2.91943600
C	1.54754200	1.79308800	0.38618700
C	-0.72042100	-0.79952000	4.13779300
C	-1.60612400	-0.67284600	2.93097300
C	-3.42359400	3.72198400	-0.38108300
C	-0.93650500	3.69581300	-0.76517300
C	-2.13544700	4.54357000	-0.34746300
C	-3.28915200	2.45896200	0.46919800
C	-0.81802600	2.46035300	0.12690300

C	-2.08859200	1.61858600	0.02777600
H	-1.31807100	-4.71683500	1.86936300
H	0.83474700	-3.09214300	1.59516300
O	0.41120300	-1.33621300	-0.51851600
O	-3.28517000	-3.95586700	0.03733200
N	-1.63676700	-2.42314200	-0.54577100
C	-0.35304000	-2.15320500	-0.07216800
C	-2.19307500	-3.49030100	0.18956300
C	-1.14790500	-3.90262900	1.18235200
C	-0.09428500	-3.11071100	1.04704900
C	-2.31025600	-1.65990200	-1.53844400
C	-3.59946600	-0.05732800	-3.40775800
C	-1.60454200	-1.16699700	-2.63067800
C	-3.66603600	-1.37552500	-1.39099600
C	-4.30335600	-0.57576800	-2.32795600
C	-2.25330400	-0.36025700	-3.55628300
H	-0.55677300	-1.40087100	-2.74794600
H	-4.21785300	-1.78968700	-0.55754400
H	-5.35706200	-0.35764900	-2.20980900
H	-1.69830600	0.02851300	-4.40041900
H	-4.09968600	0.57127200	-4.13281800
H	4.11343200	1.68655200	0.84732900
C	3.63881400	0.05206400	2.13534800
H	4.61760400	0.00172800	2.61468700
H	2.98731400	0.67709000	2.74552500
H	3.21921500	-0.95574800	2.08479900
C	4.63617300	-0.07939200	-0.22615300
C	4.77935100	0.42630600	-1.51997800
C	5.32893400	-1.23464600	0.11721700
C	5.59454600	-0.20492200	-2.44432100
H	4.23782200	1.32542500	-1.79225700
C	6.14851000	-1.87213300	-0.81044400
H	5.23877800	-1.64783300	1.11361400
C	6.28370700	-1.36116700	-2.09134600
H	5.69799100	0.20521900	-3.44126600
H	6.68243800	-2.77040000	-0.52603100
H	6.92255900	-1.85611600	-2.81180900

M-B-Maj-TS3

Total Energy= -1894.26877

Imaginary frequency= 1

XYZ coordinates

H	-3.81718100	-2.47394700	-1.91572700
H	0.35761300	-3.43920200	-1.38130000
H	-2.99783300	-3.54961400	-3.02698200
H	-3.42534000	-4.14096800	-1.42380500
H	-2.13067800	-0.64078600	4.72301000
H	-0.61002900	-2.04249100	0.16317500
H	-4.49347700	-0.52258000	1.80625200
H	-0.89570700	-1.48865900	2.52746400

H	-3.50732500	-1.60095900	2.79220800
H	-0.78418000	-4.77931200	-1.21246600
H	-0.52534500	-4.04393600	-2.79509800
H	1.99992800	0.36121700	-0.11755500
H	-2.46744500	0.54675600	0.90258600
H	0.09083200	0.68215400	0.76353200
H	-3.48375800	-1.51396700	-0.04353600
H	-3.62536000	1.44446700	3.05934000
H	-4.36942000	0.28653600	4.15538400
H	-1.05884600	1.53557100	2.86380400
H	-0.07552800	0.40871500	3.79829300
H	-2.15337700	1.08875900	5.03601900
C	3.55227900	-1.00855700	0.36138400
N	0.08125800	-0.21413100	1.24272400
N	-2.55033500	-1.45974400	0.35107500
N	2.24415500	-0.38134800	0.54210800
S	1.43072700	-2.33222200	2.18646400
C	-1.60080600	-2.13366200	-0.26108500
C	-3.07055100	-3.26471000	-1.97491200
C	1.26033000	-0.90193500	1.28852400
C	-0.60101100	-3.83201300	-1.72570500
C	-1.71668000	-2.84727200	-1.46132000
C	-3.52205600	0.44089600	3.48550600
C	-1.03185100	0.52326300	3.28461200
C	-2.20227900	0.34065100	4.24311400
C	-3.55615800	-0.59305400	2.36673400
C	-1.04430700	-0.48320800	2.12776200
C	-2.38683000	-0.42983400	1.39417200
H	-1.37879800	-1.95925100	-3.50404400
H	1.10025300	-1.22314600	-2.66046600
O	0.84184400	1.24225600	-1.32606600
O	-3.32753500	-0.29072800	-2.47123100
N	-1.41015500	0.80188400	-1.77413100
C	0.01372900	0.47625500	-1.81654800
C	-2.12535800	-0.23808800	-2.32790600
C	-1.12763900	-1.32367700	-2.66152600
C	0.14591500	-0.77587900	-2.44495500
C	-1.95727500	2.04168800	-1.35558200
C	-3.02732600	4.48045000	-0.50470500
C	-1.19928300	3.21134300	-1.44189800
C	-3.26323000	2.10752900	-0.86147100
C	-3.78845100	3.32144100	-0.44320300
C	-1.73625900	4.41521400	-1.00943800
H	-0.19398900	3.16982400	-1.83023300
H	-3.87543600	1.21817700	-0.84072900
H	-4.80512400	3.35691700	-0.07199300
H	-1.13429400	5.31273900	-1.07598200
H	-3.43953600	5.42492900	-0.17361400
H	3.78185100	-1.50448300	1.30669500
C	3.49533400	-2.06845800	-0.73196200
H	4.44564200	-2.59830200	-0.81142400

H	2.71911500	-2.79029100	-0.47895200
H	3.26318900	-1.61564300	-1.69769100
C	4.58483300	0.08274600	0.13504000
C	4.71578500	1.09403700	1.08833800
C	5.42144400	0.10171800	-0.97477700
C	5.65923900	2.09685800	0.93508900
H	4.06554900	1.08625800	1.95616700
C	6.37061300	1.10709700	-1.13107100
H	5.34155000	-0.66751700	-1.73135500
C	6.49270400	2.10610400	-0.17891000
H	5.74968300	2.87188200	1.68603800
H	7.01214000	1.10657900	-2.00344700
H	7.23096200	2.88861000	-0.30086100

M-B-Min-Cx3

Total Energy= -1894.297671

Imaginary frequency= 0

XYZ coordinates

H	-1.81831700	4.32349300	0.37085300
H	-2.36536700	3.98641000	-1.27535400
H	-5.98450400	3.42351800	-0.27520600
H	-4.91016100	3.49129500	-1.66314100
H	-3.54050700	-0.52622800	-1.36145500
H	-0.71405300	1.31959700	-1.10870000
H	-3.06041900	1.72624000	-1.89794800
H	1.33633900	1.03378000	-0.69948700
H	-3.66550700	-2.43416200	2.90169200
H	-2.06581100	-1.70155700	2.71468900
H	-4.78514400	1.42324100	0.59265100
H	-2.43070300	2.04317800	1.06031700
H	-5.32474900	1.13472600	-1.05886100
H	-1.91719300	-0.12264900	1.05669000
H	-4.08968300	3.89696800	1.25145300
H	-4.69164800	-2.03432600	-0.70329300
H	-5.23137100	-2.53495500	0.89667500
H	-4.16826500	5.14064900	0.01392300
H	-2.39756300	-3.32622000	2.06975600
H	-4.06035900	-3.51593300	0.03092700
N	-0.87525100	1.89958300	-0.29341400
N	-2.88491700	-0.00607300	-0.79291700
N	1.33207600	1.59164800	0.14676600
S	-0.06279800	2.78830300	2.09536000
C	-2.68227400	-0.61020800	0.45676300
C	-4.36228800	-2.48360900	0.23429000
C	0.14700600	2.05795800	0.58286000
C	-2.81446600	-2.32434700	2.22349600
C	-3.25274200	-1.73142400	0.91545200
C	-4.96205600	3.22358800	-0.60197500
C	-2.53157100	3.74840800	-0.21891700
C	-3.96740100	4.08060600	0.17887300

C	-4.64545800	1.73649200	-0.44768000
C	-2.24937000	2.26077700	0.00257100
C	-3.20099100	1.42733500	-0.85101200
H	-2.91207400	-3.46530200	-2.28706500
H	-1.82277700	-1.21595800	-3.33792400
O	0.46215200	-0.51749400	-1.90206100
O	-1.33517300	-4.32496600	-0.13658300
N	-0.10646900	-2.45787400	-0.77379900
C	-1.17949800	-3.37430300	-0.84728000
C	-0.26304100	-1.46911800	-1.73057400
C	-2.02552000	-2.92426000	-1.99507400
C	-1.49305100	-1.82520400	-2.51109400
C	1.03255600	-2.64081900	0.05801900
C	3.24741900	-3.14851000	1.63861200
C	2.29835900	-2.65872500	-0.51663900
C	0.86537000	-2.86804000	1.41675300
C	1.97865300	-3.13133700	2.20262300
C	3.40679300	-2.90206400	0.28047700
H	2.40638500	-2.48718100	-1.58040400
H	-0.12962500	-2.84984100	1.83952000
H	1.85180300	-3.31597000	3.26141100
H	4.39500300	-2.90274900	-0.16120300
H	4.11278500	-3.34731100	2.25751400
C	2.56260500	1.61360300	0.93171600
H	2.54076000	2.53429500	1.51417000
C	3.75610900	1.64370000	0.00265300
C	4.72855800	2.62796400	0.14138300
C	3.92108000	0.67020500	-0.98217100
C	5.84602600	2.64352000	-0.68449000
H	4.60585800	3.39166500	0.90077600
C	5.03134200	0.68807700	-1.81460800
H	3.17451900	-0.10917800	-1.10095200
C	5.99941400	1.67455600	-1.66605200
H	6.59427800	3.41695700	-0.56362800
H	5.14376600	-0.06943200	-2.58082100
H	6.86727100	1.68734700	-2.31326400
C	2.62192100	0.41904400	1.88132700
H	1.76755700	0.44761700	2.55800400
H	2.59530000	-0.50843400	1.30831000
H	3.54413300	0.43905600	2.46450100

M-B-Min-TS3

Total Energy= -1894.265605

Imaginary frequency= 1

XYZ coordinates

H	-0.75329100	3.91864600	1.07067000
H	-1.16191600	3.96992900	-0.64639000
H	-4.80877600	4.78945600	-0.09649500
H	-3.58668200	4.57537500	-1.33994900
H	-3.67341000	0.26869600	-1.68461000

H	-0.49871100	1.18617100	-0.86658300
H	-2.51967500	2.21792500	-1.63776900
H	1.46530100	0.57114900	-0.57718500
H	-5.19455400	-2.34690800	1.45539600
H	-3.46184000	-2.42107000	1.83424900
H	-4.59451100	2.41712000	0.58183300
H	-2.21546000	1.96427600	1.38568400
H	-4.94047000	2.51592300	-1.14228900
H	-2.90234400	-0.18001300	1.10396300
H	-3.13016100	4.31463500	1.67121500
H	-4.74558300	-1.35285600	-2.16317000
H	-5.89500900	-1.06436300	-0.84056900
H	-2.54100100	5.61034700	0.64354300
H	-4.16747400	-3.60605500	0.75272300
H	-5.42017600	-2.70679600	-1.28213600
N	-0.68581100	1.39461800	0.10966800
N	-3.27854100	0.51569800	-0.78711600
N	1.53585200	0.97659100	0.35372400
S	0.29863900	1.85130100	2.56144400
C	-3.38961600	-0.39034600	0.15555100
C	-5.05681200	-1.68449700	-1.16922200
C	0.40352000	1.38626900	0.93765900
C	-4.20237300	-2.55597900	1.04631700
C	-3.92928000	-1.66156800	-0.14463600
C	-3.89674600	4.24336300	-0.34355000
C	-1.54411300	3.71893500	0.34987600
C	-2.78645600	4.54727900	0.65790800
C	-4.19036700	2.74624800	-0.38142300
C	-1.85069700	2.21386700	0.38439900
C	-2.92164100	1.93048300	-0.65992700
H	-3.19705000	-3.24126100	-1.56672900
H	-2.16595500	-1.23645200	-3.06594500
O	0.31903200	-0.53674700	-1.95105400
O	-1.60564900	-3.84540400	0.54154000
N	-0.40673900	-2.08247500	-0.36683300
C	-1.51372100	-2.91560300	-0.21678500
C	-0.56721000	-1.29353300	-1.56004300
C	-2.54146700	-2.45079600	-1.21565600
C	-1.85513600	-1.58567200	-2.09491300
C	0.84282800	-2.47912000	0.18609400
C	3.14835800	-3.60461000	1.25183600
C	1.92328400	-2.76259800	-0.64564300
C	0.92565700	-2.72878800	1.55085700
C	2.07257100	-3.30433000	2.07682400
C	3.07597800	-3.31648300	-0.10554200
H	1.84609300	-2.56749900	-1.70714700
H	0.08148200	-2.49341700	2.18462400
H	2.12619700	-3.51124400	3.13792700
H	3.91525200	-3.53783400	-0.75304300
H	4.04386100	-4.05020300	1.66545200
C	2.86240700	1.10185400	0.95700000

H	2.82888600	1.99504900	1.58230000
C	3.88825000	1.30436900	-0.13693500
C	4.79187400	2.35867000	-0.06228200
C	3.97576700	0.41600700	-1.20797800
C	5.76914600	2.52564100	-1.03599600
H	4.72876000	3.05507200	0.76611100
C	4.94487500	0.58600400	-2.18667900
H	3.28221800	-0.41676400	-1.27892900
C	5.84652400	1.64024900	-2.10175900
H	6.46629600	3.35111700	-0.96377500
H	4.99733900	-0.10667100	-3.01740900
H	6.60403400	1.77098600	-2.86430100
C	3.21448900	-0.09822500	1.82708000
H	2.46341400	-0.22370300	2.60622000
H	3.25466200	-0.99914300	1.21674100
H	4.19226800	0.05321500	2.28809900

Mulliken charges (B97-D/TZVP)

Catalyst A_F
Total Energy= -1445.357189
Imaginary frequency= 0

XYZ coordinates

H	-4.86844000	1.95815300	0.43842800
H	-5.65140200	-1.70564000	1.19926000
H	-2.77932300	0.67331700	0.93473400
H	-4.92319800	-0.25351300	1.89699400
H	0.64610500	-0.45040600	-1.43873800
H	-3.84283900	-1.78331200	-0.54280700
H	-1.37061800	0.26606600	-1.36997500
H	-6.11179300	-0.50217200	-0.92387700
H	-6.82111800	0.40141200	0.42115400
H	-3.84344400	0.27987100	-1.90437300
H	-5.58521000	1.91546100	-1.18244500
C	1.98555500	-0.77241700	0.14392000
N	-1.57365400	-0.24299300	-0.51182600
N	0.66561400	-0.69946800	-0.45721600
S	-0.57897800	-0.81107100	1.93827400
C	-0.50088800	-0.56668400	0.26779700
C	-5.86843900	0.08406000	-0.02418200
C	-3.67288800	0.91587000	-1.02116700
C	-5.04213300	1.31457000	-0.43876600
C	-5.07895400	-0.80116100	0.95490000
C	-2.90428100	0.07365200	0.01798800
C	-3.71023500	-1.18757200	0.37285000
H	1.84501200	-1.17220100	1.15488400
C	2.81323600	-1.82848300	-0.61355300
C	2.68386000	0.57679200	0.23465300
C	2.88029800	1.37622800	-0.90054900
C	3.10913800	1.04242300	1.48430200

C	3.50121700	2.62215100	-0.78612400
H	2.55898800	1.02411000	-1.87859200
C	3.72921400	2.29036600	1.60089100
H	2.93861600	0.42842900	2.36638000
C	3.92733200	3.08188400	0.46563900
H	3.65426600	3.23383200	-1.67324000
H	4.05181800	2.64506100	2.57784200
H	4.40947600	4.05358500	0.55434800
H	-3.13527500	-1.78434900	1.08749500
F	4.07477300	-1.90010400	-0.12534100
F	2.26102500	-3.06107400	-0.51216400
F	2.90772700	-1.54323000	-1.95212500
N	-2.83628000	2.04350700	-1.47196600
H	-2.67739000	2.68292600	-0.69380500
H	-3.32426800	2.56876800	-2.19390400

Catalyst A
Total Energy= -1147.648910
Imaginary frequency= 0

XYZ coordinates

H	-3.98606900	1.96425500	1.04931900
H	-5.25770600	-1.63992400	0.90837100
H	-2.08188000	0.33254500	0.99376600
H	-4.28089400	-0.53651700	1.88510800
H	0.95464600	-0.59356800	-1.92617800
H	-3.58842700	-1.47087000	-0.96216100
H	-0.87358700	0.41704500	-1.43261700
H	-5.66110700	0.14017600	-0.77366400
H	-6.14472700	0.73137800	0.82202500
H	-3.35676700	0.86321700	-1.73439000
H	-4.79465100	2.44941300	-0.45175800
C	2.38713700	-1.41501300	-0.61640800
N	-1.11701800	-0.30310100	-0.75508900
N	1.01935700	-1.07283000	-1.03463100
S	-0.08645400	-1.64265900	1.36155700
C	-0.05859300	-0.96983900	-0.19204800
C	-5.27878000	0.42618400	0.21871800
C	-3.04439600	1.20865100	-0.73600400
C	-4.30394100	1.60675900	0.05676000
C	-4.57220100	-0.78384200	0.85275000
C	-2.34899900	0.02589700	-0.03160700
C	-3.31415000	-1.16865100	0.06000500
H	2.27727000	-2.13889100	0.19691600
C	3.11460700	-2.07612700	-1.79375200
C	3.11496300	-0.19031800	-0.07338500
C	3.52077900	0.84943400	-0.92416100
C	3.35470900	-0.07168600	1.30197600
C	4.15746000	1.98316500	-0.41277000
H	3.34329700	0.77317900	-1.99660300
C	3.99393400	1.06090000	1.81805800

H	3.01713900	-0.86534900	1.96476800
C	4.39717800	2.09094700	0.96264800
H	4.47008000	2.78026600	-1.08538600
H	4.17201600	1.14020900	2.88914500
H	4.89405100	2.97285800	1.36307700
H	-2.79315300	-2.00549800	0.53492700
N	-2.07903200	2.30265500	-0.95404700
H	-1.77714300	2.67476600	-0.05403000
H	-2.52825700	3.06512700	-1.45608100
H	2.58345100	-2.98422300	-2.10300600
H	4.13792900	-2.33701200	-1.50004900
H	3.17635100	-1.39588100	-2.65472200

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