

Supporting Information

Palladium-catalyzed Enantioselective Allylic Alkylation of Trifluoromethyl Group Substituted Racemic and Acyclic Unsymmetrical 1,3-Disubstituted Allylic Esters with Malonate Anions

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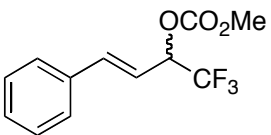
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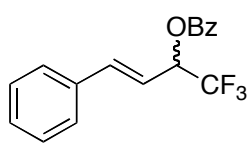
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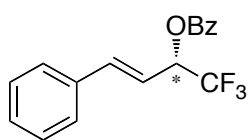
General and Materials: All manipulations were carried out under a nitrogen atmosphere. NMR spectra were recorded on a JEOL JNM-ECP500 spectrometer (500 MHz for ^1H , 125 MHz for ^{13}C and 470 MHz for ^{19}F) or JEOL EX-270 (270 MHz for ^1H , 67.8 MHz for ^{13}C). Chemical shifts are reported in δ ppm referenced to an internal SiMe_4 standard for ^1H NMR, and internal C_6F_6 standard for ^{19}F NMR. Residual chloroform (δ 77.0 for ^{13}C) was used as internal reference for ^{13}C NMR. ^1H , ^{13}C and ^{19}F NMR spectra were recorded in CDCl_3 at room temperature unless otherwise noted. The NMR yields were determined by ^1H or ^{19}F NMR using an internal standard (phenanthrene, trioxane or $\text{CF}_3\text{C}_6\text{H}_5$). $[\text{Pd}(\pi\text{-allyl})(\text{cod})]\text{BF}_4$ ¹ was prepared according to the literatures. Allyl carbonate **1a** was prepared by reaction of corresponding alcohol² with methyl chlorocarbonate. Allyl benzoates **1a'-g'** were prepared by reaction of corresponding alcohols² with benzoyl chloride. Chiral substrates (*S*)-**1a'** and (*R*)-**1a'** were prepared by reaction of corresponding chiral alcohols³ with benzoyl chloride. Allyl benzoate **6** was prepared by reaction of corresponding alcohol, which was prepared by the Luche reduction⁴ of corresponding enone,⁵ with benzoyl chloride. All other chemicals, including chiral-BINAP, chiral-Tol-BINAP, and solvents were purchased from common commercial sources and were used without further purification.

Characterization of trifluoromethylated allyl substrates:

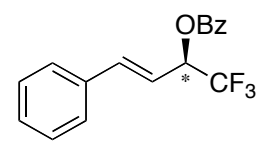
 **Methyl (1,1,1-trifluoro-4-phenylbut-3-en-2-yl) carbonate (1a):** White solid. Mp. 70–72 °C. ^1H NMR (500 MHz, CDCl_3) δ 3.86 (s, 3H), 5.63 (dq, $J_{\text{HH}} = 8.0$ Hz, $J_{\text{HF}} = 6.7$ Hz, 1H), 6.14 (dd, $J = 16.0, 8.0$ Hz, 1H), 6.91 (d, $J = 16.0$ Hz, 1H), 7.29–7.45 (m, 5H). ^{13}C NMR (125 MHz, CDCl_3) δ 55.3, 74.9 (q, $J_{\text{CF}} = 34.0$ Hz), 116.5, 122.9 (q, $J_{\text{CF}} = 280.7$ Hz), 127.0, 128.6, 129.0, 134.7, 139.2, 154.2. ^{19}F NMR (470 MHz, CDCl_3) δ 85.1 (d, $J = 6.6$ Hz). IR (KBr) 3085, 3067, 3027, 3006, 2976, 1888, 1767, 1723, 1661, 1579 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{12}\text{H}_{11}\text{F}_3\text{NaO}_3$, $[\text{M}+\text{Na}]^+$ 283.0558, found 283.0552.



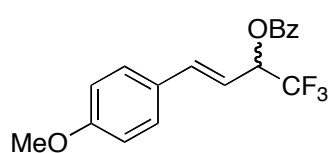
1,1,1-Trifluoro-4-phenylbut-3-en-2-yl benzoate (1a'): White solid. Mp. 62–64 °C. ¹H NMR (500 MHz, CDCl₃) δ 6.08 (dq, $J_{\text{HH}} = 7.7$ Hz, $J_{\text{HF}} = 6.7$ Hz, 1H), 6.23 (dd, $J = 15.8, 7.7$ Hz, 1H), 6.95 (d, $J = 15.8$ Hz, 1H), 7.28–7.37 (m, 3H), 7.41–7.51 (m, 4H), 7.61 (tt, $J = 7.4, 1.4$ Hz, 1H), 8.11 (dd, $J = 8.4, 1.3$ Hz, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 71.6 (q, $J_{\text{CF}} = 33.6$ Hz), 117.2, 123.3 (q, $J_{\text{CF}} = 280.7$ Hz), 127.0, 128.6, 128.7, 128.8, 129.0, 130.0, 133.8, 134.9, 138.9, 164.5. ¹⁹F NMR (470 MHz, CDCl₃) δ 85.5 (d, $J = 6.4$ Hz). IR (KBr) 3090, 3067, 3034, 2962, 1731, 1657, 1600, 1583, 1500 cm⁻¹. HRMS (ESI): m/z : calcd for C₁₇H₁₃F₃NaO₂, [M+Na]⁺ 329.0765, found 329.0768.



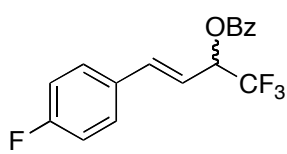
(S)-1,1,1-Trifluoro-4-phenylbut-3-en-2-yl benzoate ((S)-1a'): $[\alpha]_{\text{D}}^{25} -8.25$ (c 1.37, CHCl₃) (99% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 254 nm, 35 °C, t_{R} 5.52 min (minor); t_{R} 6.55 min (major)).



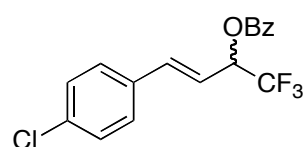
(R)-1,1,1-Trifluoro-4-phenylbut-3-en-2-yl benzoate ((R)-1a'): $[\alpha]_{\text{D}}^{24} +8.00$ (c 2.50, CHCl₃) (99% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 254 nm, 35 °C, t_{R} 5.52 min (major); t_{R} 6.55 min (minor)).



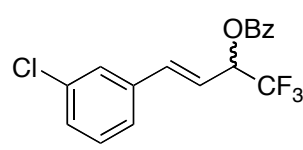
1,1,1-Trifluoro-4-(4-methoxyphenyl)but-3-en-2-yl benzoate (1b'): Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 3.81 (s, 3H), 6.01–6.12 (m, 2H), 6.84–6.92 (m, 3H), 7.37 (t, $J = 8.9$ Hz, 2H), 7.48 (t, $J = 7.7$ Hz, 2H), 7.61 (tt, $J = 7.7, 1.4$ Hz, 1H), 8.11 (dd, $J = 8.9, 1.4$ Hz, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 55.2, 71.8 (q, $J_{\text{CF}} = 33.6$ Hz), 114.0, 114.7, 123.4 (q, $J_{\text{CF}} = 280.7$ Hz), 127.7, 128.4, 128.5, 128.8, 129.9, 133.7, 138.6, 160.2, 164.5. ¹⁹F NMR (470 MHz, CDCl₃) δ 85.3 (d, $J = 6.4$ Hz). IR (neat) 3036, 3008, 2961, 2938, 2913, 2839, 1735, 1654, 1607, 1579, 1514 cm⁻¹. HRMS (ESI): m/z : calcd for C₁₈H₁₅F₃NaO₃, [M+Na]⁺ 359.0871, found 359.0867.



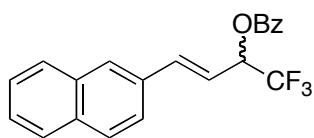
1,1,1-Trifluoro-4-(4-fluorophenyl)but-3-en-2-yl benzoate (1c'): White solid. Mp. 71–73 °C. ¹H NMR (500 MHz, CDCl₃) δ 6.06 (dq, *J*_{HH} = 6.7 Hz, *J*_{HF} = 7.7 Hz, 1H), 6.15 (dd, *J* = 15.8, 7.7 Hz, 1H), 6.91 (d, *J* = 15.8 Hz, 1H), 7.02 (t, *J* = 8.6 Hz, 2H), 7.36–7.42 (m, 2H), 7.44–7.50 (m 2H), 7.60–7.66 (m, 1H), 8.11 (dd, *J* = 8.3, 1.1 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 71.5 (q, *J*_{CF} = 33.6 Hz), 115.6 (d, *J*_{CF} = 21.6 Hz), 117.0, 123.4 (q, *J*_{CF} = 280.7 Hz), 128.5, 128.7 (d, *J*_{CF} = 8.4 Hz), 128.7, 129.9, 131.1 (q, *J*_{CF} = 3.6 Hz), 133.7, 137.6, 163.1 (d, *J*_{CF} = 249.5 Hz), 164.4. ¹⁹F NMR (470 MHz, CDCl₃) δ 49.9 (tt, *J* = 8.6, 5.3 Hz, 1F), 85.5 (d, *J* = 6.6 Hz, 3F). IR (KBr) 3075, 3064, 3042, 3014, 2958, 1736, 1693, 1660, 1600, 1512, 1454 cm⁻¹. HRMS (ESI): *m/z*: calcd for C₁₇H₁₂F₄NaO₂, [M+Na]⁺ 347.0671, found 347.0667.



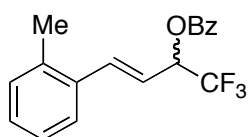
4-(4-Chlorophenyl)-1,1,1-trifluorobut-3-en-2-yl benzoate (1d'): White solid. Mp. 109–112 °C. ¹H NMR (500 MHz, CDCl₃) δ 6.06 (dq, *J*_{HH} = 7.6 Hz, *J*_{HF} = 6.7 Hz, 1H), 6.21 (dd, *J* = 15.8, 7.6 Hz, 1H), 6.90 (d, *J* = 15.8 Hz, 1H), 7.26–7.71 (m, 7H), 8.11 (d, *J* = 7.4 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 71.4 (q, *J*_{CF} = 34.0 Hz), 117.9, 123.2 (q, *J*_{CF} = 280.7 Hz), 128.2, 128.6, 128.6, 128.9, 130.0, 133.4, 133.9, 134.8, 137.5, 164.5. ¹⁹F NMR (470 MHz, CDCl₃) δ 85.6 (d, *J* = 6.2 Hz). IR (KBr) 30094, 3069, 3037, 2962, 1735, 1657, 1601 cm⁻¹. Anal. Calcd for C₁₇H₁₂ClF₃O₂: C, 59.93; H, 3.55. found (%): C, 59.81; H, 3.27.



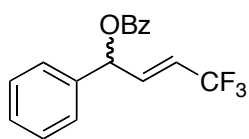
4-(3-Chlorophenyl)-1,1,1-trifluorobut-3-en-2-yl benzoate (1e'): White solid. Mp. 60–62 °C. ¹H NMR (500 MHz, CDCl₃) δ 6.06 (dq, *J*_{HH} = 7.4 Hz, *J*_{HF} = 6.6 Hz, 1H), 6.25 (dd, *J* = 16.0, 7.4 Hz, 1H), 6.89 (d, *J* = 16.0 Hz, 1H), 7.26–7.32 (m, 3H), 7.43 (s, 1H), 7.45–7.65 (m, 3H), 8.11 (dd, *J* = 1.1, 8.3 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 71.2 (q, *J*_{CF} = 33.6 Hz), 118.8, 123.2 (q, *J*_{CF} = 280.7 Hz), 125.3, 126.9, 128.6, 128.6, 128.9, 129.9, 130.0, 133.9, 134.7, 136.8, 137.2, 164.4. ¹⁹F NMR (470 MHz, CDCl₃) δ 85.5 (d, *J* = 6.6 Hz). IR (KBr) 3091, 3061, 3035, 2965, 1817, 1731, 1660, 1566 cm⁻¹. HRMS (ESI): *m/z*: calcd for C₁₇H₁₂ClF₃NaO₂, [M+Na]⁺ 363.0376, found 363.0375.



1,1,1-Trifluoro-4-(naphthalen-2-yl)but-3-en-2-yl benzoate (1f'): White solid. Mp. 180–182 °C. ^1H NMR (500 MHz, CDCl_3) δ 6.13 (dq, $J_{\text{HH}} = 7.6$ Hz, $J_{\text{HF}} = 6.7$ Hz, 1H), 6.35 (dd, $J = 15.8, 7.6$ Hz, 1H), 7.11 (d, $J = 15.8$ Hz, 1H), 7.44–7.53 (m, 4H), 7.57–7.66 (m, 2H), 7.77–7.84 (m, 4H), 8.13 (d, $J = 7.2$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 71.6 (dq, $J_{\text{CF}} = 6.0, 33.6$ Hz), 117.5, 123.2, 123.4 (q, $J_{\text{CF}} = 280.7$ Hz), 126.5, 126.6, 127.7, 127.9, 128.2, 128.4, 128.6, 128.8, 130.0, 132.4, 133.3, 133.6, 133.8, 138.9, 164.5. ^{19}F NMR (470 MHz, CDCl_3) δ 85.5 (d, $J = 6.6$ Hz). IR (KBr) 3093, 3062, 2959, 1735, 1654, 1601 cm^{-1} . HR-MS (ESI): m/z : calcd for $\text{C}_{21}\text{H}_{15}\text{F}_3\text{NaO}_2$, $[\text{M}+\text{Na}]^+$ 379.0922, found 379.0923.

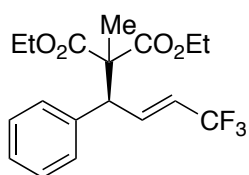


1,1,1-Trifluoro-4-(o-tolyl)but-3-en-2-yl benzoate (1g'): White solid. Mp. 59–62 °C. ^1H NMR (500 MHz, CDCl_3) δ 2.36 (s, 3H), 6.01–6.18 (m, 2H), 7.11–7.26 (m, 5H), 7.41–7.54 (m, 3H), 7.62 (t, $J = 7.4$ Hz, 1H), 8.12 (d, $J = 7.4$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 19.6, 71.8 (q, $J_{\text{CF}} = 33.6$ Hz), 118.6, 123.3 (q, $J_{\text{CF}} = 280.7$ Hz), 125.9, 126.2, 128.6, 128.8, 128.8, 130.0, 130.5, 133.8, 134.2, 136.2, 137.0, 164.5. ^{19}F NMR (470 MHz, CDCl_3) δ 85.4 (d, $J = 6.7$ Hz). IR (KBr) 3067, 3033, 2979, 2961, 2867, 1729, 1654, 1602, 1584 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{18}\text{H}_{15}\text{F}_3\text{NaO}_2$, $[\text{M}+\text{Na}]^+$ 343.0922, found 343.0924.

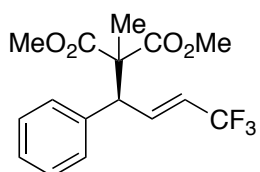


4,4,4-Trifluoro-1-phenylbut-2-en-1-yl benzoate (6): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 5.93–6.03 (m, 1H), 6.59–6.67 (m, 2H), 7.31–7.48 (m 7H), 7.57 (tt, $J = 7.4, 1.3$ Hz, 1H), 8.09 (dd, $J = 8.4, 1.3$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 73.8, 119.3 (q, $J_{\text{CF}} = 34.8$ Hz), 122.8 (q, $J_{\text{CF}} = 269.5$ Hz), 127.3, 128.5, 128.9, 129.0, 129.5, 129.7, 133.4, 136.8, 137.9 (q, $J_{\text{CF}} = 6.4$ Hz), 165.0. ^{19}F NMR (470 MHz, CDCl_3) δ 97.5 (dt, $J = 6.4, 1.8$ Hz). IR (neat) 3067, 3037, 2932, 1726, 1685, 1603, 1586, 1453 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{17}\text{H}_{13}\text{F}_3\text{NaO}_2$, $[\text{M}+\text{Na}]^+$ 329.0766, found 329.0765.

General Procedure for the Catalytic Allylic Alkylation: A typical procedure is given for the reaction of (*E*)-1,1,1-trifluoro-4-phenylbut-3-en-2-yl benzoate (**1a**) with diethyl methylmalonate (**2a**) (Table 4, entry 3). To a solution of [Pd(*p*-allyl)(cod)]BF₄ (3.4 mg, 0.010 mmol), (*S*)-Tol-BINAP (10.2 mg, 0.015 mmol) and (*E*)-1,1,1-trifluoro-4-phenylbut-3-en-2-yl benzoate (**1a**) (61.3 mg, 0.20 mmol) in dioxane (1.0 mL) was added diethyl methylmalonate (**2a**) (105 mg, 0.60 mmol) and BSA (61.0 mg, 0.30 mmol). The reaction mixture was stirred at rt for 5 min. The reaction mixture was then stirred at 60 °C for 24 h. The mixture was quenched with brine and/or H₂O (1 mL), then extracted with ethyl acetate (3 x 2 mL). The combined organic layers were dried over MgSO₄ and concentrated in vacuo. The residue was chromatographed on silica gel (hexane/Et₂O/CH₂Cl₂ = 5/1/1) to give 64.6 mg (91%) of alkylation product **3aa**. Values of ee was determined by chiral HPLC: Daicel CHIRALCEL OJ-H (hexane-2-PrOH = 19:1).

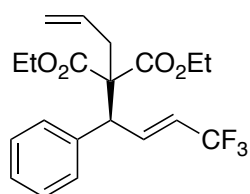


(*S*)-Diethyl 2-methyl-2-(4,4,4-trifluoro-1-phenylbut-2-en-1-yl)malonate ((*S*)-3aa): Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 1.20 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H), 1.39 (s, 3H), 4.12 (q, *J* = 7.2 Hz, 2H), 4.15–4.27 (m, 3H), 5.56 (dq, *J*_{HH} = 15.7 Hz, *J*_{HF} = 6.3 Hz, *J*_{HH} = 1.4 Hz, 1H), 6.91 (ddq, *J*_{HH} = 15.7, 7.6 Hz, *J*_{HF} = 2.2 Hz, 1H), 7.17–7.21 (m, 2H), 7.26–7.36 (m, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 13.7, 13.7, 19.3, 52.2, 58.1, 61.6, 61.6, 120.3 (q, *J*_{CF} = 33.4 Hz), 123.0 (q, *J*_{CF} = 269.6 Hz), 127.8, 128.6, 129.5, 137.0, 140.0 (q, *J*_{CF} = 6.6 Hz), 170.4, 170.9. ¹⁹F NMR (470 MHz, CDCl₃) δ 97.7 (dt, *J* = 4.2, 2.2 Hz). IR (neat) 2986, 1736, 1677, 1496, 1454, 1381 cm⁻¹. HRMS (ESI): *m/z*: calcd for C₁₈H₂₁F₃NaO₄, [M+Na]⁺ 381.1290, found 381.1281. [α]_D²⁶ +24.3 (*c* 5.96, CHCl₃) (96% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, *t*_R 4.13 min (major); *t*_R 5.14 min (minor)).



(*S*)-Dimethyl 2-methyl-2-(4,4,4-trifluoro-1-phenylbut-2-en-1-yl)malonate ((*S*)-3ab): Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 1.41 (s, 3H), 3.65 (s, 3H), 3.74 (s, 3H), 4.19 (dt, *J* = 7.9, 1.4 Hz, 1H), 5.60 (dq, *J*_{HH} = 15.8 Hz, *J*_{HF} = 6.3 Hz, *J*_{HH} = 1.4 Hz, 1H), 6.89 (ddq, *J*_{HH} = 15.8, 7.9 Hz, *J*_{HF} = 2.1 Hz, 1H), 7.17–7.21 (m, 2H), 7.26–7.35 (m,

3H). ^{13}C NMR (125 MHz, CDCl_3) δ 19.0, 52.3, 52.5, 52.6, 58.3, 120.7 (q, $J_{\text{CF}} = 33.6$ Hz), 122.9 (q, $J_{\text{CF}} = 269.5$ Hz), 127.9, 128.6, 129.4, 136.7, 139.3 (q, $J_{\text{CF}} = 6.8$ Hz), 170.8, 171.1. ^{19}F NMR (470 MHz, CDCl_3) δ 97.7 (dt, $J = 6.3, 2.0$ Hz). IR (neat) 3033, 3005, 2956, 2846, 1738, 1677, 1497, 1455, 1436 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{16}\text{H}_{18}\text{F}_3\text{O}_4$, $[\text{M}+\text{H}]^+$ 331.1157, found 331.1148. $[\alpha]_{\text{D}}^{27} +19.7$ (c 5.98, CHCl_3) (83% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_{R} 5.33 min (major); t_{R} 6.32 min (minor)).

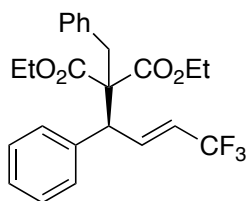


(S)-Diethyl 2-allyl-2-(4,4,4-trifluoro-1-phenylbut-2-en-1-yl)

malonate ((S)-3ac): Colorless oil. ^1H NMR (500 MHz, CDCl_3)

δ 1.25 (t, $J = 7.2$ Hz, 3H), 1.29 (t, $J = 7.2$ Hz, 3H), 2.31 (dd, $J = 14.5, 8.2$ Hz, 1H), 2.56 (dd, $J = 14.5, 6.4$ Hz, 1H), 4.13 (dt, $J = 6.7, 1.7$ Hz, 5H), 4.96–5.03 (m, 1H), 5.04–5.10 (m, 1H), 5.39

(dq, $J_{\text{HH}} = 15.8$ Hz, $J_{\text{HF}} = 6.6$ Hz, $J_{\text{HH}} = 1.7$ Hz, 1H), 5.66–5.77 (m, 1H), 6.96 (ddq, $J_{\text{HH}} = 15.8, 6.7$ Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.09–7.14 (m, 2H), 7.27–7.36 (m, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.8, 14.0, 38.7, 51.1, 61.6, 61.6, 119.3, 119.6 (q, $J_{\text{CF}} = 33.2$ Hz), 123.1 (q, $J_{\text{CF}} = 269.3$ Hz), 127.9, 128.7, 129.4, 132.3, 136.4, 141.0 (q, $J_{\text{CF}} = 6.8$ Hz), 169.7, 169.9. ^{19}F NMR (470 MHz, CDCl_3) δ 97.9 (dt, $J = 6.4, 2.3$ Hz). IR (neat) 3081, 3033, 2984, 2940, 2907, 1731, 1677, 1640, 1496 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{20}\text{H}_{23}\text{F}_3\text{NaO}_4$, $[\text{M}+\text{Na}]^+$ 407.1446, found 407.1437. $[\alpha]_{\text{D}}^{26} +31.7$ (c 6.60, CHCl_3) (92% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_{R} 3.78 min (minor); t_{R} 4.16 min (major)).



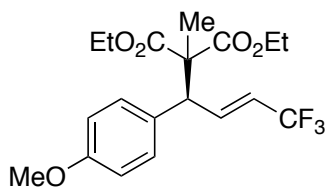
(S)-Diethyl 2-benzyl-2-(4,4,4-trifluoro-1-phenylbut-2-en-1-yl)

malonate ((S)-3ad): Colorless oil; ^1H NMR (500 MHz, CDCl_3) δ

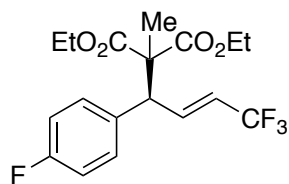
1.04 (t, $J = 7.2$ Hz, 3H), 1.25 (t, $J = 7.2$ Hz, 3H), 2.90 (d, $J = 14.0$ Hz, 1H), 3.19 (d, $J = 14.0$ Hz, 1H), 3.91 (dq, $J = 10.6, 7.2$ Hz, 1H), 4.08 (dq, $J = 10.6, 7.2$ Hz, 1H), 4.16–4.30 (m, 3H), 5.32 (dq, J_{HH}

= 15.8 Hz, $J_{\text{HF}} = 6.6$ Hz, $J_{\text{HH}} = 1.7$ Hz, 1H), 6.90 (ddq, $J_{\text{HH}} = 15.8, 6.7$ Hz, $J_{\text{HF}} = 2.1$ Hz,

1H), 7.03–7.10 (m, 2H), 7.11–7.16 (m, 2H), 7.17–7.22 (m, 3H), 7.29–7.39 (m, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 13.6, 13.7, 40.4, 52.3, 61.5, 61.6, 63.0, 119.5 (q, *J*_{CF} = 33.2 Hz), 123.1 (q, *J*_{CF} = 269.5 Hz), 126.93, 127.9, 128.0, 128.8, 129.6, 130.3, 136.0, 136.5, 141.3 (q, *J*_{CF} = 6.4 Hz), 169.8, 169.9. ¹⁹F NMR (470 MHz, CDCl₃) δ 97.9 (dt, *J* = 6.3, 2.3 Hz). IR (neat) 3064, 3033, 2984, 2940, 2906, 1728, 1676, 1603, 1496, 1454, 1369 cm⁻¹. HRMS (ESI): *m/z*: calcd for C₂₄H₂₅F₃NaO₄, [M+Na]⁺ 457.1603, found 457.1593. [α]_D²⁶ +10.6 (*c* 7.63, CHCl₃) (77% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, *t*_R 4.20 min (minor); *t*_R 5.11 min (major)).

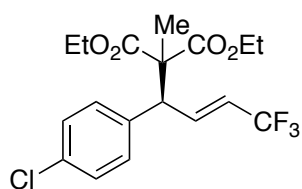


(S)-Diethyl 2-methyl-2-(4,4,4-trifluoro-1-(4-methoxyphenyl)but-2-en-1-yl)malonate ((S)-3ba): Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 1.21 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H), 1.37 (s, 3H), 3.79 (s, 3H), 4.08–4.28 (m, 5H), 5.55 (dq, *J*_{HH} = 15.7 Hz, *J*_{HF} = 6.4 Hz, *J*_{HH} = 1.5 Hz, 1H), 6.81–6.92 (m, 3H), 6.81–6.92 (m, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 13.8, 13.9, 19.2, 51.4, 55.2 (d, *J*_{CF} = 2.4 Hz), 58.1, 61.6, 61.6, 113.9, 120.1 (q, *J*_{CF} = 33.2 Hz), 123.0 (q, *J*_{CF} = 269.3 Hz), 128.7, 130.6, 140.1 (q, *J*_{CF} = 7.2 Hz), 159.1, 170.5, 171.0. ¹⁹F NMR (470 MHz, CDCl₃) δ 97.8 (dt, *J* = 4.3, 2.1 Hz). IR (neat) 2986, 2941, 2908, 2840, 1732, 1677, 1611, 1583, 1514, 1465 cm⁻¹. HRMS (ESI): *m/z*: calcd for C₁₉H₂₃F₃NaO₅, [M+Na]⁺ 411.1395, found 411.1389. [α]_D²⁶ +22.9 (*c* 6.45, CHCl₃) (91% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, *t*_R 5.06 min (major); *t*_R 6.07 min (minor)).

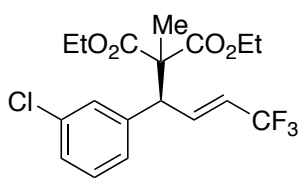


(S)-Diethyl 2-methyl-2-(4,4,4-trifluoro-1-(4-fluorophenyl)but-2-en-1-yl)malonate ((S)-3ca): Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 1.20 (t, *J* = 7.2, Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H), 1.38 (s, 3H), 4.12 (q, *J* = 7.2 Hz, 2H), 4.15–4.26 (m, 3H), 5.55 (dq, *J*_{HH} = 15.8 Hz, *J*_{HF} = 6.3 Hz, *J*_{HH} = 1.4 Hz, 1H), 6.88 (ddq, *J*_{HH} = 15.8, 7.7 Hz, *J*_{HF} = 2.2 Hz, 1H), 6.97–7.06 (m, 2H), 7.15–7.23 (m, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 13.8, 13.9, 19.2, 51.4, 58.0, 61.7, 61.7, 115.5 (d,

$J_{CF} = 21.6$ Hz), 120.6 (q, $J_{CF} = 33.6$ Hz), 122.9 (q, $J_{CF} = 269.5$ Hz), 131.1 (d, $J_{CF} = 7.2$ Hz), 132.7 (d, $J_{CF} = 3.6$ Hz), 139.5 (q, $J_{CF} = 6.8$ Hz), 162.2 (d, $J_{CF} = 247.1$ Hz), 170.3, 170.7. ^{19}F NMR (470 MHz, CDCl_3) δ 47.6 (tt, $J = 8.5, 5.3$ Hz, 1F), 97.7 (dt, $J = 4.2, 2.1$ Hz, 3F). IR (neat) 2987, 2943, 2908, 1732, 1678, 1605, 1511 cm^{-1} . HR-MS (ESI): m/z : calcd for $\text{C}_{18}\text{H}_{20}\text{F}_4\text{NaO}_4$, $[\text{M}+\text{Na}]^+$ 399.1195, found 399.1191. $[\alpha]_{\text{D}}^{26} +21.4$ (c 6.11, CHCl_3) (96% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 $^{\circ}\text{C}$, t_{R} 4.20 min (major); t_{R} 4.92 min (minor)).

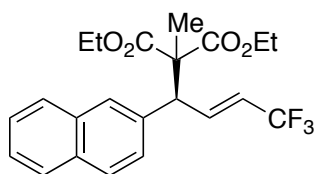


(S)-Diethyl 2-(1-(4-chlorophenyl)-4,4,4-trifluorobut-2-en-1-yl)-2-methylmalonate ((S)-3da): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.21 (t, $J = 7.2$ Hz, 3H), 1.26 (t, $J = 7.2$ Hz, 3H), 1.38 (s, 3H), 4.09–4.27 (m, 5H), 5.56 (dq, $J_{\text{HH}} = 15.6$ Hz, $J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} = 1.3$ Hz, 1H), 6.87 (ddq, $J_{\text{HH}} = 15.6, 7.7$ Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.13–7.17 (m, 2H), 7.28–7.32 (m, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.8, 13.9, 19.2, 51.5, 57.9, 61.7, 61.8, 120.7 (q, $J_{CF} = 33.6$ Hz), 122.8 (q, $J_{CF} = 269.5$ Hz), 128.8, 130.9, 133.8, 135.5, 139.2 (q, $J_{CF} = 6.4$ Hz), 170.2, 170.7. ^{19}F NMR (470 MHz, CDCl_3) δ 97.6 (dt, $J = 4.2, 2.1$ Hz). IR (neat) 2986, 2942, 2908, 2877, 1732, 1678, 1595, 1493, 1449, 1381 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{18}\text{H}_{20}\text{ClF}_3\text{NaO}_4$, $[\text{M}+\text{Na}]^+$ 415.0900, found 415.0892. $[\alpha]_{\text{D}}^{26} +24.1$ (c 6.87, CHCl_3) (94% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 9/1, flow: 1.0 mL/min, 215 nm, 35 $^{\circ}\text{C}$, t_{R} 3.88 min (major); t_{R} 4.25 min (minor)).

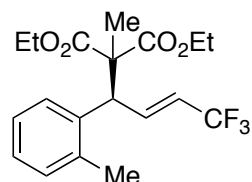


(S)-Diethyl 2-(1-(3-chlorophenyl)-4,4,4-trifluorobut-2-en-1-yl)-2-methylmalonate ((S)-3ea): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.21 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H), 1.40 (s, 3H), 4.10–4.28 (m, 5H), 5.59 (dq, $J_{\text{HH}} = 15.6$ Hz, $J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} = 1.1$ Hz, 1H), 6.87 (ddq, $J_{\text{HH}} = 15.6, 7.8$ Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.07–7.13 (m, 1H), 7.20–7.31 (m, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.9, 19.2, 51.8, 58.0, 61.8, 61.8, 120.9 (q, $J_{CF} = 33.6$ Hz), 122.8 (q, $J_{CF} = 269.9$ Hz), 127.6, 128.0, 129.7, 129.8, 134.4, 138.9 (q, $J_{CF} = 7.2$ Hz), 170.1, 170.6. ^{19}F NMR (470 MHz,

CDCl₃) δ 97.6 (dt, $J = 4.2, 2.0$ Hz). IR (neat) 3071, 2986, 2943, 2907, 2877, 1732, 1678, 1596, 1573, 1477, 1366 cm⁻¹. HRMS (ESI): m/z : calcd for C₁₈H₂₀ClF₃NaO₄, [M+Na]⁺ 415.0900, found 415.0894. $[\alpha]_D^{26} +20.6$ (c 6.26, CHCl₃) (94% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 8.08 min (major); t_R 8.65 min (minor)).

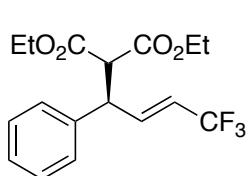


(S)-Diethyl 2-methyl-2-(4,4,4-trifluoro-1-(naphthalen-2-yl)but-2-en-1-yl)malonate ((S)-3fa): Colorless oil; ¹H NMR (500 MHz, CDCl₃) δ 1.19 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H), 1.43 (s, 3H), 4.12 (dq $J = 14.3, 1.4$ Hz, 2H), 4.18–4.31 (m, 2H), 4.36 (dd, $J = 7.4, 1.4$ Hz, 1H), 5.59 (dq, $J_{HH} = 15.8$ Hz, $J_{HF} = 6.3$ Hz, $J_{HH} = 1.4$ Hz, 1H), 7.01 (ddq, $J_{HH} = 15.8, 7.4$ Hz, $J_{HF} = 2.1$ Hz, 1H), 7.30 (dd, $J = 8.4, 1.9$ Hz, 1H), 7.44–7.51 (m, 2H), 7.68 (s, 1H), 7.76–7.85 (m, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 13.9, 19.5, 52.3, 58.1, 61.7, 61.7, 120.5 (q, $J_{CF} = 33.6$ Hz), 123.0 (q, $J_{CF} = 269.9$ Hz), 126.2, 126.3, 126.3, 126.9, 127.6, 127.8, 128.3, 129.0, 132.7, 133.2, 134.4, 139.8 (q, $J_{CF} = 6.8$ Hz), 170.5, 170.9. ¹⁹F NMR (470 MHz, CDCl₃) δ 97.8 (dt, $J = 6.3, 1.9$ Hz). IR (neat) 3060, 2985, 2941, 2906, 1731, 1677, 1600, 1508, 1463, 1381 cm⁻¹. HR-MS (ESI): m/z : calcd for C₂₂H₂₃F₃NaO₄, [M+Na]⁺ 431.1446, found 431.1443. $[\alpha]_D^{26} +28.5$ (c 5.48, CHCl₃) (96% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 99/1, flow: 1.0 mL/min, 254 nm, 35 °C, t_R 8.94 min (major); t_R 9.94 min (minor)).



(S)-Diethyl 2-methyl-2-(4,4,4-trifluoro-1-(*o*-tolyl)but-2-en-1-yl)malonate ((S)-3ga): Colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 1.16 (t, $J = 7.2$ Hz, 3H), 1.28 (t, $J = 7.2$ Hz, 3H), 1.39 (s, 3H), 2.36 (s, 3H), 4.11 (dq $J = 7.2, 2.0$ Hz, 2H), 4.20–4.31 (m, 2H), 4.55–4.61 (m, 1H), 5.38 (dq, $J_{HH} = 15.8$ Hz, $J_{HF} = 6.3$ Hz, $J_{HH} = 1.7$ Hz, 1H), 6.84 (ddq, $J_{HH} = 15.8, 6.3$ Hz, $J_{HF} = 2.0$ Hz, 1H), 7.06–7.11 (m, 1H), 7.14–7.21 (m, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 13.8, 13.8, 19.8, 20.1, 46.2, 57.9, 61.7, 61.7, 119.5 (q, $J_{CF} = 33.6$ Hz), 123.1 (q, $J_{CF} = 268.7$ Hz), 126.5, 127.5, 127.7, 130.9, 135.3, 137.2,

140.8 (q, $J_{CF} = 6.4$ Hz), 170.9, 171.3. ^{19}F NMR (470 MHz, CDCl_3) δ 98.0 (dt, $J = 4.2$, 2.1 Hz). IR (neat) 2985, 2942, 2908, 2876, 1732, 1675, 1492, 1464, 1380 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{19}\text{H}_{24}\text{F}_3\text{O}_4$, $[\text{M}+\text{H}]^+$ 373.1627, found 373.1617. $[\alpha]_{\text{D}}^{26} +29.2$ (c 5.54, CHCl_3) (86% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 $^\circ\text{C}$, t_{R} 3.80 min (major); t_{R} 6.30 min (minor)).



(R)-Diethyl 2-(4,4,4-trifluoro-1-phenylbut-2-en-1-yl)malonate

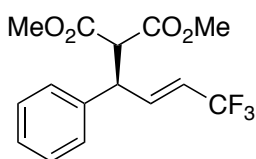
((R)-5aa)⁶: Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.00 (t,

$J = 7.2$ Hz, 3H), 1.28 (t, $J = 7.2$ Hz, 3H), 3.84 (d, $J = 10.6$ Hz, 1H), 3.93–4.00 (m, 2H), 4.17–4.26 (m, 3H), 5.66 (dq, $J_{\text{HH}} = 15.8$ Hz,

$J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} = 1.1$ Hz, 1H), 6.57 (ddq, $J_{\text{HH}} = 15.8$, 8.2 Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.20–7.36 (m, 5H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.6, 13.9, 47.3, 56.7, 61.6, 61.9, 120.2

(q, $J_{\text{CF}} = 34.0$ Hz), 122.6 (q, $J_{\text{CF}} = 269.5$ Hz), 127.7, 128.1, 128.9, 137.8, 139.5 (q, $J_{\text{CF}} = 6.4$ Hz), 166.8, 167.3. ^{19}F NMR (470 MHz, CDCl_3) δ 97.5 (dt, $J = 6.3$, 1.9 Hz). IR

(neat) 3036, 2986, 2941, 1734, 1679, 1496, 1455, 1370 cm^{-1} . $[\alpha]_{\text{D}}^{25} +15.2$ (c 4.45, CHCl_3) (87% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 $^\circ\text{C}$, t_{R} 8.21 min (major); t_{R} 9.69 min (minor)).



(R)-Dimethyl 2-(4,4,4-trifluoro-1-phenylbut-2-en-1-yl)malonate

((R)-5ab): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ

3.52 (s, 3H), 3.76 (s, 3H), 3.89 (d, $J = 10.9$ Hz, 1H), 4.21 (dd, $J = 10.9$, 8.3 Hz, 1H), 5.66 (dq, $J_{\text{HH}} = 15.8$ Hz, $J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} =$

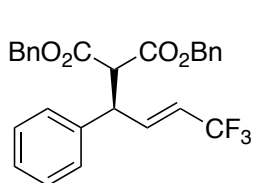
1.1 Hz, 1H), 6.56 (ddq, $J_{\text{HH}} = 15.8$, 8.3 Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.18–7.39 (m, 5H). ^{13}C

NMR (125 MHz, CDCl_3) δ 47.3, 52.6, 52.7, 56.6, 120.4 (q, $J_{\text{CF}} = 33.6$ Hz), 122.6 (q, $J_{\text{CF}} = 269.5$ Hz), 127.8, 128.0, 129.9, 137.6, 139.2 (q, $J_{\text{CF}} = 6.4$ Hz), 167.1, 167.7. ^{19}F

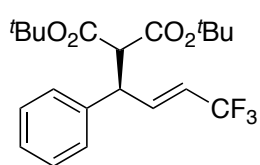
NMR (470 MHz, CDCl_3) δ 97.5 (dt, $J = 6.3$, 1.8 Hz). IR (neat) 3066, 3034, 2958, 2848, 1749, 1679, 1437 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{15}\text{H}_{15}\text{F}_3\text{NaO}_4$, $[\text{M}+\text{Na}]^+$

339.0820, found 339.0814. $[\alpha]_{\text{D}}^{26} +16.8$ (c 5.27, CHCl_3) (81% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H

(hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 8.04 min (major); t_R 8.58 min (minor)).

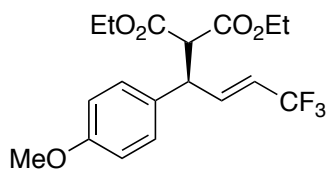


(R)-Dibenzyl 2-(4,4,4-trifluoro-1-phenylbut-2-en-1-yl)malonate ((R)-5ac): Colorless oil; ^1H NMR (500 MHz, CDCl_3) δ 3.96 (d, $J = 10.9$ Hz, 1H), 4.23 (dd, $J = 10.9, 8.1$ Hz, 1H), 4.88 (d, $J = 12.3$ Hz, 1H), 4.92 (d, $J = 12.0$ Hz, 1H), 5.13 (d, $J = 12.3$ Hz, 1H), 5.16 (d, $J = 12.0$ Hz, 1H), 5.59 (dq, $J_{\text{HH}} = 15.8$ Hz, $J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} = 1.1$ Hz, 1H), 6.55 (ddq, $J_{\text{HH}} = 15.8, 8.1$ Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.03 (dd, $J = 1.6, 7.9$ Hz, 2H), 7.14–7.18 (m, 2H), 7.21–7.37 (m, 11H). ^{13}C NMR (125 MHz, CDCl_3) δ 47.2, 56.7, 67.3, 67.6, 120.4 (q, $J_{\text{CF}} = 33.6$ Hz), 122.6 (q, $J_{\text{CF}} = 269.9$ Hz), 127.8, 128.0, 128.1, 128.3, 128.4, 128.4, 128.5, 128.6, 129.0, 134.8, 134.8, 137.5, 139.2 (q, $J_{\text{CF}} = 6.0$ Hz), 166.5, 166.9. ^{19}F NMR (470 MHz, CDCl_3) δ 97.6 (dt, $J = 6.4, 1.9$ Hz). IR (neat) 3066, 3034, 2959, 1756, 1736, 1678, 1602, 1497, 1455 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{27}\text{H}_{24}\text{F}_3\text{O}_4$, $[\text{M}+\text{H}]^+$ 469.1627, found 469.1619. $[\alpha]_{\text{D}}^{26} +9.89$ (c 7.45, CHCl_3) (78% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 17.7 min (minor); t_R 21.5 min (major)).

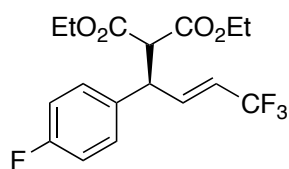


(R)-Di-tert-butyl 2-(4,4,4-trifluoro-1-phenylbut-2-en-1-yl)malonate ((R)-5ad): White solid. Mp. 99–105 °C. ^1H NMR (500 MHz, CDCl_3) δ 1.21 (s, 9H), 1.47 (s, 9H), 3.66 (d, $J = 10.9$ Hz, 1H), 4.10 (dd, $J = 10.9, 8.0$ Hz, 1H), 5.62 (dq, $J_{\text{HH}} = 15.8$ Hz, $J_{\text{HF}} = 7.9$ Hz, $J_{\text{HH}} = 1.1$ Hz, 1H), 6.57 (ddq, $J_{\text{HH}} = 15.8, 8.0$ Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.18–7.35 (m, 5H). ^{13}C NMR (125 MHz, CDCl_3) δ 27.5, 27.8, 47.2, 58.3, 82.0, 82.5, 119.8 (q, $J_{\text{CF}} = 33.6$ Hz), 122.8 (q, $J_{\text{CF}} = 269.9$ Hz), 127.5, 128.3, 128.8, 138.2, 140.1 (q, $J_{\text{CF}} = 6.4$ Hz), 166.1, 166.7. ^{19}F NMR (470 MHz, CDCl_3) δ 97.7 (dt, $J = 6.3, 1.9$ Hz). IR (KBr) 3066, 3055, 2990, 2936, 1740, 1682, 1602, 1584, 1363 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{21}\text{H}_{27}\text{F}_3\text{NaO}_4$, $[\text{M}+\text{Na}]^+$ 423.1759, found 423.1751. $[\alpha]_{\text{D}}^{26} +3.66$ (c 4.48, CHCl_3) (52% ee). Enantiomeric purity was determined by HPLC using a Daicel

CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 6.37 min (major); t_R 8.47 min (minor)).

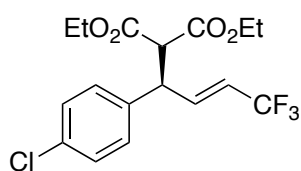


(R)-Diethyl 2-(4,4,4-trifluoro-1-(4-methoxyphenyl)but-2-en-1-yl)malonate ((R)-5ba): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.03 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H), 3.76–3.82 (m, 4H), 3.93–4.04 (m, 2H), 4.12–4.19 (m, 1H), 4.22 (d, $J = 7.2$ Hz, 2H), 5.63 (dq, $J_{\text{HH}} = 15.6$ Hz, $J_{\text{HF}} = 6.2$ Hz, $J_{\text{HH}} = 1.1$ Hz, 1H), 6.55 (ddq, $J_{\text{HH}} = 15.6$, 8.0 Hz, $J_{\text{HF}} = 2.0$ Hz, 1H), 6.86 (d, $J = 8.9$ Hz, 2H), 7.14 (d, $J = 8.9$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.7, 13.9, 46.5, 55.2 (d, $J_{\text{CF}} = 2.4$ Hz), 56.9, 61.6, 61.9, 114.2, 119.9 (q, $J_{\text{CF}} = 33.6$ Hz), 122.7 (q, $J_{\text{CF}} = 269.5$ Hz), 129.2, 129.6, 139.7 (q, $J_{\text{CF}} = 6.4$ Hz), 159.0, 166.8, 167.4. ^{19}F NMR (470 MHz, CDCl_3) δ 97.6 (dt, $J = 6.3$, 1.9 Hz). IR (neat) 2984, 2940, 2908, 2840, 1734, 1678, 1611, 1585, 1514, 1465 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{18}\text{H}_{21}\text{F}_3\text{NaO}_5$, $[\text{M}+\text{Na}]^+$ 397.1239, found 397.1234. $[\alpha]_{\text{D}}^{26} +14.0$ (c 5.41, CHCl_3) (88% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 12.0 min (major); t_R 16.9 min (minor)).

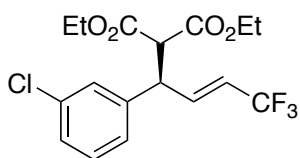


(R)-Diethyl 2-(4,4,4-trifluoro-1-(4-fluorophenyl)but-2-en-1-yl)malonate ((R)-5ca): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.04 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H), 3.80 (d, $J = 10.6$ Hz, 1H), 3.94–4.04 (m, 2H), 4.16–4.27 (m, 3H), 5.65 (dq, $J_{\text{HH}} = 15.6$ Hz, $J_{\text{HF}} = 6.2$ Hz, $J_{\text{HH}} = 1.2$ Hz, 1H), 6.54 (ddq, $J_{\text{HH}} = 15.6$, 8.2 Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 6.99–7.07 (m, 2H), 7.17–7.25 (m, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.7, 13.9, 46.5, 56.8, 61.7, 62.0, 115.8 (d, $J_{\text{CF}} = 21.6$ Hz), 120.4 (q, $J_{\text{CF}} = 33.6$ Hz), 122.6 (q, $J_{\text{CF}} = 269.5$ Hz), 129.8 (d, $J_{\text{CF}} = 8.4$ Hz), 133.6 (d, $J_{\text{CF}} = 3.6$ Hz), 139.2 (q, $J_{\text{CF}} = 6.0$ Hz), 162.1 (d, $J_{\text{CF}} = 247.1$ Hz), 166.7, 167.1. ^{19}F NMR (470 MHz, CDCl_3) δ 47.6 (tt, $J = 8.5$, 5.2 Hz), 97.5 (dt, $J = 6.2$, 1.9 Hz). IR (neat) 2986, 2942, 2909, 1734, 1680, 1605, 1511 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{17}\text{H}_{18}\text{F}_4\text{NaO}_4$, $[\text{M}+\text{Na}]^+$ 385.1039, found 385.1022. $[\alpha]_{\text{D}}^{26} +12.9$ (c 5.96, CHCl_3) (93% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H

(hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 9.33 min (major); t_R 13.23 min (minor)).

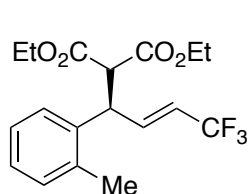


(R)-Diethyl 2-(1-(4-chlorophenyl)-4,4,4-trifluorobut-2-en-1-yl)malonate ((R)-5da): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.05 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H), 3.79 (d, $J = 10.9$ Hz, 1H), 3.97–4.03 (m, 2H), 4.14–4.25 (m, 3H), 5.65 (dq, $J_{\text{HH}} = 15.8$ Hz, $J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} = 1.1$ Hz, 1H), 6.53 (ddq, $J_{\text{HH}} = 15.8$, 8.2 Hz, $J_{\text{HF}} = 2.1$ Hz 1H), 7.17 (d, $J = 8.6$ Hz, 2H), 7.31 (d, $J = 8.6$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.7, 13.9, 46.6, 56.6, 61.8, 62.0, 120.6 (q, $J_{\text{CF}} = 34.0$ Hz), 122.5 (q, $J_{\text{CF}} = 269.5$ Hz), 129.1, 129.5, 133.7, 136.3, 138.9 (q, $J_{\text{CF}} = 6.4$ Hz), 166.6, 167.0. ^{19}F NMR (470 MHz, CDCl_3) δ 97.4 (dt, $J = 6.2$, 1.8 Hz). IR (neat) 2986, 2941, 2908, 1734, 1679, 1596, 1493, 1370 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{17}\text{H}_{18}\text{ClF}_3\text{NaO}_4$, $[\text{M}+\text{Na}]^+$ 401.0743, found 401.0735. $[\alpha]_{\text{D}}^{26} +16.0$ (c 6.60, CHCl_3) (94% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 10.8 min (major); t_R 13.7 min (minor)).

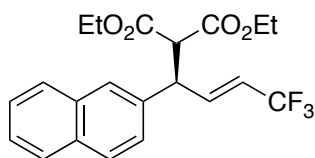


(R)-Diethyl 2-(1-(3-chlorophenyl)-4,4,4-trifluorobut-2-en-1-yl)malonate ((R)-5ea): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.05 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H), 3.82 (d, $J = 10.9$ Hz, 1H), 4.01 (qd, $J = 14.2$, 1.3 Hz, 2H), 4.16–4.27 (m, 3H), 5.68 (dq, $J_{\text{HH}} = 15.8$ Hz, $J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} = 1.1$ Hz, 1H), 6.53 (ddq, $J_{\text{HH}} = 15.8$, 8.3 Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.13 (dt, $J = 6.8$, 1.9 Hz, 1H), 7.23–7.30 (m, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.7, 13.9, 46.9, 56.5, 61.8, 62.0, 120.7 (q, $J_{\text{CF}} = 34.0$ Hz), 122.5 (q, $J_{\text{CF}} = 269.5$ Hz), 126.3, 128.0, 128.3, 130.2, 134.7, 138.7 (q, $J_{\text{CF}} = 6.8$ Hz), 139.9, 166.5, 167.0. ^{19}F NMR (470 MHz, CDCl_3) δ 97.4 (dt, $J = 4.0$, 1.9 Hz). IR (neat) 2985, 2940, 2907, 1733, 1679, 1596, 1574, 1477 cm^{-1} . HR-MS (ESI): m/z : calcd for $\text{C}_{17}\text{H}_{18}\text{ClF}_3\text{NaO}_4$, $[\text{M}+\text{Na}]^+$ 401.0743, found 401.0734. $[\alpha]_{\text{D}}^{25} +14.0$ (c 6.13, CHCl_3) (92% ee). Enantiomeric purity was determined by HPLC using a Daicel

CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 7.97 min (major); t_R 9.02 min (minor)).



(R)-Diethyl 2-(4,4,4-trifluoro-1-(o-tolyl)but-2-en-1-yl)malonate ((R)-5fa): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 0.97 (t, $J = 7.2$ Hz, 3H), 1.29 (t, $J = 7.2$ Hz, 3H), 2.40 (s, 3H), 3.88–4.00 (m, 3H), 4.19–4.29 (m, 2H), 4.49 (dd, $J = 11.5, 7.8$ Hz, 1H), 5.57 (dq, $J_{\text{HH}} = 15.8$ Hz, $J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} = 1.4$ Hz, 1H), 6.46 (ddq, $J_{\text{HH}} = 15.8, 7.8$ Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.12–7.22 (m, 4H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.5, 13.9, 19.6, 42.5, 56.2, 61.5, 61.9, 119.9 (q, $J_{\text{CF}} = 33.6$ Hz), 122.6 (q, $J_{\text{CF}} = 269.5$ Hz), 126.4, 126.5, 127.4, 130.9, 135.9, 136.6, 139.3 (q, $J_{\text{CF}} = 6.4$ Hz), 166.7, 167.5. ^{19}F NMR (470 MHz, CDCl_3) δ 97.6 (dt, $J = 4.2, 2.1$ Hz). IR (neat) 2984, 2940, 2908, 2876, 1736, 1677, 1493, 1466, 1447 cm^{-1} . HRMS (ESI): m/z : calcd for $\text{C}_{18}\text{H}_{22}\text{F}_3\text{O}_4$, $[\text{M}+\text{H}]^+$ 359.1470, found 359.1465. $[\alpha]_{\text{D}}^{25} +43.4$ (c 2.84, CHCl_3) (83% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, t_R 4.78 min (major); t_R 7.06 min (minor)).

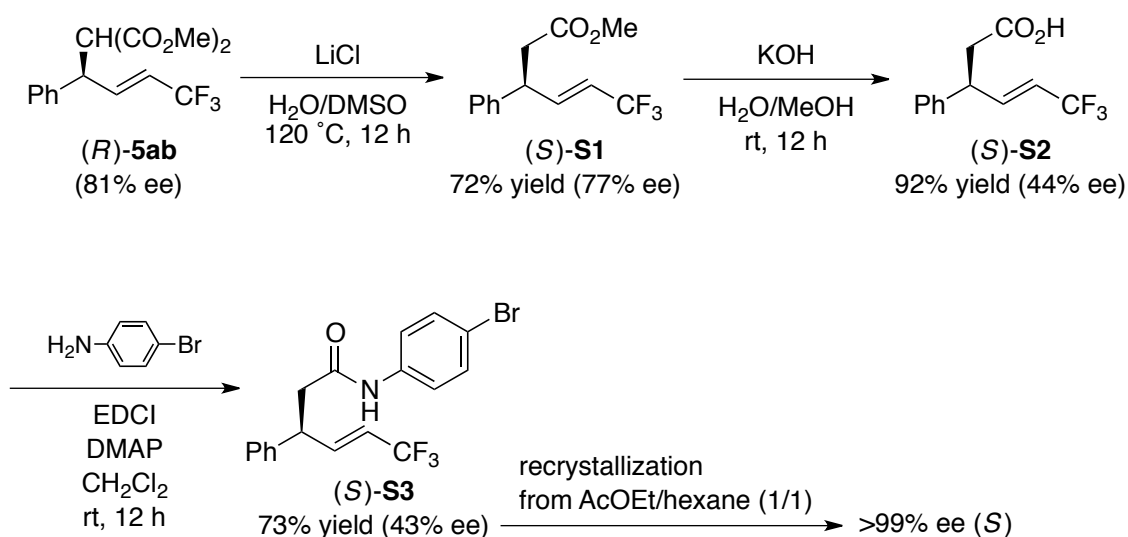


(R)-Diethyl 2-(4,4,4-trifluoro-1-(naphthalen-2-yl)but-2-en-1-yl)malonate ((R)-5ga): Colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 0.94 (t, $J = 7.2$ Hz, 3H), 1.29 (t, $J = 7.2$ Hz, 3H), 3.88–4.01 (m, 3H), 4.25 (qd, $J = 7.2, 0.9$ Hz, 2H), 4.40 (dd, $J = 10.9, 8.2$ Hz, 1H), 5.71 (dq, $J_{\text{HH}} = 15.8$ Hz, $J_{\text{HF}} = 6.3$ Hz, $J_{\text{HH}} = 1.1$ Hz, 1H), 6.67 (ddq, $J_{\text{HH}} = 15.8, 8.2$ Hz, $J_{\text{HF}} = 2.1$ Hz, 1H), 7.35 (dd, $J = 8.4, 1.9$ Hz, 1H), 7.44–7.50 (m, 2H), 7.70 (d, $J = 1.7$ Hz, 1H), 7.76–7.85 (m, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 13.6, 14.0, 47.4, 56.7, 61.6, 62.0, 120.4 (q, $J_{\text{CF}} = 34.0$ Hz), 122.6 (q, $J_{\text{CF}} = 269.9$ Hz), 125.7, 126.2, 126.4, 127.1, 127.6, 127.8, 128.7, 132.7, 133.3, 135.2, 139.4 (q, $J_{\text{CF}} = 6.8$ Hz), 166.8, 167.3. ^{19}F NMR (470 MHz, CDCl_3) δ 97.6 (dt, $J = 4.0, 2.3$ Hz). IR (neat) 3058, 2984, 2940, 2907, 1733, 1678, 1600, 1508, 1465, 1370 cm^{-1} . H-MS (ESI): m/z : calcd for $\text{C}_{21}\text{H}_{21}\text{F}_3\text{NaO}_4$, $[\text{M}+\text{Na}]^+$ 417.1290, found 417.1280. $[\alpha]_{\text{D}}^{26} +22.1$ (c 6.75, CHCl_3) (82% ee). Enantiomeric purity was determined by HPLC using

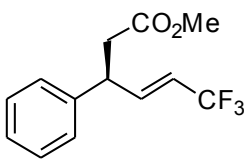
a Daicel CHIRALCEL OJ-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 254 nm, 35 °C, t_R 7.81 min (major); t_R 9.01 min (minor)).

Determination of the absolute configuration of the alkylated product **5ab** and **3ab**:

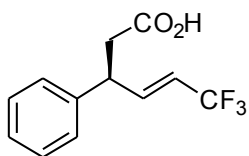
The absolute configuration of **5ab** was assigned to be *R* by the X-ray crystallography of its brominated derivative (*S*)-**S3** (Scheme S1), and the absolute configuration of other alkylated products were estimated by comparison with (*R*)-**5ab**. Furthermore, we also confirmed that the methylation of (*R*)-**5ab** by MeI and NaH in MeOH at reflux temperature provided (*S*)-**3ab** in 83% yield.



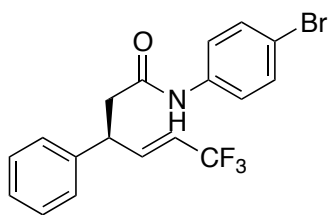
Scheme S1.


(*R*)-Methyl 6,6,6-trifluoro-3-phenylhex-4-enoate ((*S*)-S1**):**
 Isolated yield: 72%. Colorless oil. ^1H NMR (500 MHz, CDCl_3): δ 2.78 (d, $J = 7.5$ Hz, 2H), 3.64 (s, 3H), 3.98 (dt, $J = 7.0, 7.5$), 5.59 (dq, $J_{\text{HH}} = 16.0$ Hz, $J_{\text{HF}} = 6.5$ Hz, 1H), 6.54 (dd, $J_{\text{HH}} = 16.0, 6.5$ Hz, 1H), 7.19 (d, $J = 7.5$ Hz, 2H), 7.28 (d, $J = 7.0$ Hz, 1H), 7.34 (t, $J = 7.5$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ 39.4, 43.5, 51.8, 119.0 (q, $J_{\text{CF}} = 33.4$), 122.9 (q, $J_{\text{CF}} = 268$ Hz), 127.5, 129.0, 140.0, 141.7 (q, $J_{\text{CF}} = 6.0$ Hz), 171.4. ^{19}F NMR (CDCl_3): δ 97.80 (d, $J = 7.5$ Hz). IR (neat) 3033, 2955, 1740, 1678, 1439 cm^{-1} . HRMS (ESI): m/z : Calcd for $\text{C}_{13}\text{H}_{13}\text{F}_3\text{O}_2^+$ [$\text{M}+\text{H}$] $^+$ 259.0940, found 259.0933. $[\alpha]_{\text{D}}^{22}$

-12.2 (*c* 0.66, CHCl₃) (77% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 49/1, flow: 0.7 mL/min, 215 nm, 35 °C, *t*_R 7.77 min (minor); *t*_R 8.38 (major)).



(*R*)-6,6,6-trifluoro-3-phenylhex-4-enoic acid ((*S*)-S2): Isolated yield: 92%. White solid. Mp 85–87 °C. ¹H NMR (500 MHz, CDCl₃): δ 2.83 (d, *J* = 7.7 Hz, 2H), 3.96 (dt, *J* = 6.5, 7.7 Hz, 1H), 5.60 (dq, *J*_{HH} = 16.0 Hz, *J*_{HF} = 6.5 Hz, 1H), 6.54 (dd, *J*_{HH} = 16.0, 6.5 Hz, 1H), 7.19 (d, *J* = 7.5 Hz, 2H), 7.29 (d, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃): δ 39.2, 43.1, 119.3 (q, *J*_{CF} = 33.4 Hz), 122.9 (q, *J*_{CF} = 268 Hz), 127.6, 127.6, 129.1, 139.7, 141.5 (q, *J*_{CF} = 6.4 Hz), 177.0. ¹⁹F NMR (470 MHz, CDCl₃): δ 97.73 (d, *J* = 7.5 Hz). IR (neat) 3033, 1723, 1284 cm⁻¹. HRMS (ESI): *m/z*: Calcd for C₁₂H₁₁F₃O₂⁺ [M+Na]⁺ 267.0603, found 259.0608. [*α*]_D²⁸ +15.0 (*c* 0.35, CHCl₃) (44% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 9/1, flow: 0.7 mL/min, 215 nm, 35 °C, *t*_R 9.76 min (minor); *t*_R 11.39 min (major)).



(*R*)-*N*-(4-bromophenyl)-6,6,6-trifluoro-3-phenylhex-4-enamide ((*S*)-3S): Isolated yield 73%. White solid. Mp 160–164 °C. ¹H NMR (500 MHz, CDCl₃): δ 2.73 (m, 2H), 4.09 (dt, *J* = 6.0, 7.5 Hz, 1H), 5.62 (dq, *J*_{HH} = 15.5 Hz, *J*_{HF} = 6.0 Hz, 1H), 6.60 (dd, *J*_{HH} = 15.5, 6.0 Hz, 1H), 7.08 (br, 1H), 7.11-7.22 (m, 4H), 7.28-7.29 (m, 1H), 7.35-7.37 (m, 4H). ¹³C NMR (125 MHz, CDCl₃): δ 43.1, 43.7, 117.3, 119.3 (q, *J*_{CF} = 34.2 Hz), 121.7, 122.9 (q, *J* = 276 Hz), 127.6, 127.7, 129.2, 132.0, 136.3, 140.0, 141.7 (q, *J*_{CF} = 6.0 Hz), 168.2. ¹⁹F NMR (470 MHz, CDCl₃): δ 97.84 (d, *J* = 5.2 Hz). IR (neat) 3033, 1722, 1284 cm⁻¹. HRMS (ESI): *m/z*: Calcd for C₁₈H₁₅BrF₃NO⁺ [M+H]⁺ 398.0362, found 398.0334. [*α*]_D²⁷ -36.0 (*c* 0.66, CHCl₃) (99% ee). Enantiomeric purity was determined by HPLC using a Daicel CHIRALPAK AD-H (hexane/2-propanol = 19/1, flow: 1.0 mL/min, 215 nm, 35 °C, *t*_R 49.31 min (minor); *t*_R 55.39 min (major)). Recrystallization from AcOEt/hexane (1/1) at room temperature gave an enantiomerically pure **S3**, which is a

suitable for X-ray study, and the absolute configuration was determined to be *S*.

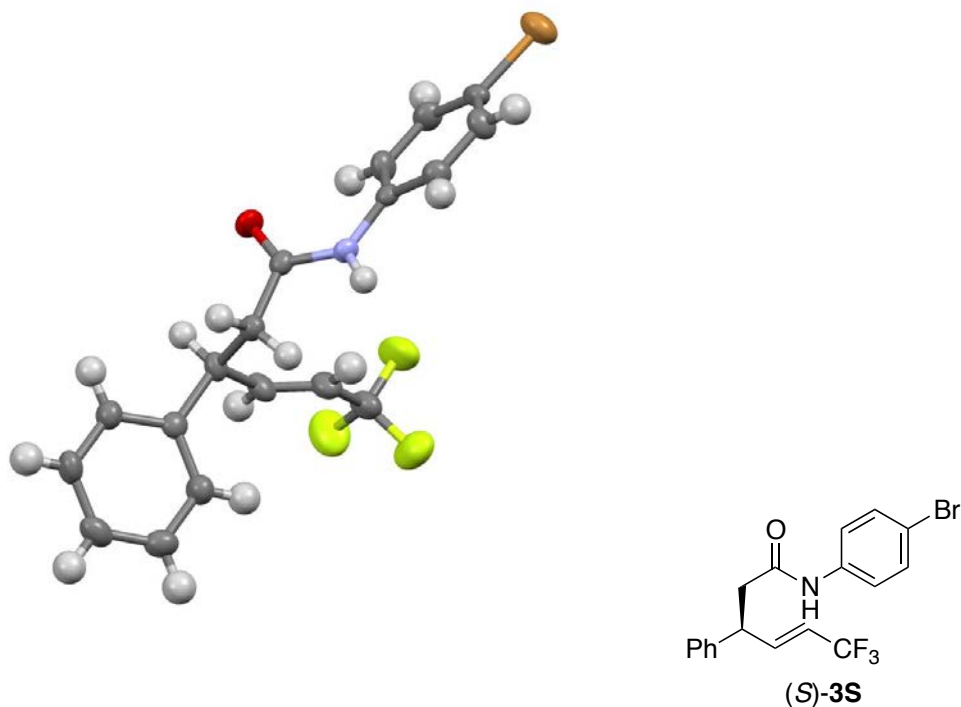


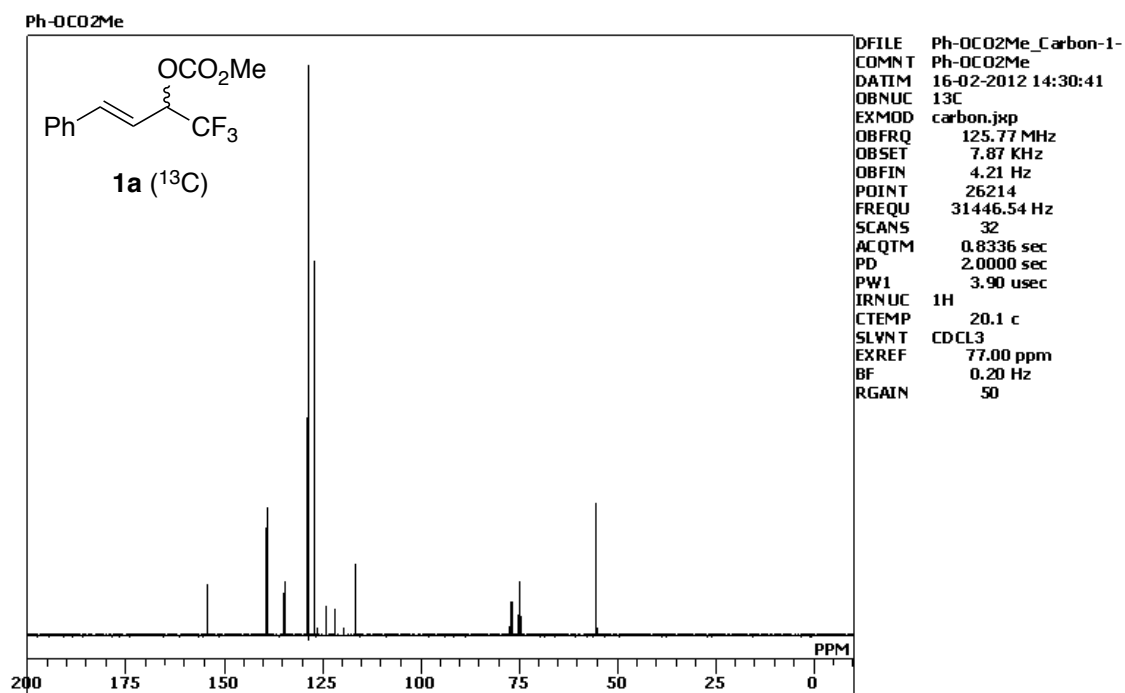
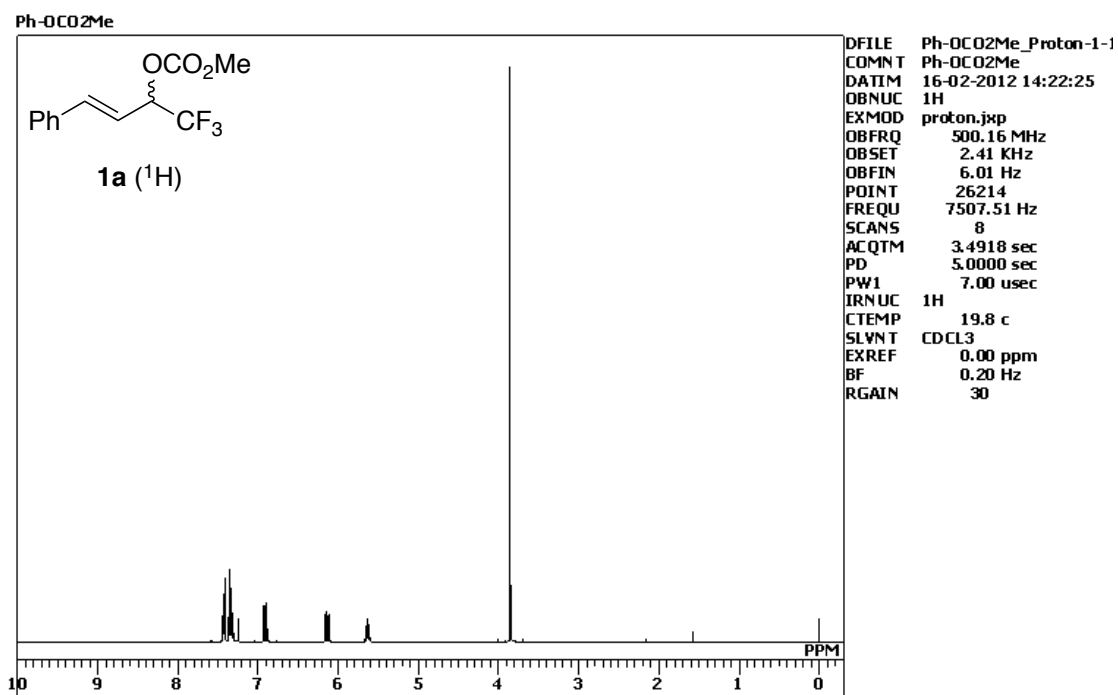
Figure S1. X-ray crystal structure of (*S*)-3S. CCDC 1451796 contains the supplementary crystallographic data for the compound (S)-3S. This data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

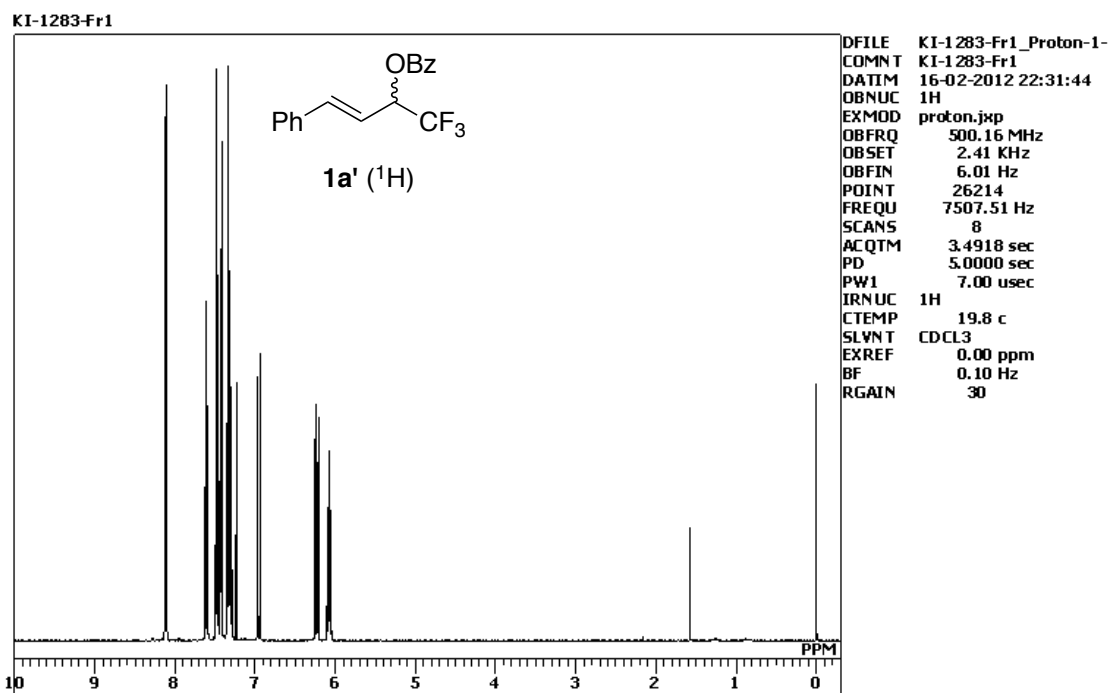
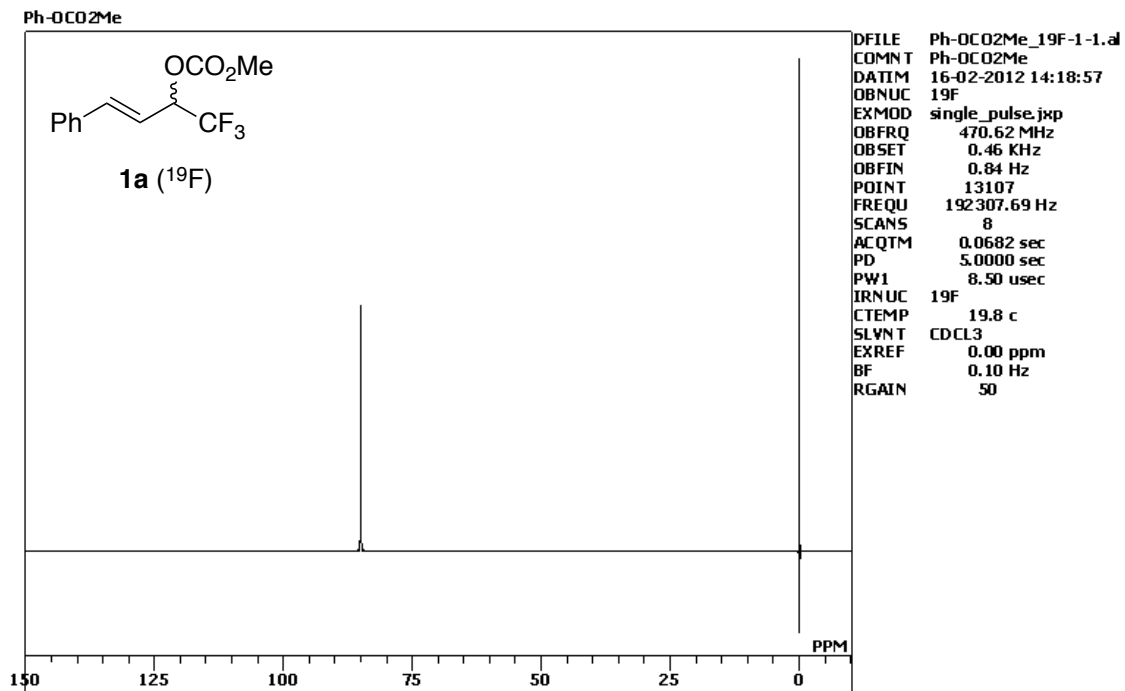
References

- (1) White, D. A.; Doyle, J. R.; Lewis, H. *Inorg. Synth.* **1972**, *13*, 55–65.
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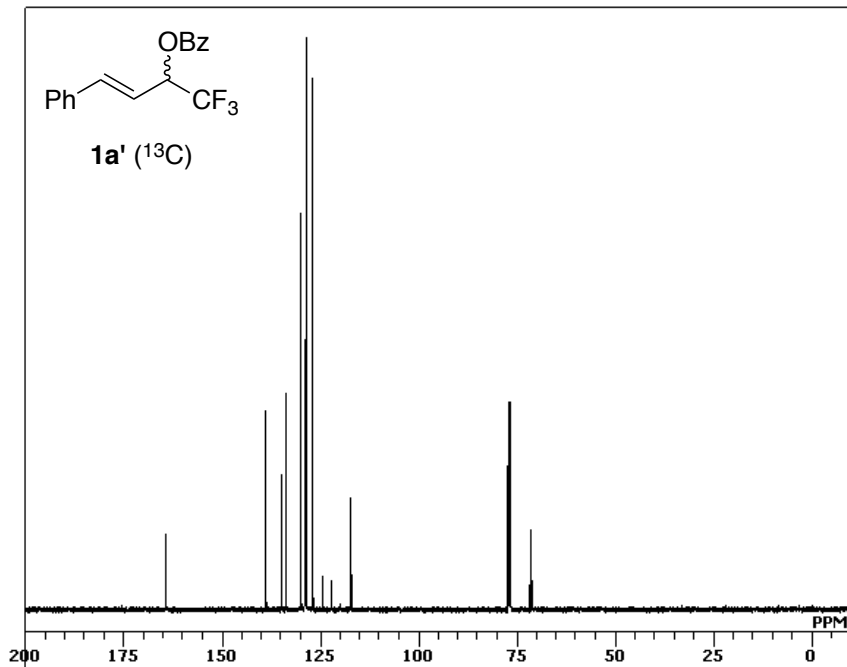
- (5) (a) Yamazaki, T.; Mizutani, K.; Kitazume, T. *J. Org. Chem.* **1995**, *60*, 6046–6056.
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Copies of ^1H , ^{13}C , and ^{19}F NMR spectra



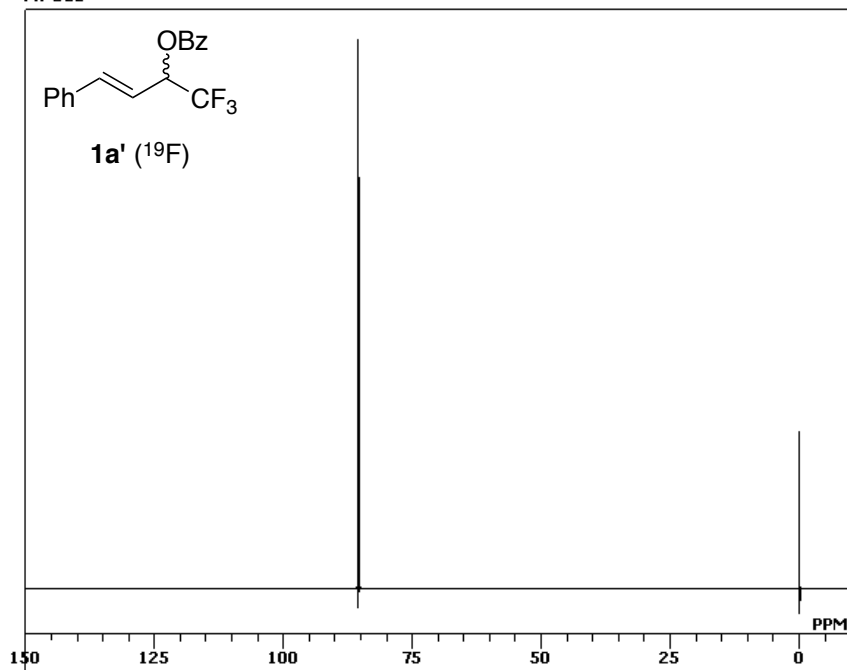


Ph-OBz



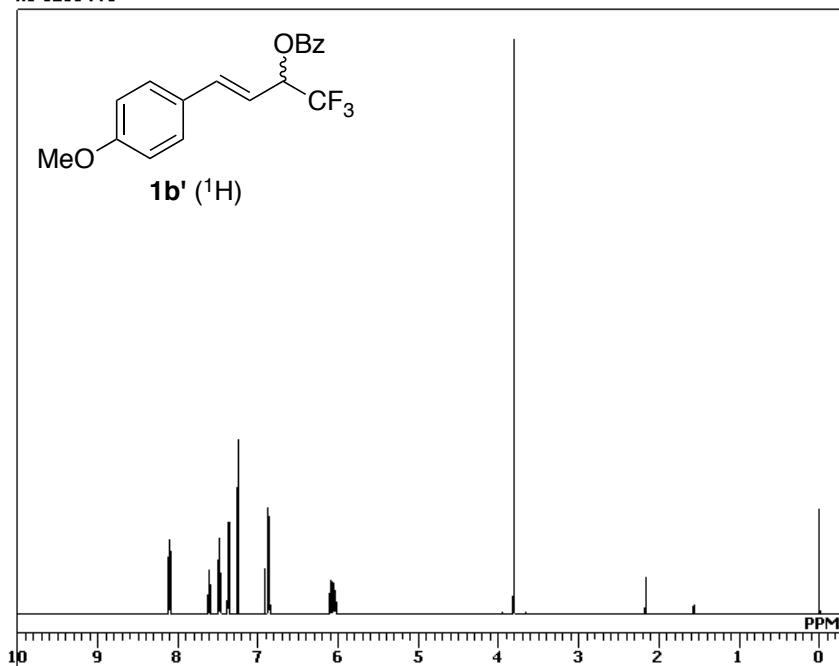
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POINT 26214
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PD 2.0000 sec
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CTEMP 20.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

Ph-OBz



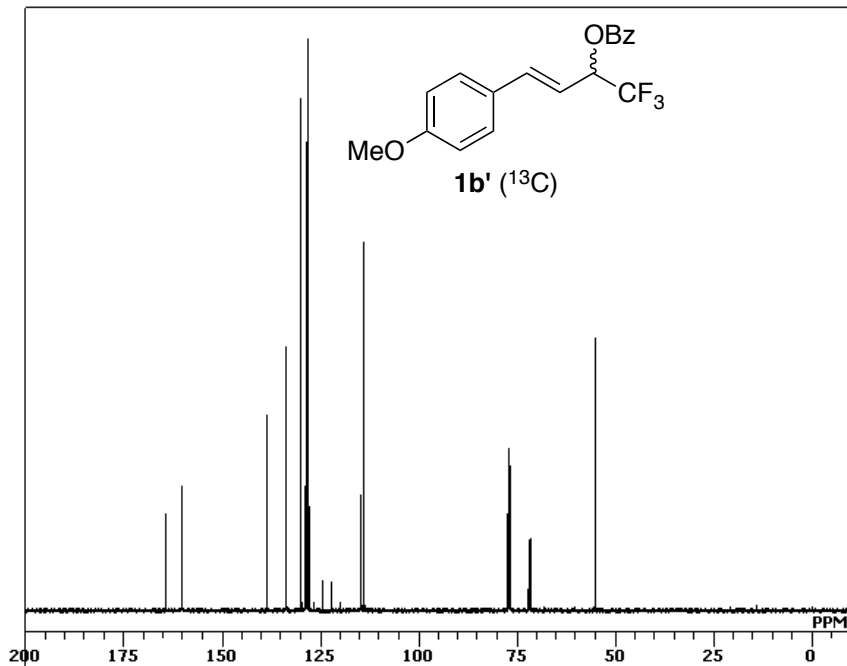
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OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
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EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 50

KI-1261-Fr1



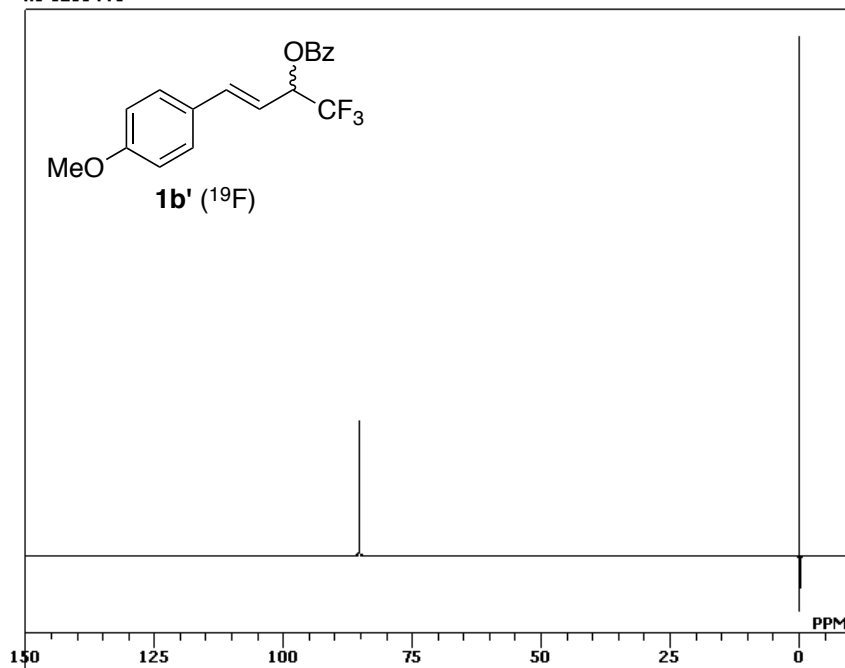
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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
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CTEMP 19.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 34

KI-1261-Fr1



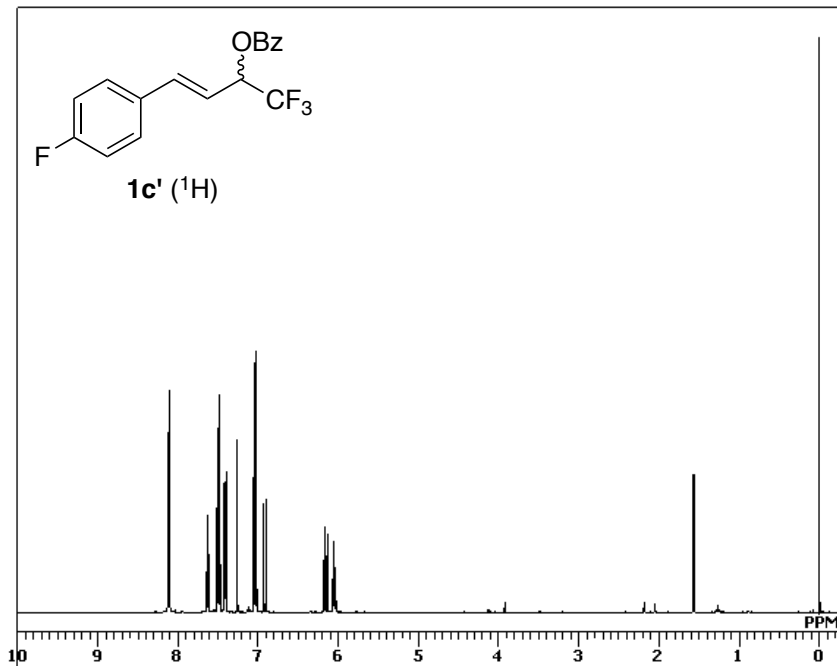
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OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 128
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

KI-1261-Fr1

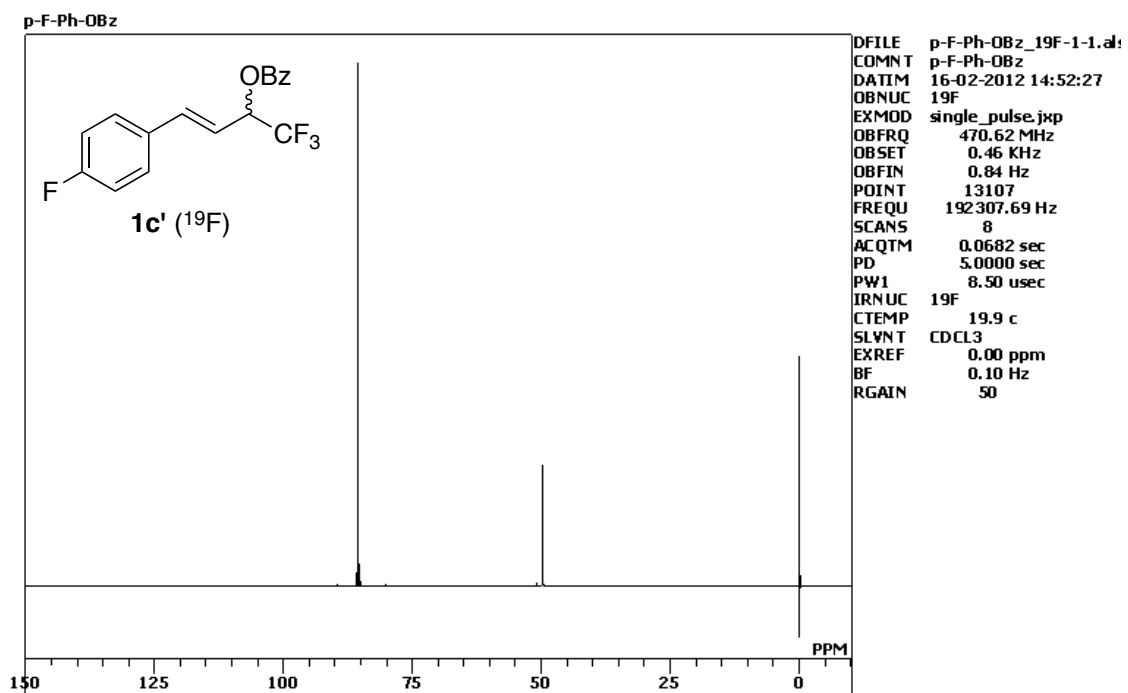
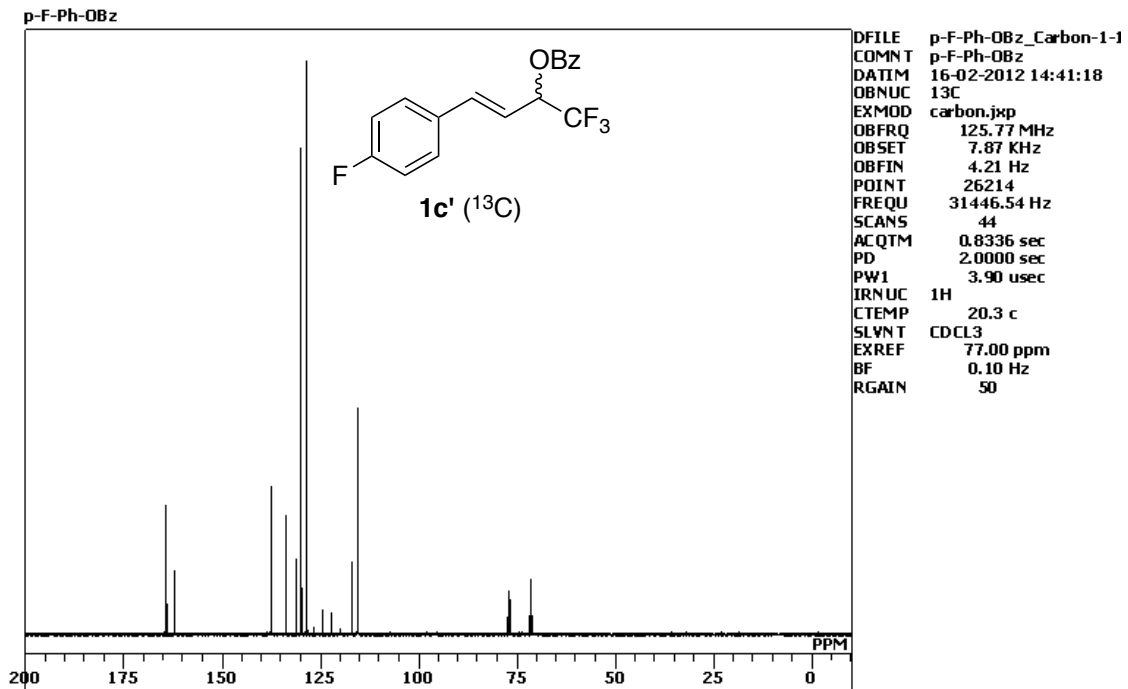


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OBFIN 0.84 Hz
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SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
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IRNUC 19F
CTEMP 19.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 50

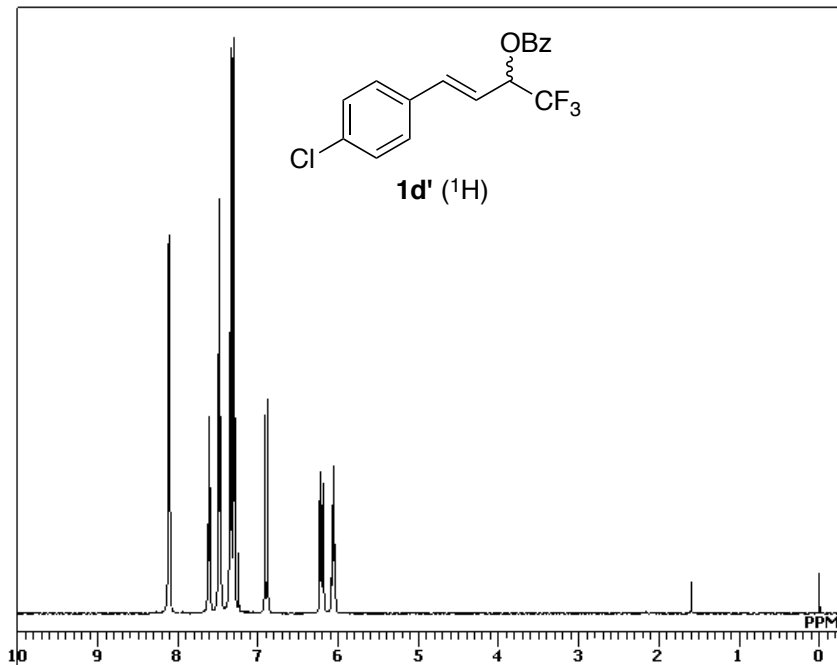
KI-683-Fr1



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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 16384
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SCANS 8
ACQTM 1.7459 sec
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IRNUC 1H
CTEMP 17.1 c
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BF 0.10 Hz
RGAIN 48

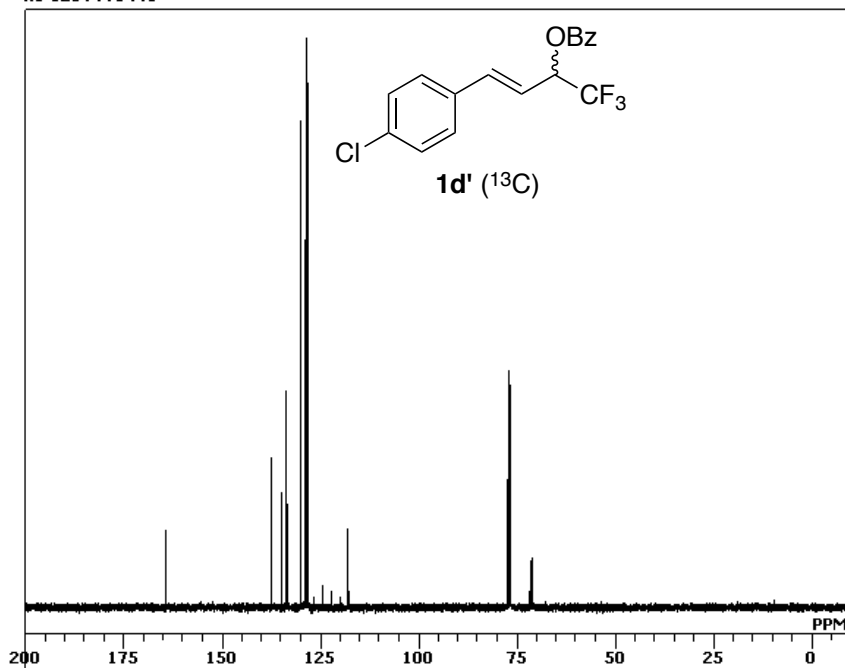


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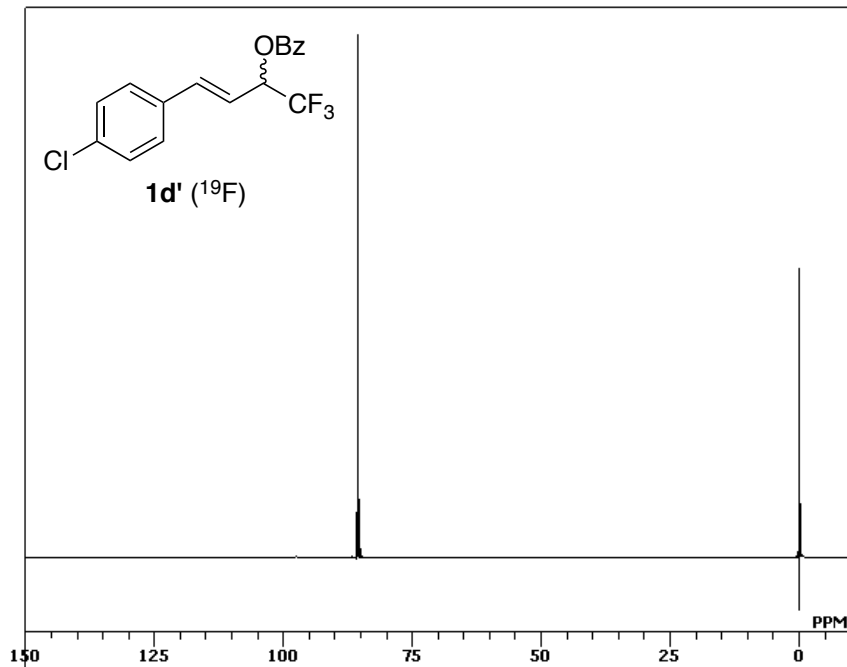
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EXMOD proton.jxp
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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 19.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 30

KI-1284-Fr1-Fr1



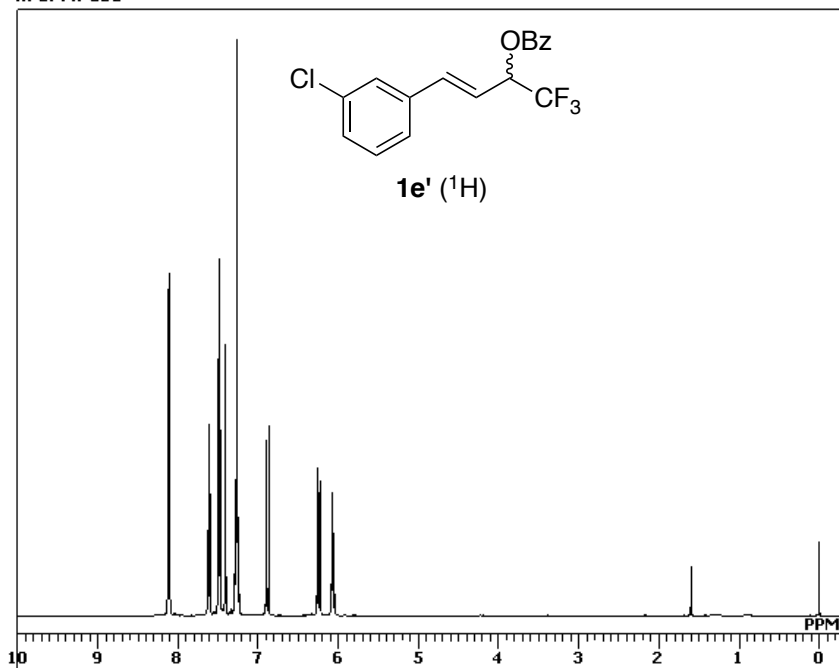
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OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 243
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PD 2.0000 sec
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CTEMP 20.4 c
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EXREF 77.00 ppm
BF 0.10 Hz
RGAIN 50

KI-1284-Fr1



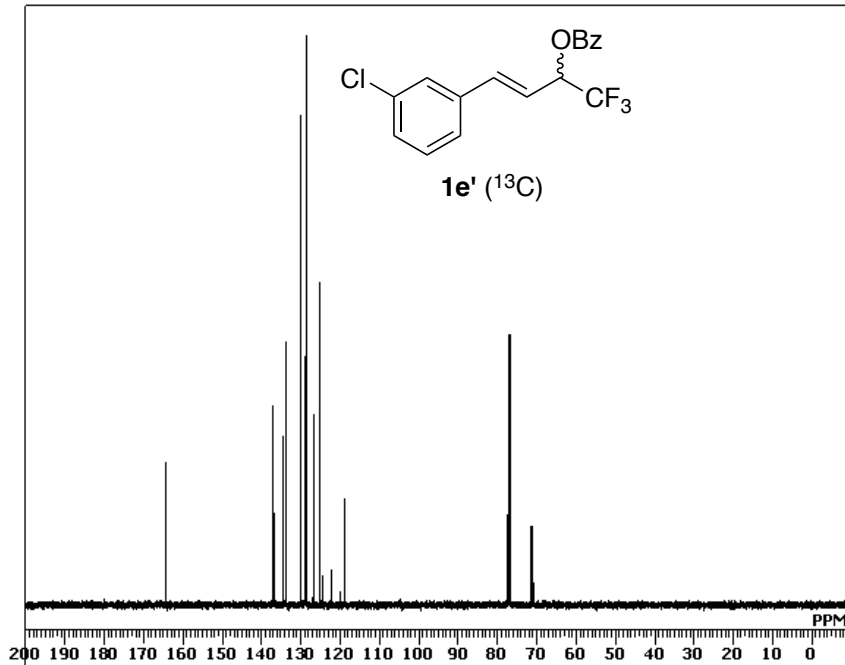
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OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 8.50 usec
IRNUC 19F
CTEMP 19.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 50

m-Cl-Ph-OBz



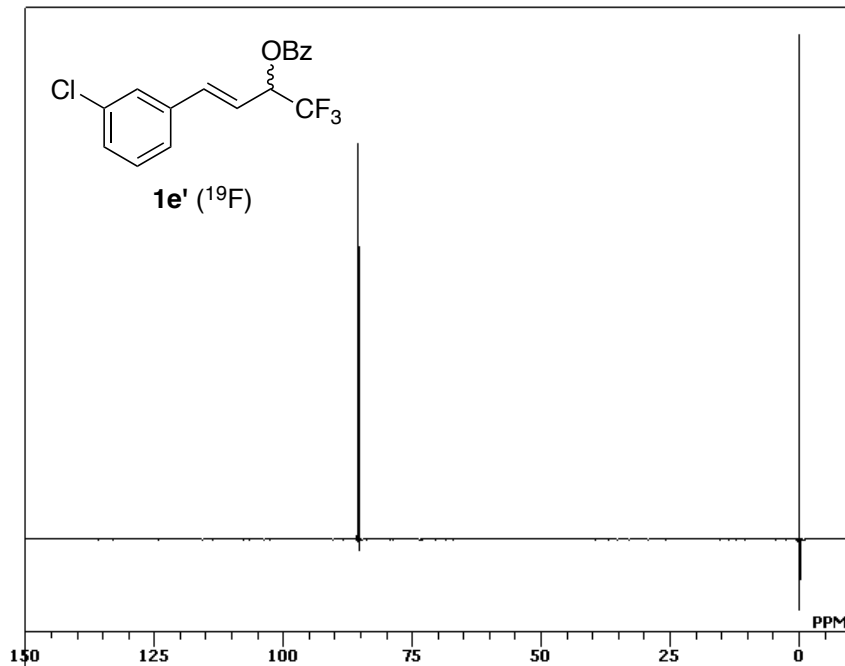
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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 19.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.30 Hz
RGAIN 30

m-Cl-Ph-OBz



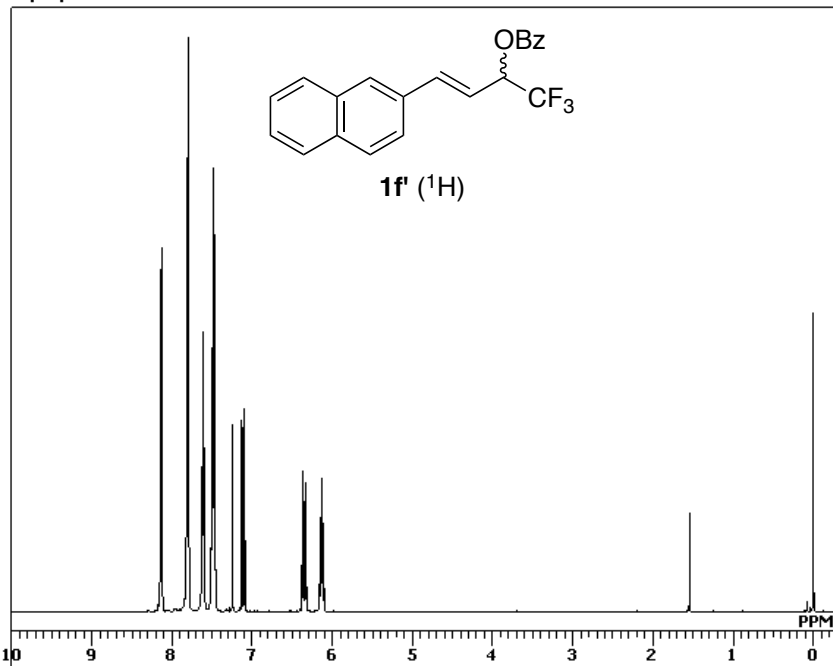
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POINT 26214
FREQU 31446.54 Hz
SCANS 200
ACQTM 0.8336 sec
PD 2.0000 sec
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BF 0.30 Hz
RGAIN 50

KI-1190



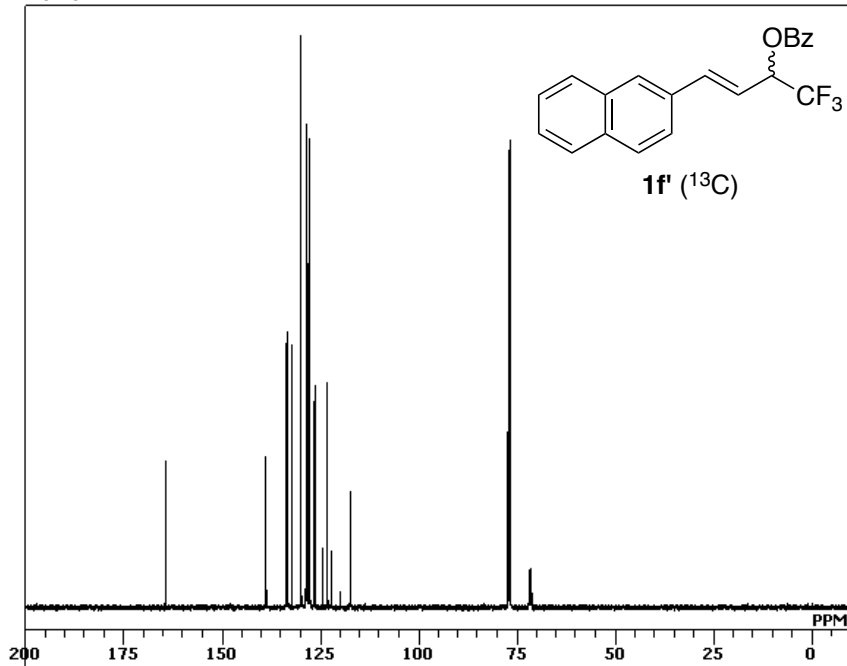
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OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 50

naphtyl-OBz



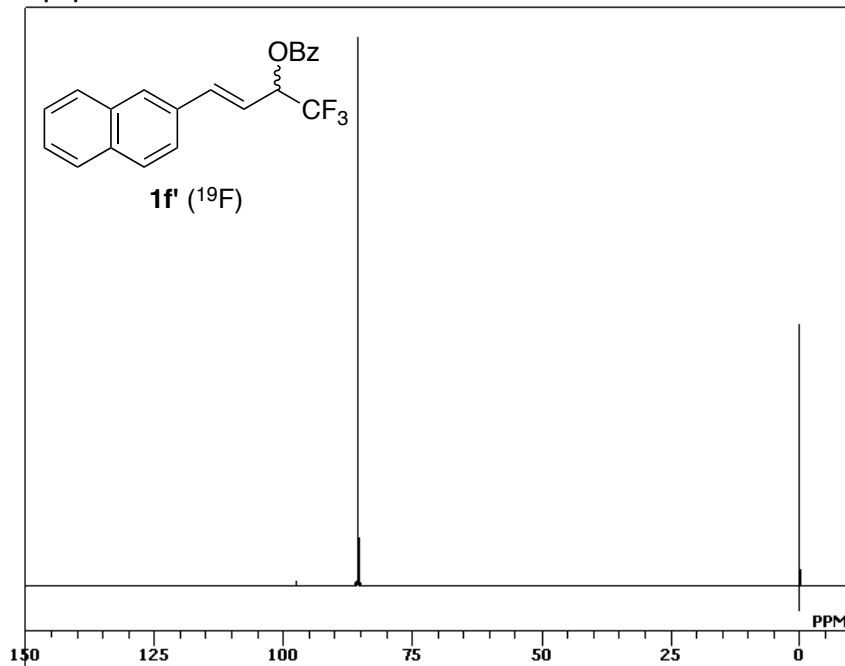
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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 6.80 usec
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CTEMP 23.4 c
SLVNT CDCL3
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BF 1.00 Hz
RGAIN 36

naphtyl-OBz



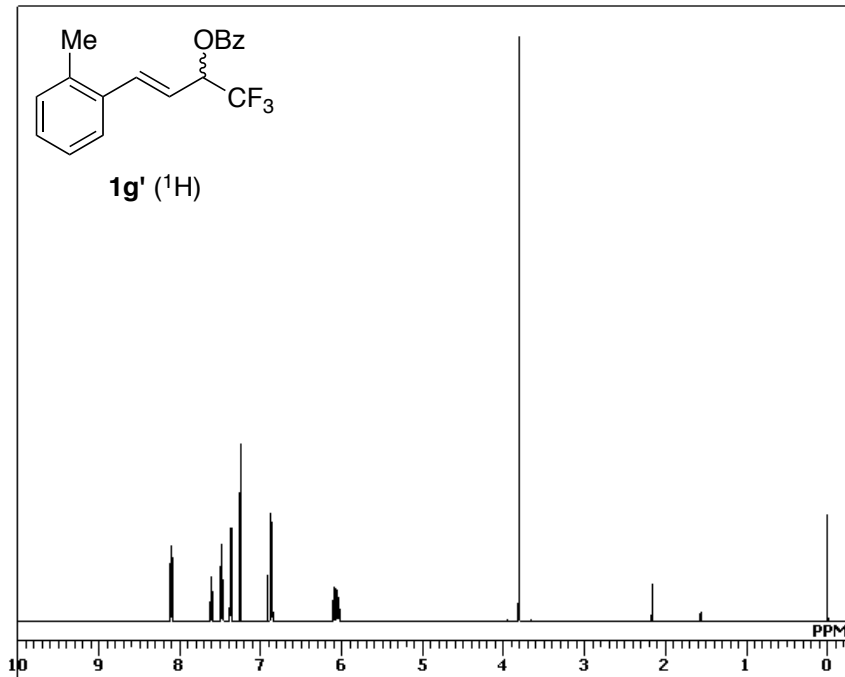
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OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
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PD 2.0000 sec
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BF 1.00 Hz
RGAIN 50

naphtyl-OBz



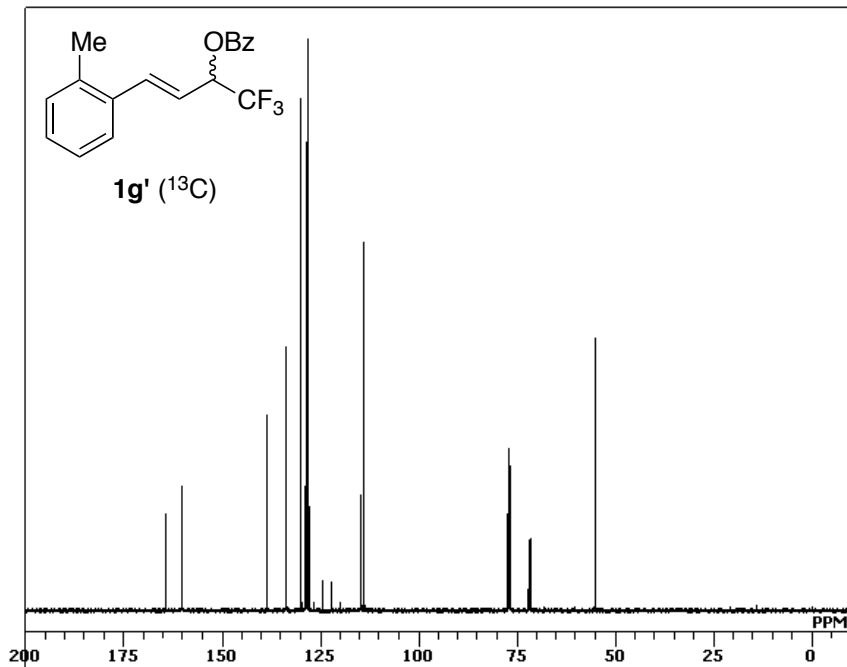
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OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 26214
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.1363 sec
PD 5.0000 sec
PW1 7.00 usec
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CTEMP 23.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 50

KI-1261-Fr1



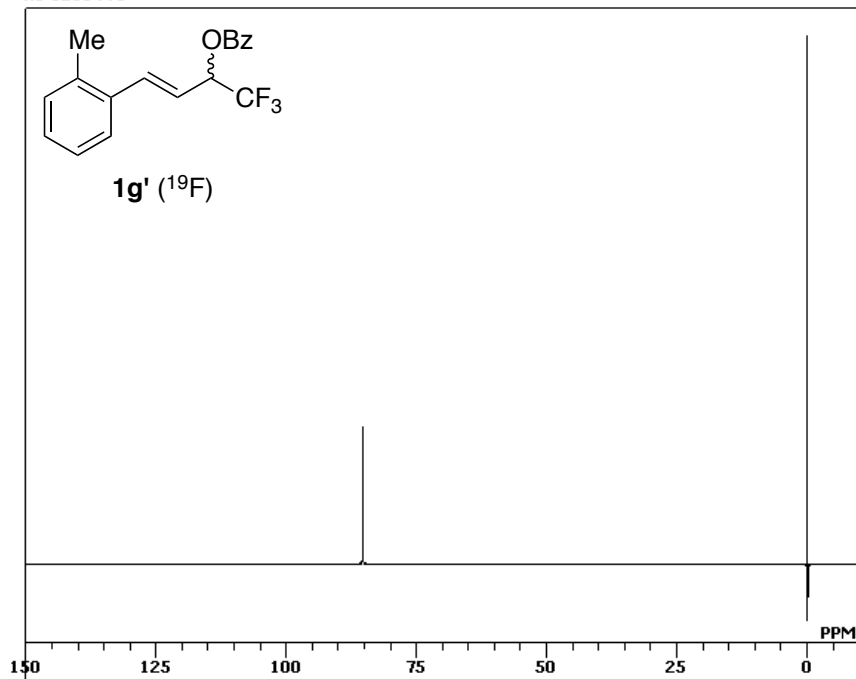
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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 19.8 c
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BF 0.10 Hz
RGAIN 34

KI-1261-Fr1



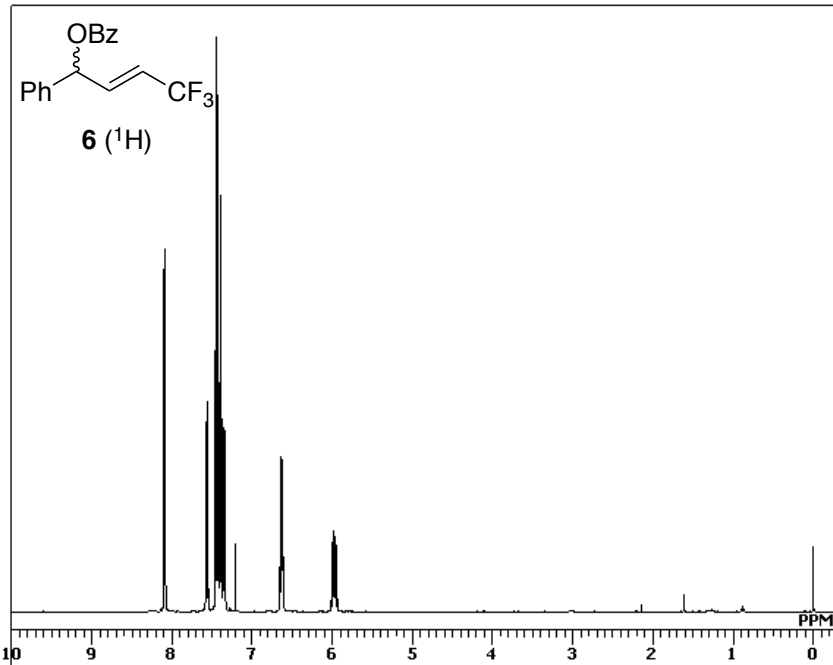
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OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
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CTEMP 20.5 c
SLVNT CDCL3
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BF 1.00 Hz
RGAIN 50

KI-1261-Fr1



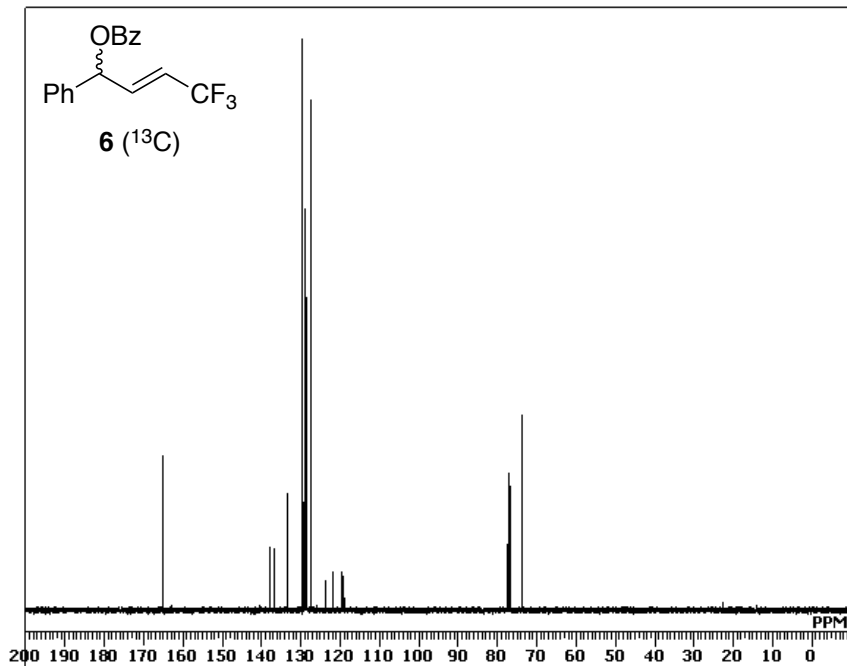
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OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 8.50 usec
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EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 50

KI-1210



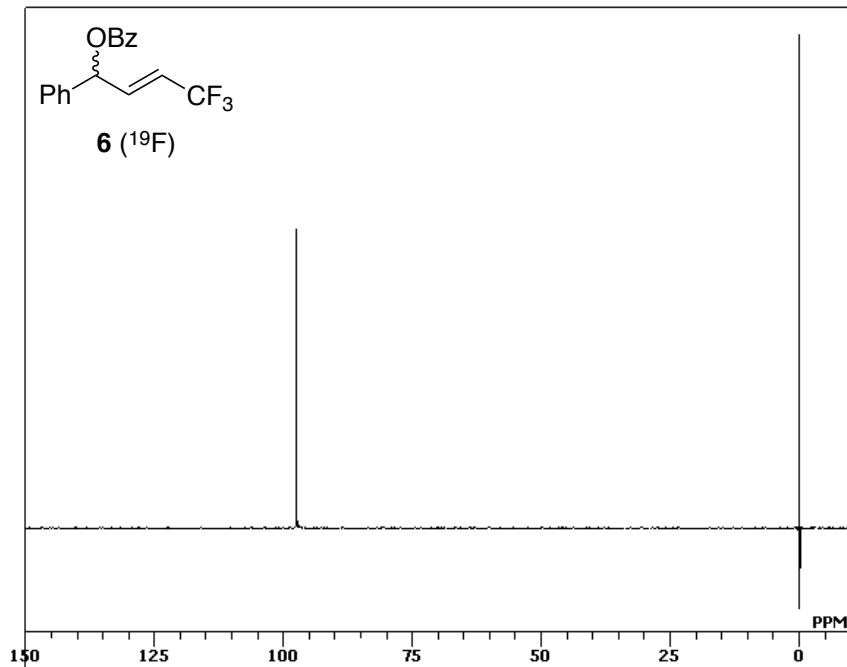
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OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 4
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 6.80 usec
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CTEMP 21.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 30

KI-1191-Fr1



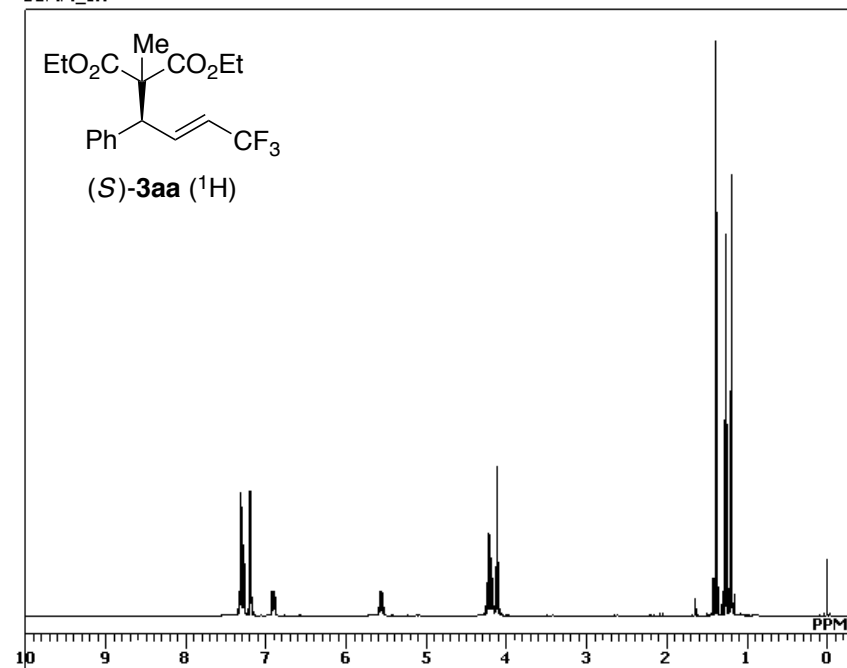
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OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 128
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
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CTEMP 20.1 c
SLVNT CDCL3
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BF 0.20 Hz
RGAIN 50

KI-1191-Fr1



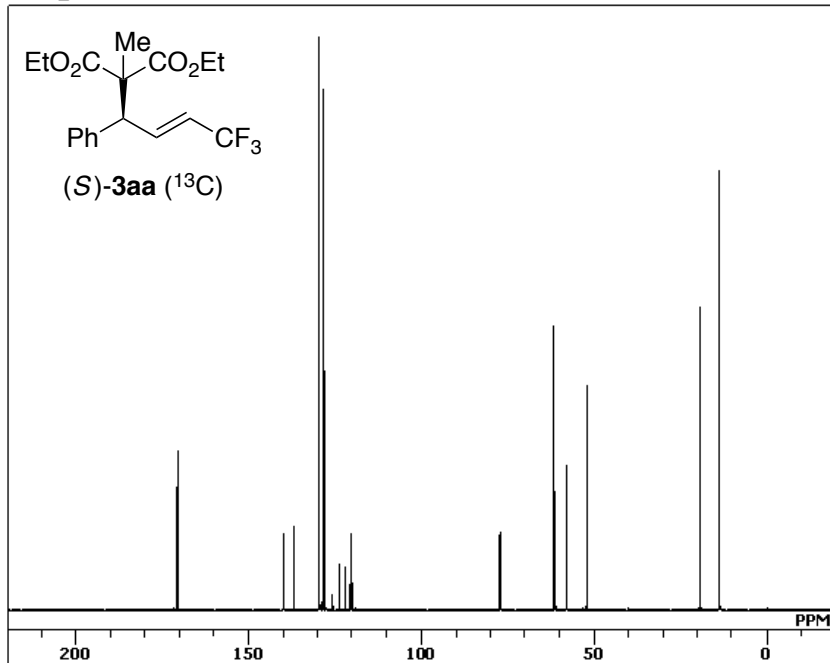
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OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 19.9 c
SLVNT CDCL3
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BF 0.20 Hz
RGAIN 50

DEMM_1H



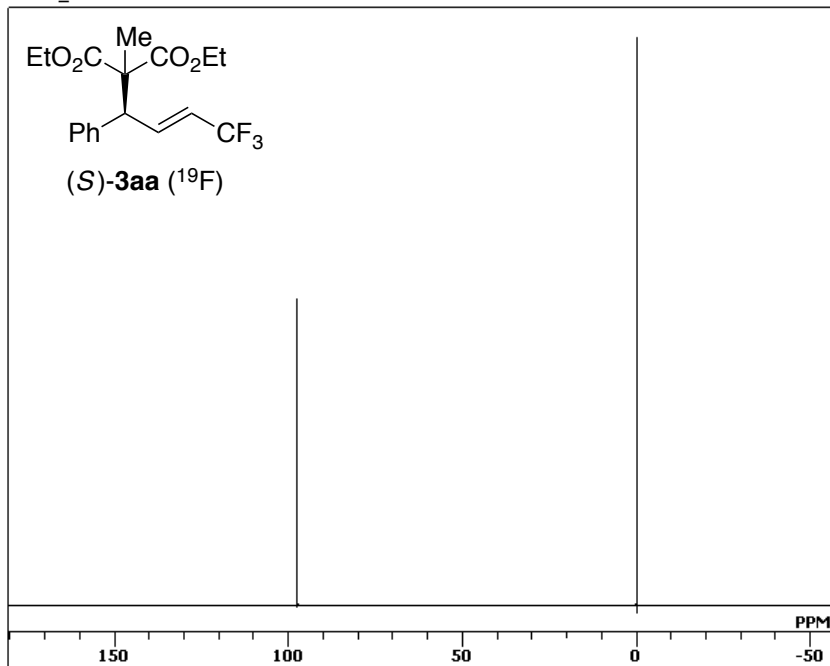
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OBSET 3.70 KHz
OBFIN 6.05 Hz
POINT 32768
FREQU 12335.53 Hz
SCANS 16
ACQTM 2.6564 sec
PD 1.0000 sec
PW1 13.00 usec
IRNUC
CTEMP 19.3 c
SLVNT CDCL3
EXREF 16.43 ppm
BF 0.30 Hz
RGAIN 36

DEMM_13C



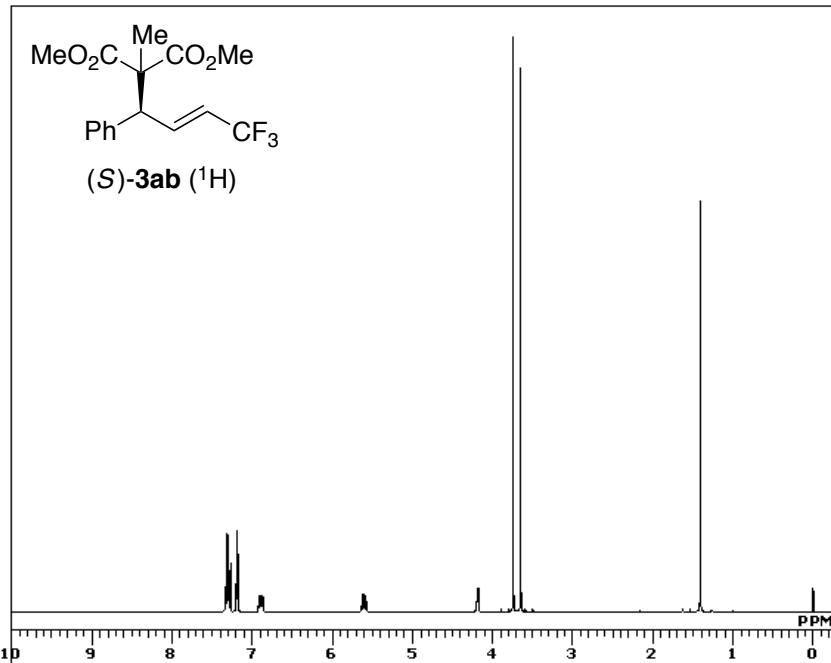
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 OBSET 7.89 KHz
 OBFIN 8.81 Hz
 POINT 32768
 FREQU 36057.69 Hz
 SCANS 128
 ACQTM 0.9088 sec
 PD 2.0000 sec
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 CTEMP 20.7 c
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 BF 1.00 Hz
 RGAIN 203

DEMM_19F



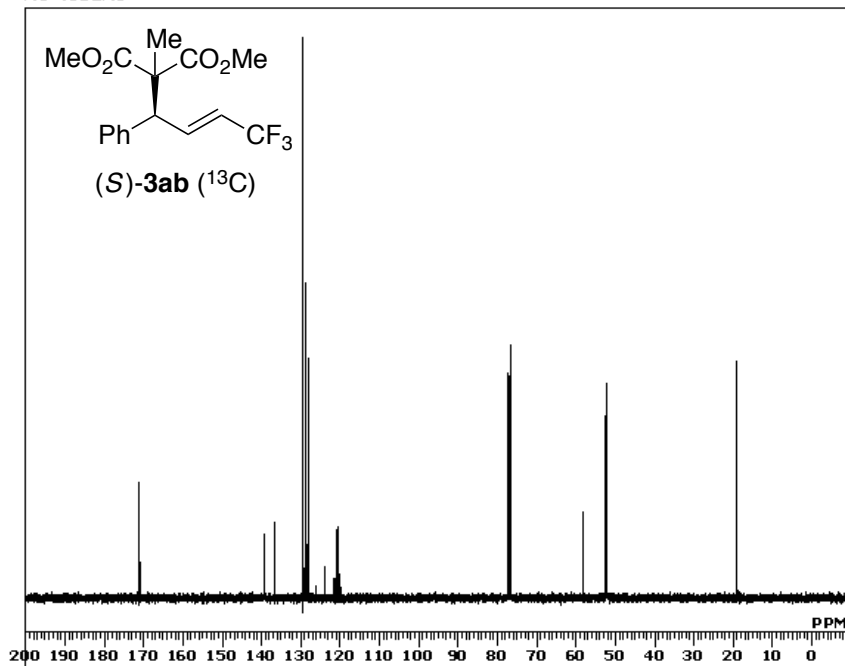
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 OBNUC 19F
 EXMOD zgfgqn
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 OBSET 9.91 KHz
 OBFIN 9.58 Hz
 POINT 65536
 FREQU 133928.58 Hz
 SCANS 16
 ACQTM 0.4894 sec
 PD 1.0000 sec
 PW1 14.20 usec
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 BF 0.30 Hz
 RGAIN 90

Me- <CO2Me



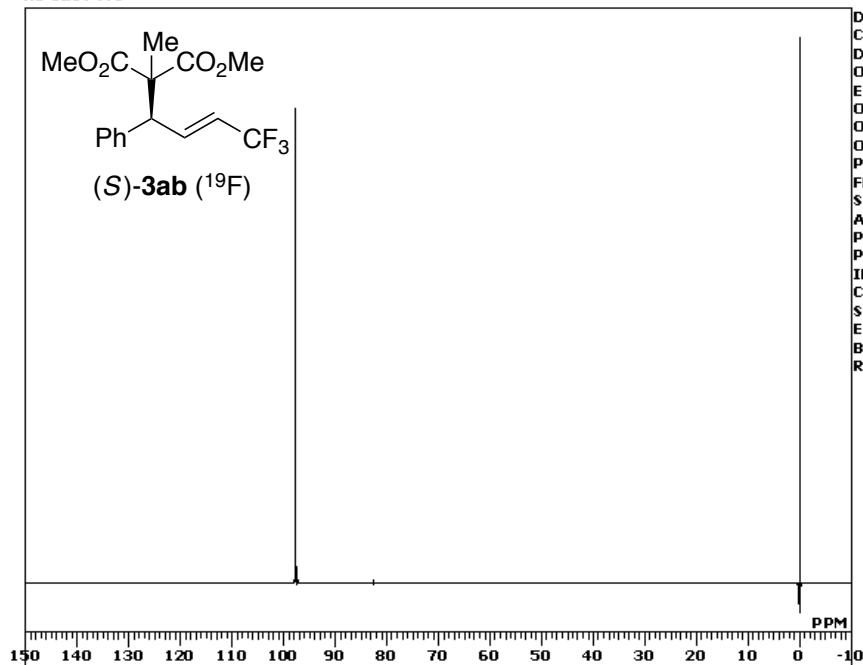
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OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 19.5 c
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EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 30

Me- <CO2Me

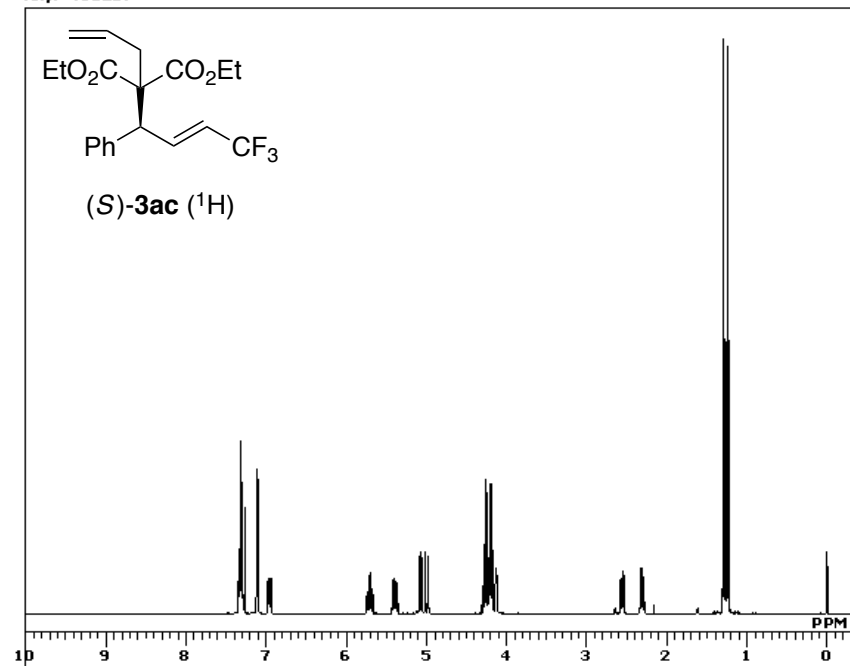


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OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 128
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50

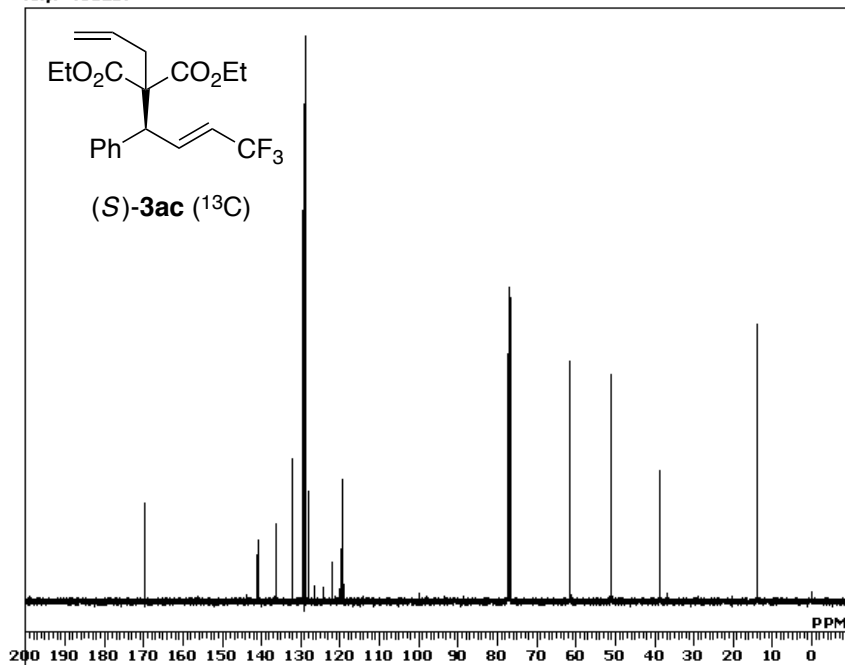
KI-1234-Fr1



Allyl-<CO2Et

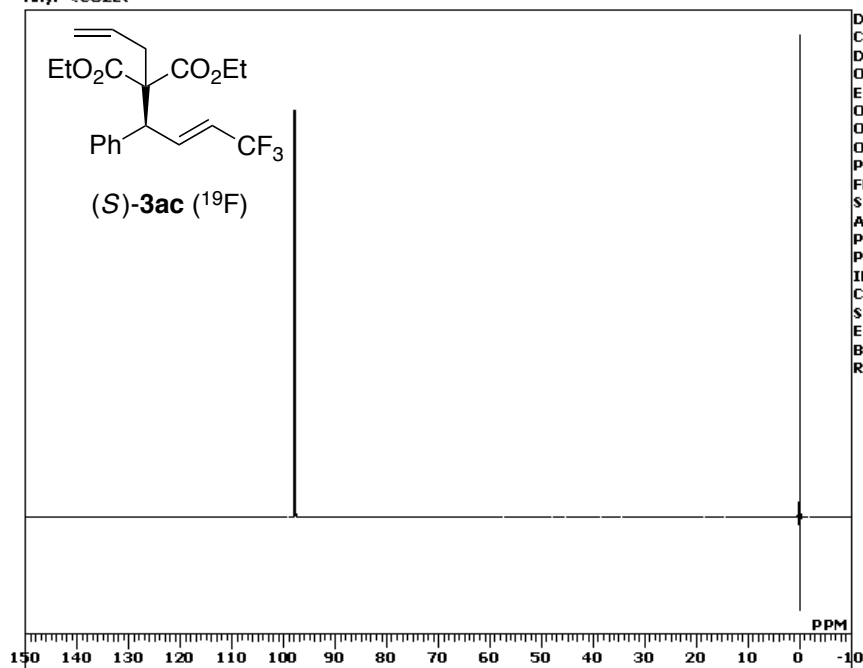


Allyl-<CO2Et



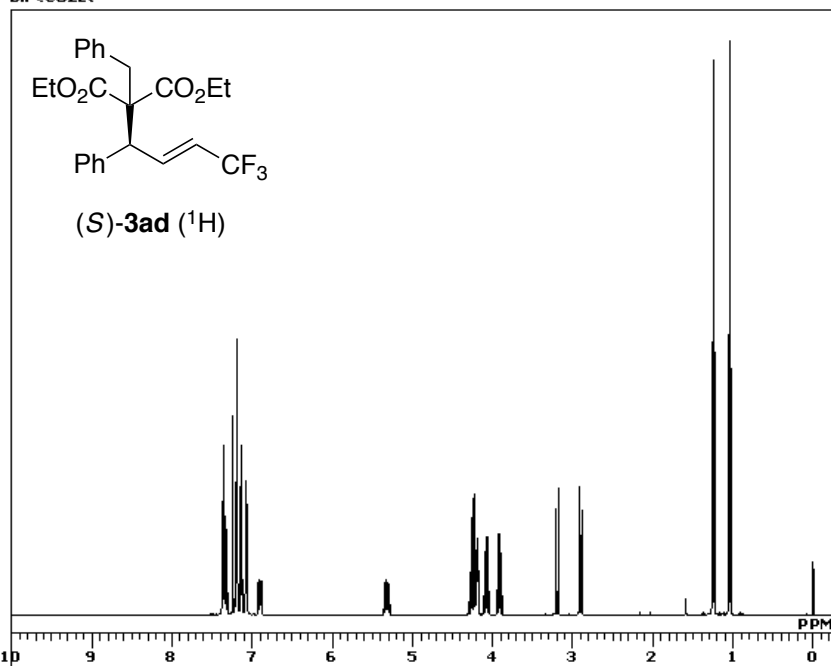
DFILE Allyl-fCO2Et_Carbon-
COMNT Allyl-<CO2Et
DATIM 21-02-2012 23:32:56
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 291
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50

Allyl-<CO2Et



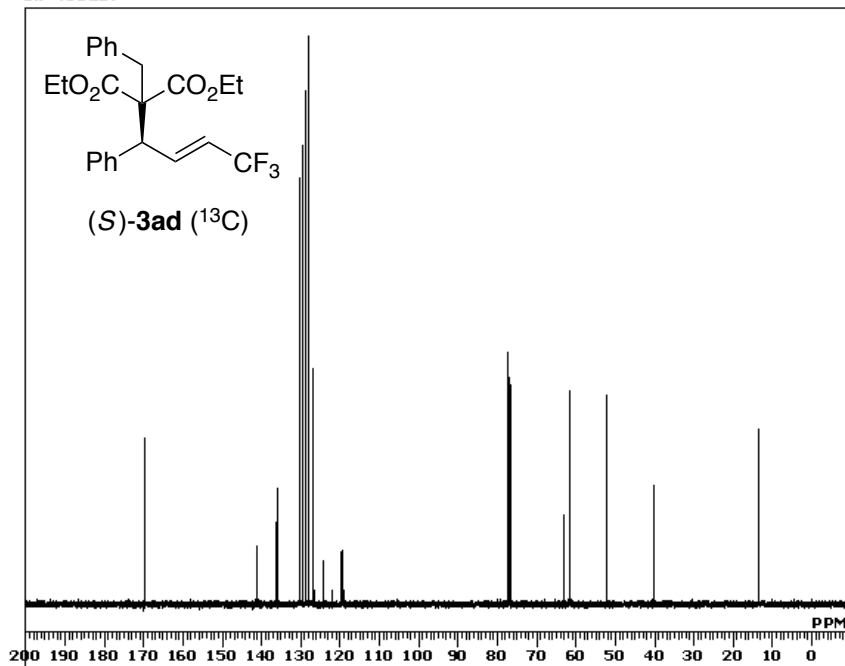
DFILE Allyl-fCO2Et_19F-1-1
COMNT Allyl-<CO2Et
DATIM 20-02-2012 16:44:17
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 8.50 usec
IRNUC 19F
CTEMP 18.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 50

Bn <CO2Et



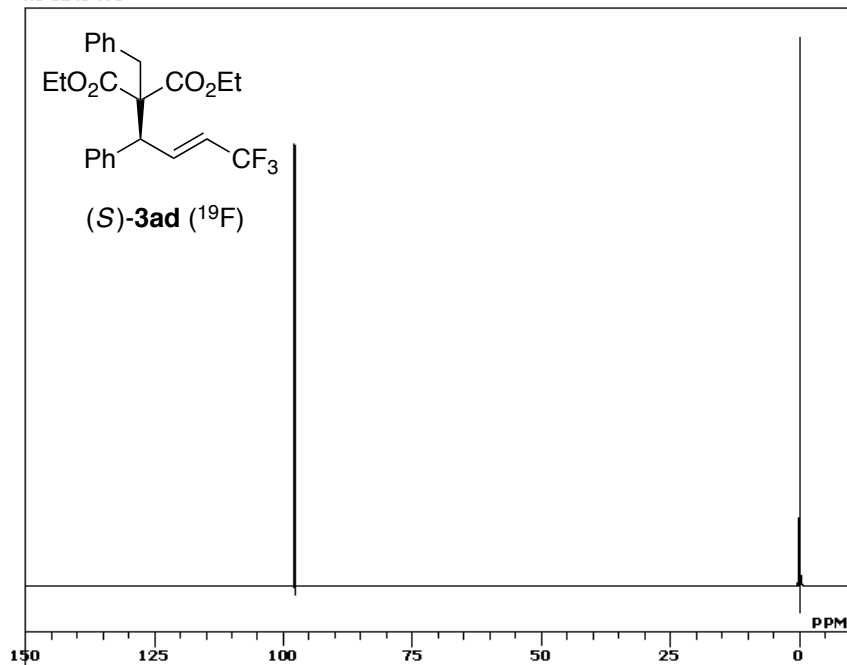
DFILE Bn-fCO2Et_Proton-1-
COMNT Bn <CO2Et
DATIM 21-02-2012 23:14:53
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 19.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 28

Bn <CO2Et



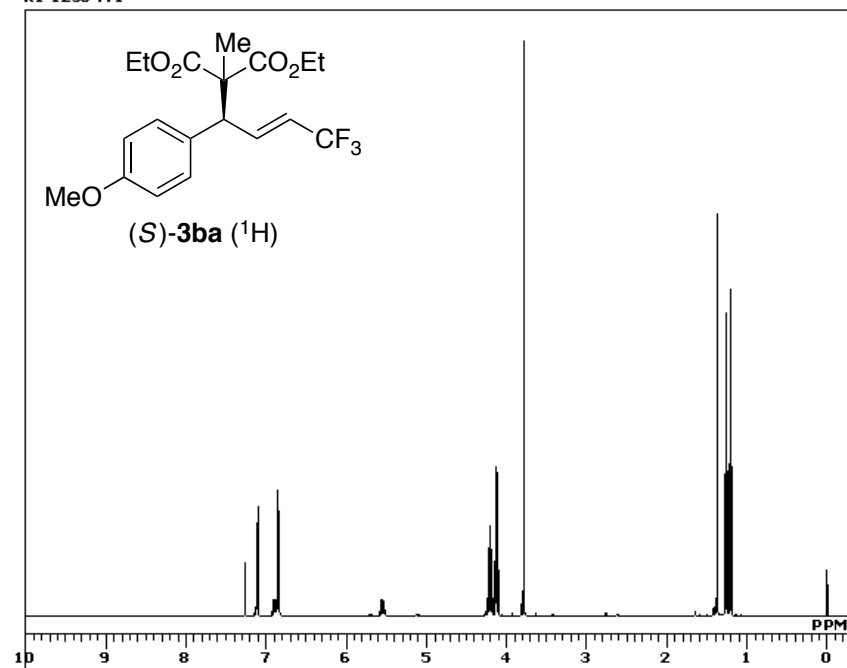
DFILE Bn-fCO2Et_Carbon-1-
COMNT Bn <CO2Et
DATIM 21-02-2012 23:16:27
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 201
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50

KI-1245-Fr1



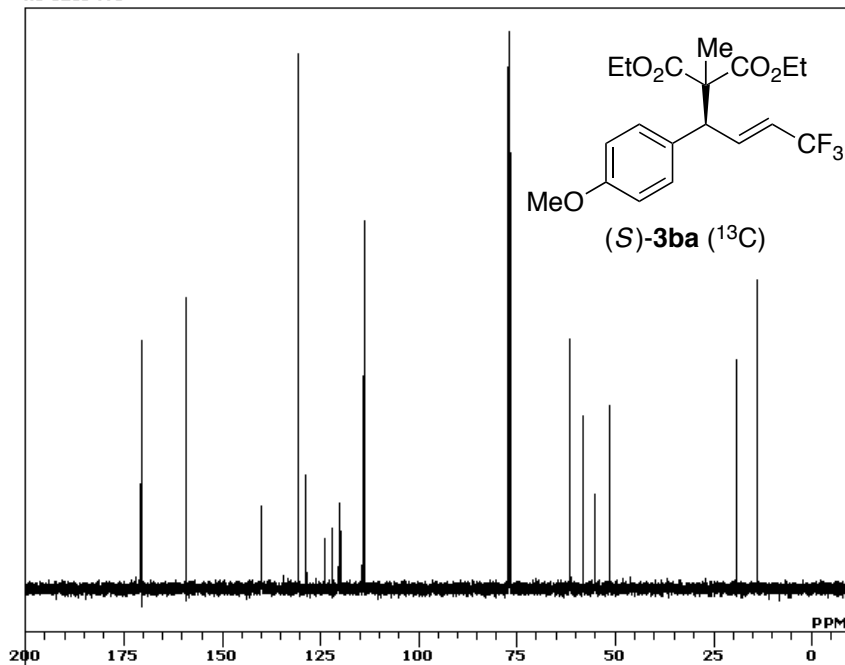
DFILE KI-1245-Fr1_19F-1-1.a
COMNT KI-1245-Fr1
DATIM 24-01-2012 20:20:17
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 50

KI-1256-Fr1



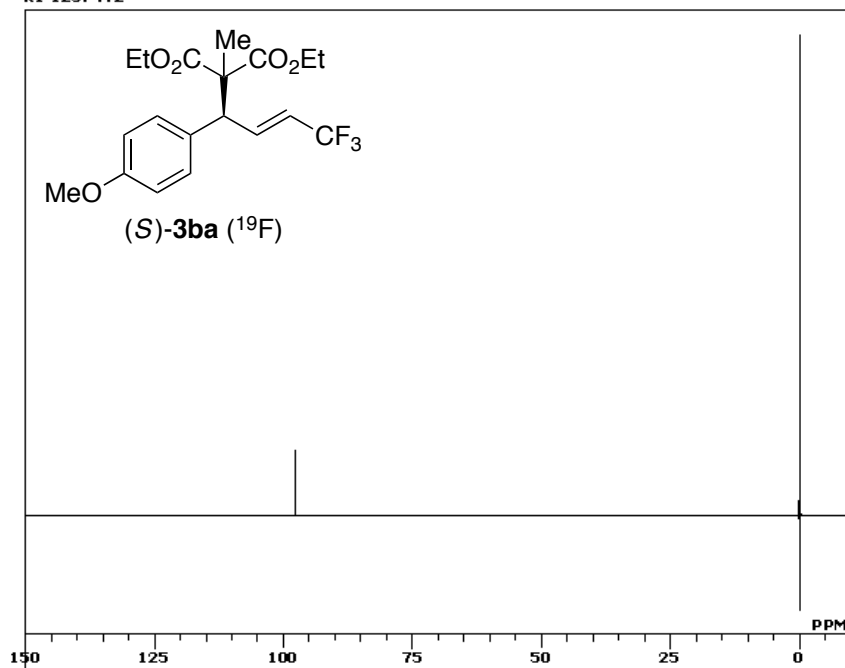
DFILE KI-1256-Fr1_Proton-1-
COMNT KI-1256-Fr1
DATIM 25-01-2012 15:36:41
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 4
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 6.80 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 32

KI-1256-Fr1



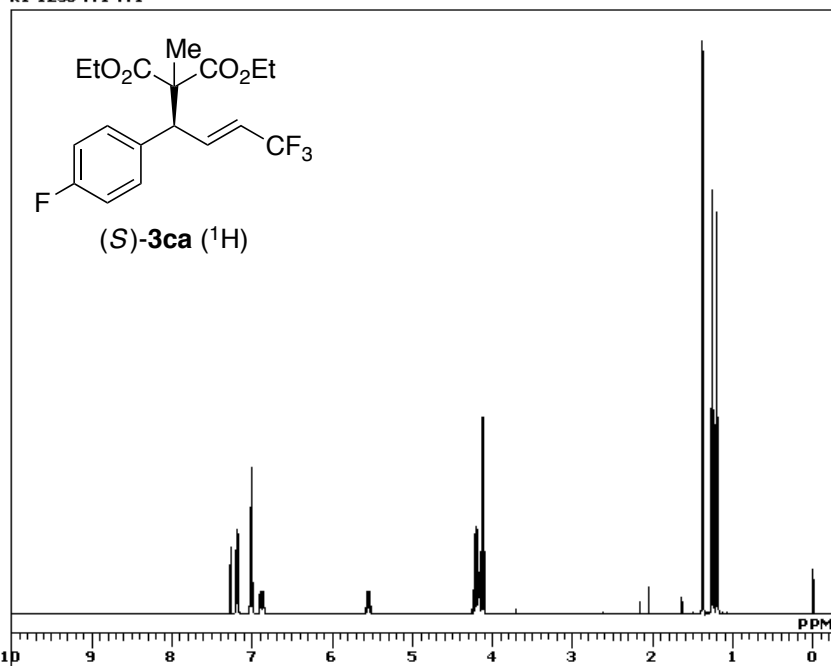
DFILE KI-1256-Fr1_Carbon-1-
 COMNT KI-1256-Fr1
 DATIM 25-01-2012 15:42:60
 OBNUC 13C
 EXMOD carbon.jsp
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 400
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.90 usec
 IRNUC 1H
 CTEMP 20.9 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 50

KI-1237-Fr2



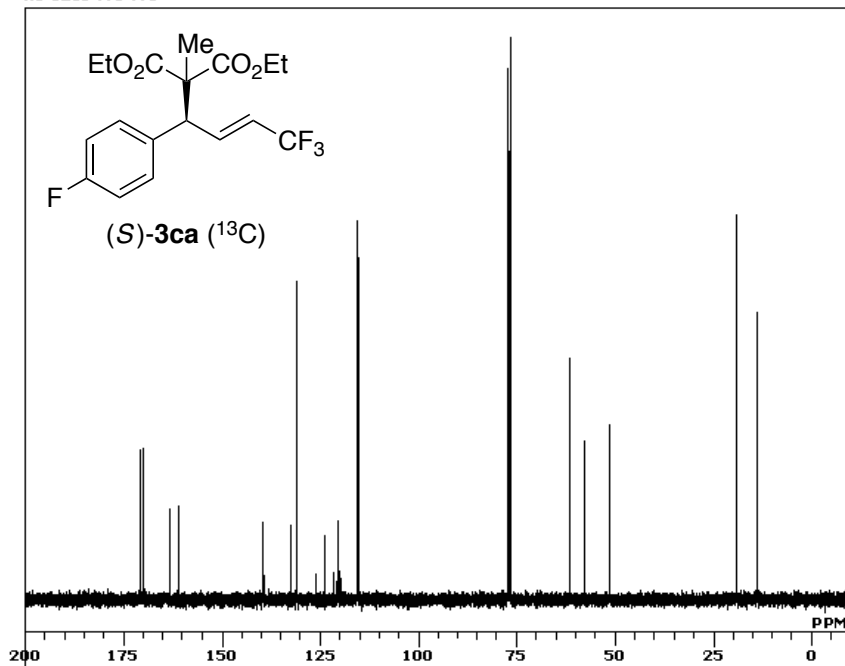
DFILE KI-1237-Fr2_19F-1-1.a
 COMNT KI-1237-Fr2
 DATIM 19-01-2012 23:38:21
 OBNUC 19F
 EXMOD single_pulse.jsp
 OBFRQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 13107
 FREQU 192307.69 Hz
 SCANS 8
 ACQTM 0.0682 sec
 PD 5.0000 sec
 PW1 7.00 usec
 IRNUC 19F
 CTEMP 21.3 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.20 Hz
 RGAIN 50

KI-1236-Fr1-Fr1



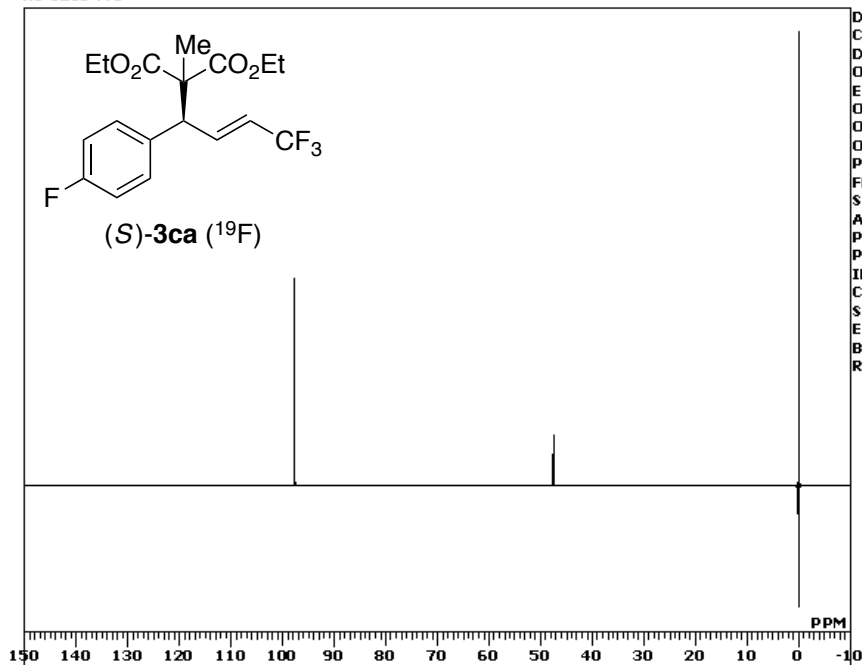
DFILE KI-1236-Fr1-Fr1_Proto
 COMNT KI-1236-Fr1-Fr1
 DATIM 23-01-2012 23:35:41
 OBNUC 1H
 EXMOD proton.jsp
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.51 Hz
 SCANS 4
 ACQTM 3.4918 sec
 PD 5.0000 sec
 PW1 6.80 usec
 IRNUC 1H
 CTEMP 21.3 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 34

KI-1236-Fr1-Fr1



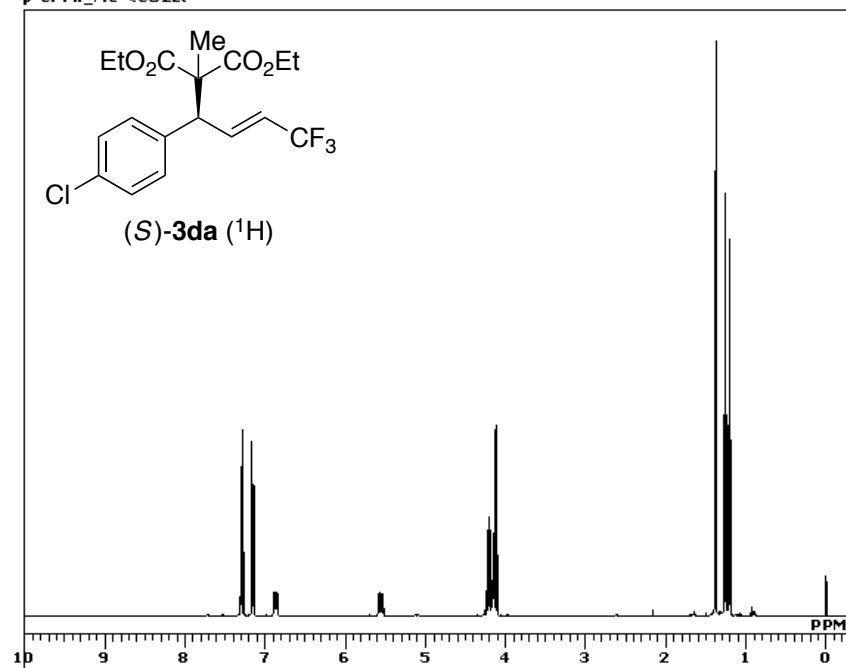
DFILE KI-1236-Fr1-Fr1_Carbo
 COMNT KI-1236-Fr1-Fr1
 DATIM 23-01-2012 23:36:39
 OBNUC 13C
 EXMOD carbon.jsp
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 316
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.90 usec
 IRNUC 1H
 CTEMP 21.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 50

KI-1236-Fr1



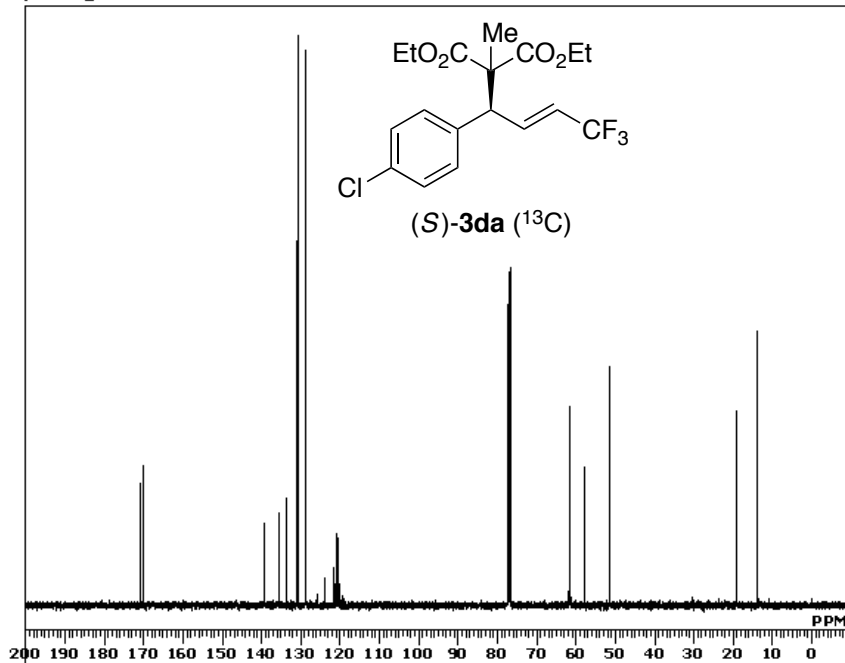
DFILE KI-1236-Fr1_19F-1-1.a
COMNT KI-1236-Fr1
DATIM 19-01-2012 23:29:59
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 50

p-Cl-Ph_Me-<CO2Et



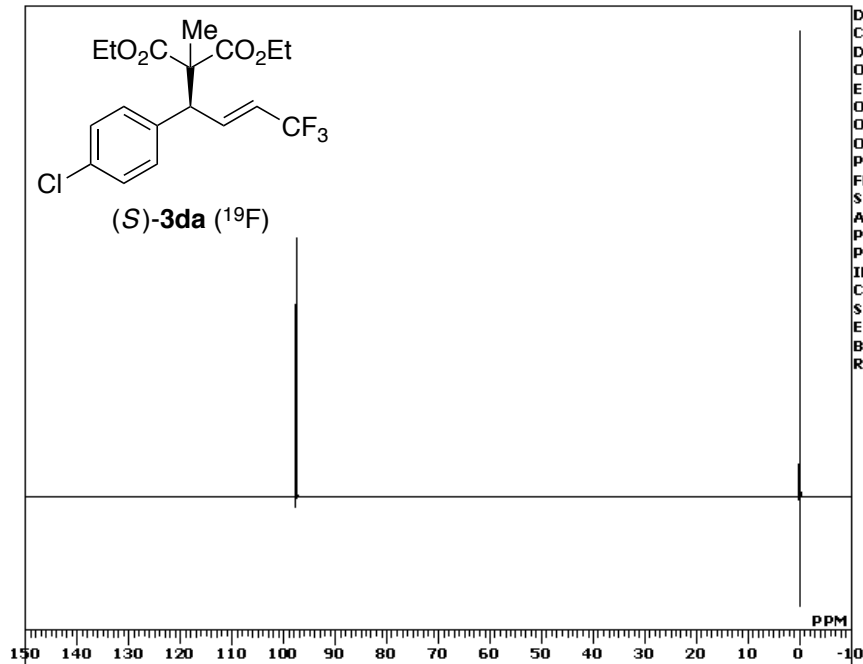
DFILE p-Cl-Ph_Me-fCO2Et_1
COMNT p-Cl-Ph_Me-<CO2Et
DATIM 21-02-2012 23:52:19
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 30

p-Cl-Ph_Me-<CO2Et



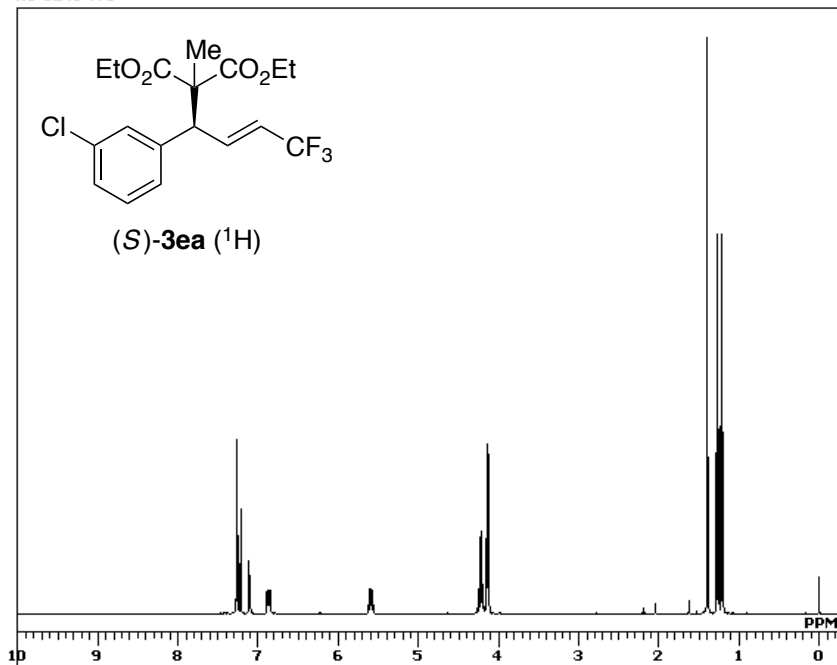
DFILE p-Cl-Ph_Me-fCO2Et_1
COMNT p-Cl-Ph_Me-<CO2Et
DATIM 21-02-2012 23:53:51
OBNUC 13C
EXMOD carbon.jsp
OBFREQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 200
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

KI-1239-Fr1



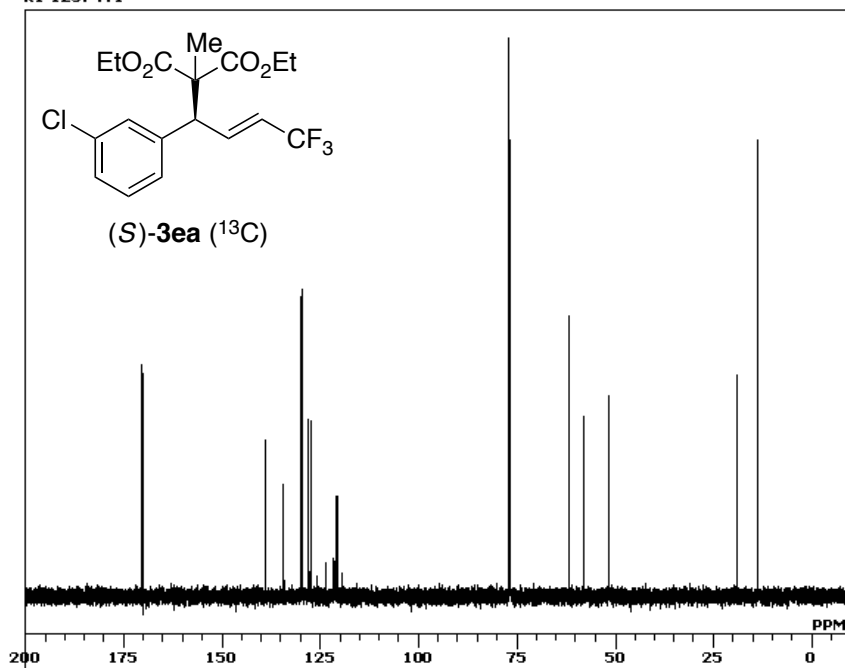
DFILE KI-1239-Fr1_19F-1-1.a
COMNT KI-1239-Fr1
DATIM 19-01-2012 23:53:22
OBNUC 19F
EXMOD single_pulse.jsp
OBFREQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 50

KI-1246-Fr1



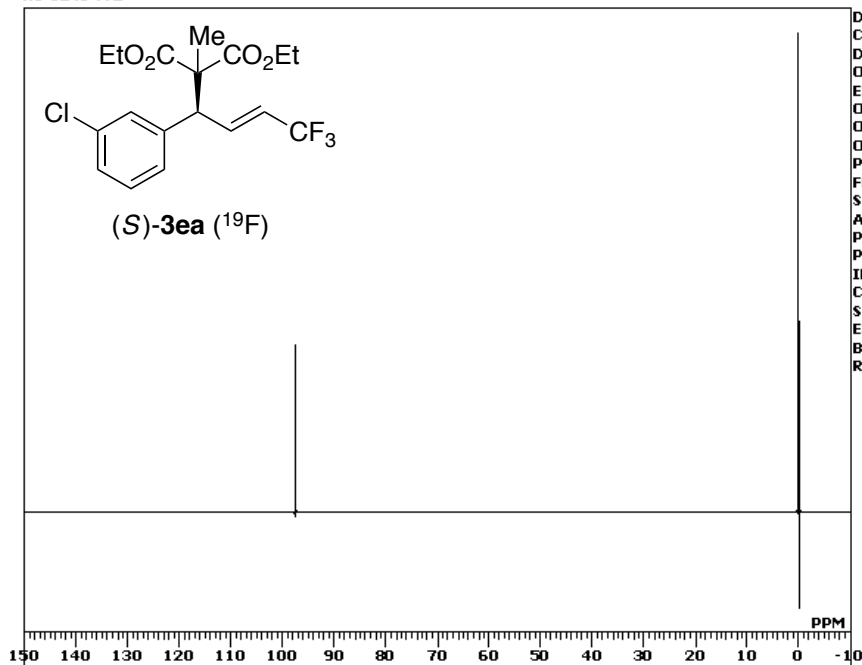
DFILE KI-1246-Fr1_Proton-2-
COMNT KI-1246-Fr1
DATIM 18-01-2012 15:57:53
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 4
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 6.80 usec
IRNUC 1H
CTEMP 21.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 32

KI-1257-Fr1



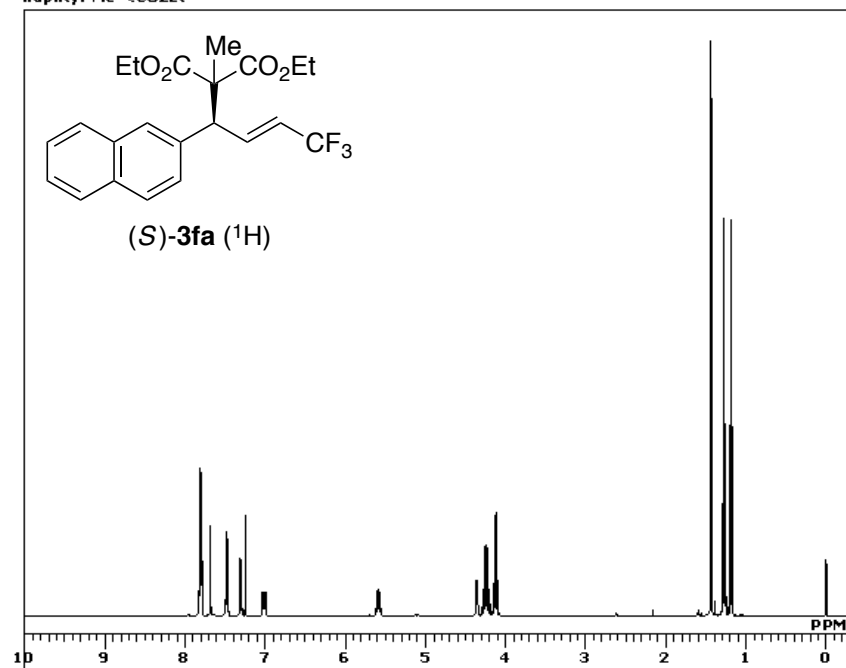
DFILE KI-1257-Fr1_Carbon-1-
COMNT KI-1257-Fr1
DATIM 25-01-2012 16:08:29
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 206
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50

KI-1240-Fr2



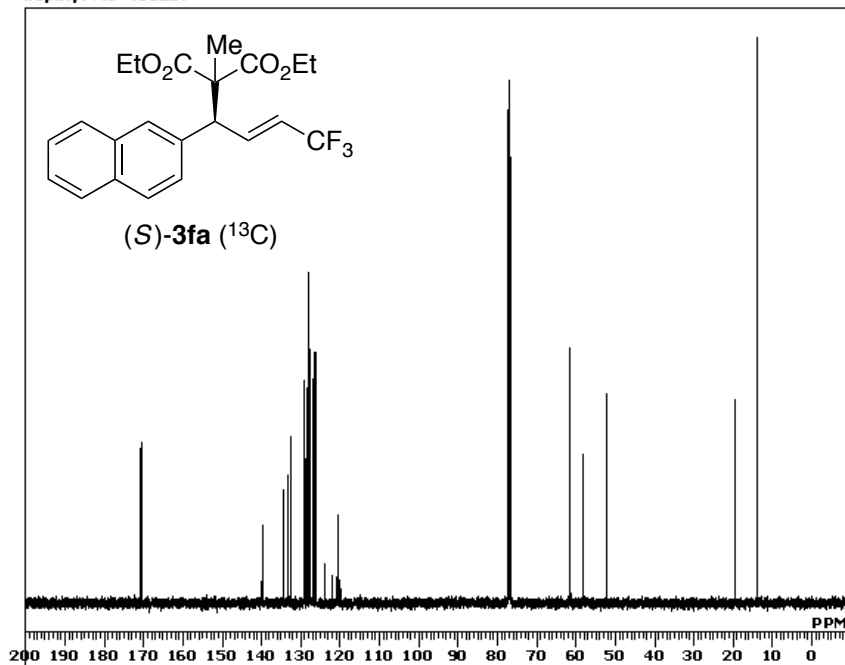
DFILE KI-1240-Fr2_19F-1-1.a
 COMNT KI-1240-Fr2
 DATIM 20-01-2012 00:00:45
 OBNUC 19F
 EXMOD single_pulse.jsp
 OBFRQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 13107
 FREQU 192307.69 Hz
 SCANS 8
 ACQTM 0.0682 sec
 PD 5.0000 sec
 PW1 7.00 usec
 IRNUC 19F
 CTEMP 21.3 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.20 Hz
 RGAIN 50

naphtyl-Me-<CO2Et



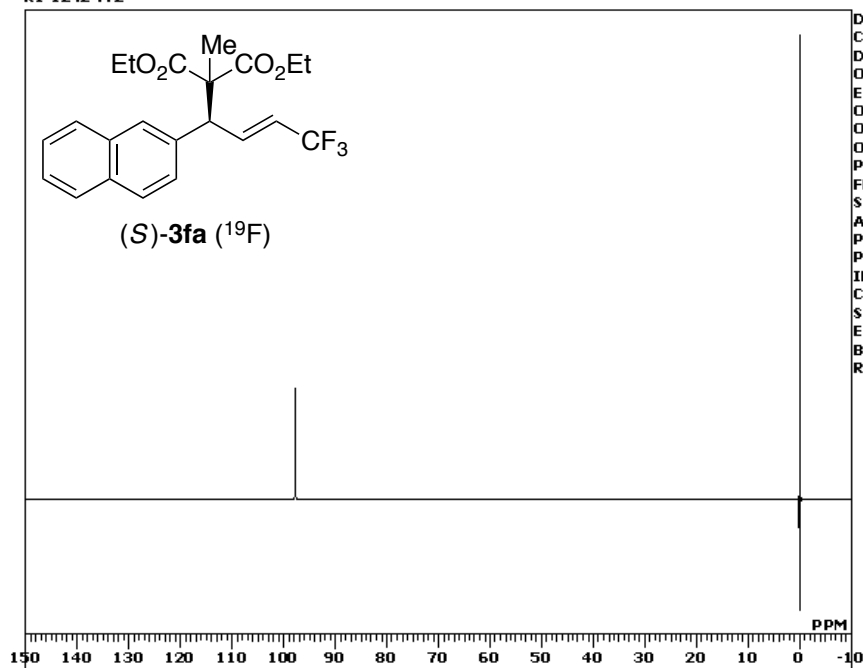
DFILE naphtyl-Me- \square fCO2Et_f
 COMNT naphtyl-Me-<CO2Et
 DATIM 22-02-2012 00:34:27
 OBNUC 1H
 EXMOD proton.jsp
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.51 Hz
 SCANS 8
 ACQTM 3.4918 sec
 PD 5.0000 sec
 PW1 7.00 usec
 IRNUC 1H
 CTEMP 19.6 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 30

naphtyl-Me-<CO2Et



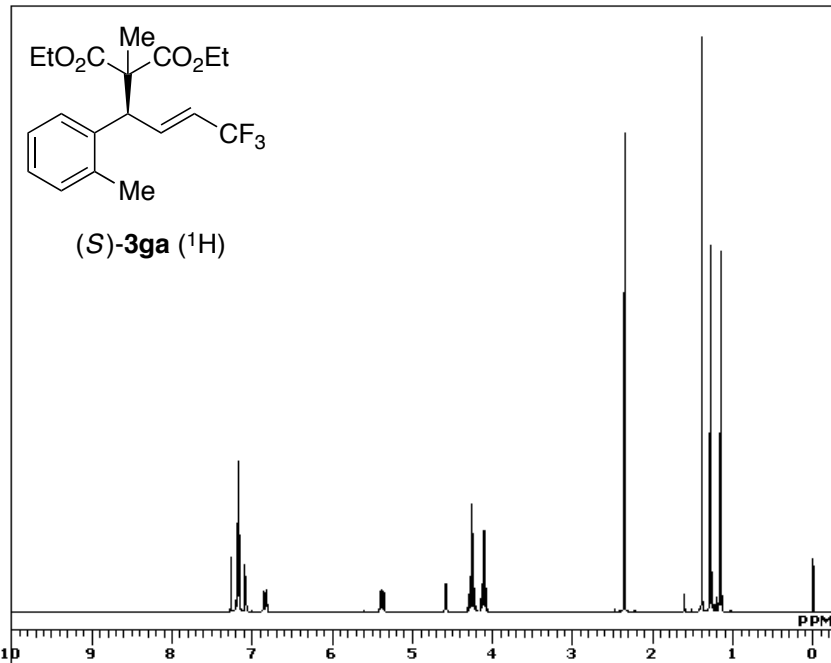
DFILE naphtyl-Me-fCO2Et_C
COMNT naphtyl-Me-<CO2Et
DATIM 22-02-2012 00:35:60
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 200
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

KI-1242-Fr2



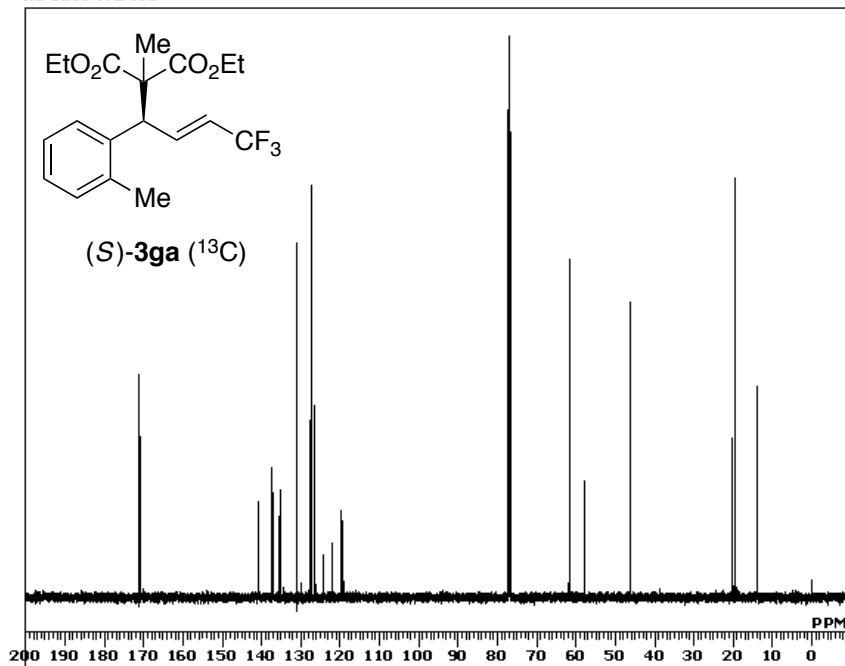
DFILE KI-1242-Fr2_19F-1-1.al
COMNT KI-1242-Fr2
DATIM 20-01-2012 00:04:28
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 50

KI-1238-Fr2-Fr1



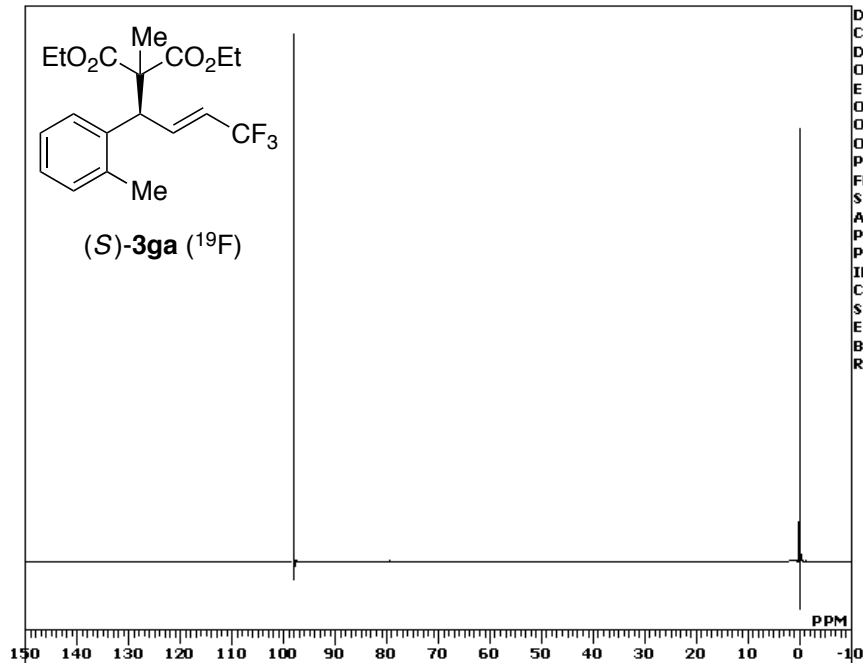
DFILE KI-1238-Fr2-Fr1_Proto
COMNT KI-1238-Fr2-Fr1
DATIM 23-02-2012 09:10:12
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 30

KI-1238-Fr2-Fr1



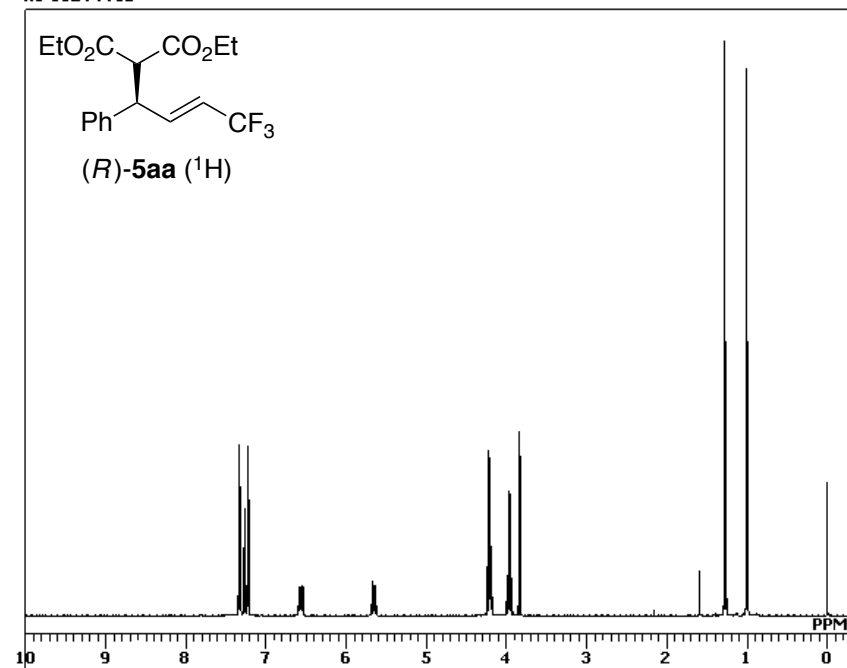
DFILE KI-1238-Fr2-Fr1_Carbo
COMNT KI-1238-Fr2-Fr1
DATIM 23-02-2012 09:11:44
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 560
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 21.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.10 Hz
RGAIN 50

KI-1238-Fr2



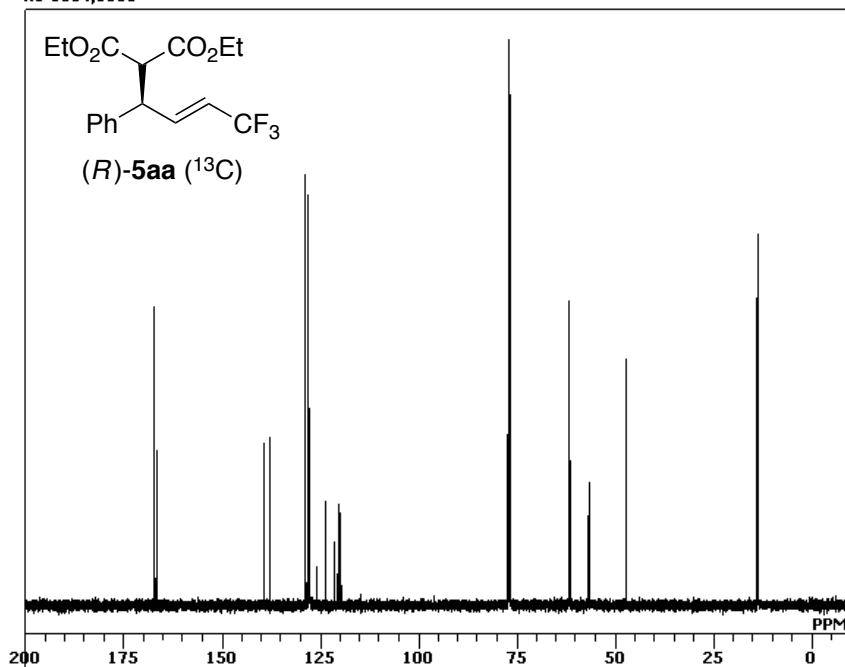
DFILE KI-1238-Fr2_19F-1-1.a
COMNT KI-1238-Fr2
DATIM 19-01-2012 23:46:09
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 50

KI-1124-Fr1D



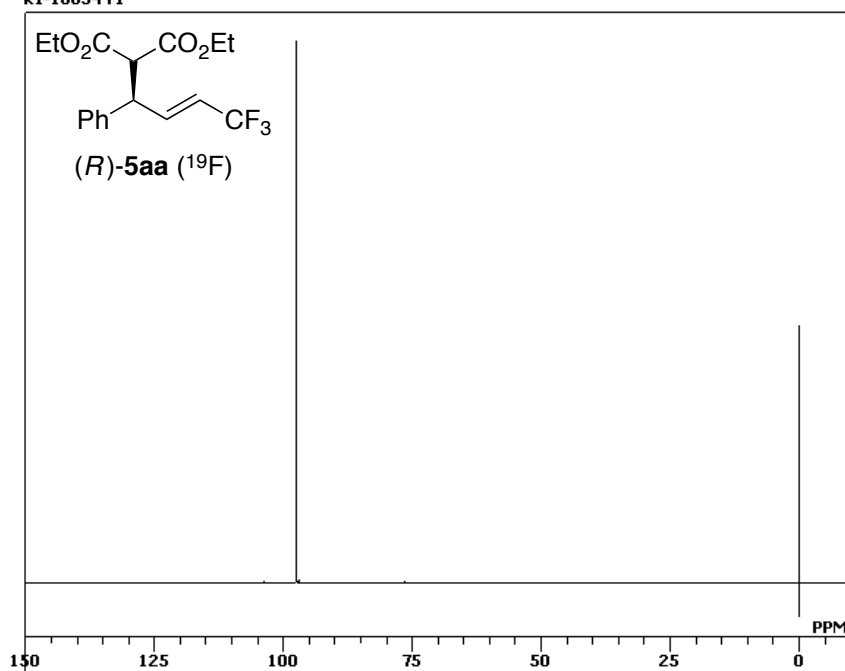
DFILE KI-1124-Fr1D_Proton-1
COMNT KI-1124-Fr1D
DATIM 24-11-2011 20:34:44
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 6.80 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 36

KI-1004,1005

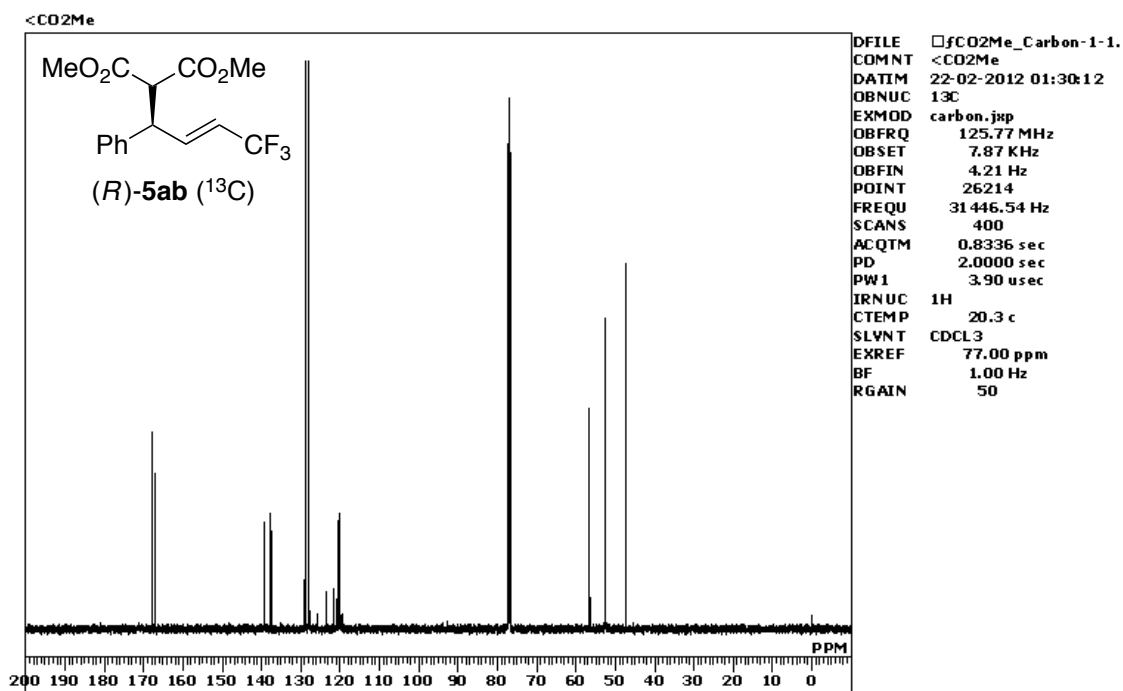
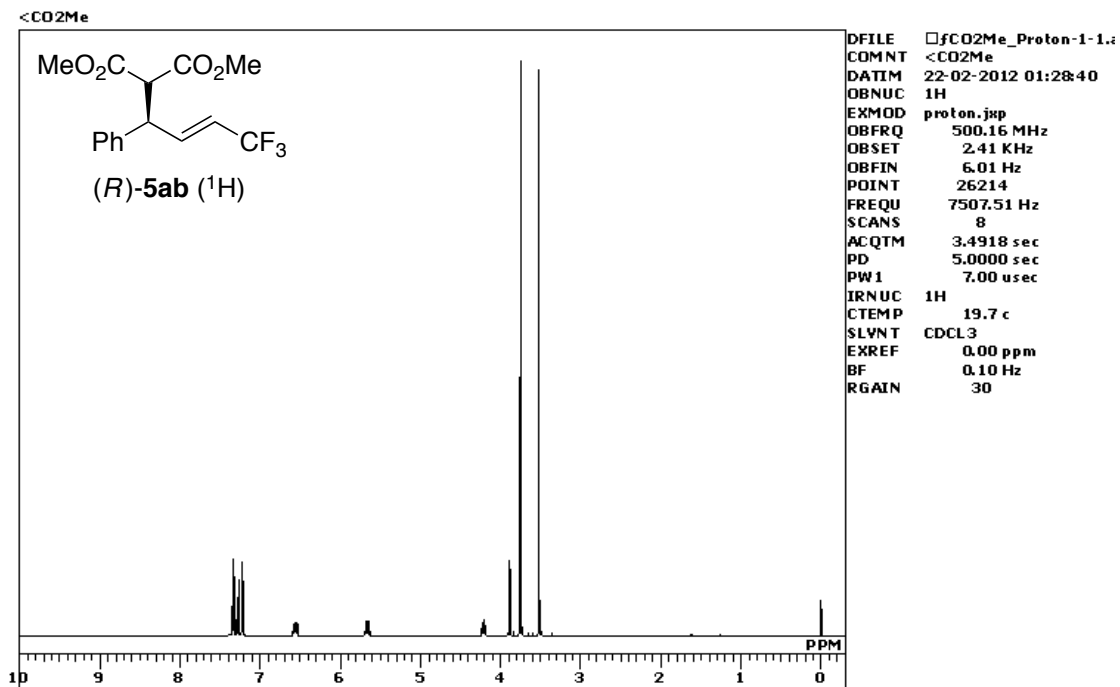


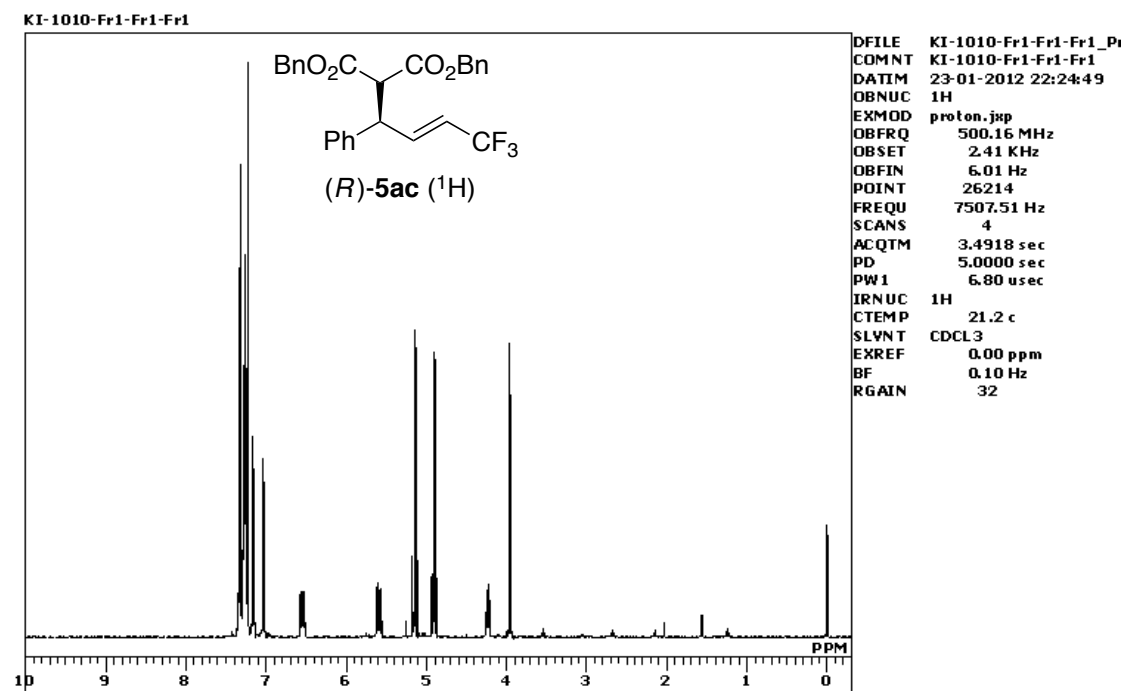
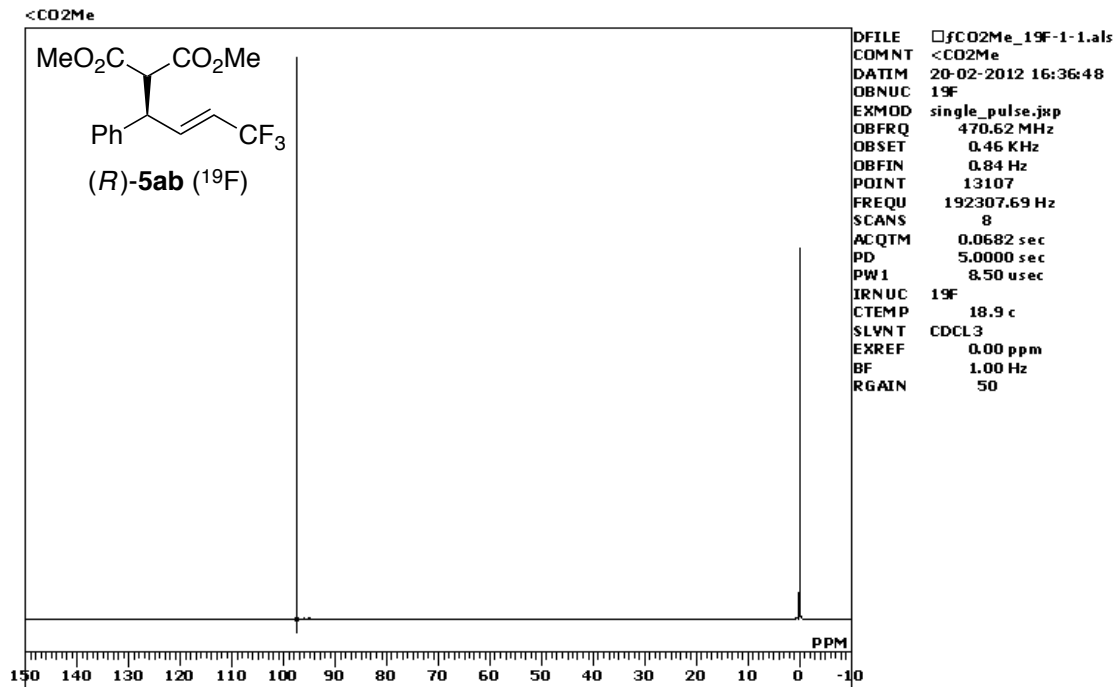
DFILE KI-1004,1005_Carbon-
 COMNT KI-1004,1005
 DATIM 21-09-2011 14:16:25
 OBNUC 13C
 EXMOD carbon.jxp
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 512
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.90 usec
 IRNUC 1H
 CTEMP 26.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.10 Hz
 RGAIN 50

KI-1005-Fr1

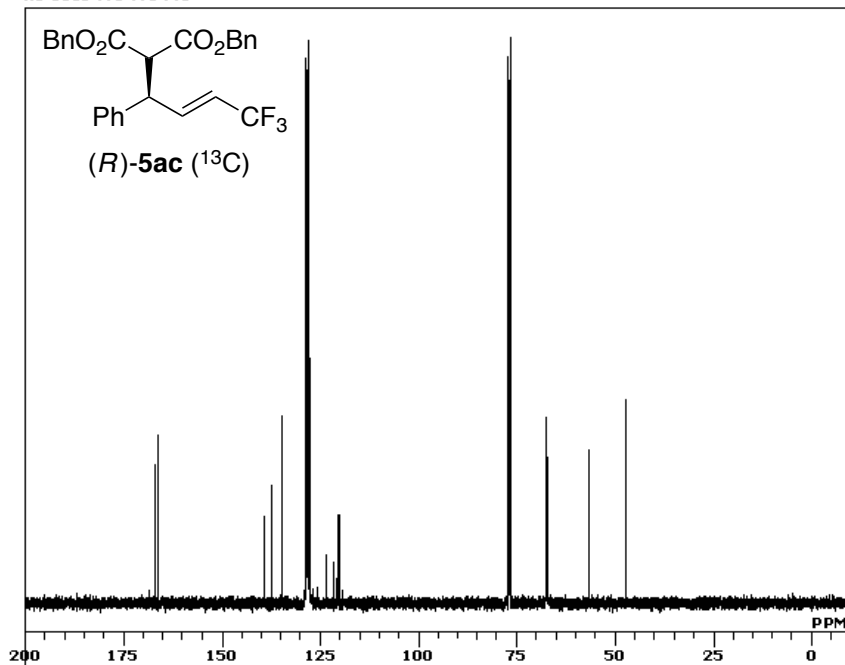


DFILE KI-1005-Fr1_19F-1-1.al
 COMNT KI-1005-Fr1
 DATIM 20-09-2011 15:56:40
 OBNUC 19F
 EXMOD single_pulse.jxp
 OBFREQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 52428
 FREQU 192307.69 Hz
 SCANS 16
 ACQTM 0.2726 sec
 PD 5.0000 sec
 PW1 7.00 usec
 IRNUC 19F
 CTEMP 24.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.30 Hz
 RGAIN 50



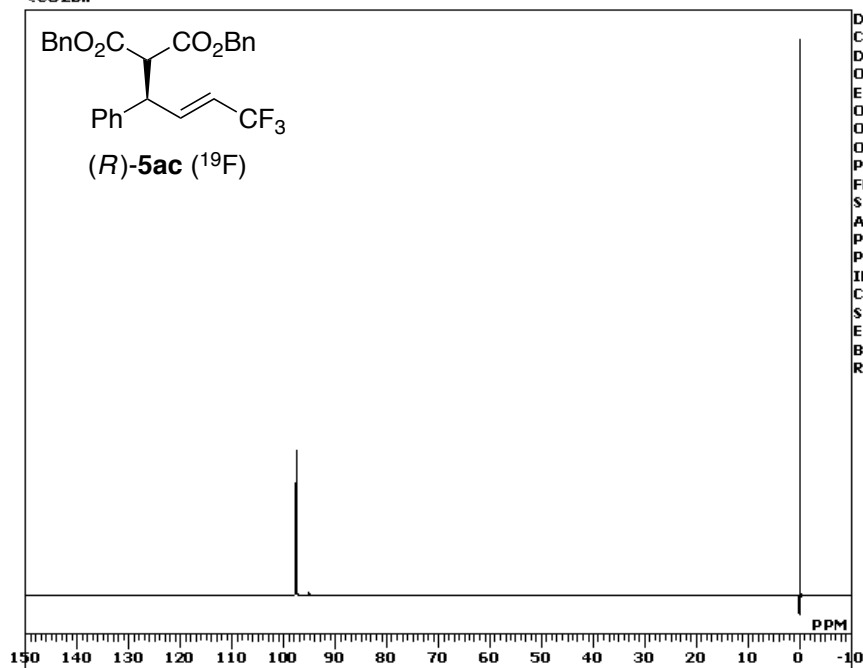


KI-1010-Fr1-Fr1-Fr1



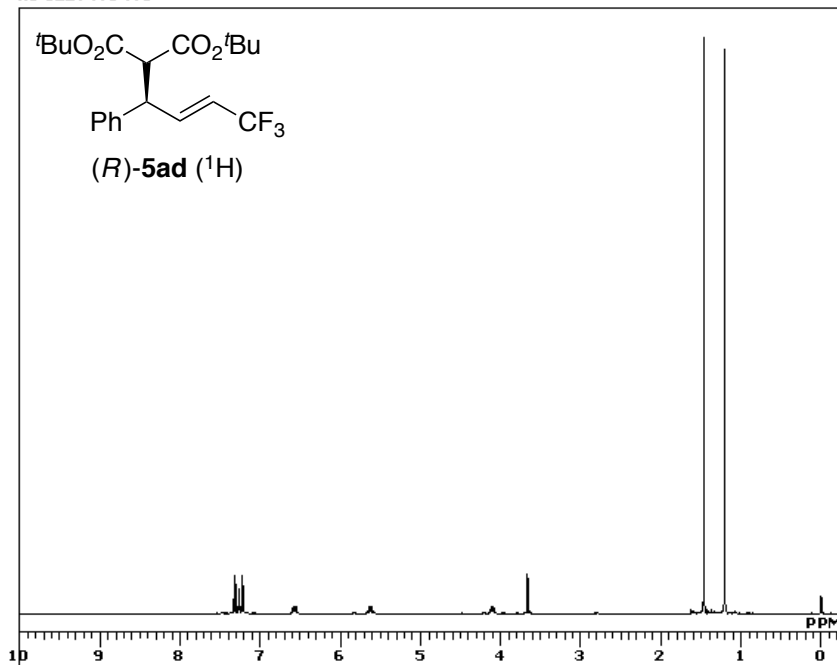
DFILE KI-1010-Fr1-Fr1-Fr1_C
 COMNT KI-1010-Fr1-Fr1-Fr1
 DATIM 23-01-2012 22:25:47
 OBNUC 13C
 EXMOD carbon.jsp
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 256
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.90 usec
 IRNUC 1H
 CTEMP 21.6 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.00 Hz
 RGAIN 50

<CO2Bn



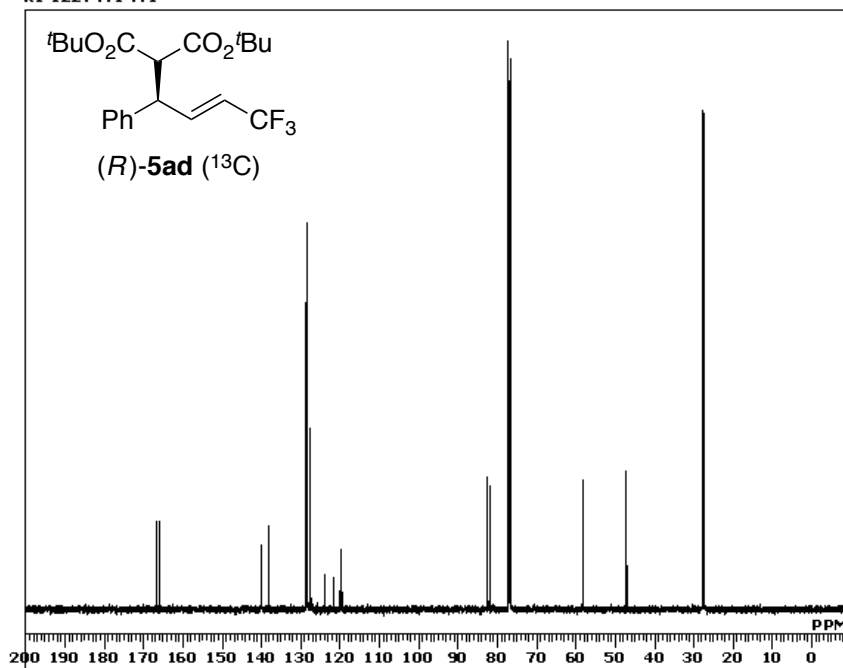
DFILE fCO2Bn_19F-1-1.als
 COMNT <CO2Bn
 DATIM 20-02-2012 16:56:06
 OBNUC 19F
 EXMOD single_pulse.jsp
 OBFREQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 13107
 FREQU 192307.69 Hz
 SCANS 8
 ACQTM 0.0682 sec
 PD 5.0000 sec
 PW1 8.50 usec
 IRNUC 19F
 CTEMP 18.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.00 Hz
 RGAIN 50

KI-1224-Fr1-Fr1



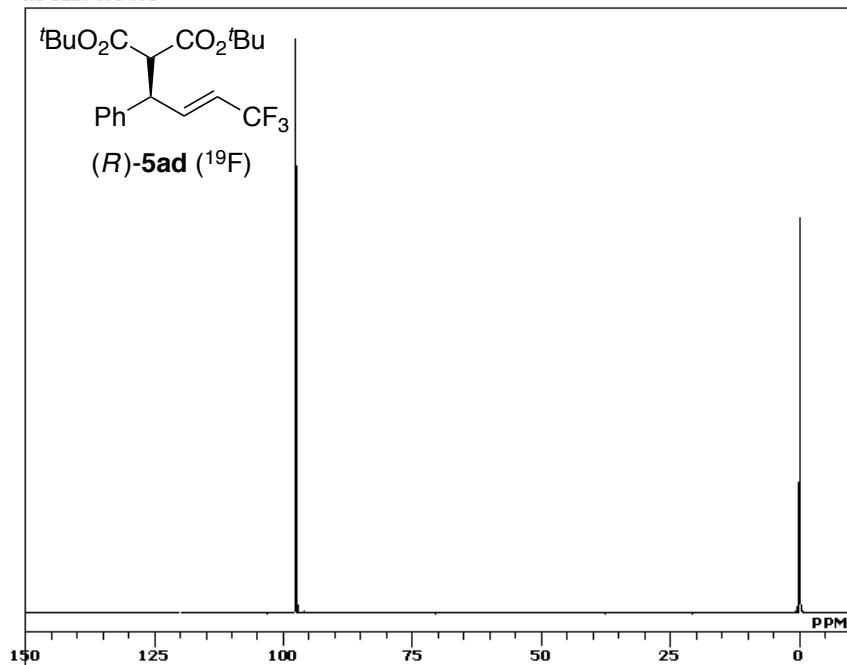
DFILE KI-1224-Fr1-Fr1_Proto
 COMNT KI-1224-Fr1-Fr1
 DATIM 25-01-2012 16:23:50
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 26214
 FREQU 7507.51 Hz
 SCANS 8
 ACQTM 3.4918 sec
 PD 5.0000 sec
 PW1 6.80 usec
 IRNUC 1H
 CTEMP 20.6 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 34

KI-1224-Fr1-Fr1



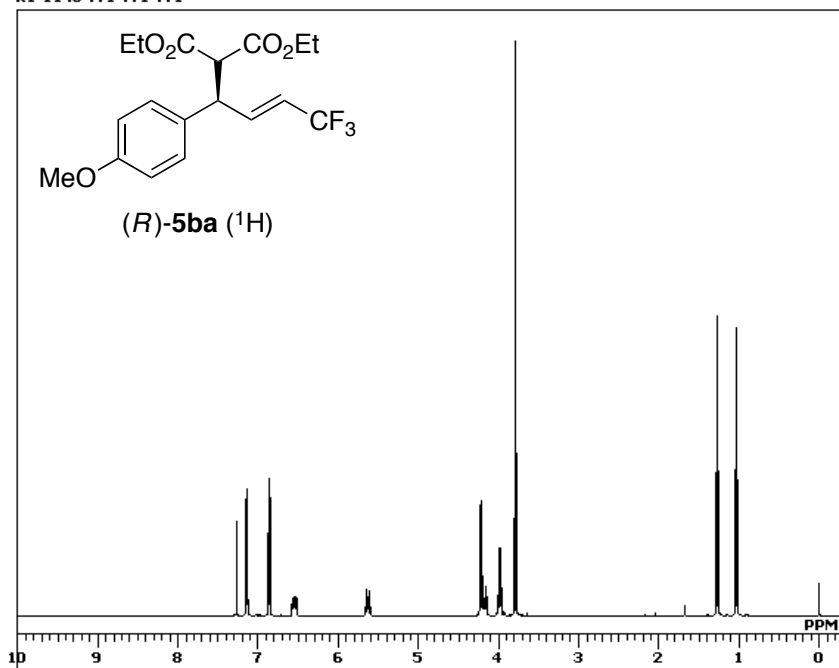
DFILE KI-1224-Fr1-Fr1_Carbo
 COMNT KI-1224-Fr1-Fr1
 DATIM 25-01-2012 16:25:27
 OBNUC 13C
 EXMOD carbon.jsp
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 26214
 FREQU 31446.54 Hz
 SCANS 754
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.90 usec
 IRNUC 1H
 CTEMP 20.9 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.00 Hz
 RGAIN 50

KI-1224-Fr1-Fr1



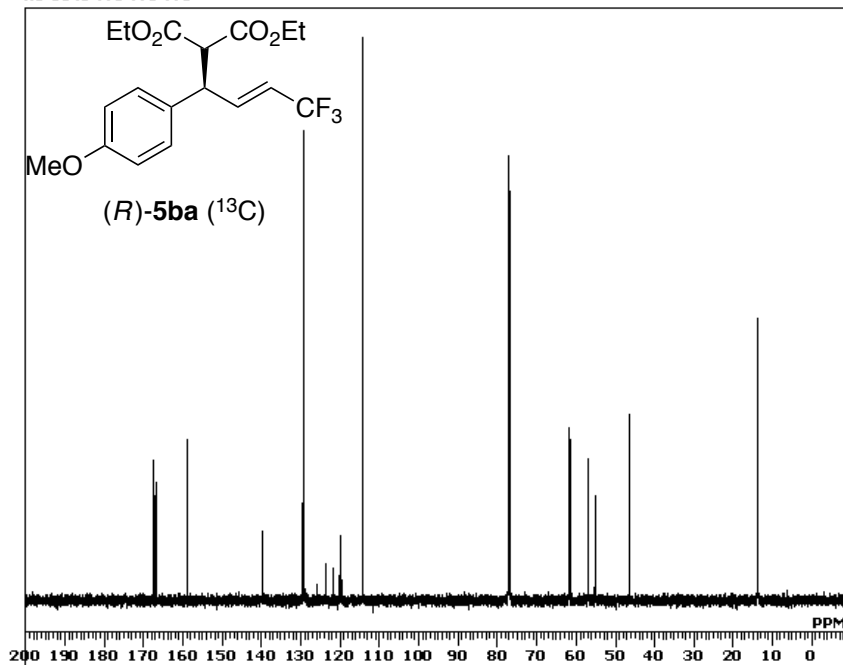
DFILE KI-1224-Fr1-Fr1_19F-1
COMNT KI-1224-Fr1-Fr1
DATIM 25-01-2012 22:25:34
OBNUC ¹⁹F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC ¹⁹F
CTEMP 20.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 50

KI-1146-Fr1-Fr1-Fr1



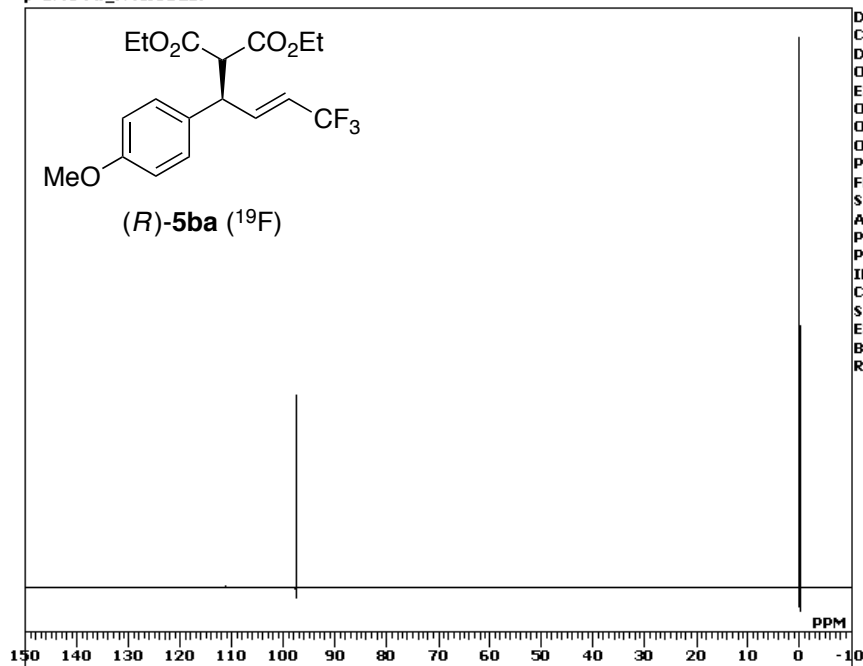
DFILE KI-1146-Fr1-Fr1-Fr1_P1
COMNT KI-1146-Fr1-Fr1-Fr1
DATIM 23-01-2012 23:03:17
OBNUC ¹H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 4
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 6.80 usec
IRNUC ¹H
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 32

KI-1146-Fr1-Fr1-Fr1



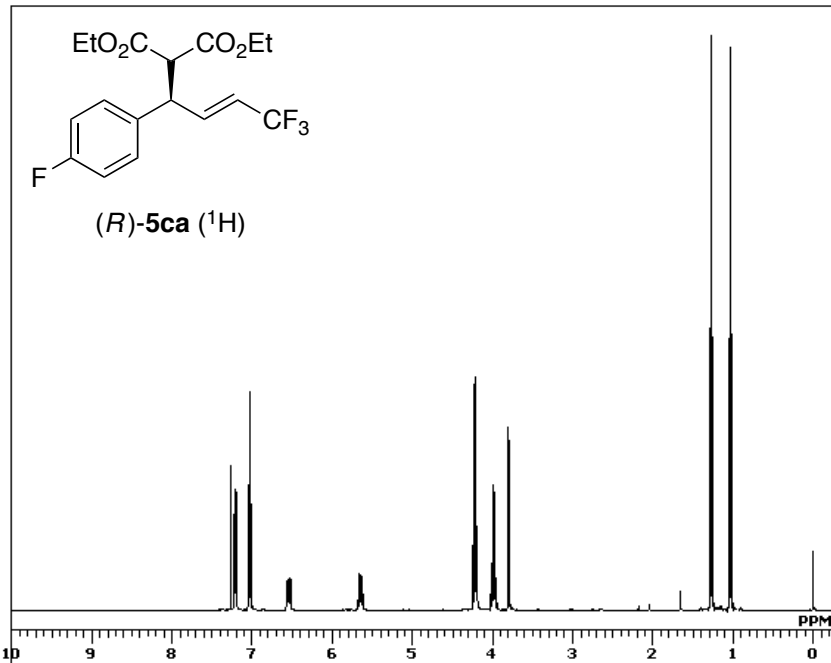
DFILE KI-1146-Fr1-Fr1-Fr1_C
COMNT KI-1146-Fr1-Fr1-Fr1
DATIM 23-01-2012 23:04:15
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 167
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 21.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

p-OMe-Ph_14oCO2Et



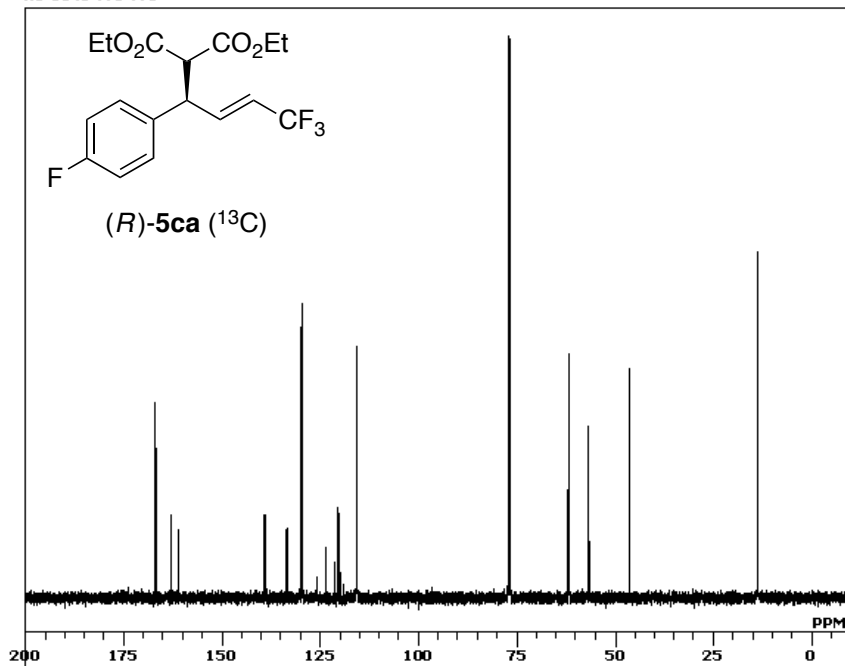
DFILE p-OMe-Ph_14oCO2Et_1!
COMNT p-OMe-Ph_14oCO2Et
DATIM 20-02-2012 17:13:58
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 8.50 usec
IRNUC 19F
CTEMP 18.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 50

KI-1145-Fr1-Fr1



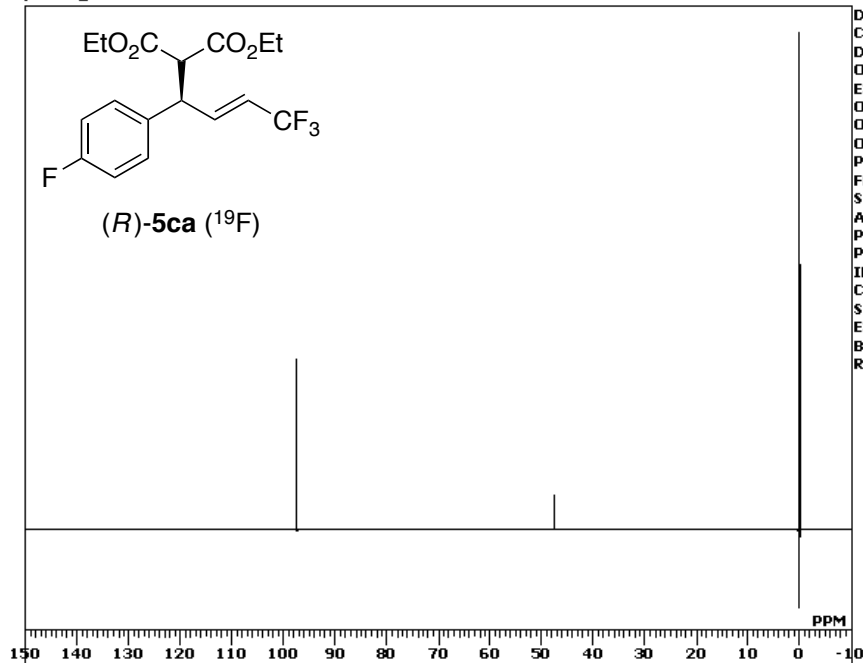
DFILE KI-1145-Fr1-Fr1_Proto
COMNT KI-1145-Fr1-Fr1
DATIM 23-01-2012 22:43:33
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 4
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 6.80 usec
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 34

KI-1145-Fr1-Fr1



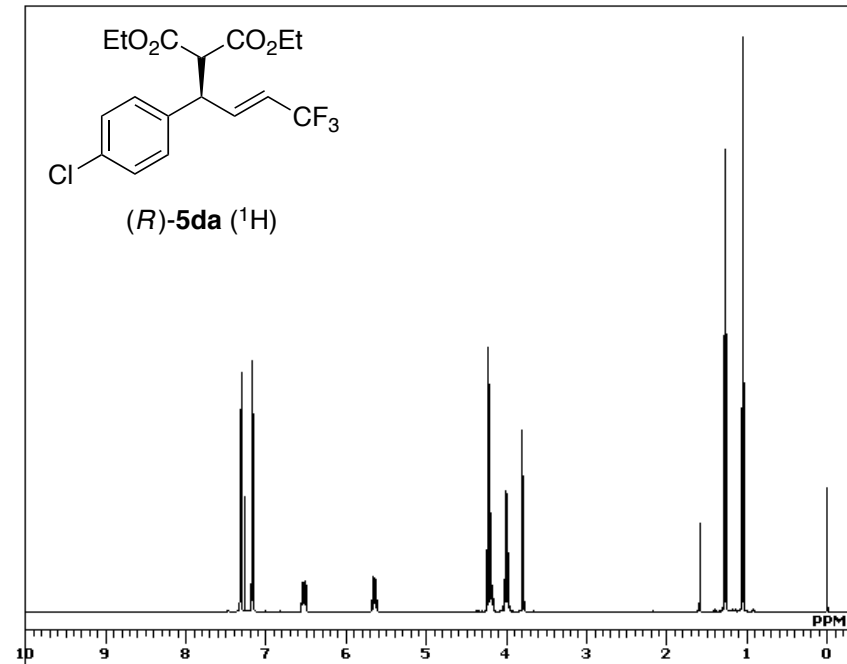
DFILE KI-1145-Fr1-Fr1_Carbo
COMNT KI-1145-Fr1-Fr1
DATIM 23-01-2012 22:44:33
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 277
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 21.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

p-F-Ph_<CO2Et



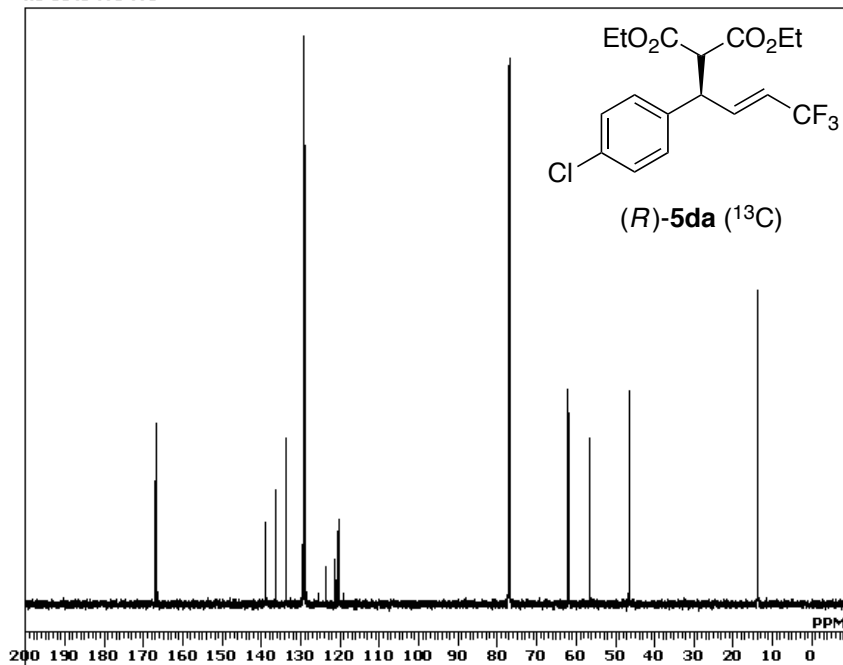
DFILE p-F-Ph_<fCO2Et_19F-1
COMNT p-F-Ph_<CO2Et
DATIM 20-02-2012 17:02:00
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 8.50 usec
IRNUC 19F
CTEMP 18.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 50

KI-924-Fr1



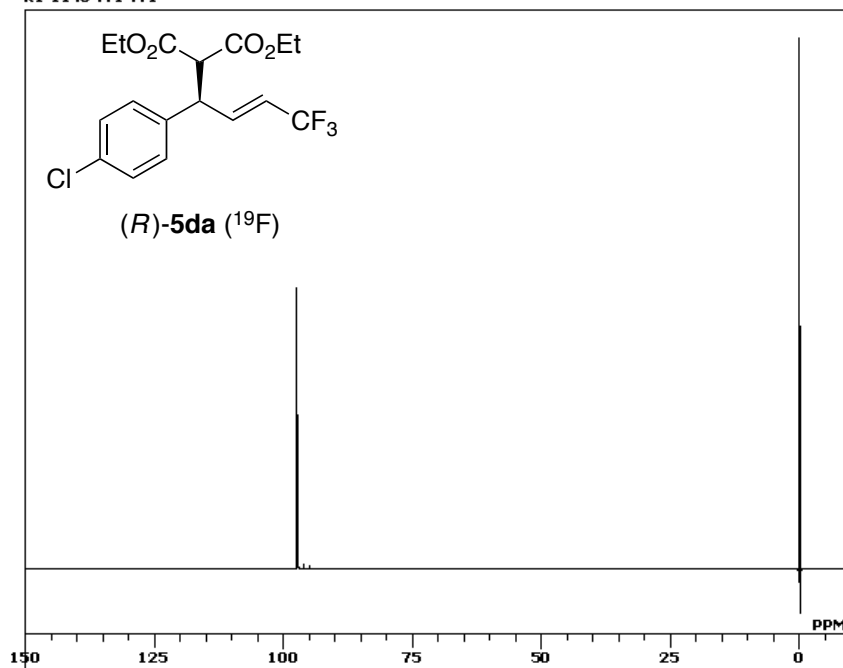
DFILE KI-924-Fr1_Proton-1-1.
COMNT KI-924-Fr1
DATIM 14-07-2011 19:48:42
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 4
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 6.80 usec
IRNUC 1H
CTEMP 24.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 36

KI-1148-Fr1-Fr1



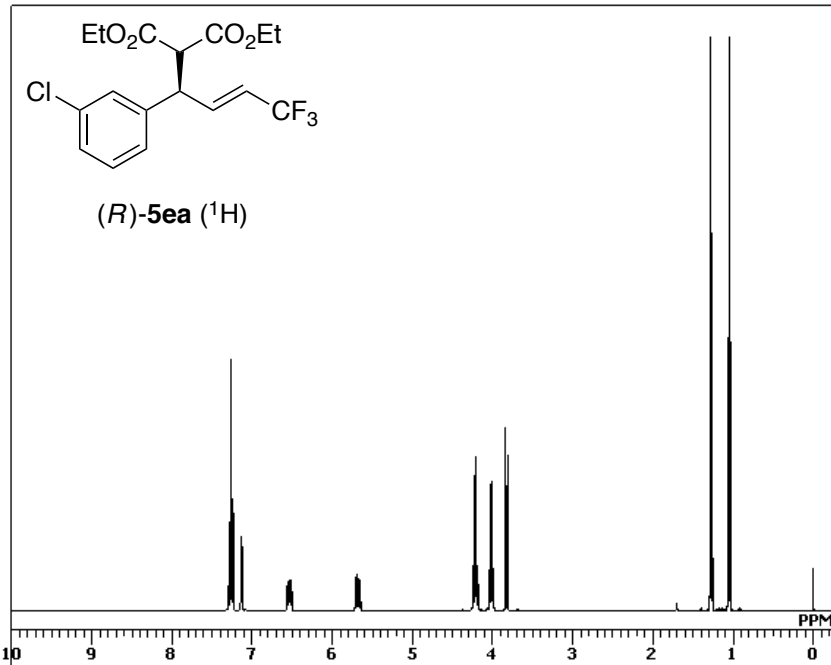
DFILE KI-1148-Fr1-Fr1_Carbo
COMNT KI-1148-Fr1-Fr1
DATIM 25-01-2012 19:27:28
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 512
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

KI-1148-Fr1-Fr1



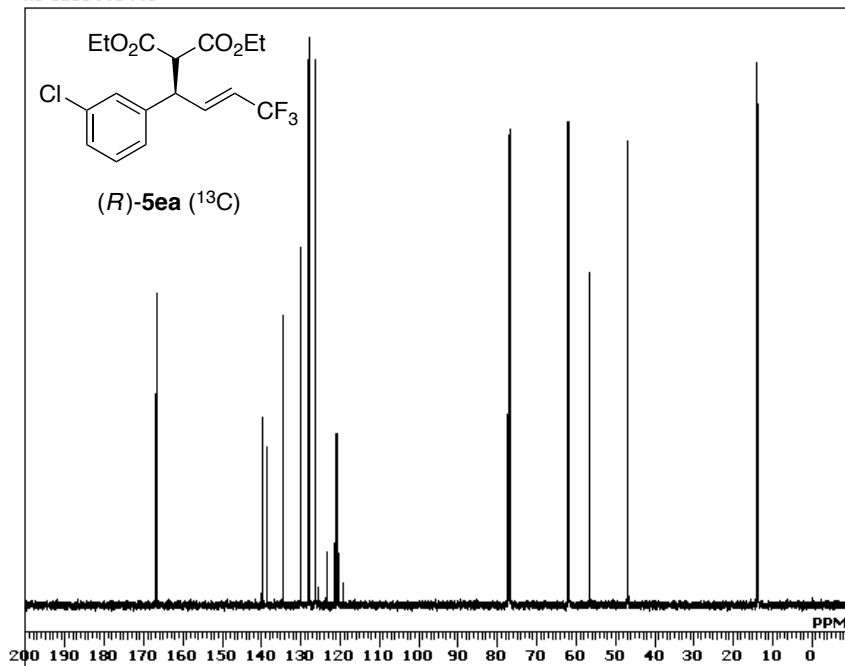
DFILE KI-1148-Fr1-Fr1_19F-1
COMNT KI-1148-Fr1-Fr1
DATIM 25-01-2012 22:22:11
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 20.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 50

KI-1216-Fr1-Fr1



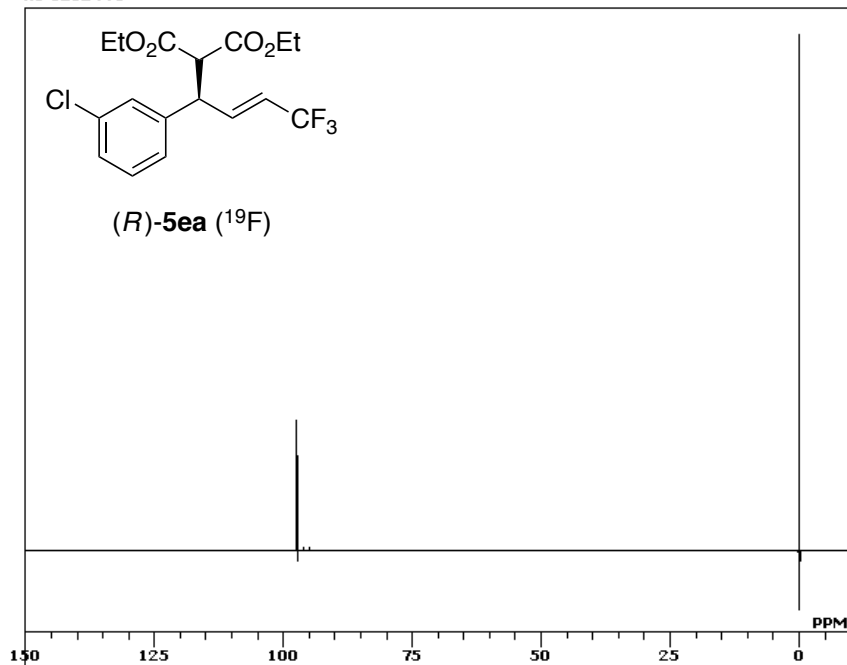
DFILE KI-1216-Fr1-Fr1_Proton
COMNT KI-1216-Fr1-Fr1
DATIM 23-02-2012 08:50:60
OBNUC 1H
EXMOD proton.jxp
OBFREQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 28

KI-1216-Fr1-Fr1



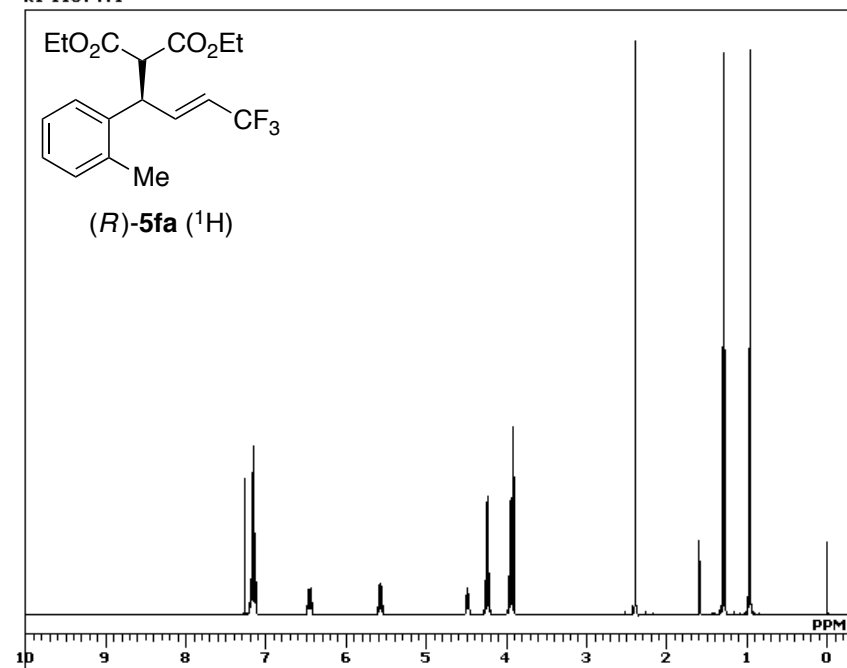
DFILE KI-1216-Fr1-Fr1_Carbon
COMNT KI-1216-Fr1-Fr1
DATIM 23-02-2012 08:52:32
OBNUC 13C
EXMOD carbon.jxp
OBFREQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 256
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

KI-1262-Fr1

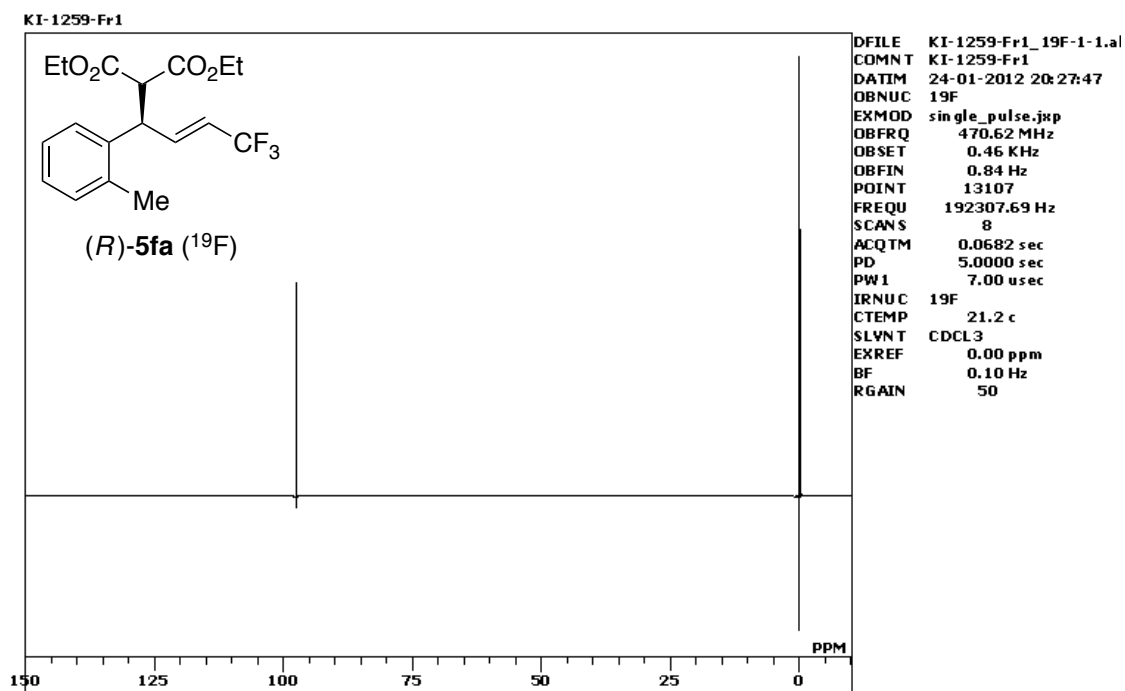
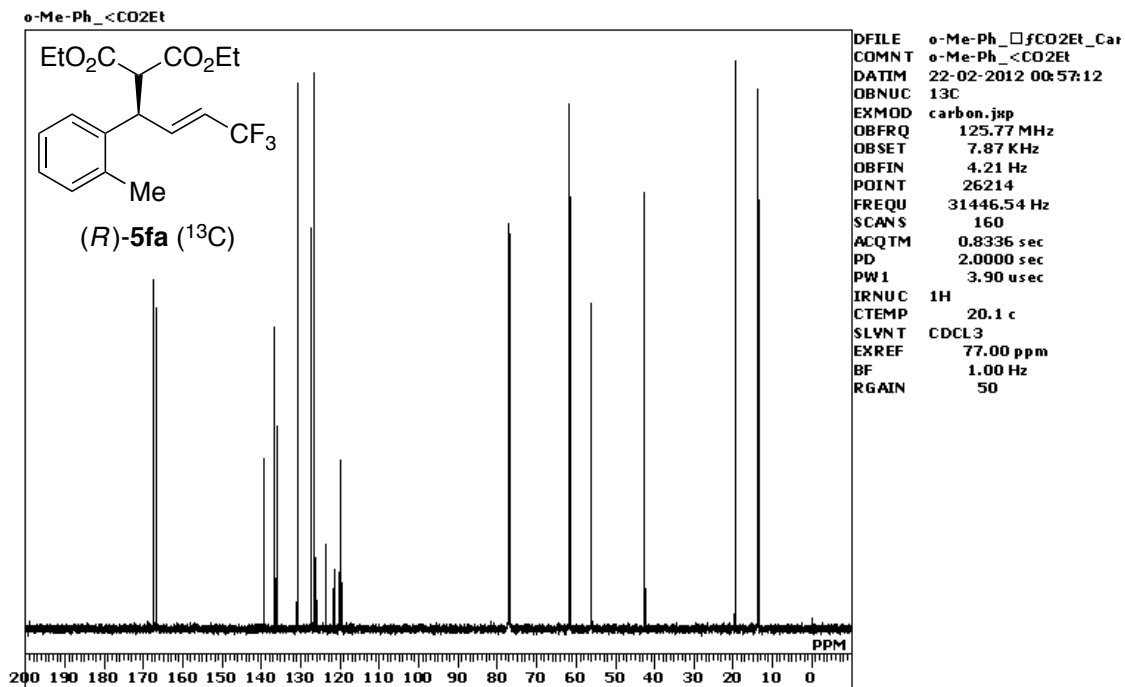


DFILE KI-1262-Fr1_19F-1-1.al
COMNT KI-1262-Fr1
DATIM 24-01-2012 20:39:19
OBNUC 19F
EXMOD single_pulse.jsp
OBFRQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 19F
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 50

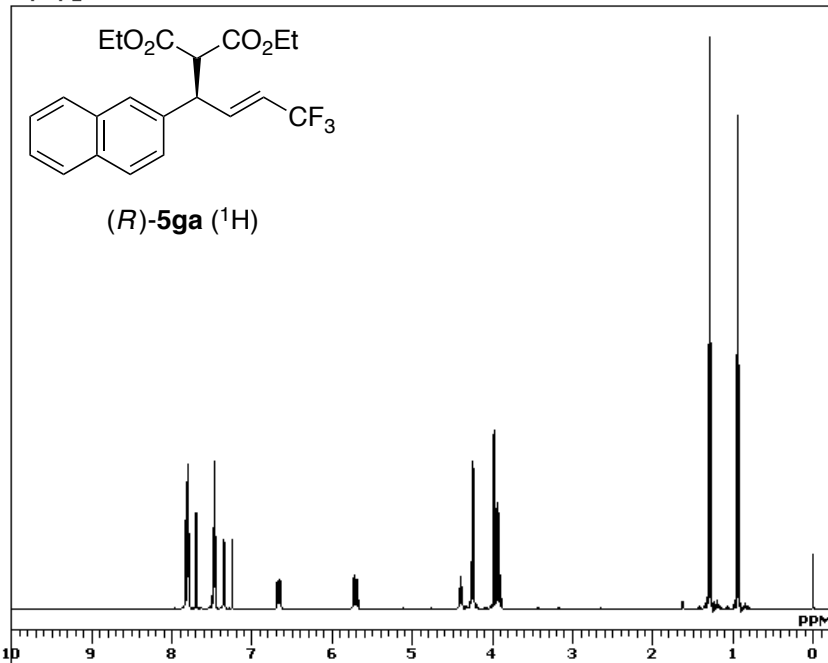
KI-1164-Fr1



DFILE KI-1153-Fr1_Proton-1-
COMNT KI-1164-Fr1
DATIM 20-12-2011 19:02:20
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 4
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 6.80 usec
IRNUC 1H
CTEMP 21.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 38

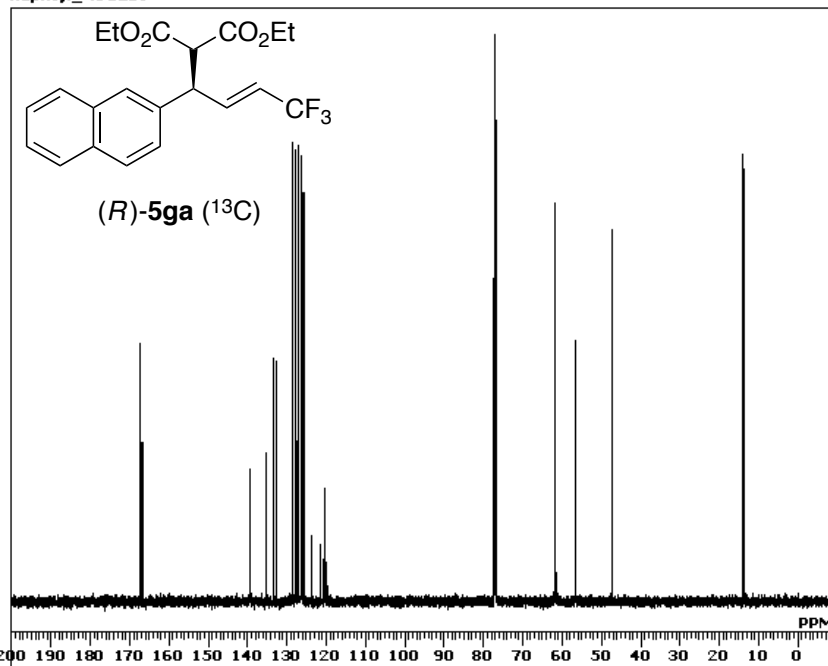


naphtyl_i%aeCO2Et



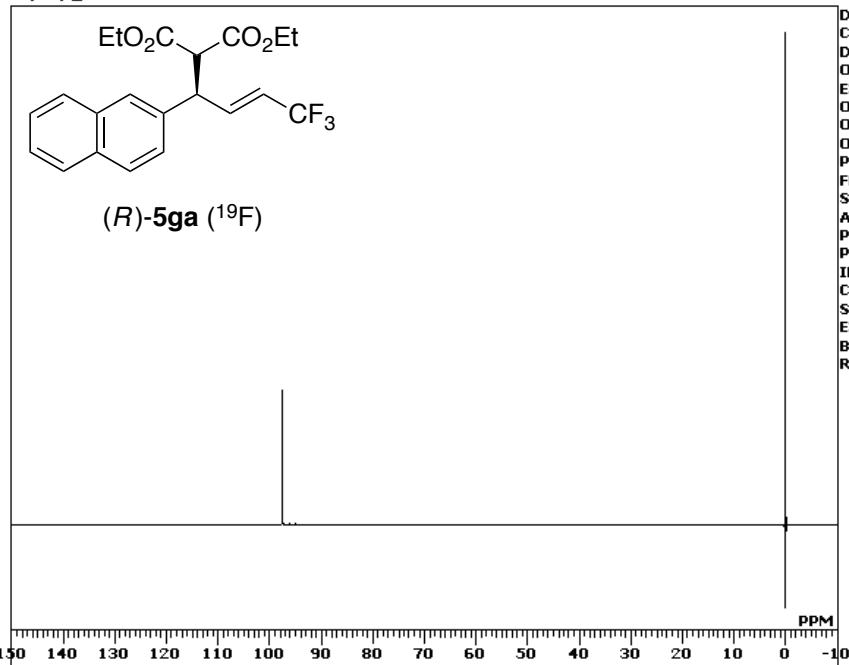
DFILE n aphtyl_ fCO2Et_Prot
COMNT n aphtyl_i%aeCO2Et
DATIM 20-02-2012 17:24:57
OBNUC 1H
EXMOD proton.jsp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 26214
FREQU 7507.51 Hz
SCANS 8
ACQTM 3.4918 sec
PD 5.0000 sec
PW1 7.00 usec
IRNUC 1H
CTEMP 18.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 30

naphtyl_<CO2Et

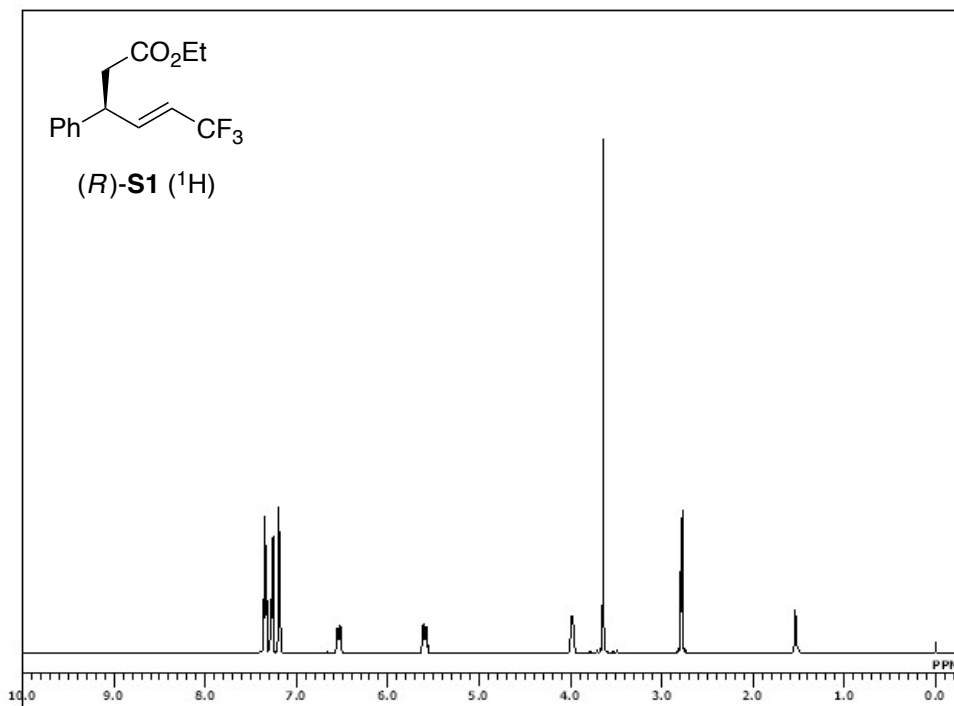


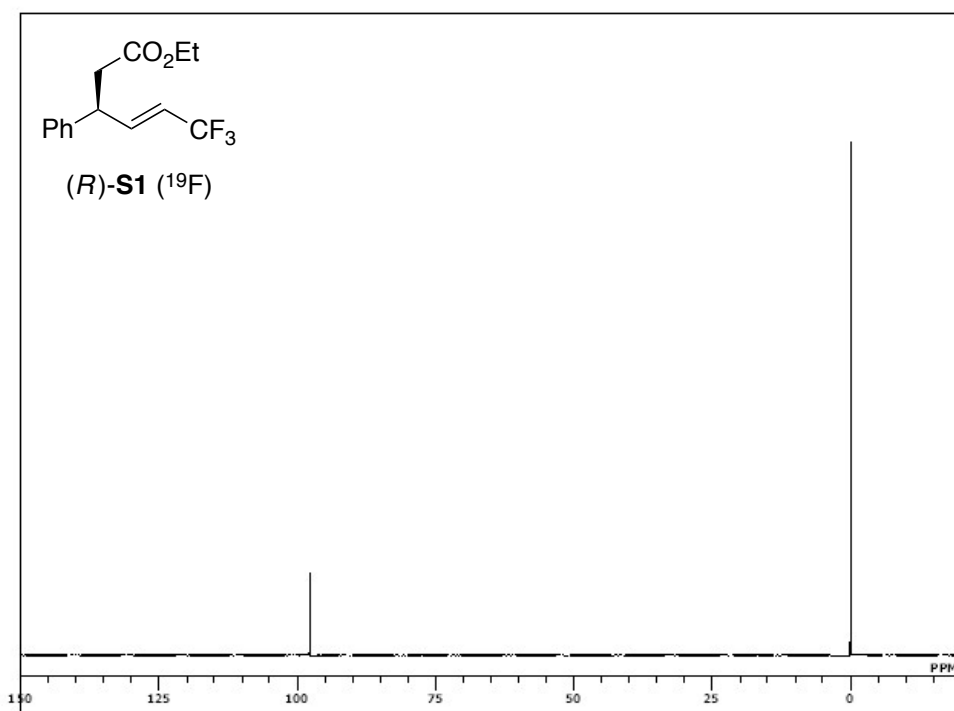
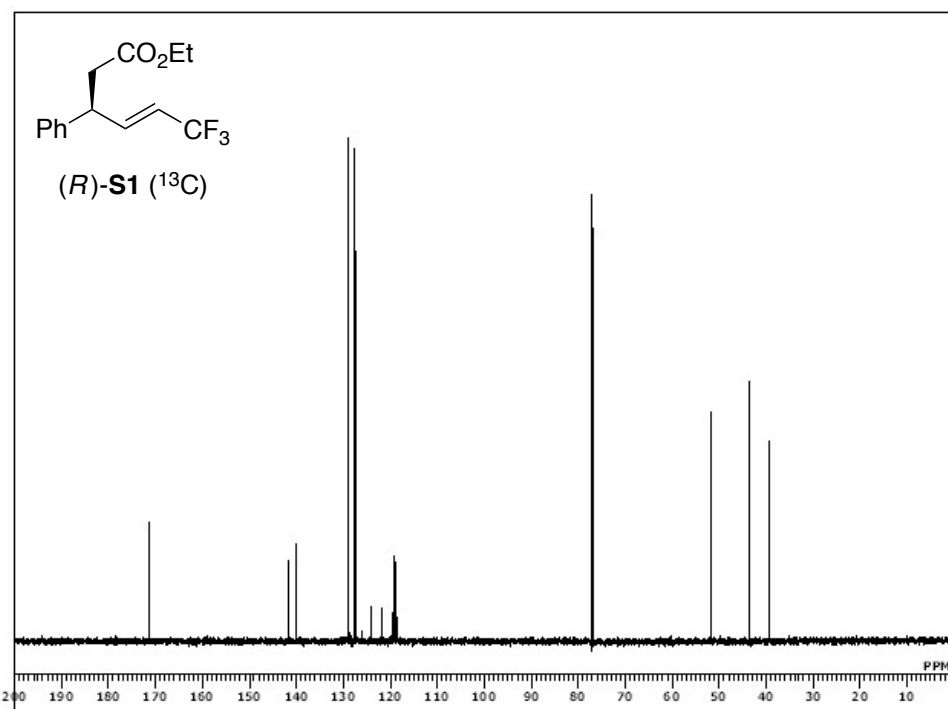
DFILE n aphtyl_ fCO2Et_Cart
COMNT n aphtyl_<CO2Et
DATIM 22-02-2012 01:11:58
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 236
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.90 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

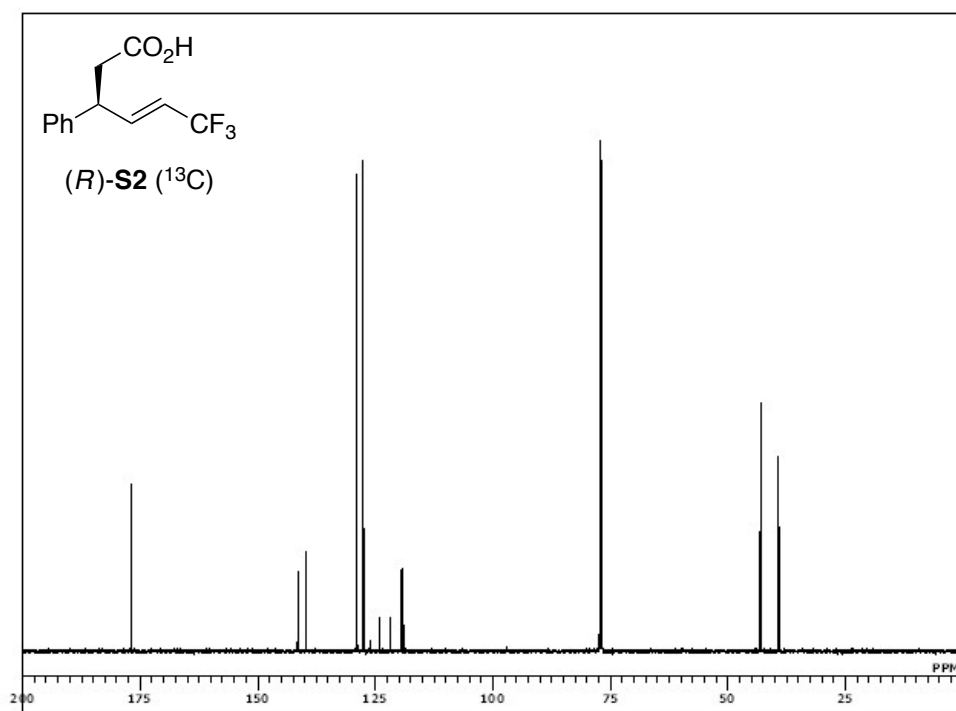
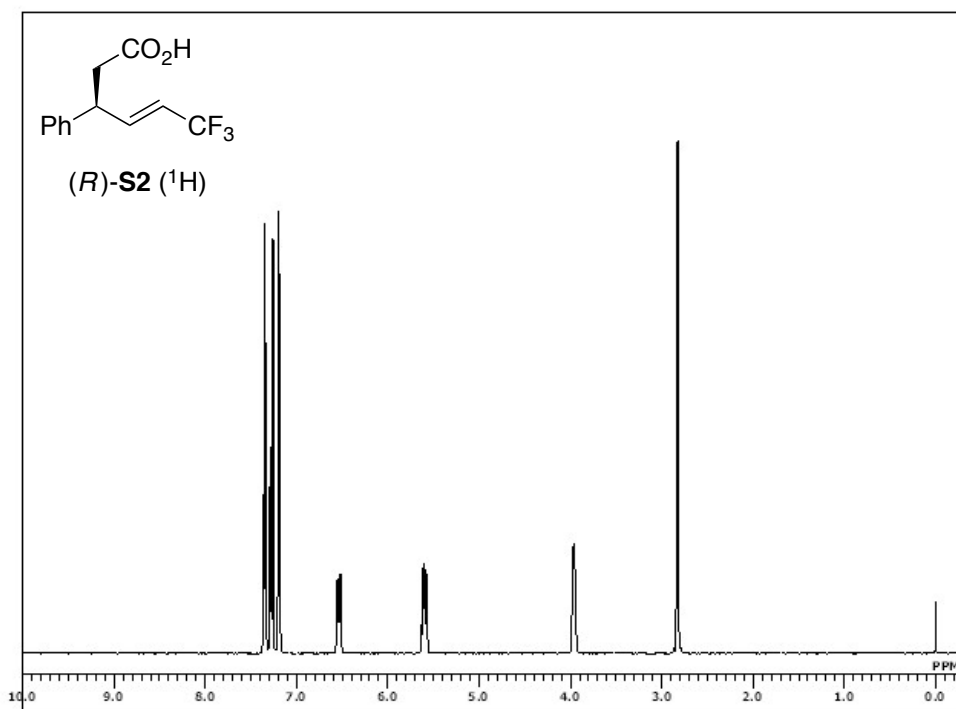
naphtyl_<CO2Et

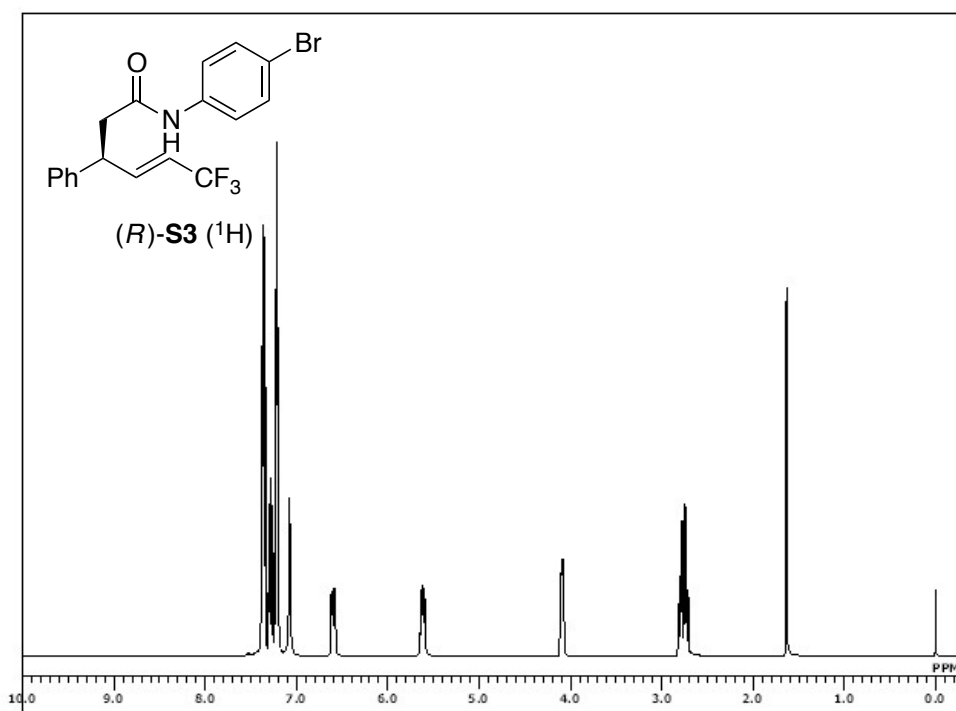
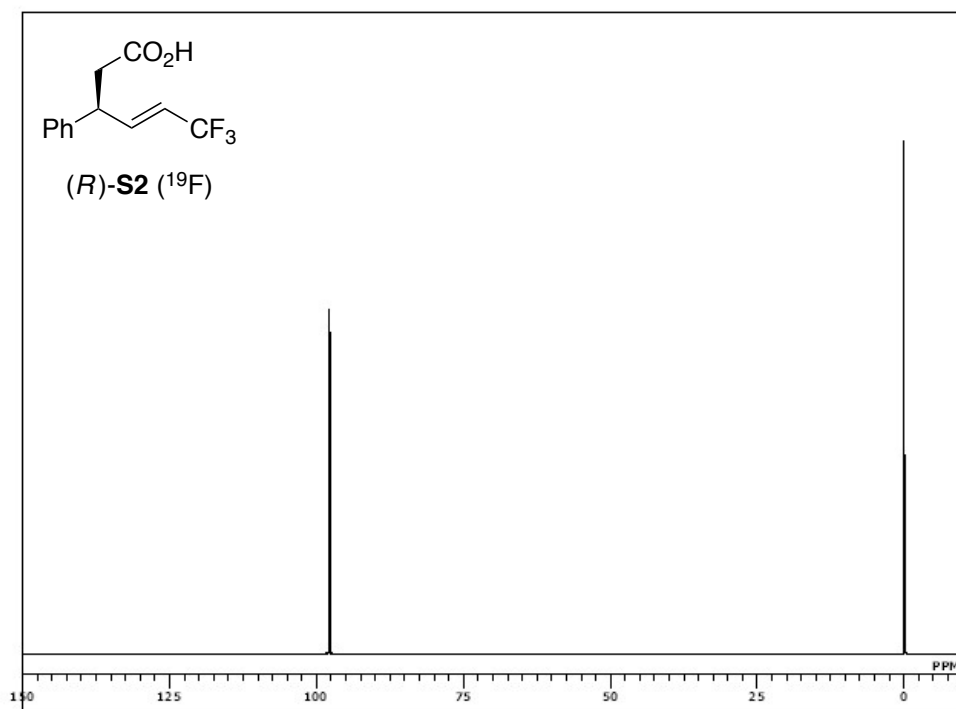


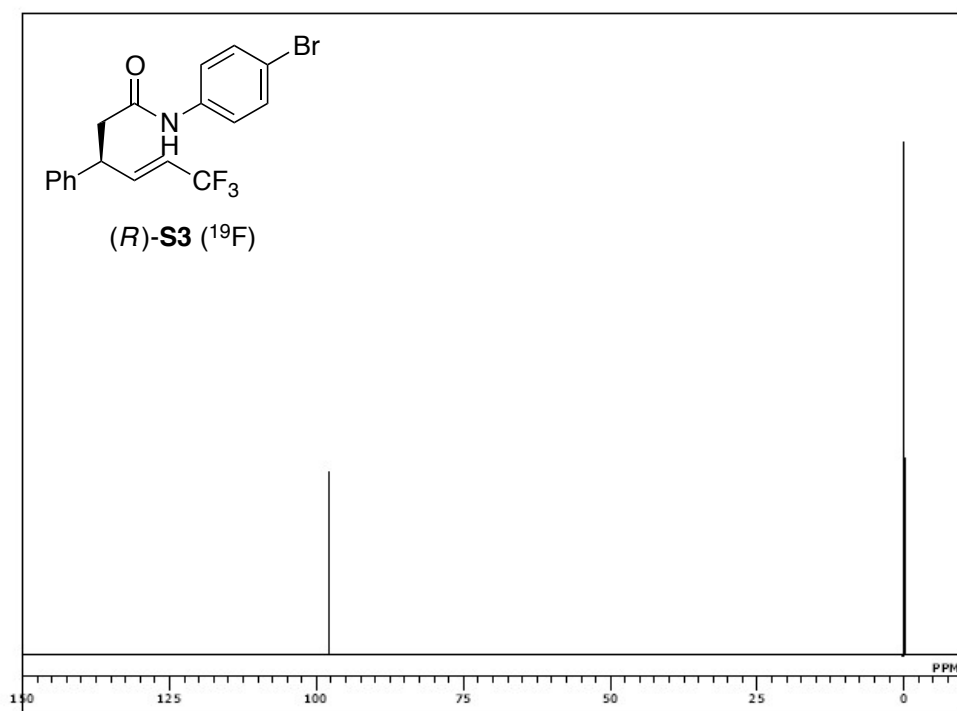
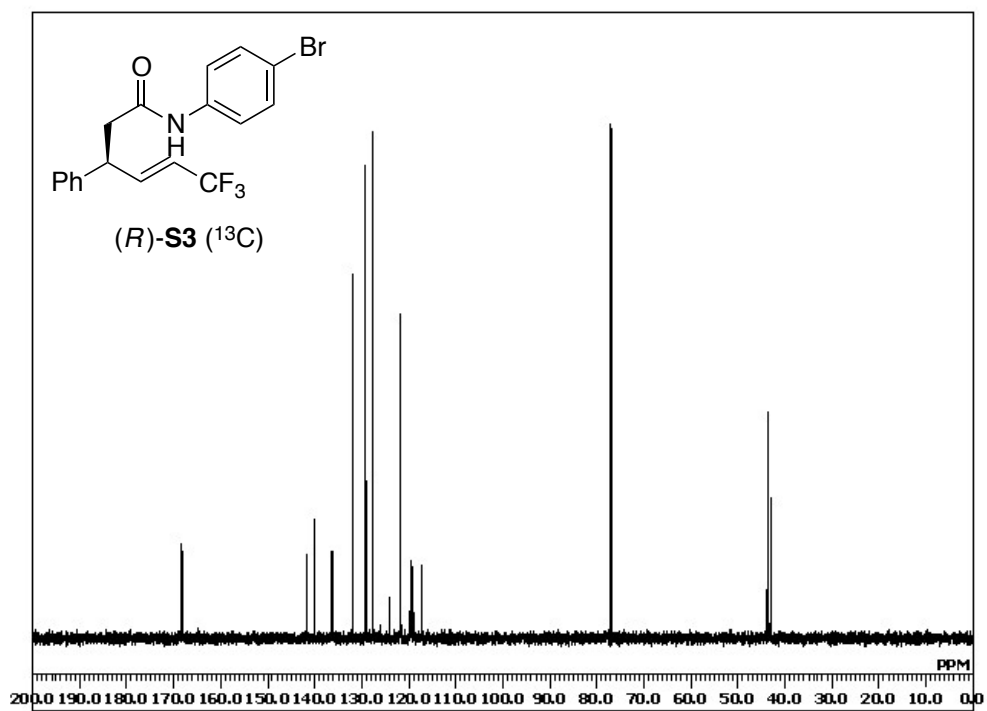
DFILE naphtyl_<CO2Et_19F-
COMNT naphtyl_<CO2Et
DATIM 20-02-2012 17:20:20
OBNUC 19F
EXMOD single_pulse.jxp
OBFREQ 470.62 MHz
OBSET 0.46 KHz
OBFIN 0.84 Hz
POINT 13107
FREQU 192307.69 Hz
SCANS 8
ACQTM 0.0682 sec
PD 5.0000 sec
PW1 8.50 usec
IRNUC 19F
CTEMP 18.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 50



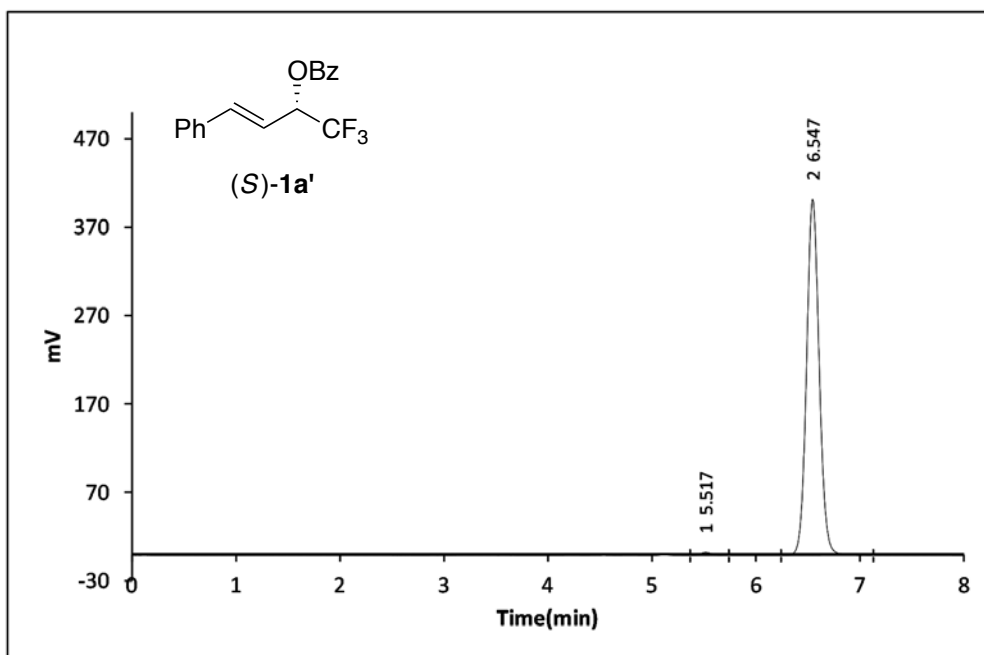
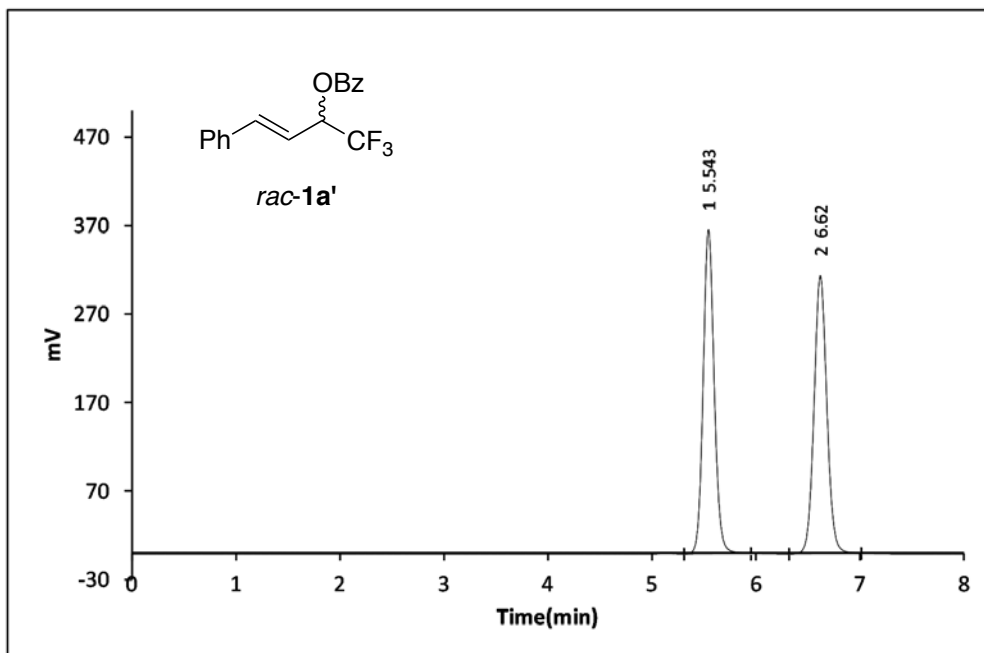


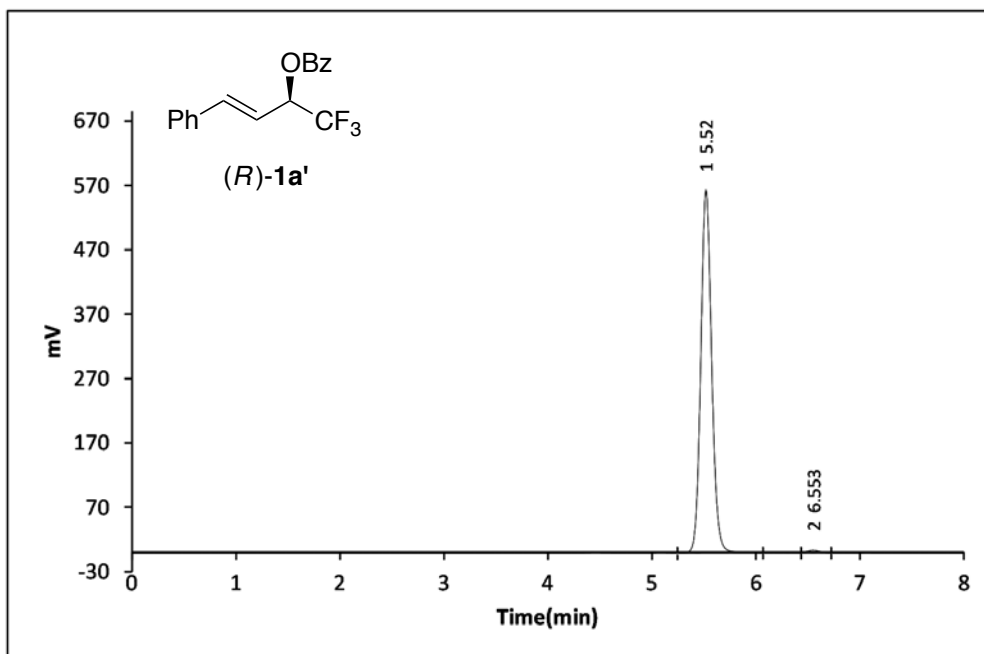


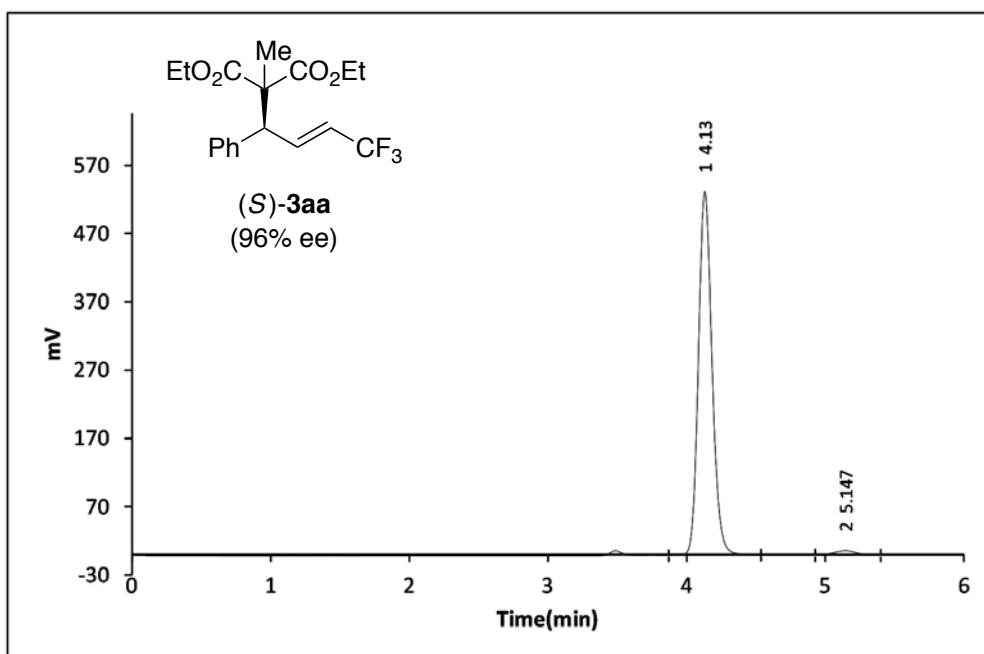
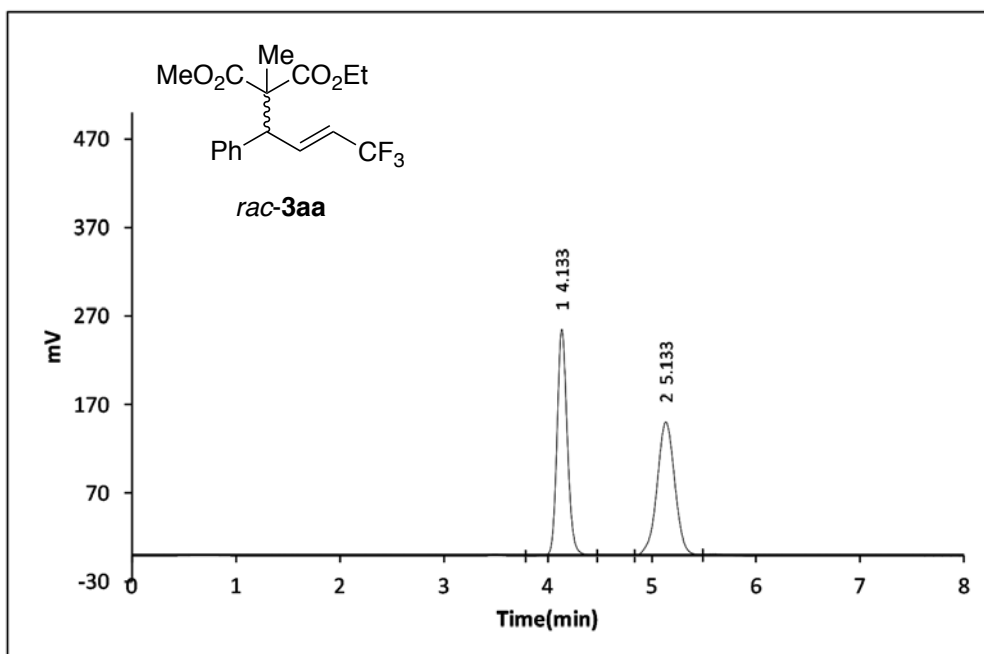


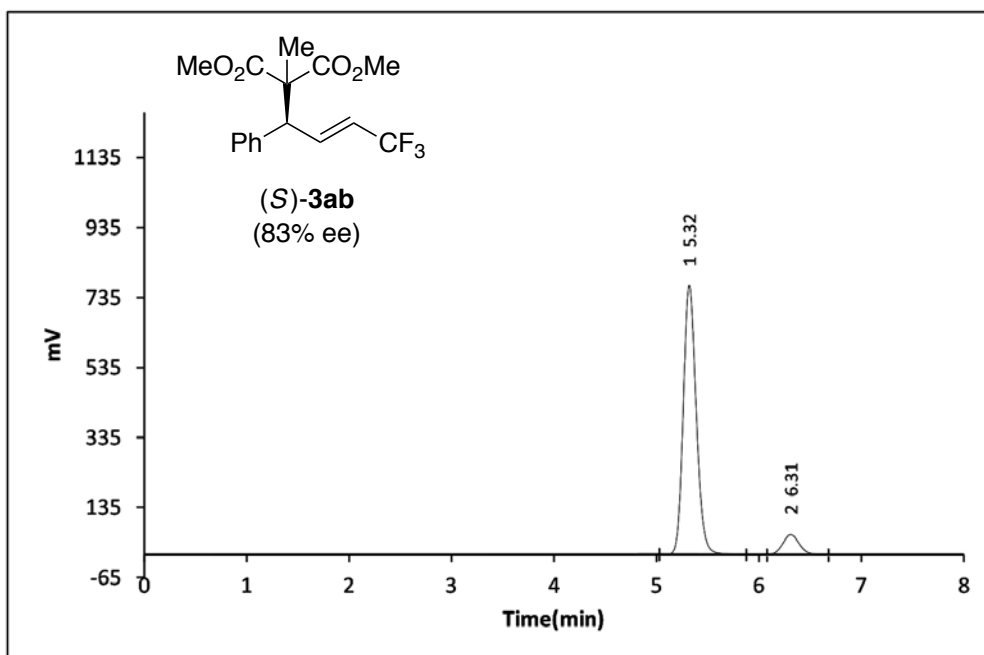
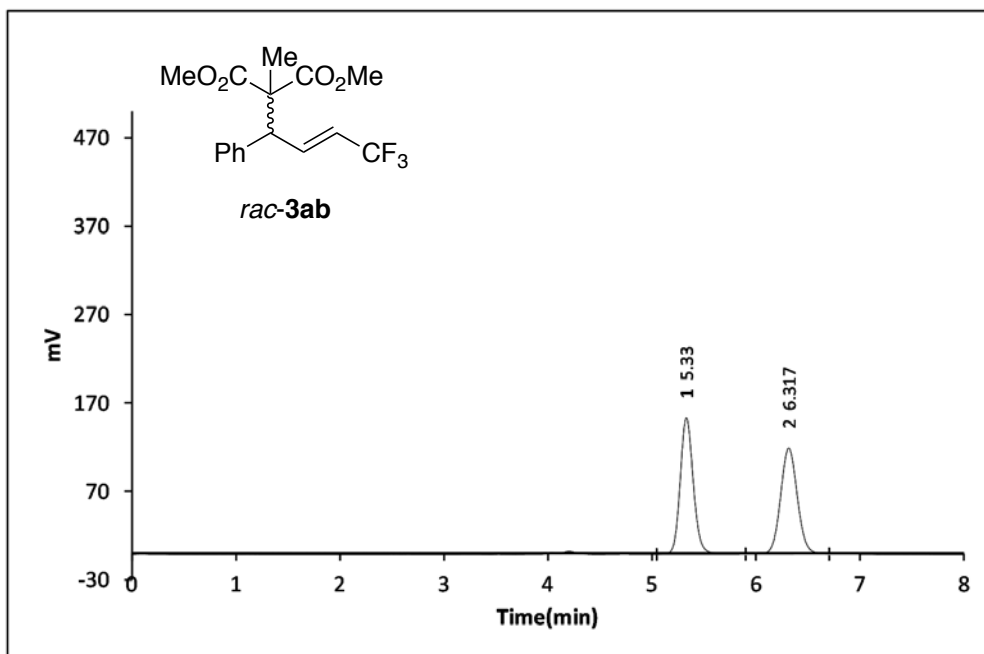


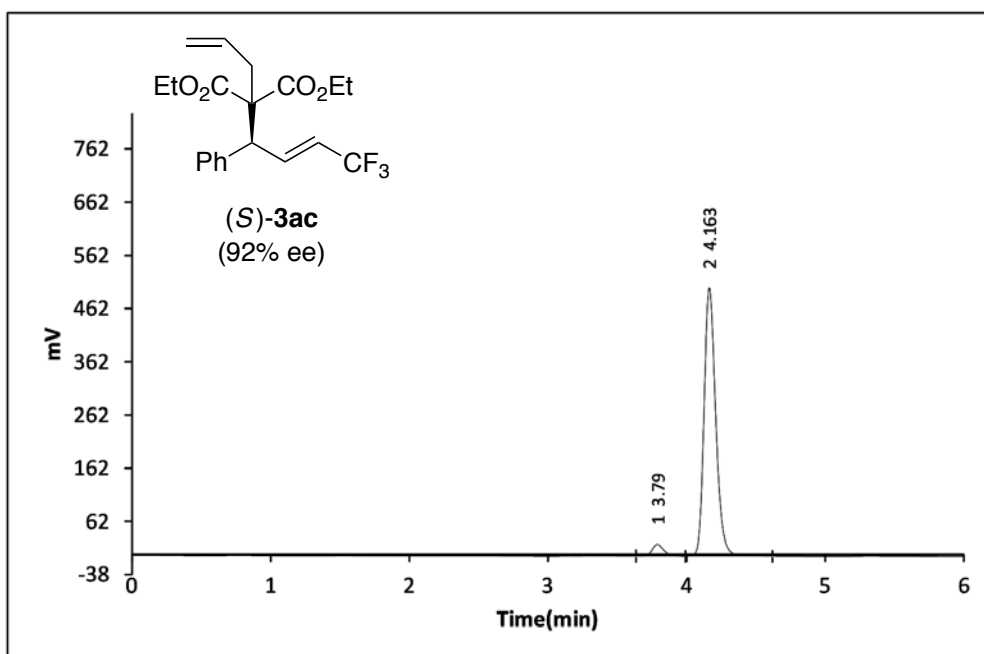
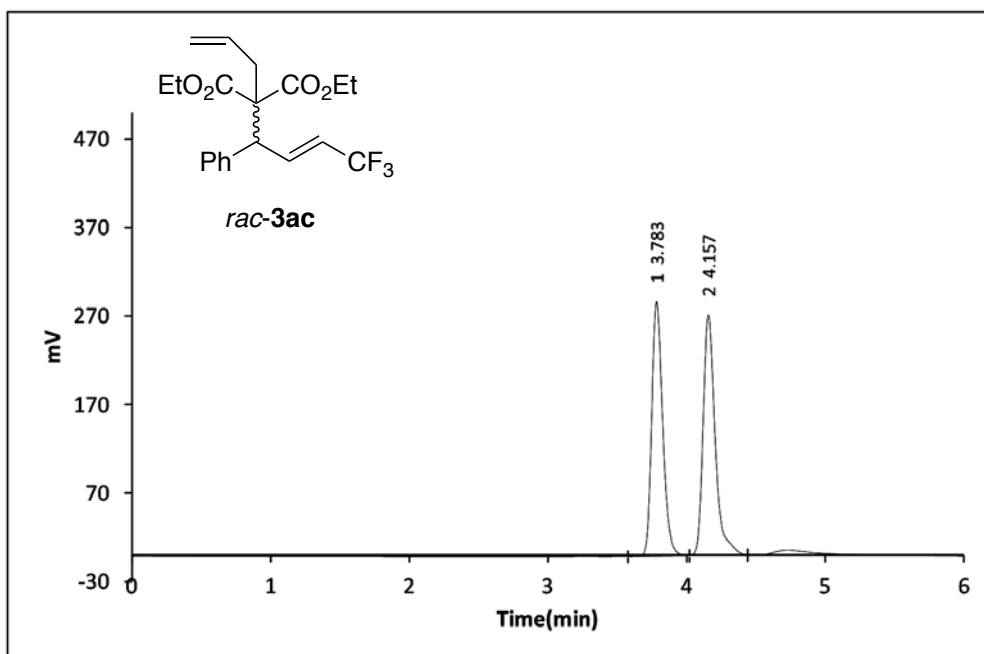
Copies of chiral HPLC chart of products

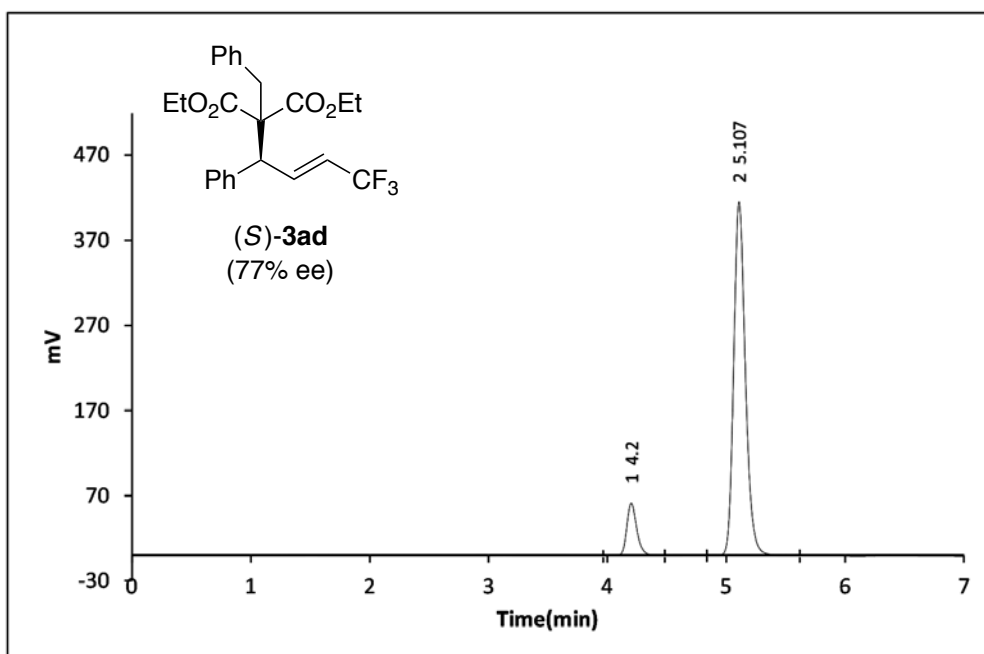
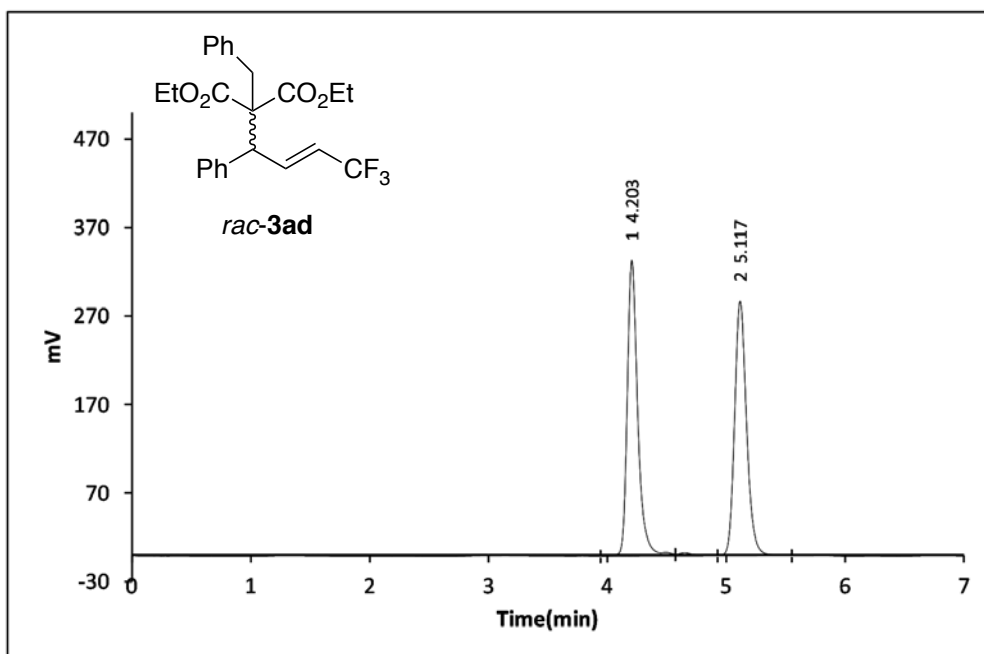


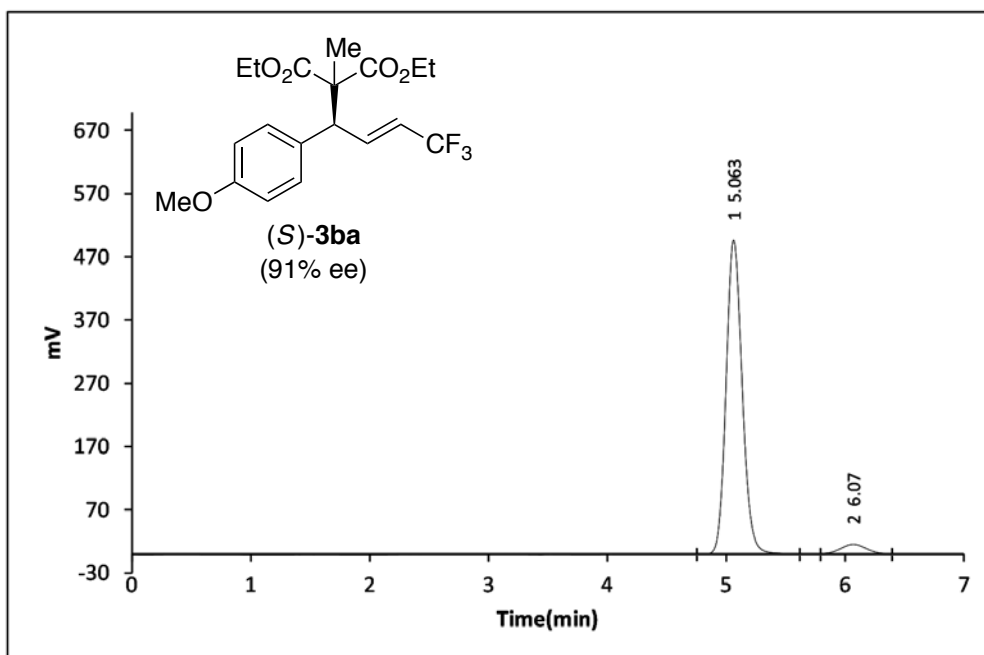
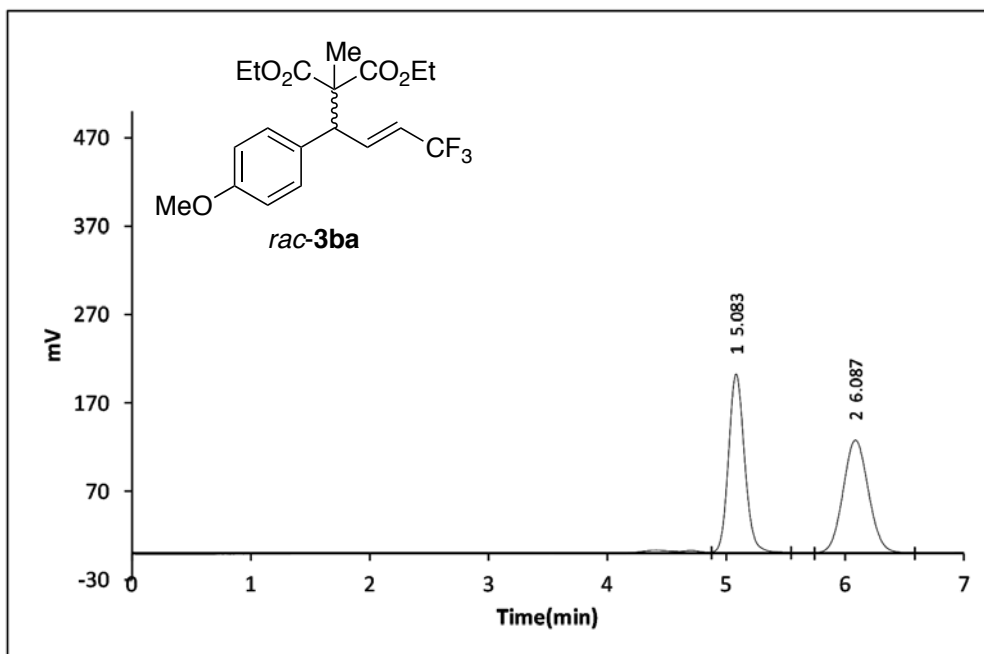


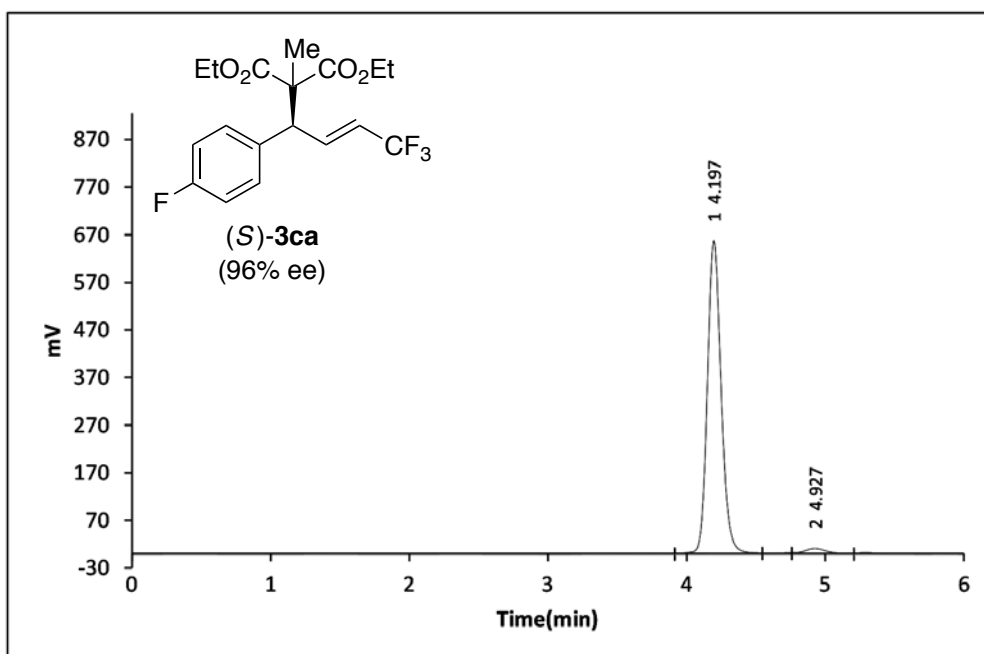
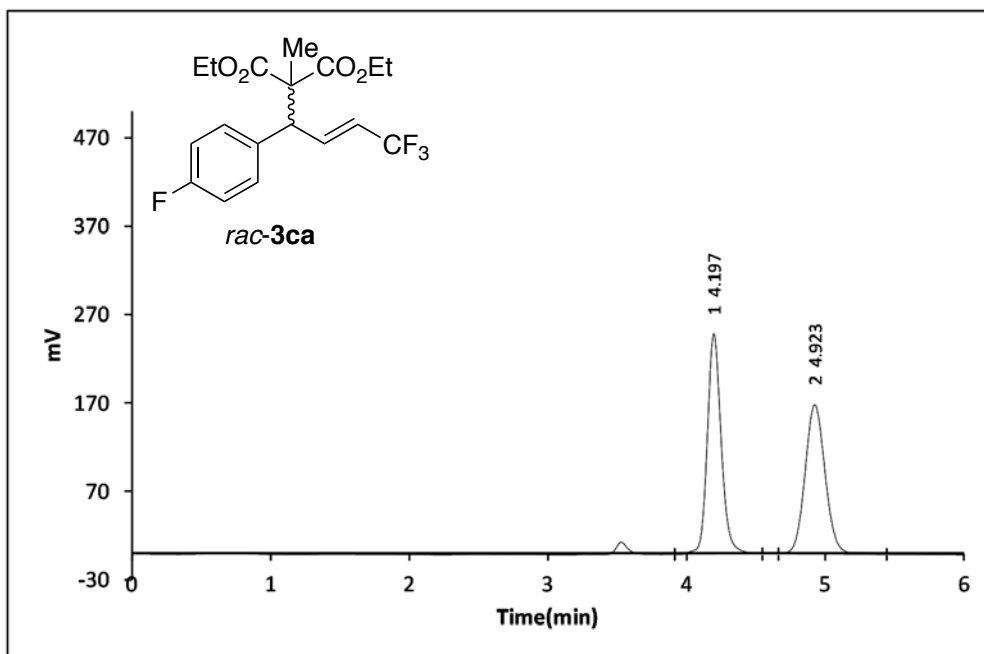


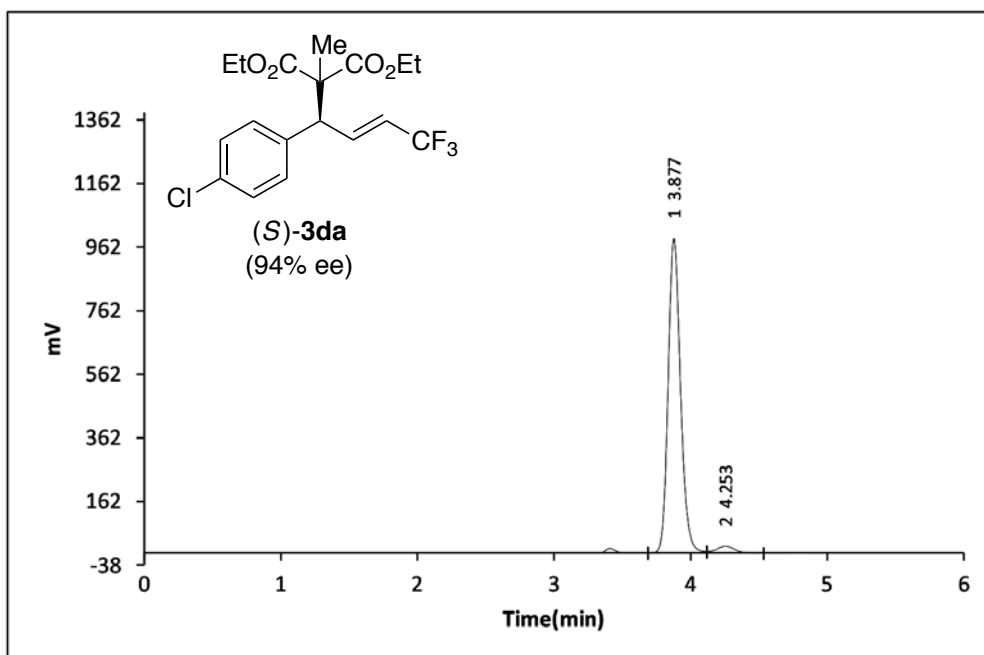
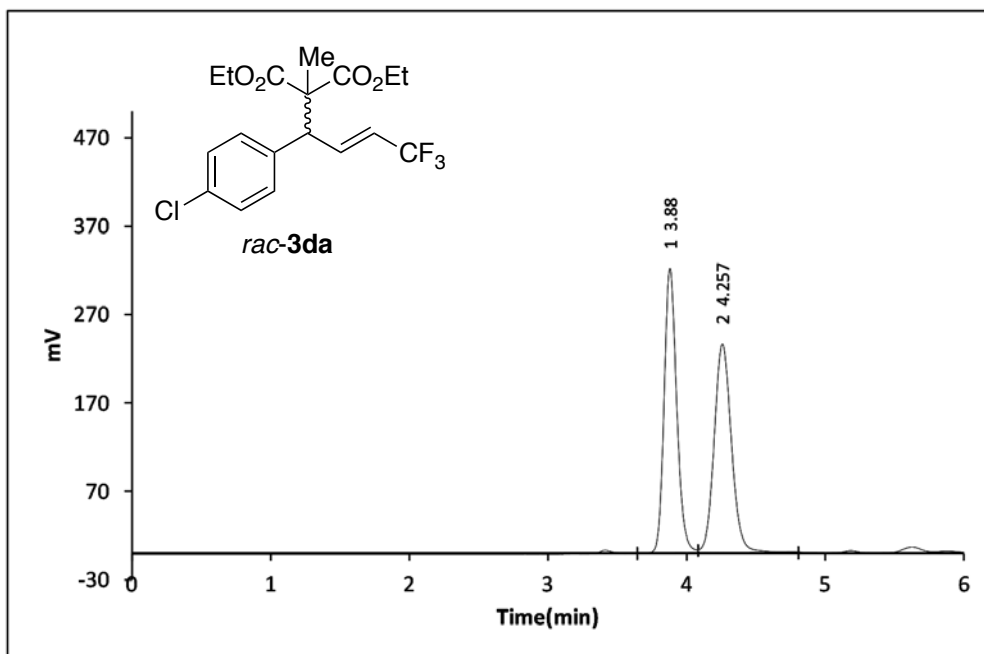


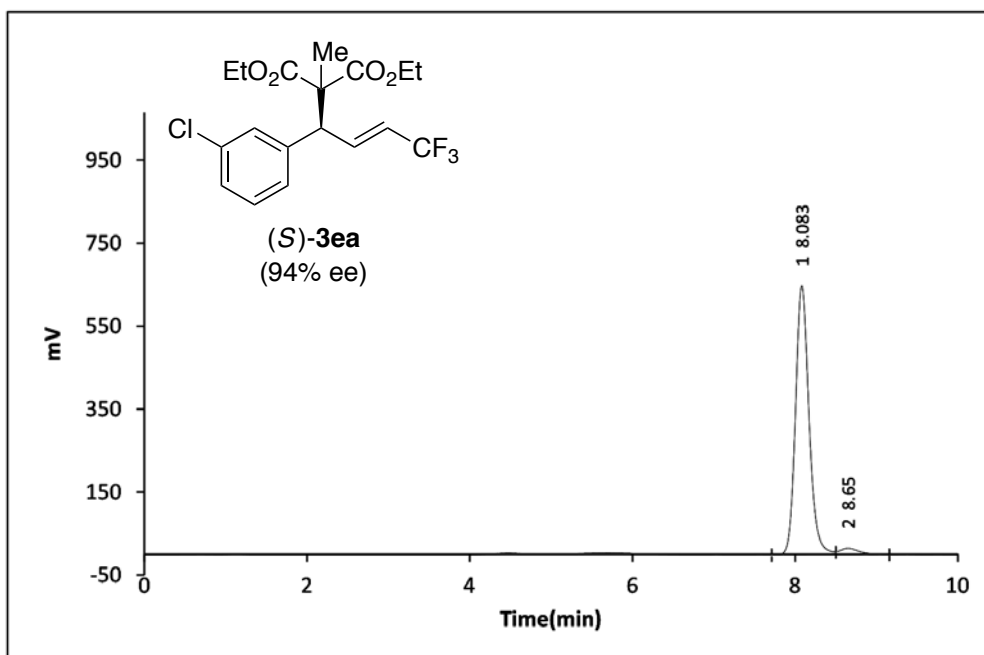
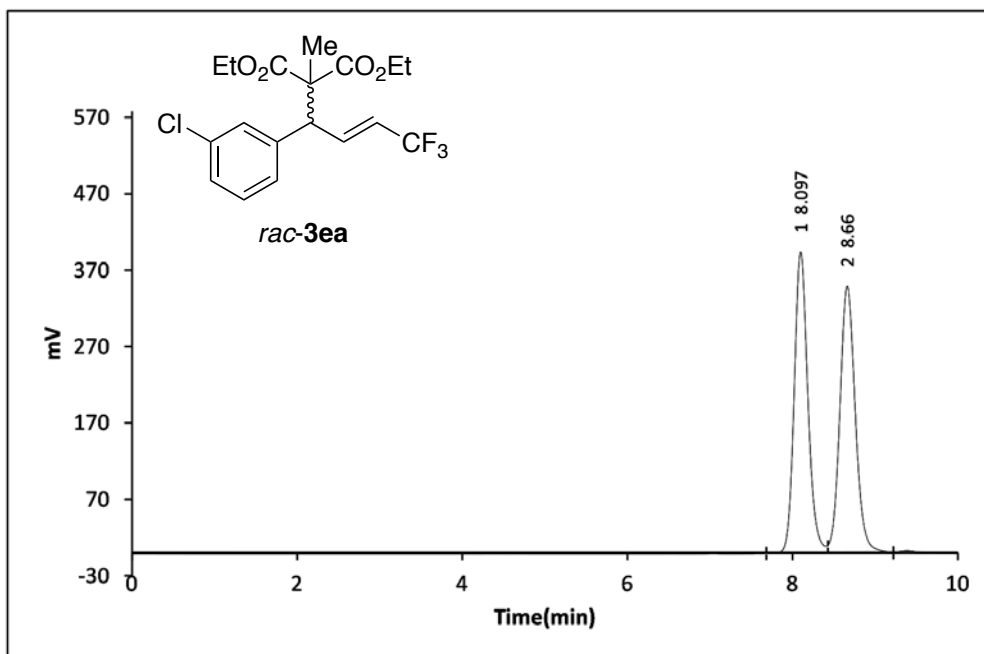


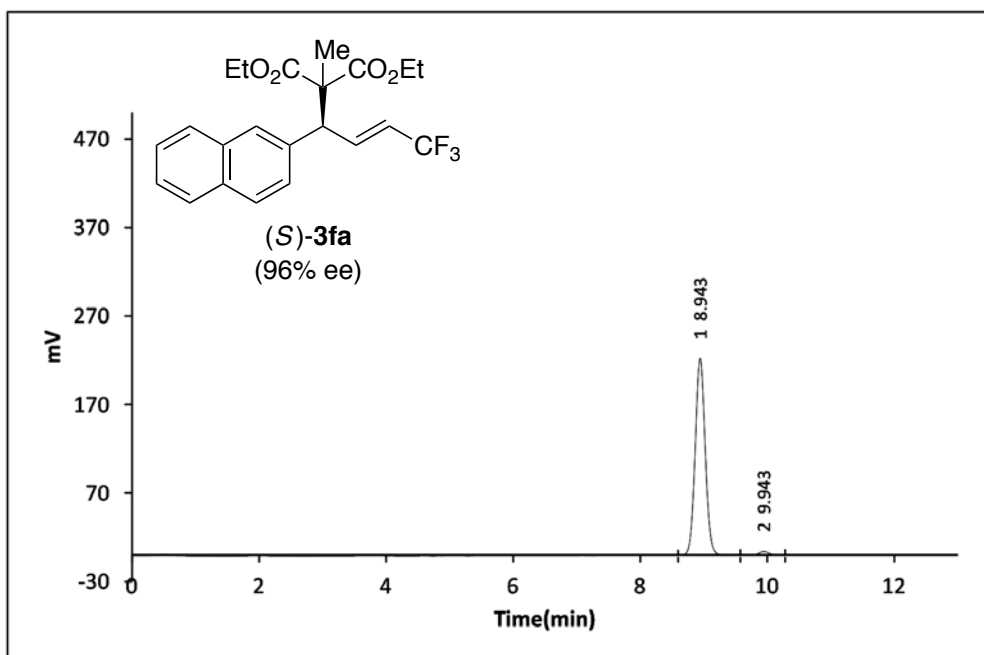
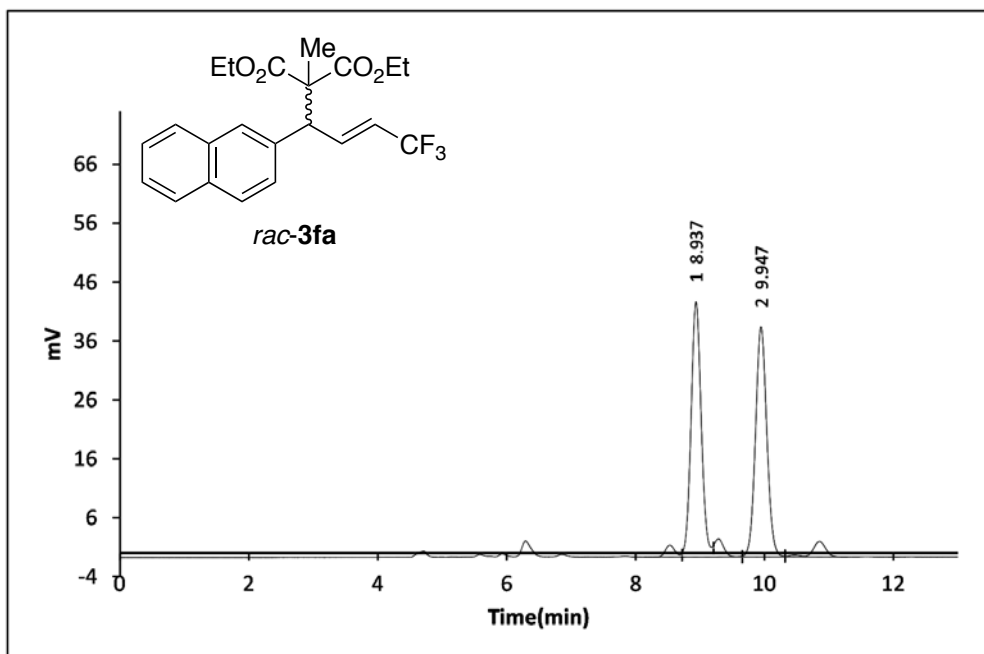


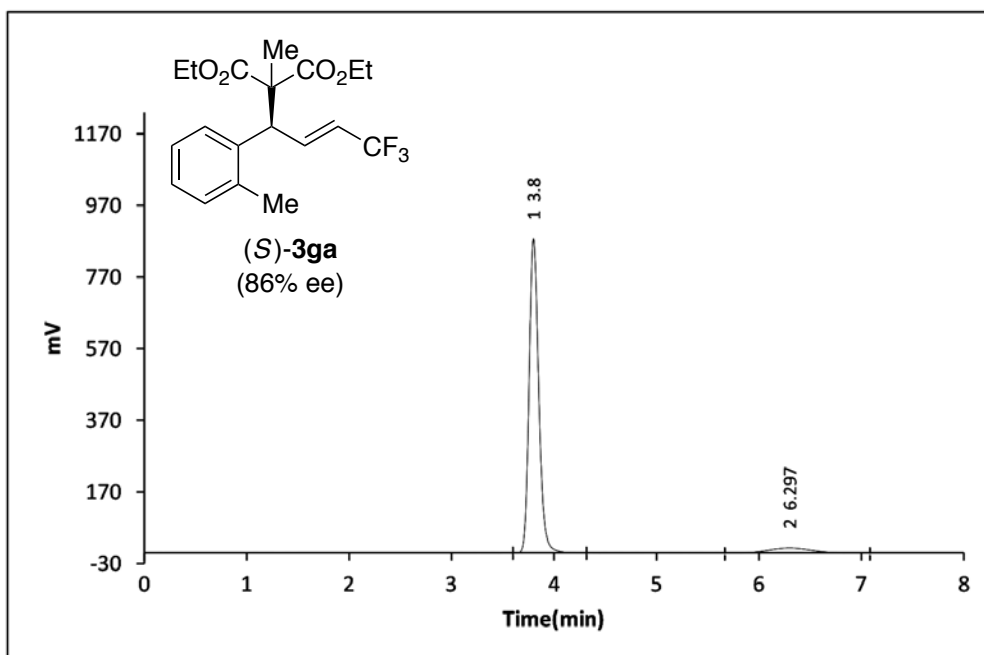
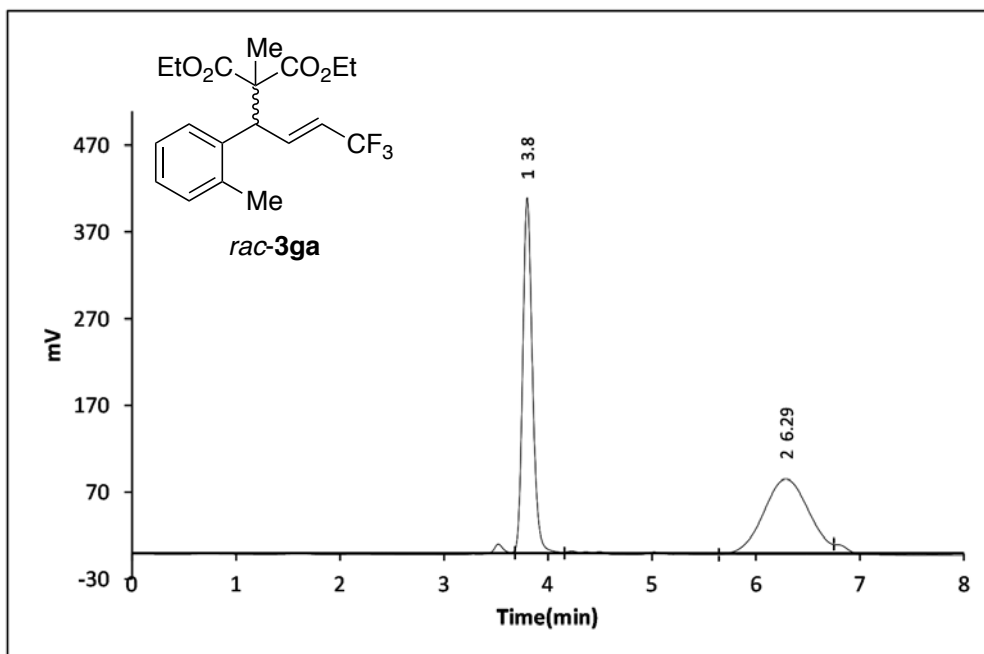


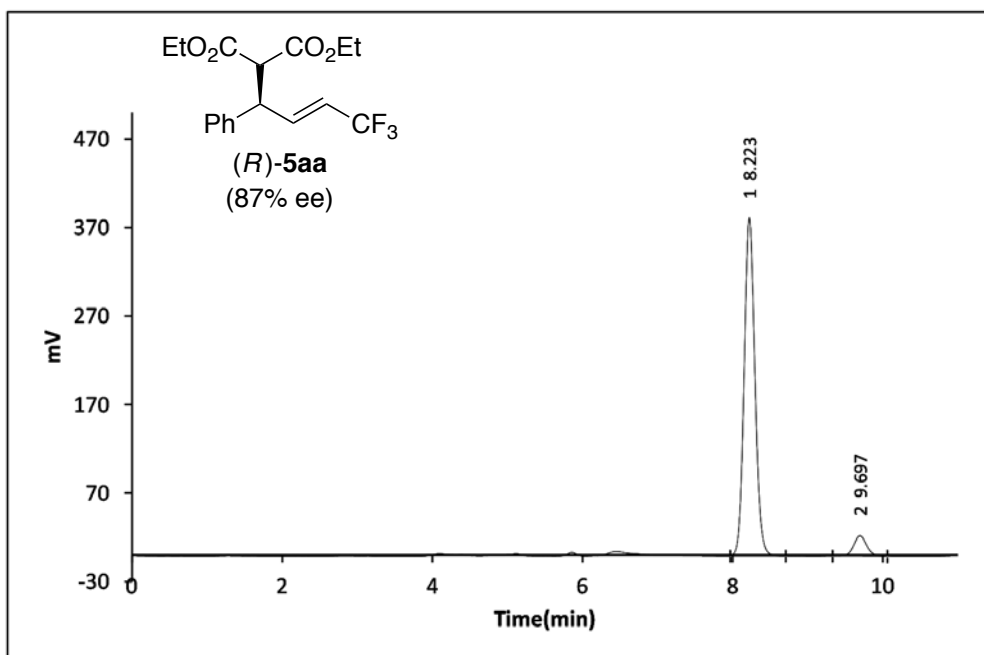
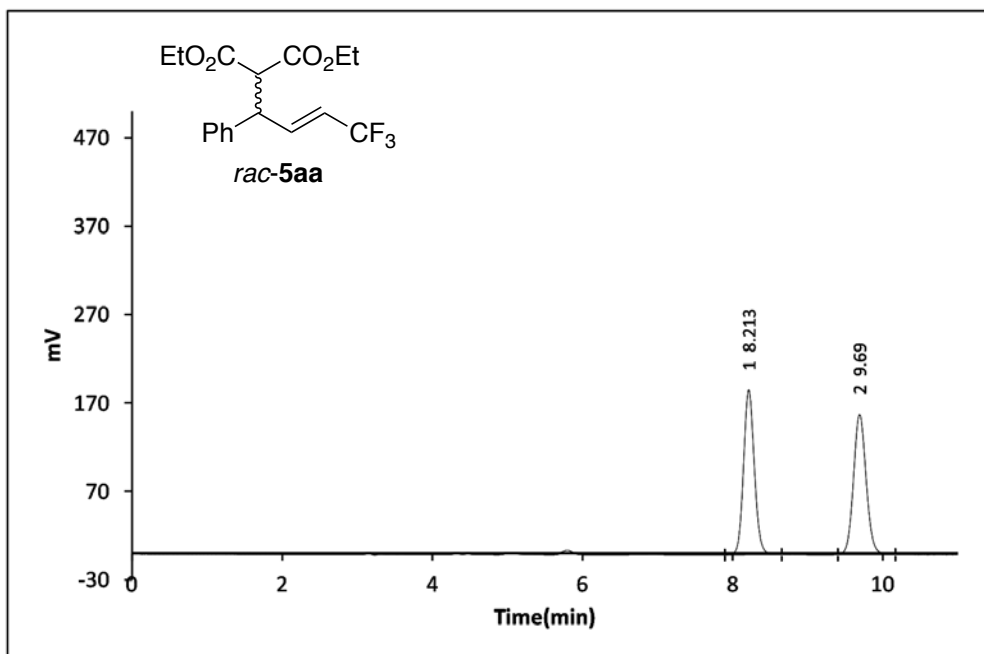


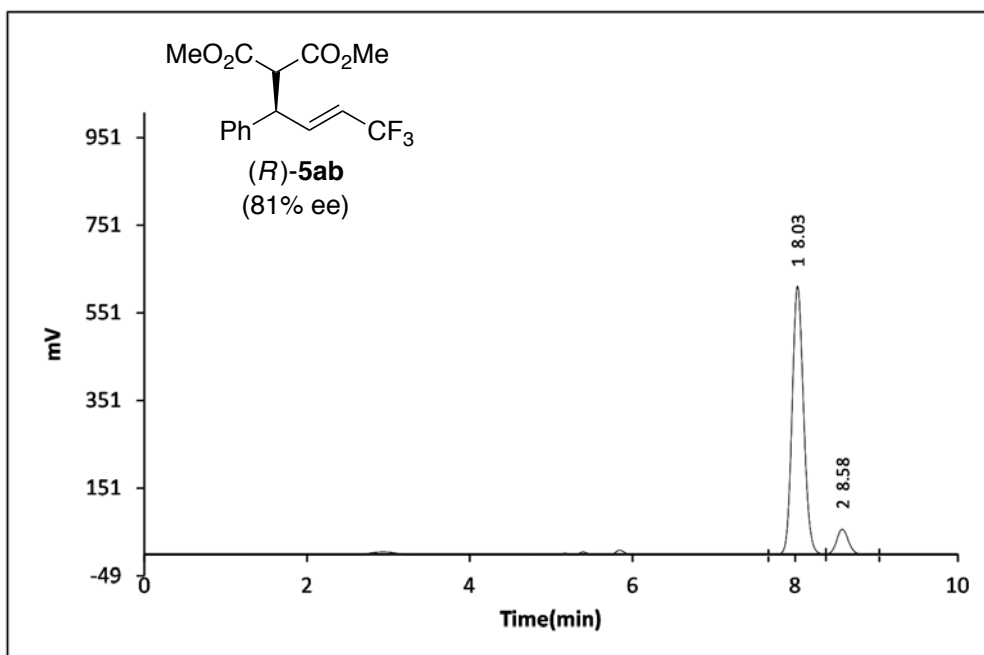
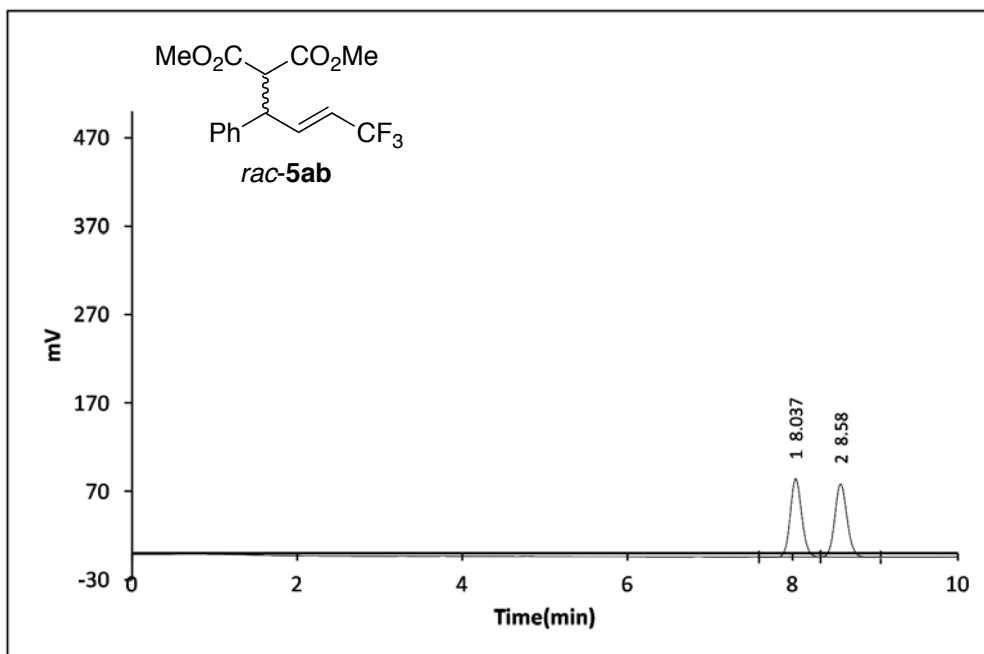


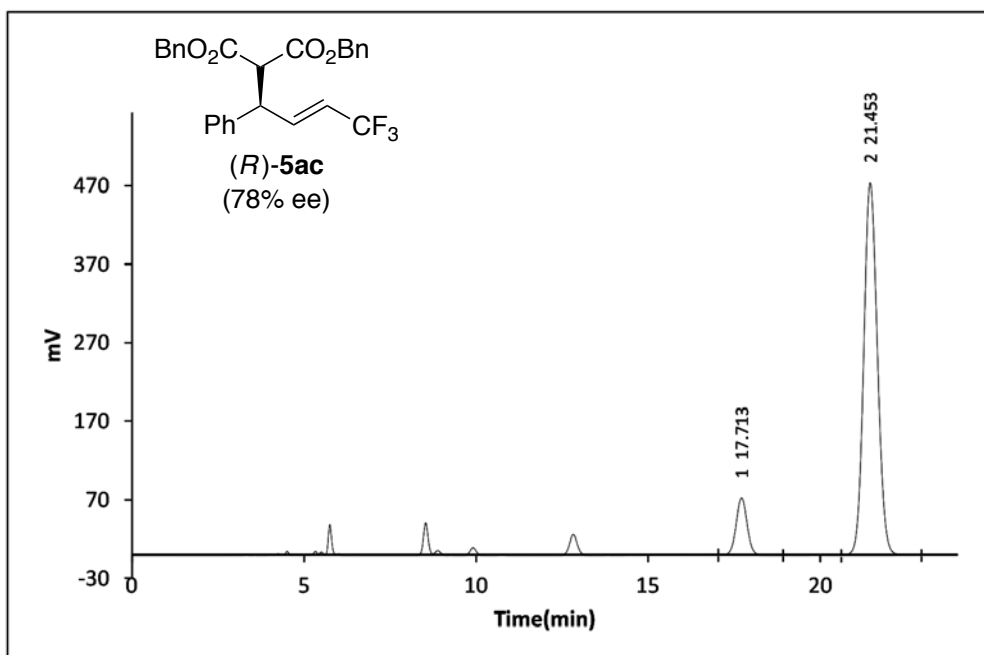
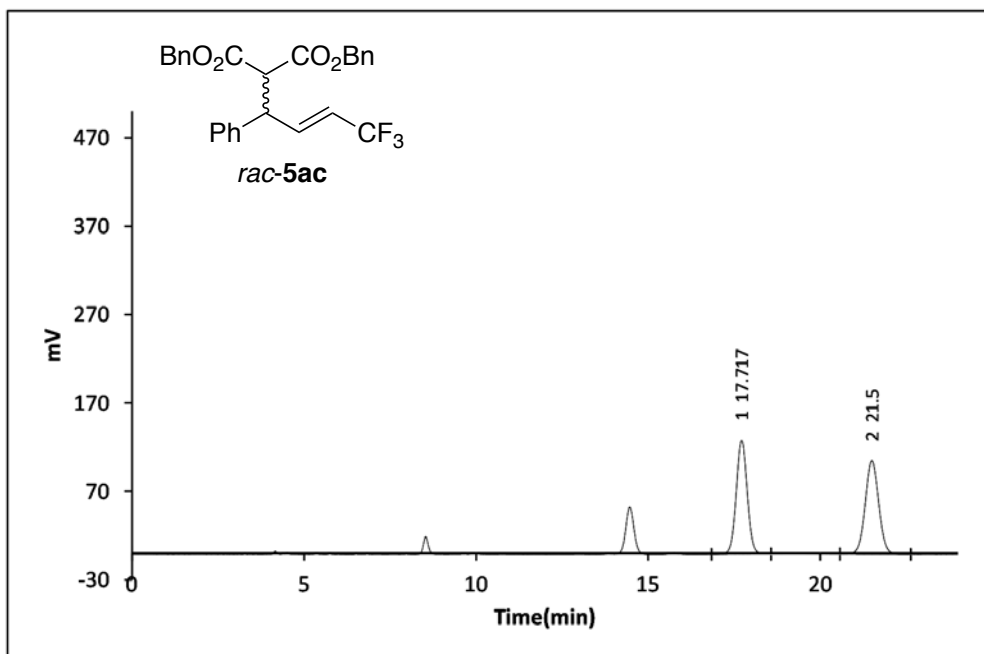


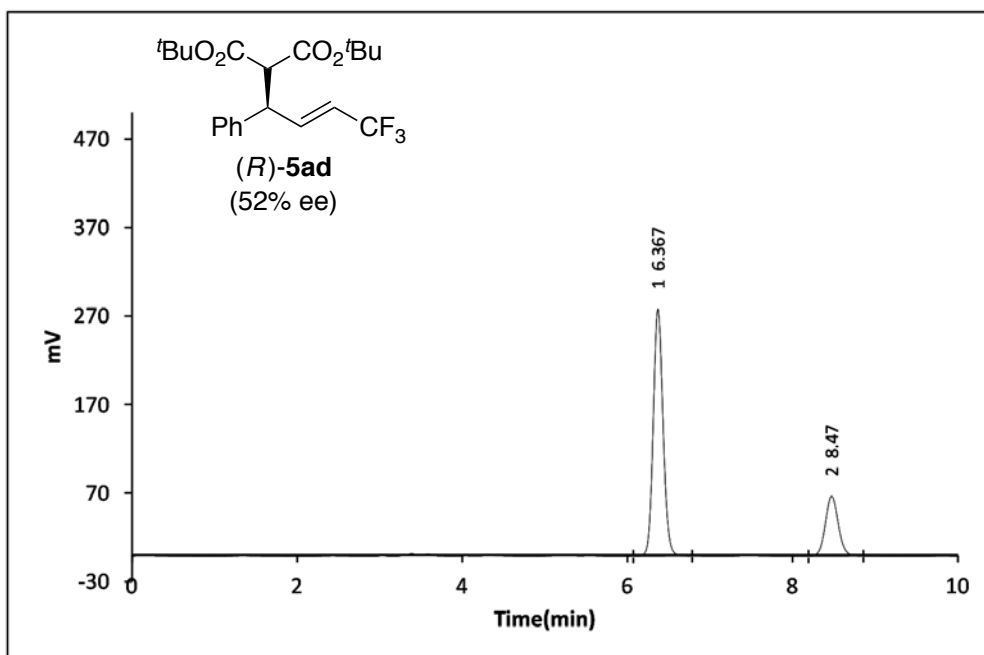
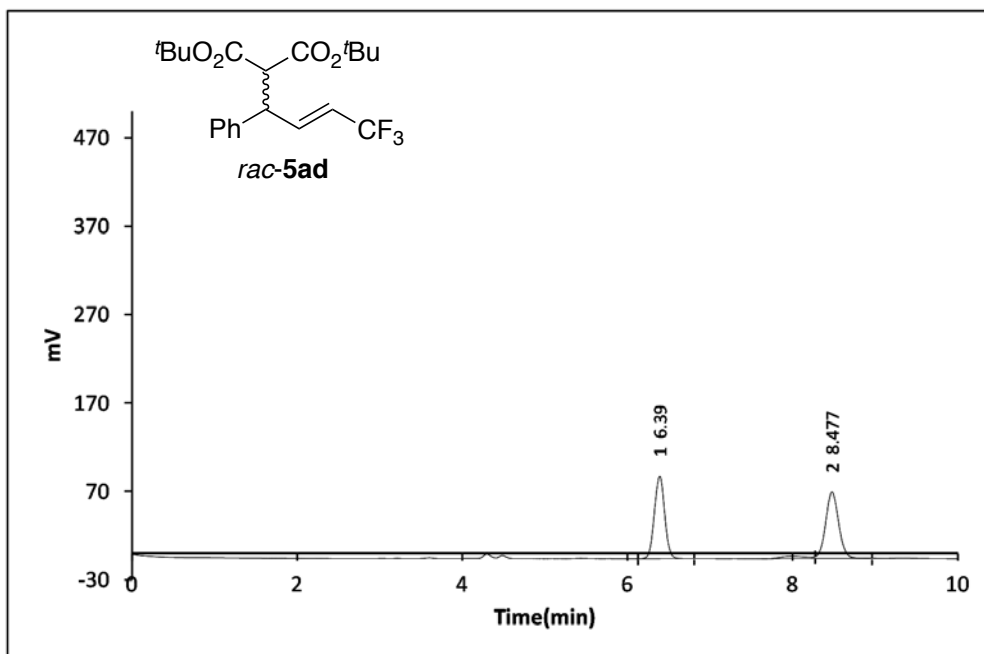


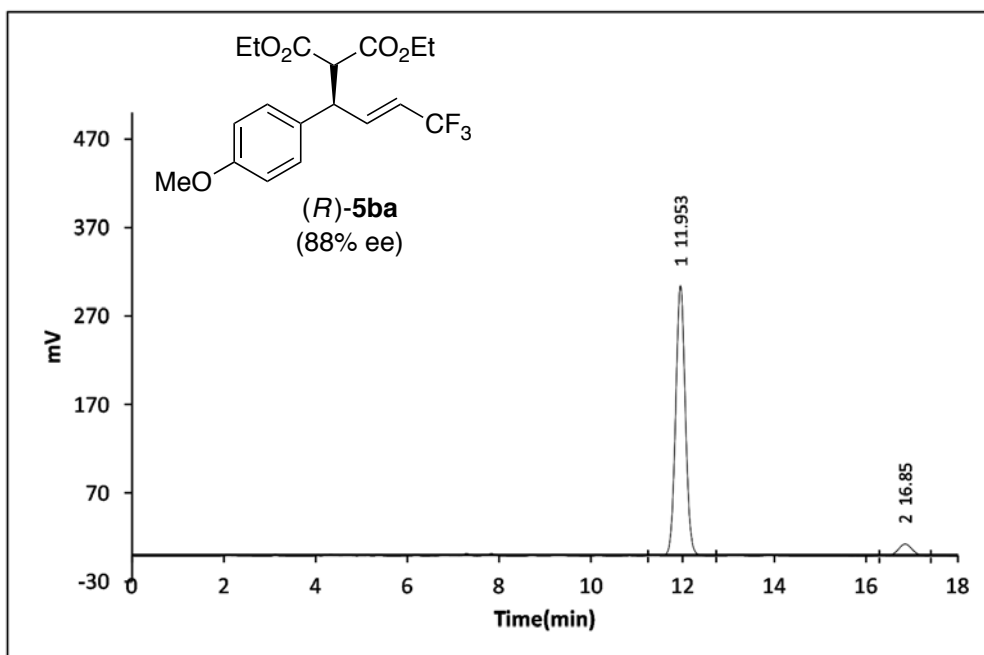
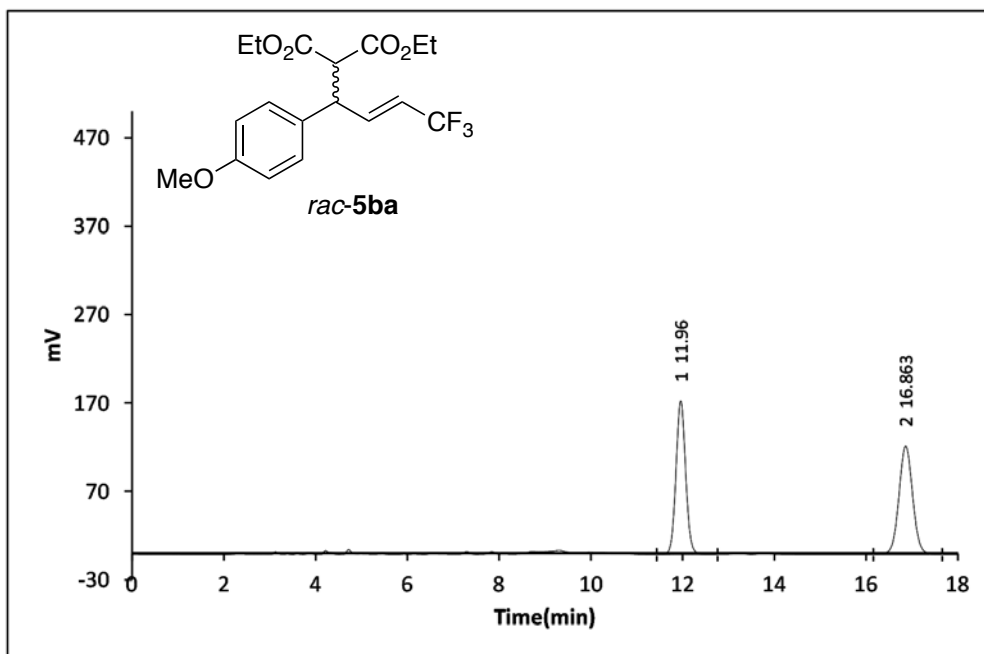


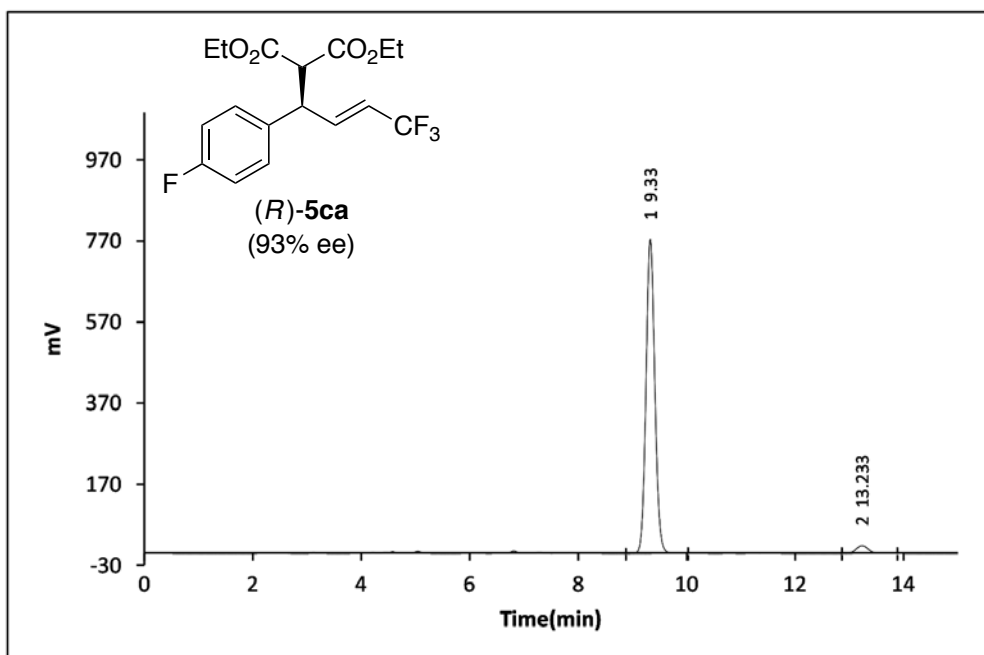
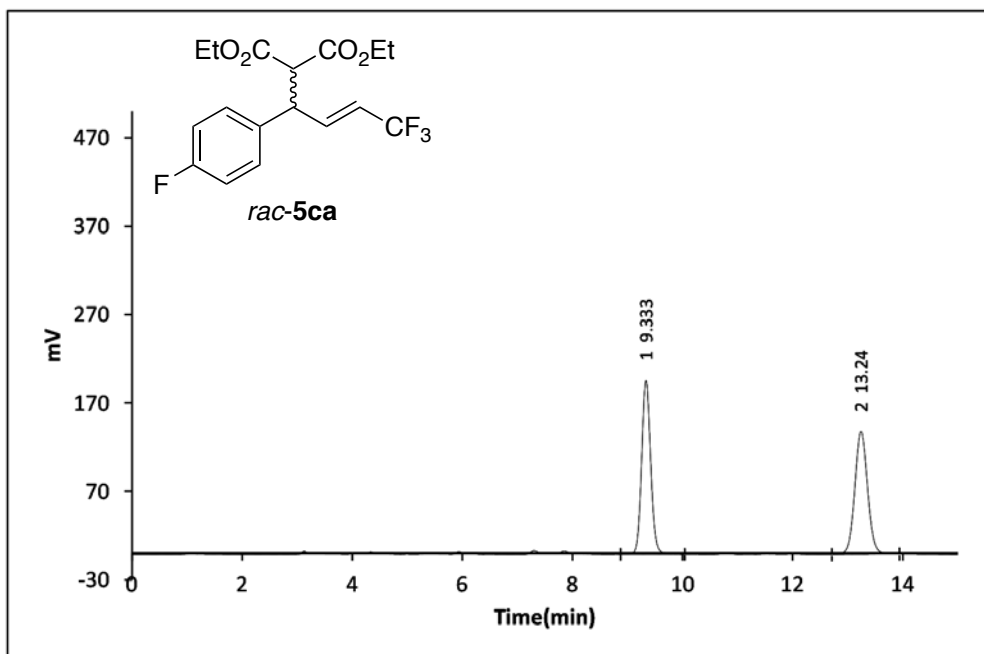


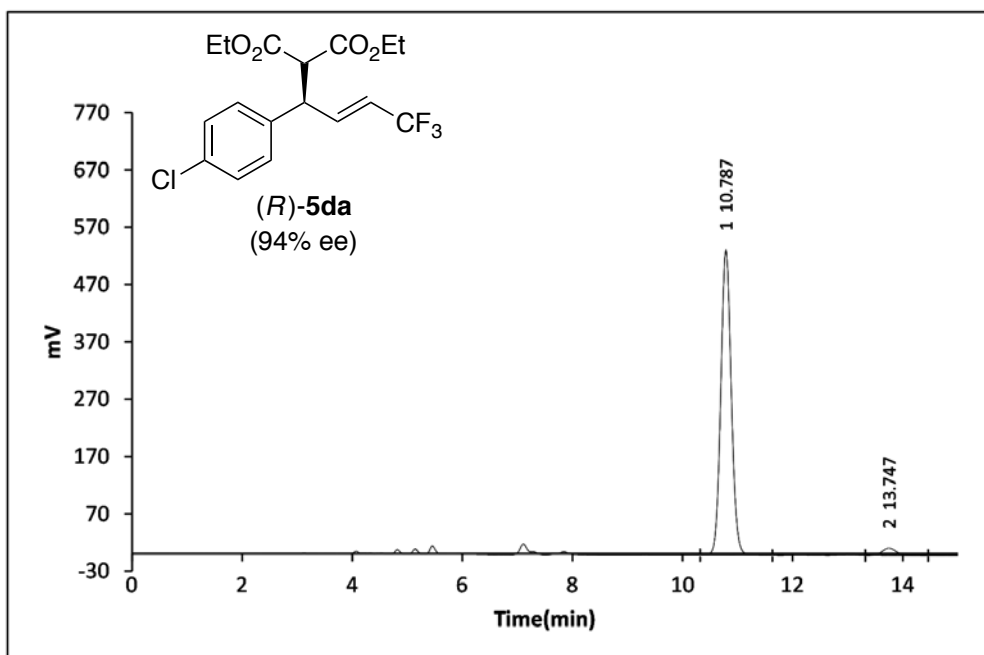
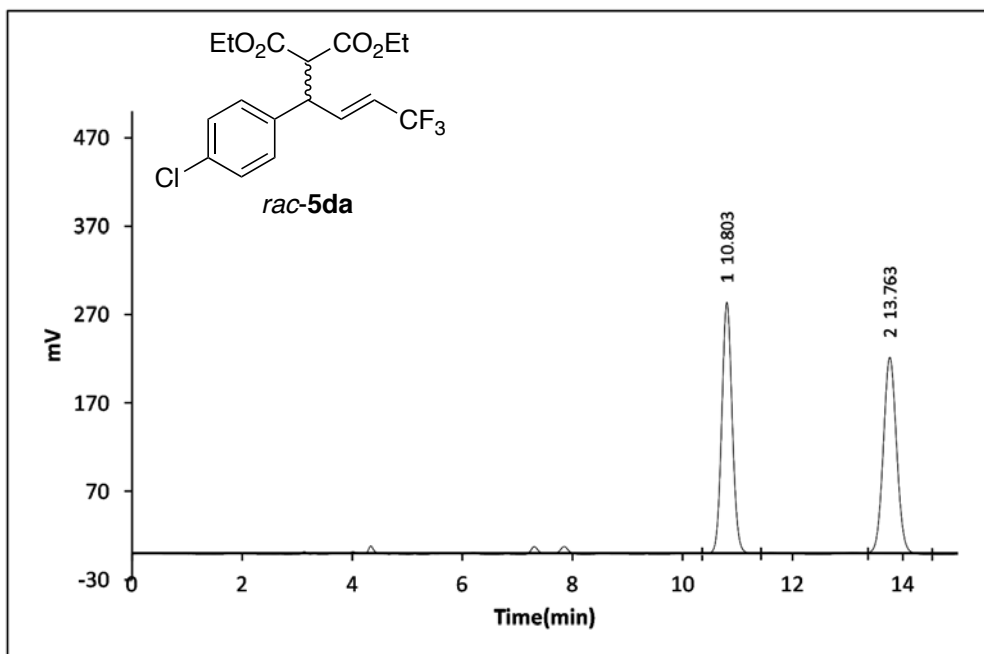


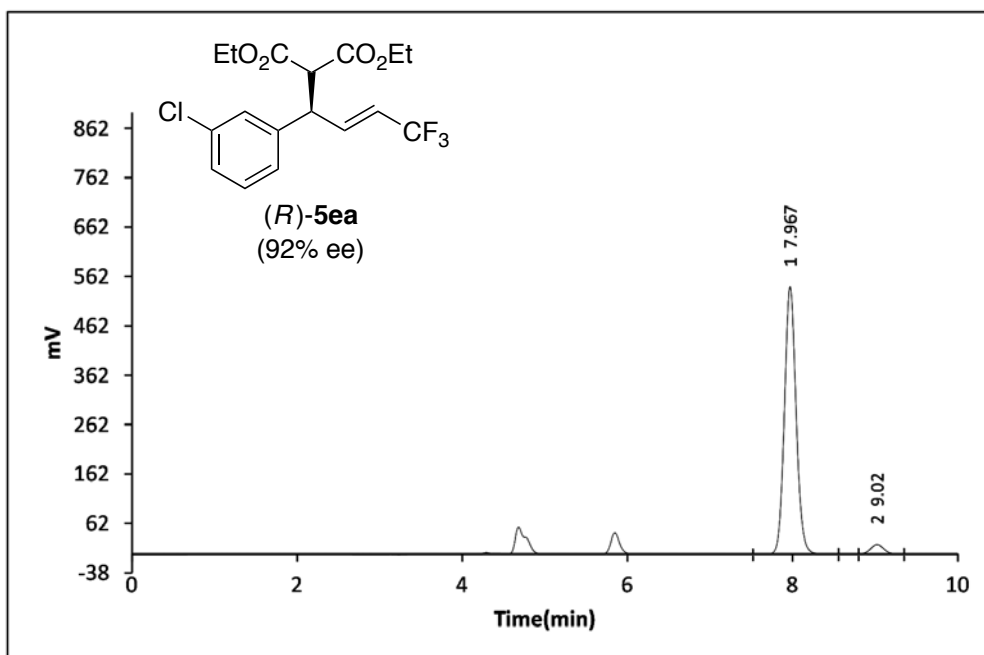
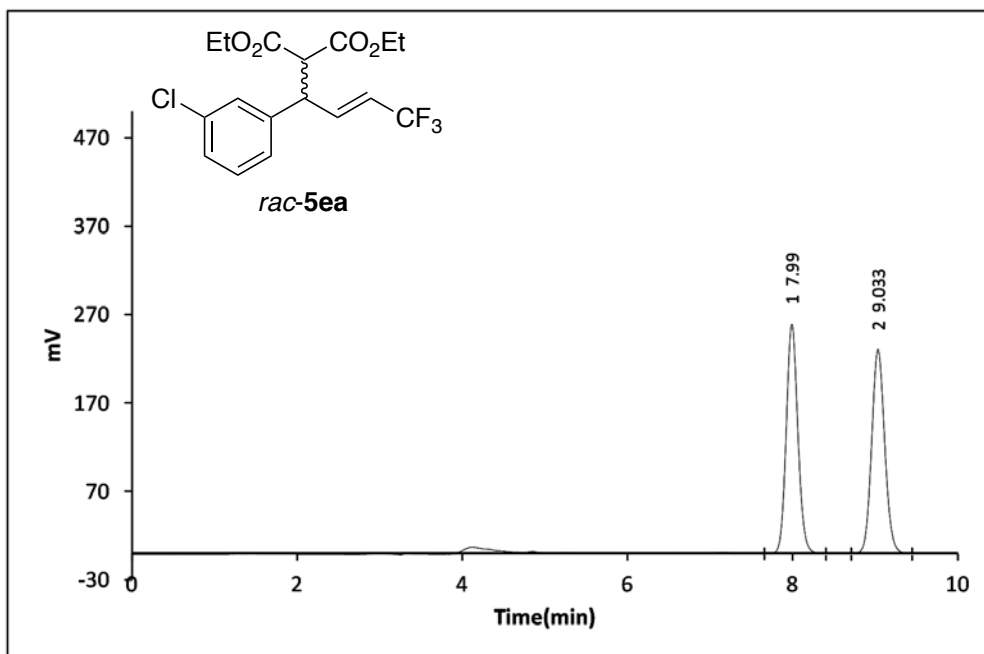


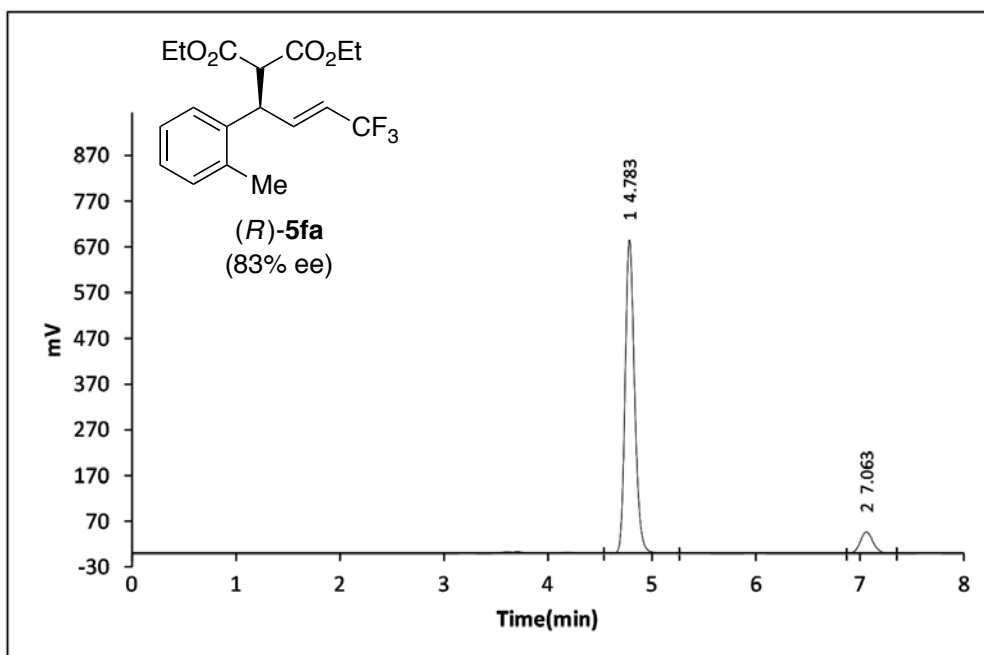
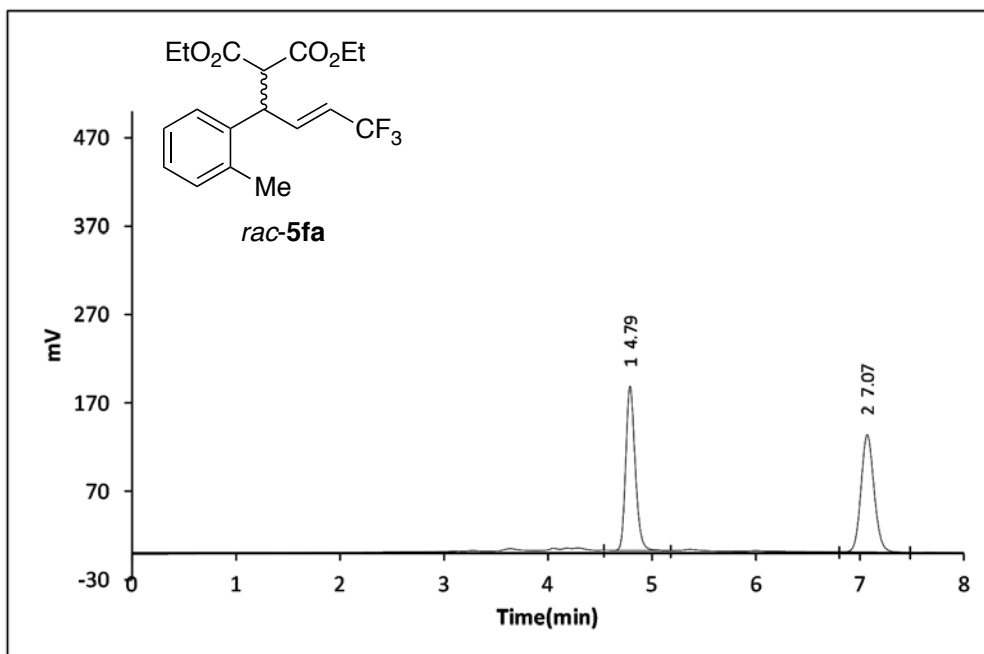


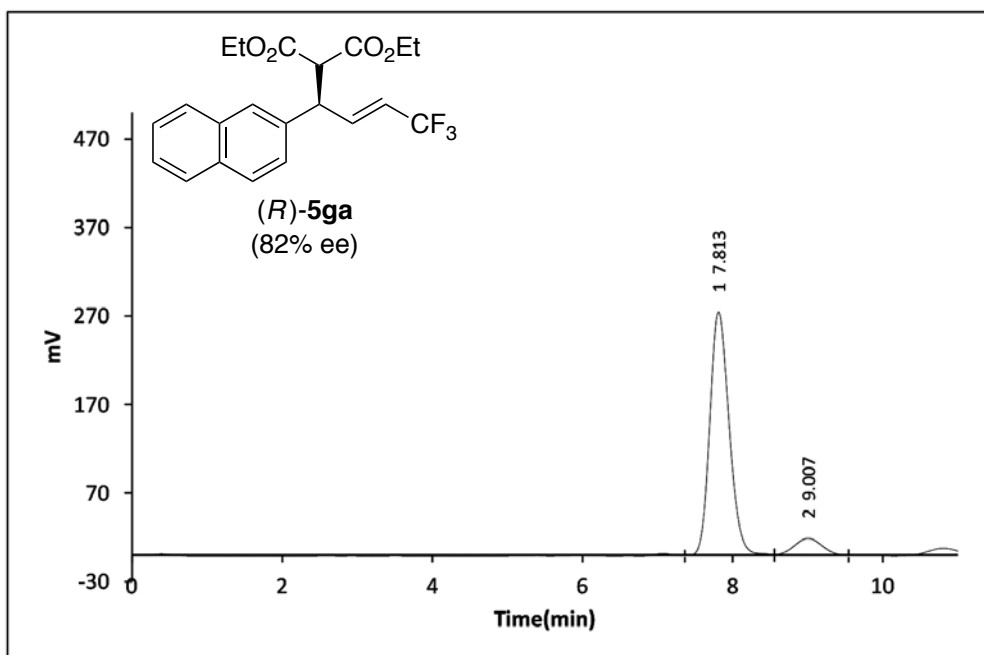
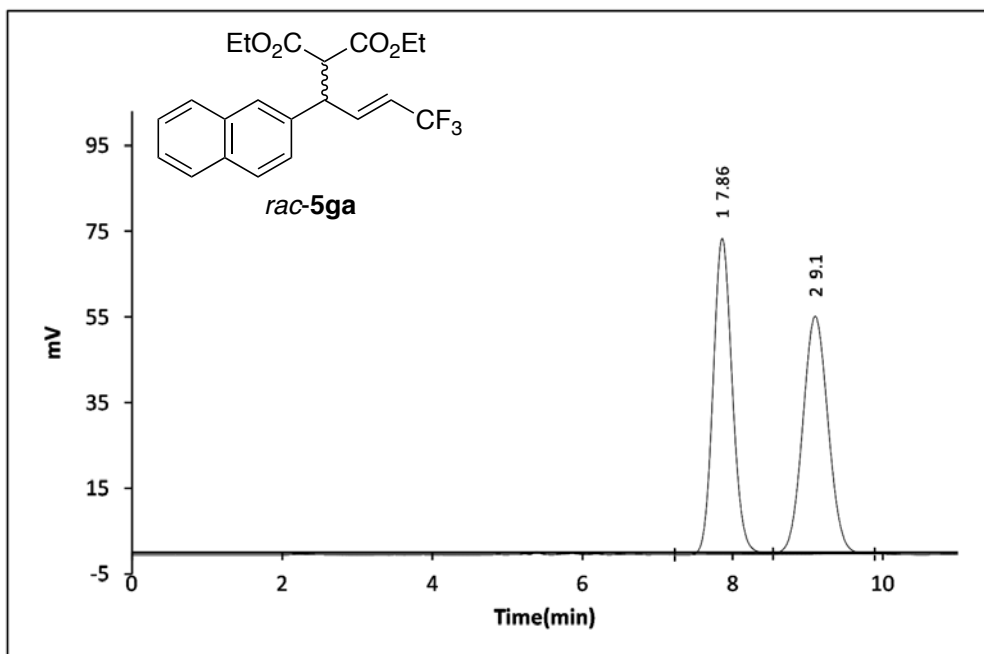


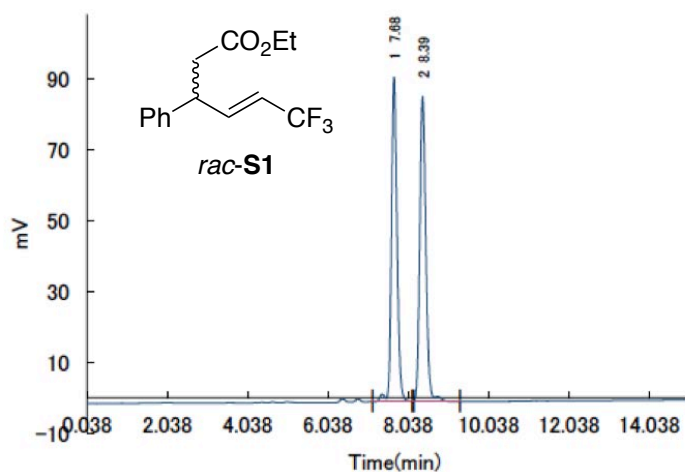






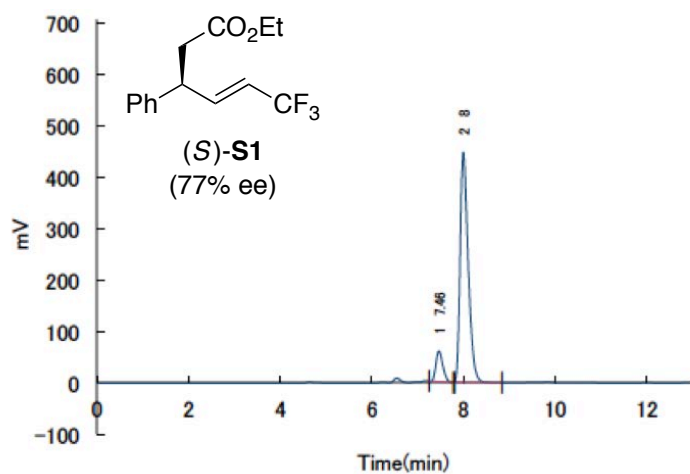






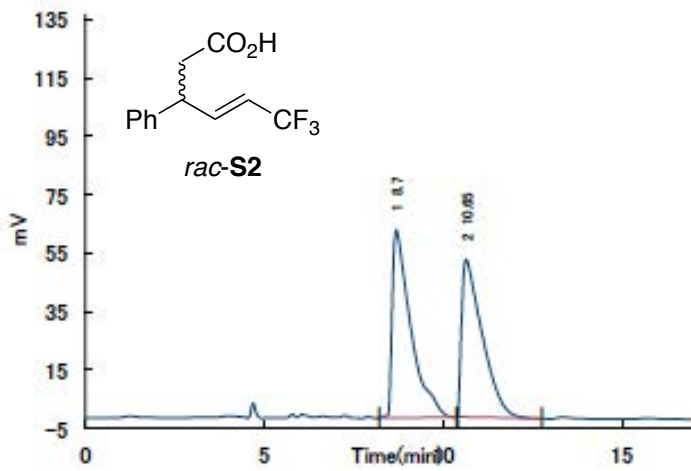
comment AD-H, H/i-PrOH=49/1, 0.7mL/min, 215nm

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	7.68		892238.4	49.5832	91343	---	14033.6	1.169	2.628
2	8.39		907239.8	50.4168	85895	---	14283.4	1.165	---
			1799478.2	100	177238				



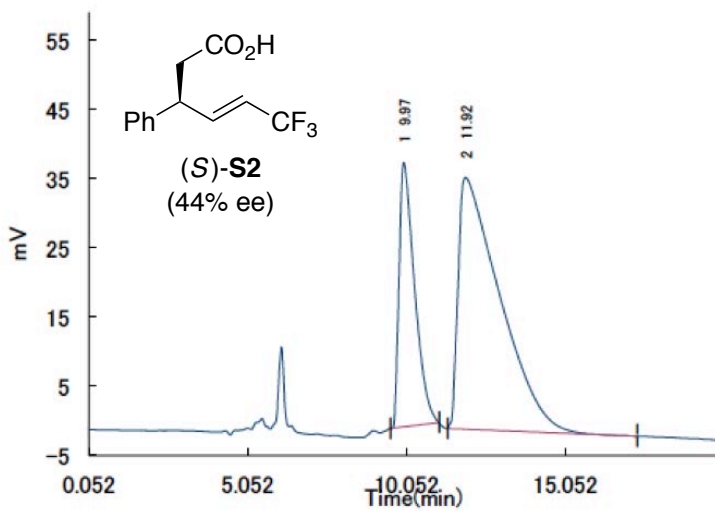
comment AD-H, H/i-PrOH=49/1, 0.7mL/min, 215nm

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	7.46		616662.2	10.1465	58954	---	11086.1	1.269	1.726
2	8		5460906.4	89.8535	448619	---	9154.2	1.419	---
			6077568.6	100	507573				



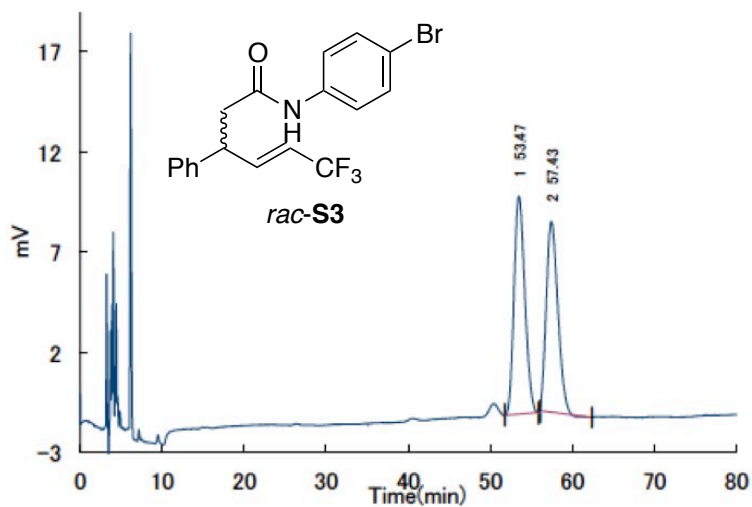
comment AD-H, H/i-PrOH=9/1, 0.7mL/min, 215nm

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	8.7		2314161.4	51.7283	64309	—	977.9	3.423	1.747
2	10.65		2159520	48.2717	53929	—	1436.6	3.004	—
			4473681.4	100	118238				



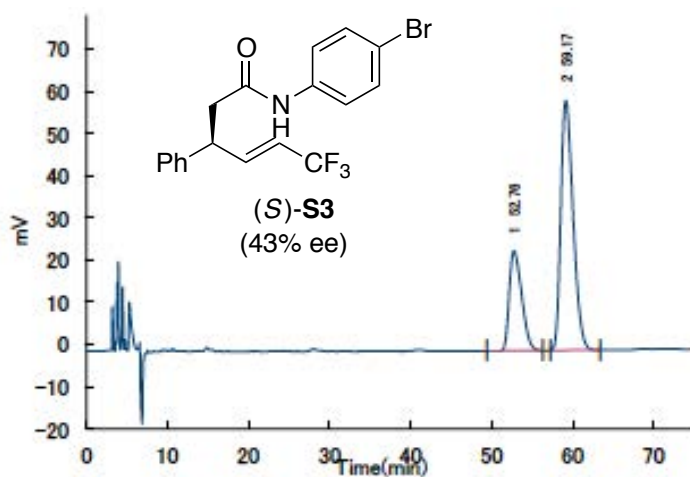
comment AD-H, H/i-PrOH=9/1, 0.7mL/min, 215nm

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	9.97		1294366.3	28.0177	38174	—	1775.4	2.02	1.107
2	11.92		3325453.6	71.9823	36358	—	345.9	3.687	—
			4619819.9	100	74532				



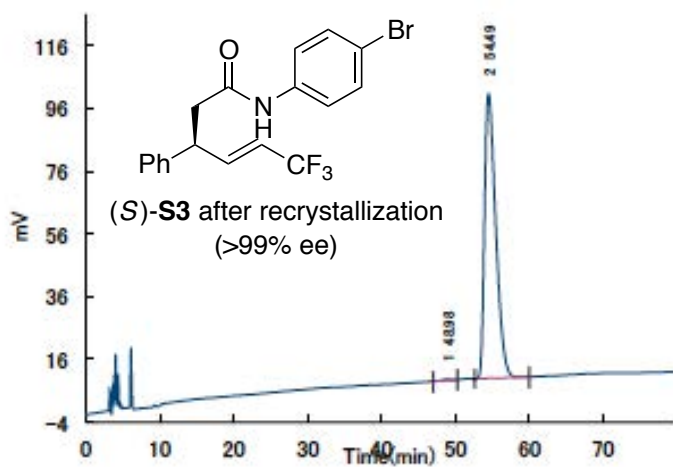
comment AD-H, H/i-PrOH=19/1, 1.0mL/min, 215nm

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	53.47		991779.8	51.5716	10880	—	7576.4	1.193	1.552
2	57.43		931331.6	48.4284	9528	—	7537.8	1.248	—
			1923111.4	100	20408				



comment AD-H, H/i-PrOH=19/1, 1.0mL/min, 215nm

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	52.76		2501024.2	28.6156	23616	—	5700	1.443	2.277
2	59.17		6239036.9	71.3844	59188	—	6989.9	1.364	—
			8740061.1	100	82804				



comment AD-H, H/i-PrOH=19/1, 1.0mL/min, 215nm

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	48.98		27670.2	0.2892	331	—	8709.7	0.824	2.23
2	54.49		9540997.5	99.7108	90655	—	5884.8	1.611	—
			9568667.7	100	90986				