Supporting Information

Catalytic Asymmetric Trifluoromethylthiolation of Carbonyl Compounds via Diastereo- and Enantioselective Cu-Catalyzed Tandem Reaction

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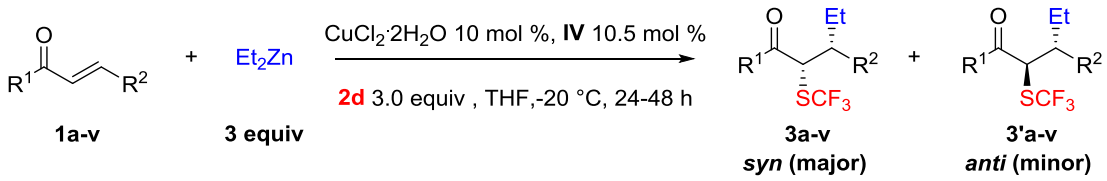
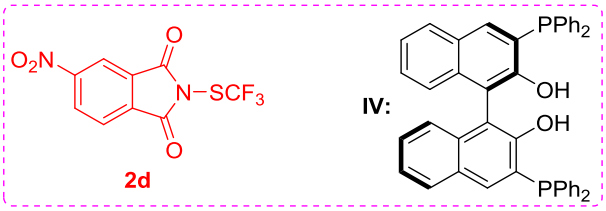
General Information

Unless Stated otherwise, the reactions and manipulations were performed under an atmosphere of argon by using standard Schlenk techniques and Drybox (Mikrouna, Supper 1220/750). Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 GF254 plates. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040-0.063 mm). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker at 500 MHz, 125 MHz and 376 MHz. Chemical shift values are reported in ppm from tetramethylsilane as the internal standard (TMS: δ 7.26 for ^{1}H and δ 77.16 for ^{13}C). Data are reported as follows: chemical shifts, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dq = doublet of quartets, m = multiplet), and coupling constants (Hz). The enantiomeric excess values were determined by chiral HPLC with an Agilent 1200 LC instrument and a Daicel CHIRALCEL OJ-3 column. High resolution mass spectroscopy (HRMS) analyses were performed at a Bruker Daltonics. Inc mass instrument (ESI). Optical rotations were determined on a Atopol I from Rudolph Research Analytical model 343 plus at 589 nm. Circular dichroism (CD) spectra were recorded on an Applied PhotoPhysics Chirascan CD spectropolarimeter, using a 10 mm quartz cuvette. Commercial grade reagents and solvents were used without further purification except as indicated below. Toluene was distilled from sodium. Tetrahydrofuran and Diethyl ether were distilled from sodium and benzophenone. Dichloromethane was distilled from calcium hydride. Acetonitrile was distilled from both P_2O_5 and calcium hydride according to general method prior to use. Diethyl zinc solution 1.0 M in hexanes was purchased from Sigma-Aldrich Chemicals. The chiral ligands were prepared according to the known method [1] or purchased from Strem Chemicals. All of the α,β-unsaturated ketones were known compounds and prepared according to the reported procedure. [2]

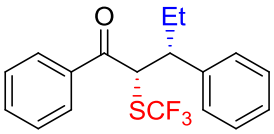
General Procedure for Asymmetric Trifluoromethylthiolation of Carbonyl Compounds via Diastereo- and Enantioselective Cu-Catalyzed Tandem Reaction





An oven-dried vial fitted with a stirrer bar was charged with 10 mol% $CuCl_2{\cdot}2H_2O$ (4.26 mg, 0.1 equiv) and 10.5 mol% (*R*)-Binol-phos (17.2 mg, 0.105 equiv) in dry THF (4.0 mL) and the mixture was stirred at room temperature for 1 h. Diethyl zinc (1.0 M solution in Hexanes, 0.75 mL, 0.75 mmol) was added dropwise to the vial at -20 ^{o}C, after 10 minutes, α,β-unsaturated ketones **1** (0.25 M solution in THF, 0.25 mmol, 1.0 mL) was added slowly. Stirring was continued at -20 ^{o}C for 1 h. Then SCF_3 reagent **2d** (0.75 M solution in THF, 219.1 mg, 0.75 mmol) was added and the reaction mixture was stirred for 24-48 h at -20 ^{o}C. The reaction was quenched with 1.0 mL Sat. NH_4Cl aq at -20 ^{o}C. After stirring at –20 ℃ for 5 min, the mixture was passed through a pad of silica gel with EtOAc (100 mL). Concentration and purification by silica gel column chromatography gave the product.

Analytic Data for Products



3a

(2*S*,3*R*)-1,3-diphenyl-2-(trifluoromethylthio)pentan-1-one (3a)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 93% yield, 78.7 mg), *dr* = 16:1, 92% ee of **3a**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 5.0 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.9 Hz, 2H), 7.19-7.11 (m, 4H), 7.10-7.04 (m, 1H), 4.90 (d, *J* = 10.0 Hz, 1H), 3.15-3.05 (m, 1H),

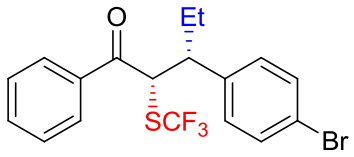
2.41-2.29 (m, 1H), 1.80-1.67 (m, 1H), 0.76 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.16, 139.83, 135.76, 133.55, 130.63 (q, J_{CF} = 305.0 Hz), 128.64, 128.61, 128.39, 127.38, 53.01, 49.34, 25.66, 11.86.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.44 (s, 3F).

HRMS (ESI) calcd for $C_{18}H_{16}F_3OS$ $(M-H)^-$ 337.0879, found 377.0885.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 0.8mL/min, λ = 254 nm, T_R = 17.9 min (minor) and T_R = 19.78 min (major).



3b

(2*S*,3*R*)-3-(4-bromophenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3b)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 92% yield, 96.0 mg), *dr* = 8:1, 91% ee of **3b**. The major product was separated by Pre-TLC.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70-7.64 (m, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 2H), 7.29 (d, *J* = 10.0 Hz, 2H), 7.02 (d, *J* = 10.0 Hz, 2H), 4.85 (d, *J* = 10.0 Hz, 1H), 3.14-3.04 (m, 1H), 2.40-2.28 (m, 1H), 1.75-1.61 (m, 1H), 0.75 (t, *J* = 7.3 Hz, 3H).

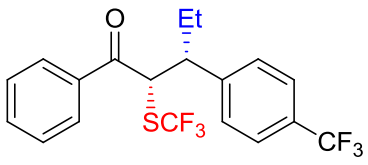
^{13}C NMR (125 MHz, $CDCl_3$) δ 196.64, 139.02, 135.55, 133.84, 131.79, 130.50 (q, J_{CF} = 306.3 Hz), 130.29, 128.83, 128.39, 121.27, 52.60, 48.79, 25.65, 11.81.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.37 (s, 3F).

HRMS (ESI) calcd for $C_{18}H_{15}BrF_3OS$ $(M-H)^-$ 414.9985, found 414.9992.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0mL/min, λ = 230 nm, T_R = 15.3 min (minor) and T_R = 33.3 min (major).

$[\alpha]^{25}_D$ = -42.43 (*c* = 0.5, $CHCl_3$).



3c

(2*S*,3*R*)-1-phenyl-3-(4-(trifluoromethyl)phenyl)-2-(trifluoromethylthio)pentan-1-one (3c)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 87% yield, 88.4 mg), *dr* = 5:1, 94% ee of **3c**. The major product was separated by Pre-TLC.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70-7.61 (m, 2H), 7.55-7.48 (m, 1H), 7.42 (d, *J* = 10.0 Hz, 2H), 7.39-7.33 (m, 2H), 7.26 (d, *J* = 10.0 Hz, 2H), 4.89 (d, *J* = 10.0 Hz, 1H), 3.24-3.15 (m, 1H), 2.45-2.33 (m, 1H), 1.81-1.67 (m, 1H), 0.76 (t, *J* = 7.4 Hz, 3H).

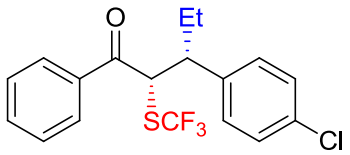
^{13}C NMR (125 MHz, $CDCl_3$) δ 196.53, 144.22, 135.55, 133.90, 130.47 (q, J_{CF} = 306.25 Hz), 129.67 (q, J_{CF} = 32.5 Hz), 129.0, 128.83, 128.33, 125.60 (q, J_{CF} = 3.75 Hz), 124.02 (q, J_{CF} = 270.0 Hz), 52.61, 49.22, 25.69, 11.79.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.34 (s, 3F), -62.70 (s, 3F).

HRMS (ESI) calcd for $C_{19}H_{15}F_6OS$ $(M-H)^-$ 405.0753, found 405.0757.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0mL/min, λ = 254 nm, T_R = 13.1 min (minor) and T_R = 21.9 min (major).

$[\alpha]^{20}_D$ = -31.21 (*c* = 0.5, $CHCl_3$).



3d

(2*S*,3*R*)-3-(4-chlorophenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3d)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 91% yield, 84.6 mg), *dr* = 7:1, 92% ee of **3d**. The major product was separated by Pre-TLC.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70-7.65 (m, 2H), 7.56-7.48 (m, 1H), 7.41-7.34 (m, 2H), 7.16-7.11 (m, 2H), 7.10-7.04 (m, 2H), 4.85 (d, *J* = 10.0 Hz, 1H), 3.15-3.05 (m, 1H), 2.41-2.28 (m, 1H), 1.74-1.61 (m, 1H), 0.75 (t, *J* = 7.3 Hz, 3H).

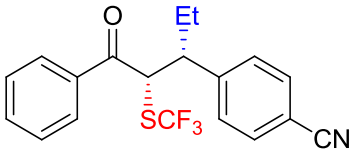
^{13}C NMR (125 MHz, $CDCl_3$) δ 196.71, 138.47, 135.57, 133.83, 133.14, 130.52 (q, J_{CF} = 305.0 Hz), 129.93, 128.84, 128.81, 128.39, 52.68, 48.74, 25.68, 11.81.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.38 (s, 3F).

HRMS (ESI) calcd for $C_{18}H_{15}ClF_3OS$ $(M-H)^-$ 371.0490, found 371.0495.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0mL/min, λ = 254 nm, T_R = 14.9 min (minor) and T_R = 28.5 min (major).

$[\alpha]^{25}_D$ = -36.59 (*c* = 0.5, $CHCl_3$).



3e

4-((2*S*,3*R*)-1-oxo-1-phenyl-2-(trifluoromethylthio)pentan-3-yl)benzonitrile (3e)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 89% yield, 80.9 mg), *dr* = 4:1, 93% ee of **3e**.

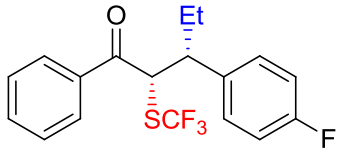
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70-7.65 (m, 2H), 7.58-7.52 (m, 1H), 7.50-7.44 (m, 2H), 7.42-7.36 (m, 2H), 7.29-7.25 (m, 2H), 4.87 (d, *J* = 10.0 Hz, 1H), 3.26-3.16 (m, 1H), 2.45-2.34 (m, 1H), 1.79-1.65 (m, 1H), 0.75 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.14, 145.78, 135.28, 134.13, 132.43, 130.36 (q, J_{CF} = 305.0 Hz), 129.44, 129.14, 128.34, 118.58, 111.36, 52.18, 49.42, 25.60, 11.77.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.27 (s, 3F).

HRMS (ESI) calcd for $C_{19}H_{15}F_3NOS$ $(M-H)^-$ 362.0832, found 362.0834.

HPLC: OJ-3, 2-PrOH: *n*-hexane = 5:95, 25 °C, flow rate: 1.0mL/min, λ = 254 nm, T_R = 12.23 min(minor) and T_R = 15.4 min (major).



3f

(2*S*,3*R*)-3-(4-fluorophenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3f)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 87% yield, 81.1 mg), *dr* = 7:1, 91% ee of **3f**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70-7.62 (m, 2H), 7.54-7.48 (m, 1H), 7.40-7.33 (m, 2H), 7.13-7.07 (m, 2H), 6.88-6.81 (m, 2H), 4.85 (d, *J* = 10.0 Hz, 1H), 3.14-3.06 (m, 1H), 2.41-2.29 (m,

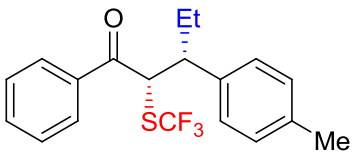
1H), 1.75-1.62 (m, 1H), 0.75 (t, J = 7.4 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.02, 161.93 (d, J_{CF} = 243.75 Hz), 135.66, 135.52 (d, J_{CF} = 2.5 Hz), 133.76, 130.57 (q, J_{CF} = 305.0 Hz), 130.14 (d, J_{CF} = 8.75 Hz), 128.77, 128.35, 115.57 (d, J_{CF} = 21.25 Hz), 52.89, 48.70, 25.75, 11.82.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.42 (s, 3F), -115.08 (s, F).

HRMS (ESI) calcd for $C_{18}H_{15}F_4OS$ $(M-H)^-$ 355.0785, found 355.0790.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0 mL/min, λ = 254 nm, T_R = 18.4 min (minor) and T_R = 23.6 min (major).



3g

(2*S*,3*R*)-1-phenyl-3-*p*-tolyl-2-(trifluoromethylthio)pentan-1-one (3g)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 89% yield, 78.3 mg), *dr* = 19:1, 88% ee of **3g**.

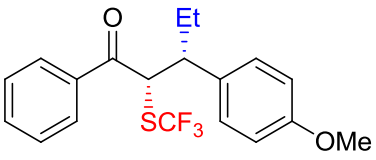
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, J = 10.0 Hz, 2H), 7.49 (t, J = 7.4 Hz, 1H), 7.35 (t, J = 7.85 Hz, 2H), 7.02 (d, J = 5.0 Hz, 2H), 6.96 (d, J = 5.0 Hz, 2H), 4.89 (d, J = 10.0 Hz, 1H), 3.12-3.02 (m, 1H), 2.36-2.26 (m, 1H), 2.19 (s, 3H), 1.76-1.64 (m, 1H), 0.76 (t, J = 7.3 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.16, 136.94, 136.70, 135.79, 133.47, 130.64 (q, J_{CF} = 305.0 Hz), 129.31, 128.61, 128.43, 53.10, 48.87, 25.66, 21.07, 11.87.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.46 (s, 3F).

HRMS (ESI) calcd for $C_{19}H_{18}F_3OS$ $(M-H)^-$ 351.1036, found 351.1039.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0 mL/min, λ = 254 nm, T_R = 16.7 min (minor) and T_R = 20.5 min (major).



3h

(2*S*,3*R*)-3-(4-methoxyphenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3h)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 71% yield, 65.4 mg), *dr* = 16:1, 79% ee of **3h**.

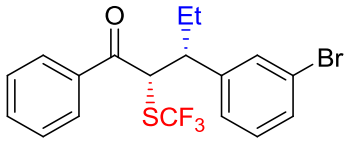
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 5.0 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.85 Hz, 2H), 7.04 (d, *J* = 10.0 Hz, 2H), 6.96 (d, *J* = 10.0 Hz, 2H), 4.86 (d, *J* = 10.0 Hz, 1H), 3.69 (s, 3H), 3.12-3.02 (m, 1H), 2.38-2.25 (m, 1H), 1.74-1.62 (m, 1H), 0.76 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.32, 158.70, 135.81, 133.52, 131.66, 130.65 (q, J_{CF} = 305.0 Hz), 129.62, 128.65, 128.40, 114.02, 55.25, 53.13, 48.55, 25.71, 11.86.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.46 (s, 3F).

HRMS (ESI) calcd for $C_{19}H_{18}F_3O_2S$ $(M-H)^-$ 367.0985, found 367.0986.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0mL/min, λ = 254 nm, T_R = 14.1 min (minor) and T_R = 14.3 min (major).



3i

(2*S*,3*R*)-3-(3-bromophenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3i)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 88% yield, 91.8 mg), *dr* = 11:1, 94% ee of **3i**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 5.0 Hz, 2H), 7.52 (t, *J* = 7.35 Hz, 1H), 7.37 (t, *J* = 7.85 Hz, 2H), 7.29-7.27 (m, 1H), 7.23-7.18 (m, 1H), 7.09-6.99 (m, 2H), 4.86 (d, *J* = 10.0 Hz, 1H), 3.12-3.03 (m, 1H), 2.44-2.28 (m, 1H), 1.76-1.63 (m, 1H), 0.77 (t, *J* = 7.35 Hz, 3H).

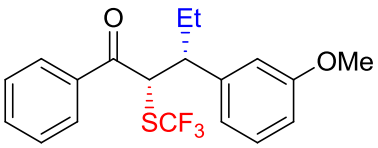
^{13}C NMR (125 MHz, $CDCl_3$) δ 196.76, 142.31, 135.62, 133.81, 131.47, 130.52 (q, J_{CF} = 305.0

Hz), 130.56, 130.19, 128.78, 128.36, 127.46, 52.69, 49.16, 25.67, 11.83.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.37 (s, 3F).

HRMS (ESI) calcd for $C_{18}H_{15}BrF_3OS$ $(M-H)^-$ 414.9985, found 414.9999.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0mL/min, λ = 254 nm, T_R = 19.9 min (minor) and T_R = 21.6 min (major).



3j

(2*S*,3*R*)-3-(3-methoxyphenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3j)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 86% yield, 79.2 mg), *dr* = 20:1, 88% ee of **3j**.

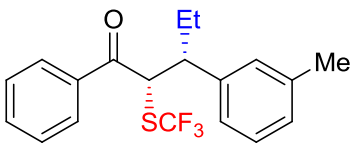
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 5.0 Hz, 2H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.9 Hz, 2H), 7.07 (t, *J* = 6.1 Hz, 1H), 6.73 (d, *J* = 10.0 Hz, 1H), 6.67-6.64 (m, 1H), 6.63-6.59 (m, 1H), 4.89 (d, *J* = 10.0 Hz, 1H), 3.68 (s, 3H), 3.12-3.02 (m, 1H), 2.38-2.26 (m, 1H), 1.78-1.65 (m, 1H), 0.78 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.07, 159.68, 141.49, 135.80, 133.54, 130.61 (q, J_{CF} = 306.25 Hz), 129.65, 128.65, 128.41, 120.90, 114.57, 112.59, 55.27, 52.94, 49.37, 25.70, 11.86.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.43 (s, 3F).

HRMS (ESI) calcd for $C_{19}H_{18}F_3O_2S$ $(M-H)^-$ 367.0985, found 367.0985.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0 mL/min, λ = 254 nm, T_R = 17.2 min (minor) and T_R = 19.3 min (major).



3k

(2*S*,3*R*)-1-phenyl-3-*m*-tolyl-2-(trifluoromethylthio)pentan-1-one (3k)

The compound was prepared according to the general procedure. Flash chromatography

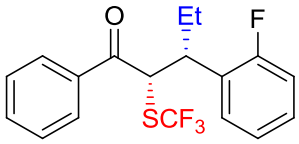
purification afforded the desired product (***syn*** + ***anti*** : 90% yield, 79.3 mg), *dr* = 11:1, 90% ee of after reduction of **3k**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 5.0 Hz, 2H), 7.48 (t, *J* = 7.30 Hz, 1H), 7.34 (t, *J* = 7.50 Hz, 2H), 7.03 (t, *J* = 7.50 Hz, 1H), 6.93-6.89 (m, 2H), 6.86 (d, *J* = 10.0 Hz, 1H), 4.90 (d, *J* = 10.0 Hz, 1H), 3.10-3.00 (m, 1H), 2.38-2.28 (m, 1H), 2.18 (s, 3H), 1.80-1.65 (m, 1H), 0.76 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.34, 139.66, 138.16, 135.92, 133.45, 130.55 (q, J_{CF} = 305.0 Hz), 129.40, 128.56, 128.48, 128.36, 128.08, 125.59, 53.04, 49.36, 25.74, 21.43, 11.89.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.44 (s, 3F).

HRMS (ESI) calcd for $C_{19}H_{18}F_3OS$ $(M-H)^-$ 351.1036, found 351.1043.



3l

(2*S*,3*R*)-3-(2-fluorophenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3l)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 88% yield, 78.4 mg), *dr* = 11:1, 95% ee of **3l**.

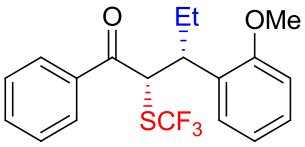
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 5.0 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.9 Hz), 7.17-7.04 (m, 2H), 6.97 (t, *J* = 7.45 Hz, 1H), 6.90-6.82 (m, 1H), 5.13 (*d*, *J* = 10.0 Hz, 1H), 3.40-3.30 (m, 1H), 2.34-2.22 (m, 1H), 190-1.75 (m, 1H), 0.78 (t, *J* = 7.35 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.77, 161.21 (d, J_{CF} = 245.0 Hz), 135.39, 133.78, 130.52 (q, J_{CF} = 306.25 Hz), 131.06 (d, J_{CF} = 3.75 Hz), 129.15, 129.09, 128.75, 128.46, 126.66 (d, J_{CF} = 12.5 Hz), 124.33 (d, J_{CF} = 3.75 Hz), 115.84 (d, J_{CF} = 22.5 Hz), 51.53, 44.75, 24.01, 11.94.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.50 (s, 3F), -115.73 (s, F).

HRMS (ESI) calcd for $C_{18}H_{15}F_4OS$ $(M-H)^-$ 355.0785, found 355.0789.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 ^{o}C, flow rate: 1.0 mL/min, λ = 214 nm, T_R = 19.6 min (minor) and T_R = 20.9 min (major).



3m

(2*S*,3*R*)-3-(2-methoxyphenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3m)

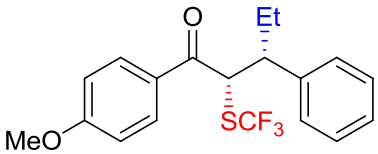
The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 85% yield, 78.2 mg), *dr* = 17:1, 76% ee of after reduction of **3m**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 10.0 Hz, 2H), 7.50 (t, *J* = 7.30 Hz, 1H), 7.37 (t, *J* = 7.65 Hz, 2H), 7.13-7.03 (m, 2H), 6.81 (t, *J* = 7.85 Hz, 1H), 6.66 (d, *J* = 10.0 Hz, 1H), 5.31 (d, *J* = 10.0 Hz, 1H), 3.73 (s, 3H), 2.20-2.05 (m, 1H), 2.01-1.85 (m, 1H), 0.73 (t, *J* = 7.40 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.55, 157.43, 135.82, 133.42, 130.76 (q, J_{CF} = 305.0 Hz), 128.49, 128.46, 127.16, 120.66, 110.65, 55.12, 22.85, 12.12.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.75 (s, 3F).

HRMS (ESI) calcd for $C_{19}H_{18}F_3O_2S$ $(M-H)^-$ 367.0985, found 367.0986.



3n

(2*S*,3*R*)-1-(4-methoxyphenyl)-3-phenyl-2-(trifluoromethylthio)pentan-1-one (3n)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 50% yield, 46.1 mg), *dr* = 17:1, 86% ee of **3n**.

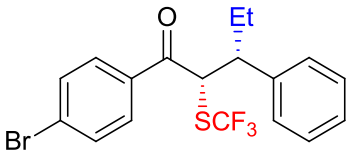
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 10.0 Hz, 2H), 7.20-7.11 (m, 4H), 7.10-7.05 (m, 1H), 6.81 (d, *J* = 10.0 Hz, 2H), 4.86 (d, *J* = 10.0 Hz, 1H), 3.82 (s, 3H), 3.15-3.05 (m, 1H), 2.40-2.29 (m, 1H), 1.80-1.66 (m, 1H), 0.76 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.45, 163.96, 140.02, 130.90, 130.74 (q, J_{CF} = 305.0 Hz), 128.59, 128.58, 127.31, 113.88, 55.59, 52.61, 49.39, 25.64, 11.90.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.49 (s, 3F).

HRMS (ESI) calcd for $C_{19}H_{18}F_3O_2S$ $(M-H)^-$ 367.0985, found 367.0992.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 0.8mL/min, λ = 254 nm, T_R = 15.7 min (minor) and T_R = 15.9 min (major).



3o

(2*S*,3*R*)-1-(4-bromophenyl)-3-phenyl-2-(trifluoromethylthio)pentan-1-one (3o)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 85% yield, 88.7 mg), *dr* = 15:1, 95% ee of **3o**.

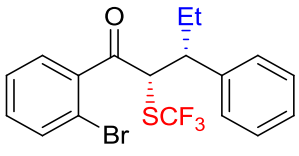
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52-7.45 (m, 4H), 7.19-7.13 (m, 2H), 7.12-7.06 (m, 3H), 4.82 (d, *J* = 15 Hz, 1H), 3.12-3.03 (m, 1H), 2.41-2.28 (m, 1H), 1.79-1.67 (m, 1H), 0.76 (t, *J* = 7.30 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.38, 139.64, 134.48, 131.98, 130.5 (q, J_{CF} = 305.0 Hz), 129.81, 128.76, 128.55, 127.55, 52.83, 49.34, 25.75, 11.82.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.39 (s, 3F).

HRMS (ESI) calcd for $C_{18}H_{15}BrF_3OS$ $(M-H)^-$ 414.9985, found 414.9987.

HPLC: OD-H, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0mL/min, λ = 254 nm, T_R = 12.0 min (minor) and T_R = 12.6 min (major).



3p

(2*S*,3*R*)-1-(2-bromophenyl)-3-phenyl-2-(trifluoromethylthio)pentan-1-one (3p)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 83% yield, 86.6 mg), *dr* = 1:1, 95% ee of **3p**.

^{1}H NMR (500 MHz, $CDCl_3$) *syn*+*anti*: δ 7.64 (d, *J* = 5.0 Hz, 1H), 7.58-7.54 (m, 1H), 7.43-7.12 (m, 18H), 5.01 (d, *J* = 10.0 Hz, 1H), 4.75 (d, *J* = 10.0 Hz, 1H), 3.30-3.15 (m, 2H), 2.35-2.20 (m,

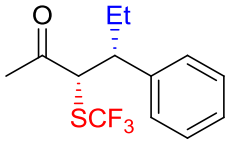
1H), 2.07-1.96 (m, 1H), 1.94-1.82 (m, 1H), 1.79-1.66 (m, 1H), 0.84-0.75 (m, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) *syn*+*anti*: δ 198.11, 196.78, 140.20, 139.55, 139.02, 138.90, 134.29, 134.26, 132.70, 132.38, 130.0 (q, J_{CF} = 306.3 Hz), 130.91, 129.28, 128.86, 128.83, 128.76, 128.63, 127.54, 127.51, 127.24, 120.40, 119.85, 57.40, 56.45, 49.31, 47.95, 26.84, 24.99, 12.61, 11.97.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.69, -39.87 (s, 3F).

HRMS (ESI) calcd for $C_{18}H_{15}BrF_3OS$ $(M-H)^-$ 414.9985, found 414.9988.

HPLC: OD-H, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0mL/min, λ = 230 nm, T_R = 14.6 min (minor) and T_R = 15.3 min (major).



3q

(3*S*,4*R*)-4-phenyl-3-(trifluoromethylthio)hexan-2-one (3q)

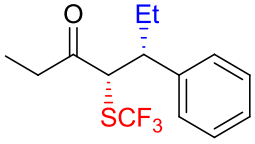
The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 82% yield, 56.6 mg), *dr* = 9:1, 76% ee of after reduction of **3q**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35-7.29 (m, 2H), 7.27-7.21 (m, 1H), 7.19-7.11 (m, 2H), 3.98 (d, *J* = 10.0 Hz, 1H), 2.86-2.78 (m, 1H), 2.28-2.18 (m, 1H), 1.92 (s, 3H), 1.70-1.62 (m, 1H), 0.74 (t, *J* = 7.25 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 204.10, 139.64, 130.31 (q, J_{CF} = 305.0 Hz), 128.96, 128.41, 127.71, 58.07, 48.22, 28.22, 26.32, 11.57.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.85 (s, 3F).

HRMS (ESI) calcd for $C_{13}H_{14}F_3OS$ $(M-H)^-$ 275.0723, found 275.0725.



3r

(4*S*,5*R*)-5-phenyl-4-(trifluoromethylthio)heptan-3-one (3r)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 60% yield, 43.6 mg), *dr* = 10:1, 81% ee of

3r.

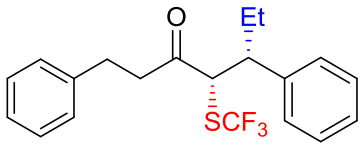
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.27 (m, 2H), 7.26-7.21 (m, 1H), 7.16-7.11 (m, 2H), 3.95 (d, *J* = 10.0 Hz, 1H), 2.89-2.80 (m, 1H), 2.36-2.20 (m, 2H), 2.05-1.95 (m, 1H), 1.72-1.63 (m, 1H), 0.77-0.71 (m, 6H)

^{13}C NMR (125 MHz, $CDCl_3$) δ 207.20, 139.84, 131.69, 130.47 (q, J_{CF} = 305.0 Hz), 128.91, 128.48, 127.62, 57.44, 48.46, 35.10, 26.06, 11.67, 7.45.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.86 (s, 3F).

HRMS (ESI) calcd for $C_{14}H_{16}F_3OS$ $(M-H)^-$ 289.0879, found 289.0881

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 0.8 mL/min, λ = 220 nm, T_R =17.0 min (minor) and T_R = 17.9 min (major).



3s

(4*S*,5*R*)-1,5-diphenyl-4-(trifluoromethylthio)heptan-3-one (3s)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 66% yield, 60.5 mg), *dr* = 12:1, 68% ee of **3s**.

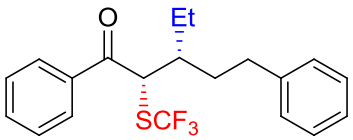
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.28 (m, 2H), 7.28-7.23 (m, 1H), 7.22-7.18 (m, 2H), 7.17-7.11 (m, 3H), 6.96-6.91 (m, 2H), 3.95 (d, *J* = 10.0 Hz, 1H), 2.86-2.80 (m, 1H), 2.64-2.46 (m, 3H), 2.36-2.28 (m, 1H), 2.28-2.19 (m,1H), 1.70-1.60 (m, 1H), 0.73 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 205.58, 140.63, 139.73, 130.41 (q, J_{CF} = 305.0 Hz), 129.02, 128.54, 128.53, 128.28, 127.74, 126.19, 57.64, 48.49, 43.53, 29.32, 26.13, 11.64

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.80 (s, 3F).

HRMS (ESI) calcd for $C_{20}H_{20}F_3OS$ $(M-H)^-$ 365.1192, found 365.1195.

HPLC: OD-H, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 0.8 mL/min, λ = 214 nm, T_R =16.0 min (major) and T_R = 18.7 min (minor).



3t

(2*S*,3*R*)-3-ethyl-1,5-diphenyl-2-(trifluoromethylthio)pentan-1-one (3t)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 89% yield, 81.5 mg), *dr* = 2:1, 96% ee of **3t**.

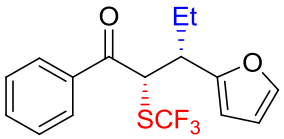
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 10.0 Hz, 2H), 7.48 (t, *J* = 7.50 Hz, 1H), 7.22-7.18 (m, 2H), 7.14 (d, *J* = 5.0 Hz, 2H), 7.06 (d, *J* = 10.0 Hz, 2H), 4.98 (d, *J* = 5.0 Hz, 1H), 2.82-2.69 (m, 1H), 2.53-2.43 (m, 1H), 2.05-1.95 (m, 1H), 1.66-1.54 (m, 4H), 1.02 (t, *J* = 7.35 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.72, 141.39, 135.54, 133.88, 130.89 (q, J_{CF} = 305.0 Hz), 129.10, 128.69, 128.54, 128.50, 128.45, 128.36, 126.08, 51.97, 41.47, 32.91, 31.47, 24.17, 11.51.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.87 (s, 3F).

HRMS (ESI) calcd for $C_{20}H_{20}F_3OS$ $(M-H)^-$ 365.1192, found 365.1192.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 ^{o}C, flow rate: 0.8 mL/min, λ = 254 nm, T_R = 29.5 min (minor) and T_R = 51.8 min (major).



3u

(2*S*,3*R*)-3-(furan-2-yl)-1-phenyl-2-(trifluoromethylthio)pentan-1-one (3u)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (***syn*** + ***anti*** : 82% yield, 82.1 mg), *dr* = 7:1, 91% ee of **3u**.

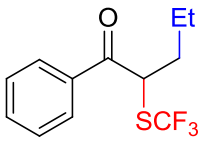
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, *J* = 5.0 Hz, 2H), 7.55 (t, *J* = 7.30 Hz, 1H), 7.42 (t, *J* = 7.60 Hz, 2H), 7.18 (s, 1H), 6.13-6.08 (m, 1H), 6.06-6.01 (m, 1H), 5.05 (d, *J*= 10.0 Hz, 1H), 3.30-3.22 (m, 1H), 2.24-2.10 (m, 1H), 1.88-1.75 (m, 1H), 0.84 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 197.11, 152.47, 141.95, 135.12, 133.78, 130.56 (q, J_{CF} = 305.0 Hz), 128.77, 128.55, 110.31, 108.94, 51.15, 43.17, 23.66, 11.77.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.63 (s, 3F).

HRMS (ESI) calcd for $C_{16}H_{14}F_3O_2S$ $(M-H)^-$ 327.0672, found 327.0672.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 0.8 mL/min, λ = 254 nm, T_R =24.5 min (minor) and T_R = 25.3 min (major).



3v

1-phenyl-2-(trifluoromethylthio)pentan-1-one (3v)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product (82% yield, 53.7 mg).

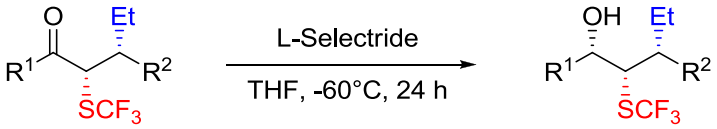
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00-7.94 (m, 2H), 7.66-7.60 (m, 1H), 7.55-7.48 (m, 2H), 4.86 (t, *J* = 6.85 Hz, 1H), 2.16-2.05 (m, 1H), 1.99-1.86 (m, 1H), 1.49-1.39 (m, 2H), 0.93 (t, J = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 196.72, 135.05, 134.15, 130.78 (q, J_{CF} = 306.25 Hz), 129.13, 128.71, 48.23, 35.12, 20.13, 13.79.

^{19}F NMR (376 MHz, $CDCl_3$) δ -39.83 (s, 3F).

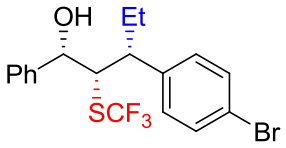
HRMS (ESI) calcd for $C_{12}H_{12}F_3OS$ $(M-H)^-$ 261.0566, found 261.0567.

General Procedure for Reduction of α-SCF_3-β-carbonyl Compounds 3b, 3k, 3m, 3q



3b, 3k, 3m, 3q **4b, 4k, 4m, 4q**

To a cooled (-60 °C) solution of α-SCF_3-β-carbonyl compounds (0.22 mmol, 1.0 equiv) in 1.0 mL of THF was added dropwise a solution of L-Selectride (0.44 mmol, 1.0 M solution in THF) under argon atmosphere and the mixture was stirred for 24 hours. The reaction was quenched with a saturated aqueous NH_4Cl. After extraction with dichloromethane, the combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. Concentration and purification by silica gel column chromatography gave the reduction product.



4b

(1*S*,2*S*,3*R*)-3-(4-bromophenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-ol (4b)

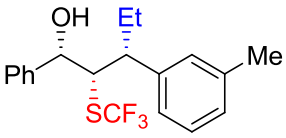
The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product, 73% yield, 67.3 mg, 92% ee of **4b**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 10.0 Hz, 2H), 7.33 (t, *J* = 7.20 Hz, 2H), 7.28 (d, *J* = 10.0 Hz, 1H), 7.23 (d, *J* = 5.0 Hz, 2H), 7.15 (d, *J* = 10.0 Hz, 2H), 4.70 (s, 1H), 3.28-3.21 (m, 1H), 2.90-2.80 (m, 1H), 2.34-2.21 (m, 1H), 2.04-1.98 (m, 1H), 1.68-1.58 (m, 1H), 0.73 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 141.41, 141.27, 132.15, 130.06, 128.35, 128.11, 126.13, 121.02, 72.94, 60.72, 49.81, 26.07, 12.34.

HRMS (ESI) calcd for $C_{19}H_{19}BrF_3O_3S$ (M+COOH) 463.0196, found 463.0201.

HPLC: OJ-3, two combined, 2-PrOH: *n*-hexane = 5:95, 25 °C, flow rate: 1.0 mL/min, λ = 210 nm, T_R = 15.9 min (minor) and T_R = 19.7 min (major).



4k

(1*S*,2*S*,3*R*)-1-phenyl-3-*m*-tolyl-2-(trifluoromethylthio)pentan-1-ol (4k)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product, 72% yield, 56.1 mg, 92% ee of **4b**.

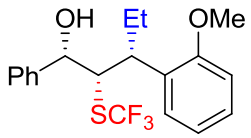
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.29 (m, 3H), 7.28-7.24 (m, 1H), 7.22 (d, *J* = 10.0 Hz, 2H), 7.13-7.06 (m, 3H), 4.76 (s, 1H), 3.34-3.28 (m, 1H), 2.89-2.80 (m, 1H), 3.28 (s, 3H), 2.34-2.25 (m, 1H), 1.95 (d, *J* = 5.0 Hz, 1H), 1.71-1.61 (m, 1H), 0.76 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 142.10, 141.73, 138.70, 129.11, 128.97, 128.19, 128.07, 127.81, 126.06, 125.16, 72.55, 60.97, 50.55, 26.49, 21.70, 12.48.

HRMS (ESI) calcd for $C_{20}H_{22}F_3O_3S$ (M+COOH) 399.1247, found 399.1250.

HPLC: OD-H, three combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0 mL/min, λ = 214

nm, T_R = 25.27 min (minor) and T_R = 28.56 min (major).



4m

(1*S*,2*S*,3*R*)-3-(2-methoxyphenyl)-1-phenyl-2-(trifluoromethylthio)pentan-1-ol (4m)

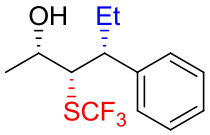
The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product, 74% yield, 60.3 mg, 76% ee of **4m**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35-7.26 (m, 5H), 7.22-7.15 (m, 1H), 7.14 (d, *J* = 10.0 Hz, 1H), 6.91 (t, *J* = 7.45 Hz, 1H), 6.78 (d, *J* = 10.0 Hz, 1H), 5.02-4.96 (m, 1H), 3.84 (s, 1H), 3.66 (s, 3H), 3.15 (s, 1H), 2.56 (d, *J* = 5.0 Hz, 1H), 2.21-2.10 (m, 1H), 1.75-1.65 (m, 1H), 0.66 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 157.40, 140.55, 129.32, 128.11, 127.93, 127.85, 126.91, 120.53, 110.59, 75.60, 58.23, 55.14, 23.50, 11.91.

HRMS (ESI) calcd for $C_{20}H_{22}F_3O_4S$ (M+COOH) 415.1196, found 415.1198.

HPLC: OD-H, three combined, 2-PrOH: *n*-hexane = 1:99, 25 ^{o}C, flow rate: 1.0 mL/min, λ = 210 nm, T_R = 37.5 min (major) and T_R = 41.7min (minor).



4q

(2*S*,3*S*,4*R*)-4-phenyl-3-(trifluoromethylthio)hexan-2-ol (4q)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product, 58% yield, 30.5 mg, 57% ee of **4q**.

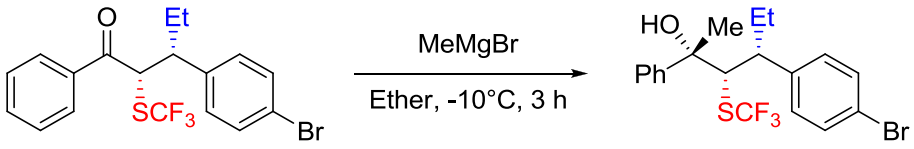
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38-7.32 (m, 2H), 7.30-7.24 (m, 1H), 7.21 (d, *J* = 5.0 Hz, 2H), 3.80-3.70 (m, 1H), 3.11 (d, *J* = 10.0 Hz, 1H), 2.84-2.75 (m, 1H), 2.41-2.30 (m, 1H), 1.70-1.60 (m, 1H), 1.25 (d, *J* = 5.0 Hz, 3H), 0.72 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 142.13, 129.02, 128.81, 128.30, 127.10, 66.60, 59.87, 50.62, 26.94, 22.09, 12.34.

HRMS (ESI) calcd for $C_{14}H_{18}F_3O_3S$ (M+COOH) 323.0934, found 323.0935.

HPLC: OD-H, two combined, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0 mL/min, λ = 210 nm, T_R = 13.4 min (major) and T_R = 25.7 min (minor).

General Procedure for Grignard reaction of compound 3b



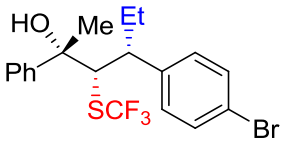
3b

d.r. >20:1, 92 % ee

5

82 % yield
d.r = 5:1, 92 % ee

To a solution of **3b** (0.12 mmol, 1.0 equiv) in anhydrous Et_2O (2.0 mL) at -10 ℃, a 1.0 M solution of methylmagnesium bromide in THF (0.24 mmol, 2.0 equiv) was slowly added. The mixture was stirred at this temperature for 3 h. The solution was quenched with H_2O (5 mL) and extracted with Et_2O (3 x 5 mL). The organic phase was washed successively with water, brine and dried over anhydrous Na_2SO_4. Concentration and purification by silica gel column chromatography gave the reduction product.



5

(2*S*,3*S*,4*R*)-4-(4-bromophenyl)-2-phenyl-3-(trifluoromethylthio)hexan-2-ol (5)

The compound was prepared according to the general procedure. Flash chromatography purification afforded the desired product, 82% yield, 42.6 mg, *dr* = 5:1, 92% ee of **5**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.40 (m, 4H), 7.39-7.30 (m, 3H), 6.80 (d, *J* = 10.0 Hz, 2H), 3.37 (s, 1H), 2.60 (d, *J* = 15.0 Hz, 1H), 2.10-2.02 (m, 1H), 1.75 (s, 3H), 1.74-1.67 (m, 1H), 0.51 (t, *J* = 7.30 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 145.52, 141.75, 131.35, 130.04, 128.81, 127.52, 124.99, 120.42, 78.55, 47.15, 31.60, 22.20, 12.18.

HRMS (ESI) calcd for $C_{20}H_{21}BrF_3O_3S$ (M+COOH) 477.0352, found 477.0356.

HPLC: OD-H, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 1.0 mL/min, λ = 220 nm, T_R = 18.4 min (major) and T_R = 23.3 min (minor).

General Procedure for Synthesis the quaternary carbon compound 6

To a solution of **3b** (0.185 mmol, 1.0 equiv) in anhydrous CH_2Cl_2 (2.0 mL) at room temperature, NBS (0.222 mmol, 1.2 equiv) and DBU (0.0185 mmol, 0.1 equiv) were added, then the mixture was stirred at this temperature for 5 h. The solution was quenched with H_2O (5 mL) and extracted with CH_2Cl_2 (3 x 5 mL). The organic phase was washed successively with water, brine and dried over anhydrous Na_2SO_4. Concentration and purification by silica gel column chromatography gave the quaternary carbon product **6**.

6 **6'**

(2*R*,3*R*)-2-bromo-3-(4-bromophenyl)-1-phenyl-2-((trifluoromethyl)thio)pentan-1-one (6)

(2*S*,3*R*)-2-bromo-3-(4-bromophenyl)-1-phenyl-2-((trifluoromethyl)thio)pentan-1-one (6')

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73-7.68 (m, 2H), 7.51-7.45 (m, 1H), 7.39-7.31 (m, 4H), 7.19-7.12 (m, 2H), 3.64 (dd, *J* = 15.0, 5.0 Hz, 1H), 2.44-2.32 (m, 1H), 2.08-1.96 (m, 1H), 0.79 (t, *J* = 7.3 Hz, 3H).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24-8.18 (m, 2H), 7.62-7.57 (m, 1H), 7.55-7.46 (m, 4H), 7.42-7.36 (m, 2H), 3.64 (dd, *J* = 15.0, 5.0 Hz, 1H), 1.98-1.87 (m, 1H), 1.61-1.51 (m, 1H), 0.63 (t, J = 7.3 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 191.75, 135.76, 135.68, 132.59, 132.43, 131.10, 129.40, 122.07, 76.59, 54.10, 25.56, 11.72.

^{13}C NMR (125 MHz, $CDCl_3$) δ 191.26, 135.64, 134.93, 133.12, 132.32, 131.58, 130.17, 128.45, 122.79, 77.64, 54.96, 27.31, 12.05.

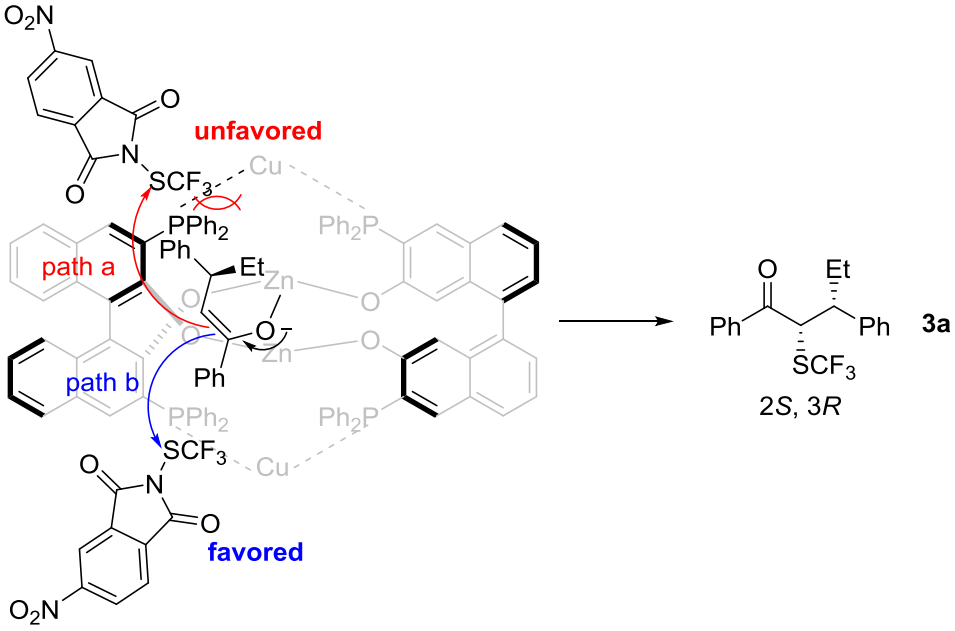
HRMS (ESI) calcd for $C_{18}H_{14}Br_2F_3O_3S$ $(M-H)^-$ 492.9090, found 477.9076.

HRMS (ESI) calcd for $C_{18}H_{15}BrF_3O_3S$ $(M-Br)^-$ 414.9985, found 414.9965.

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 ^oC, flow rate: 0.8 mL/min, λ = 254 nm, T_R = 15.9 min (major) and T_R = 17.3 min (minor).

HPLC: OJ-3, three combined, 2-PrOH: *n*-hexane = 1:99, 25 ^oC, flow rate: 0.8 mL/min, λ = 254 nm, T_R = 19.2 min (minor) and T_R = 28.9 min (major)

A plausible reaction mechanism and stereochemical model



In order to explain the configuration of product, a steochemical pathway has been proposed on the basis of our experimental results. The configuration of 1,4-addition adduct was obtained according to the multinuclear Cu/Zn complex-catalyst system reported by Shibata[1]. In the pre-transition-state assembly, forming the zinc enolate intermediate attacked the electrophilic SCF_3 reagent, path a showed the steric effect between SCF_3 reagent and PPh_2 group of ligand **IV**; path b was less hindered leading to the tandem reaction product with 2*S*, 3*R* configuration.

Quantum chemical ECD calculation method

All calculations were carried out by Gaussian16 software[3]. Density functional theory (DFT) method B3LYP-D3[4] along with 6-31G* basis set were used for geometry optimization calculations by using Gaussian09 defaults settings. Fourteen conformers of (2*R*, 3*R*)-**3d'** and thirteen conformers of (2*S*, 3*R*)-**3d** were located. TD-B3LYP-D3/6-311+G* calculations[5] were performed on several stable optimized conformers (which are not higher in free energy than the most stable one by ~3 kcal/mol: three and six lowest-energy conformers for **3d'** and **3d**, respectively) to obtain overall ECD spectra by including ECD spectra of each conformers weighted by Boltzmann distribution..

Table S1. Energies (Hartree) of the optimized conformers of (2*S*, 3*R*)-**3d** at B3LYP/6-31G* level.

Conformer	Electronic energy (E)	E + ZPE	Free energy (G)
1S	-1928.784241	-1928.481511	-1928.536114
2S	-1928.781438	-1928.478721	-1928.534726
3S	-1928.781642	-1928.478444	-1928.534119
4S	-1928.779463	-1928.476679	-1928.531870
5S	-1928.779692	-1928.476535	-1928.531454
6S	-1928.779515	-1928.476329	-1928.531300
7S	-1928.778323	-1928.475404	-1928.530895
8S	-1928.777690	-1928.475107	-1928.530827
9S	-1928.777506	-1928.474729	-1928.529996
10S	-1928.777049	-1928.474002	-1928.529279
11S	-1928.773911	-1928.470562	-1928.526202
12S	-1928.772651	-1928.469487	-1928.524798
13S	-1928.773901	-1928.470676	-1928.524148

Table S2. Relative energies (kcal/mol) of the optimized conformers of (2*S*, 3*R*)-**3d** at B3LYP/6-31G* level.

Conformer	ΔE	ΔE+ZPE	ΔG	Boltzmann distribution factor at 298.15 K
1S	0.0	0.0	0.0	72.2107%
2S	1.8	1.8	0.9	16.5901%
3S	1.6	1.9	1.3	8.7198%
4S	3.0	3.0	2.7	0.8045%
5S	2.9	3.1	2.9	0.5177%
6S	3.0	3.3	3.0	0.4398%
7S	3.7	3.8	3.3	0.2863%
8S	4.1	4.0	3.3	0.2664%
9S	4.2	4.3	3.8	0.1104%
10S	4.5	4.7	4.3	0.0517%
11S	6.5	6.9	6.2	0.0020%
12S	7.3	7.5	7.1	0.0004%
13S	6.5	6.8	7.5	0.0002%

Table S3. Energies (Hartree) of the optimized conformers of (2*R*, 3*R*)-**3d'** at B3LYP/6-31G* level.

Conformer	Electronic energy (E)	E + ZPE	Free energy (G)
1R	-1928.781776	-1928.478726	-1928.534852
2R	-1928.782176	-1928.479335	-1928.534058
3R	-1928.781239	-1928.478626	-1928.533937
4R	-1928.778661	-1928.475773	-1928.531653
5R	-1928.779622	-1928.476437	-1928.531507
6R	-1928.778667	-1928.475716	-1928.530666
7R	-1928.777924	-1928.4749	-1928.530039
8R	-1928.777425	-1928.474445	-1928.529265
9R	-1928.776483	-1928.47381	-1928.528411
10R	-1928.774385	-1928.471085	-1928.527445
11R	-1928.775402	-1928.472693	-1928.527161
12R	-1928.773258	-1928.470205	-1928.524705
13R	-1928.773576	-1928.469588	-1928.523079
14R	-1928.770677	-1928.467882	-1928.522722

Table S4. Relative energies (kcal/mol) of the optimized conformers of (2*R*, 3*R*)-**3d'** at B3LYP/6-31G* level.

Conformer	ΔE	ΔE+ZPE	ΔG	Boltzmann distribution factor at 298.15 K
1R	0.4	0.1	0.0	63.1708%
2R	0.0	0.0	0.6	23.0361%
3R	0.8	0.5	0.9	12.8754%
4R	2.8	2.7	3.1	0.3189%
5R	2.4	2.5	3.4	0.2033%
6R	2.4	2.4	3.5	0.1738%
7R	2.8	2.7	3.6	0.1565%
8R	3.2	3.2	4.2	0.0549%
9R	5.0	5.2	5.4	0.0070%
10R	5.0	4.8	6.1	0.0020%
11R	5.4	5.2	6.5	0.0010%
12R	6.0	6.0	7.3	0.0003%
13R	6.4	6.9	8.6	0.0000%
14R	8.8	8.8	10.1	0.0000%

Cartesian Coordinates of optimized conformers

1S

C	0.464611	0.734258	1.295758
C	1.357797	-0.148743	0.414708
C	0.791827	-1.596387	0.448225
C	-0.697057	-1.505531	0.147115
C	-1.153234	-1.108263	-1.116300
H	-0.444807	-0.947604	-1.924045
C	-2.504979	-0.879286	-1.357545
H	-2.848288	-0.551854	-2.332394
C	-3.416606	-1.057298	-0.318895
C	-2.997631	-1.479042	0.940132
H	-3.720283	-1.619198	1.736388
C	-1.639080	-1.699333	1.161868
H	-1.302575	-1.992009	2.152001
C	-0.445849	1.700747	0.625595
C	-1.691111	1.945368	1.221409
H	-1.922664	1.452089	2.158727
C	-2.615662	2.773329	0.593913
H	-3.590903	2.935565	1.042930
C	-2.290022	3.391020	-0.616289
H	-3.011796	4.038405	-1.106042
C	-1.037475	3.179961	-1.196332
H	-0.777167	3.675623	-2.126910
C	-0.121440	2.325996	-0.586873
H	0.855217	2.176566	-1.035798
O	0.442055	0.540527	2.500526
Cl	-5.120286	-0.732438	-0.600634
C	1.542773	-2.553270	-0.489381
H	2.608063	-2.525582	-0.239943
C	1.024091	-3.989283	-0.392012
H	-0.032467	-4.052498	-0.672675
H	1.590901	-4.654146	-1.052014
H	1.120235	-4.371764	0.631161
H	0.904803	-1.952909	1.478760
H	1.461668	-2.193915	-1.523292
S	3.090751	-0.025761	1.051421
H	1.370229	0.199263	-0.617194
C	3.887142	0.455060	-0.501730
F	3.745550	-0.461202	-1.483162
F	3.397183	1.614439	-1.002601
F	5.195897	0.623157	-0.272684

2S

C	-0.833865	0.702245	-0.488561
C	-0.806839	-0.404300	0.579984
C	0.078636	-1.592698	0.140397
C	1.508826	-1.079773	0.047197
C	2.236031	-0.750710	1.198250
H	1.787632	-0.879314	2.179946
C	3.540785	-0.268676	1.118397
H	4.098240	-0.019390	2.014596
C	4.127121	-0.111813	-0.135861
C	3.428984	-0.427364	-1.298780
H	3.897825	-0.296355	-2.267819
C	2.124142	-0.907025	-1.196695
H	1.566141	-1.134071	-2.099243

C	-1.006355	2.124348	-0.075565	C	1.063359	-0.327087	0.474396
C	-0.952615	3.097774	-1.085846	C	0.226695	-1.599699	0.713623
H	-0.802618	2.767224	-2.107588	C	-1.230175	-1.342991	0.355505
C	-1.083792	4.446096	-0.774785	C	-1.612813	-0.636557	-0.792262
H	-1.036657	5.191339	-1.563346	H	-0.862909	-0.230376	-1.462816
C	-1.275569	4.840853	0.551985	C	-2.956486	-0.424794	-1.099255
H	-1.378492	5.894194	0.796790	H	-3.240573	0.129304	-1.986990
C	-1.336428	3.881165	1.563402	C	-3.934087	-0.931621	-0.247992
H	-1.491114	4.184329	2.594572	C	-3.586519	-1.639329	0.900903
C	-1.201068	2.529961	1.252967	H	-4.358606	-2.021218	1.559663
H	-1.266154	1.800600	2.052318	C	-2.238607	-1.833937	1.192405
O	-0.710336	0.395713	-1.663661	H	-1.964151	-2.370994	2.096288
Cl	5.773008	0.495776	-0.249552	C	0.207914	2.142522	0.478869
C	-0.044791	-2.825761	1.052112	C	-0.723849	3.043866	1.016394
H	-1.086592	-3.156980	1.048183	H	-1.230494	2.772597	1.936148
C	0.857251	-3.977504	0.604094	C	-0.992857	4.244447	0.369290
H	1.915776	-3.703334	0.651966	H	-1.726294	4.930677	0.782282
H	0.705031	-4.858140	1.236893	C	-0.318270	4.566861	-0.811668
H	0.634443	-4.265423	-0.430289	H	-0.525788	5.506086	-1.316511
H	-0.239294	-1.876077	-0.864872	C	0.625328	3.685108	-1.341189
H	0.184568	-2.550677	2.090600	H	1.161701	3.941958	-2.249835
S	-2.546144	-0.795366	1.094899	C	0.883960	2.472548	-0.705150
H	-0.411741	-0.002961	1.517486	H	1.638751	1.810463	-1.114016
C	-3.297837	-1.418043	-0.443554	O	0.084872	0.720927	2.372147
F	-3.441104	-0.482391	-1.391505	Cl	-5.631163	-0.668223	-0.623014
F	-2.611850	-2.441077	-0.990566	C	0.783955	-2.852368	0.002424
F	-4.521807	-1.867162	-0.114788	H	0.182530	-3.707294	0.334722
				C	0.782519	-2.804879	-1.527541
3S				H	1.389358	-1.980571	-1.916347
C	0.425009	0.864051	1.208252	H	1.204741	-3.730298	-1.932664

H	-0.231585	-2.697036	-1.924027	H	-3.192984	3.952040	-0.773639
H	0.261595	-1.786721	1.791577	C	-1.215087	3.126851	-0.996796
H	1.801972	-3.029293	0.364512	H	-1.006626	3.665771	-1.916333
S	2.784959	-0.417862	1.161977	C	-0.259187	2.261358	-0.470286
H	1.170116	-0.120795	-0.587350	H	0.696008	2.150836	-0.972065
C	3.752568	-0.699761	-0.350712	O	0.456233	0.335135	2.504684
F	3.726892	-1.973699	-0.788736	Cl	-5.142288	-0.816223	-0.703314
F	3.341515	0.065143	-1.391463	C	1.546060	-2.602589	-0.645604
F	5.028838	-0.391069	-0.083129	H	2.158109	-1.994507	-1.320445
				C	2.435624	-3.622103	0.070413
4S				H	1.838368	-4.274354	0.718695
C	0.436854	0.595221	1.312509	H	2.962252	-4.257200	-0.650354
C	1.310282	-0.226729	0.355201	H	3.184870	-3.122251	0.691895
C	0.768882	-1.684984	0.335182	H	0.878129	-2.070792	1.354599
C	-0.719344	-1.592146	0.038183	H	0.825247	-3.135107	-1.275561
C	-1.173897	-1.175604	-1.219663	S	3.076916	-0.132315	0.897140
H	-0.462396	-1.004640	-2.023226	H	1.271114	0.163264	-0.660550
C	-2.525568	-0.945045	-1.459021	C	3.733967	0.727316	-0.554082
H	-2.868784	-0.603917	-2.429242	F	3.543380	0.051881	-1.710566
C	-3.438163	-1.141480	-0.424160	F	3.171999	1.944291	-0.740502
C	-3.020223	-1.582239	0.828453	F	5.050826	0.899164	-0.385344
H	-3.743997	-1.736556	1.621061				
C	-1.661351	-1.802183	1.049436	**5S**			
H	-1.325440	-2.107841	2.035911	C	1.449322	-1.144600	-0.071510
C	-0.515089	1.578005	0.727118	C	0.787310	0.120203	0.497398
C	-1.733851	1.778067	1.391317	C	-0.478360	-0.086528	1.373861
H	-1.913279	1.240519	2.315608	C	-1.783312	-0.307805	0.624946
C	-2.697718	2.620171	0.847760	C	-2.148414	-1.541474	0.071551
H	-3.651476	2.748675	1.350669	H	-1.464373	-2.377772	0.127745
C	-2.439955	3.294745	-0.348408	C	-3.369556	-1.704089	-0.580339

H	-3.643157	-2.662536	-1.007793	F	-0.152476	3.091523	0.829114
C	-4.239698	-0.621297	-0.682284	F	1.973330	2.919474	0.492884
C	-3.905768	0.617819	-0.143913	F	0.702177	3.802013	-1.042733
H	-4.590366	1.454301	-0.230755				
C	-2.681611	0.759922	0.506738	**6S**			
H	-2.415164	1.728234	0.919917	C	1.415130	-1.117689	-0.141183
C	2.921888	-1.140287	-0.325356	C	0.706804	0.106287	0.455838
C	3.505175	-2.357629	-0.713275	C	-0.500329	-0.169839	1.396318
H	2.862143	-3.224265	-0.819093	C	-1.842051	-0.386428	0.716219
C	4.872553	-2.443095	-0.947967	C	-2.165607	-1.558779	0.021537
H	5.313642	-3.390794	-1.242509	H	-1.422505	-2.338031	-0.085917
C	5.676673	-1.309397	-0.804497	C	-3.420584	-1.724744	-0.561708
H	6.745387	-1.373552	-0.988419	H	-3.662222	-2.634167	-1.101062
C	5.105549	-0.092849	-0.428089	C	-4.366810	-0.708934	-0.448940
H	5.726339	0.792051	-0.324615	C	-4.074988	0.468300	0.233688
C	3.736174	-0.005229	-0.187635	H	-4.818485	1.253917	0.311222
H	3.312444	0.954640	0.079431	C	-2.814644	0.616426	0.809732
O	0.784879	-2.145656	-0.291625	H	-2.580210	1.539912	1.331260
Cl	-5.782675	-0.822729	-1.503351	C	2.880712	-1.038831	-0.422065
C	-0.210993	-1.137040	2.472509	C	3.520770	-2.226826	-0.811937
H	0.775318	-0.936707	2.914908	H	2.923387	-3.127740	-0.897151
C	-1.276271	-1.114733	3.570395	C	4.885463	-2.240412	-1.075395
H	-2.265270	-1.346374	3.162387	H	5.371088	-3.165728	-1.371003
H	-1.049906	-1.850183	4.349604	C	5.629625	-1.063316	-0.960181
H	-1.334227	-0.127875	4.045512	H	6.695964	-1.071412	-1.167368
H	-0.591344	0.874374	1.888385	C	5.001550	0.124321	-0.582408
H	-0.151717	-2.133437	2.026584	H	5.575188	1.042738	-0.501493
S	0.510893	1.242977	-0.955885	C	3.635060	0.140073	-0.311976
H	1.531000	0.626411	1.116830	H	3.165692	1.078651	-0.045607
C	0.770027	2.831507	-0.123758	O	0.797321	-2.148944	-0.360809

Cl	-5.953070	-0.915252	-1.182047
C	-0.182564	-1.273004	2.430990
H	-0.144146	-2.245574	1.932811
C	1.114720	-1.037428	3.210929
H	1.130026	-0.040473	3.669369
H	1.221180	-1.773854	4.014161
H	2.002807	-1.125332	2.574080
H	-0.598738	0.764350	1.960993
H	-1.027293	-1.310645	3.128570
S	0.291492	1.202139	-0.983690
H	1.448972	0.661606	1.030337
C	0.507834	2.805643	-0.168230
F	-0.366471	3.011712	0.840405
F	1.740552	2.967078	0.372234
F	0.325751	3.767818	-1.080445

7S

C	2.154574	1.234649	-0.180771
C	0.759121	0.645898	0.114709
C	-0.367226	1.708701	0.039072
C	-1.689771	1.033221	-0.282348
C	-2.577361	0.603441	0.709781
H	-2.346733	0.773778	1.755243
C	-3.762270	-0.055511	0.384605
H	-4.442056	-0.386894	1.161813
C	-4.065440	-0.288660	-0.953782
C	-3.204854	0.129215	-1.966872
H	-3.457105	-0.051909	-3.005894
C	-2.027624	0.787518	-1.619624
H	-1.357684	1.122240	-2.408397
C	3.271334	0.331331	-0.592293
C	4.532820	0.921443	-0.774013
H	4.633152	1.985503	-0.591178
C	5.619460	0.155968	-1.180787
H	6.590766	0.622703	-1.315790
C	5.459614	-1.211957	-1.416421
H	6.307215	-1.812210	-1.734870
C	4.209534	-1.807263	-1.241828
H	4.081429	-2.870256	-1.422998
C	3.119855	-1.043032	-0.830437
H	2.164519	-1.530926	-0.690542
O	2.327397	2.441227	-0.103275
Cl	-5.557830	-1.117531	-1.373493
C	-0.420628	2.656843	1.249049
H	0.590758	3.030220	1.427254
C	-1.371807	3.834471	1.027755
H	-2.398863	3.496161	0.854968
H	-1.377066	4.498787	1.898364
H	-1.064389	4.426841	0.157727
H	-0.097288	2.323025	-0.829678
H	-0.714372	2.101499	2.146341
S	0.882511	-0.233213	1.746652
H	0.558548	-0.134966	-0.620175
C	0.054992	-1.827149	1.409017
F	-1.240621	-1.836996	1.757526
F	0.115703	-2.198057	0.110762
F	0.670137	-2.770362	2.140388

8S

C	-0.689124	0.667786	-0.462394

C	-0.739690	-0.449639	0.593560	H	-2.046451	-3.597739	0.455012
C	0.083024	-1.688606	0.167799	H	-0.255057	-1.971872	-0.830544
C	1.533839	-1.242142	0.059257	H	0.899921	-3.348321	1.288302
C	2.285993	-0.962317	1.207787	S	-2.500624	-0.763063	1.083628
H	1.840228	-1.087864	2.191421	H	-0.332190	-0.077891	1.538148
C	3.609251	-0.534945	1.121436	C	-3.329735	-0.982851	-0.524765
H	4.185668	-0.322315	2.015081	F	-3.479519	0.162945	-1.206970
C	4.189048	-0.385207	-0.136701	F	-2.695811	-1.851074	-1.332530
C	3.466670	-0.653622	-1.296689	F	-4.555700	-1.469377	-0.263341
H	3.931690	-0.529321	-2.268468				
C	2.142627	-1.076164	-1.188735	**9S**			
H	1.566028	-1.262492	-2.088777	C	-1.759752	-0.160169	0.982270
C	-0.781285	2.092748	-0.037062	C	-0.392004	-0.045559	0.286348
C	-0.636985	3.070782	-1.033867	C	0.730458	0.508247	1.206748
H	-0.478176	2.741873	-2.054790	C	2.078179	0.033285	0.688628
C	-0.692233	4.421365	-0.710330	C	2.762522	0.705622	-0.332711
H	-0.574970	5.170319	-1.487983	H	2.350633	1.617355	-0.750281
C	-0.898451	4.813438	0.615076	C	3.973609	0.225598	-0.828843
H	-0.942551	5.868608	0.869536	H	4.496528	0.753808	-1.618539
C	-1.049999	3.849167	1.612595	C	4.511169	-0.944153	-0.296776
H	-1.217189	4.151054	2.642180	C	3.858380	-1.633577	0.722157
C	-0.990205	2.495368	1.290134	H	4.292444	-2.538506	1.133057
H	-1.128227	1.762310	2.076527	C	2.648428	-1.136801	1.204024
O	-0.570797	0.364424	-1.638897	H	2.139562	-1.670541	2.003163
Cl	5.858468	0.153204	-0.259532	C	-2.750979	-1.158455	0.482425
C	-0.085129	-2.898063	1.126203	C	-3.974344	-1.244300	1.165425
H	-0.427845	-2.554683	2.111038	H	-4.140148	-0.580199	2.006389
C	-1.033246	-3.978792	0.599904	C	-4.941651	-2.159693	0.767346
H	-0.680825	-4.363938	-0.364183	H	-5.884997	-2.218312	1.302259
H	-1.084620	-4.820861	1.298997	C	-4.699153	-3.002539	-0.320628

H	-5.454415	-3.717994	-0.633347	H	-4.245389	-1.514607	-0.256714
C	-3.486975	-2.923442	-1.007591	C	-4.122205	0.631662	-0.154029
H	-3.297223	-3.573634	-1.856309	C	-3.349669	1.739610	0.182182
C	-2.516626	-2.006372	-0.610087	H	-3.745254	2.740731	0.050778
H	-1.590389	-1.946313	-1.169349	C	-2.065648	1.538224	0.688461
O	-1.995510	0.522639	1.965832	H	-1.459278	2.401489	0.950998
Cl	6.039071	-1.555038	-0.915276	C	2.342880	1.456414	-0.159022
C	0.675695	2.018757	1.483318	C	3.589591	2.085551	-0.015921
H	-0.330537	2.261904	1.827027	H	4.386057	1.537125	0.475006
C	1.702875	2.451622	2.531855	C	3.788593	3.375201	-0.495283
H	2.727677	2.246795	2.204645	H	4.757200	3.852705	-0.379895
H	1.620841	3.524872	2.733498	C	2.742827	4.055406	-1.125508
H	1.543272	1.921634	3.478724	H	2.897764	5.062817	-1.501220
H	0.557252	0.004421	2.167113	C	1.499617	3.439232	-1.274042
H	0.834679	2.574664	0.553274	H	0.685667	3.963055	-1.766423
S	-0.495168	0.753674	-1.387803	C	1.298288	2.146209	-0.794663
H	-0.095291	-1.060038	0.001553	H	0.322540	1.690106	-0.920098
C	-1.809166	2.006945	-1.219321	O	3.164337	-0.515530	0.860168
F	-3.020038	1.480554	-0.964208	Cl	-5.741339	0.867397	-0.795103
F	-1.576184	2.927164	-0.270984	C	-0.145016	-0.635807	2.782062
F	-1.871703	2.635143	-2.406199	H	-0.885362	-0.118640	3.404054
				H	0.258110	1.083059	1.588957
10S				S	0.855139	-2.397296	0.450881
C	2.208408	0.066496	0.382572	H	0.369038	-0.351354	-0.642296
C	0.804102	-0.562065	0.335401	C	1.156798	-2.714294	-1.308274
C	-0.140112	0.076455	1.413377	F	0.146393	-2.281583	-2.094594
C	-1.543602	0.251554	0.864542	F	2.273220	-2.114891	-1.762135
C	-2.346809	-0.844615	0.520202	F	1.282022	-4.037234	-1.482424
H	-1.965116	-1.852713	0.640521	C	1.208332	-0.650704	3.497781
C	-3.630343	-0.662394	0.010517	H	1.963827	-1.212010	2.942202

H	1.590071	0.368278	3.634959
H	1.107386	-1.105243	4.488994
H	-0.522328	-1.659005	2.661748

11S

C	1.505368	-1.012230	-0.302218
C	0.774553	0.144200	0.394830
C	-0.449953	-0.157064	1.301730
C	-1.805548	-0.322804	0.638542
C	-2.052841	-1.178278	-0.442919
H	-1.234611	-1.743579	-0.870293
C	-3.332369	-1.303491	-0.981272
H	-3.513314	-1.964493	-1.821917
C	-4.381759	-0.571294	-0.431518
C	-4.168416	0.288264	0.642120
H	-4.991153	0.860443	1.056516
C	-2.880881	0.405576	1.162391
H	-2.711109	1.086694	1.992597
C	2.997559	-0.985618	-0.352521
C	3.644566	-2.174473	-0.727899
H	3.035169	-3.040511	-0.961202
C	5.031865	-2.233809	-0.790594
H	5.522402	-3.161210	-1.071065
C	5.792295	-1.099219	-0.495512
H	6.876473	-1.142505	-0.547461
C	5.158264	0.091976	-0.139362
H	5.746026	0.979321	0.075676
C	3.768547	0.151101	-0.061540
H	3.297691	1.094026	0.188443
O	0.889148	-1.939902	-0.806926
Cl	-5.998637	-0.728662	-1.107265
C	-0.138767	-1.257150	2.360688
H	-0.750461	-1.022603	3.240514
C	-0.400731	-2.715612	1.975294
H	0.204928	-3.040883	1.128023
H	-0.175317	-3.365821	2.828004
H	-1.451146	-2.864957	1.708434
H	-0.533023	0.769264	1.878939
H	0.905973	-1.137520	2.682341
S	0.411147	1.355533	-0.967633
H	1.503735	0.641843	1.034472
C	0.624094	2.890799	-0.027214
F	-0.281713	3.036080	0.961668
F	1.840606	2.988168	0.563125
F	0.489769	3.920773	-0.871364

12S

C	-2.245608	1.000120	0.067995
C	-0.767139	0.612452	-0.041224
C	0.161755	1.520784	0.820464
C	1.545514	0.893316	0.872372
C	2.581646	1.250580	0.003293
H	2.434141	2.039584	-0.722350
C	3.815924	0.603155	0.045204
H	4.611448	0.886466	-0.635131
C	4.017744	-0.419522	0.967329
C	3.009338	-0.794625	1.852258
H	3.182385	-1.586483	2.572643
C	1.786121	-0.132162	1.795719
H	0.998106	-0.423966	2.486715

C	-3.244856	-0.022641	0.499066	C	-0.275591	-0.068420	0.332502
C	-4.520940	0.445184	0.856703	C	0.811073	0.628018	1.203041
H	-4.711595	1.510883	0.795263	C	2.177738	0.169081	0.719493
C	-5.504638	-0.439781	1.280437	C	2.820955	0.766423	-0.372768
H	-6.484719	-0.066488	1.562617	H	2.359358	1.606067	-0.880230
C	-5.231964	-1.809561	1.340401	C	4.052774	0.299588	-0.829082
H	-6.000715	-2.503366	1.668644	H	4.543487	0.768463	-1.674998
C	-3.973621	-2.286124	0.972532	C	4.652584	-0.780174	-0.185142
H	-3.763145	-3.350967	1.003581	C	4.040662	-1.393708	0.905177
C	-2.980888	-1.399382	0.558986	H	4.522196	-2.228835	1.402016
H	-2.024802	-1.798322	0.245872	C	2.808666	-0.912618	1.345731
O	-2.591478	2.150636	-0.158582	H	2.330389	-1.387808	2.198893
Cl	5.568254	-1.245971	1.021535	C	-2.582545	-1.317821	0.460911
C	0.134283	3.046603	0.547589	C	-3.850696	-1.374224	1.059519
H	0.981204	3.471097	1.101159	H	-4.040479	-0.745981	1.922759
C	0.156648	3.561051	-0.896045	C	-4.834243	-2.215276	0.551546
H	-0.755511	3.269743	-1.423017	H	-5.815471	-2.243734	1.016108
H	0.186906	4.656497	-0.883129	C	-4.557782	-3.024258	-0.553667
H	1.015761	3.215484	-1.476261	H	-5.324258	-3.683881	-0.950486
H	-0.252232	1.404490	1.833103	C	-3.295667	-2.985372	-1.147575
H	-0.771144	3.445105	1.013125	H	-3.075352	-3.616585	-2.003211
S	-0.312159	0.538423	-1.840996	C	-2.313663	-2.132340	-0.648494
H	-0.619141	-0.399987	0.328535	H	-1.343404	-2.110626	-1.130138
C	0.208053	-1.198170	-1.941355	O	-1.736809	0.003045	2.224360
F	1.147993	-1.530401	-1.039241	Cl	6.206674	-1.374052	-0.753703
F	-0.813516	-2.068090	-1.760183	C	0.738122	2.162502	1.323945
F	0.704953	-1.401040	-3.169823	H	1.676028	2.480318	1.795387
				H	0.659826	0.213185	2.206003
13S				S	-0.524224	0.637862	-1.362800
C	-1.575812	-0.410677	1.089349	H	0.141409	-1.041499	0.042028

C	-1.798333	1.932047	-1.186093	C	0.995170	4.496072	-0.221195
F	-2.761740	1.618799	-0.300718	H	1.423953	5.423201	-0.590743
F	-1.311263	3.134634	-0.828521	C	0.106624	3.773102	-1.018135
F	-2.364810	2.080221	-2.394951	H	-0.167121	4.141900	-2.002057
H	0.739723	2.608744	0.324290	C	-0.432603	2.574593	-0.555219
C	-0.432026	2.722116	2.136091	H	-1.143228	2.040724	-1.175979
H	-0.438300	2.313408	3.150915	O	-0.610159	0.614678	2.491625
H	-0.343223	3.812279	2.204010	Cl	5.238020	-0.772227	-1.191229
H	-1.400303	2.492987	1.690323	C	-0.773257	-2.332489	1.821873
				H	-1.850839	-2.341645	2.020338
1R				C	-0.242710	-3.768047	1.804076
C	-0.637757	0.833962	1.288645	H	-0.451026	-4.271532	2.753942
C	-1.204902	-0.223475	0.336202	H	-0.712930	-4.353975	1.004668
H	-1.053433	0.094096	-0.693891	H	0.840065	-3.792985	1.640291
C	-0.541644	-1.620378	0.480924	H	-1.014449	-2.232414	-0.296732
C	0.923596	-1.460098	0.100546	H	-0.321523	-1.766167	2.638981
C	1.885813	-1.017119	1.017941	S	-3.042802	-0.224583	0.599925
H	1.604569	-0.824968	2.047431	C	-3.525958	-0.401978	-1.137277
C	3.207364	-0.806236	0.629971	F	-3.004140	-1.504575	-1.716681
H	3.946221	-0.463024	1.345728	F	-4.860543	-0.483978	-1.201950
C	3.573528	-1.039284	-0.693852	F	-3.135076	0.643236	-1.904339
C	2.641049	-1.482573	-1.628488				
H	2.941808	-1.664801	-2.654367	**2R**			
C	1.324191	-1.688140	-1.220863	C	-2.257956	0.871182	0.709536
H	0.592223	-2.033549	-1.947049	C	-0.837662	0.432245	0.316646
C	-0.097755	2.100100	0.721882	H	-0.830165	0.001926	-0.684319
C	0.777666	2.846405	1.526508	C	0.179607	1.587418	0.408438
H	1.014021	2.470941	2.516160	C	1.581884	1.091103	0.120328
C	1.329954	4.030799	1.053707	C	1.948224	0.665506	-1.162831
H	2.019060	4.594514	1.675633	H	1.226684	0.702923	-1.974448

C	3.227352	0.184433	-1.427916	F	1.679766	-2.014199	0.361456
H	3.502637	-0.146637	-2.423154	F	0.124280	-3.395488	0.949686
C	4.156713	0.128245	-0.390997	F	-0.112774	-2.169487	-0.840982
C	3.824659	0.547997	0.893930				
H	4.559209	0.498020	1.690068	**3R**			
C	2.538353	1.027510	1.137027	C	2.010066	-0.439653	0.624196
H	2.271536	1.348759	2.139754	C	0.615562	-0.442071	-0.024438
C	-3.430778	0.271746	0.012754	H	0.614754	-1.113486	-0.889179
C	-4.684585	0.863314	0.233608	C	-0.491164	-0.883213	0.958257
H	-4.740026	1.716105	0.901425	C	-1.875309	-0.659754	0.382607
C	-5.819000	0.364288	-0.396205	C	-2.322864	-1.378111	-0.732967
H	-6.783921	0.833091	-0.226932	H	-1.676951	-2.118518	-1.197540
C	-5.715925	-0.741539	-1.244586	C	-3.591568	-1.168849	-1.268321
H	-6.601915	-1.134442	-1.735267	H	-3.930542	-1.728667	-2.133073
C	-4.475647	-1.345253	-1.457885	C	-4.429046	-0.226672	-0.674048
H	-4.395891	-2.212833	-2.106061	C	-4.013853	0.501779	0.437350
C	-3.335082	-0.840342	-0.837396	H	-4.676200	1.233015	0.887408
H	-2.385498	-1.337903	-0.993771	C	-2.738543	0.278814	0.954895
O	-2.396626	1.705838	1.591404	H	-2.403419	0.856593	1.810892
Cl	5.773885	-0.480858	-0.713427	C	3.225367	-0.580068	-0.229007
C	-0.233887	2.741847	-0.532174	C	4.470333	-0.563756	0.419561
H	-1.249039	3.058087	-0.274607	H	4.485180	-0.439259	1.496636
C	0.707899	3.944136	-0.439081	C	5.646726	-0.704163	-0.307534
H	0.367792	4.755604	-1.091020	H	6.604764	-0.689859	0.203761
H	0.744508	4.330726	0.586141	C	5.594845	-0.862203	-1.695018
H	1.727753	3.676362	-0.732112	H	6.513278	-0.971166	-2.264811
H	0.141299	1.965397	1.435194	C	4.362410	-0.876777	-2.349966
H	-0.270418	2.377902	-1.567792	H	4.319262	-0.993423	-3.428690
S	-0.490540	-0.961779	1.498408	C	3.182999	-0.736081	-1.622294
C	0.352436	-2.177866	0.431465	H	2.237363	-0.730936	-2.152152

O	2.099469	-0.319690	1.835769	H	-2.627572	0.874761	2.034793
Cl	-6.033967	0.043887	-1.339214	C	3.245794	-0.518103	-0.038183
C	-0.272650	-2.357763	1.367109	C	4.489840	-0.378351	0.597332
H	0.748395	-2.472704	1.742500	H	4.508228	0.031855	1.600940
C	-1.259724	-2.821869	2.439910	C	5.659819	-0.759356	-0.049277
H	-1.063158	-3.860319	2.726788	H	6.616901	-0.648643	0.451888
H	-1.172692	-2.202927	3.340483	C	5.602920	-1.283503	-1.343488
H	-2.293796	-2.756097	2.087039	H	6.516318	-1.581025	-1.850647
H	-0.381287	-0.271645	1.855894	C	4.372098	-1.422103	-1.986666
H	-0.359857	-3.000026	0.479951	H	4.325486	-1.822422	-2.994971
S	0.315254	1.191994	-0.852800	C	3.198852	-1.042565	-1.338620
C	0.673852	2.374460	0.483183	H	2.255670	-1.140663	-1.863956
F	1.978174	2.450592	0.795912	O	2.132187	0.368555	1.852902
F	0.284559	3.582943	0.043831	Cl	-6.122555	-0.608614	-1.019600
F	0.009256	2.108096	1.624539	C	-0.181481	-1.716986	2.051771
				H	-1.023645	-1.803568	2.748385
4R				C	-0.000225	-3.045909	1.314192
C	2.035904	-0.104075	0.731211	H	0.873940	-3.034298	0.651578
C	0.644312	-0.278648	0.107379	H	0.156051	-3.856308	2.033838
H	0.655833	-1.136471	-0.568581	H	-0.879296	-3.302944	0.714647
C	-0.456533	-0.467234	1.167207	H	-0.395993	0.391211	1.837918
C	-1.851507	-0.499124	0.574294	H	0.705090	-1.510875	2.658424
C	-2.185741	-1.276633	-0.542046	S	0.341638	1.091496	-1.106677
H	-1.424139	-1.857842	-1.052577	C	0.383231	2.586669	-0.067781
C	-3.488043	-1.316661	-1.036048	F	1.582855	2.834118	0.477586
H	-3.734193	-1.919668	-1.903096	F	0.074554	3.613782	-0.878331
C	-4.476331	-0.565797	-0.403957	F	-0.514636	2.566653	0.936468
C	-4.176421	0.223060	0.703399				
H	-4.952955	0.811192	1.179946	**5R**			
C	-2.866650	0.250119	1.178749	C	2.215174	-0.765651	0.896603

C	0.786927	-0.370080	0.496698	H	0.902264	-3.790844	-1.726141
H	0.763367	-0.042200	-0.539265	H	-0.278799	-2.513123	-2.016471
C	-0.232130	-1.498751	0.740392	H	-0.247896	-1.675975	1.820026
C	-1.629196	-1.089413	0.315005	H	1.071891	-3.211813	0.661184
C	-1.914107	-0.613253	-0.971910	S	0.459968	1.138003	1.534877
H	-1.118564	-0.485173	-1.697884	C	-0.399693	2.244002	0.367080
C	-3.209317	-0.262749	-1.345578	F	-1.730325	2.090763	0.358127
H	-3.416750	0.111159	-2.342131	F	-0.143677	3.508360	0.739293
C	-4.239910	-0.386311	-0.417310	F	0.024746	2.089966	-0.911131
C	-3.990674	-0.851423	0.871176				
H	-4.801083	-0.934689	1.586935	**6R**			
C	-2.687659	-1.197877	1.223363	C	-1.458616	-1.237944	0.458303
H	-2.489225	-1.553951	2.230593	C	-0.770991	0.131969	0.636711
C	3.363922	-0.282840	0.078419	H	-1.484922	0.802402	1.120908
C	4.617593	-0.867171	0.319002	C	0.511223	0.044240	1.514310
H	4.689869	-1.629521	1.087040	C	1.780163	-0.303390	0.752520
C	5.729830	-0.475356	-0.417016	C	2.538295	0.679776	0.102633
H	6.694222	-0.938790	-0.230914	H	2.209627	1.712837	0.111896
C	5.605420	0.516563	-1.393761	C	3.712293	0.358962	-0.575078
H	6.474306	0.826206	-1.967551	H	4.291123	1.127322	-1.075587
C	4.366154	1.114041	-1.628973	C	4.136578	-0.967406	-0.603982
H	4.270708	1.894794	-2.377620	C	3.404780	-1.967523	0.029747
C	3.246806	0.715125	-0.901601	H	3.746399	-2.996269	-0.002040
H	2.299518	1.210363	-1.079415	C	2.232964	-1.626029	0.703784
O	2.383376	-1.472734	1.879184	H	1.648445	-2.402998	1.183202
Cl	-5.876588	0.060759	-0.876688	C	-2.903782	-1.298903	0.085345
C	0.214270	-2.839861	0.093211	C	-3.463764	-2.575060	-0.088235
H	-0.599258	-3.558163	0.248993	H	-2.820618	-3.439178	0.035701
C	0.574530	-2.799866	-1.394825	C	-4.809124	-2.719302	-0.406909
H	1.396600	-2.103933	-1.601649	H	-5.231018	-3.711076	-0.540466

C	-5.615811	-1.588040	-0.553962	C	3.907076	0.413613	-0.148090
H	-6.667468	-1.698205	-0.802955	H	4.571510	1.215944	-0.449638
C	-5.069252	-0.315281	-0.382820	C	4.254746	-0.912191	-0.393904
H	-5.692685	0.566068	-0.499935	C	3.411334	-1.954855	-0.020152
C	-3.720709	-0.167785	-0.066542	H	3.695053	-2.982710	-0.218142
H	-3.315885	0.830278	0.042106	C	2.204547	-1.657970	0.611471
O	-0.820540	-2.260897	0.650271	H	1.533451	-2.462622	0.889349
Cl	5.620136	-1.382853	-1.453688	C	-2.868330	-1.258782	-0.065520
C	0.652577	1.305586	2.391085	C	-3.490793	-2.509874	-0.207530
H	-0.298859	1.456242	2.919294	H	-2.905039	-3.400279	-0.008295
C	1.784634	1.199183	3.414271	C	-4.824702	-2.596690	-0.588478
H	1.814634	2.086708	4.055201	H	-5.295704	-3.569496	-0.694517
H	1.649137	0.322445	4.058903	C	-5.556892	-1.432041	-0.833017
H	2.757417	1.101986	2.923109	H	-6.599599	-1.497178	-1.130735
H	0.318343	-0.792393	2.195081	C	-4.947137	-0.184084	-0.696790
H	0.794034	2.192585	1.766791	H	-5.511973	0.722752	-0.891169
S	-0.554273	0.803736	-1.078800	C	-3.610111	-0.094157	-0.316222
C	-0.880124	2.567890	-0.807389	H	-3.153629	0.883870	-0.237822
F	0.154738	3.233704	-0.246944	O	-0.864275	-2.308341	0.612859
F	-1.115480	3.127392	-2.001585	Cl	5.781876	-1.273667	-1.189830
F	-1.949851	2.800180	-0.011762	C	0.568359	1.175133	2.508746
				H	0.575836	2.104230	1.930349
7R				C	-0.576951	1.212556	3.524657
C	-1.443280	-1.258063	0.380828	H	-0.477541	2.075933	4.190870
C	-0.705995	0.080190	0.589226	H	-1.560408	1.288244	3.044791
H	-1.426087	0.792823	0.994272	H	-0.582104	0.307998	4.144208
C	0.504165	-0.043566	1.564032	H	0.277344	-0.918507	2.182673
C	1.827717	-0.335897	0.874264	H	1.522425	1.137427	3.046688
C	2.696300	0.690876	0.483361	S	-0.309979	0.710605	-1.110492
H	2.426228	1.726786	0.654262	C	-0.591775	2.487683	-0.882959

F	0.383811	3.110427	-0.184611
F	-0.641762	3.051885	-2.096399
F	-1.748434	2.770230	-0.236609

8R

C	0.839684	0.413802	-0.475073
C	0.677970	-0.558278	0.704089
H	0.307388	0.020746	1.554644
C	-0.338056	-1.713653	0.492912
C	-1.720477	-1.099838	0.312353
C	-2.205378	-0.690378	-0.937010
H	-1.594492	-0.824071	-1.821742
C	-3.459970	-0.097128	-1.062955
H	-3.828184	0.215351	-2.033973
C	-4.241789	0.094443	0.074223
C	-3.789349	-0.302563	1.329672
H	-4.410807	-0.154307	2.205881
C	-2.533238	-0.897624	1.434191
H	-2.181895	-1.217562	2.412537
C	1.104311	1.852879	-0.190372
C	1.017805	2.747850	-1.268245
H	0.770474	2.351072	-2.246589
C	1.239918	4.106436	-1.075849
H	1.162582	4.792459	-1.914174
C	1.563772	4.587075	0.195771
H	1.739736	5.648266	0.347318
C	1.665052	3.703362	1.271290
H	1.927309	4.072967	2.258059
C	1.432651	2.343015	1.082264
H	1.540281	1.667741	1.923480
O	0.719936	0.011918	-1.621628
Cl	-5.824709	0.843915	-0.078180
C	0.031045	-2.769223	-0.561050
H	1.037047	-3.134793	-0.336454
C	-0.948205	-3.945395	-0.557781
H	-0.638081	-4.709498	-1.278346
H	-0.995287	-4.418514	0.431141
H	-1.962237	-3.626425	-0.820550
H	-0.355611	-2.234640	1.460205
H	0.086068	-2.313302	-1.551115
S	2.317758	-1.138645	1.362945
C	3.419887	-1.169763	-0.090236
F	3.657900	0.053772	-0.594757
F	4.588953	-1.673655	0.342306
F	2.979628	-1.934472	-1.099161

9R

C	-1.578959	0.411036	0.846180
C	-0.850021	1.196479	-0.258468
H	-1.541506	1.982350	-0.583752
C	0.446974	1.907459	0.225129
C	1.674994	1.017978	0.325255
C	2.482654	0.753067	-0.788236
H	2.243397	1.189544	-1.751151
C	3.599226	-0.075376	-0.693659
H	4.213840	-0.278732	-1.563622
C	3.919262	-0.640940	0.537220
C	3.147326	-0.381826	1.666782
H	3.411733	-0.824698	2.620670
C	2.034297	0.447637	1.550991

H	1.414700	0.629148	2.421267	C	-1.144687	-0.373426	0.363087
C	-3.029715	0.094925	0.688727	H	-0.966862	-0.181708	-0.693186
C	-3.634550	-0.657222	1.707937	C	-0.238524	-1.576588	0.745880
H	-3.019786	-0.982573	2.539729	C	1.187386	-1.299697	0.297046
C	-4.986733	-0.972849	1.644859	C	1.933074	-0.211768	0.774460
H	-5.443962	-1.557940	2.437358	H	1.512949	0.453464	1.519037
C	-5.755210	-0.537174	0.562159	C	3.226541	0.034341	0.319970
H	-6.812203	-0.782656	0.511331	H	3.791601	0.880839	0.694109
C	-5.163498	0.211630	-0.456058	C	3.791260	-0.821732	-0.623084
H	-5.756871	0.548803	-1.300665	C	3.081269	-1.914264	-1.112993
C	-3.807489	0.524796	-0.396339	H	3.532096	-2.573373	-1.846702
H	-3.362278	1.088292	-1.207720	C	1.785383	-2.139021	-0.650135
O	-0.979290	0.104155	1.863011	H	1.227238	-2.987371	-1.037822
Cl	5.325063	-1.690654	0.668683	C	-0.660616	2.185485	0.437034
C	0.688295	3.169234	-0.628979	C	-0.150677	3.252450	1.194568
H	-0.232540	3.768153	-0.620931	H	-0.016409	3.108407	2.261251
C	1.850884	4.028949	-0.129894	C	0.178219	4.456240	0.582971
H	1.950184	4.937013	-0.733913	H	0.586152	5.271272	1.173519
H	1.691970	4.332915	0.911602	C	-0.020208	4.617103	-0.791396
H	2.798473	3.484514	-0.175215	H	0.234433	5.558080	-1.270632
H	0.212872	2.245508	1.241917	C	-0.551669	3.571632	-1.547367
H	0.854975	2.886027	-1.676421	H	-0.722960	3.700638	-2.611785
S	-0.661326	0.232098	-1.828338	C	-0.864104	2.356886	-0.940569
C	-0.386202	-1.482914	-1.260282	H	-1.304855	1.567912	-1.538766
F	-1.507109	-2.053188	-0.778720	O	-1.073550	0.898476	2.379315
F	-0.003915	-2.179112	-2.344281	Cl	5.422232	-0.516123	-1.202595
F	0.550722	-1.607776	-0.315746	C	-0.366684	-2.141492	2.188226
				H	-0.173540	-3.218616	2.108558
10R				C	0.546701	-1.582568	3.282094
C	-0.966680	0.919162	1.161234	H	0.356367	-2.119133	4.218497

H	1.603233	-1.720033	3.031414
H	0.363016	-0.522702	3.464054
H	-0.612752	-2.368821	0.089905
H	-1.413008	-2.044743	2.498092
S	-2.957723	-0.763510	0.505075
C	-3.229563	-1.254855	-1.218442
F	-2.446027	-2.285045	-1.603716
F	-4.508508	-1.625631	-1.356940
F	-2.987820	-0.252546	-2.095637

11R

C	1.512017	0.264706	-0.874703
C	0.824159	1.133955	0.191179
H	1.563403	1.883409	0.490590
C	-0.426815	1.901300	-0.326066
C	-1.707511	1.086950	-0.385142
C	-2.543723	0.959304	0.731243
H	-2.283186	1.443418	1.665421
C	-3.716670	0.208283	0.675885
H	-4.353708	0.109820	1.547911
C	-4.063543	-0.416715	-0.518147
C	-3.261978	-0.294553	-1.650409
H	-3.547861	-0.782757	-2.575593
C	-2.092014	0.457306	-1.574214
H	-1.450060	0.531658	-2.443984
C	2.941973	-0.125339	-0.693240
C	3.512144	-0.944752	-1.680024
H	2.886654	-1.264978	-2.505800
C	4.844597	-1.331035	-1.593789
H	5.274829	-1.967429	-2.361479
C	5.628086	-0.900021	-0.520049
H	6.669709	-1.200618	-0.451218
C	5.070987	-0.084528	0.465947
H	5.675864	0.249536	1.303615
C	3.734713	0.299897	0.382950
H	3.315967	0.915629	1.170216
O	0.902250	-0.048300	-1.883795
Cl	-5.541279	-1.368664	-0.599669
C	-0.608865	3.210788	0.474656
H	-0.614835	2.990741	1.550534
C	0.446558	4.277590	0.171240
H	0.247775	5.191499	0.740846
H	1.461929	3.953516	0.429072
H	0.444560	4.538652	-0.893499
H	-0.176050	2.179493	-1.356803
H	-1.600628	3.614166	0.242576
S	0.567645	0.249227	1.798068
C	0.191794	-1.467709	1.298877
F	1.280361	-2.123361	0.853100
F	-0.240627	-2.094525	2.406105
F	-0.742889	-1.574587	0.350360

12R

C	0.698514	0.496117	-0.481375
C	0.669842	-0.519562	0.673143
H	0.220068	-0.018112	1.534503
C	-0.193254	-1.789036	0.427513
C	-1.631561	-1.314357	0.257878
C	-2.158511	-0.957285	-0.990293
H	-1.538178	-1.032835	-1.875734

C	-3.464557	-0.487011	-1.112002	F	3.518372	0.423173	-0.705668
H	-3.865055	-0.212594	-2.081732	F	4.700120	-1.084992	0.322062
C	-4.255647	-0.368342	0.028747	F	3.146614	-1.672435	-1.082765
C	-3.761137	-0.715091	1.283421				
H	-4.390440	-0.624814	2.161951	**13R**			
C	-2.452537	-1.184298	1.384413	C	-1.362492	-0.962418	-0.518995
H	-2.066684	-1.463311	2.362412	C	-0.587374	0.039255	0.349332
C	0.751909	1.951487	-0.161622	H	-1.280241	0.541364	1.017858
C	0.585568	2.848390	-1.228672	C	0.474199	-0.673924	1.259794
H	0.434597	2.441218	-2.222165	C	1.906351	-0.638374	0.720450
C	0.609891	4.220321	-1.007233	C	2.996576	-0.274305	1.520857
H	0.472820	4.906050	-1.838121	H	2.850286	0.022072	2.552148
C	0.811879	4.715162	0.283964	C	4.300158	-0.281621	1.024850
H	0.833016	5.787153	0.458423	H	5.132175	0.007917	1.657304
C	0.989324	3.831997	1.349923	C	4.523177	-0.662901	-0.294123
H	1.155738	4.213729	2.352761	C	3.463608	-1.044043	-1.112947
C	0.955967	2.456826	1.131003	H	3.647907	-1.348546	-2.137327
H	1.118737	1.787345	1.967745	C	2.168311	-1.035535	-0.601132
O	0.652484	0.110820	-1.639127	H	1.344781	-1.343028	-1.236304
Cl	-5.904469	0.224273	-0.117557	C	-2.815472	-1.171033	-0.242190
C	0.275334	-2.770955	-0.675229	C	-3.393421	-2.357693	-0.724250
H	0.787828	-2.227296	-1.467780	H	-2.763150	-3.050529	-1.270859
C	1.153013	-3.908534	-0.144297	C	-4.737113	-2.631585	-0.499351
H	1.436626	-4.584917	-0.958260	H	-5.170792	-3.556743	-0.867394
H	2.071135	-3.537084	0.315759	C	-5.528698	-1.714409	0.197688
H	0.615773	-4.498732	0.608518	H	-6.579982	-1.925268	0.371947
H	-0.158669	-2.331421	1.381318	C	-4.969743	-0.524265	0.663983
H	-0.619282	-3.210952	-1.129982	H	-5.586161	0.198153	1.190528
S	2.378225	-0.836986	1.336163	C	-3.619311	-0.253300	0.452463
C	3.467719	-0.787920	-0.125849	H	-3.219601	0.694269	0.792161

O	-0.791999	-1.634320	-1.364829	H	-1.478386	-0.099315	-2.586127
Cl	6.161662	-0.669049	-0.931071	C	3.013283	-0.201502	-0.700845
C	0.310296	-0.165575	2.708761	C	3.625245	-1.224204	-1.442283
H	1.015729	-0.705329	3.351112	H	3.018592	-1.777723	-2.150231
C	0.460518	1.347106	2.917636	C	4.973487	-1.513454	-1.267009
H	0.380785	1.588200	3.983121	H	5.436638	-2.308049	-1.844550
H	1.421803	1.720447	2.555085	C	5.730243	-0.782296	-0.347517
H	-0.317202	1.911070	2.394002	H	6.783897	-1.007363	-0.208789
H	0.184129	-1.733159	1.273099	C	5.131124	0.235967	0.395211
H	-0.688136	-0.471233	3.047476	H	5.715217	0.803239	1.113676
S	0.187476	1.386181	-0.652242	C	3.779566	0.525334	0.222163
C	-1.291340	2.419088	-0.823242	H	3.328496	1.305117	0.824404
F	-0.948375	3.545291	-1.461185	O	0.969168	-0.551160	-1.836025
F	-2.279137	1.822064	-1.520869	Cl	-5.529285	-1.518546	-0.283682
F	-1.836219	2.769648	0.372192	C	-0.554392	3.245871	-0.695295
				H	-1.483024	3.562091	-1.184375
14R				C	-0.517403	3.811859	0.729587
C	1.567301	0.060000	-0.966075	H	-0.562213	4.905734	0.688713
C	0.839832	1.160866	-0.171843	H	-1.355006	3.474926	1.343892
H	1.549475	1.988397	-0.066986	H	0.406714	3.549947	1.257644
C	-0.415550	1.713773	-0.905044	H	-0.167577	1.597894	-1.965188
C	-1.698704	0.923809	-0.709096	H	0.261697	3.717469	-1.260275
C	-2.512368	1.047290	0.424814	S	0.589236	0.685398	1.602936
H	-2.230173	1.710312	1.230927	C	0.260436	-1.110385	1.537496
C	-3.684880	0.305702	0.562193	F	1.354366	-1.829839	1.222451
H	-4.302287	0.407652	1.447901	F	-0.118873	-1.461665	2.778494
C	-4.053941	-0.574517	-0.450031	F	-0.700310	-1.463615	0.678896
C	-3.271177	-0.718004	-1.592475				
H	-3.568044	-1.408720	-2.374008				
C	-2.104428	0.032667	-1.710846				

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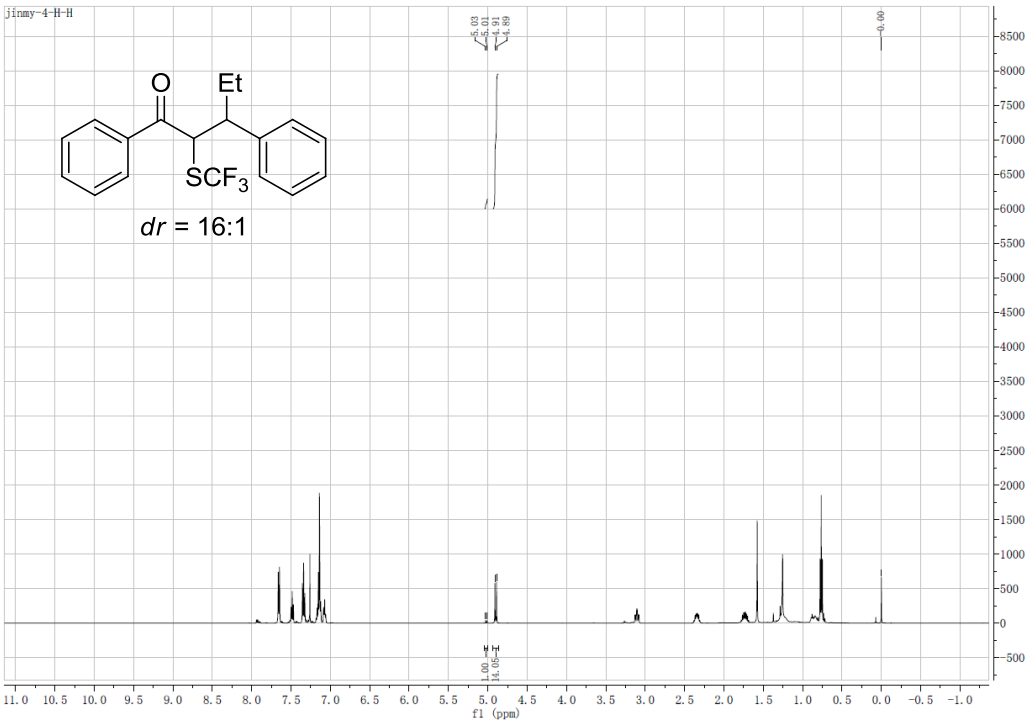
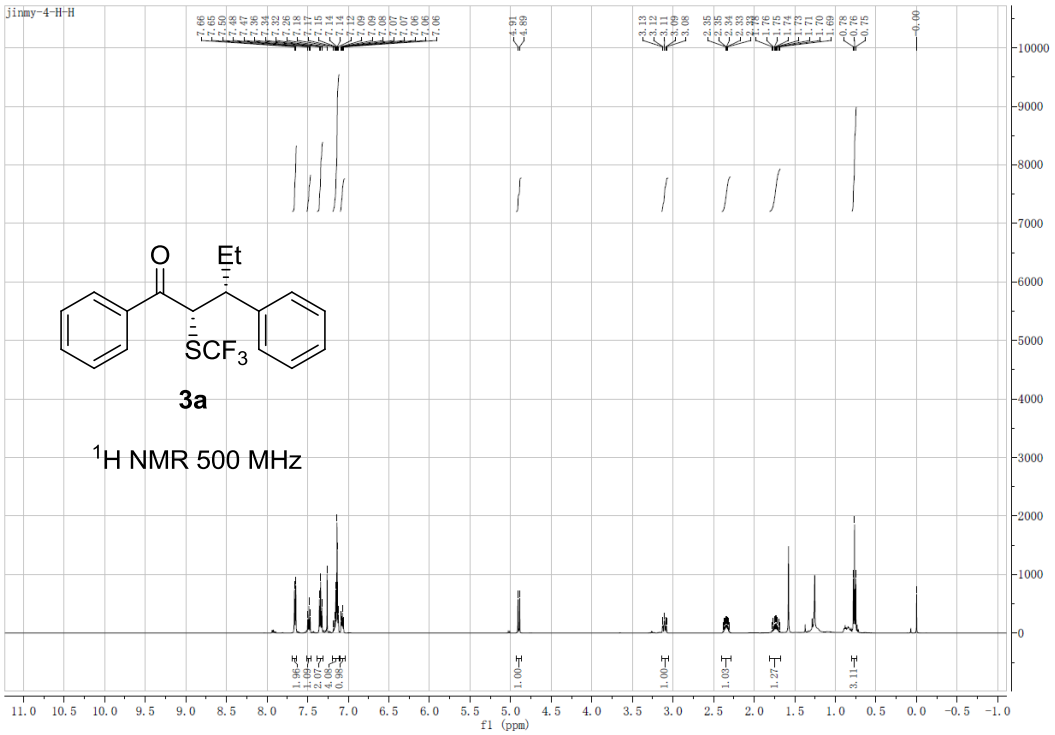
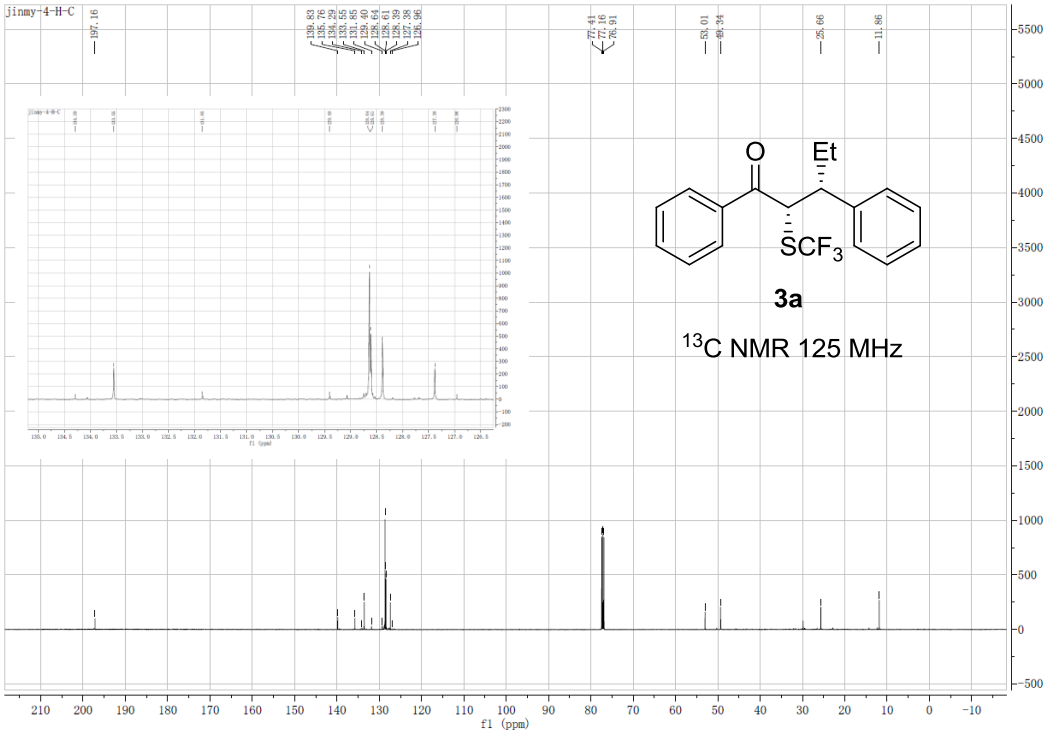
^{1}H NMR, ^{13}C NMR, ^{19}F NMR and HPLC Spectra



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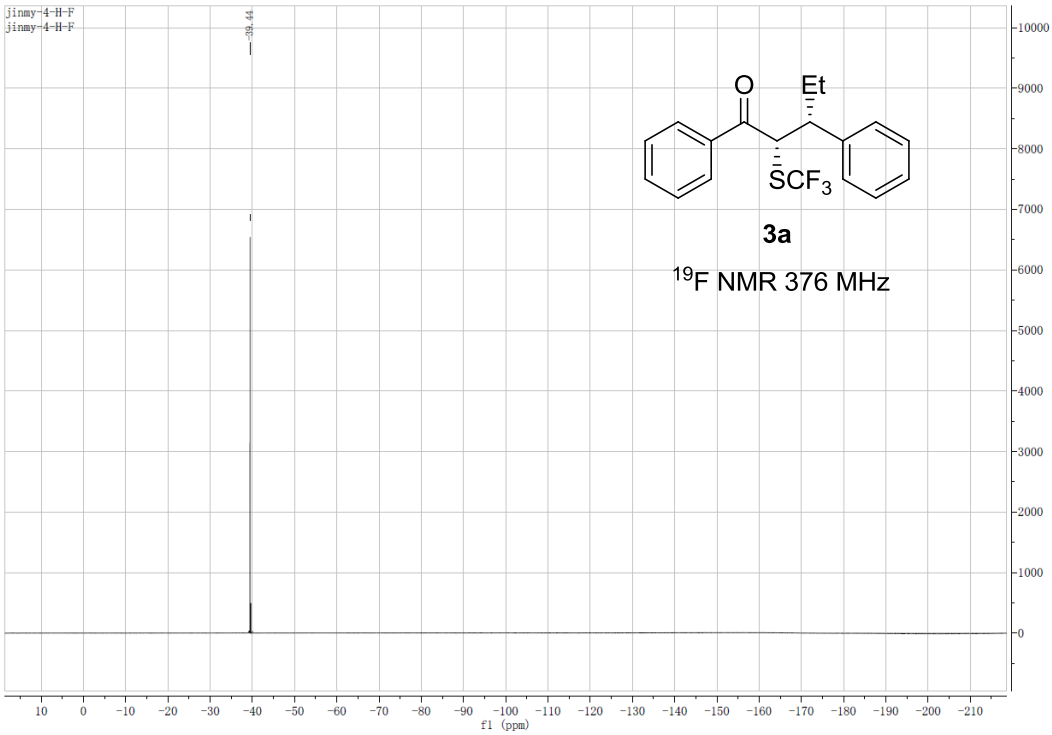
O
Et
SCF3
3a
13C NMR 125 MHz
f1 (ppm)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jinmy-4-H-F
O
Et
SCF3
3a
19F NMR 376 MHz
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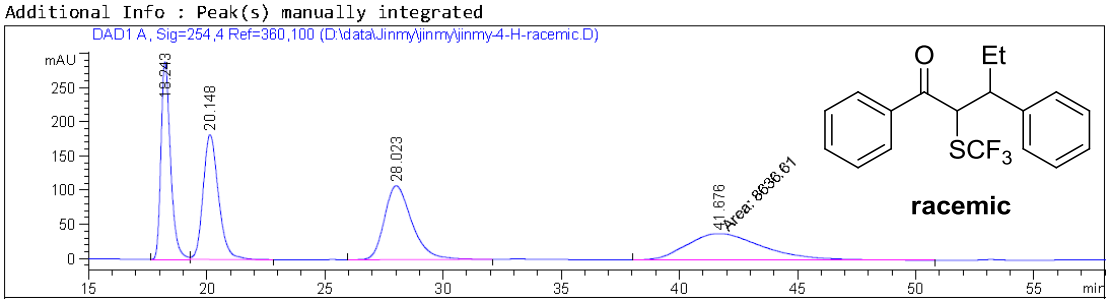
Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

Additional Info : Peak(s) manually integrated

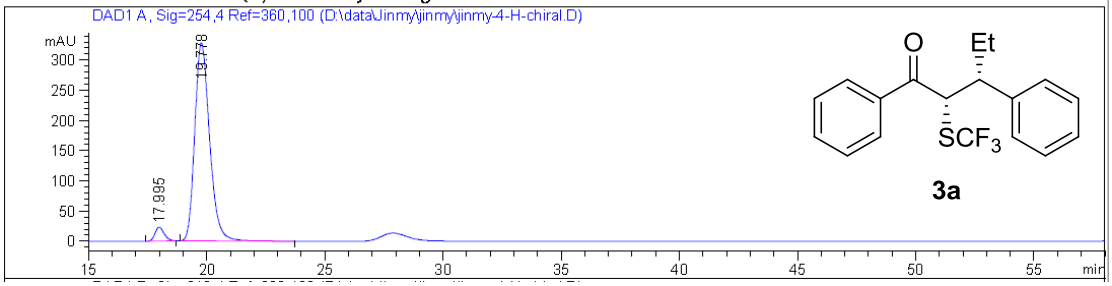


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.243	BV	0.4311	8139.96143	288.60196	24.1202
2	20.148	VB	0.6969	8266.49219	182.34087	24.4951
3	28.023	BB	1.2359	8704.40820	107.59158	25.7928
4	41.676	MM	3.7183	8636.61035	38.71251	25.5919
Totals :				3.37475e4	617.24691	

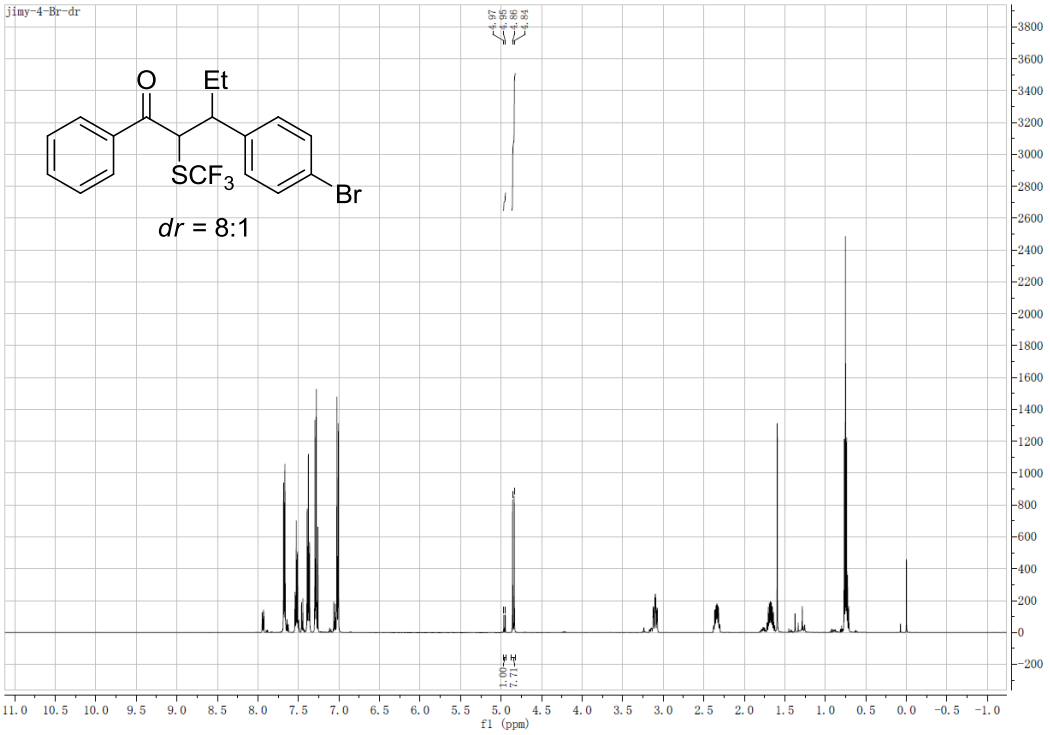
Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

Additional Info : Peak(s) manually integrated



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.995	BB	0.4109	609.71539	22.88046	4.0967
2	19.778	BB	0.6697	1.42732e4	327.97577	95.9033
Totals :				1.48829e4	350.85623	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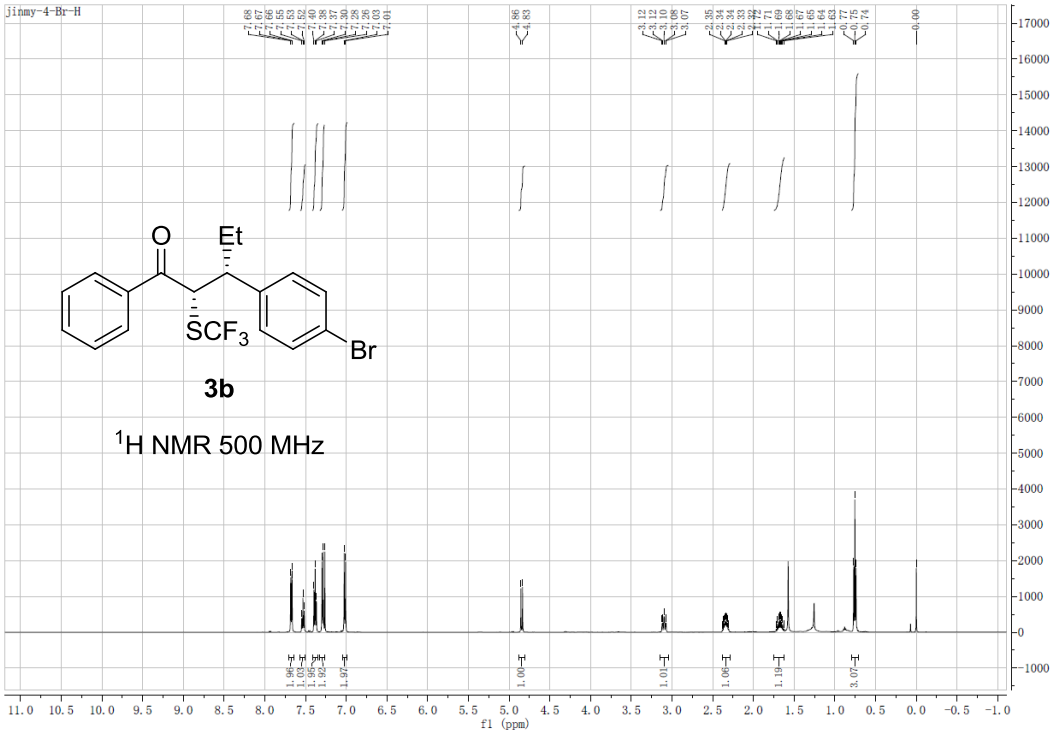
Et
SCF3
Br
dr = 8:1
f1 (ppm)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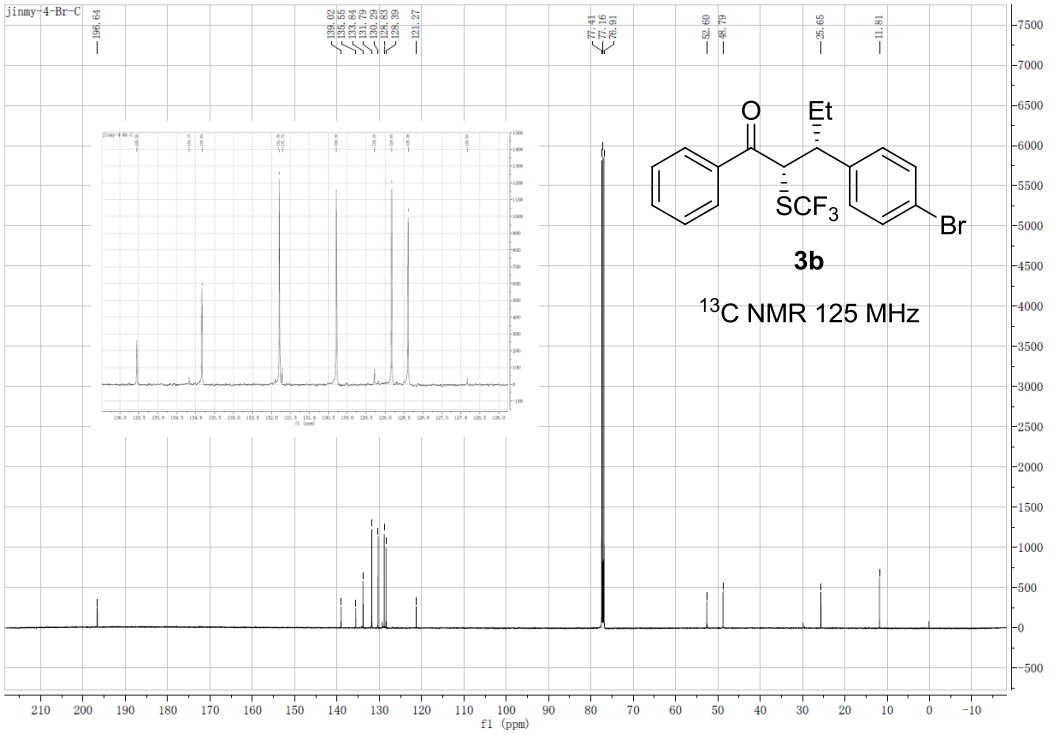
O
Et
SCF3
Br
3b
1H NMR 500 MHz
f1 (ppm)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133.95
131.84
131.79
130.29
128.83
128.39
121.27
77.41
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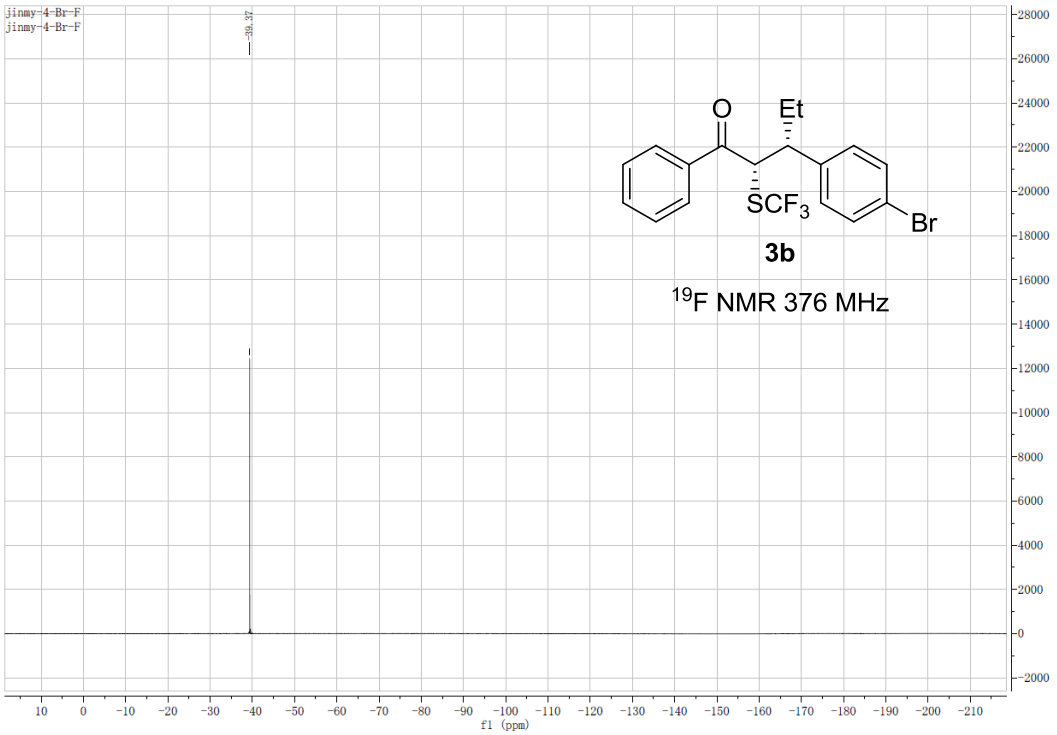
76.91
52.60
48.79
25.65
11.81
O
Et
SCF3
Br
3b
13C NMR 125 MHz
f1 (ppm)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3b
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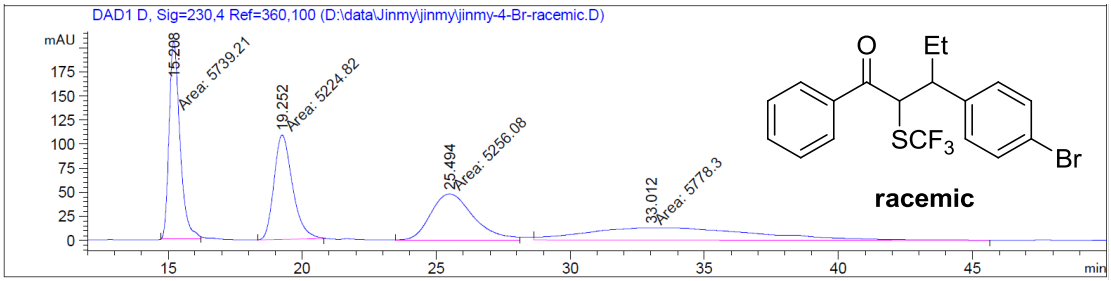
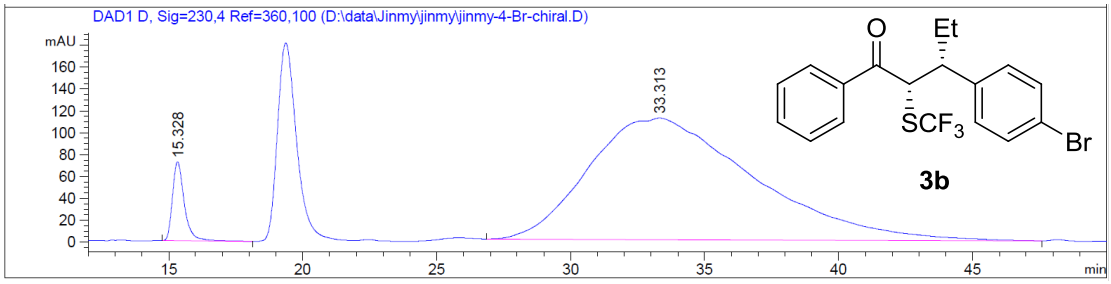
f1 (ppm)



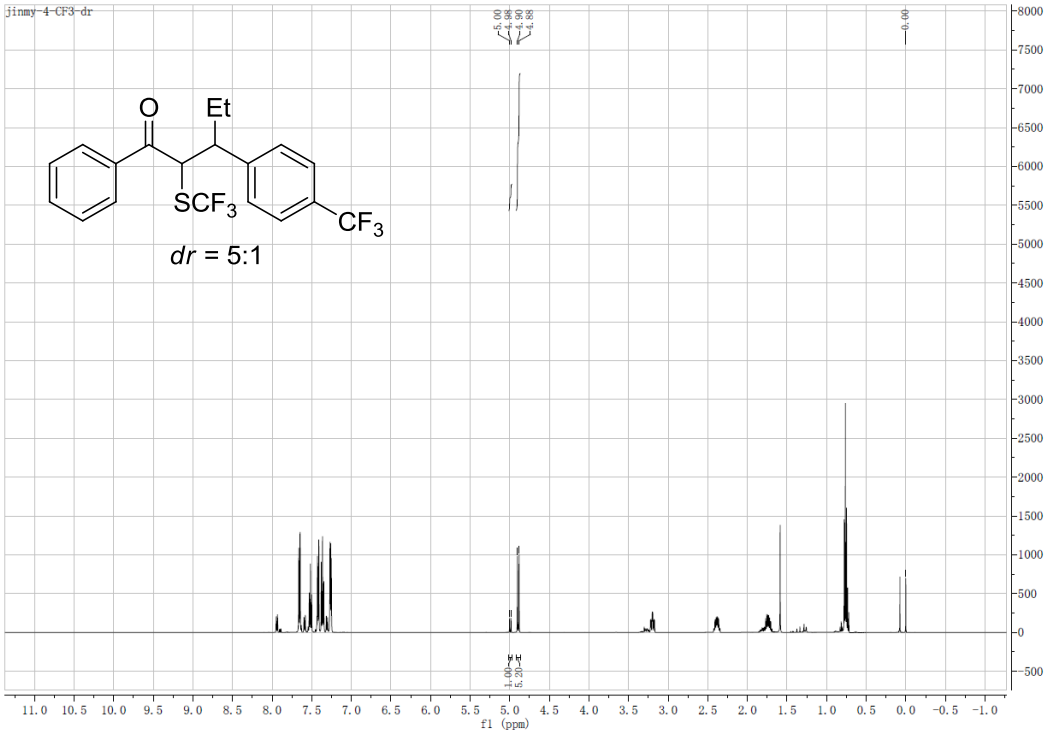
Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.208	MM	0.4679	5739.21289	204.41205	26.0892
2	19.252	MM	0.8020	5224.81934	108.58484	23.7509
3	25.494	MM	1.8419	5256.07666	47.55970	23.8930
4	33.012	MM	7.4654	5778.29834	12.90022	26.2669
Totals :				2.19984e4	373.45681	



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.328	BB	0.4664	2215.03394	72.11260	4.4500
2	33.313	BB	5.1608	4.75613e4	111.09157	95.5500
Totals :				4.97764e4	183.20417	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Et
SCF3
CF3
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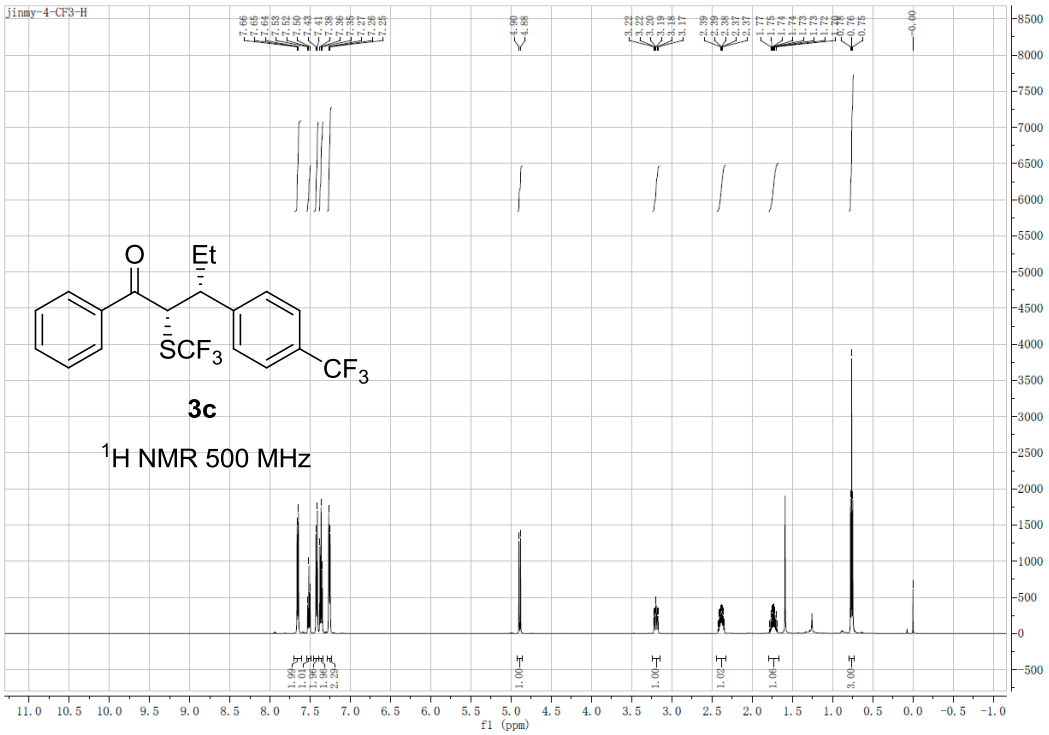
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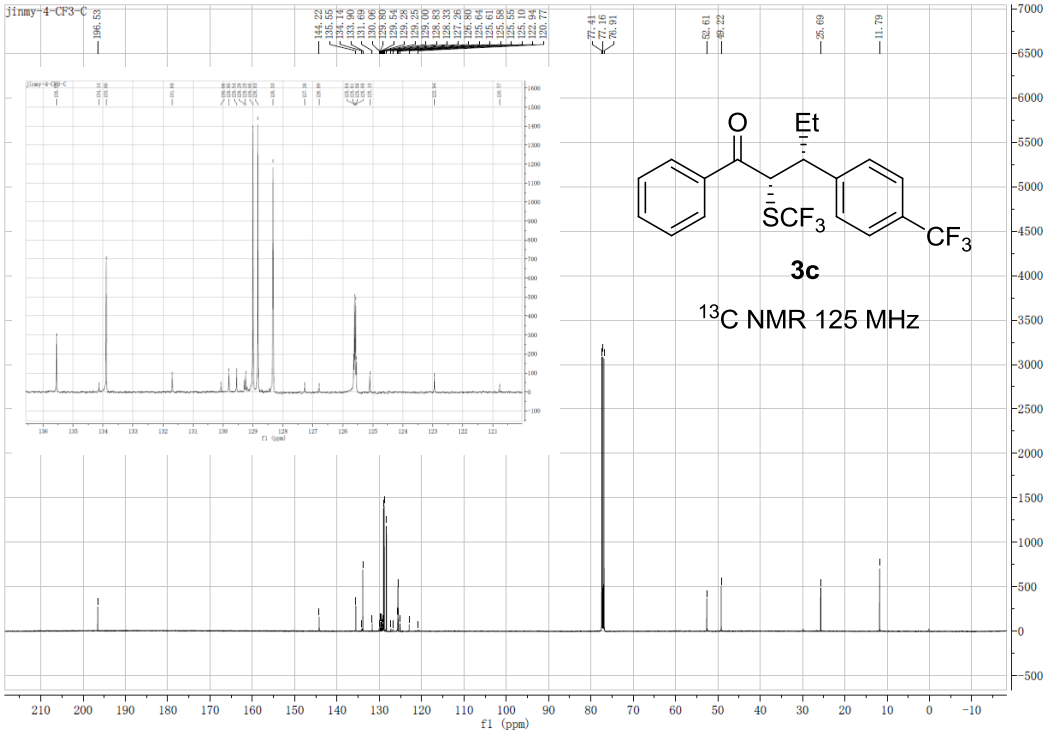
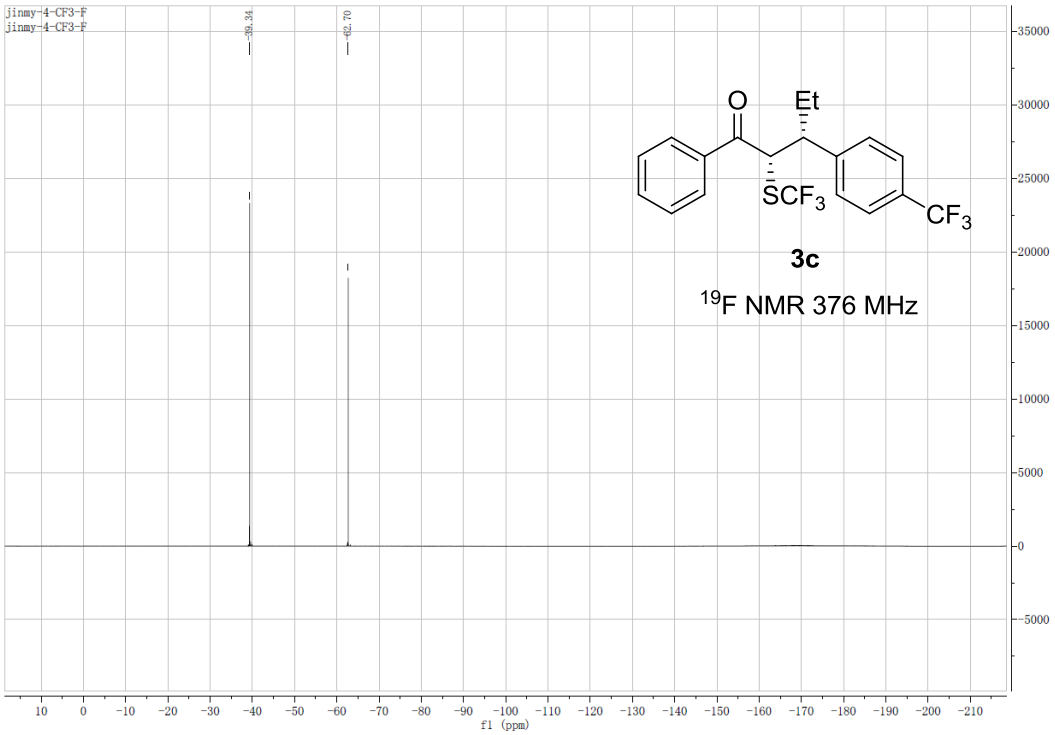
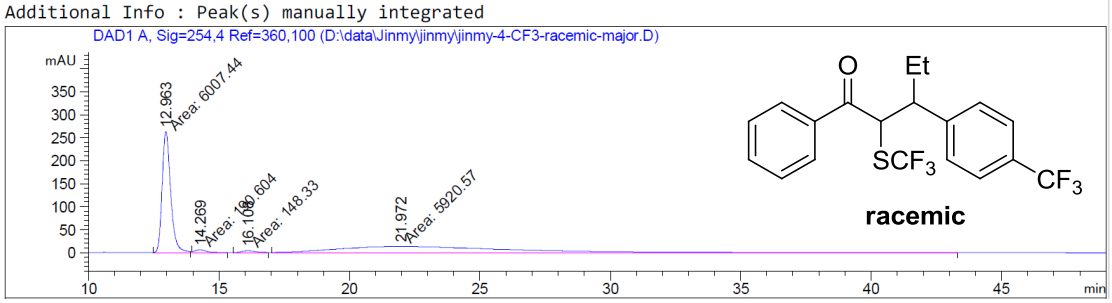
Et
SCF3
CF3
3c
1H NMR 500 MHz
f1 (ppm)


jinmy-4-CF3-C
O
Et
SCF3
CF3
3c
13C NMR 125 MHz
f1 (ppm)


jinmy-4-CF3-F
jinmy-4-CF3-F
O
Et
SCF3
CF3
3c
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, iPA:Hex=1:99, Flow: 1.0ml/min

Additional Info : Peak(s) manually integrated

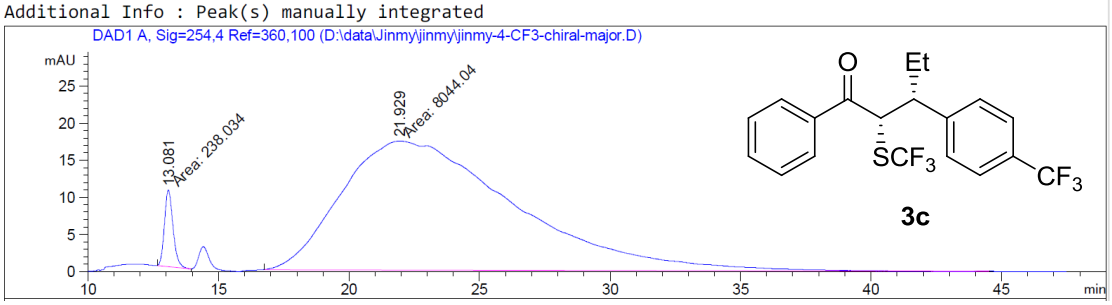


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.963	MM	0.3799	6007.44092	263.54495	48.9726
2	14.269	MM	0.5231	190.60379	6.07285	1.5538
3	16.108	MM	0.6411	148.33015	3.85584	1.2092
4	21.972	MM	7.4496	5920.57031	13.24587	48.2644
Totals :				1.22669e4	286.71952	

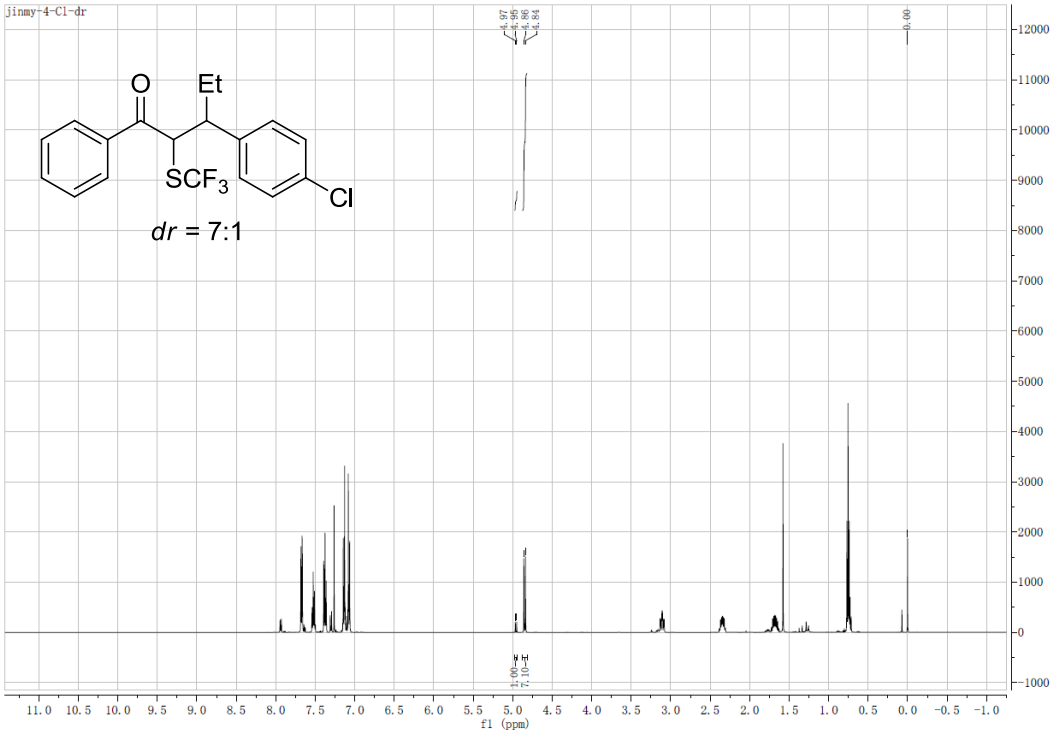
Sample Info : OJ-3, three combined, iPA:Hex=1:99, Flow: 1.0ml/min

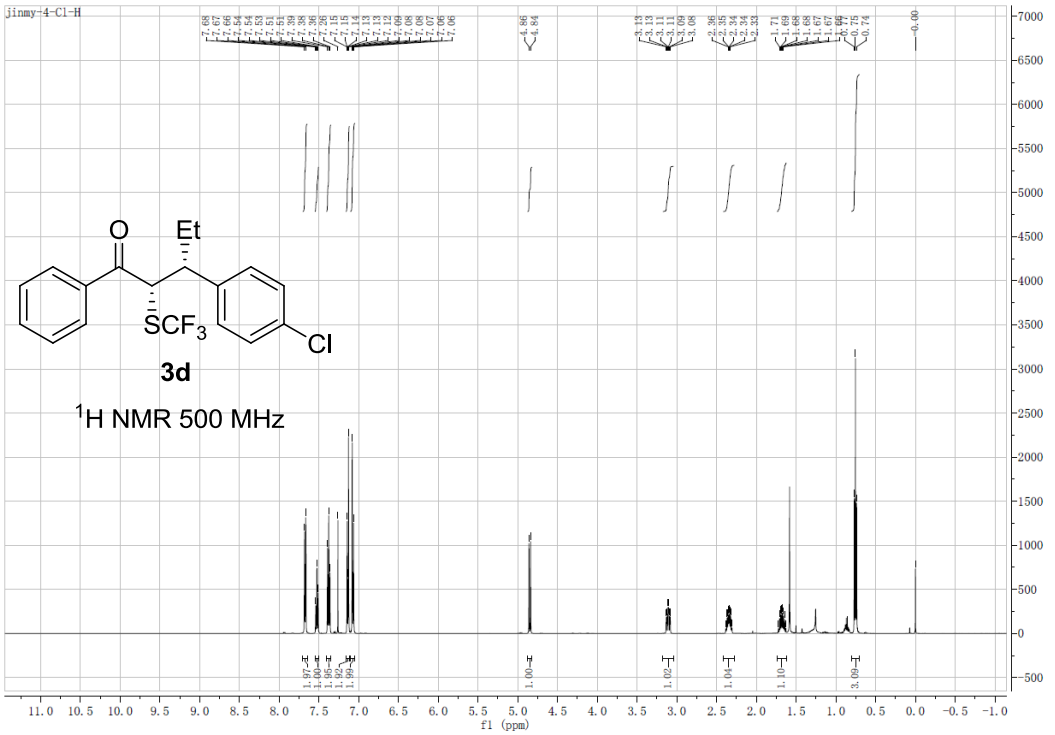
Additional Info : Peak(s) manually integrated

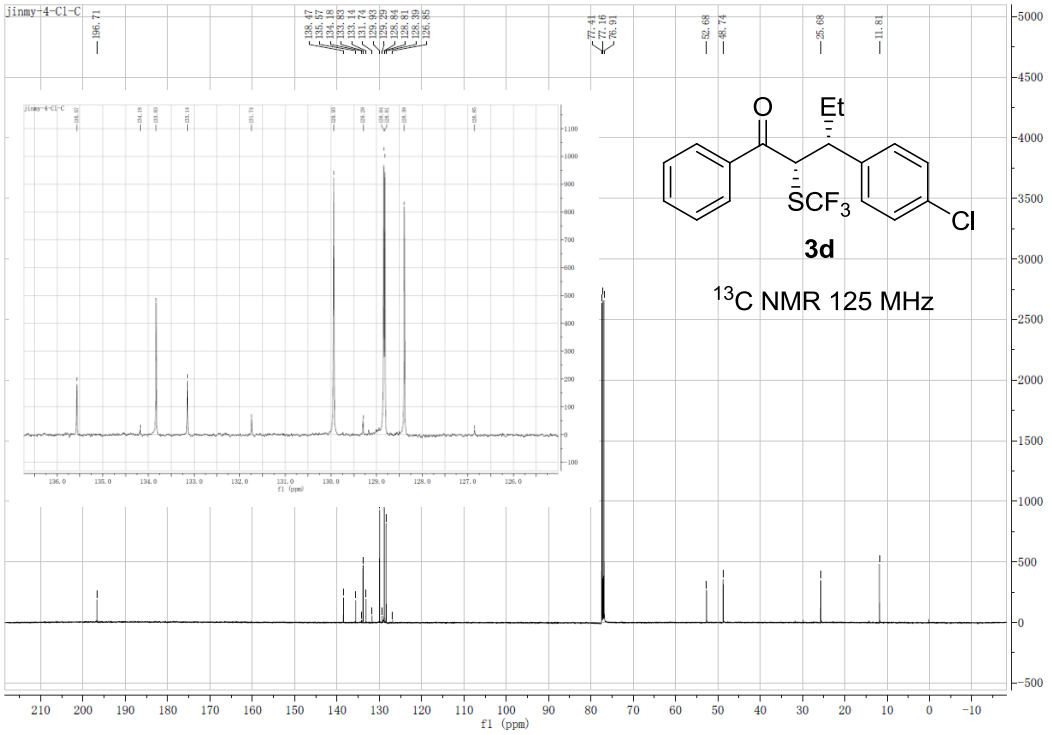


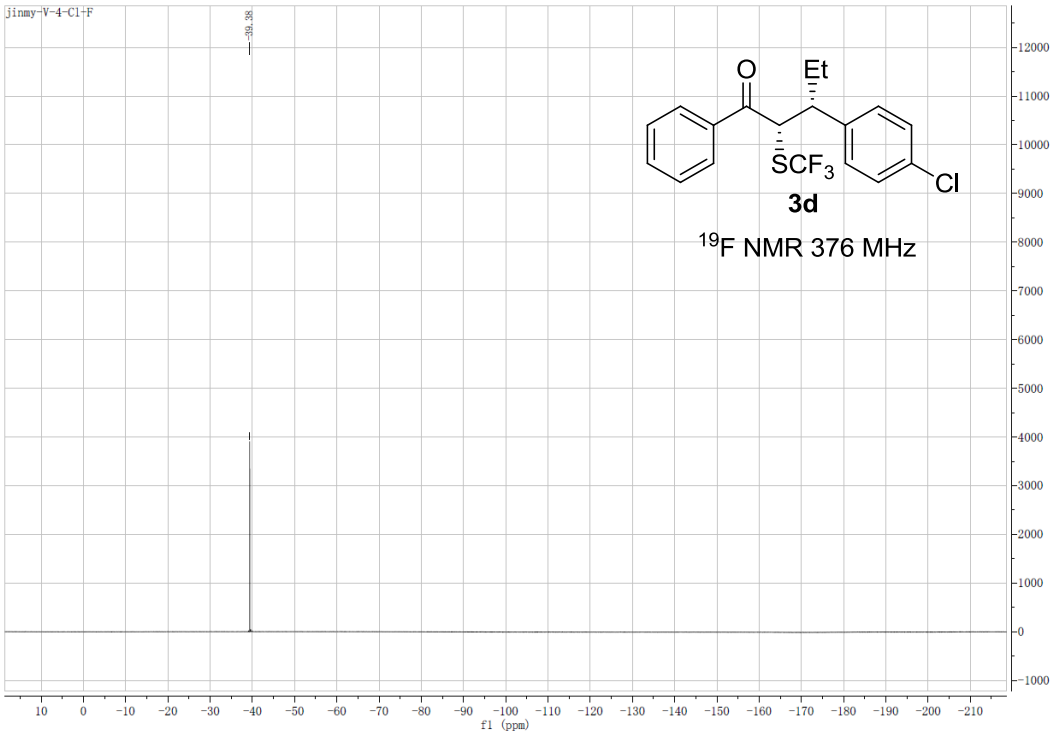
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.081	MM	0.3830	238.03368	10.35817	2.8741
2	21.929	MM	7.7026	8044.03906	17.40554	97.1259
Totals :				8282.07274	27.76372	


jinmy-4-Cl-dr
O
Et
SCF3
Cl
dr = 7:1
f1 (ppm)

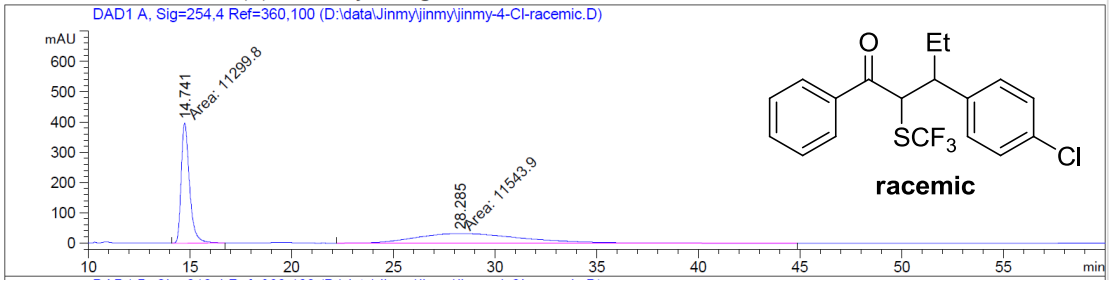

jinmy-4-Cl-H
O
Et
SCF3
Cl
3d
1H NMR 500 MHz
f1 (ppm)


jinmy-4-Cl-C
O
Et
SCF3
Cl
3d
13C NMR 125 MHz
f1 (ppm)


jinmy-V-4-Cl+F
-39.38
O
Et
SCF3
Cl
3d
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, IPALHEX=1:99, Flow: 1.0mL/min

Additional Info : Peak(s) manually integrated

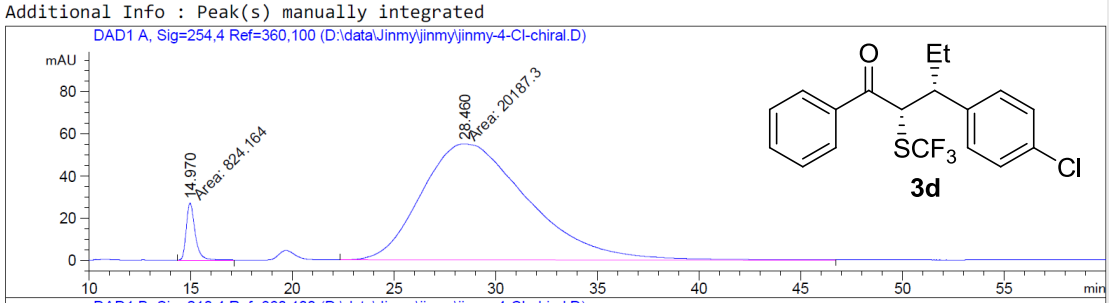


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.741	MM	0.4754	1.12998e4	396.12329	49.4657
2	28.285	MM	6.0306	1.15439e4	31.90364	50.5343
Totals :				2.28437e4	428.02693	

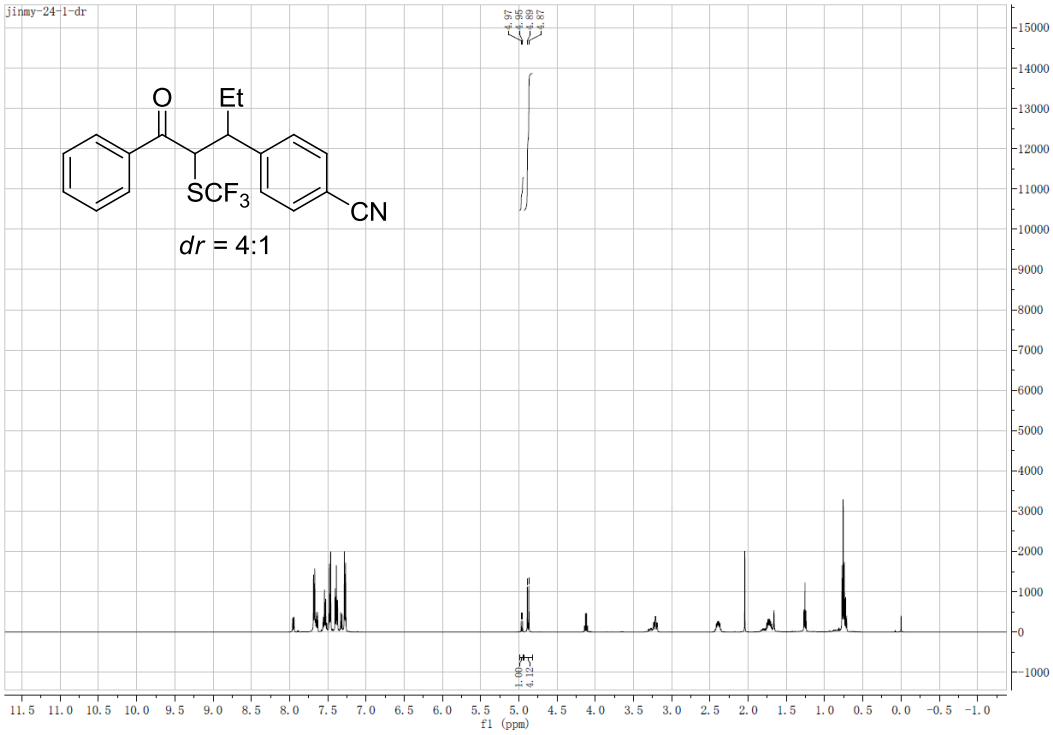
Sample Info : OJ-3, three combined, IPALHEX=1:99, Flow: 1.0mL/min

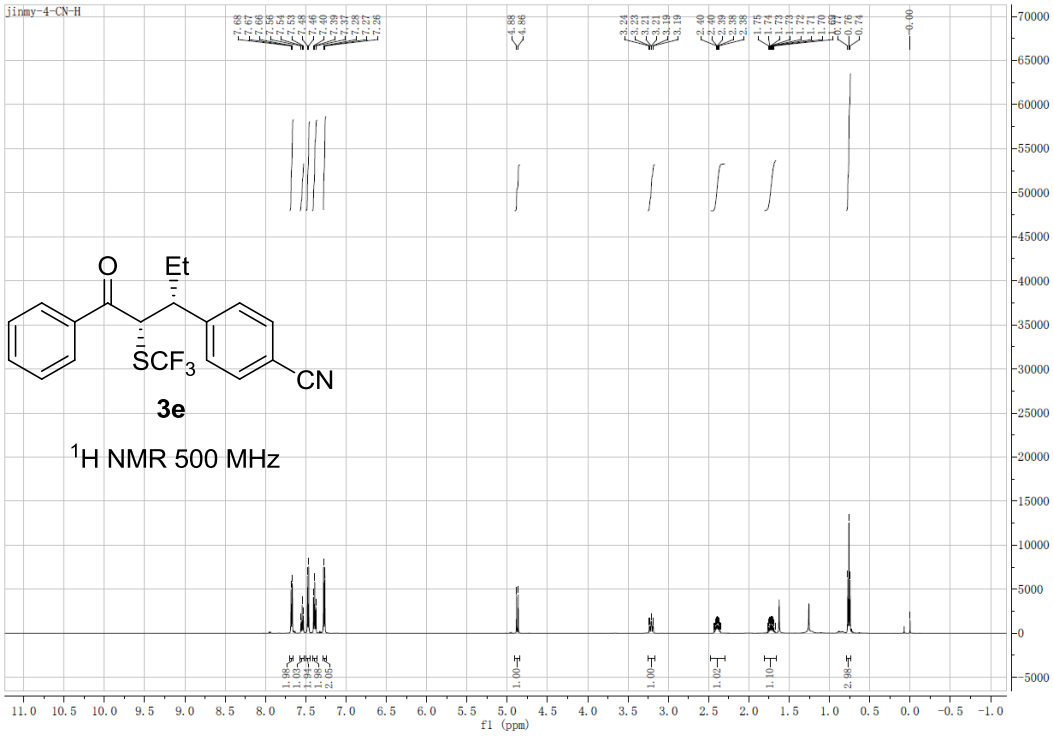
Additional Info : Peak(s) manually integrated

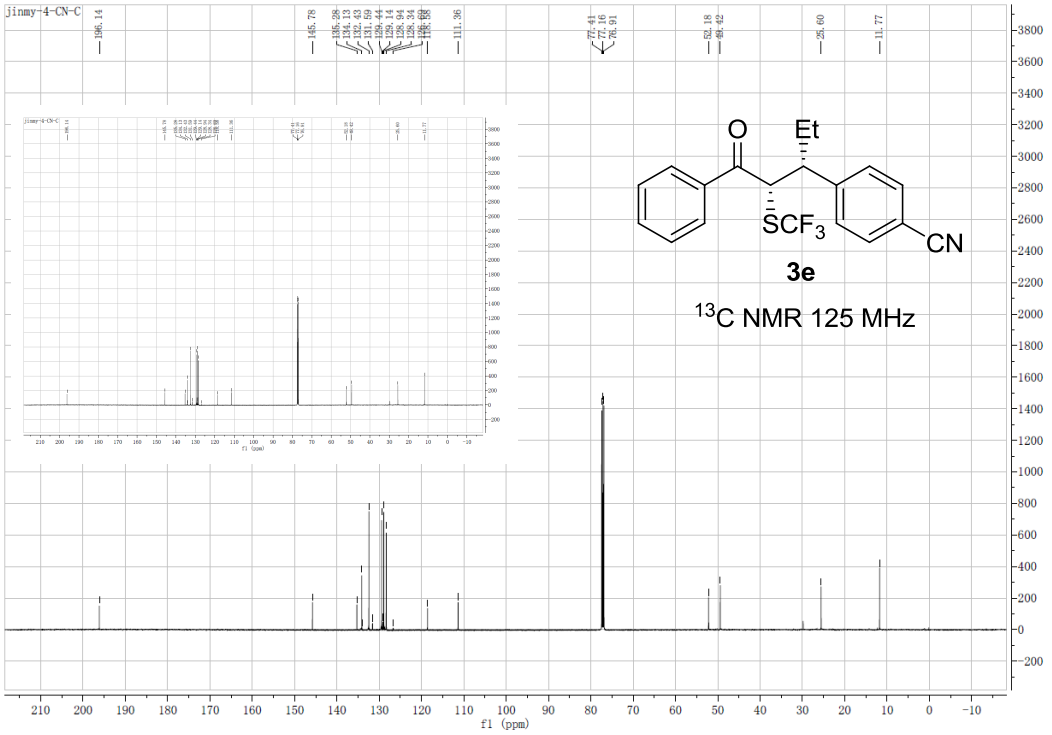


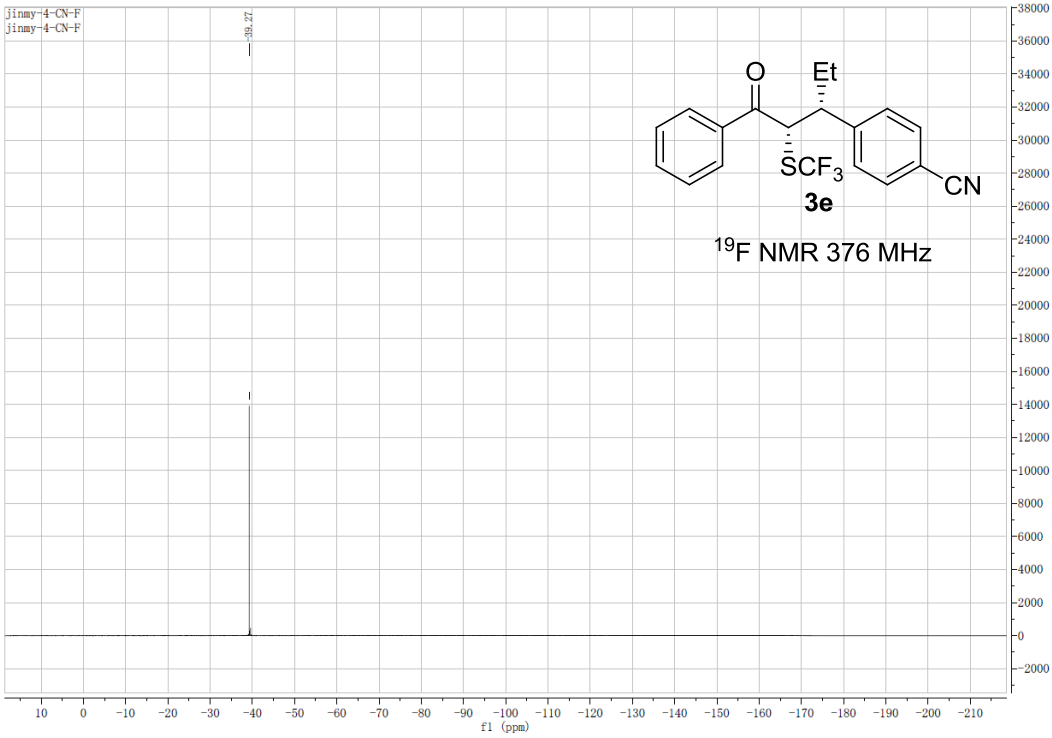
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.970	MM	0.5047	824.16357	27.21499	3.9224
2	28.460	MM	6.1068	2.01873e4	55.09532	96.0776
Totals :				2.10115e4	82.31031	


jinmy-24-1-dr
O
Et
SCF3
CN
dr = 4:1
f1 (ppm)

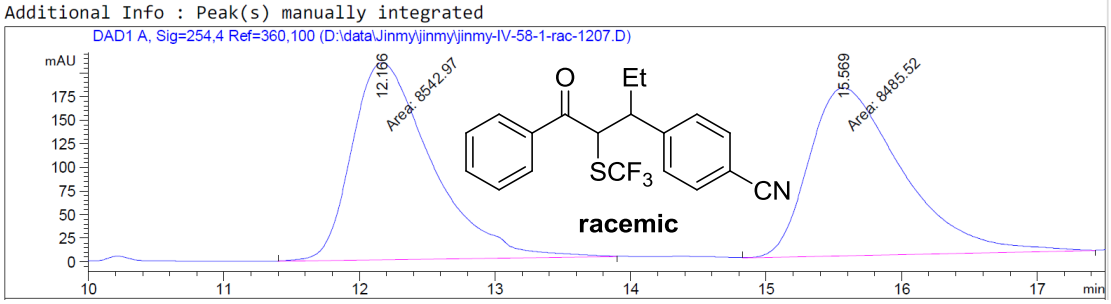

jinmy-4-CN-H
O
Et
SCF3
CN
3e
1H NMR 500 MHz
f1 (ppm)


jinmy-4-CN-C
O
Et
SCF3
CN
3e
13C NMR 125 MHz
f1 (ppm)


jinmy-4-CN-F
jinmy-4-CN-F
O
Et
SCF3
CN
3e
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, IPA:HEX=5:95, Flow=1.0mL/min

Additional Info : Peak(s) manually integrated

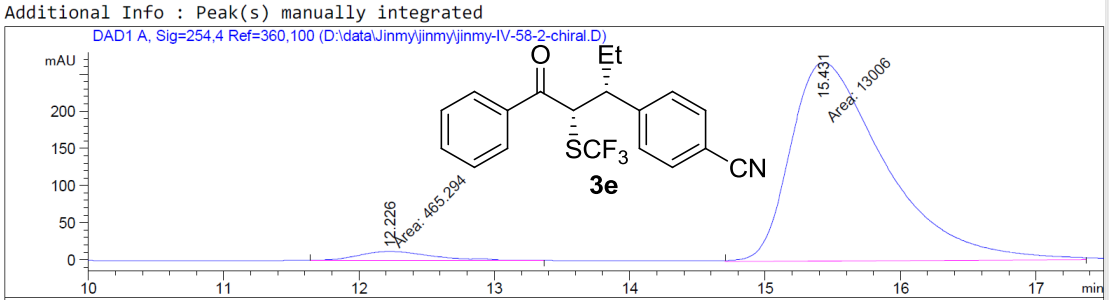


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.166	MM	0.6828	8542.96875	208.51917	50.1687
2	15.569	MM	0.7958	8485.51660	177.70700	49.8313
Totals :				1.70285e4	386.22617	

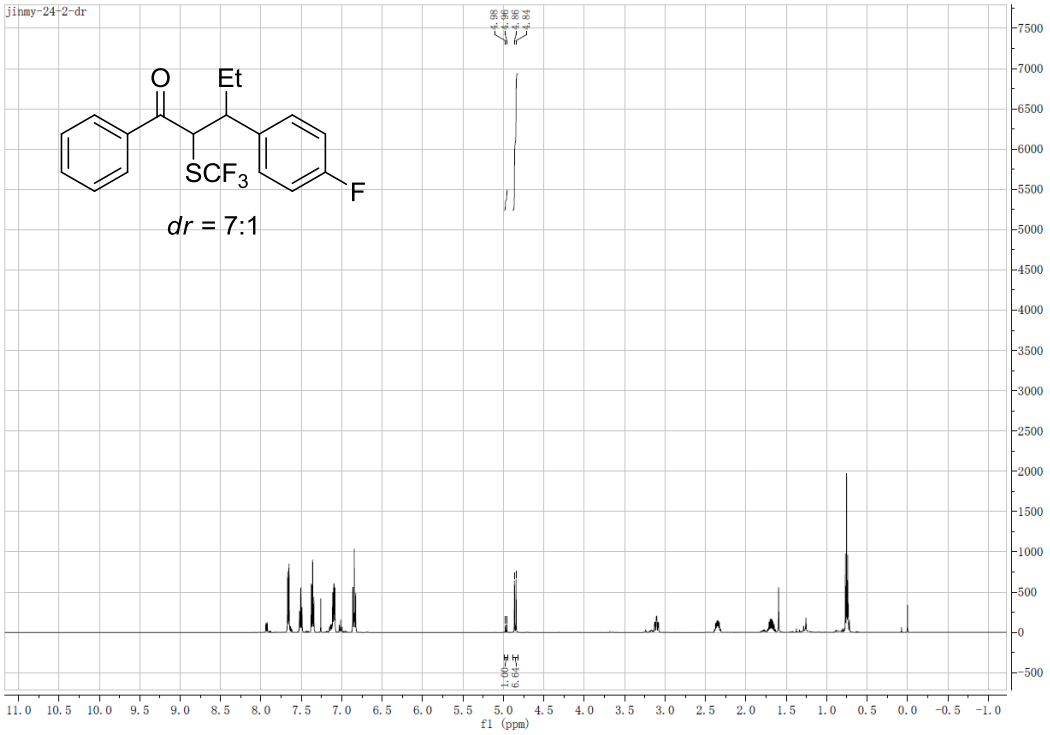
Sample Info : OJ-3, IPA:HEX=5:95, Flow=1.0mL/min

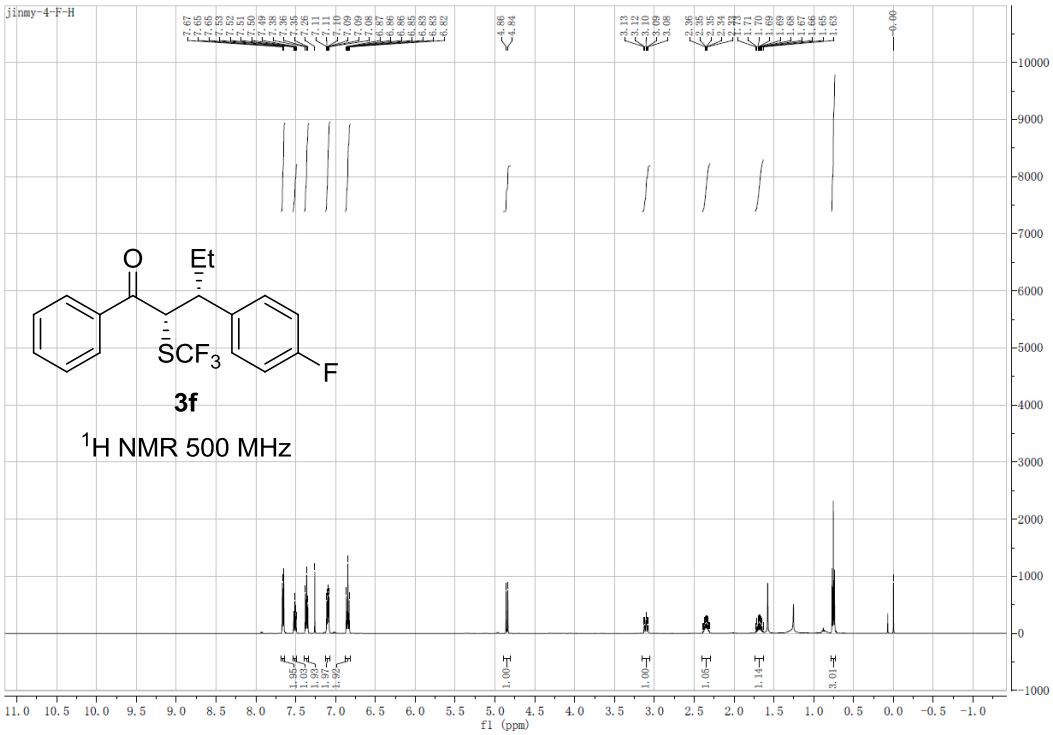
Additional Info : Peak(s) manually integrated

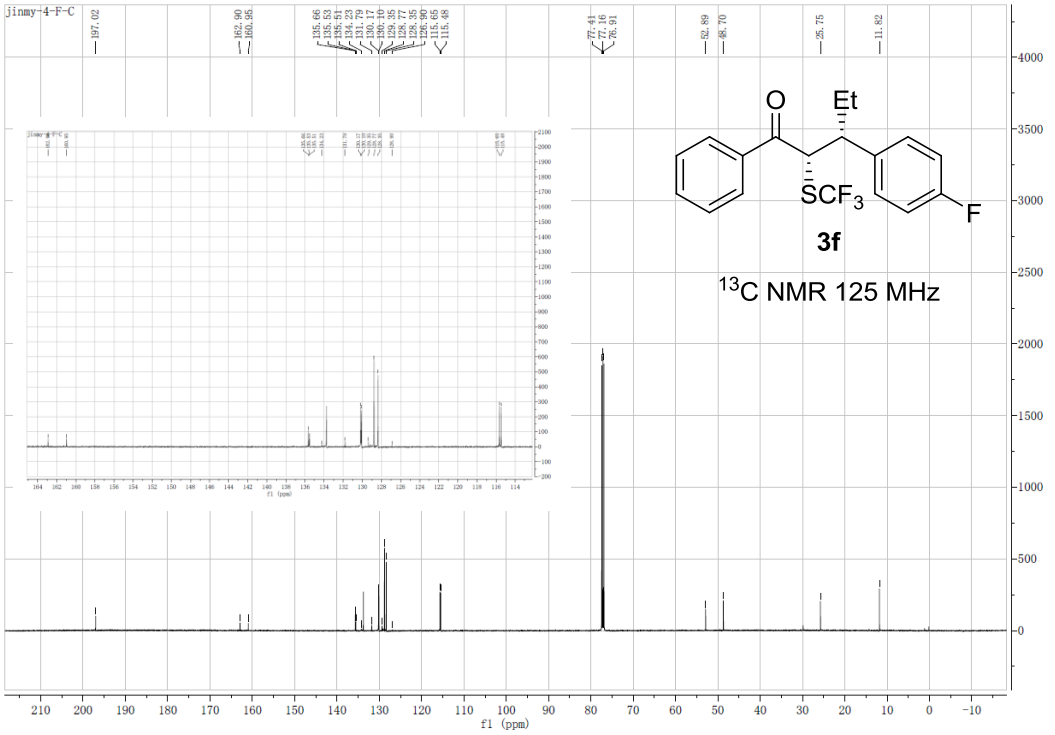


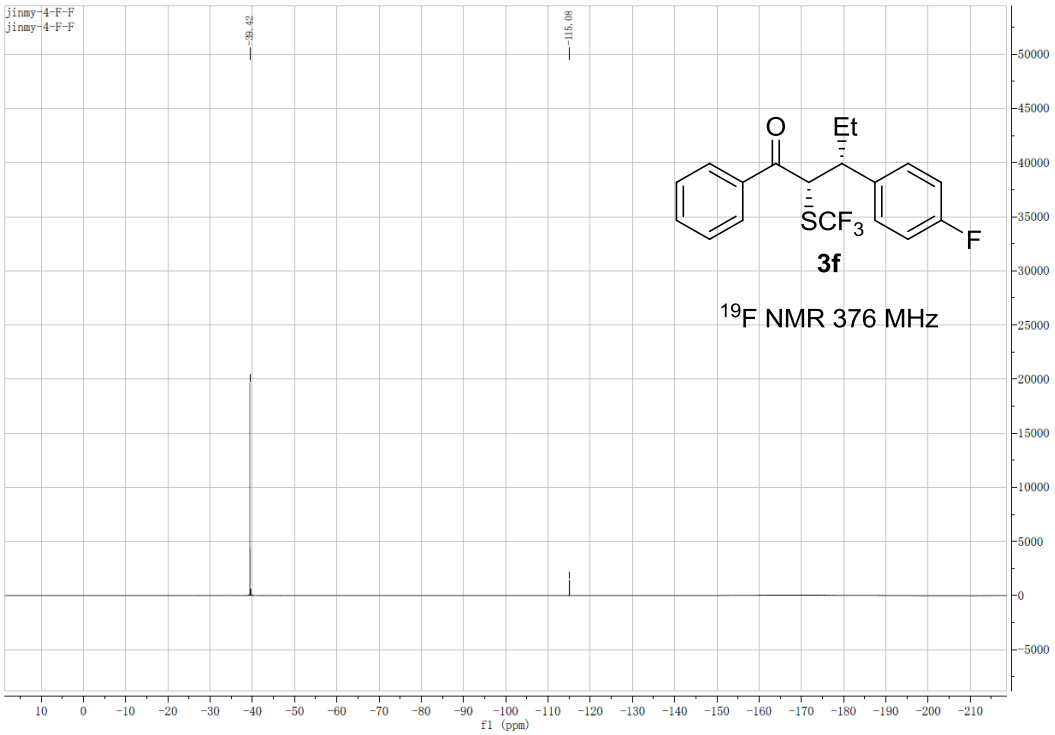
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.226	MM	0.6391	465.29370	12.13491	3.4540
2	15.431	MM	0.8097	1.30060e4	267.69907	96.5460
Totals :				1.34713e4	279.83397	


jinmy-24+2-dr
O
Et
SCF3
F
dr = 7:1
f1 (ppm)

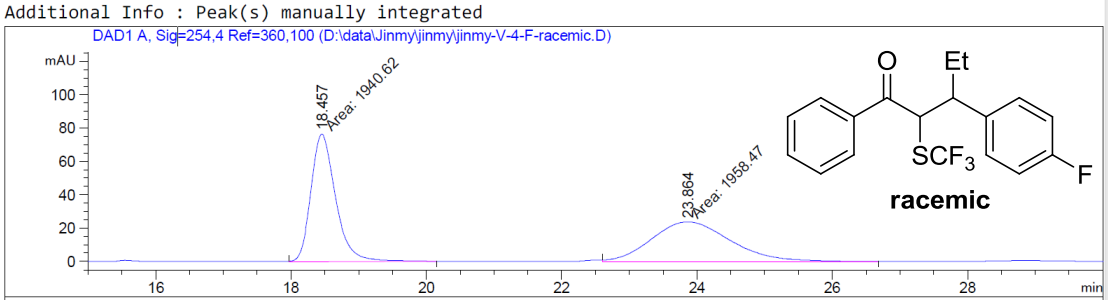

jinmy-4-F-H
O
Et
SCF3
F
3f
1H NMR 500 MHz
f1 (ppm)


jinmy-4-F-C
197.02
162.90
160.95
135.66
135.63
135.51
134.23
131.79
130.17
130.09
129.35
128.77
128.35
126.69
115.65
115.48
77.41
77.16
76.91
52.89
48.70
25.75
11.82
O
Et
SCF3
F
3f
13C NMR 125 MHz
f1 (ppm)


jinmy-4-F-F
jinmy-4-F-F
-39.62
-115.08
O
Et
SCF3
F
3f
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined,IPA:HEX=1:99, Flow:1.0mL/min

Additional Info : Peak(s) manually integrated

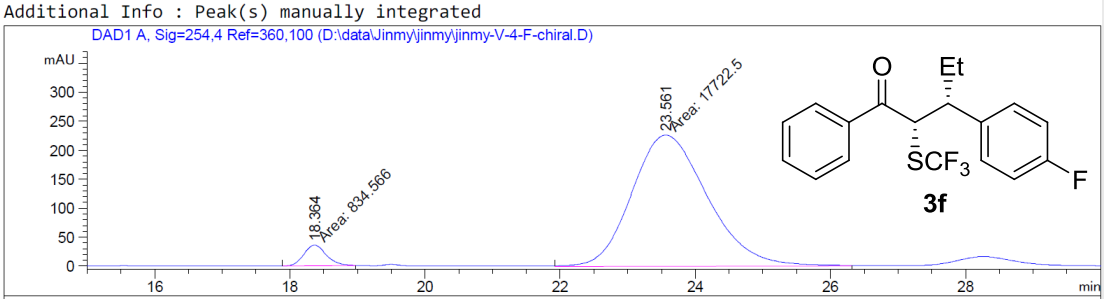


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.457	MM	0.4230	1940.62219	76.46241	49.7711
2	23.864	MM	1.3641	1958.46936	23.92804	50.2289
Totals :				3899.09155	100.39045	

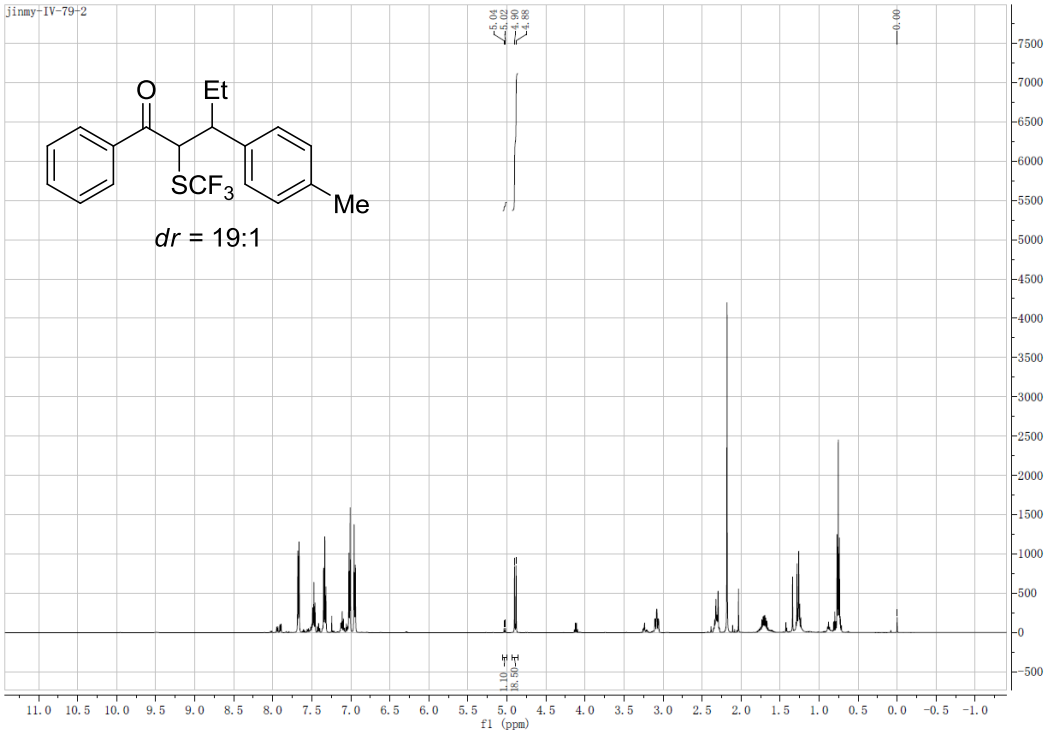
Sample Info : OJ-3, three combined,IPA:HEX=1:99, Flow:1.0mL/min

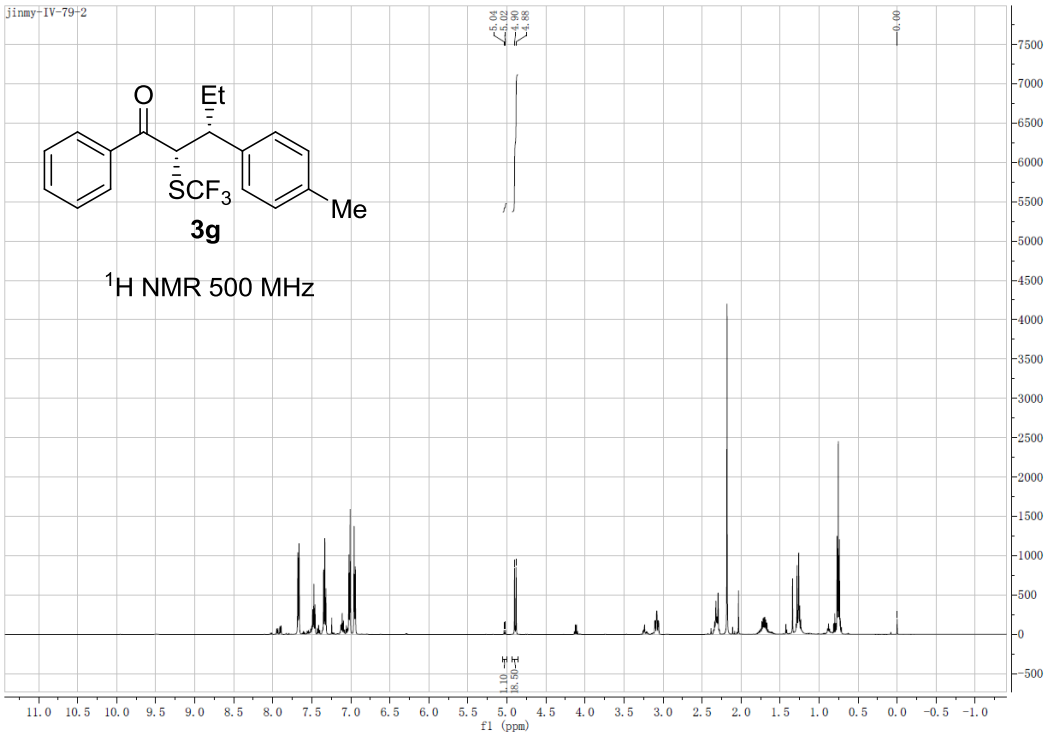
Additional Info : Peak(s) manually integrated

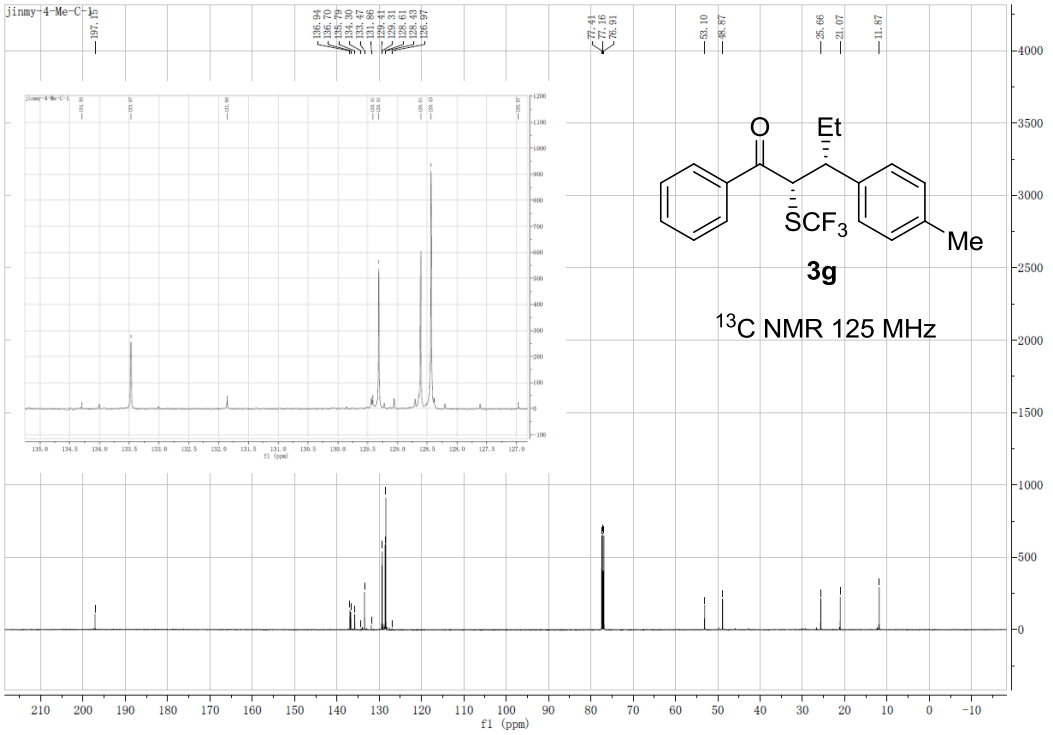


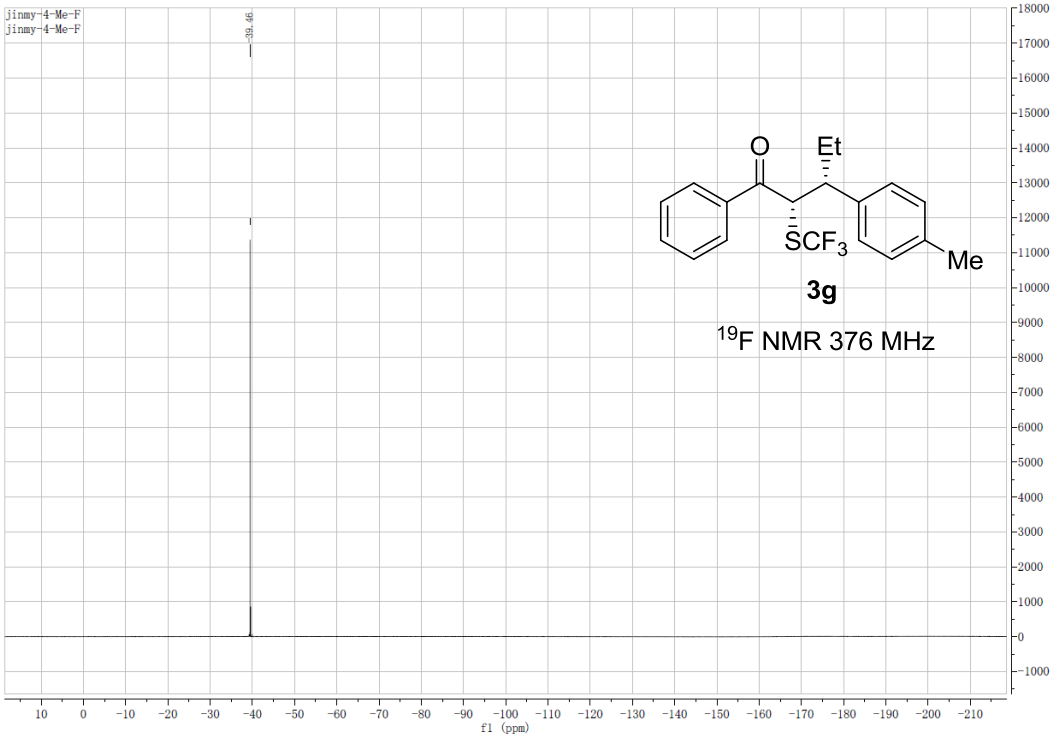
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.364	MM	0.3884	834.56567	35.81388	4.4973
2	23.561	MM	1.3027	1.77225e4	226.74712	95.5027
Totals :				1.85570e4	262.56100	


jinmy-IV-79-2
O
Et
SCF3
Me
dr = 19:1
f1 (ppm)

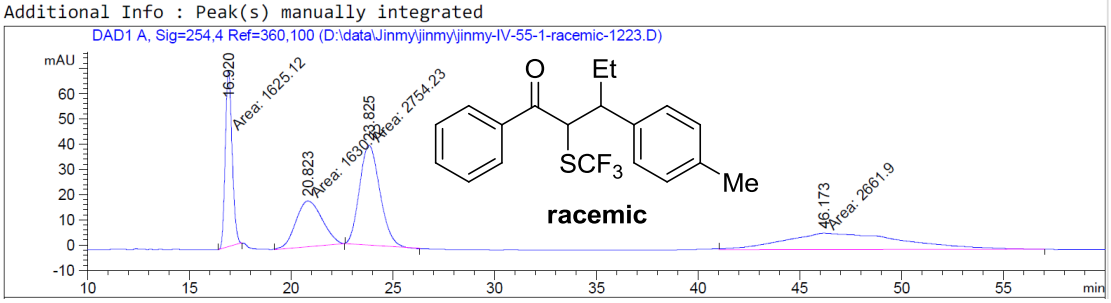

jinmy-IV-79-2
O
Et
SCF3
Me
3g
1H NMR 500 MHz
f1 (ppm)


jinmy-4-Me-C-1
197.15
136.94
135.70
135.29
134.30
133.47
131.96
129.31
128.61
128.43
126.97
77.41
77.16
76.91
53.10
46.87
25.66
21.07
11.87
O
Et
SCF3
Me
3g
13C NMR 125 MHz
f1 (ppm)


jinmy-4-Me-F
jinmy-4-Me-F
-39.46
O
Et
SCF3
Me
3g
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:1.0mL/min

Additional Info : Peak(s) manually integrated

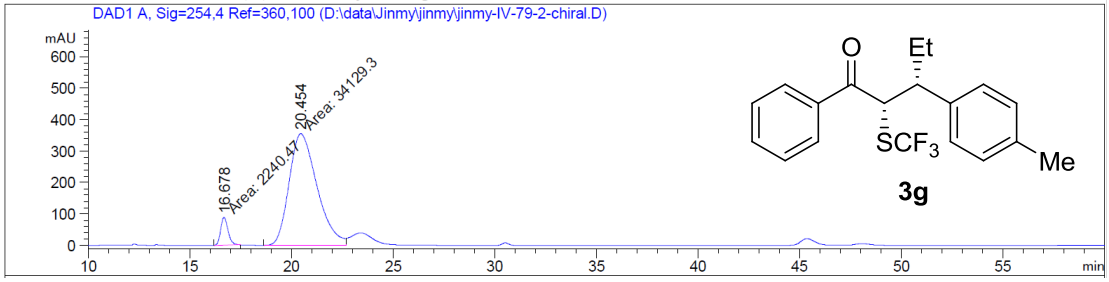


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.920	MM	0.3880	1625.11853	69.80933	18.7412
2	20.823	MM	1.5009	1630.12329	18.10116	18.7989
3	23.825	MM	1.1614	2754.23145	39.52479	31.7623
4	46.173	MM	6.8003	2661.90454	6.52399	30.6976
Totals :				8671.37781	133.95928	

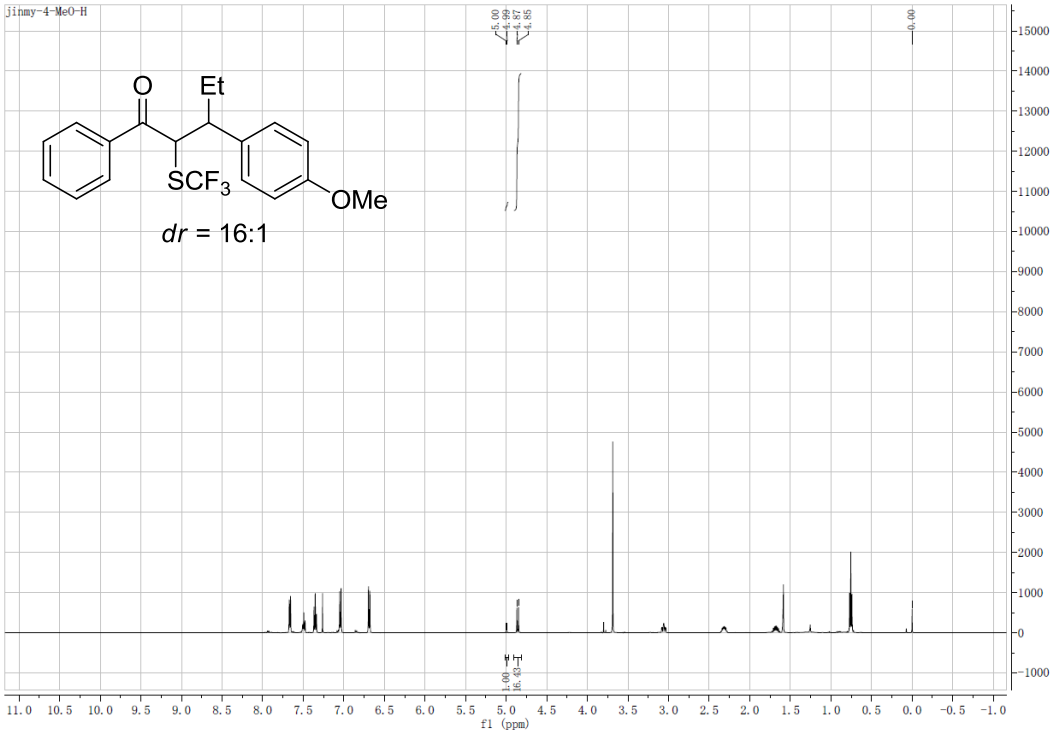
Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:1.0mL/min

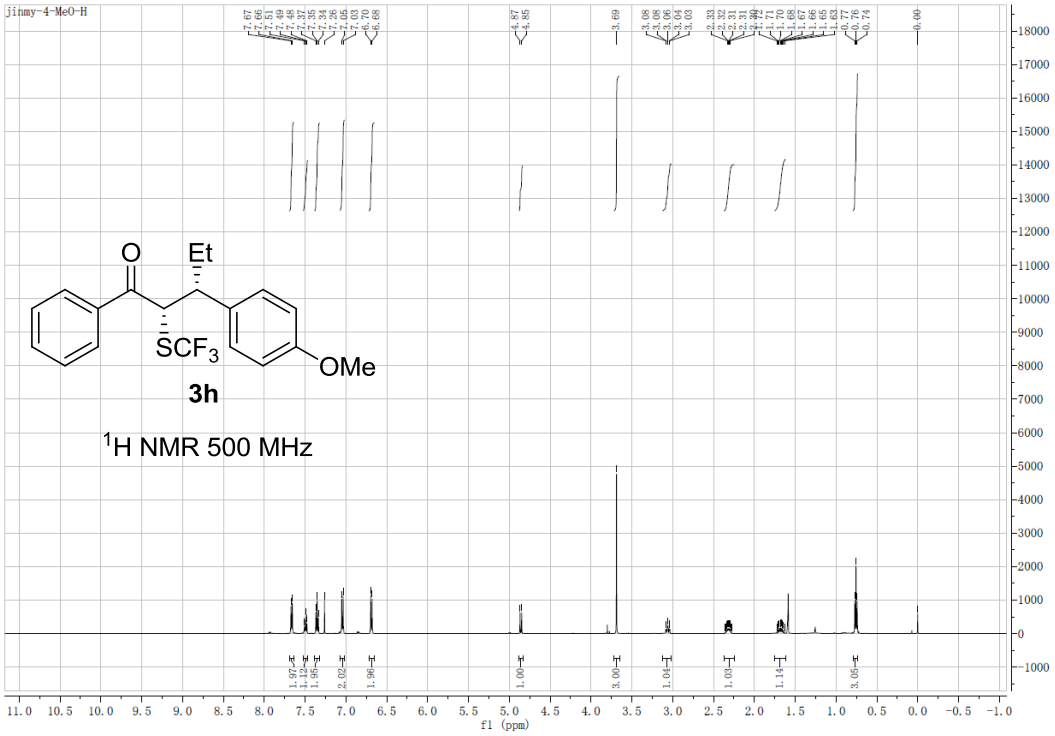
Additional Info : Peak(s) manually integrated

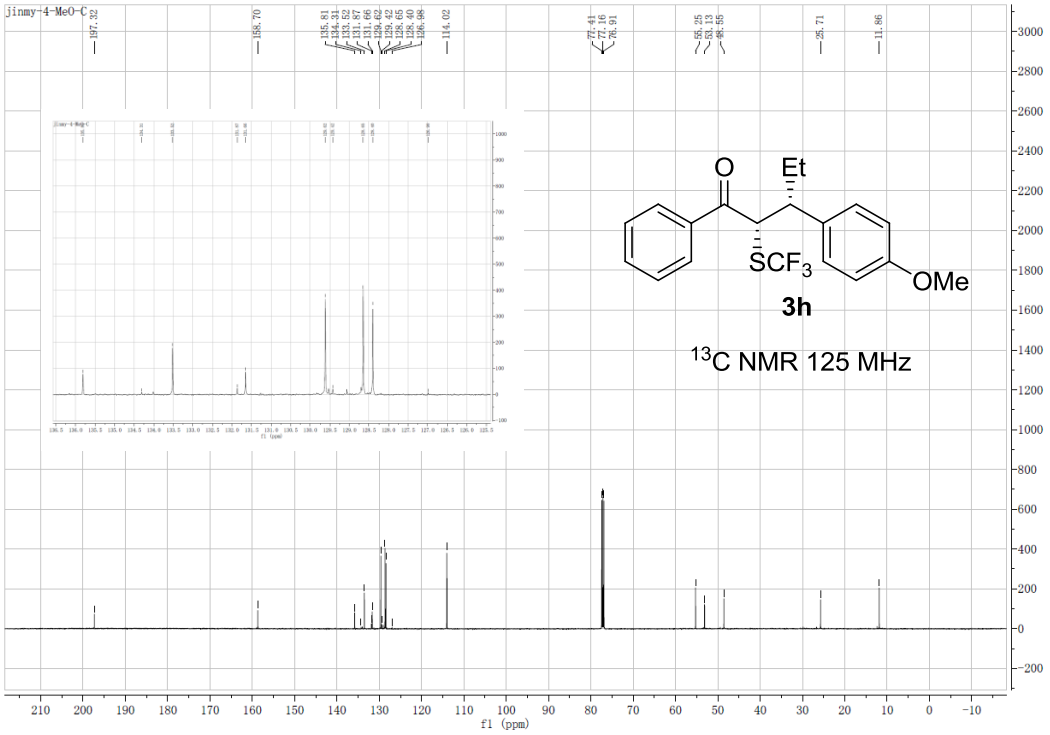


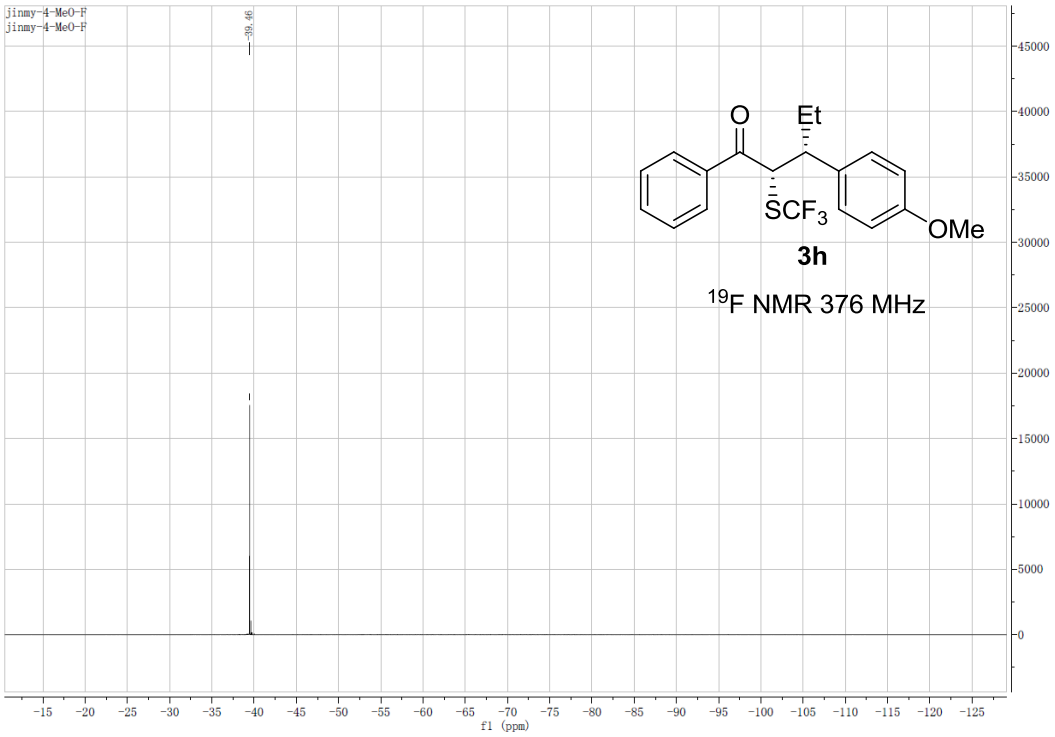
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.678	MM	0.4187	2240.46899	89.17694	6.1603
2	20.454	MM	1.5965	3.41293e4	356.29288	93.8397
Totals :				3.63698e4	445.46982	

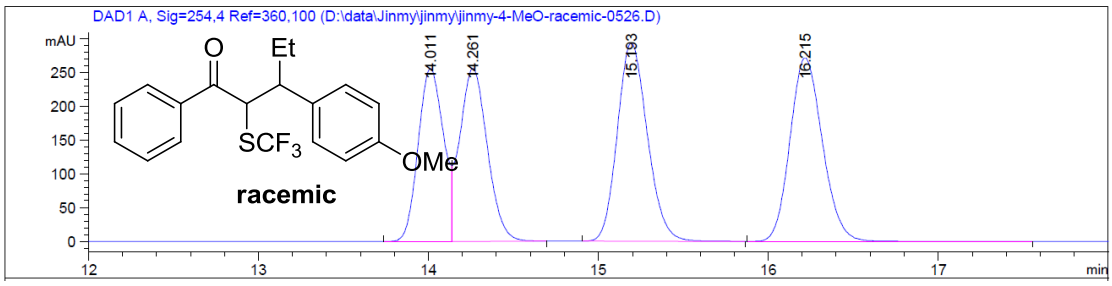

jinmy-4-MeO-H
O
Et
SCF3
OMe
dr = 16:1
f1 (ppm)


jinmy-4-MeO-H
O
Et
SCF3
OMe
3h
1H NMR 500 MHz
f1 (ppm)


jinmy-4-MeO-C
197.32
158.70
135.81
134.31
133.52
131.67
131.05
129.62
129.42
128.65
128.40
126.98
114.02
77.41
77.16
76.91
55.25
53.13
46.55
25.71
11.86
O
Et
SCF3
OMe
3h
13C NMR 125 MHz
f1 (ppm)


jinmy-4-MeO-F
jinmy-4-MeO-F
-39.46
O
Et
SCF3
OMe
3h
19F NMR 376 MHz
f1 (ppm)

Sample Info : OD-H, three combined, IPA:HEX=1:99, Flow = 1.0mL/min

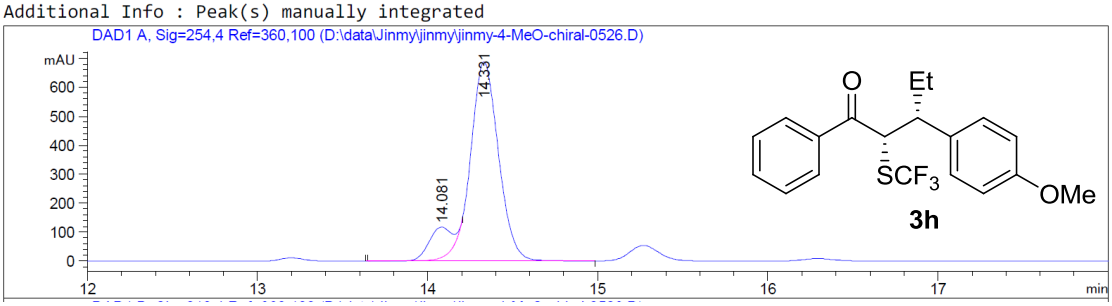


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.011	BV	0.1588	2648.86548	255.82014	20.7819
2	14.261	VB	0.1721	2896.66455	255.81833	22.7260
3	15.193	BB	0.1890	3596.22168	293.30872	28.2144
4	16.215	BB	0.2067	3604.29077	271.79233	28.2777
Totals :				1.27460e4	1076.73952	

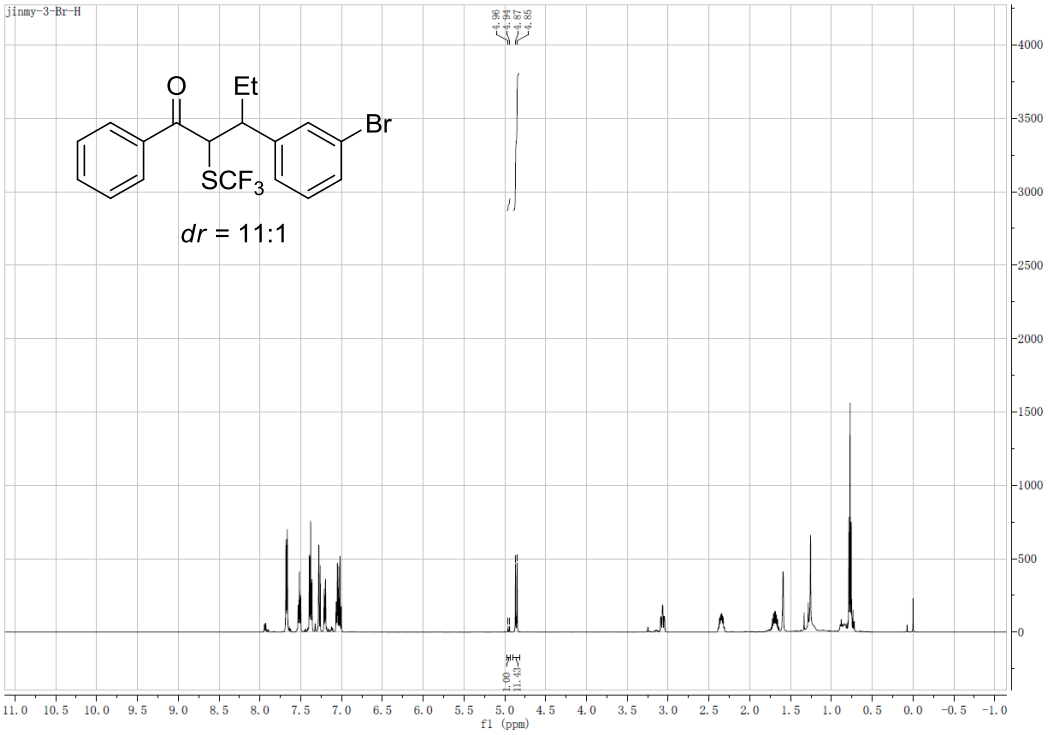
Sample Info : OD-H, three combined, IPA:HEX=1:99, Flow = 1.0mL/min

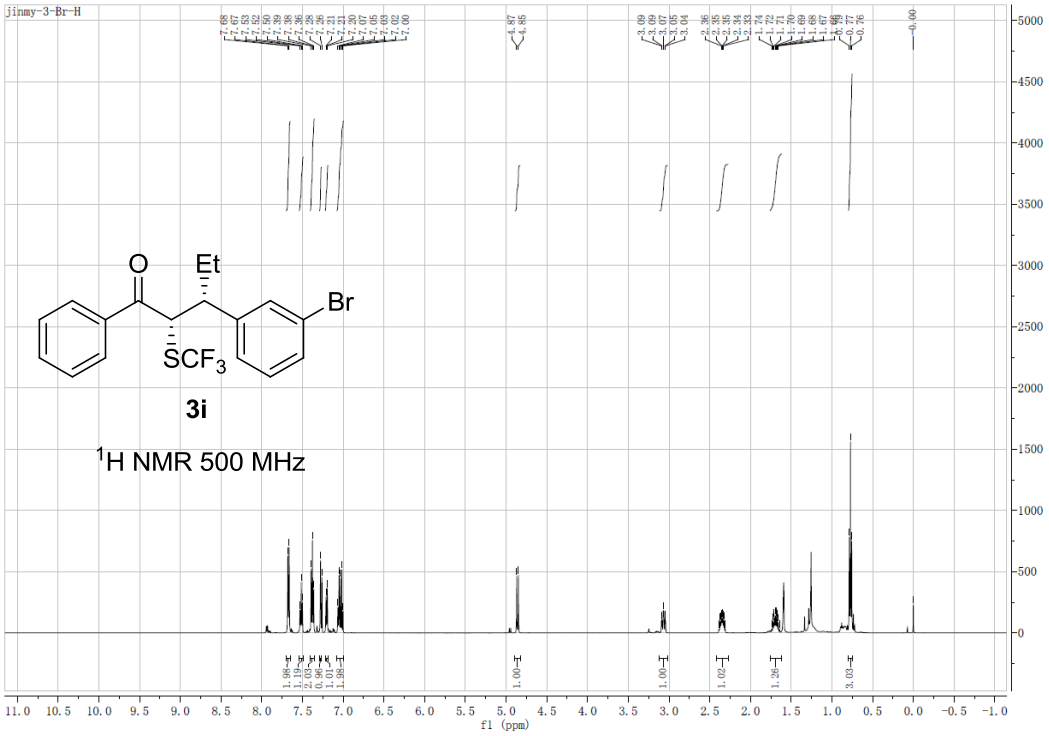
Additional Info : Peak(s) manually integrated

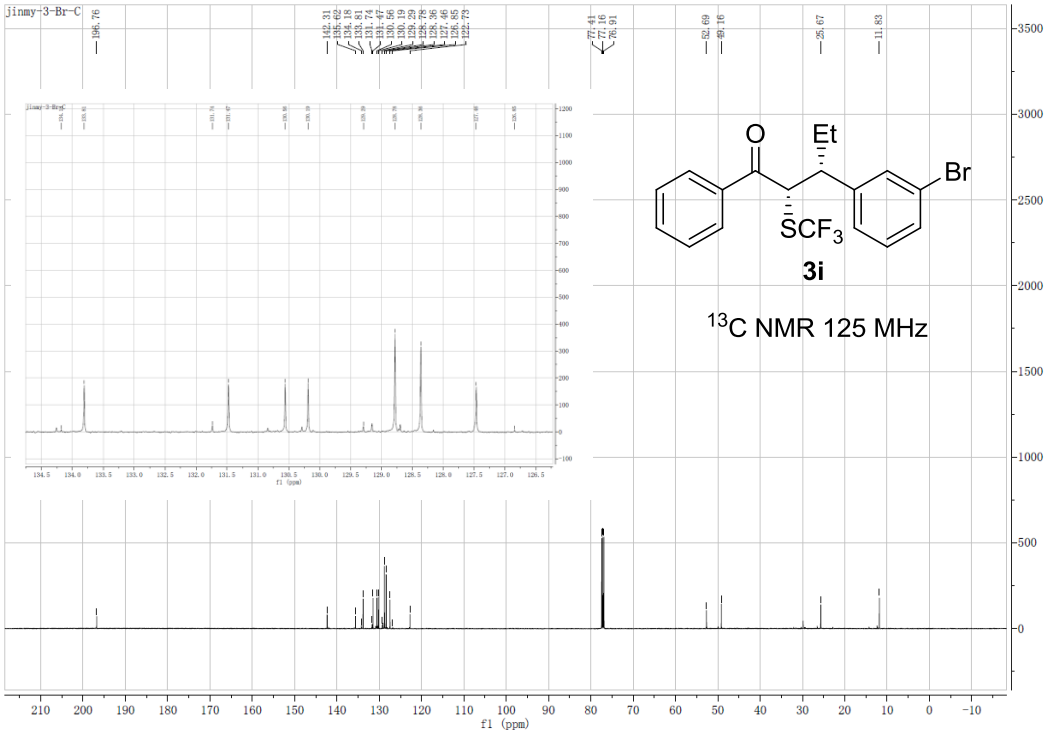


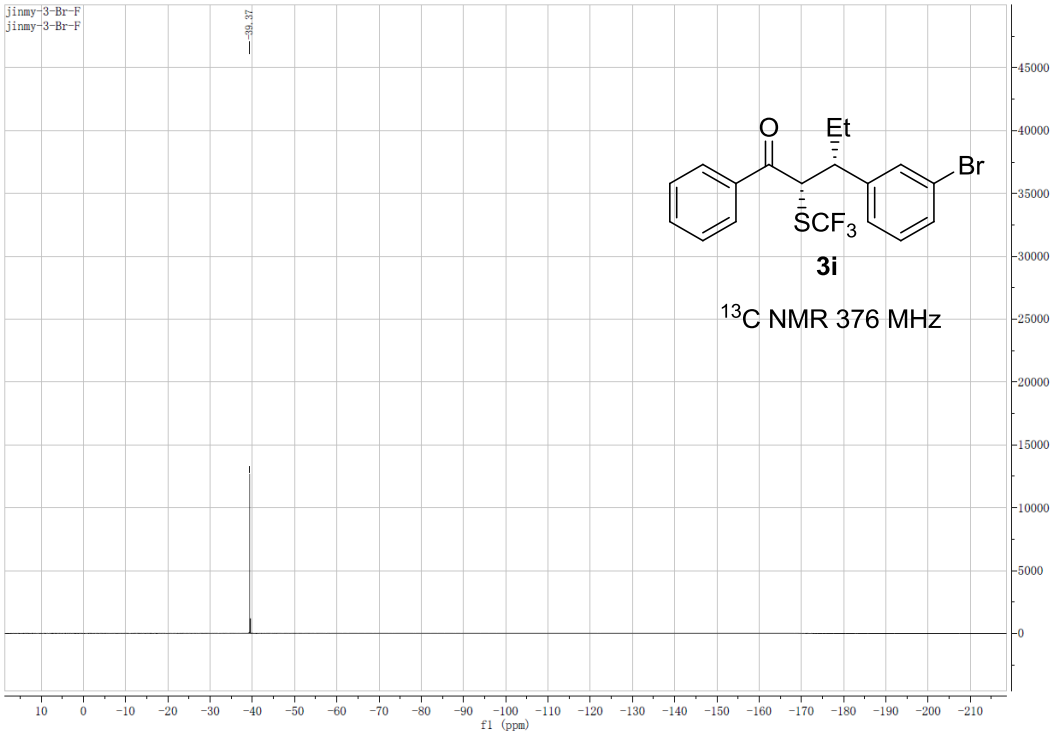
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.081	BV E	0.1386	940.68152	104.89614	10.5459
2	14.331	VV R	0.1772	7979.19824	688.29517	89.4541
Totals :				8919.87976	793.19131	


jinmy-3-Br-H
O
Et
Br
SCF3
dr = 11:1
f1 (ppm)

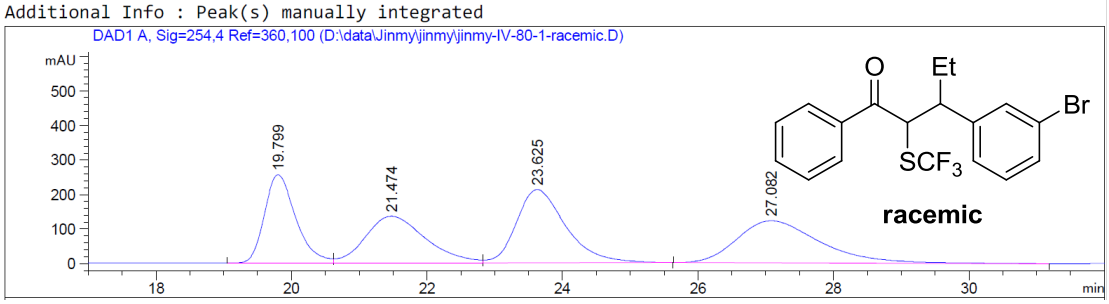

jinmy-3-Br-H
O
Et
Br
SCF3
3i
1H NMR 500 MHz
f1 (ppm)


jinmy-3-Br-C
O
Et
Br
SCF3
3i
13C NMR 125 MHz
f1 (ppm)


jinmy-3-Br-F
jinmy-3-Br-F
O
Et
Br
SCF3
3i
13C NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:1.0mL/min

Additional Info : Peak(s) manually integrated

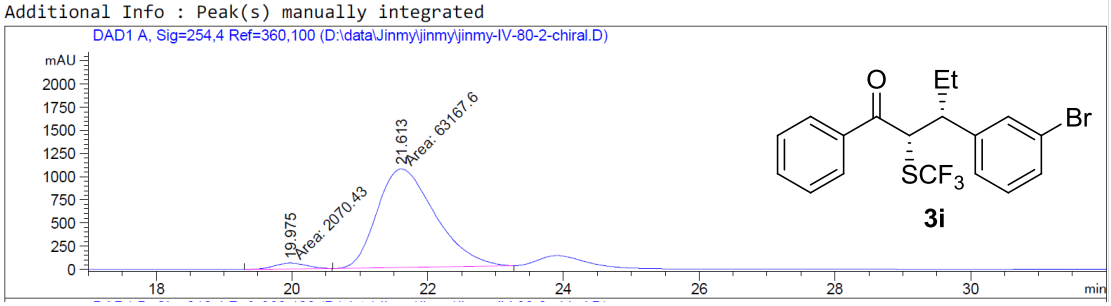


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.799	BV	0.4917	8171.18604	255.12025	21.8231
2	21.474	VV	0.9421	8276.66504	134.83638	22.1048
3	23.625	VB	0.7651	1.06422e4	211.46750	28.4226
4	27.082	BB	1.2921	1.03528e4	121.74805	27.6496
Totals :				3.74429e4	723.17218	

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:1.0mL/min

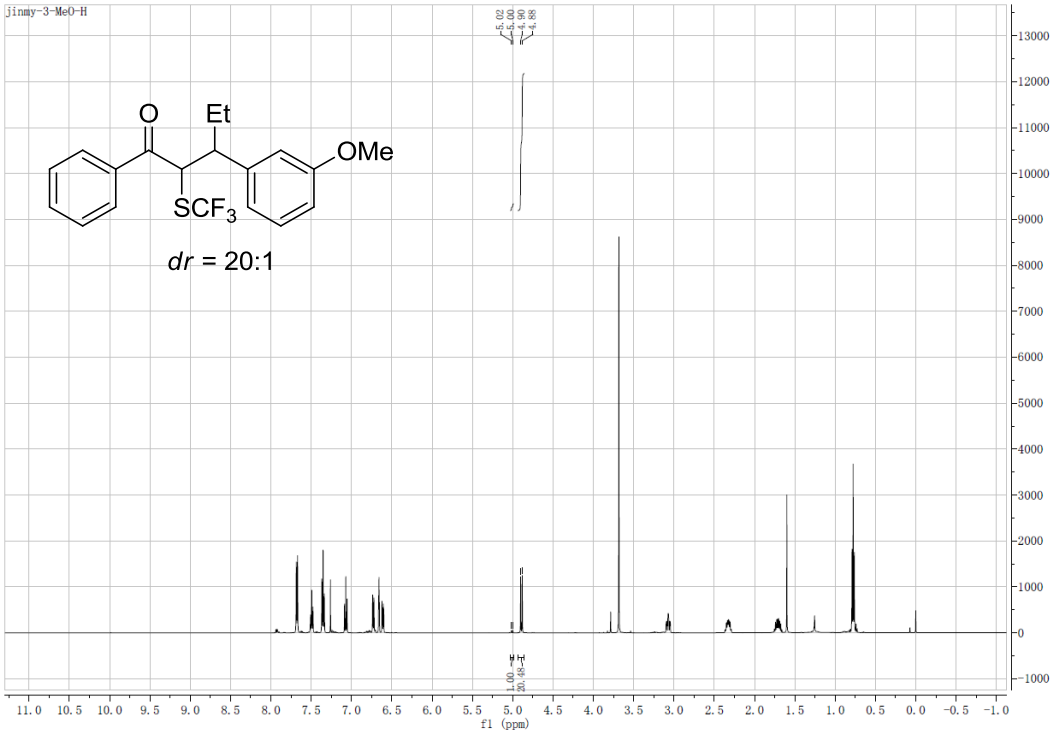
Additional Info : Peak(s) manually integrated

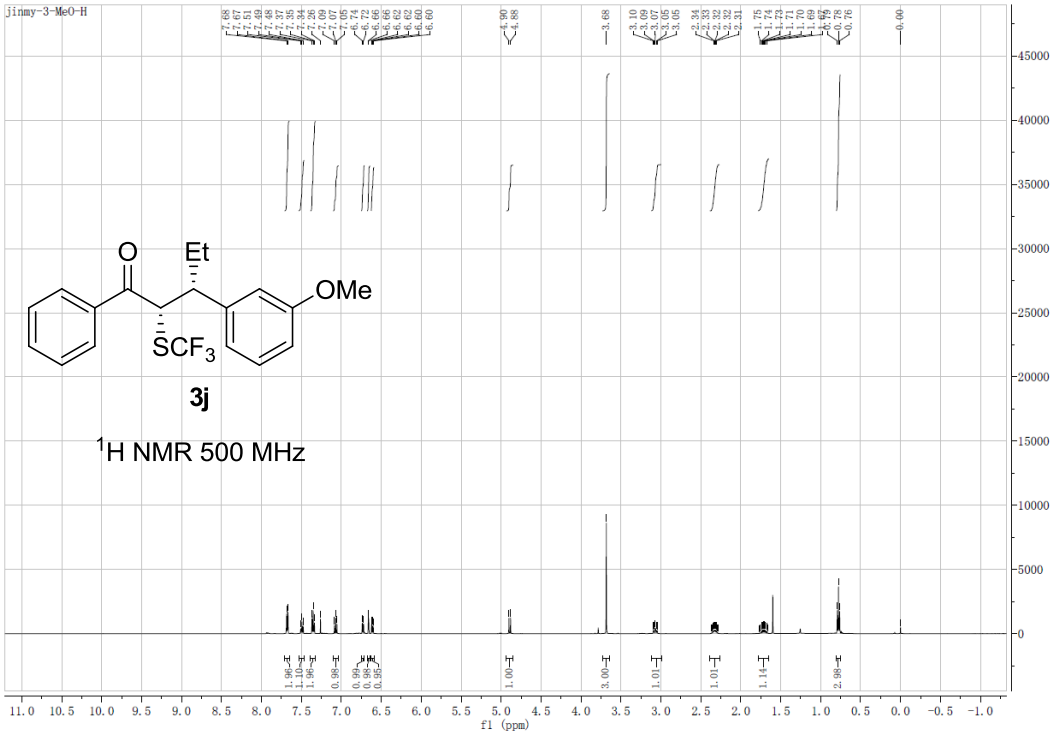


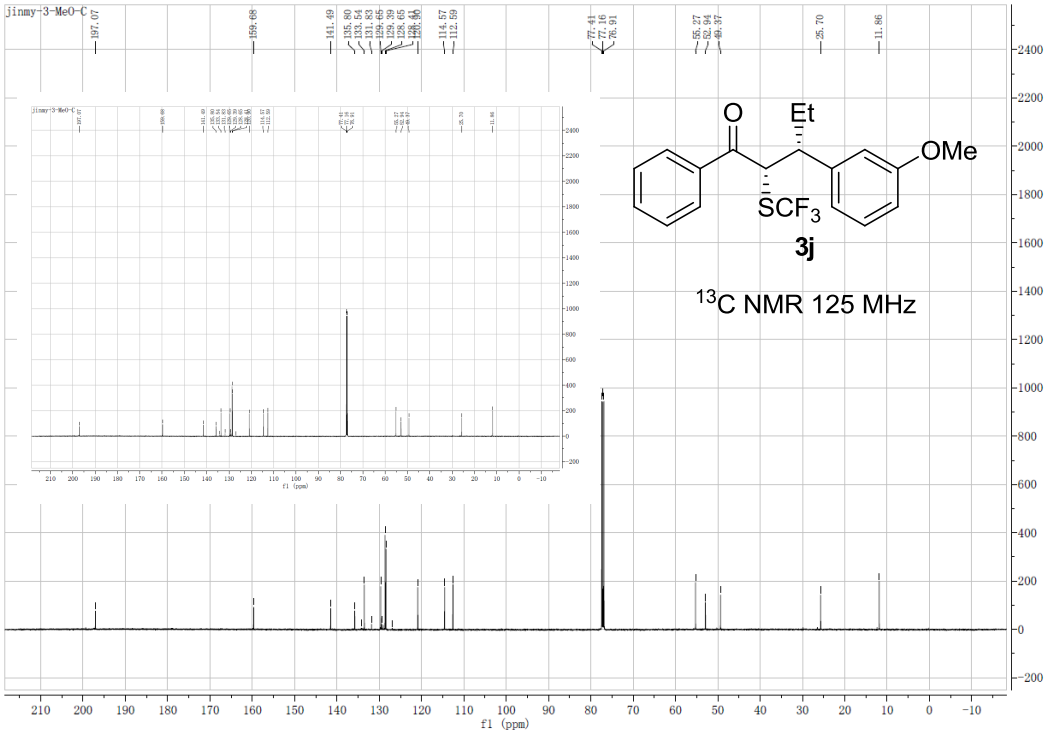
,

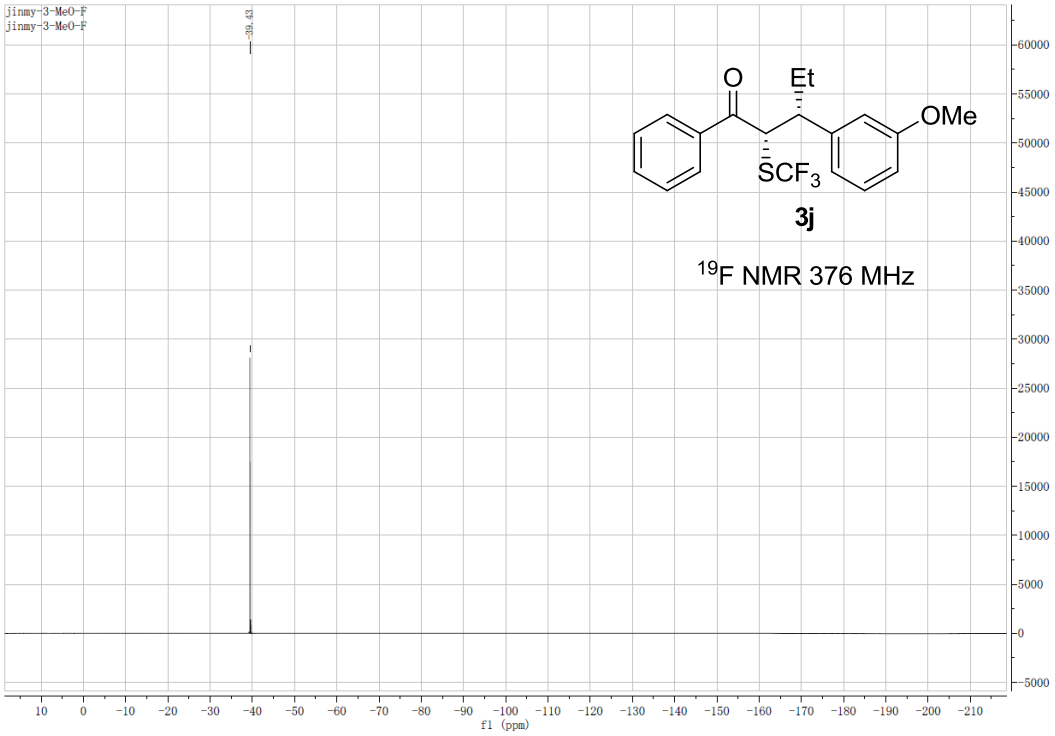
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.975	MM	0.5469	2070.42798	63.09276	3.1737
2	21.613	MM	0.9894	6.31676e4	1064.10095	96.8263
Totals :				6.52380e4	1127.19371	


jinmy-3-MeO-H
O
Et
OMe
SCF3
dr = 20:1
f1 (ppm)

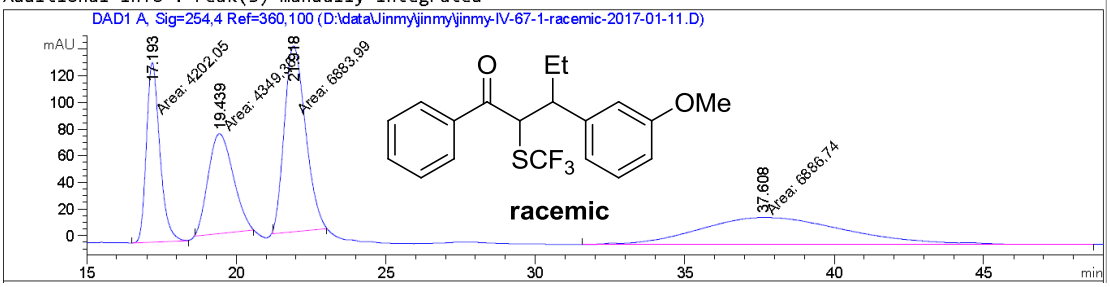

jinmy-3-MeO-H
O
Et
OMe
SCF3
3j
1H NMR 500 MHz
f1 (ppm)


jinmy-3-MeO-C
197.07
159.68
141.49
135.80
133.54
131.63
129.46
129.39
128.65
114.67
112.09
77.41
77.16
76.91
55.27
52.94
40.37
25.70
11.86
O
Et
OMe
SCF3
3j
13C NMR 125 MHz
f1 (ppm)


jinmy-3-MeO-F
jinmy-3-MeO-F
-39.43
O
Et
OMe
SCF3
3j
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:1.0mL/min

Additional Info : Peak(s) manually integrated

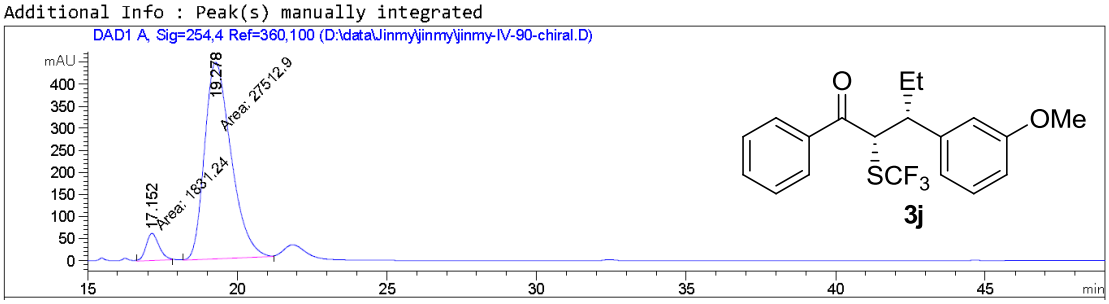


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.193	MM	0.5195	4202.04541	134.80524	18.8246
2	19.439	MM	0.9662	4349.36133	75.02186	19.4845
3	21.918	MM	0.8206	6883.99268	139.80779	30.8393
4	37.608	MM	5.6690	6886.74219	20.24688	30.8516
Totals :				2.23221e4	369.88176	

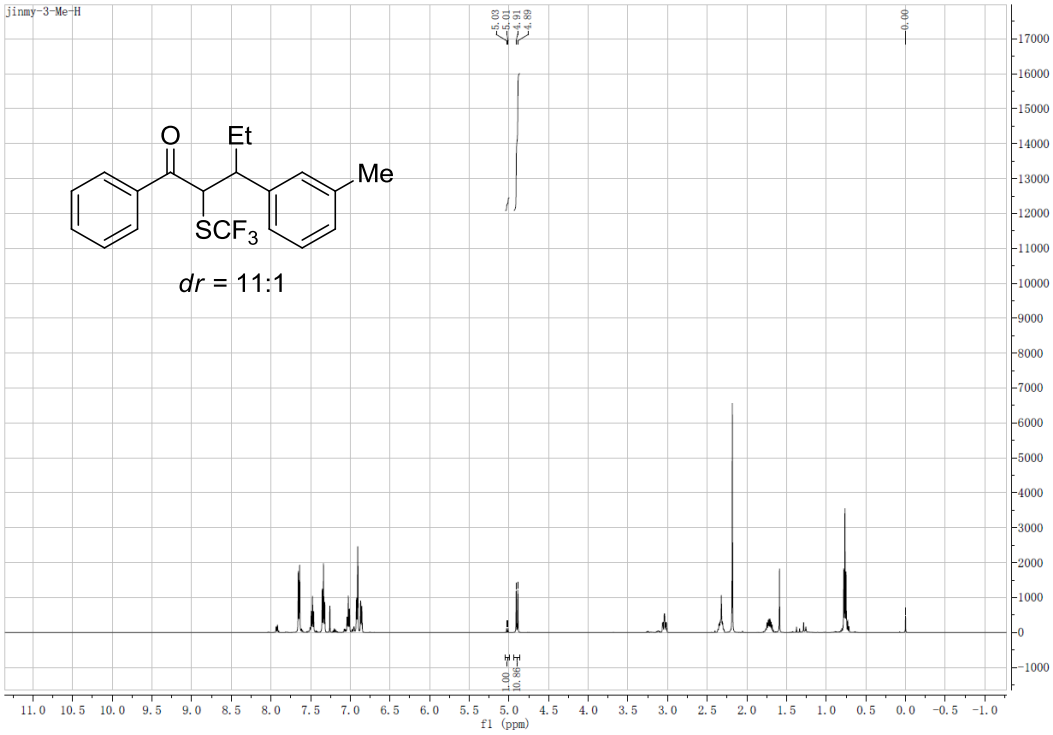
Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:1.0mL/min

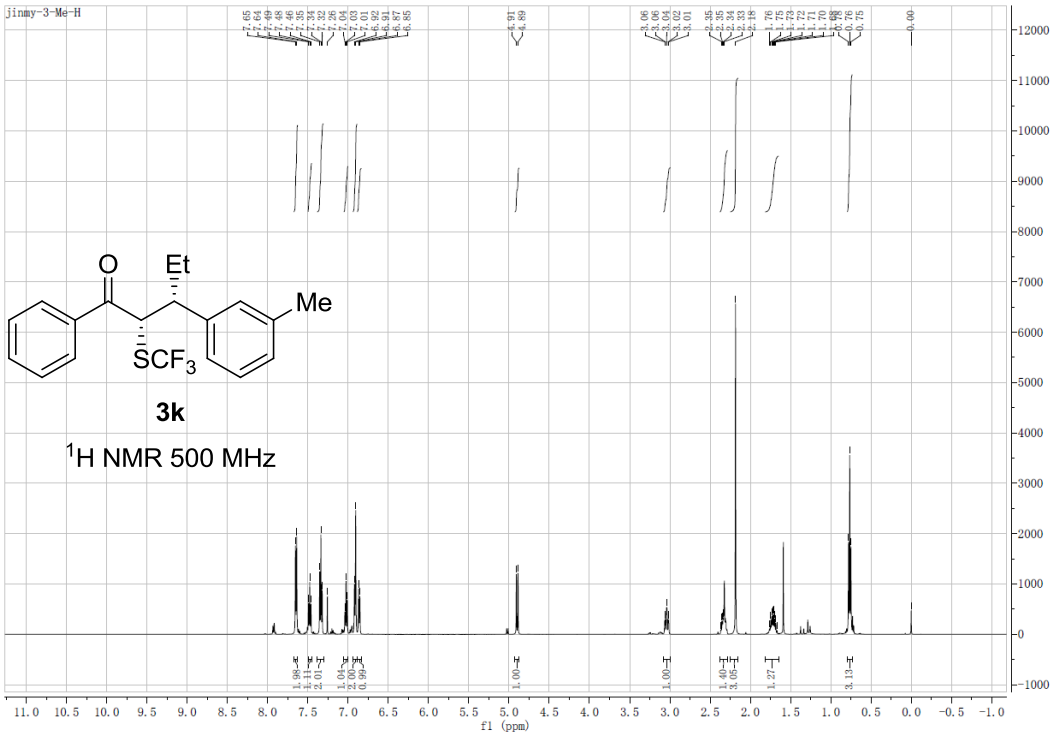
Additional Info : Peak(s) manually integrated

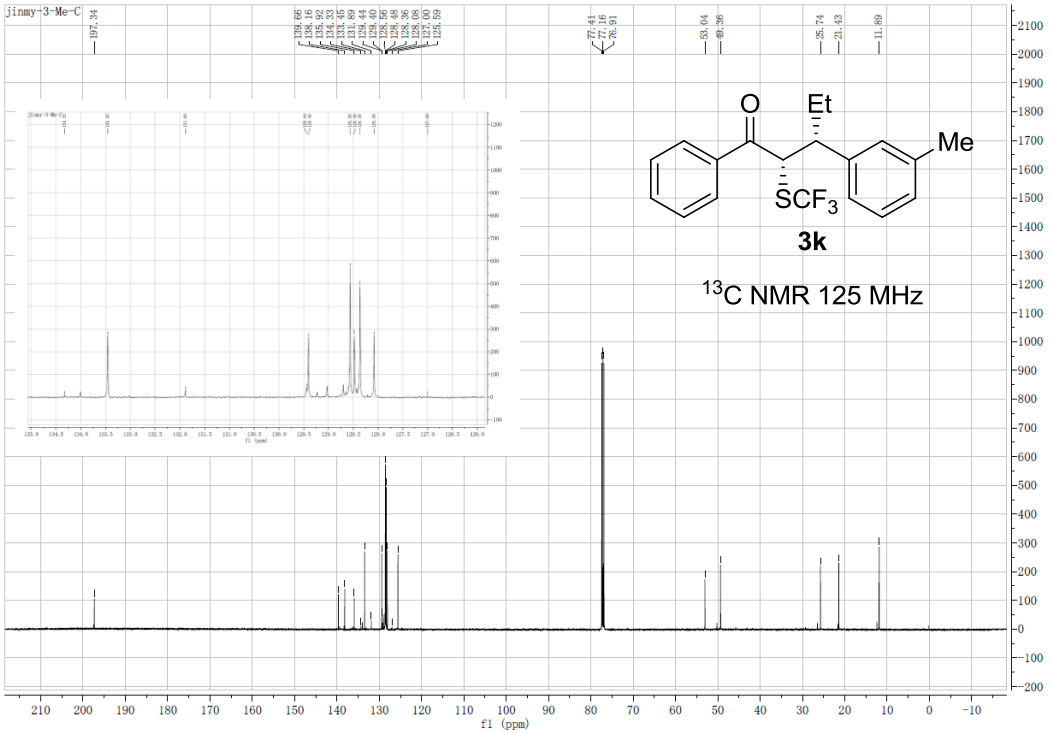


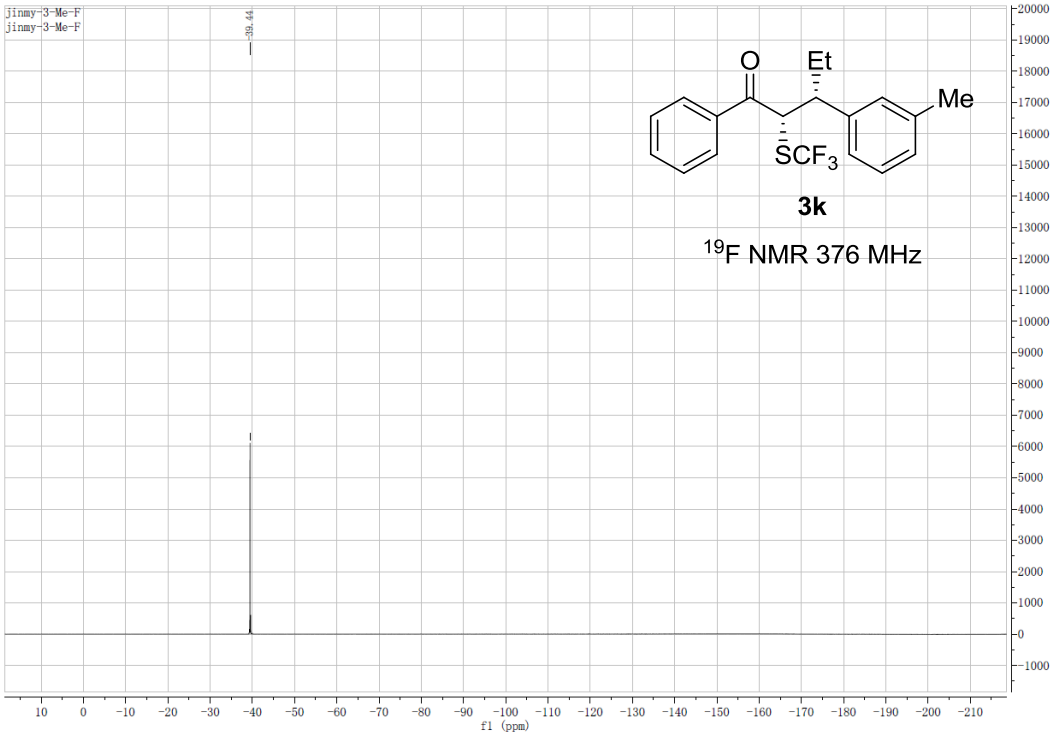
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

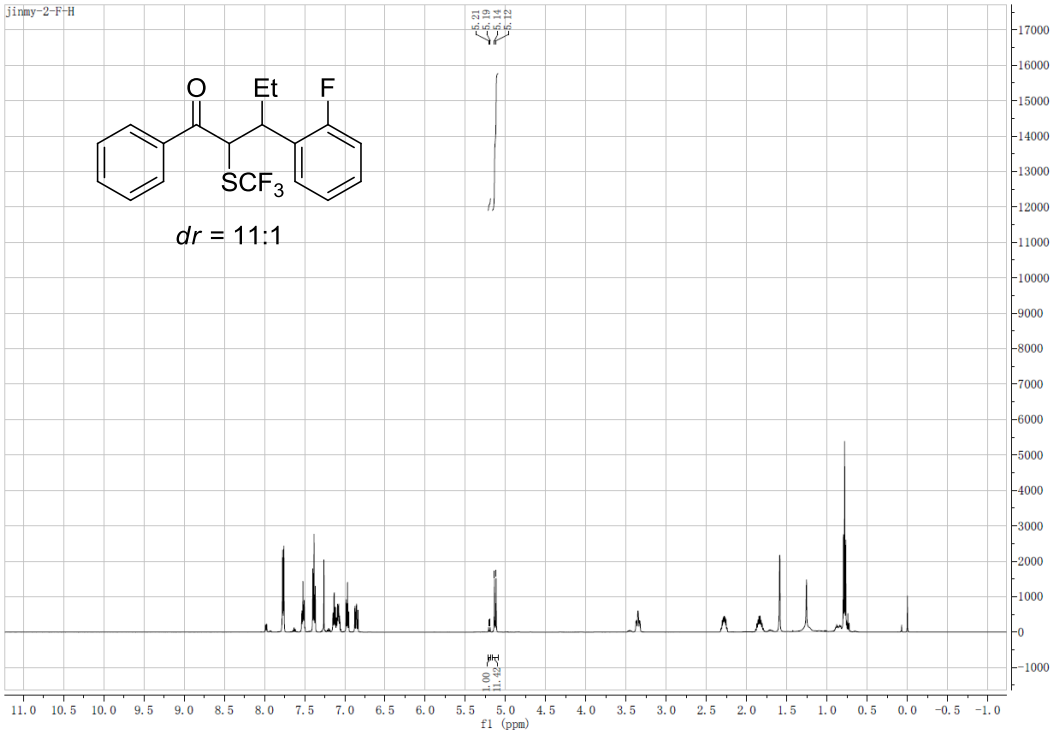
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.152	MM	0.4982	1831.24121	61.25579	6.2406
2	19.278	MM	1.0277	2.75129e4	446.17194	93.7594
Totals :				2.93442e4	507.42773	

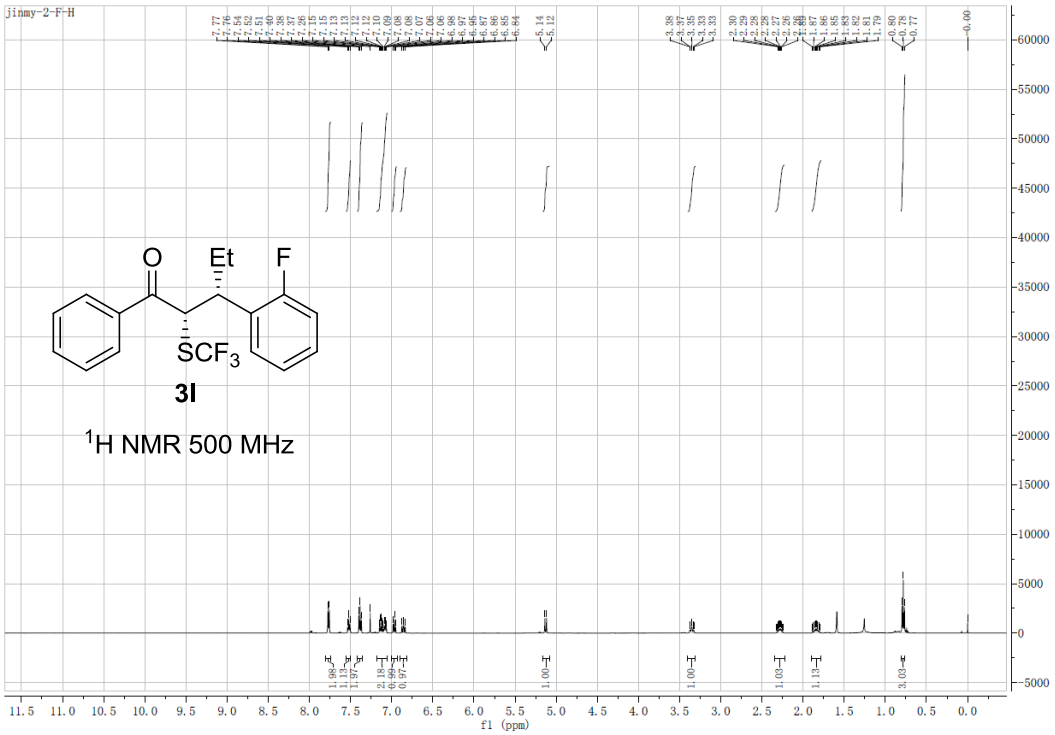

jinmy-3-Me-H
O
Et
Me
SCF3
dr = 11:1
f1 (ppm)

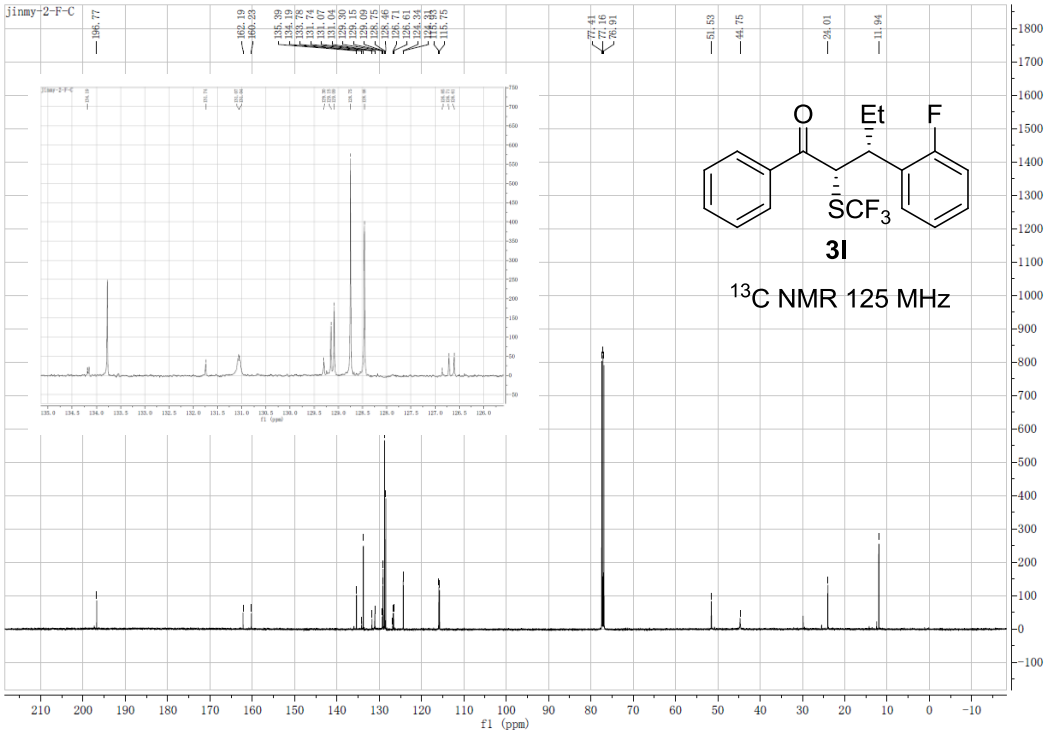

jinmy-3-Me-H
O
Et
Me
SCF3
3k
1H NMR 500 MHz
f1 (ppm)

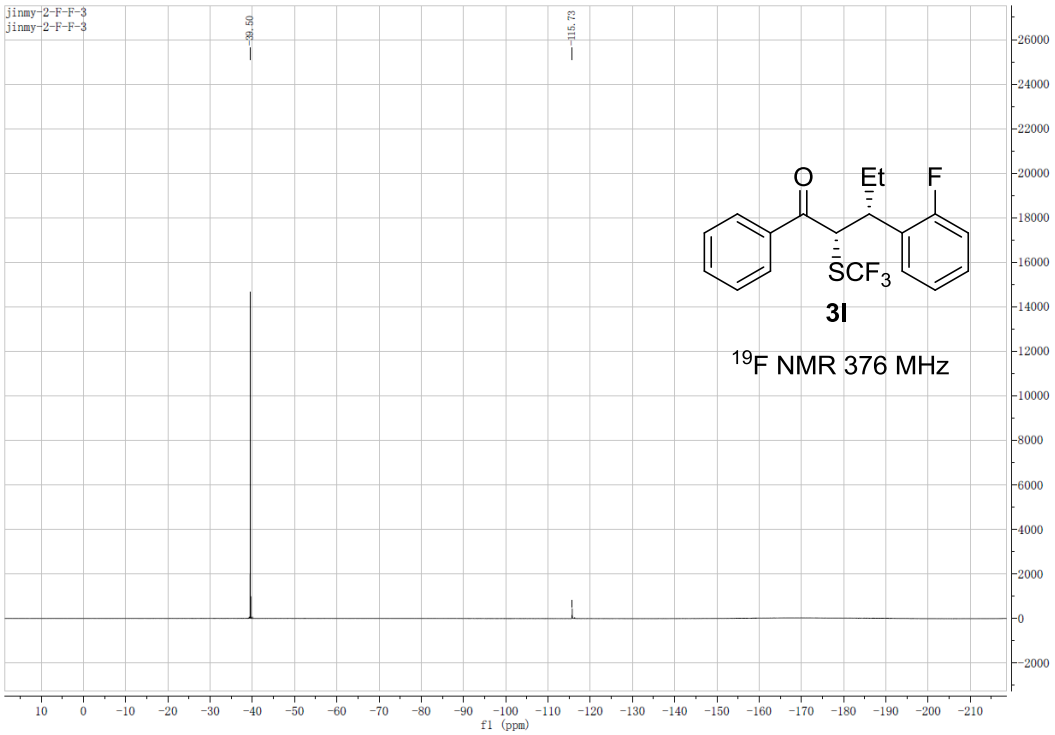

jinmy-3-Me-C
O
Et
Me
SCF3
3k
13C NMR 125 MHz
f1 (ppm)

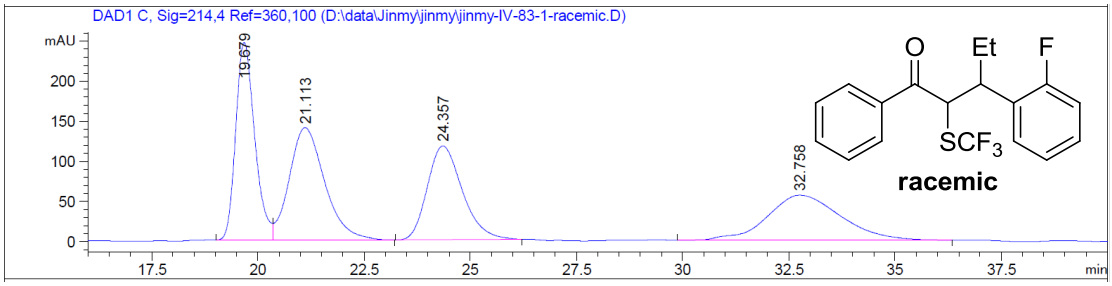

jinmy-3-Me-F
jinmy-3-Me-F
O
Et
Me
SCF3
3k
19F NMR 376 MHz
f1 (ppm)


jinmy-2-F-H
O
Et
F
SCF3
dr = 11:1
f1 (ppm)


jinmy-2-F-H
O
Et
F
SCF3
3l
1H NMR 500 MHz
f1 (ppm)

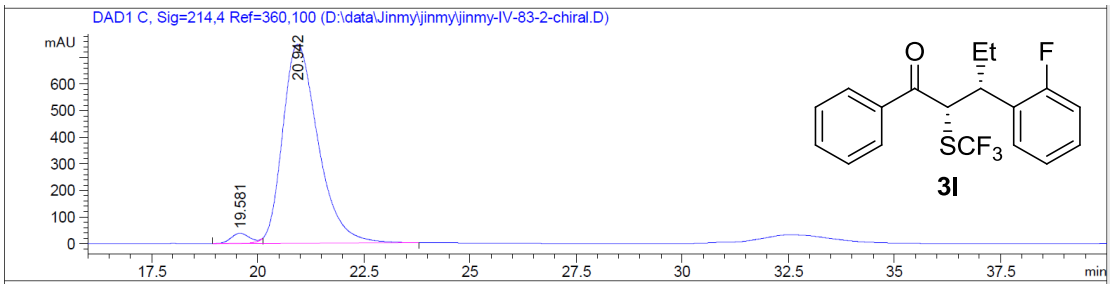

jinmy-2-F-C
196.77
162.19
160.23
135.39
134.19
133.78
131.74
131.07
131.04
129.30
129.15
128.69
128.75
128.46
126.71
126.01
125.24
118.83
115.75
77.41
77.16
76.91
51.53
44.75
26.01
11.94
O
Et
F
SCF3
3l
13C NMR 125 MHz
f1 (ppm)


jinmy-2-F-F-3
jinmy-2-F-F-3
-39.50
-115.73
O
Et
F
SCF3
3l
19F NMR 376 MHz
f1 (ppm)



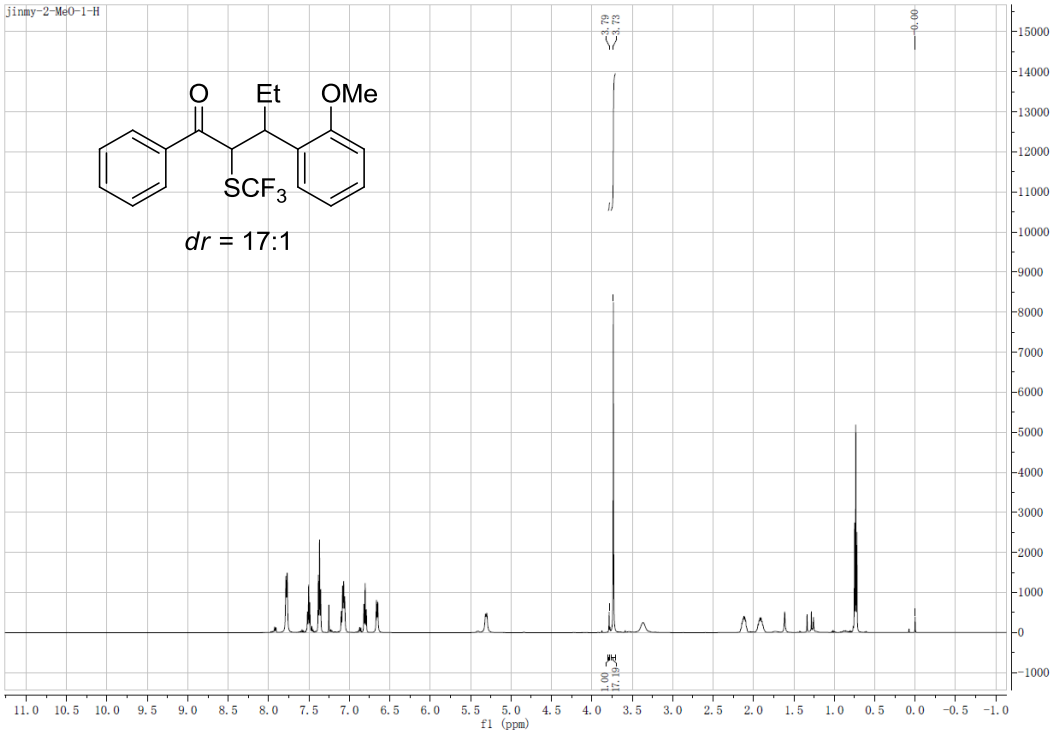
Signal 3: DAD1 C, Sig=214,4 Ref=360,100

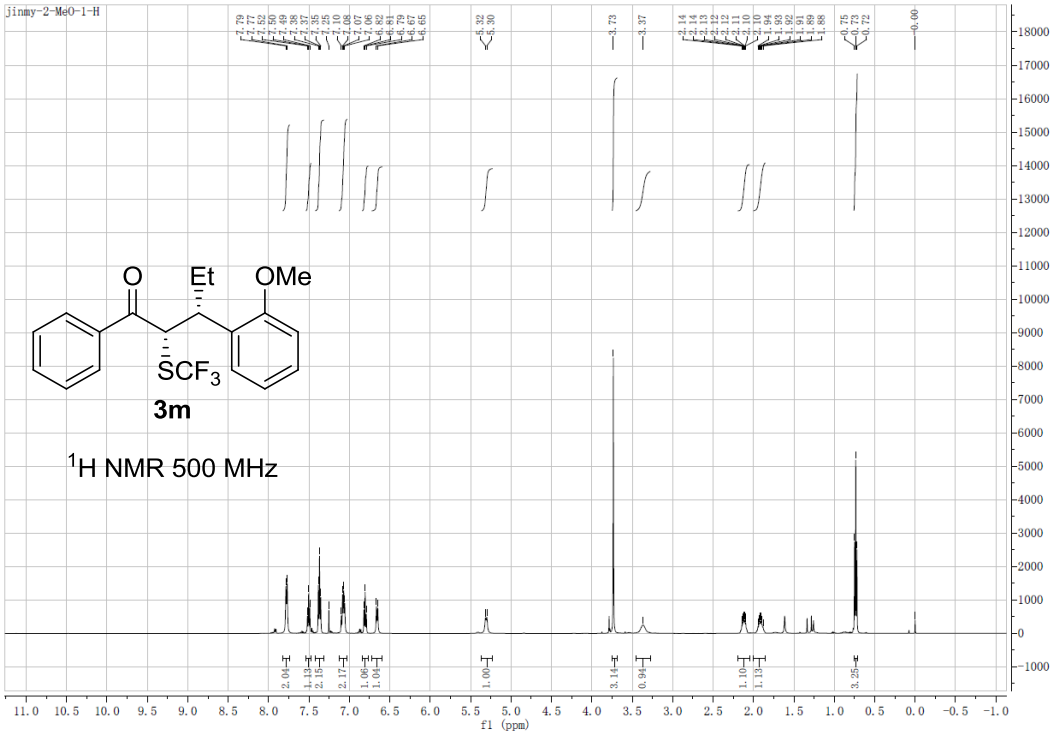
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.679	BV	0.4769	7663.17383	246.35909	26.1343
2	21.113	VB	0.8866	8125.17725	140.10373	27.7099
3	24.357	BB	0.8830	6711.62695	117.03589	22.8892
4	32.758	BB	1.8316	6822.30420	56.30644	23.2666
Totals :				2.93223e4	559.80515	

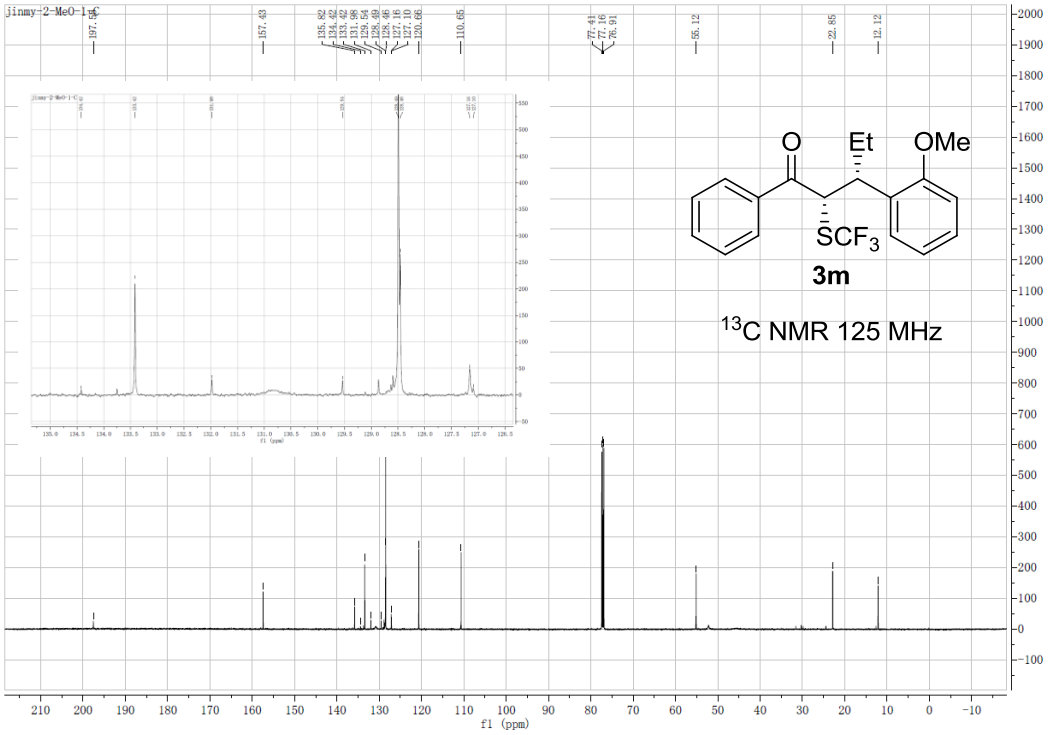


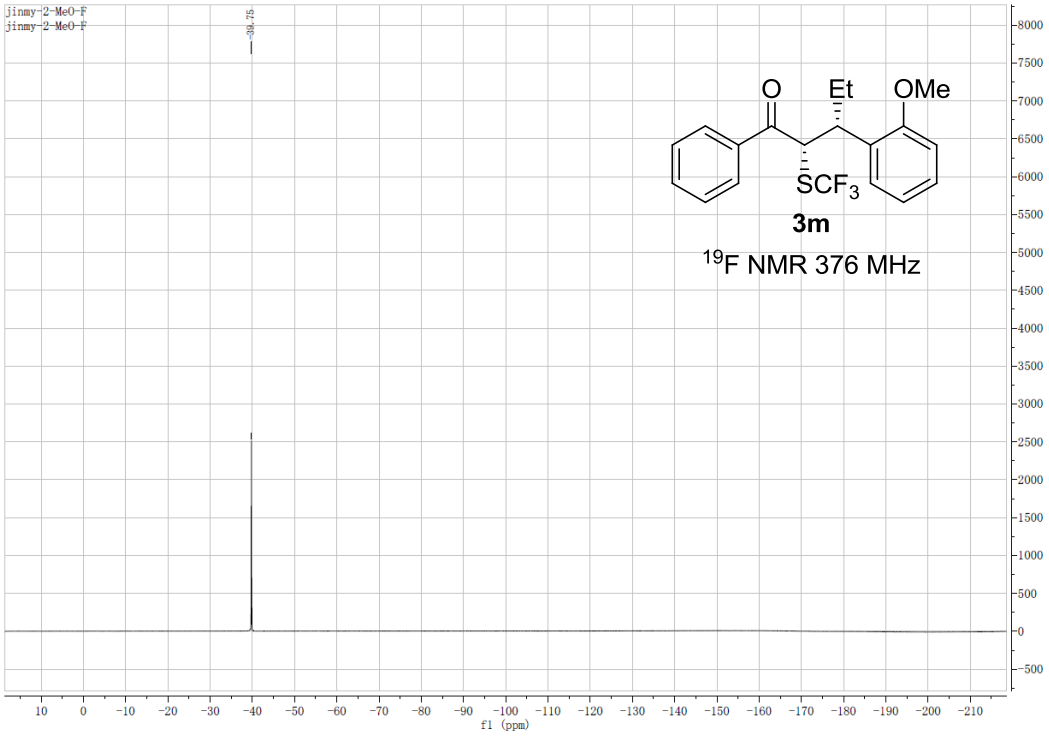
Signal 3: DAD1 C, Sig=214,4 Ref=360,100

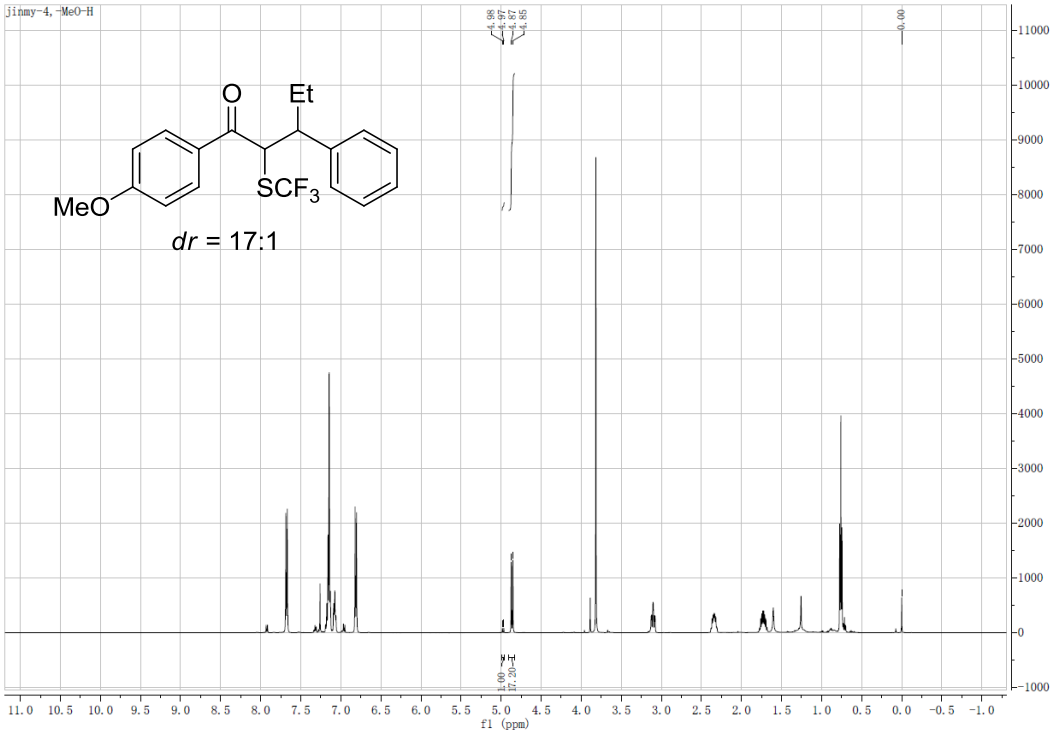
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.581	BV E	0.4541	1099.33887	37.70794	2.4707
2	20.942	VB R	0.8901	4.33966e4	748.79095	97.5293
Totals :				4.44959e4	786.49889	

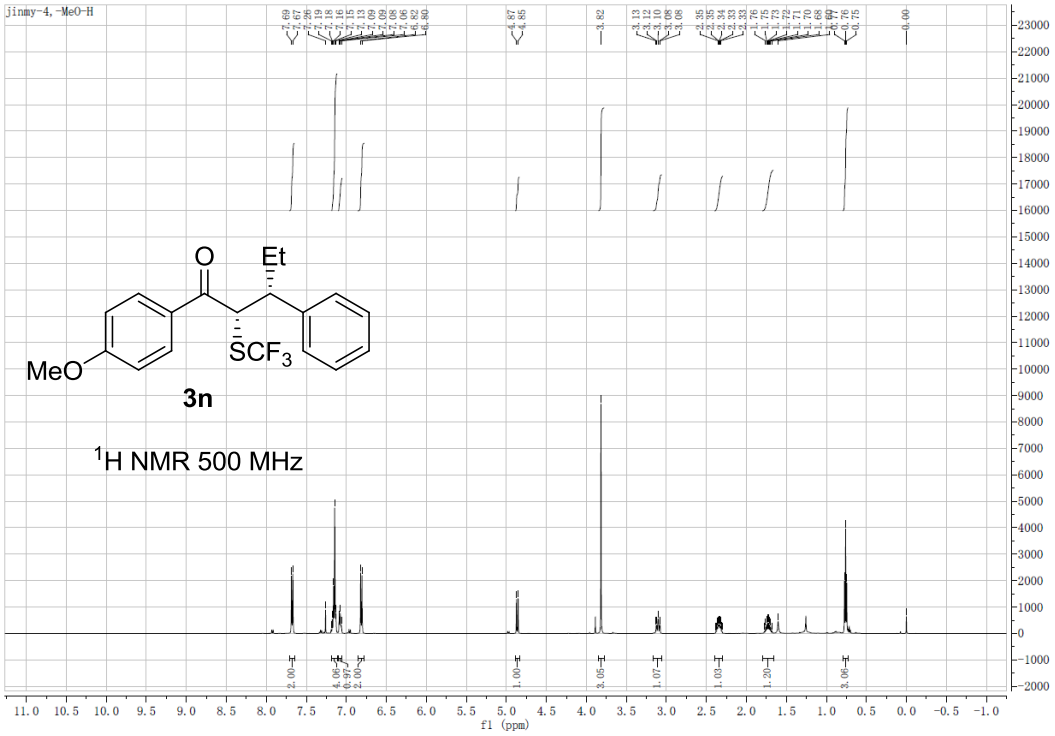

jinmy-2-MeO-1-H
O
Et
OMe
SCF3
dr = 17:1
f1 (ppm)

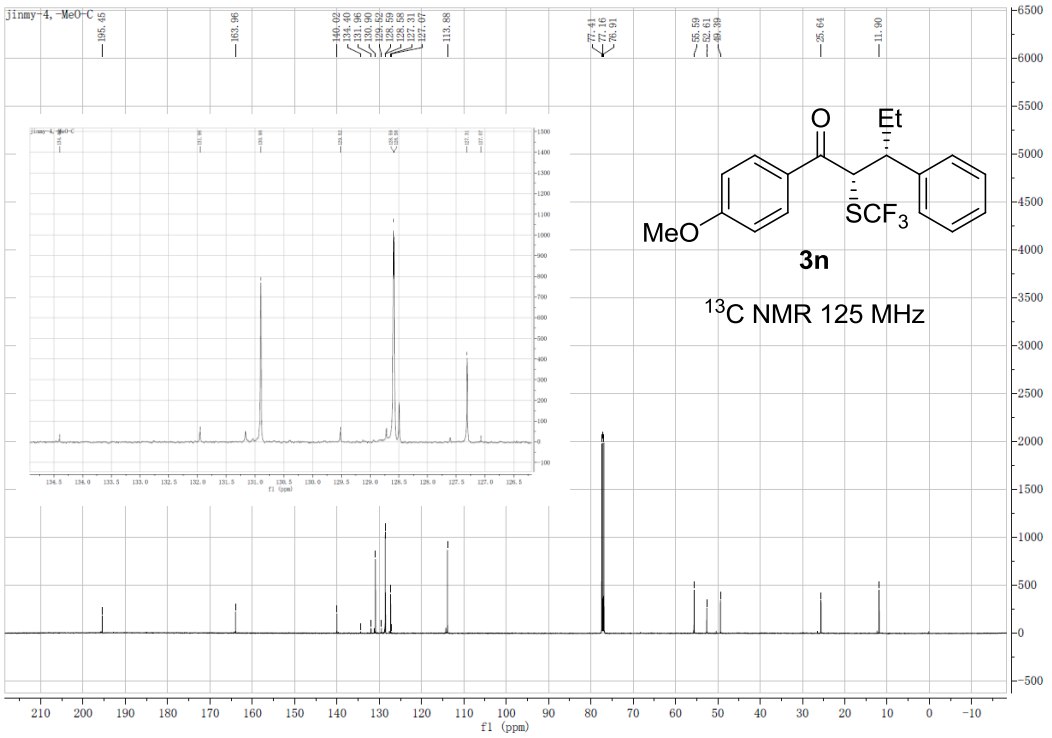

jinmy-2-MeO-1-H
O
Et
OMe
SCF3
3m
1H NMR 500 MHz
f1 (ppm)

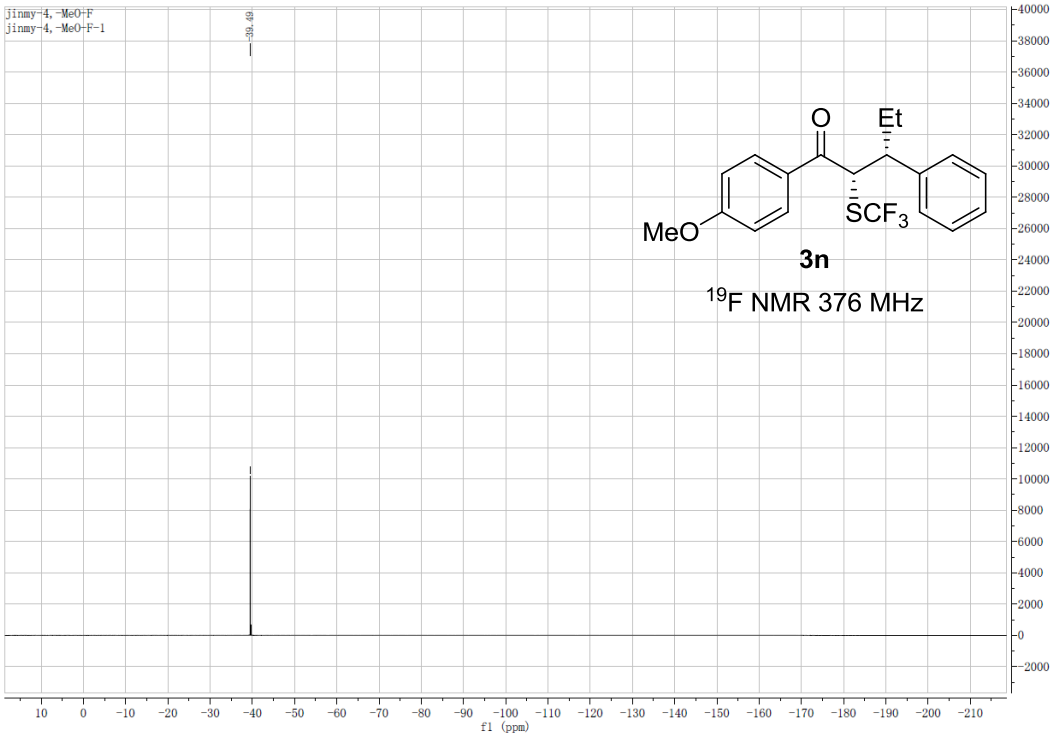

O
Et
OMe
SCF3
3m
13C NMR 125 MHz
f1 (ppm)


jinmy-2-MeO-F
O
Et
OMe
SCF3
3m
19F NMR 376 MHz
f1 (ppm)

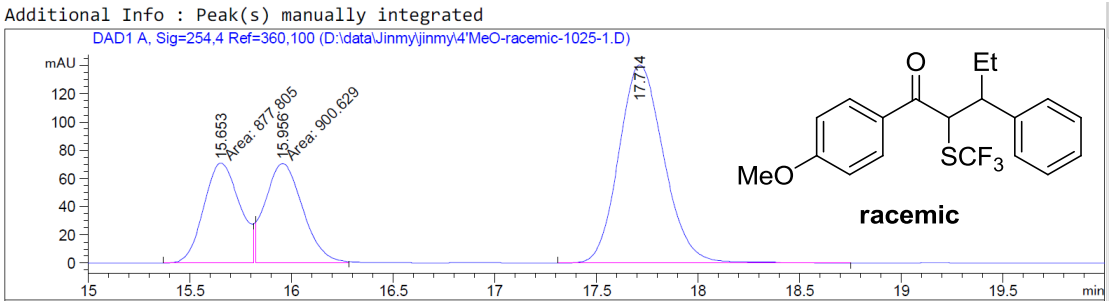

jinmy-4, -MeO-H
O
Et
SCF3
MeO
dr = 17:1
f1 (ppm)


jinmy-4, -MeO-H
O
Et
SCF3
MeO
3n
1H NMR 500 MHz
f1 (ppm)


jinmy-4, -MeO-C
195.45
163.96
140.02
134.40
131.96
130.69
129.82
128.59
128.59
127.31
127.07
113.88
77.41
77.16
76.91
55.59
52.61
40.39
25.64
11.90
O
Et
SCF3
MeO
3n
13C NMR 125 MHz
f1 (ppm)


jinmy-4, -MeO-F
jinmy-4, -MeO-F-1
-39.49
O
Et
SCF3
MeO
3n
19F NMR 376 MHz
f1 (ppm)

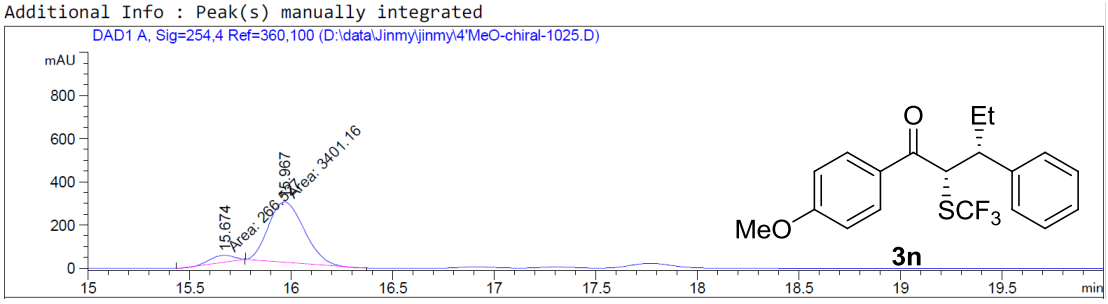
Additional Info : Peak(s) manually integrated



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

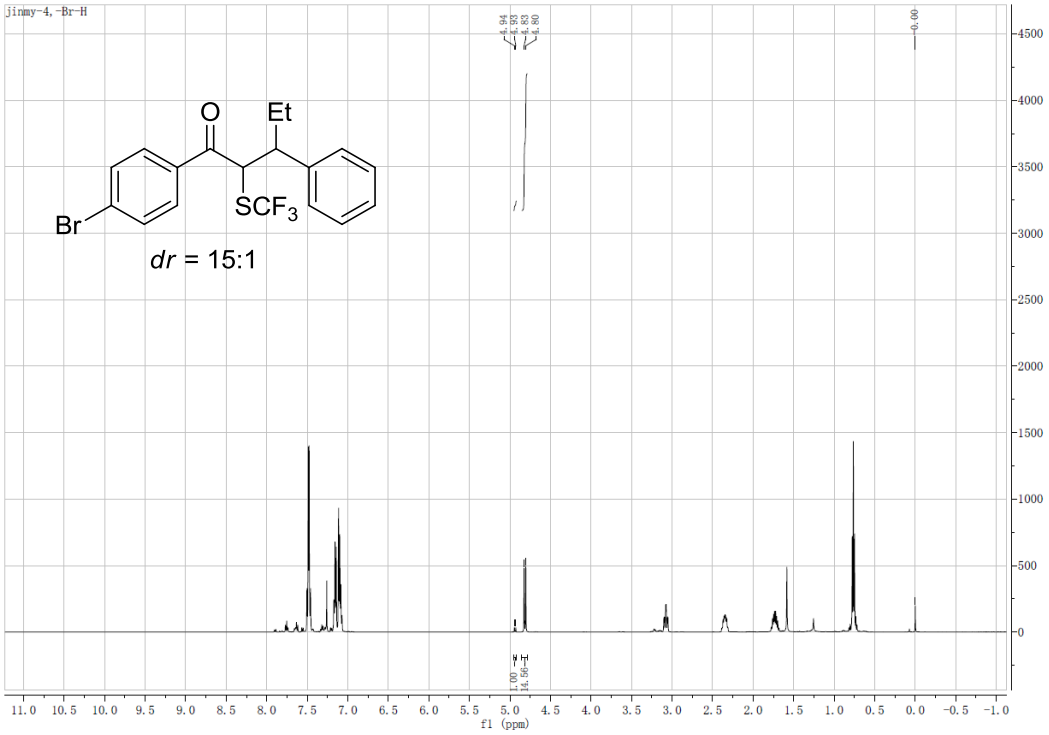
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.653	MM	0.2067	877.80450	70.76807	22.3055
2	15.956	MM	0.2128	900.62872	70.52351	22.8855
3	17.714	BB	0.2373	2156.93457	140.31815	54.8090
Totals :				3935.36780	281.60972	

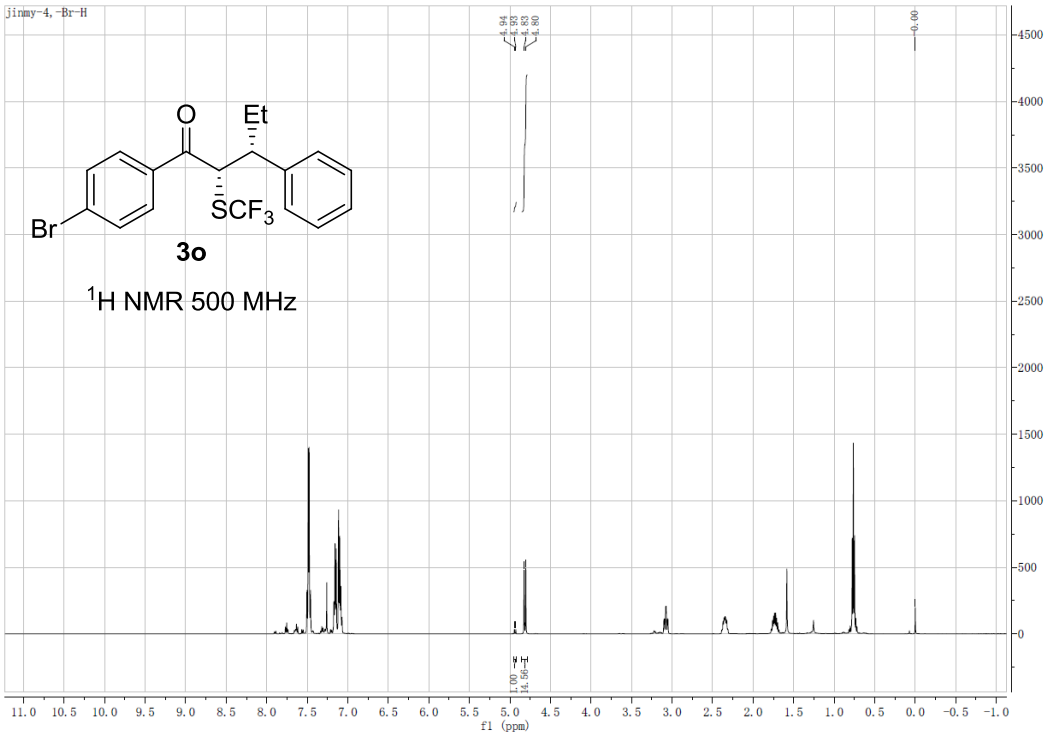
Additional Info : Peak(s) manually integrated

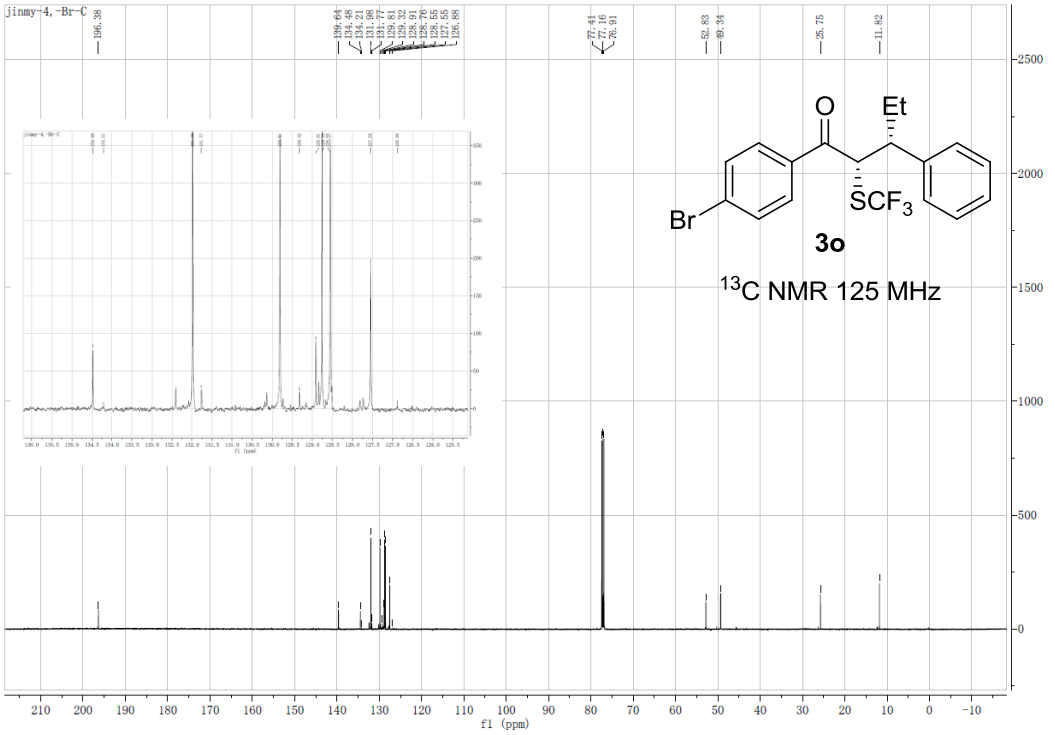


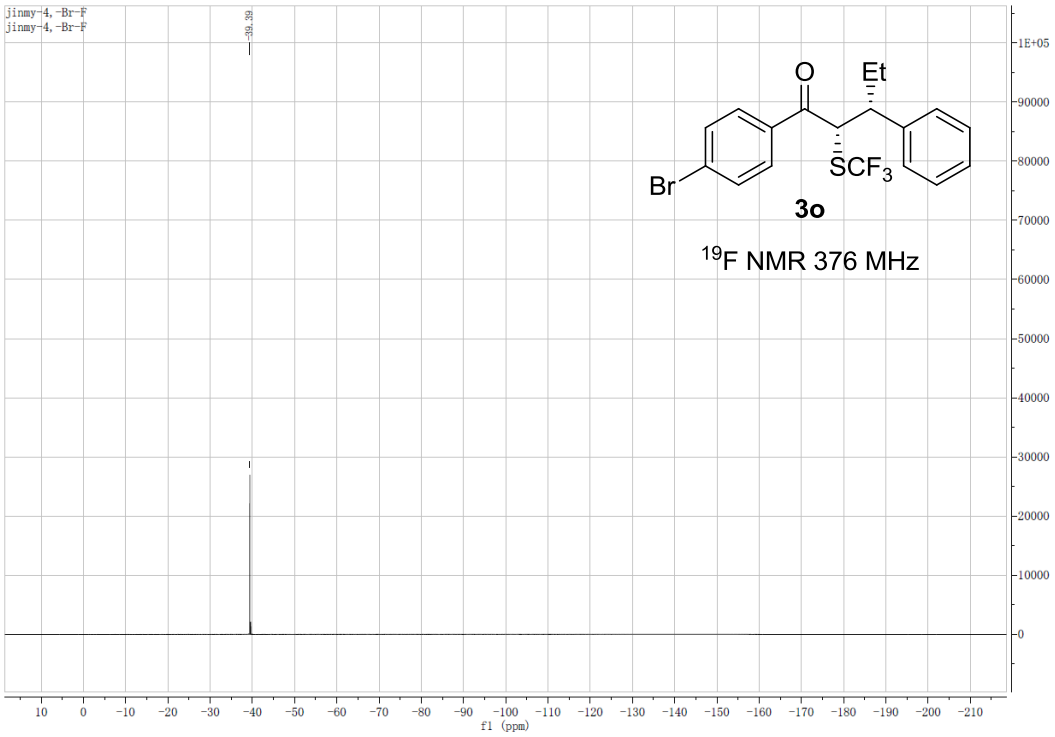
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.674	MM	0.1392	266.52725	31.90391	7.2669
2	15.967	MM	0.2034	3401.16235	278.70737	92.7331
Totals :				3667.68961	310.61128	


jinmy-4,-Br-H
O
Et
Br
SCF3
dr = 15:1
f1 (ppm)

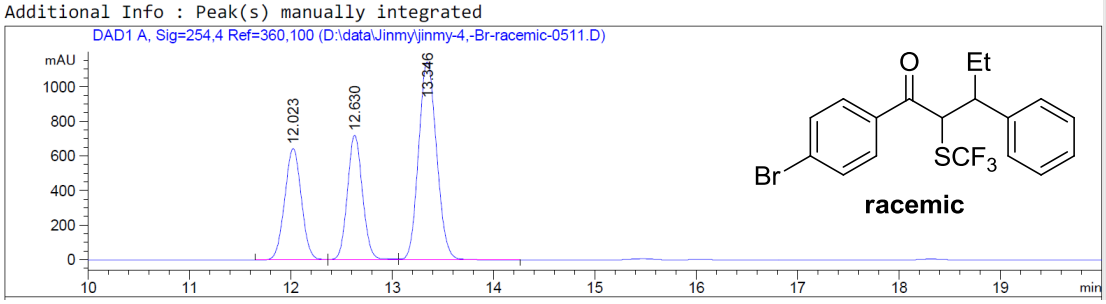

jinmy-4,-Br-H
O
Et
Br
SCF3
3o
1H NMR 500 MHz
f1 (ppm)


jinmy-4,-Br-C
196.38
139.64
134.48
134.21
131.98
131.77
129.61
129.32
128.91
128.79
128.55
127.55
126.88
77.41
77.16
76.91
52.83
49.34
25.75
11.82
O
Et
SCF3
Br
3o
13C NMR 125 MHz
f1 (ppm)


jinmy-4,-Br-F
jinmy-4,-Br-F
-39.39
O
Et
SCF3
Br
3o
19F NMR 376 MHz
f1 (ppm)

Sample Info : OD-H, three combined, IPA:HEX=1:99, Flow: 1.0mL/min

Additional Info : Peak(s) manually integrated

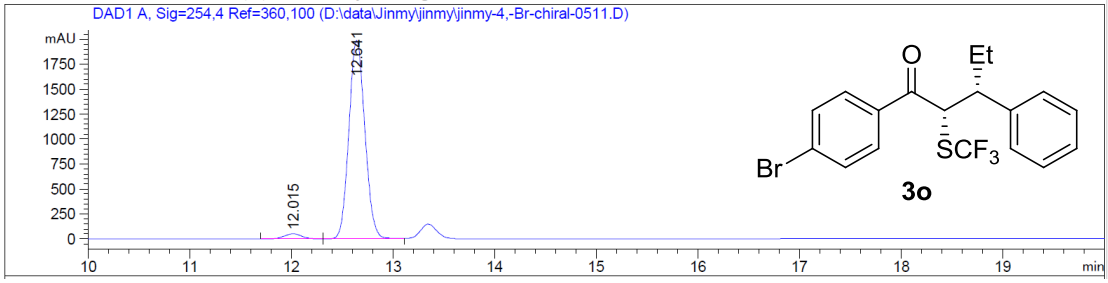


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.023	BV	0.1776	7373.11279	643.93463	25.4226
2	12.630	VV	0.1614	7502.62891	721.00360	25.8691
3	13.346	VB	0.1942	1.41265e4	1143.16296	48.7083
Totals :				2.90022e4	2508.10120	

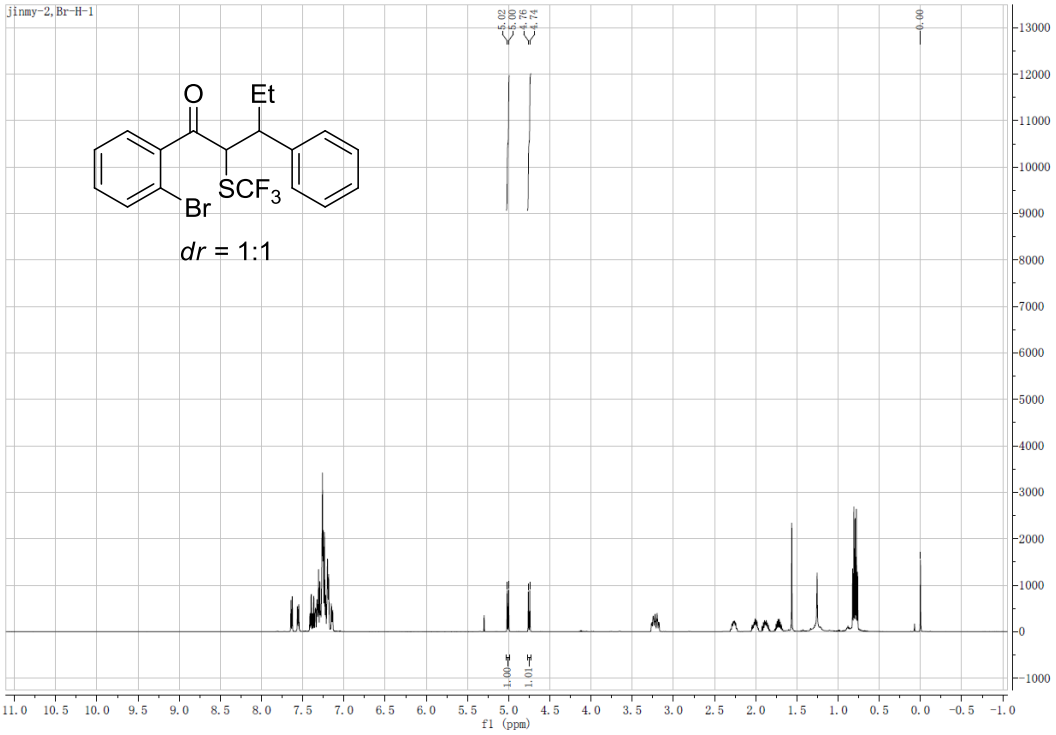
Sample Info : OD-H, three combined, IPA:HEX=1:99, Flow: 1.0mL/min

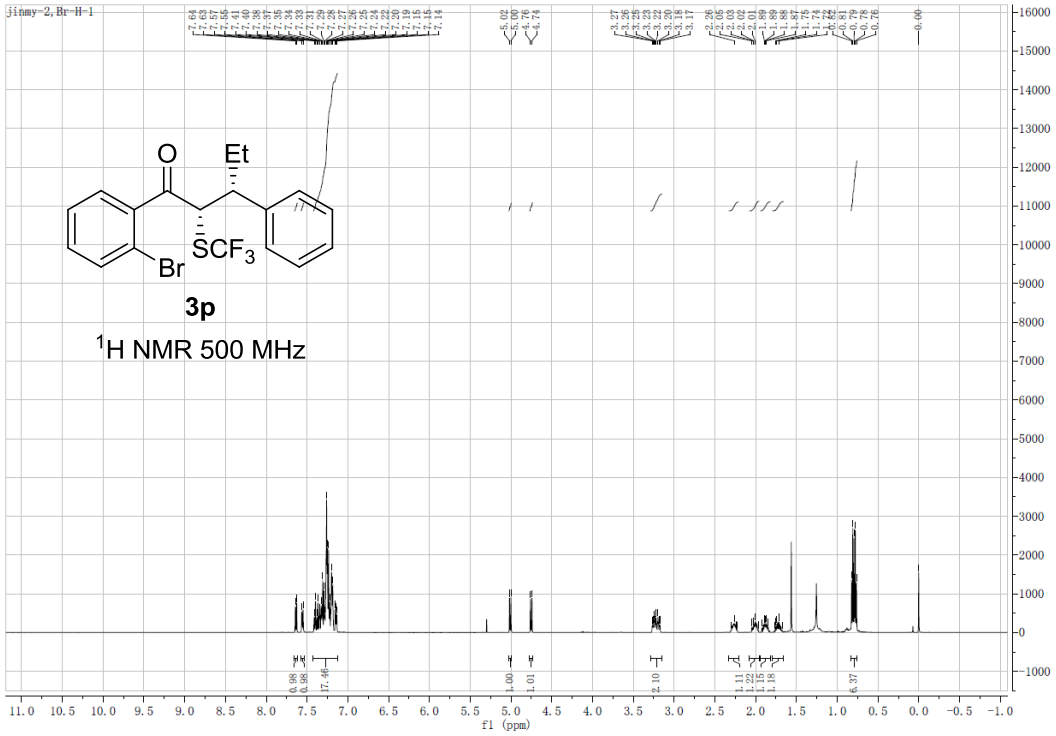
Additional Info : Peak(s) manually integrated

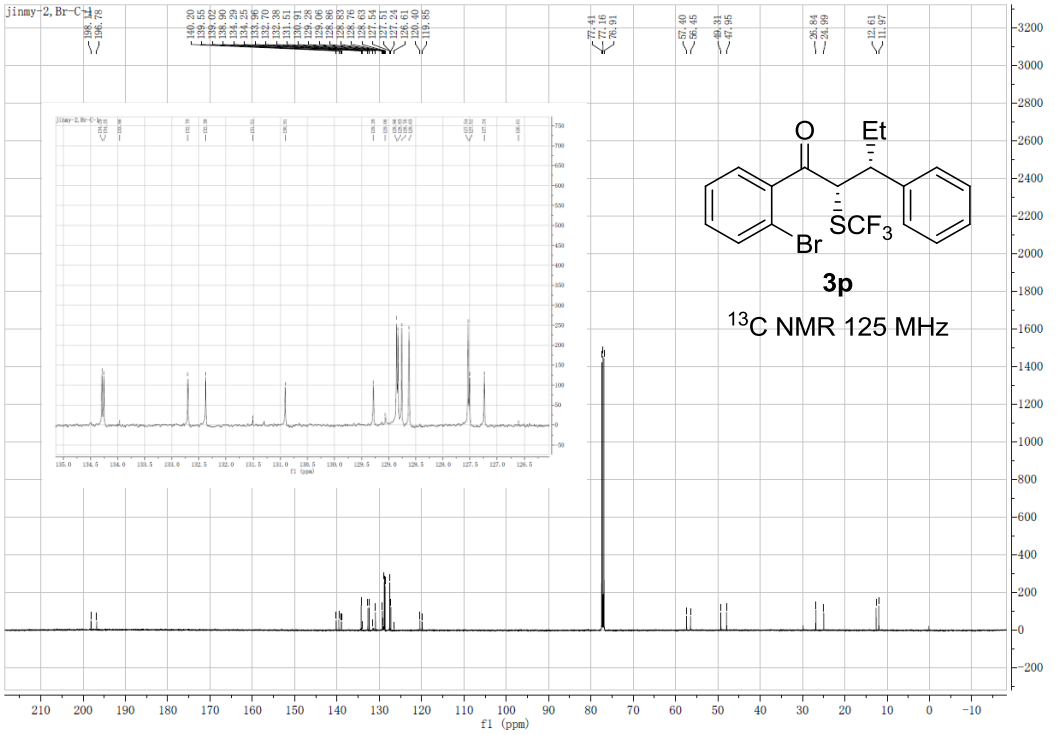


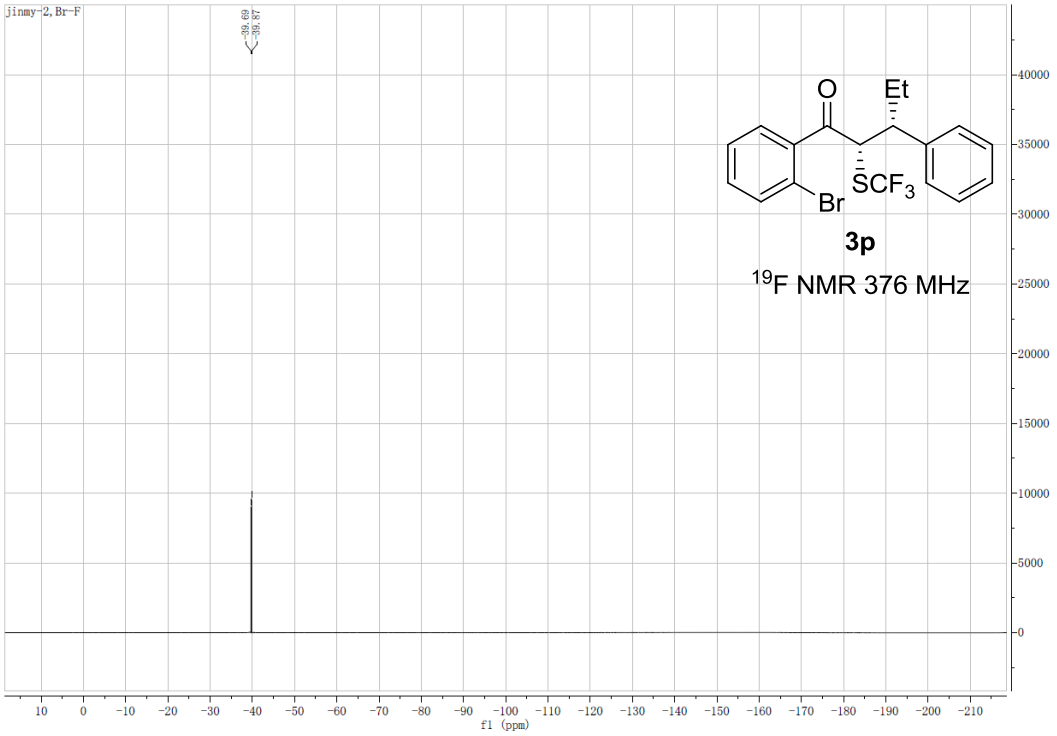
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

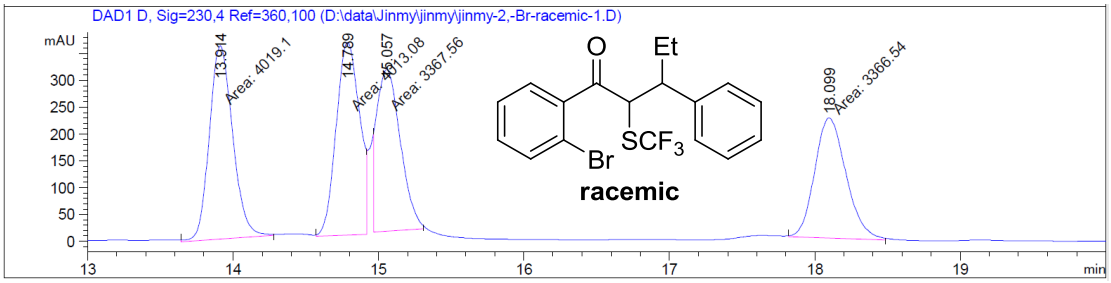
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.015	BV	0.1843	611.29681	51.56868	2.7307
2	12.641	VV	0.1716	2.17747e4	1991.00195	97.2693
Totals :				2.23860e4	2042.57063	


jinmy-2,Br-H-1
O
Et
SCF3
Br
dr = 1:1
f1 (ppm)


jinmy-2,Br-H-1
O
Et
SCF3
Br
3p
1H NMR 500 MHz
f1 (ppm)

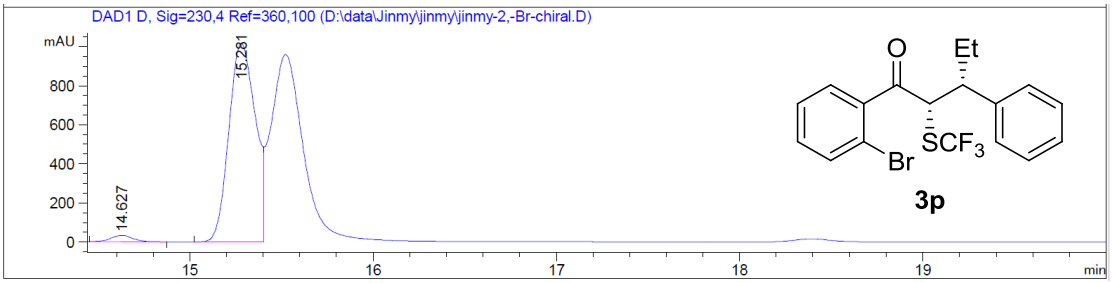

jinmy-2, Br-C-1
O
Et
SCF3
Br
3p
13C NMR 125 MHz
f1 (ppm)


jinmy-2, Br-F
-39.69
-39.87
O
Et
SCF3
Br
3p
19F NMR 376 MHz
f1 (ppm)



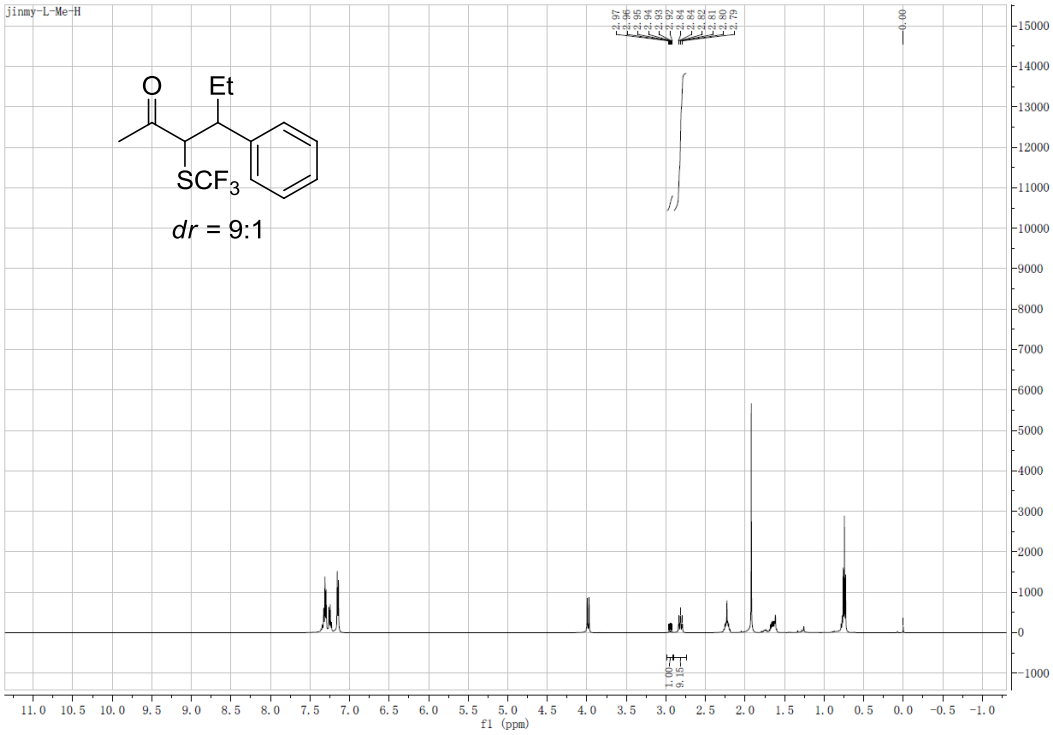
Signal 4: DAD1 D, Sig=230,4 Ref=360,100

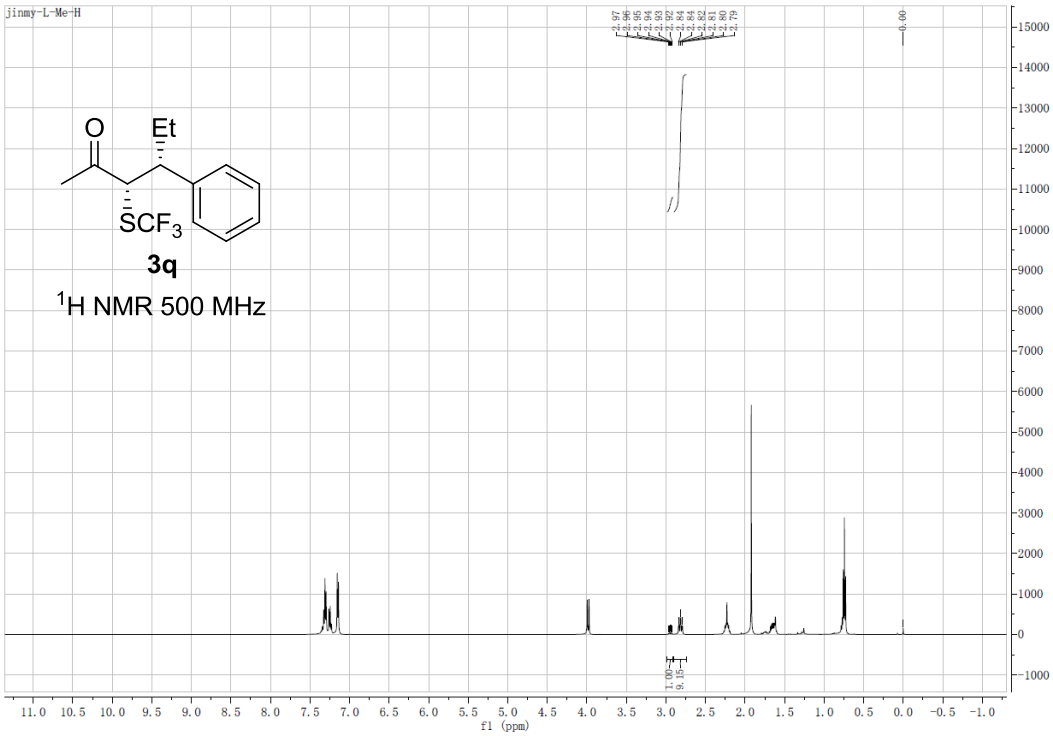
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.914	MM	0.1859	4019.09546	360.32767	27.2181
2	14.789	MM	0.1861	4013.07813	359.30582	27.1773
3	15.057	MM	0.1859	3367.56177	301.94159	22.8058
4	18.099	MM	0.2501	3366.53857	224.38652	22.7988
Totals :				1.47663e4	1245.96159	
Totals :				2108.31601	170.48021	

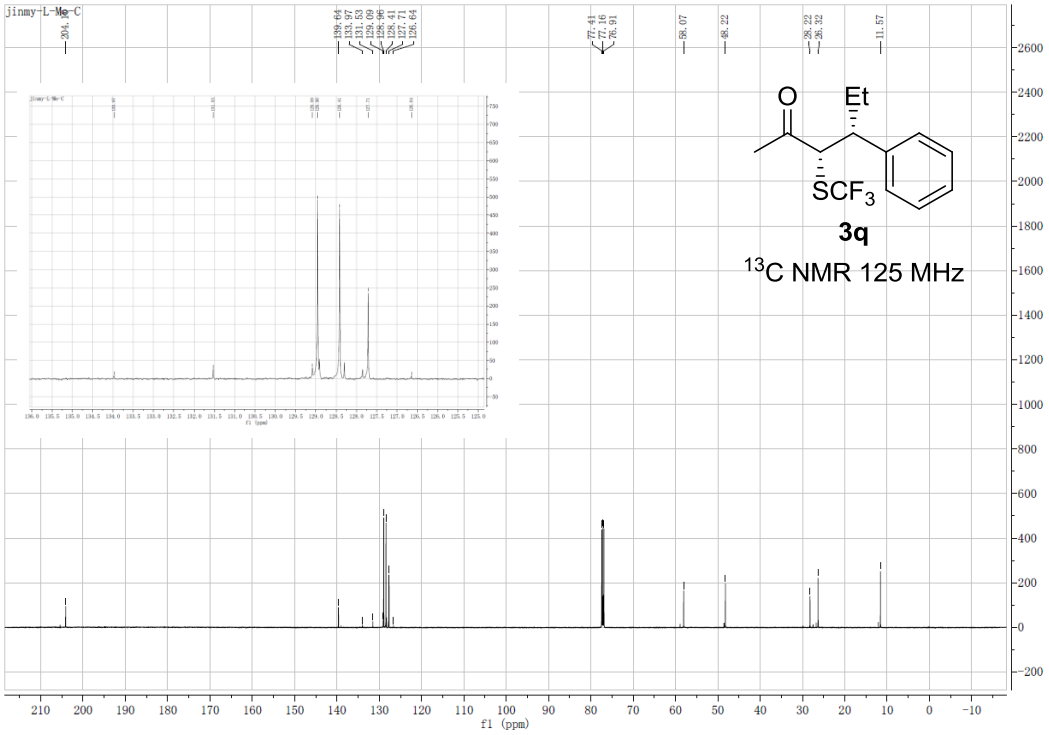


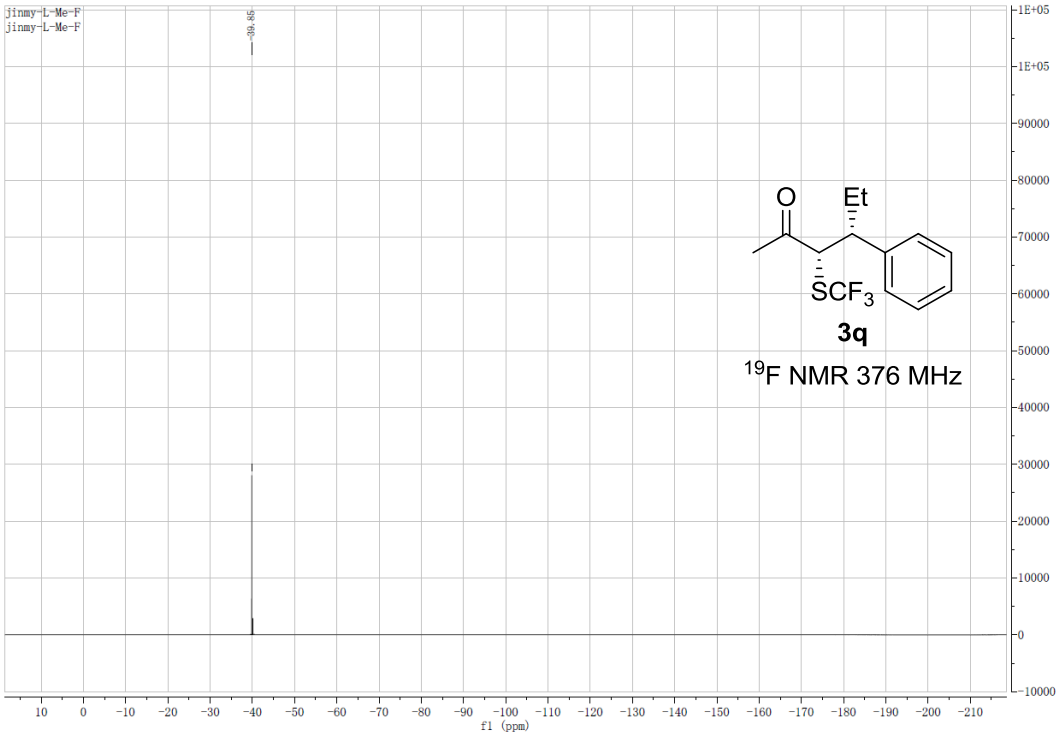
Signal 4: DAD1 D, Sig=230,4 Ref=360,100

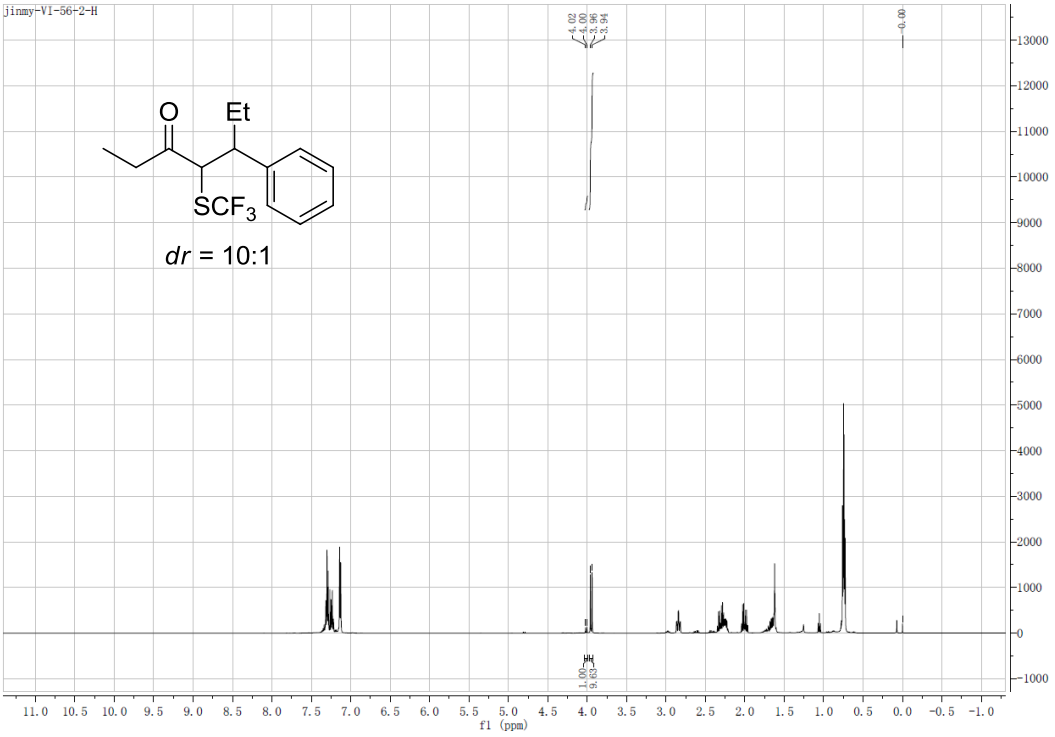
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.627	BB	0.1256	267.95401	32.68599	2.5470
2	15.281	BV	0.1534	1.02524e4	1018.96661	97.4530
Totals :				1.05203e4	1051.65260	

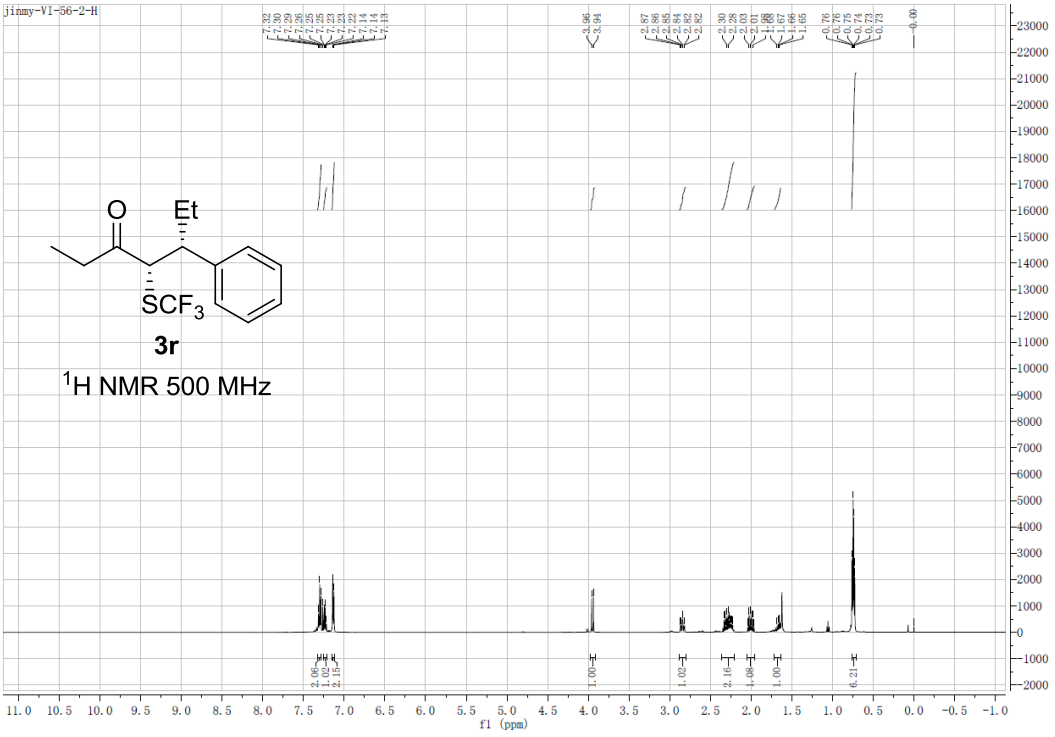

jinmy-L-Me-H
O
Et
SCF3
dr = 9:1
f1 (ppm)

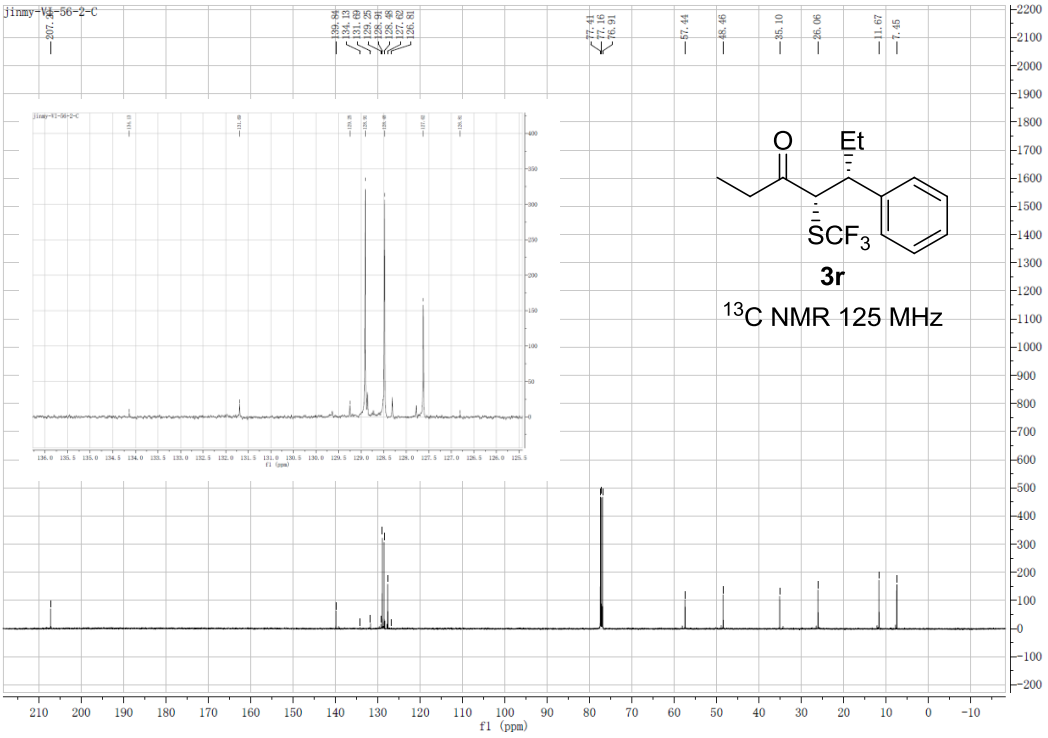

jinmy-L-Me-H
O
Et
SCF3
3q
1H NMR 500 MHz
f1 (ppm)

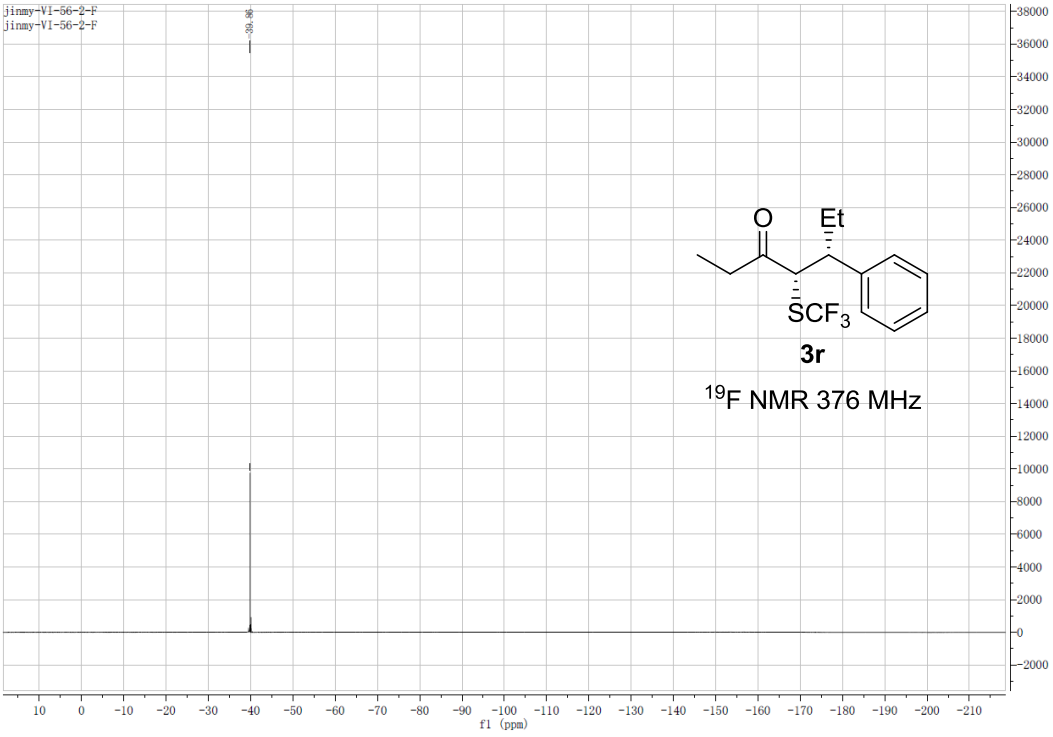

jinmy-L-Me-C
O
Et
SCF3
3q
13C NMR 125 MHz
f1 (ppm)

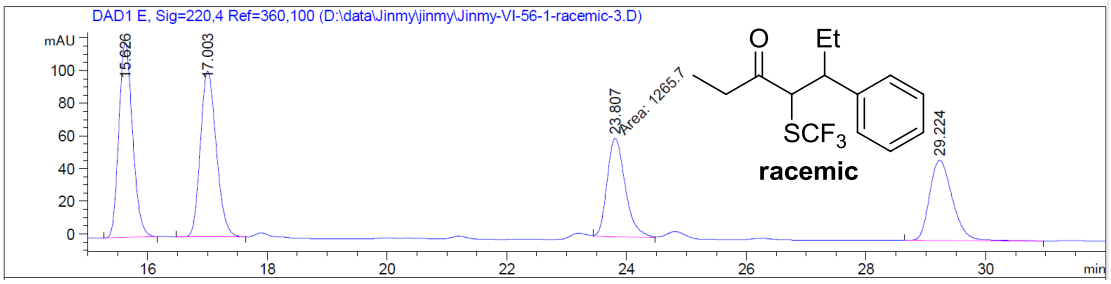

jinmy-L-Me-F
jinmy-L-Me-F
-39.86
O
Et
SCF3
3q
19F NMR 376 MHz
f1 (ppm)


jinmy-V1-56+2-H
O
Et
SCF3
dr = 10:1
f1 (ppm)


jinmy-V1-56-2-H
O
Et
SCF3
3r
1H NMR 500 MHz
f1 (ppm)

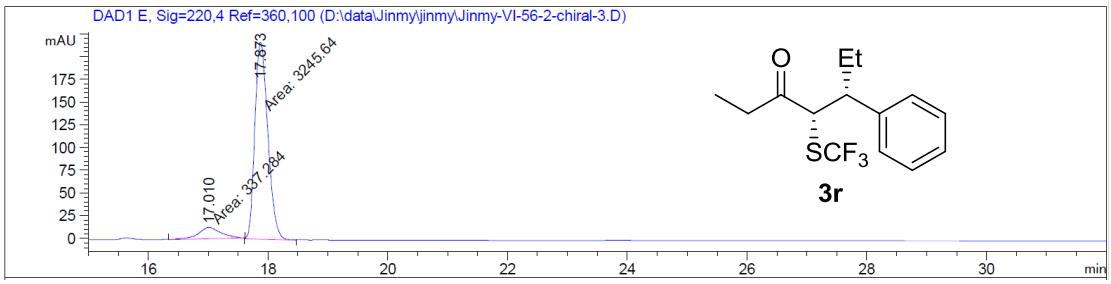

jinmy-V1-56-2-C
O
Et
SCF3
3r
13C NMR 125 MHz
f1 (ppm)


jinmy-V1-56-2-F
jinmy-V1-56-2-F
O
Et
SCF3
3r
19F NMR 376 MHz
f1 (ppm)



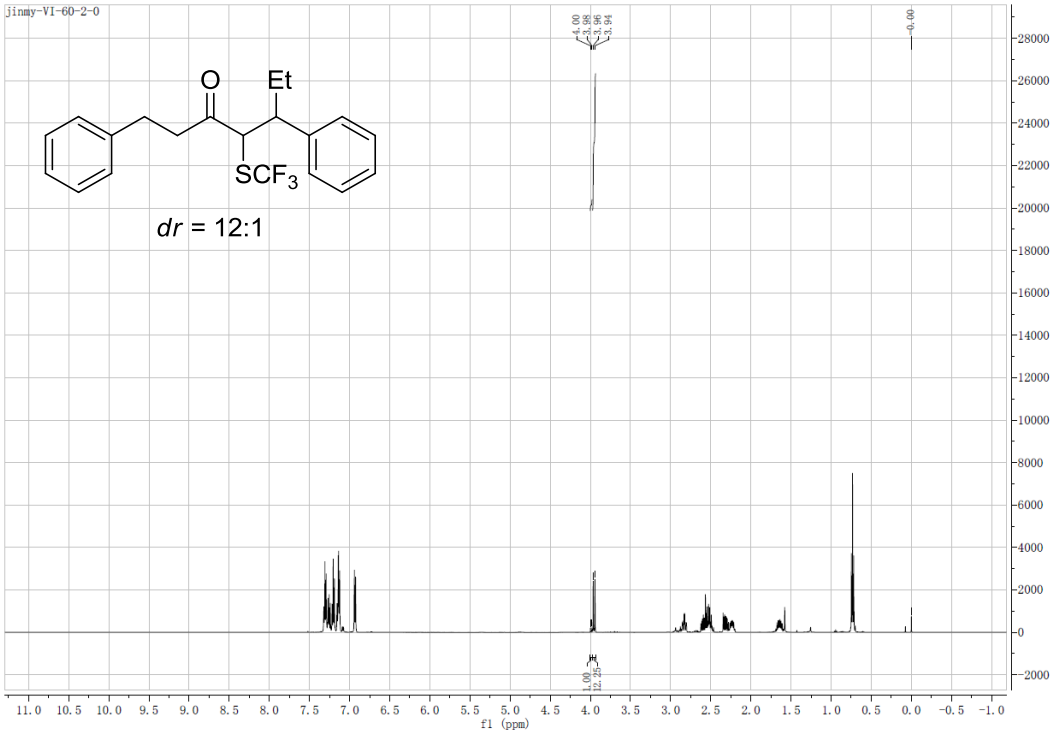
Signal 5: DAD1 E, Sig=220,4 Ref=360,100

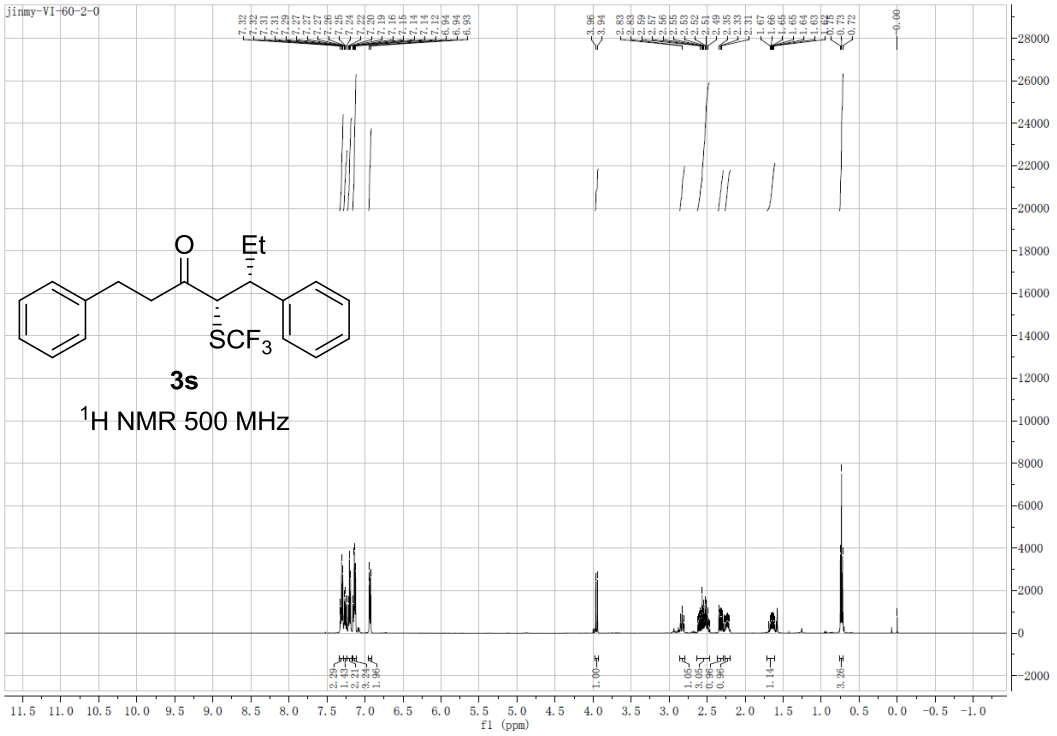
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.626	BB	0.2477	1897.62854	119.19968	30.0114
2	17.003	BB	0.2871	1869.73047	101.38798	29.5702
3	23.807	MM	0.3502	1265.69812	60.23948	20.0173
4	29.224	BB	0.4112	1289.97009	48.98400	20.4011
Totals :				6323.02722	329.81113	

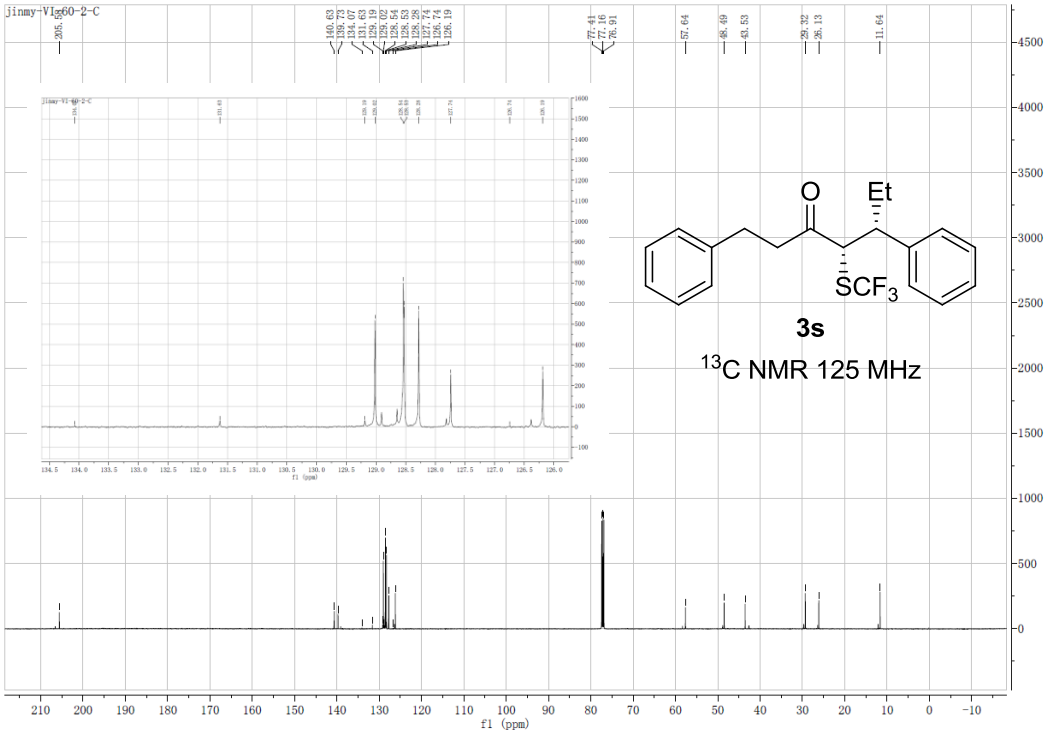


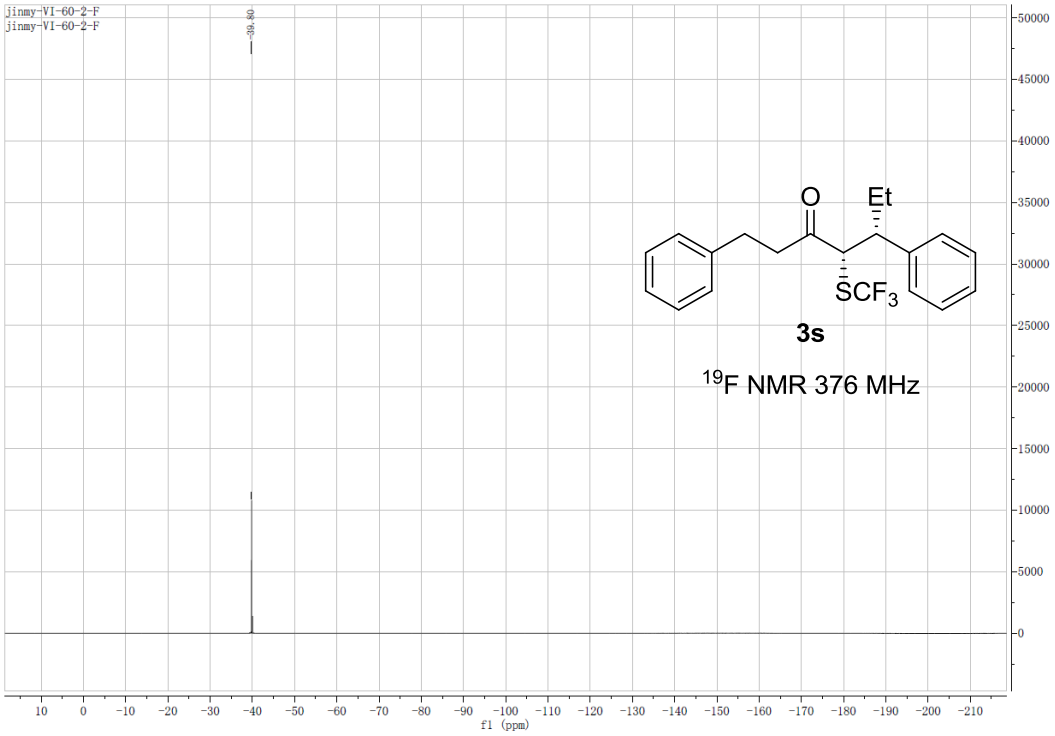
Signal 5: DAD1 E, Sig=220,4 Ref=360,100

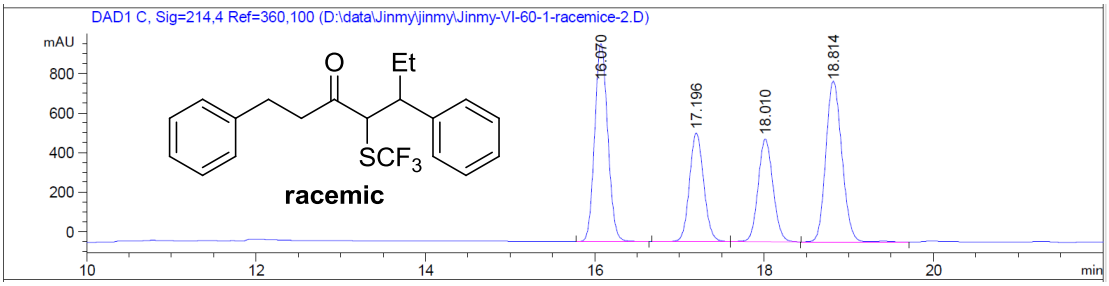
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.010	MM	0.4522	337.28418	12.43009	9.4136
2	17.873	MM	0.2502	3245.64355	216.18810	90.5864
Totals :				3582.92773	228.61819	


jinmy-VI-60-2-0
O
Et
SCF3
dr = 12:1
f1 (ppm)


jinmy-VI-60-2-0
O
Et
SCF3
3s
1H NMR 500 MHz
f1 (ppm)

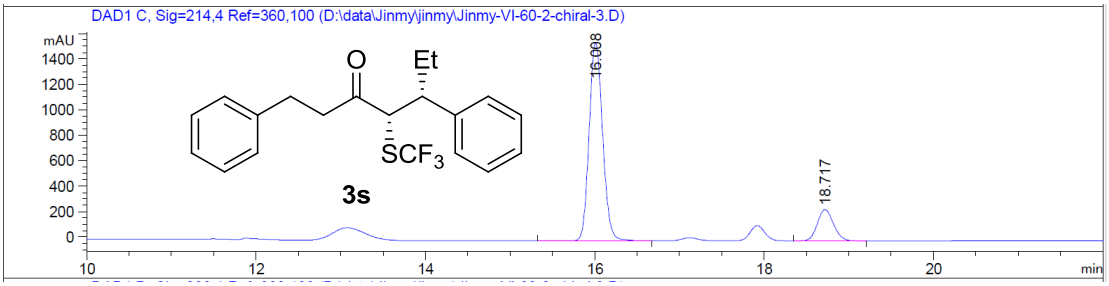

jinmy-VI-60-2-C
O
Et
SCF3
3s
13C NMR 125 MHz
f1 (ppm)


jinmy-VI-60-2-F
jinmy-VI-60-2-F
-39.80
O
Et
SCF3
3s
19F NMR 376 MHz
f1 (ppm)



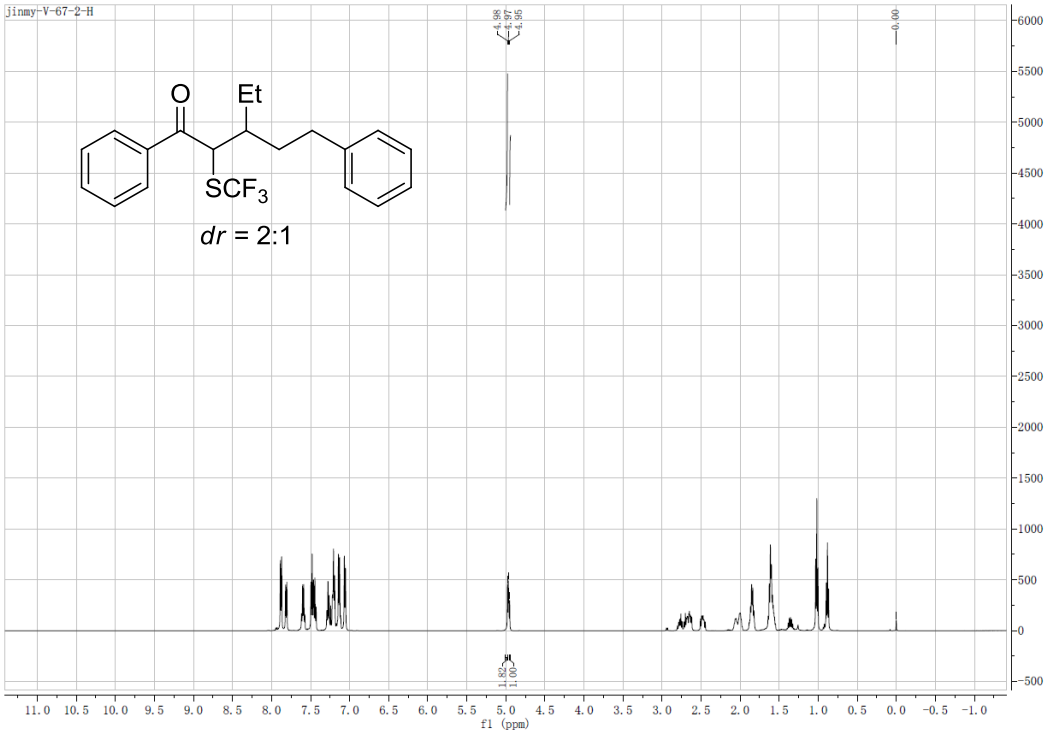
Signal 3: DAD1 C, Sig=214,4 Ref=360,100

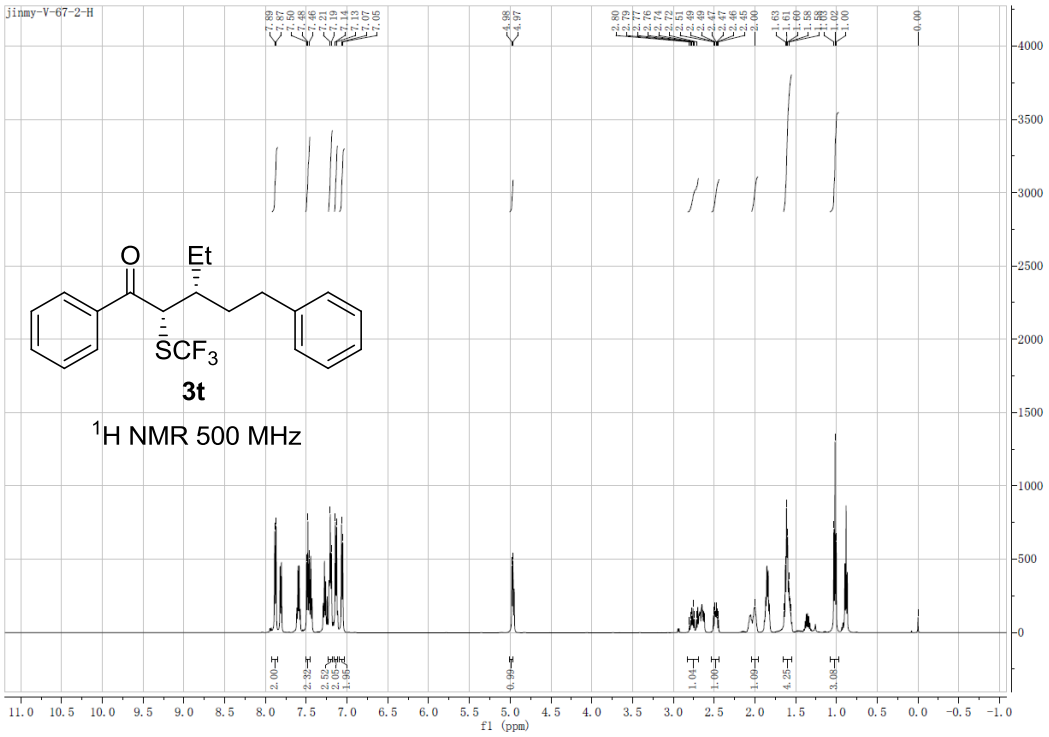
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.070	BB	0.1673	1.07411e4	1000.28418	31.3651
2	17.196	BB	0.1803	6410.46240	548.59351	18.7193
3	18.010	BB	0.1905	6341.50635	519.21130	18.5179
4	18.814	BV R	0.2055	1.07522e4	812.37714	31.3977
Totals :				3.42452e4	2880.46613	

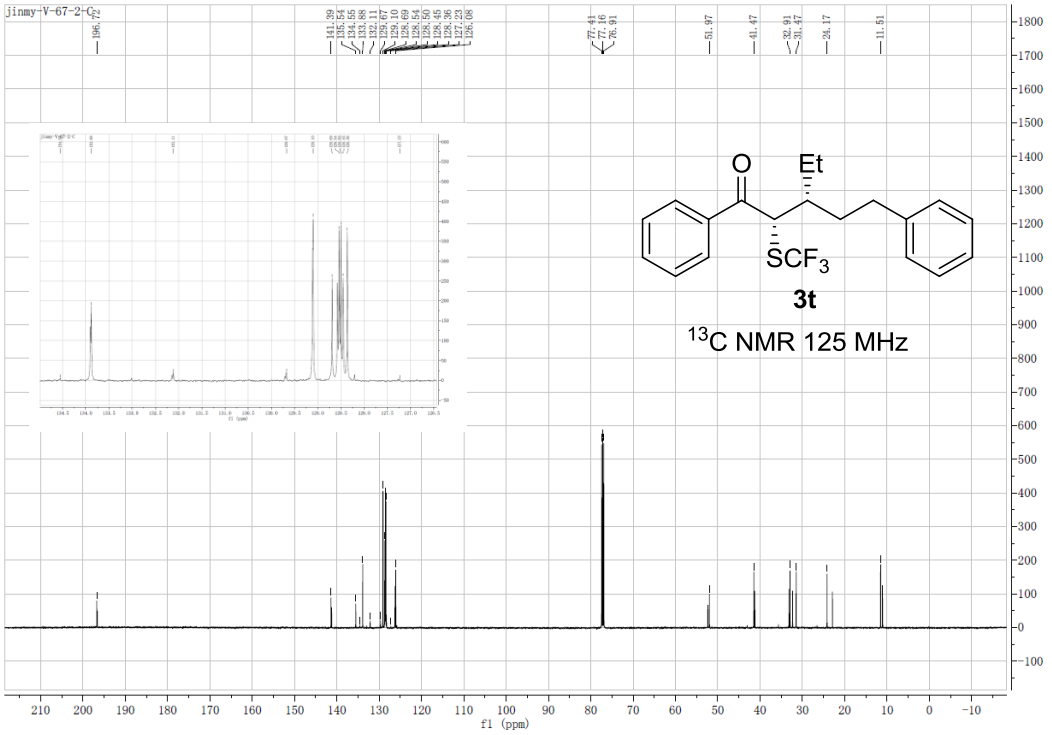


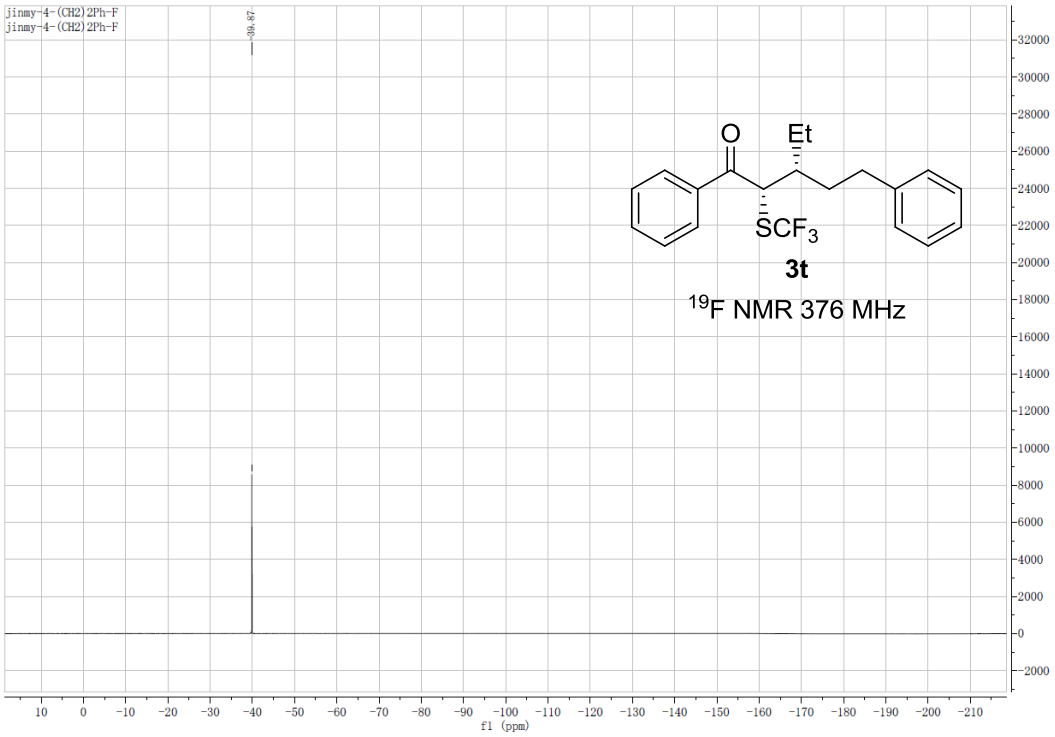
Signal 3: DAD1 C, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.008	BB	0.1703	1.71281e4	1558.08276	84.0485
2	18.717	BB	0.2063	3250.72852	245.76860	15.9515
Totals :				2.03788e4	1803.85136	


jinmy-V-67-2-H
O
Et
SCF3
dr = 2:1
f1 (ppm)

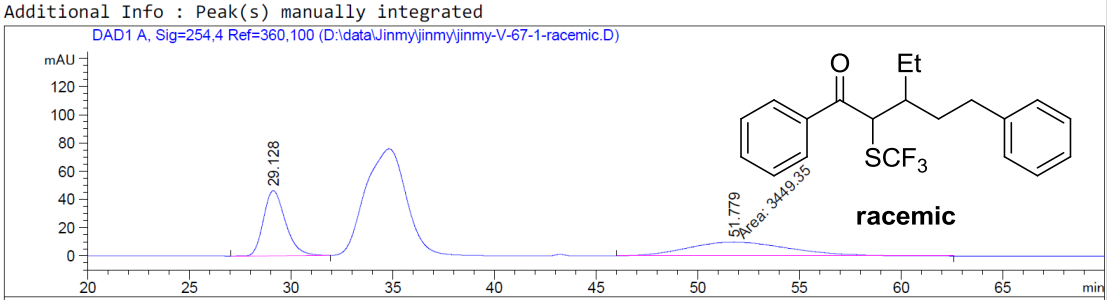

jinmy-V-67-2-H
O
Et
SCF3
3t
1H NMR 500 MHz
f1 (ppm)


jinmy-V-67-2-C13
196.47
141.39
135.54
134.55
133.88
132.11
129.67
129.10
128.69
128.54
128.50
128.45
128.36
127.23
126.08
77.41
77.16
76.91
51.97
41.47
32.91
32.47
26.17
11.51
O
Et
SCF3
3t
13C NMR 125 MHz
f1 (ppm)


jinmy-4-(CH2)2Ph-F
jinmy-4-(CH2)2Ph-F
-39.87
O
Et
SCF3
3t
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

Additional Info : Peak(s) manually integrated

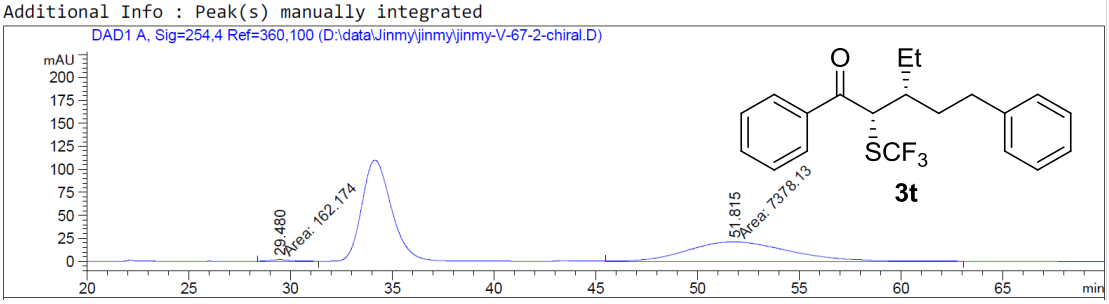


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.128	BB	1.1430	3463.46875	46.18130	50.1021
2	51.779	MM	5.8408	3449.34985	9.84266	49.8979
Totals :				6912.81860	56.02396	

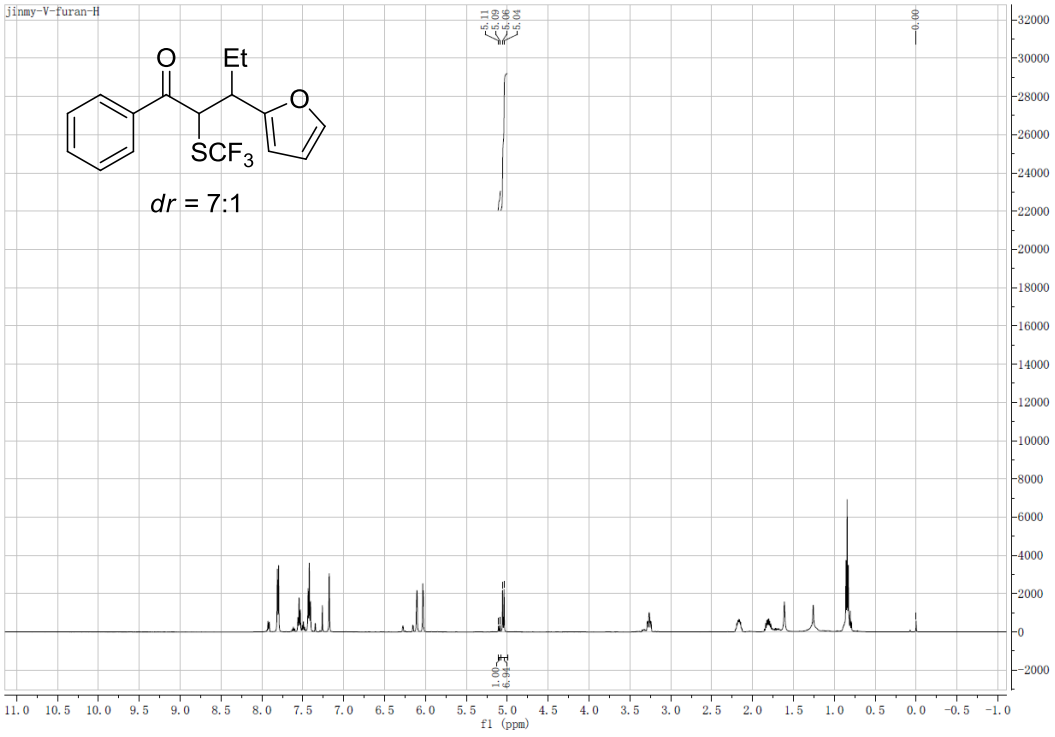
Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

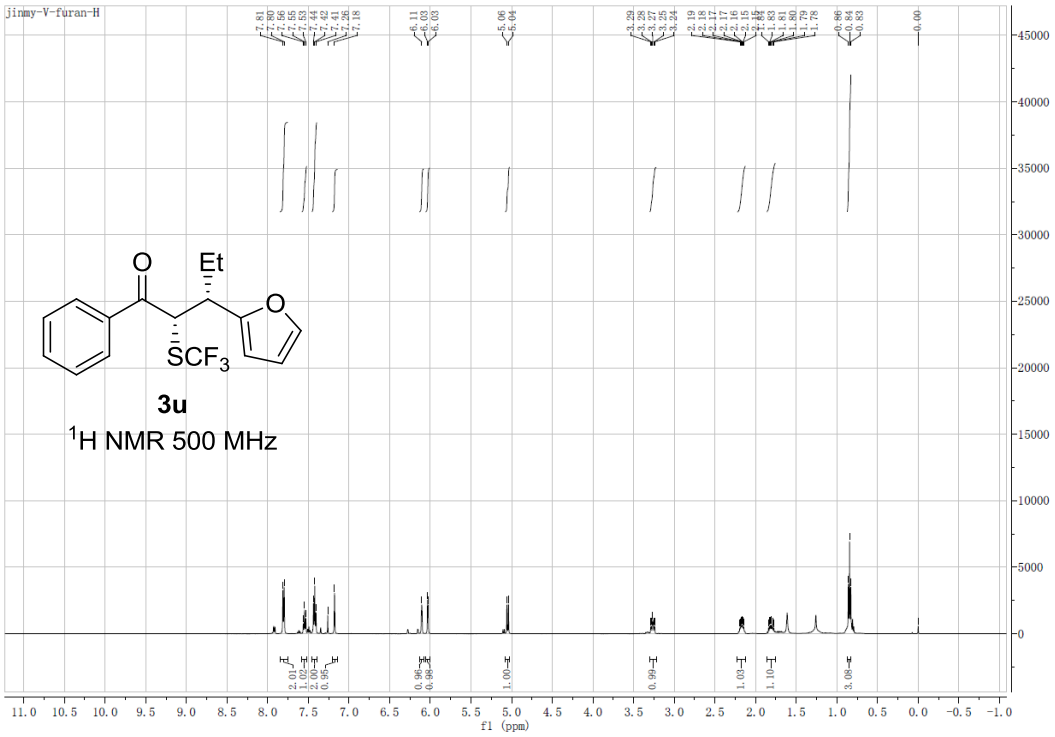
Additional Info : Peak(s) manually integrated

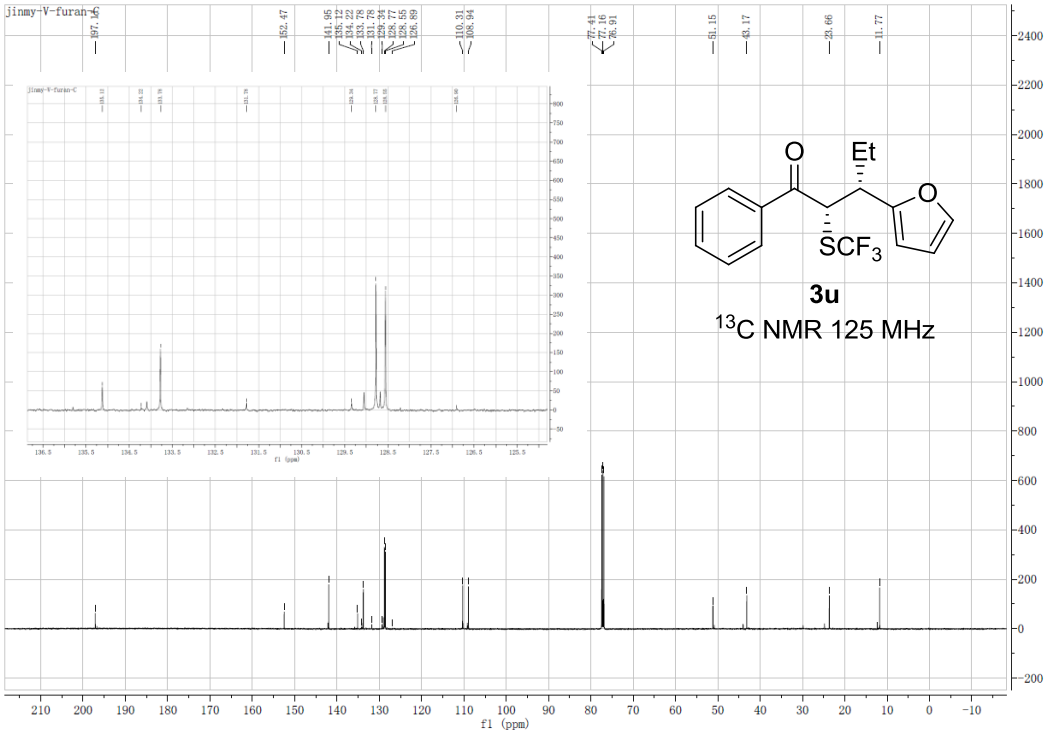


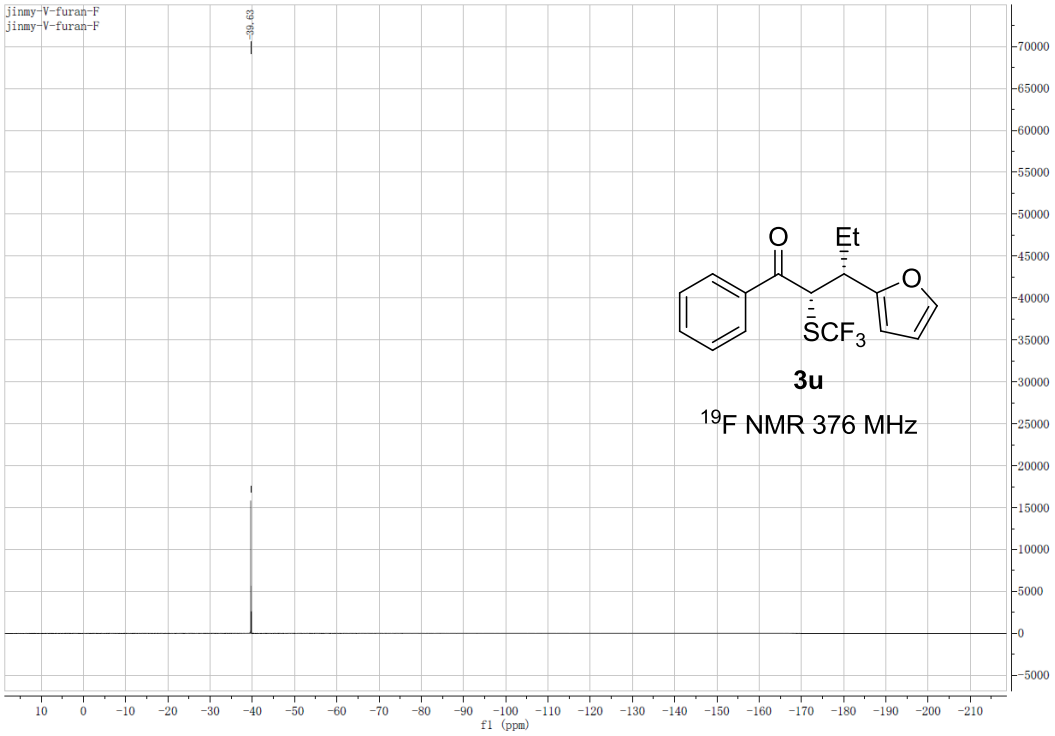
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.480	MM	1.4477	162.17418	1.86698	2.1508
2	51.815	MM	5.8323	7378.13086	21.08426	97.8492
Totals :				7540.30504	22.95124	


jinmy-V-furan-H
O
Et
O
SCF3
dr = 7:1
f1 (ppm)

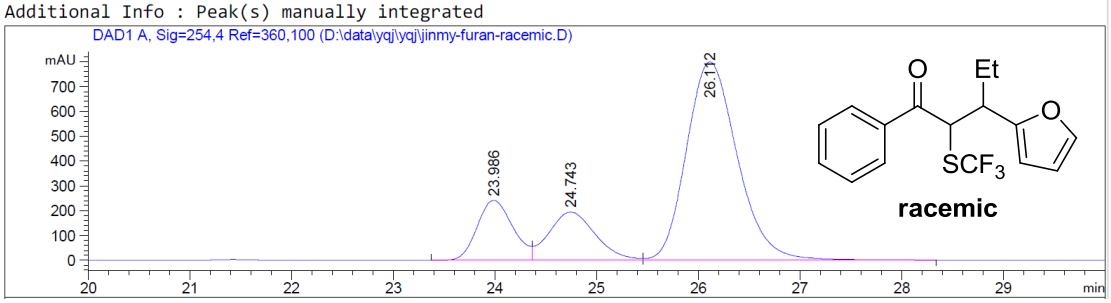

jinmy-V-furan-H
O
Et
O
SCF3
3u
1H NMR 500 MHz
f1 (ppm)


jinmy-V-furan-C
O
Et
O
SCF3
3u
13C NMR 125 MHz
f1 (ppm)


jinmy-V-furan-F
jinmy-V-furan-F
-39.63
O
Et
O
SCF3
3u
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

Additional Info : Peak(s) manually integrated

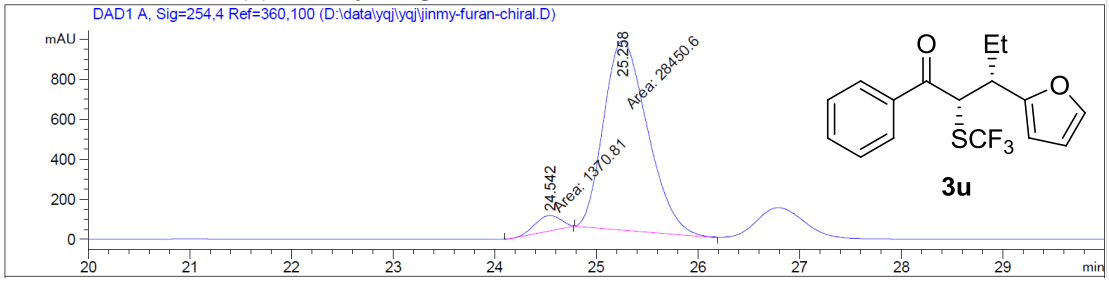


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.986	BV	0.3755	5882.55420	242.11627	14.7851
2	24.743	VV	0.4861	6157.98145	194.13998	15.4774
3	26.112	VB	0.5389	2.77465e4	799.55847	69.7375
Totals :				3.97870e4	1235.81473	

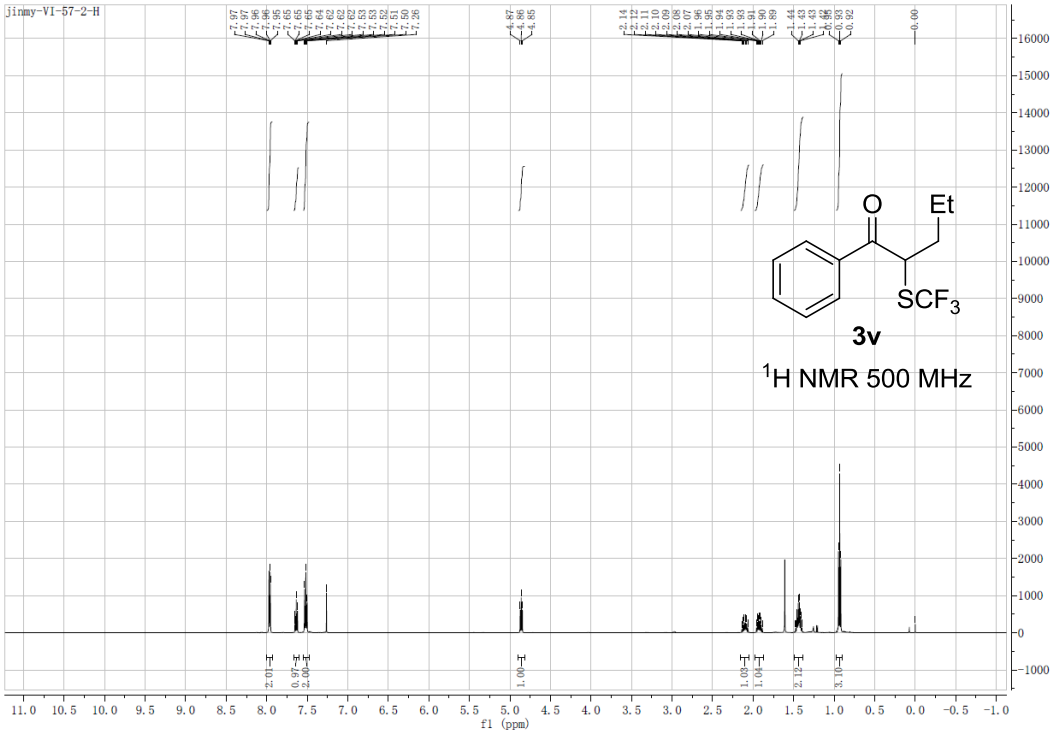
Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

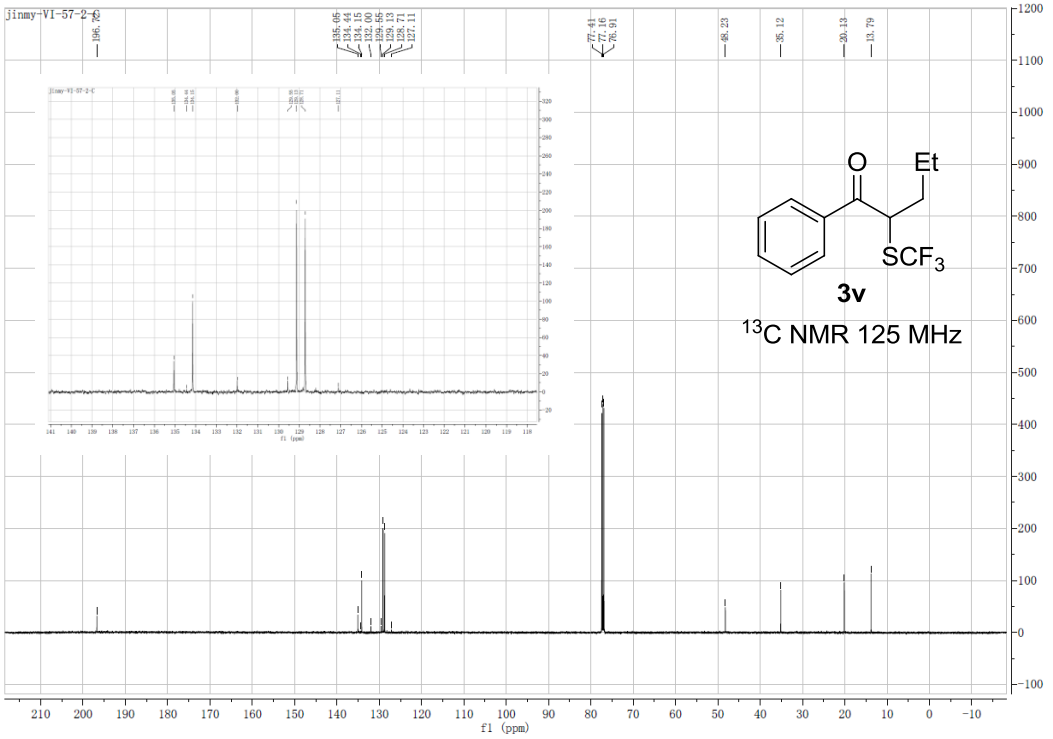
Additional Info : Peak(s) manually integrated

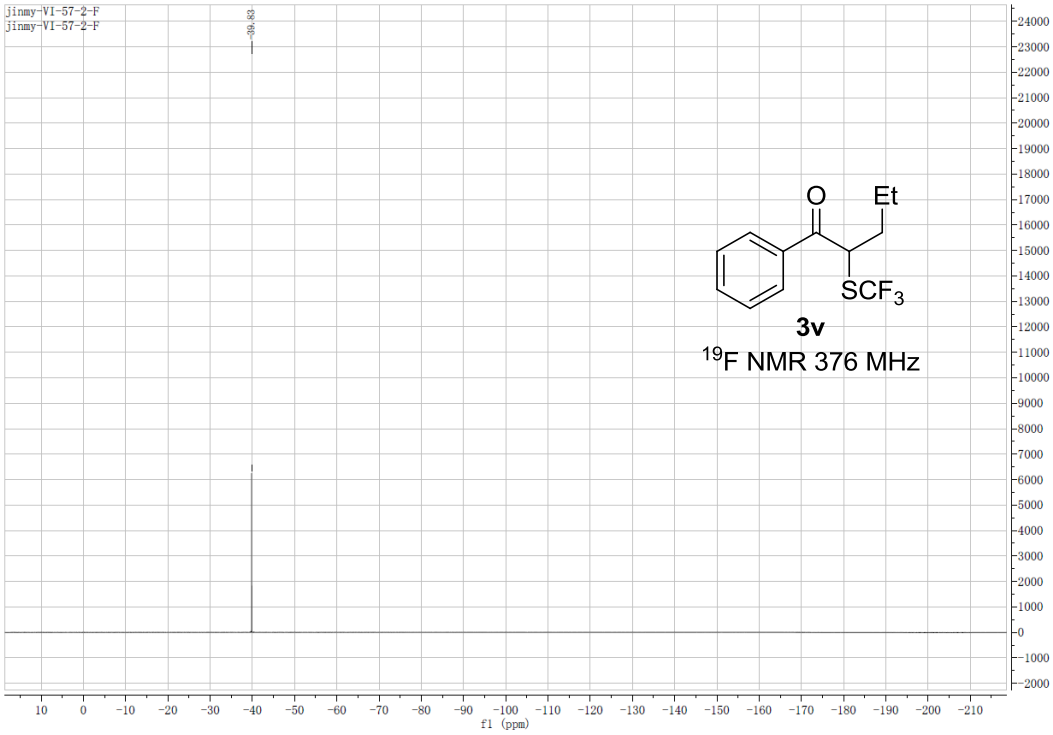


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.542	MM	0.2961	1370.81189	77.15406	4.5967
2	25.258	MM	0.5007	2.84506e4	946.95856	95.4033
Totals :				2.98214e4	1024.11262	

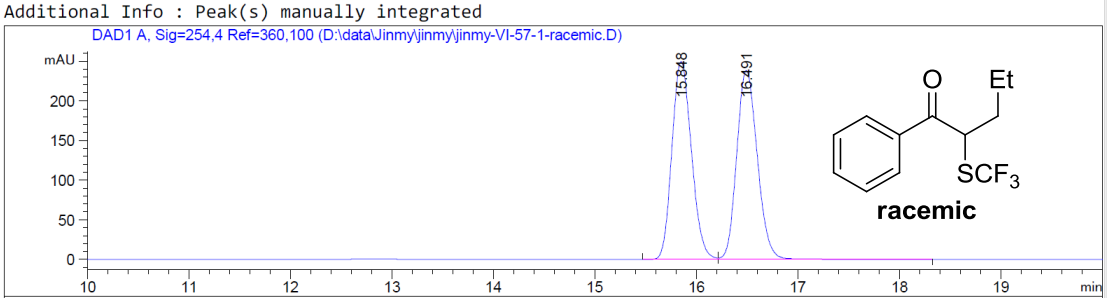

jinmy-VI-57-2-H
O
Et
SCF3
3v
1H NMR 500 MHz
f1 (ppm)


jinmy-VI-57-2-C
O
Et
SCF3
3v
13C NMR 125 MHz
f1 (ppm)


jinmy-VI-57-2-F
jinmy-VI-57-2-F
-39.83
O
Et
SCF3
3v
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

Additional Info : Peak(s) manually integrated

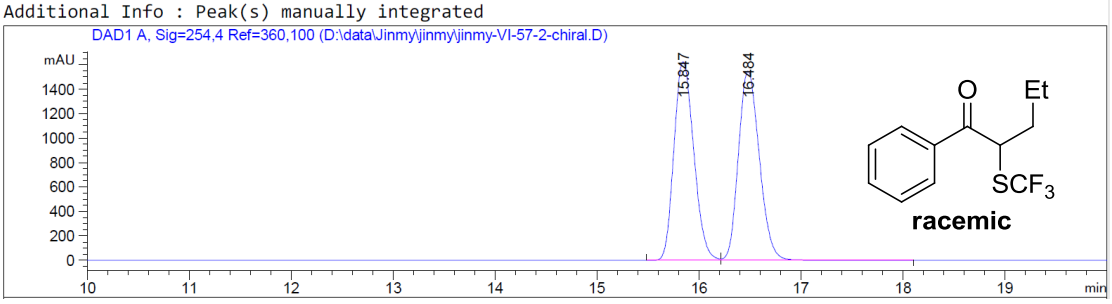


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.848	BV	0.2097	3326.15869	249.30450	49.7929
2	16.491	VB	0.2203	3353.83228	238.11264	50.2071
Totals :				6679.99097	487.41714	

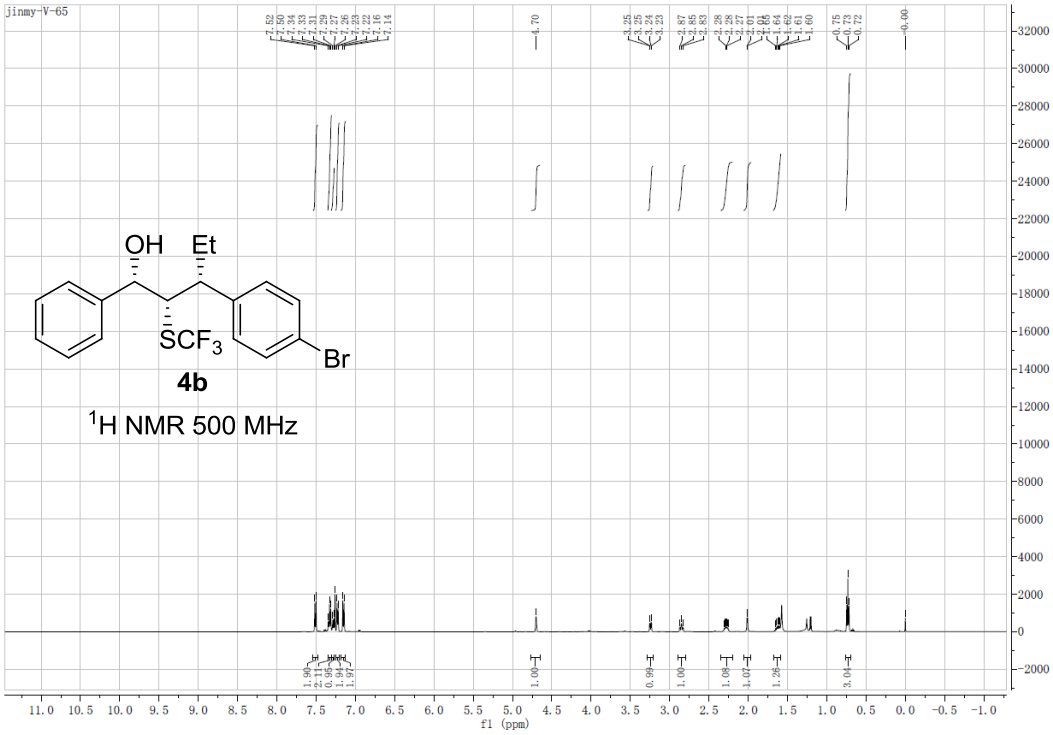
Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

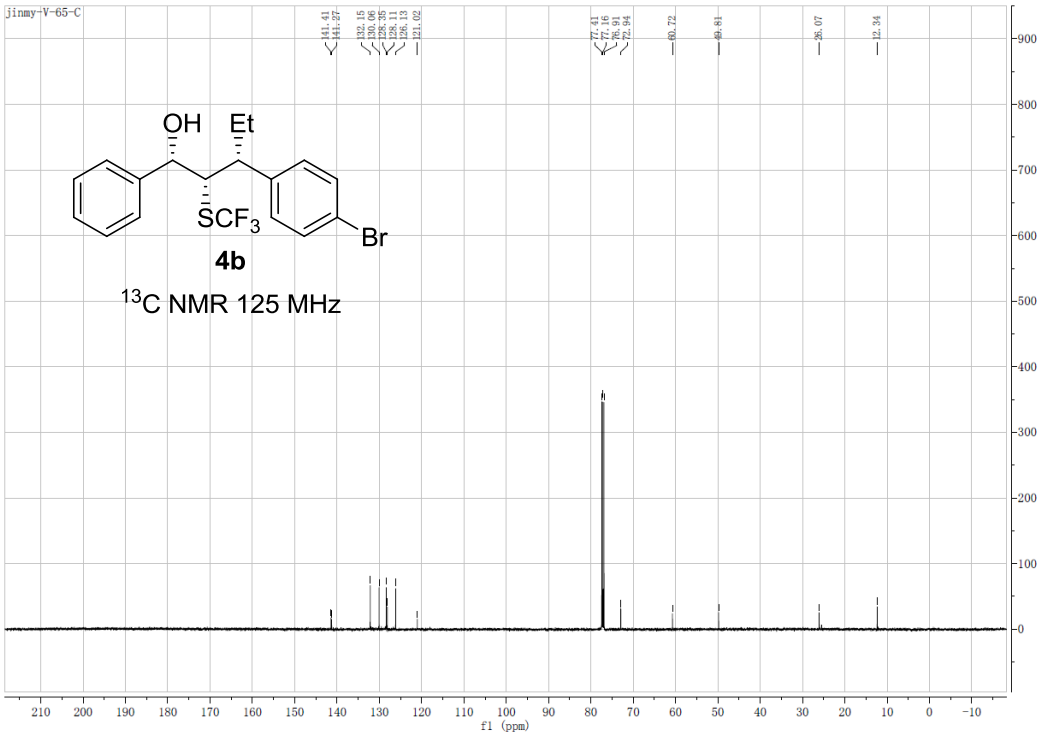
Additional Info : Peak(s) manually integrated

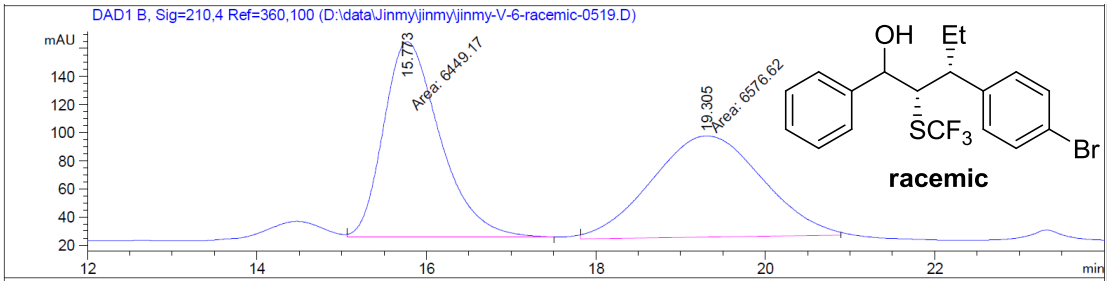


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.847	BV	0.2132	2.18741e4	1623.91028	49.8263
2	16.484	VB	0.2242	2.20266e4	1546.38965	50.1737
Totals :				4.39007e4	3170.29993	

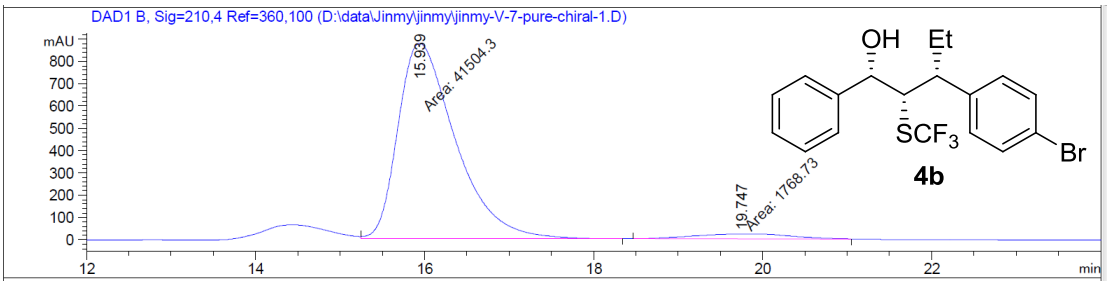

jinmy-V-65
OH
Et
SCF3
Br
4b
1H NMR 500 MHz
f1 (ppm)


jinmy-V-65-C
OH
Et
SCF3
Br
4b
13C NMR 125 MHz
f1 (ppm)



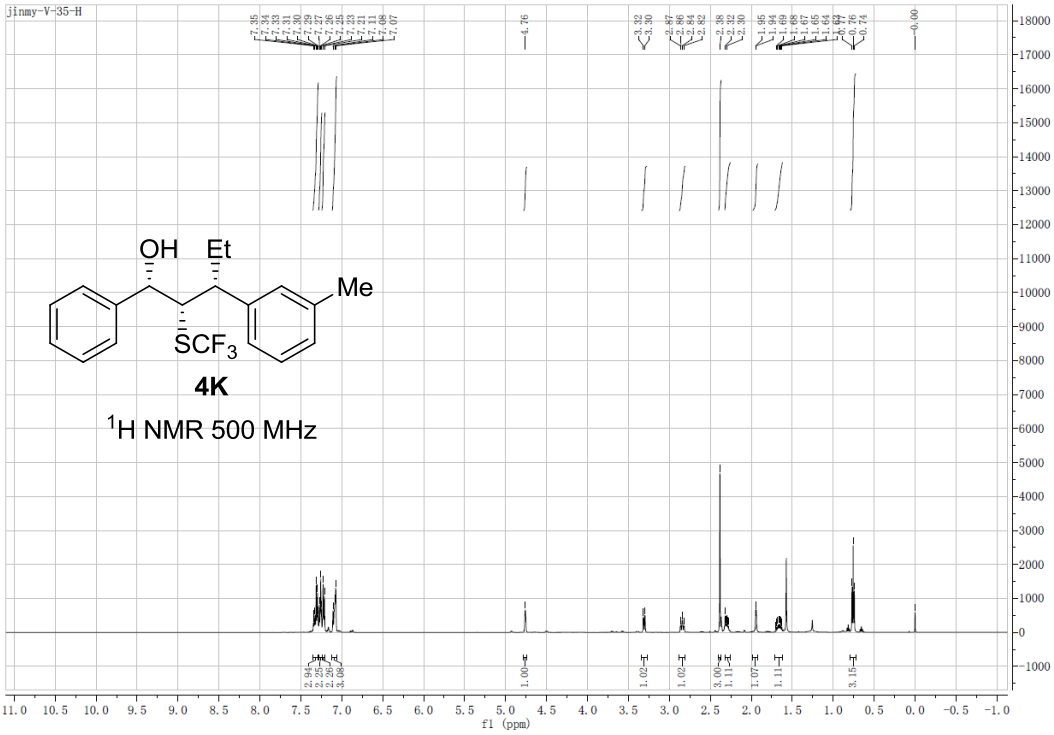
Signal 2: DAD1 B, Sig=210,4 Ref=360,100

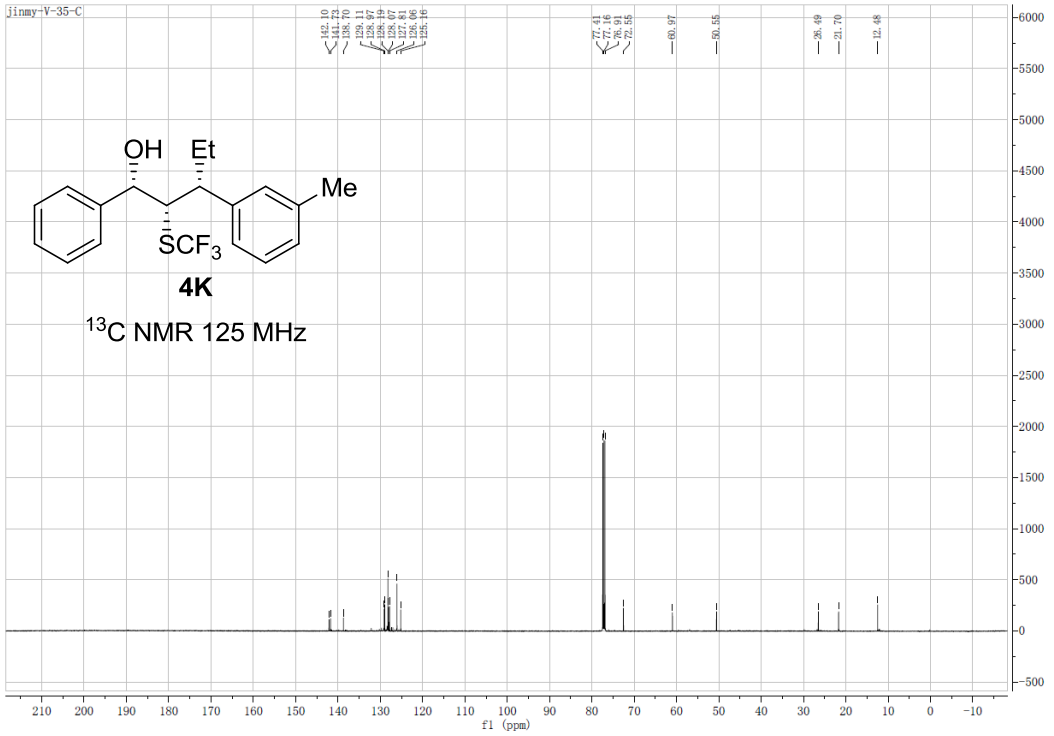
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.773	MM	0.7734	6449.17188	138.97356	49.5108
2	19.305	MM	1.5213	6576.61523	72.05170	50.4892
Totals :				1.30258e4	211.02525	

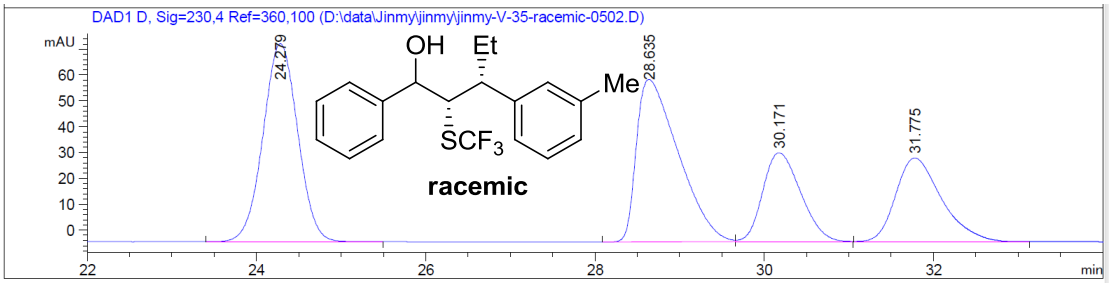


Signal 2: DAD1 B, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.939	MM	0.7882	4.15043e4	877.56958	95.9126
2	19.747	MM	1.3379	1768.72864	22.03446	4.0874
Totals :				4.32731e4	899.60404	

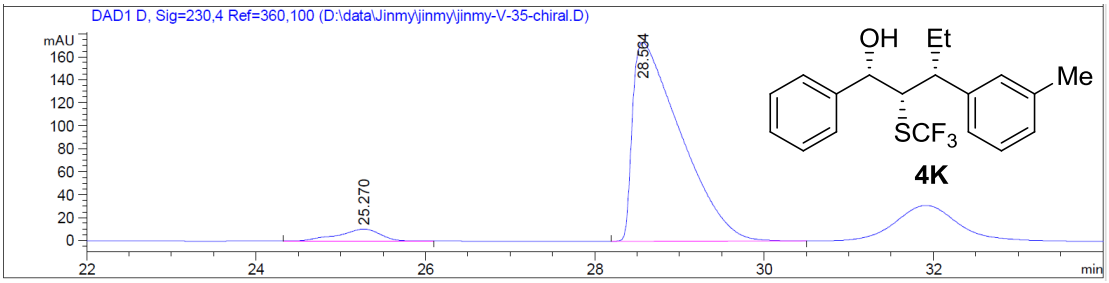

jinmy-V-35-H
OH
Et
Me
SCF3
4K
1H NMR 500 MHz
f1 (ppm)


jinmy-V-35-C
OH
Et
Me
SCF3
4K
13C NMR 125 MHz
f1 (ppm)



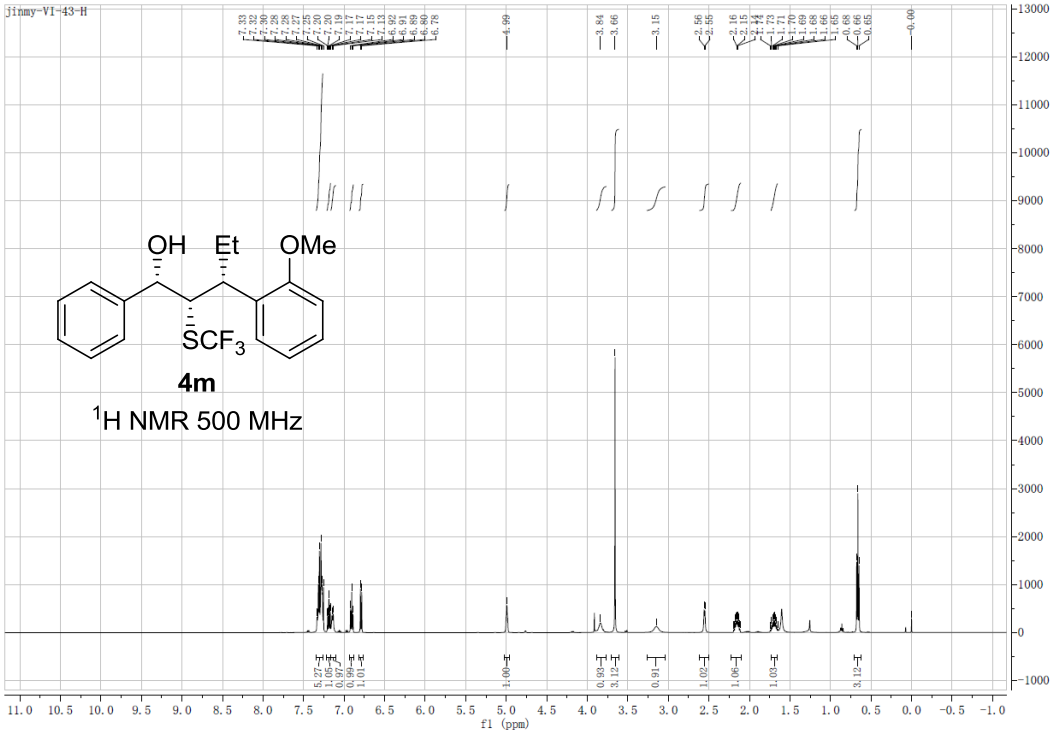
Signal 4: DAD1 D, Sig=230,4 Ref=360,100

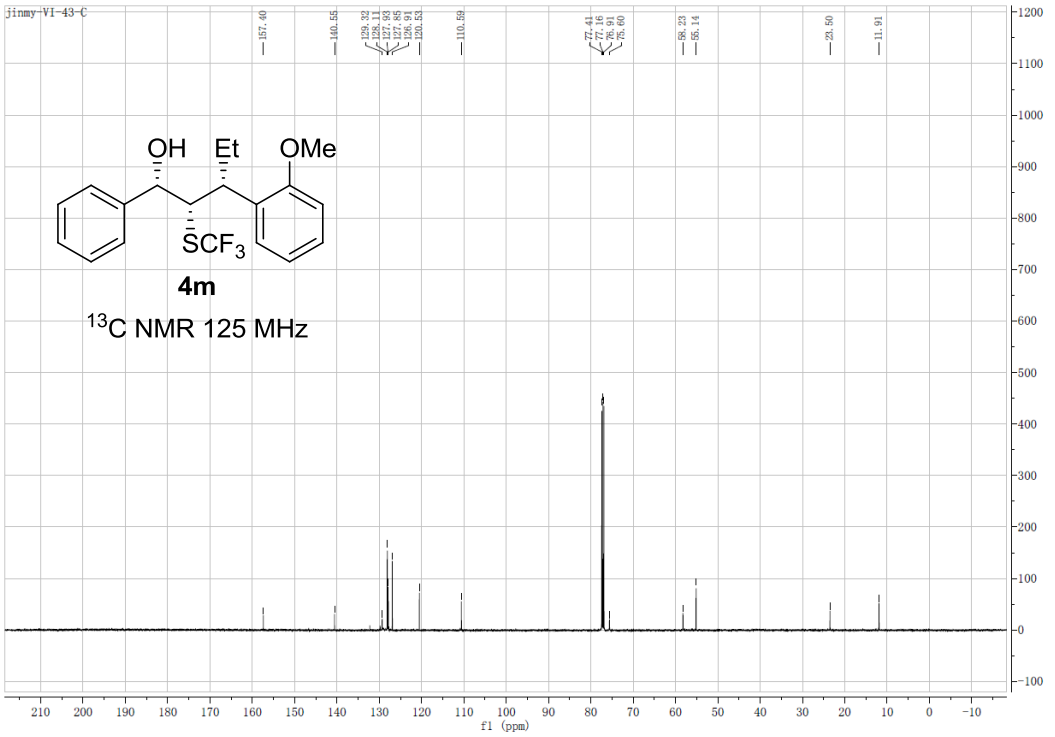
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.279	BB	0.4445	2184.55518	76.66001	32.9312
2	28.635	BV	0.5257	2165.48560	62.89725	32.6437
3	30.171	VB	0.4881	1067.77283	34.40182	16.0962
4	31.775	BB	0.5726	1215.88977	32.34079	18.3290
Totals :				6633.70337	206.29987	

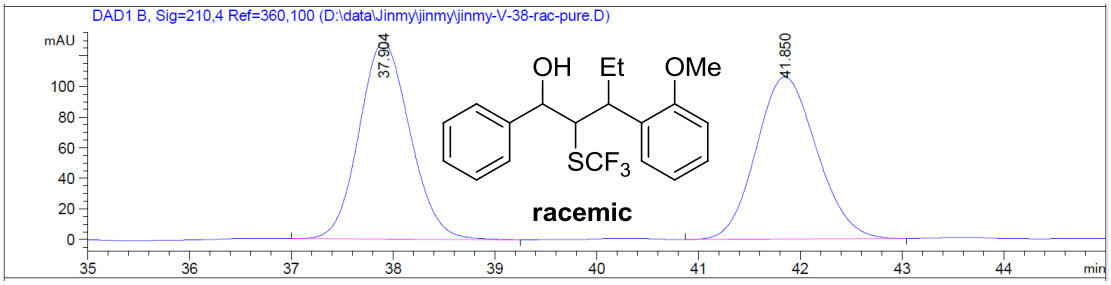


Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.270	BB	0.5105	356.16232	10.32475	4.9238
2	28.564	BB	0.5912	6877.34326	173.21690	95.0762
Totals :				7233.50558	183.54165	

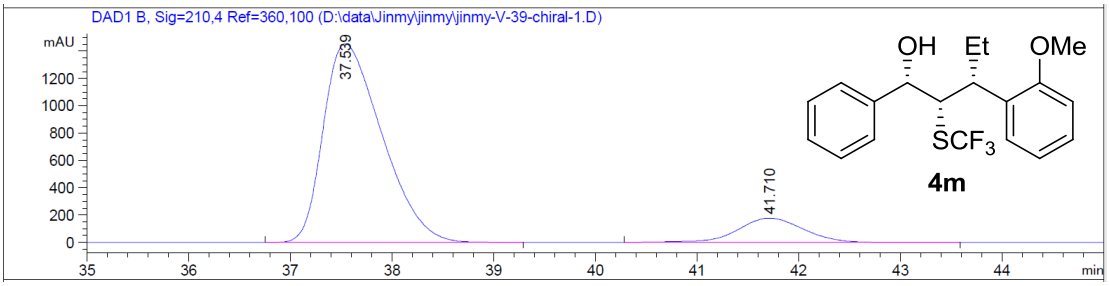

jinmy-VI-43-H
OH
Et
OMe
SCF3
4m
1H NMR 500 MHz
f1 (ppm)


jinmy-VI-43-C
OH
Et
OMe
SCF3
4m
13C NMR 125 MHz
f1 (ppm)



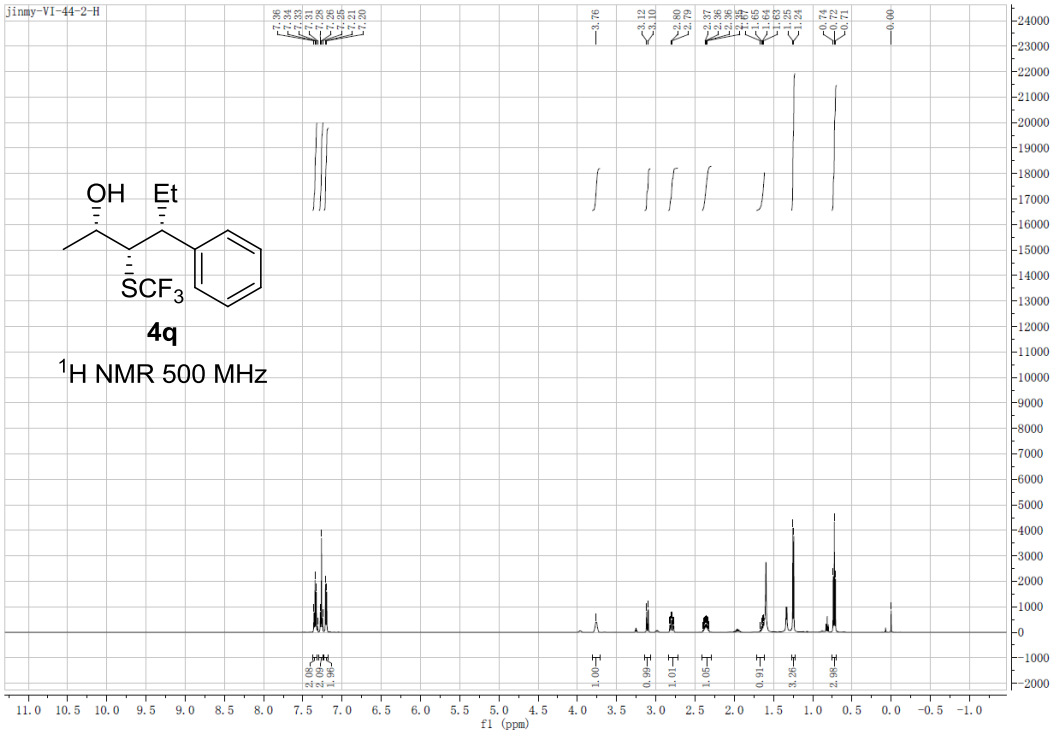
Signal 2: DAD1 B, Sig=210,4 Ref=360,100

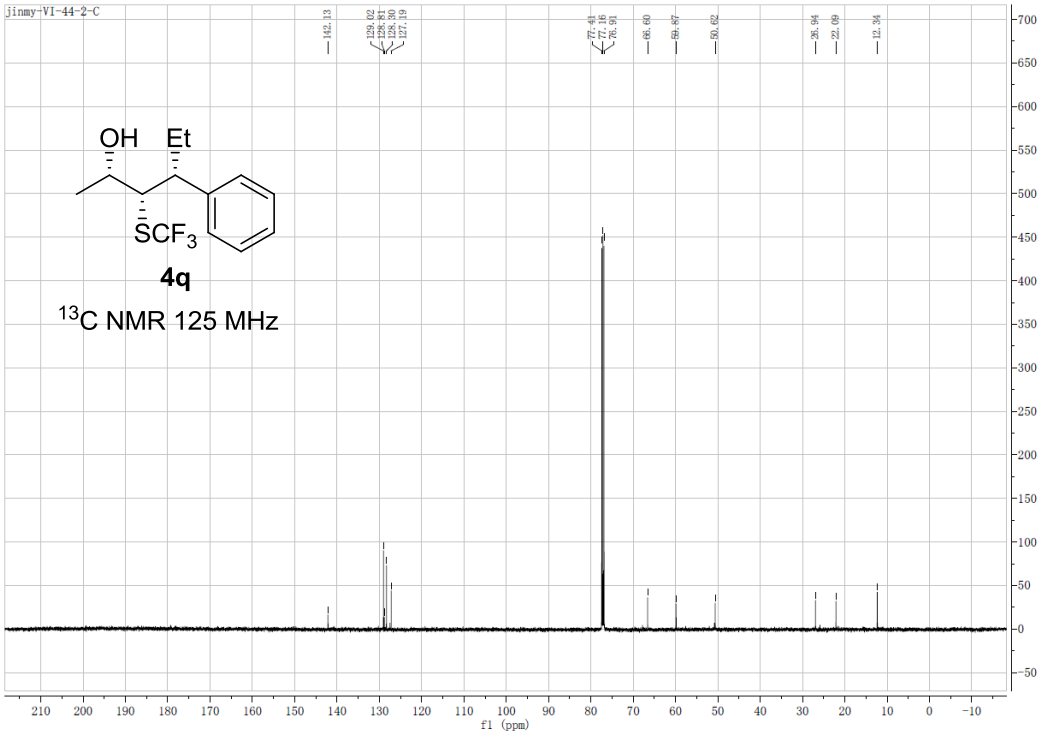
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.904	BB	0.5396	4468.42920	128.54424	50.4650
2	41.850	BB	0.6447	4386.07764	106.00964	49.5350
Totals :				8854.50684	234.55387	

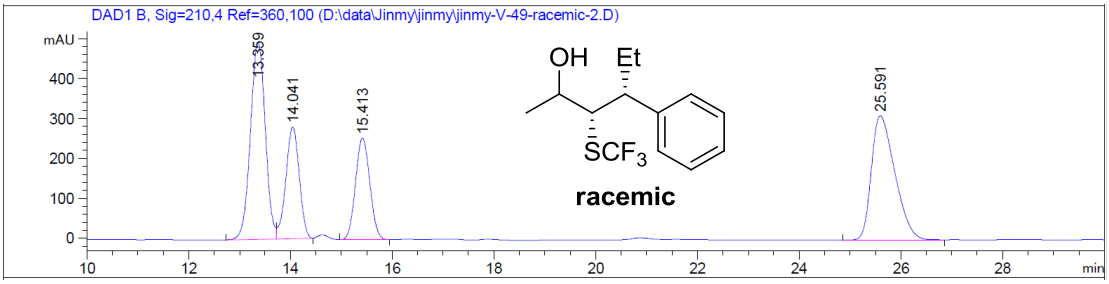


Signal 2: DAD1 B, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.539	BB	0.6215	5.82157e4	1452.84729	87.9505
2	41.710	BB	0.6933	7975.73486	177.80048	12.0495
Totals :				6.61914e4	1630.64777	

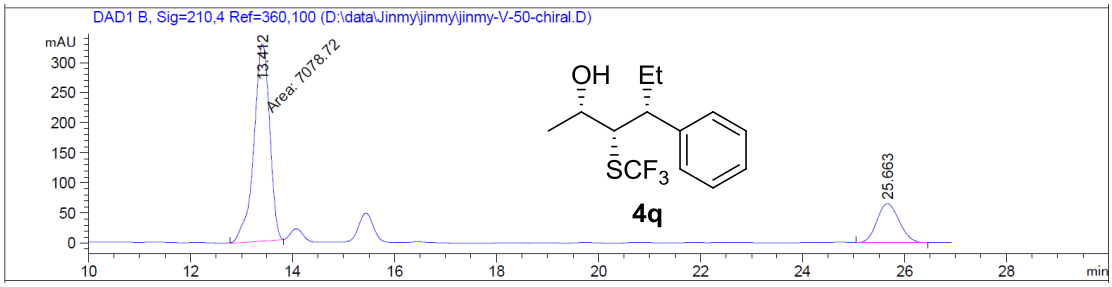

jinmy-VI-44-2-H
OH
Et
SCF3
4q
1H NMR 500 MHz
f1 (ppm)


jinmy-VI-44-2-C
OH
Et
SCF3
4q
13C NMR 125 MHz
f1 (ppm)



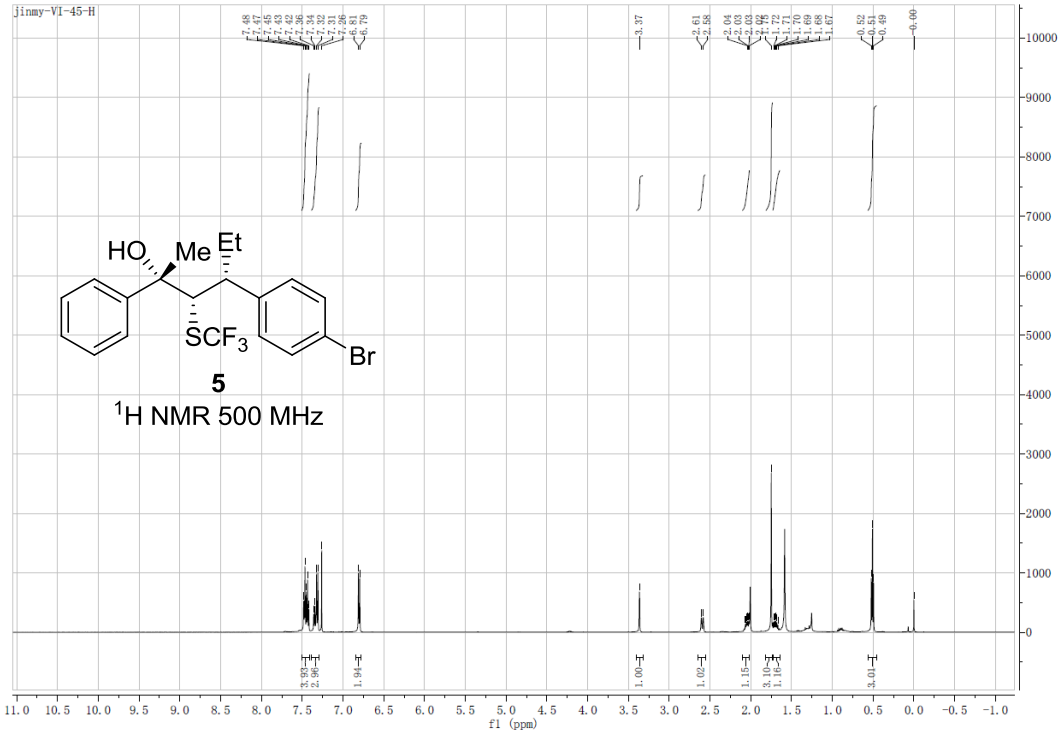
Signal 2: DAD1 B, Sig=210,4 Ref=360,100

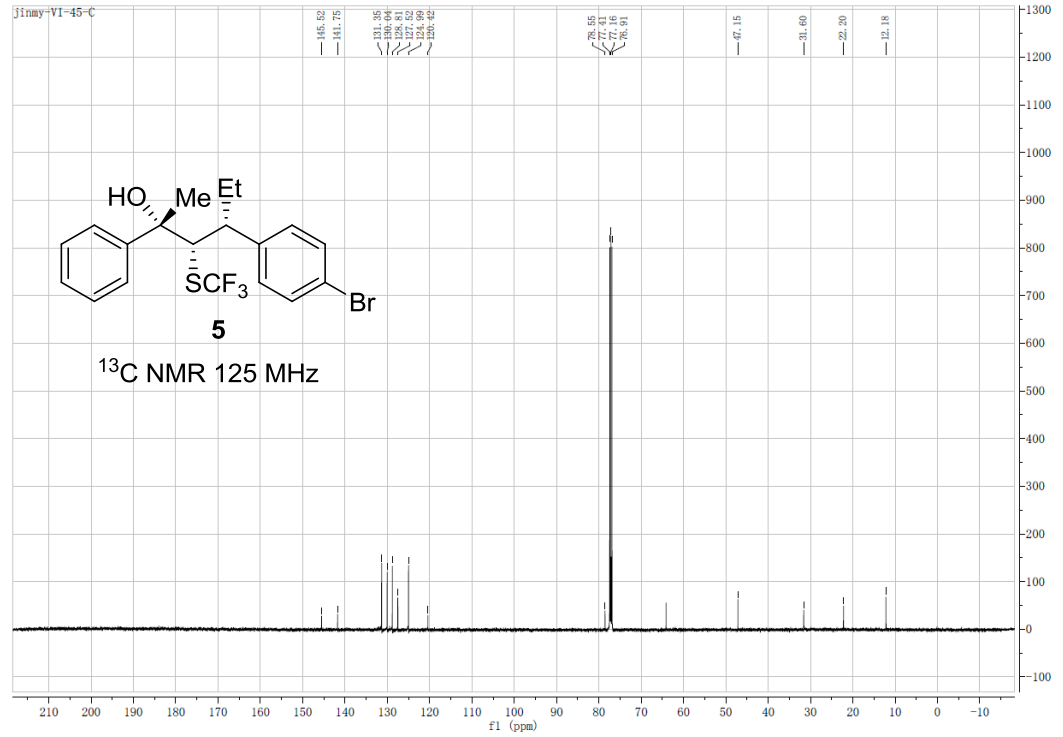
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.359	BV	0.3202	1.00030e4	494.02087	33.3150
2	14.041	VB	0.2854	5112.09375	279.49051	17.0258
3	15.413	BB	0.3077	4960.36621	254.17244	16.5205
4	25.591	BB	0.4955	9950.08398	310.77939	33.1387
Totals :				3.00256e4	1338.46321	

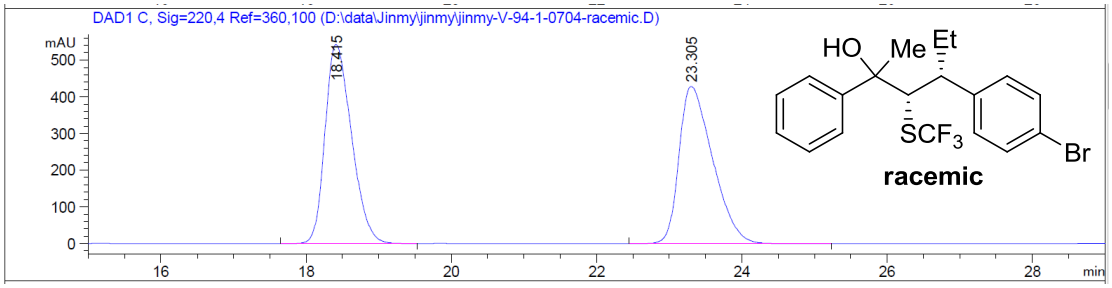


Signal 2: DAD1 B, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.412	MM	0.3599	7078.71533	327.77188	78.4211
2	25.663	BB	0.4735	1947.83264	64.64543	21.5789
Totals :				9026.54797	392.41731	

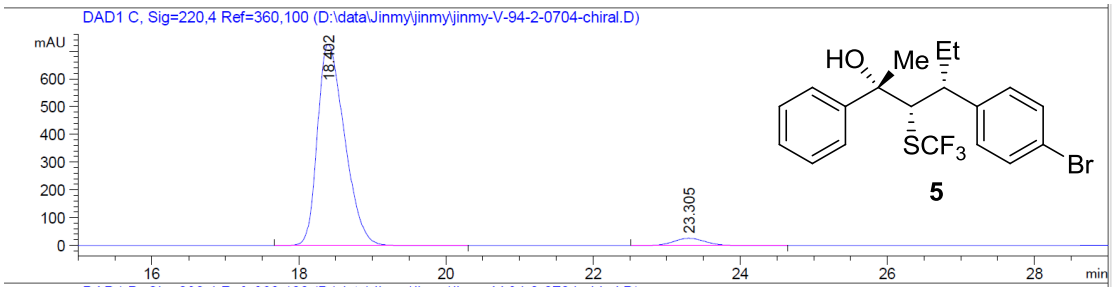

jinmy-VI-45-H
HO
Me
Et
SCF3
Br
5
1H NMR 500 MHz
f1 (ppm)


jinmy-VI-45-C
HO
Me
Et
SCF3
Br
5
13C NMR 125 MHz
f1 (ppm)



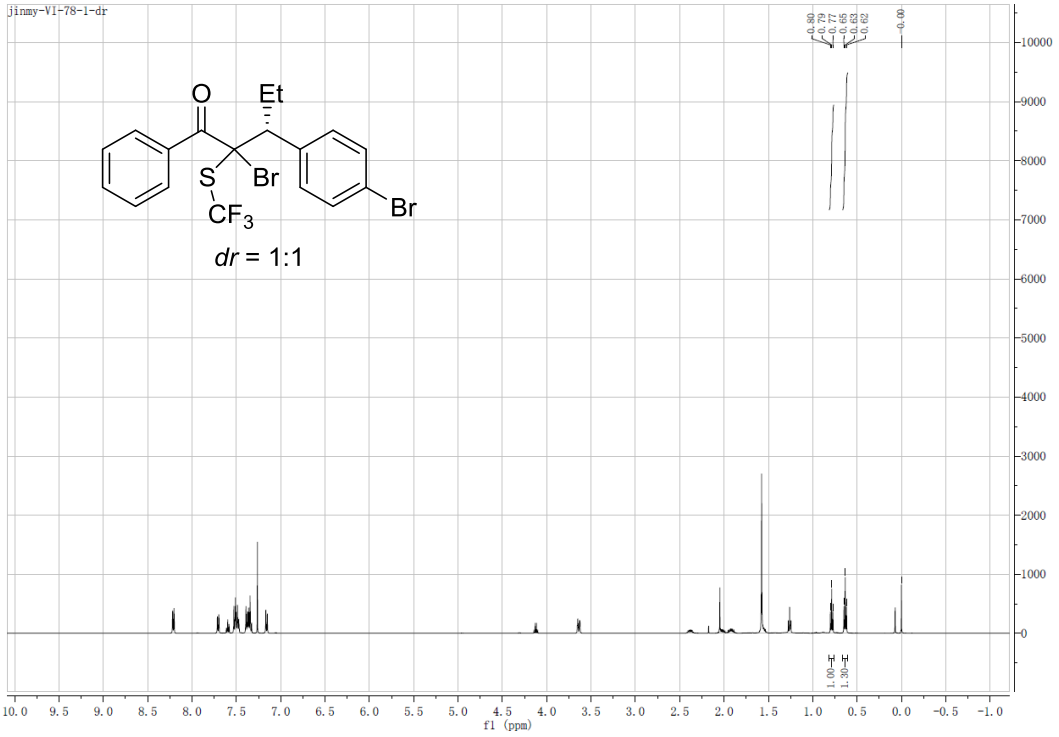
Signal 3: DAD1 C, Sig=220,4 Ref=360,100

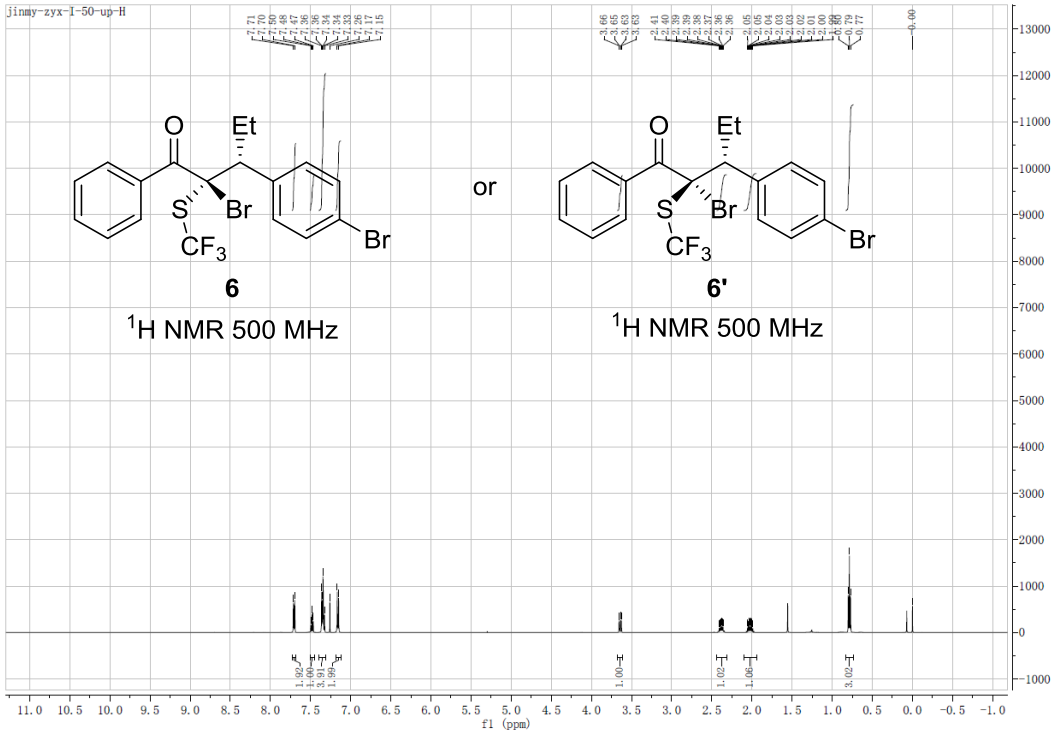
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.415	BB	0.3940	1.37660e4	542.54773	50.0121
2	23.305	BB	0.4904	1.37593e4	428.77686	49.9879
Totals :				2.75253e4	971.32458	

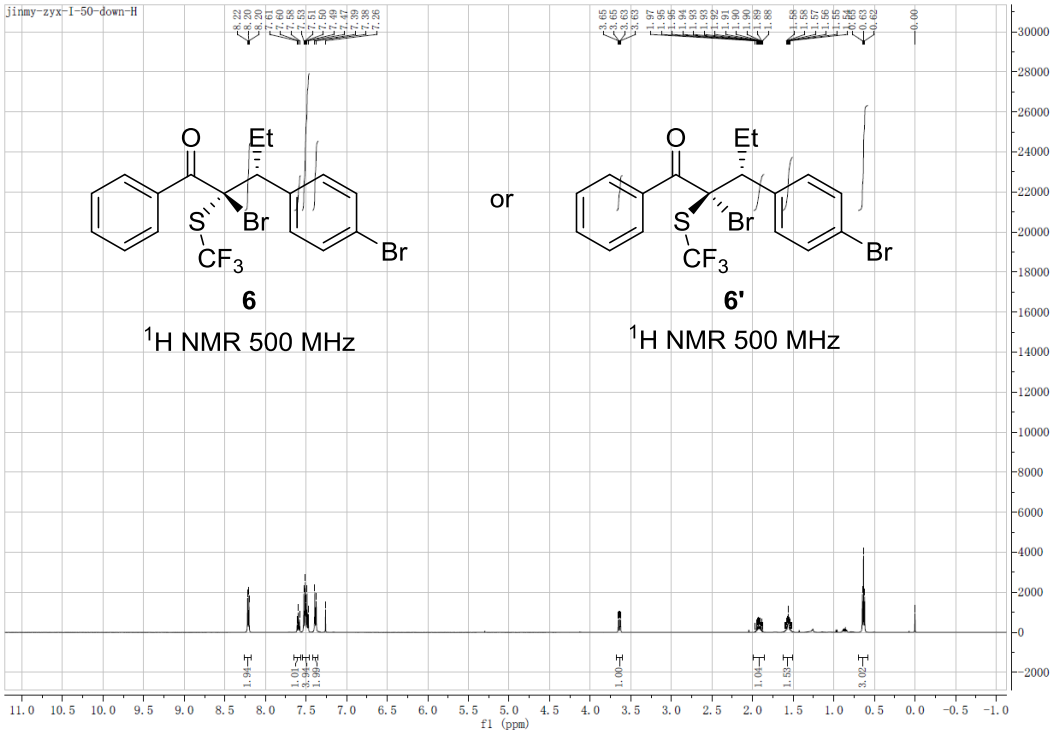


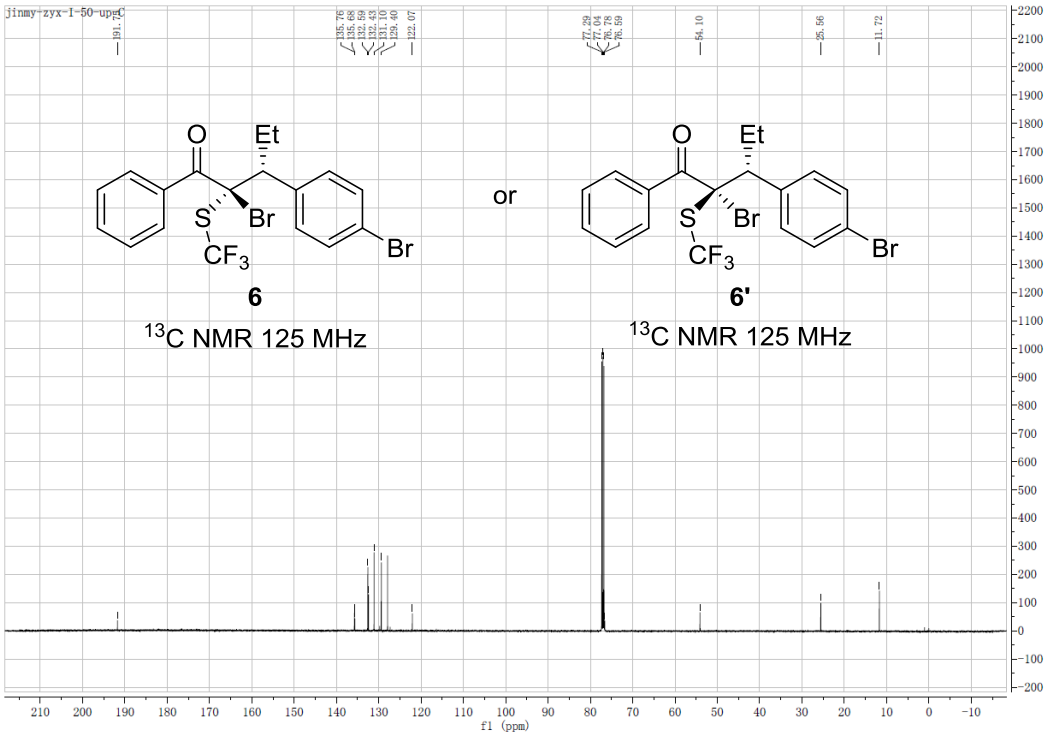
Signal 3: DAD1 C, Sig=220,4 Ref=360,100

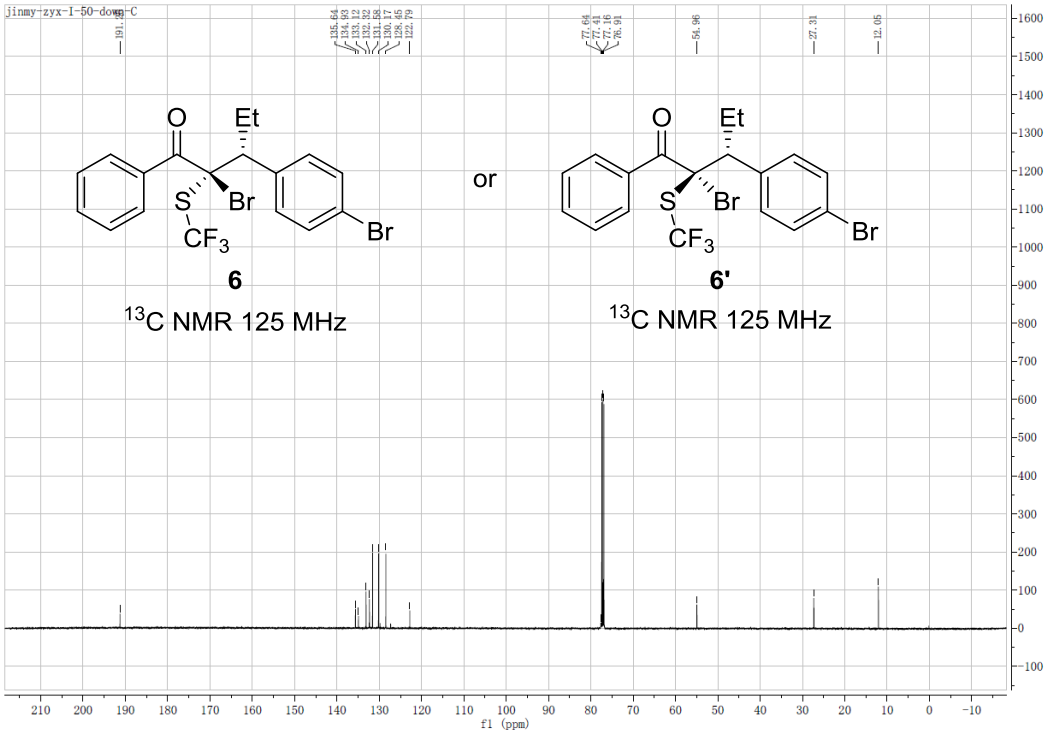
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.402	BB	0.3985	1.85542e4	725.19690	95.9363
2	23.305	BB	0.4625	785.91876	26.46395	4.0637
Totals :				1.93401e4	751.66085	


jinmy-V1-78-1-dr
O
Et
S
Br
CF3
Br
dr = 1:1
f1 (ppm)


jinmy-zyx-1-50-up-H
O
Et
S
Br
CF3
Br
6
1H NMR 500 MHz
or
O
Et
S
Br
CF3
Br
6'
1H NMR 500 MHz
f1 (ppm)

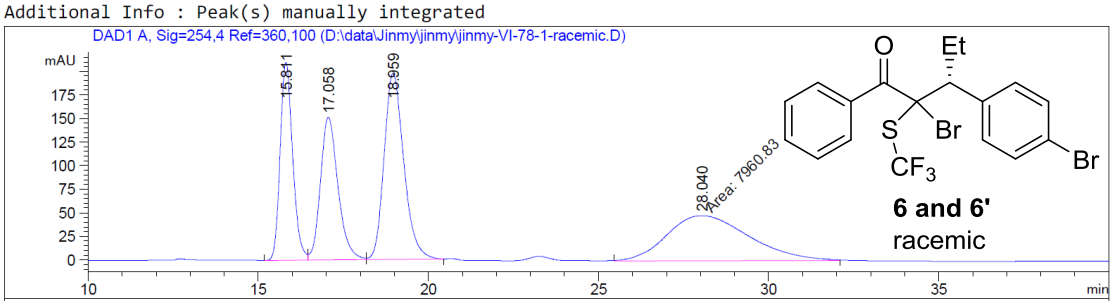

jinmy-zyx-I-50-down-H
O
Et
S
Br
CF3
Br
6
1H NMR 500 MHz
or
O
Et
S
Br
CF3
Br
6'
1H NMR 500 MHz
f1 (ppm)


jinmy-zyx-I-50-upc
O
Et
S
Br
CF3
Br
6
13C NMR 125 MHz
or
O
Et
S
Br
CF3
Br
6'
13C NMR 125 MHz
f1 (ppm)



Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

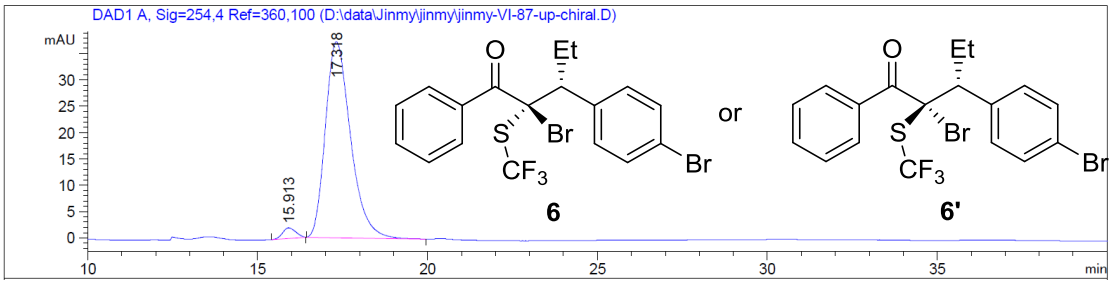
Additional Info : Peak(s) manually integrated



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

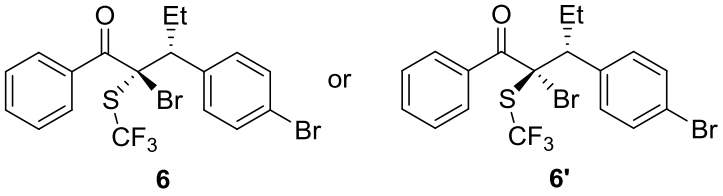
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.811	BV	0.3943	5361.31543	209.68294	20.0765
2	17.058	VV	0.5511	5427.38916	151.07356	20.3239
3	18.959	VB	0.6208	7954.90479	197.11475	29.7887
4	28.040	MM	2.7792	7960.82910	47.74095	29.8109
Totals :				2.67044e4	605.61220	

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8 mL/min

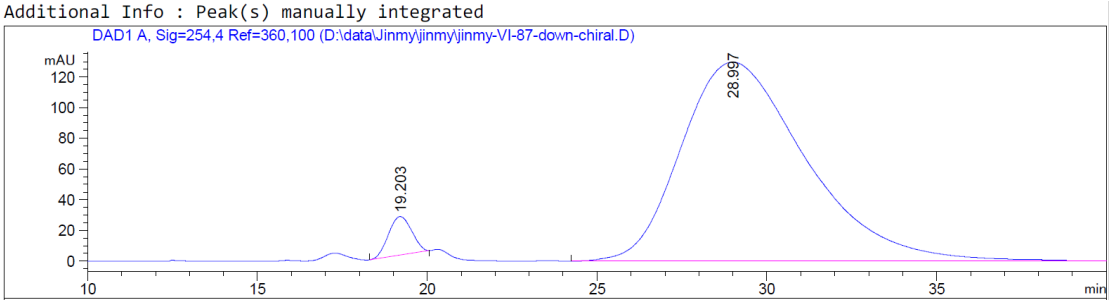


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.913	BB	0.4130	53.79772	2.03099	2.7303
2	17.318	BB	0.7843	1916.56934	37.25008	97.2697
Totals :				1970.36705	39.28108	

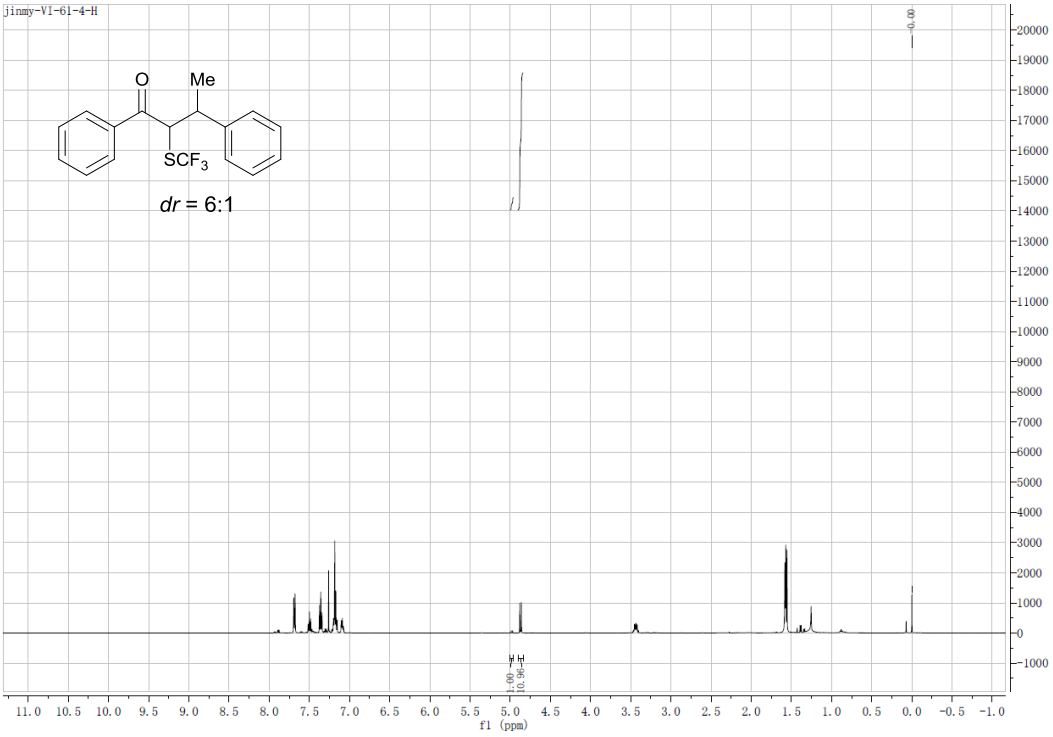


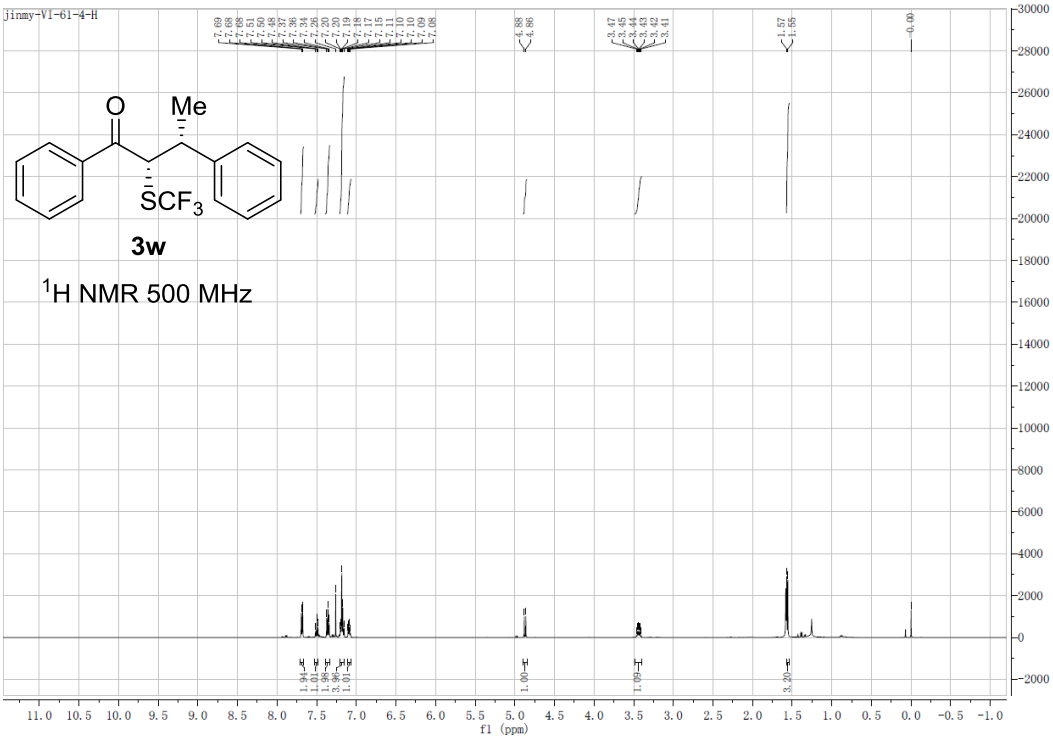
Additional Info : Peak(s) manually integrated

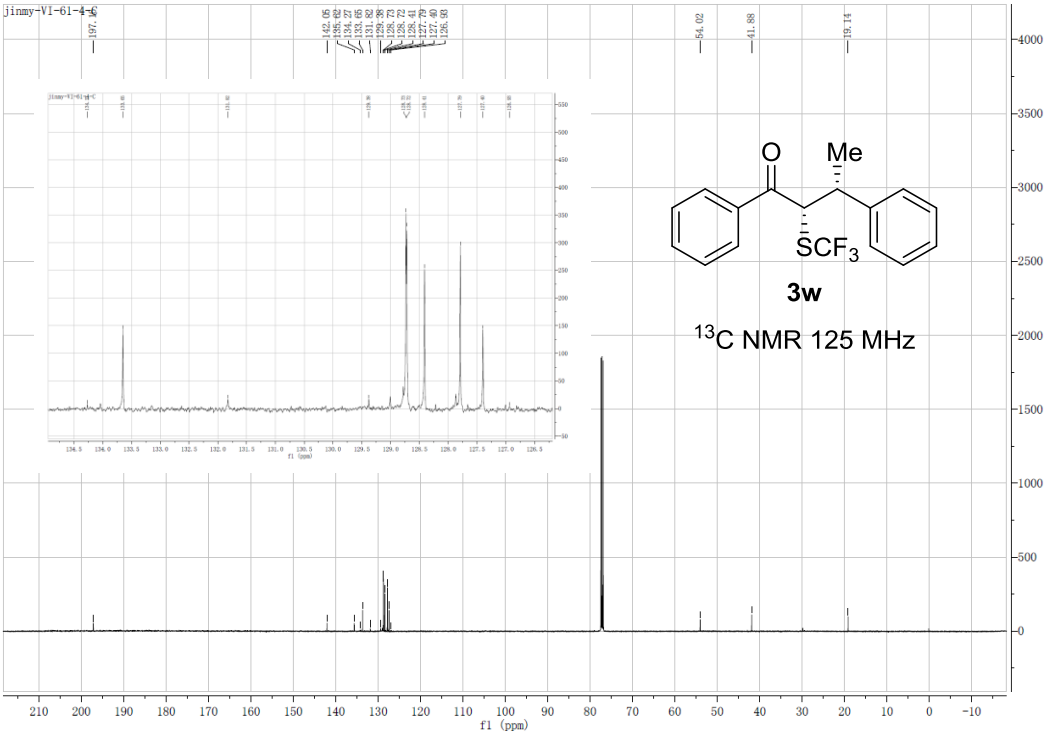


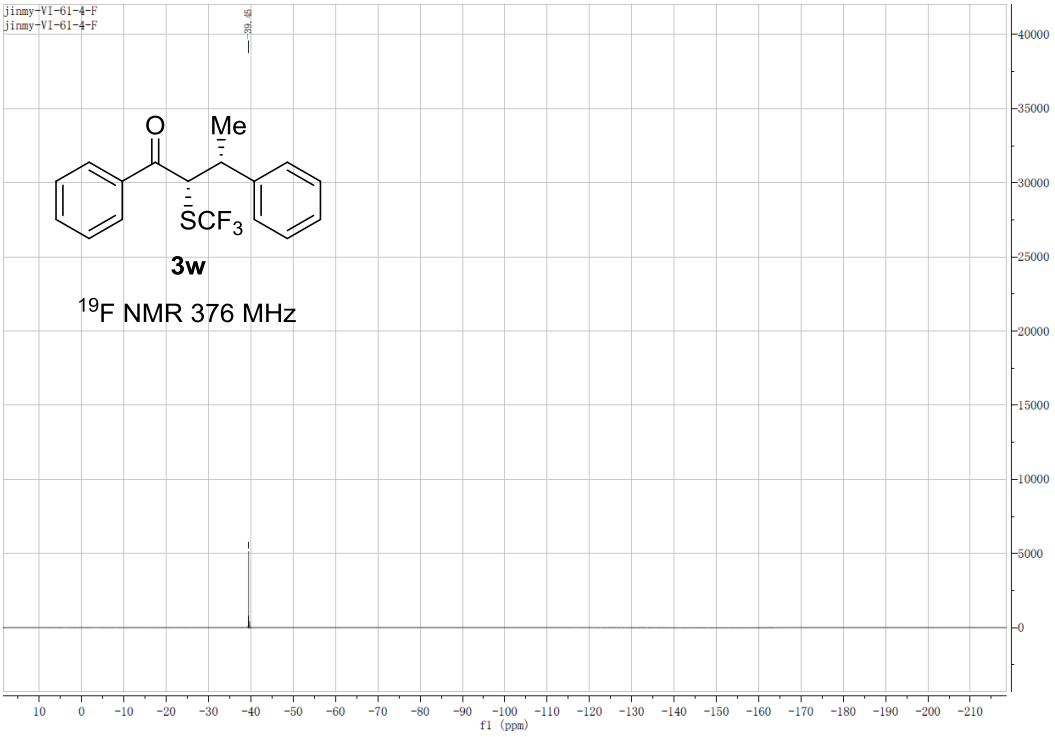
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.203	BB	0.7633	1193.27026	25.15869	3.4744
2	28.997	BB	3.7295	3.31516e4	129.63588	96.5256
Totals :				3.43448e4	154.79457	


jinmy-V1-61-4-H
O
Me
SCF3
dr = 6:1
f1 (ppm)

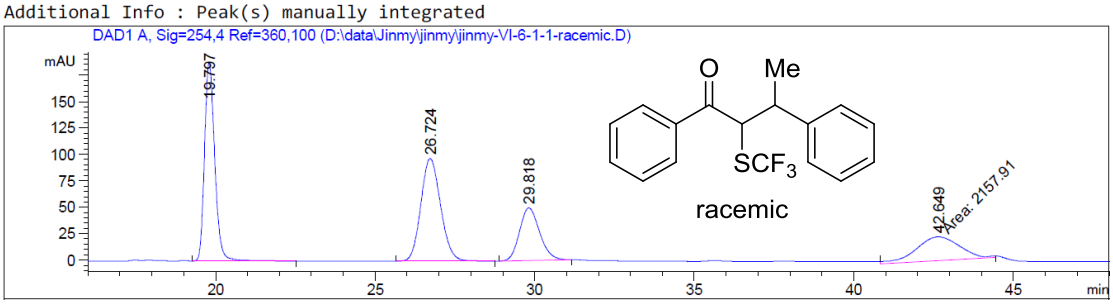

jinmy-V1-61-4-H
O
Me
SCF3
3w
1H NMR 500 MHz
f1 (ppm)


O
Me
SCF3
3w
13C NMR 125 MHz
f1 (ppm)


O
Me
SCF3
3w
19F NMR 376 MHz
f1 (ppm)

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

Additional Info : Peak(s) manually integrated

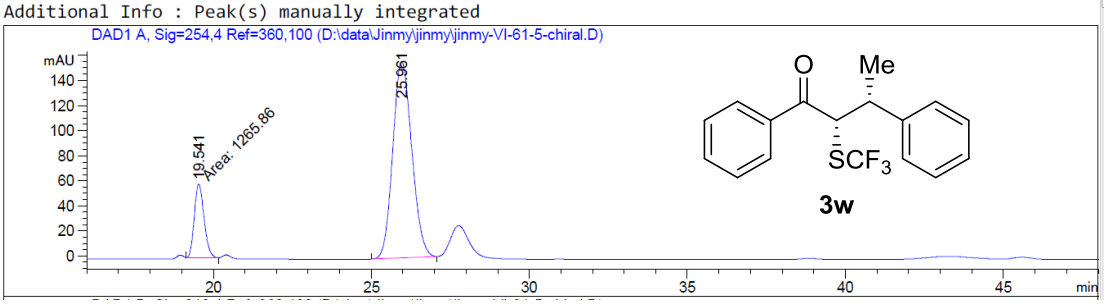


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.797	BB	0.3425	4163.70313	187.93834	32.9001
2	26.724	BB	0.6683	4161.33057	97.03346	32.8814
3	29.818	BB	0.6769	2172.65332	49.80930	17.1675
4	42.649	MM	1.5937	2157.90576	22.56645	17.0510
Totals :				1.26556e4	357.34755	

Sample Info : OJ-3, three combined, IPA:HEX=1:99, Flow:0.8mL/min

Additional Info : Peak(s) manually integrated



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.541	MM	0.3588	1265.85889	58.79857	16.1940
2	25.961	BB	0.6541	6550.98535	156.59074	83.8060
Totals :				7816.84424	215.38932	