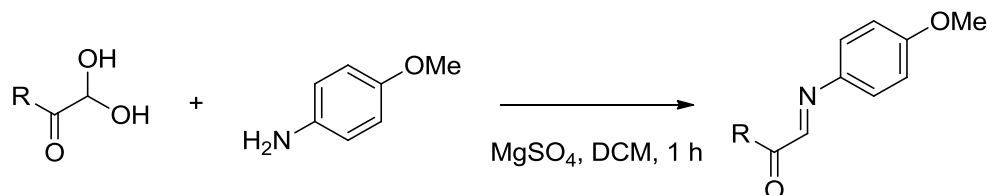


Preparation of Trifluoromethyl-Substituted Aziridines with in situ Generated CF_3CHN_2

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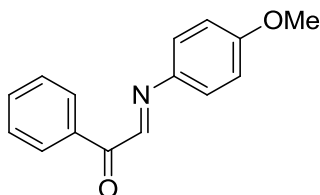
General. All reactions were carried out under an atmosphere of Ar. For flash chromatography technical grade solvents were used, which were distilled prior to use. Chromatographic purification was performed as flash chromatography using Brunschwig silica 32-63, 60Å, using hexane / ethyl acetate as eluent with 0.3-0.5 bar pressure. TLC was performed on Merck silica gel 60 F254 TLC glass plates and visualized with UV light and cerium ammonium molybdate stain. ^1H -NMR spectra were recorded on a VARIAN Mercury 300 MHz spectrometer in chloroform-d, all signals are reported in ppm with the internal chloroform signal at 7.26 ppm. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad signal, coupling constant(s) in Hz, integration). ^{13}C -NMR spectra were recorded with ^1H -decoupling on a Bruker 100 MHz spectrometer in chloroform-d, all signals are reported in ppm with the internal chloroform signal at 77.0 ppm as standard. Infrared spectra were recorded neat on a Perkin-Elmer spectrum RX-I FT-IR spectrometer. The data is reported as absorption maxima (ν , cm^{-1}). Mass spectrometric measurements were performed by the mass spectrometry service of the LOC at the ETHZ on a VG-TRIBRID for electron impact ionization (EI) and on a Varian IonSpec for electron spray ionization (ESI). Chemicals were purchased from commercial suppliers and used without further purification if not noted otherwise.

General procedure for imine condensation:



Arylglyoxals were produced according to known procedures^{1,2,3,4,5} or purchased from commercial sources. MgSO_4 (10 g) was suspended in 50 mL CH_2Cl_2 . Then, the corresponding arylglyoxal monohydrate (11 mmol) and *p*-anisidine (11 mmol) were added in one portion to the stirred suspension. After 1 h the suspension was filtered, and the solvent was evaporated under reduced pressure to give the desired product (quantitative yield). The crude product was used without further purification.

(*E*)-2-((4-methoxyphenyl)imino)-1-phenylethanone (3a)



The title compound was obtained in quantitative yield as a brown solid following the general procedure for condensation.

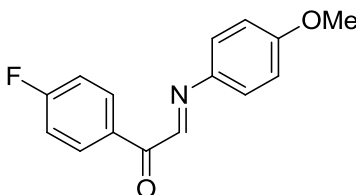
¹H-NMR (300 MHz, CDCl₃): δ = 8.36 (s, 1H), 8.32 – 8.26 (m, 2H), 7.66 – 7.57 (m, 1H), 7.55 – 7.46 (m, 2H), 7.44 – 7.36 (m, 2H), 7.01 – 6.94 (m, 2H), 3.86 (s, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 190.9, 160.6, 154.2, 141.7, 135.5, 133.4, 130.6, 128.3, 123.5, 114.7, 55.6.

HRMS (ESI): calcd for C₁₅H₁₄NO₂⁺ ([M+H]⁺) 240.1019, found 240.1016.

IR (neat): 3061, 2837, 1649, 1574, 1503, 1245, 1024, 829 cm⁻¹.

(*E*)-1-(4-fluorophenyl)-2-((4-methoxyphenyl)imino)ethanone (3b)



The title compound was obtained in quantitative yield as a green solid following the general procedure for condensation.

¹H-NMR (300 MHz, CDCl₃): δ = 8.43 – 8.35 (m, 2H), 8.31 (s, 1H), 7.44 – 7.36 (m, 2H), 7.22 – 7.11 (m, 2H), 7.01 – 6.92 (m, 2H), 3.86 (s, 3H).

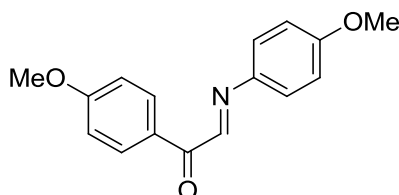
¹³C-NMR (100 MHz, CDCl₃): δ = 189.2, 166.0 (d, *J* = 255.5 Hz), 160.7, 154.1, 141.4, 133.5 (d, *J* = 9.3 Hz), 131.8 (d, *J* = 3.0 Hz), 123.6, 115.5 (d, *J* = 21.7 Hz), 114.7, 55.6.

¹⁹F-NMR (282 MHz, CDCl₃): δ = -104.12 (m).

HRMS (ESI): calcd for C₁₅H₁₃FNO₂⁺ ([M+H]⁺) 258.0925, found 258.0924.

IR (neat): 1694, 1651, 1598, 1581, 1504, 1229, 1158, 824 cm⁻¹.

(E)-1-(4-methoxyphenyl)-2-((4-methoxyphenyl)imino)ethanone (3c)



The title compound was obtained in quantitative yield as a red-brown solid following the general procedure for condensation.

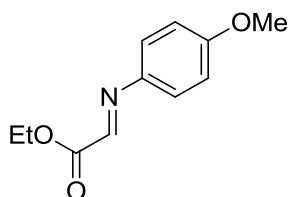
¹H-NMR (300 MHz, CDCl₃): δ = 8.39 – 8.33 (m, 2H), 8.33 (s, 1H), 7.42 – 7.35 (m, 2H), 7.02 – 6.90 (m, 4H), 3.90 (s, 3H), 3.86 (s, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 189.0, 164.0, 160.4, 154.8, 141.9, 133.1, 128.4, 123.4, 114.6, 113.7, 55.6, 55.5.

HRMS (ESI): calcd for C₁₆H₁₆NO₃⁺ ([M+H]⁺) 270.1125, found 270.1121.

IR (neat): 2935, 2838, 1648, 1596, 1504, 1244, 1021, 822 cm⁻¹.

(E)-ethyl 2-((4-methoxyphenyl)imino)acetate (3d)



The title compound was obtained in quantitative yield as an oil following the general procedure for condensation.

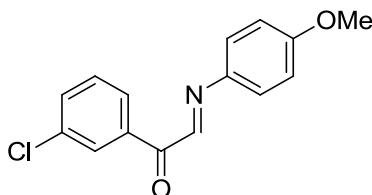
¹H-NMR (300 MHz, CDCl₃): δ = 7.93 (s, 1H), 7.40 – 7.31 (m, 2H), 6.98 – 6.86 (m, 2H), 4.41 (q, J = 7.1 Hz, 2H), 3.84 (s, 1H), 1.41 (t, J = 7.1 Hz, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 163.6, 160.5, 148.0, 141.4, 123.6, 114.5, 61.9, 55.5, 14.2.

HRMS (ESI): calcd for C₁₁H₁₄NO₃⁺ ([M+H]⁺) 208.0968, found 208.0973.

IR (neat): 2979, 2836, 1730, 1508, 1244, 1027, 831 cm⁻¹.

(E)-1-(3-chlorophenyl)-2-((4-methoxyphenyl)imino)ethanone (3e)



The title compound was obtained in quantitative yield as a green solid following the general procedure for condensation.

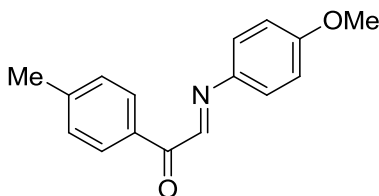
¹H-NMR (300 MHz, CDCl₃): δ = 8.31 (s, 1H), 8.31 – 8.29 (m, 1H), 8.20 (ddd, J = 7.8, 1.6, 1.1 Hz, 1H), 7.58 (ddd, J = 8.0, 2.1, 1.1 Hz, 1H), 7.47 – 7.38 (m, 3H), 7.02 – 6.93 (m, 2H), 3.87 (s, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 189.5, 160.9, 153.6, 141.3, 137.0, 134.5, 133.2, 130.7, 129.6, 128.8, 123.7, 114.7, 55.6.

HRMS (ESI): calcd for C₁₅H₁₃ClNO₂⁺ ([M+H]⁺) 274.0629, found 274.0625.

IR (neat): 3087, 3000, 2949, 2839, 1641, 1561, 1505, 1250, 1163, 827 cm⁻¹.

(E)-2-((4-methoxyphenyl)imino)-1-(p-tolyl)ethanone (3f)



The title compound was obtained in quantitative yield as a brown solid following the general procedure for condensation.

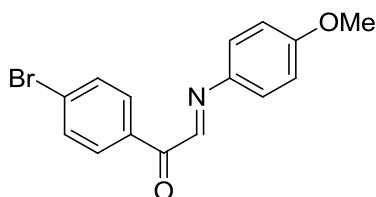
¹H-NMR (300 MHz, CDCl₃): δ = 8.35 (s, 1H), 8.23 – 8.18 (m, 2H), 7.44 – 7.35 (m, 2H), 7.33 – 7.27 (m, 2H), 7.01 – 6.91 (m, 2H), 3.86 (s, 3H), 2.44 (s, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 190.4, 160.4, 154.4, 144.4, 141.8, 133.0, 130.7, 129.1, 123.5, 114.6, 55.6, 21.8.

HRMS (EI/ESI): calcd for C₁₆H₁₆NO₂⁺ ([M+H]⁺) 254.1176, found 254.1172.

IR (neat): 2934, 2836, 1648, 1602, 1503, 1243, 1027, 822 cm⁻¹.

(E)-1-(4-bromophenyl)-2-((4-methoxyphenyl)imino)ethanone (3g)



The title compound was obtained in quantitative yield as a green solid following the general procedure for condensation.

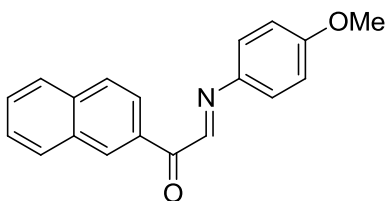
¹H-NMR (300 MHz, CDCl₃): δ = 8.30 (s, 1H), 8.25 – 8.14 (m, 2H), 7.66 – 7.60 (m, 2H), 7.44 – 7.35 (m, 2H), 7.01 – 6.92 (m, 2H), 3.86 (s, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 189.9, 160.8, 153.8, 141.3, 134.2, 132.2, 131.6, 128.7, 123.7, 114.7, 55.6.

HRMS (ESI): calcd for C₁₅H₁₃BrNO₂ ([M+H]⁺) 318.0124, found 318.0128.

IR (neat): 1650, 1582, 1504, 1256, 823 cm⁻¹.

(E)-2-((4-methoxyphenyl)imino)-1-(naphthalen-1-yl)ethanone (3h)



The title compound was obtained in quantitative yield as a green solid following the general procedure for condensation.

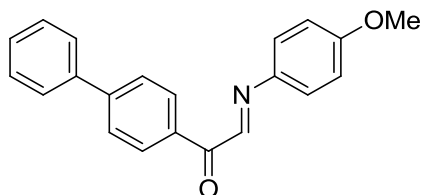
¹H-NMR (300 MHz, CDCl₃): δ = 8.98 (s, 1H), 8.46 (s, 1H), 8.26 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.04 – 7.85 (m, 3H), 7.59 (dddd, *J* = 19.1, 8.2, 6.9, 1.4 Hz, 2H), 7.49 – 7.42 (m, 2H), 7.03 – 6.96 (m, 2H), 3.88 (s, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 190.6, 160.6, 154.4, 141.8, 135.8, 133.3, 132.8, 132.4, 130.0, 128.7, 128.2, 127.8, 126.7, 125.6, 123.6, 114.7, 55.6.

HRMS (ESI): calcd for C₁₉H₁₆NO₂⁺ ([M+H]⁺) 290.1176, found 290.1169.

IR (neat): 3048, 1652, 1574, 1504, 1258, 811 cm⁻¹.

(*E*)-1-([1,1'-biphenyl]-4-yl)-2-((4-methoxyphenyl)imino)ethanone (3i)



The title compound was obtained in quantitative yield as an orange solid following the general procedure for condensation.

¹H-NMR (300 MHz, CDCl₃): δ = 8.40 (s, 1H), 8.37 (s, 2H), 7.77 – 7.57 (m, 4H), 7.54 – 7.34 (m, 5H), 7.04 – 6.92 (m, 2H), 3.86 (s, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 190.4, 160.6, 154.4, 146.1, 141.7, 140.0, 134.2, 131.2, 129.0, 128.3, 127.3, 127.0, 123.6, 114.7, 55.6.

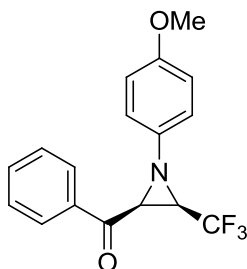
HRMS (ESI): calcd for C₂₁H₁₈NO₂⁺ ([M+H]⁺) 316.1332, found 316.1333.

IR (neat): 3003, 1645, 1592, 1574, 1502, 1246, 833 cm⁻¹.

General procedure for aziridination:

To a mixture of 7.5 mL CH₂Cl₂ and 0.25 mL H₂O cooled to 0 °C was added trifluoroethylamine hydrochloride (203 mg, 1.5 mmol) and NaNO₂ (124 mg, 1.8 mmol). After being stirred at this temperature for 1 h, the reaction mixture was cooled to -78 °C. Then, after 20-25 min the appropriate imine (0.5 mmol) and BF₃·OEt₂ (111 µL, 0.9 mmol) were added consecutively. After the indicated time, the reaction was quenched with MeOH and sat. NaHCO₃. The reaction mixture was extracted with CH₂Cl₂ (3x), dried over MgSO₄ and the solvent was evaporated under reduced pressure. The residue was purified by flash column chromatography (hexane/ethyl acetate) to afford the pure *cis*-isomer

((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)(phenyl)methanone (4a)



The title compound was obtained as an amorphous solid (103 mg, 64 %) following the general procedure (dr 17:1).

¹H-NMR (300 MHz, CDCl₃): δ = 8.14 – 8.05 (m, 2H), 7.66 – 7.57 (m, 1H), 7.54 – 7.41 (m, 2H), 7.07 – 6.97 (m, 2H), 6.89 – 6.76 (m, 2H), 3.77 (s, 3H), 3.60 (d, *J* = 6.6 Hz, 1H), 3.14 (dq, *J* = 6.7, 5.6 Hz, 1H).

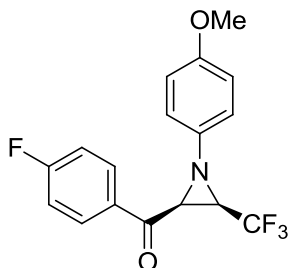
¹³C-NMR (100 MHz, CDCl₃): δ = 190.5, 156.6, 143.5, 135.2, 134.1, 128.8, 128.7, 123.3 (q, *J* = 274.7 Hz), 120.7, 114.7, 55.5, 45.7, 44.4 (q, *J* = 40.2 Hz).

¹⁹F-NMR (282 MHz, CDCl₃): δ = -67.7 (d, *J* = 5.4 Hz).

HRMS (EI): calcd for C₁₇H₁₄F₃NO₂⁺ (*M*⁺) 321.0977, found 321.0972.

IR (neat): 2957, 2837, 2359, 1692, 1597, 1240, 1142 cm⁻¹.

(4-fluorophenyl)((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)methanone (4b)



The title compound was obtained as an amorphous solid (132 mg, 78 %) following the general procedure for aziridination (dr 19:1).

¹H-NMR (300 MHz, CDCl₃): δ = 8.20 – 8.12 (m, 2H), 7.22 – 7.10 (m, 2H), 7.06 – 6.98 (m, 2H), 6.90 – 6.78 (m, 2H), 3.79 (s, 3H), 3.54 (d, J = 6.5 Hz, 1H), 3.11 (dq, J = 6.6, 5.5 Hz, 1H).

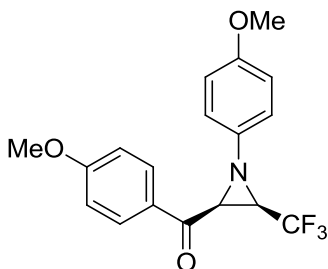
¹³C-NMR (100 MHz, CDCl₃): δ = 189.1, 166.3 (d, J = 256.8 Hz), 156.7, 143.3, 131.7 (d, J = 2.9 Hz), 131.5 (d, J = 9.5 Hz), 123.2 (q, J = 274.6 Hz), 120.7, 116.1 (d, J = 22.0 Hz), 114.7, 55.6, 45.4, 44.3 (q, J = 40.2 Hz).

¹⁹F-NMR (282 MHz, CDCl₃): δ = -67.8 (d, J = 5.5 Hz) , -102.6 (m).

HRMS (ESI): calcd for C₁₇H₁₄F₄NO₂ ([M+H]⁺) 340.0955, found 340.0957.

IR (neat): 3003, 1688, 1595, 1509, 1146 cm⁻¹.

(4-methoxyphenyl)((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)methanone (4c)



The title compound was obtained as an amorphous solid (87 mg, 50 %) following the general procedure for aziridination (dr 12:1).

¹H-NMR (300 MHz, CDCl₃): δ = 8.13 – 8.06 (m, 2H), 7.05 – 6.91 (m, 4H), 6.87 – 6.78 (m, 2H), 3.87 (s, 3H), 3.77 (s, 3H), 3.54 (d, J = 6.7 Hz, 2H), 3.09 (dq, J = 6.3, 5.5 Hz, 1H).

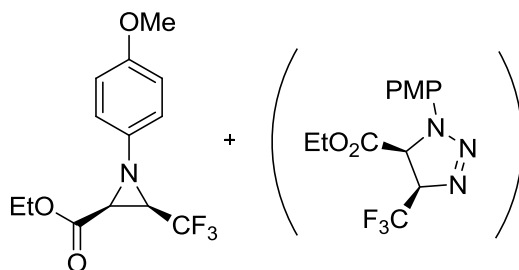
¹³C-NMR (100 MHz, CDCl₃): δ = 188.9, 164.3, 156.6, 143.7, 131.1, 128.4, 123.3 (q, J = 274.8 Hz), 120.7, 114.7, 114.0, 55.57, 55.55, 45.5, 44.3 (q, J = 40.1 Hz).

¹⁹F-NMR (282 MHz, CDCl₃): δ = -67.8 (d, J = 5.3 Hz).

HRMS (ESI): calcd for C₁₈H₁₇F₃NO₃⁺ ([M+H]⁺) 352.1155, found 352.1148.

IR (neat): 1961, 2841, 1681, 1597, 1509, 1241, 1141 cm⁻¹.

(2*SR*,3*RS*)-ethyl 1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-carboxylate (4d)



The title compound was obtained as an oil (104 mg total, 83 % purity (17 % cycloaddition product, designed as minor below), 87 mg, 60%) following the general procedure for aziridination (dr 11:1).

¹H-NMR (300 MHz, CDCl₃): δ = 6.99 – 6.85 (m, 2H), 6.83 – 6.76 (m, 2H), 5.23 (dq, J = 8.5, 7.4 Hz, 1H, minor), 4.56 (d, J = 8.4 Hz, 1H, minor), 4.40 – 4.17 (m, 2H), 3.79 (s, 3H, minor), 3.75 (s, 3H), 3.05 (d, J = 6.6 Hz, 1H), 2.88 (dq, J = 6.6, 5.5 Hz, 1H), 1.31 (t, J = 7.1 Hz, 3H).

¹³C-NMR (100 MHz, CDCl₃): δ = 167.8 (minor), 165.8, 157.0 (minor), 156.6, 143.2, 132.5 (minor), 123.1 (q, J = 274.4 Hz), 120.5, 117.8 (minor), 114.8 (minor), 114.6, 82.1 (q, J = 29.9 Hz, minor), 63.0 (minor), 62.1, 57.9 (minor), 55.5, 43.1 (q, J = 40.8 Hz), 41.4, 13.9.

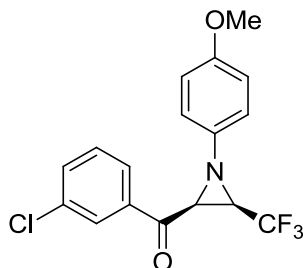
¹⁹F-NMR (282 MHz, CDCl₃): δ = -68.0 (d, J = 5.6 Hz, major), -73.2 (d, J = 7.7 Hz, minor).

HRMS (ESI): calcd for C₁₃H₁₅F₃NO₃⁺ ([M+H]⁺) 290.0999, found 290.1009.

IR (neat): 2986, 2838, 1751, 1508, 1240, 1143 cm⁻¹.

Spectral data in accordance with literature values.⁶

(3-chlorophenyl)((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)methanone (4e)



The title compound was obtained as yellow oil (79 mg, 61 %) following the general procedure for aziridination on a 0.365 mmol scale (dr 16:1).

¹H-NMR (300 MHz, CDCl₃): δ = 8.07 (t, J = 1.7 Hz, 1H), 7.99 (ddd, J = 7.8, 1.6, 1.1 Hz, 1H), 7.59 (ddd, J = 8.0, 2.1, 1.1 Hz, 1H), 7.52 – 7.39 (m, 1H), 7.05 – 6.96 (m, 2H), 6.89 – 6.78 (m, 2H), 3.77 (s, 3H), 3.56 (d, J = 6.6 Hz, 1H), 3.14 (dq, J = 6.7, 5.5 Hz, 1H).

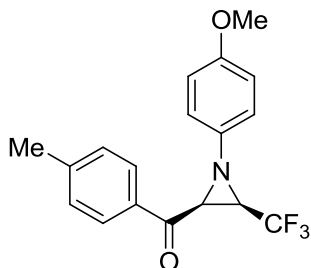
¹³C-NMR (100 MHz, CDCl₃): δ = 189.6, 156.7, 143.2, 136.7, 135.2, 134.1, 130.2, 128.7, 126.8, 123.1 (q, J = 274.7 Hz), 120.7, 114.7, 55.5, 45.5, 44.4 (q, J = 40.2 Hz).

¹⁹F-NMR (282 MHz, CDCl₃): δ = -67.7 (d, J = 5.9 Hz).

HRMS (ESI): calcd for C₁₇H₁₄ClF₃NO₂⁺ ([M+H]⁺) 356.0660, found 356.0647.

IR (neat): 2959, 2837, 1698, 1572, 1508, 1240, 1144 cm⁻¹.

((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)(*p*-tolyl)methanone (4f)



The title compound was obtained as an amorphous solid (100 mg, 60 %) following the general procedure for aziridination (dr 16:1).

¹H-NMR (300 MHz, CDCl₃): δ = 8.05 – 7.96 (m, 2H), 7.35 – 7.21 (m, 2H), 7.08 – 6.94 (m, 2H), 6.91 – 6.77 (m, 2H), 3.77 (s, 3H, major), 3.57 (d, *J* = 6.6 Hz, 1H), 3.12 (dq, *J* = 6.7, 5.6 Hz, 1H), 2.42 (s, 3H).

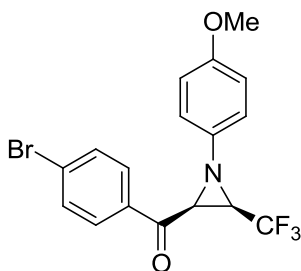
¹³C-NMR (100 MHz, CDCl₃): δ = 190.0, 156.6, 145.2, 143.7, 132.8, 129.5, 128.8, 123.29 (q, *J* = 274.7 Hz), 120.7, 114.6, 55.5, 45.7, 44.4 (q, *J* = 40.1 Hz), 21.8.

¹⁹F-NMR (282 MHz, CDCl₃): δ = -67.8 (d, *J* = 5.7 Hz).

HRMS (ESI): calcd for C₁₈H₁₇F₃NO₂⁺ ([M+H]⁺) 336.1206, found 336.1207.

IR (neat): 2963, 2838, 2360, 1685, 1605, 1508, 1240, 1143 cm⁻¹.

(4-bromophenyl)((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)methanone (4g)



The title compound was obtained as an amorphous solid (94 mg, 47 %) following the general procedure for aziridination (dr 13:1).

¹H-NMR (300 MHz, CDCl₃): δ = 8.01 – 7.93 (m, 2H), 7.69 – 7.56 (m, 2H), 7.06 – 6.95 (m, 2H), 6.90 – 6.78 (m, 2H), 3.78 (s, 3H), 3.53 (d, *J* = 6.6 Hz, 1H), 3.11 (dq, *J* = 6.7, 5.5 Hz, 1H).

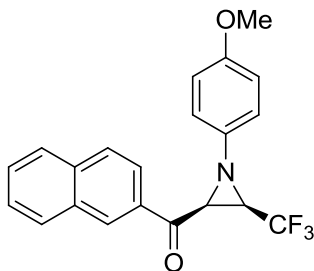
¹³C-NMR (100 MHz, CDCl₃): δ = 189.9, 156.7, 143.2, 134.0, 132.2, 130.2, 129.5, 123.2 (q, *J* = 274.7 Hz), 120.7, 114.7, 55.6, 45.4, 44.4 (q, *J* = 40.1 Hz).

¹⁹F-NMR (282 MHz, CDCl₃): δ = -67.56 (d, *J* = 5.3 Hz).

HRMS (ESI): calcd for C₁₇H₁₄BrF₃NO₂⁺ ([M+H]⁺) 400.0155, found 400.0162.

IR (neat): 1691, 1582, 1508, 1144 cm⁻¹.

((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)(naphthalen-1-yl)methanone (4h)



The title compound was obtained as an amorphous solid (130 mg, 70 %) following the general procedure for aziridination (dr 15:1).

¹H-NMR (300 MHz, CDCl₃): δ = 8.76 – 8.61 (m, 1H), 8.13 (dd, J = 8.6, 1.7 Hz, 1H), 8.03 – 7.84 (m, 3H), 7.60 (dddd, J = 21.2, 8.1, 6.9, 1.3 Hz, 2H), 7.12 – 7.00 (m, 2H), 6.93 – 6.78 (m, 2H), 3.80 (s, 3H), 3.72 (d, J = 6.6 Hz, 1H), 3.22 (dq, J = 6.6, 5.5 Hz, 1H).

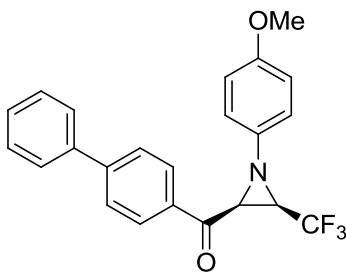
¹³C-NMR (100 MHz, CDCl₃): δ = 190.4, 156.7, 143.6, 136.1, 132.6, 132.4, 131.0, 129.8, 129.1, 128.8, 127.9, 123.3 (q, J = 274.7 Hz), 127.0, 123.8, 120.7, 114.7, 55.6, 45.8, 44.5 (q, J = 40.1 Hz).

¹⁹F-NMR (282 MHz, CDCl₃): δ = -67.65 (d, J = 5.5 Hz).

HRMS (ESI): calcd for C₂₁H₁₇F₃NO₂⁺ ([M+H]⁺) 372.1206, found 372.1197.

IR (neat): 1694, 1624, 1508, 1142 cm⁻¹.

[1,1'-biphenyl]-4-yl((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)methanone (4i)



The title compound was obtained as an amorphous solid (144 mg, 73 %) following the general procedure for aziridination (dr 15:1).

¹H-NMR (300 MHz, CDCl₃): δ = 8.28 – 8.12 (m, 2H), 7.76 – 7.67 (m, 2H), 7.67 – 7.59 (m, 2H), 7.53 – 7.31 (m, 3H), 7.11 – 6.97 (m, 2H), 6.92 – 6.78 (m, 2H), 3.79 (s, 3H), 3.62 (d, J = 6.6 Hz, 1H), 3.22 – 3.05 (m, 1H).

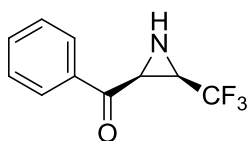
¹³C-NMR (100 MHz, CDCl₃): δ = 190.1, 156.7, 146.8, 143.6, 139.6, 133.9, 129.3, 129.0, 128.5, 127.4, 127.3, 127.2 – 118.8 (m), 120.7, 114.7, 55.6, 45.7, 44.4 (q, J = 40.0 Hz).

¹⁹F-NMR (282 MHz, CDCl₃): δ = -67.51 (d, J = 5.6 Hz).

HRMS (ESI): calcd for C₂₃H₁₉F₃NO₂⁺ ($[M+H]^+$) 398.1362, found 398.1362.

IR (neat): 1682, 1603, 1506, 1143 cm⁻¹.

phenyl((2*SR*,3*RS*)-3-(trifluoromethyl)aziridin-2-yl)methanone (5)



To a solution of ((2*SR*,3*RS*)-1-(4-methoxyphenyl)-3-(trifluoromethyl)aziridin-2-yl)(phenyl)methanone (100 mg, 0.31 mmol) in 8 ml CH₃CN was added (NH₄)₂Ce(NO₃)₆ (427 mg, 0.78 mmol) in 2.7 ml H₂O at 0 °C. After 1 h 30 min the reaction was quenched with sat. Na₂SO₃ and sat. NaHCO₃, extracted 3 times with dichloromethane, dried over MgSO₄ and the solvent evaporated under reduced pressure.

The residue was purified on silica gel (hexane/ethyl acetate 70:30) to give the product as white solid (50 mg, 75 %).

¹H-NMR (300 MHz, CD₃CN): δ = 8.13 – 8.03 (m, 2H), 7.70 – 7.62 (m, 1H), 7.59 – 7.48 (m, 2H), 3.62 (dd, J = 9.8, 6.6 Hz, 1H), 3.35 – 3.11 (m, 1H), 2.24 (br, 1H).

¹³C-NMR (100 MHz, CD₃CN): δ = 191.7, 135.9, 133.7, 128.7, 128.5, 124.6 (q, J = 273.2 Hz), 37.6, 35.0 (q, J = 39.3 Hz).

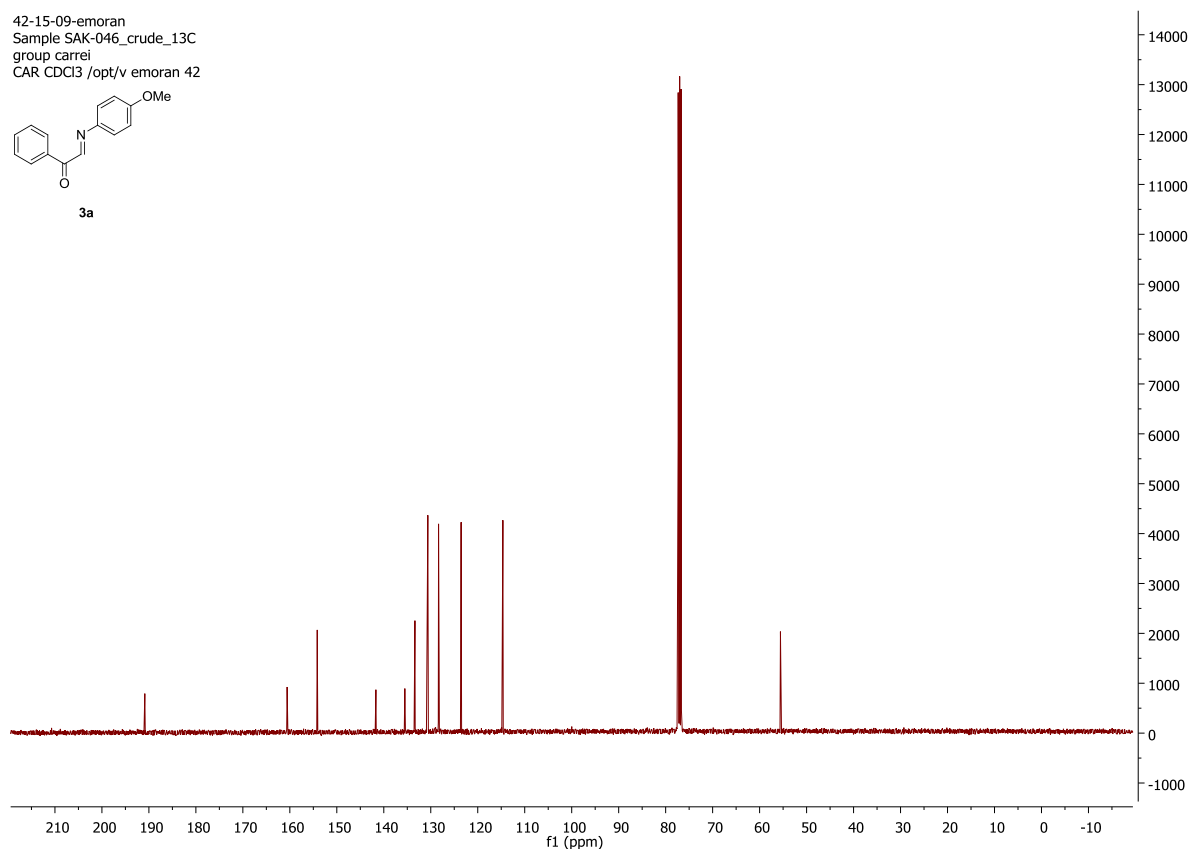
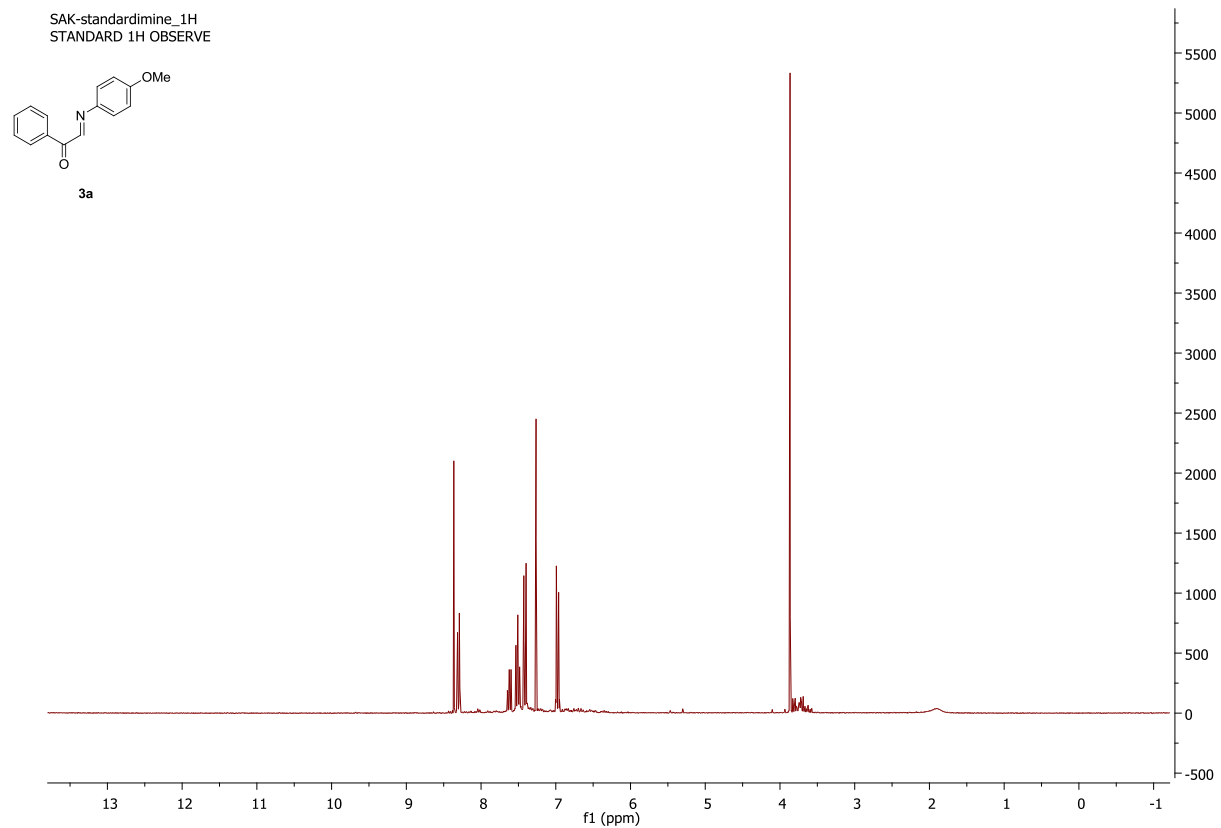
¹⁹F-NMR (282 MHz, CD₃CN): δ = -66.94 (d, J = 6.2 Hz).

HRMS (ESI): calcd for C₁₀H₉F₃NO⁺ ($[M+H]^+$) 216.0631, found 216.0633.

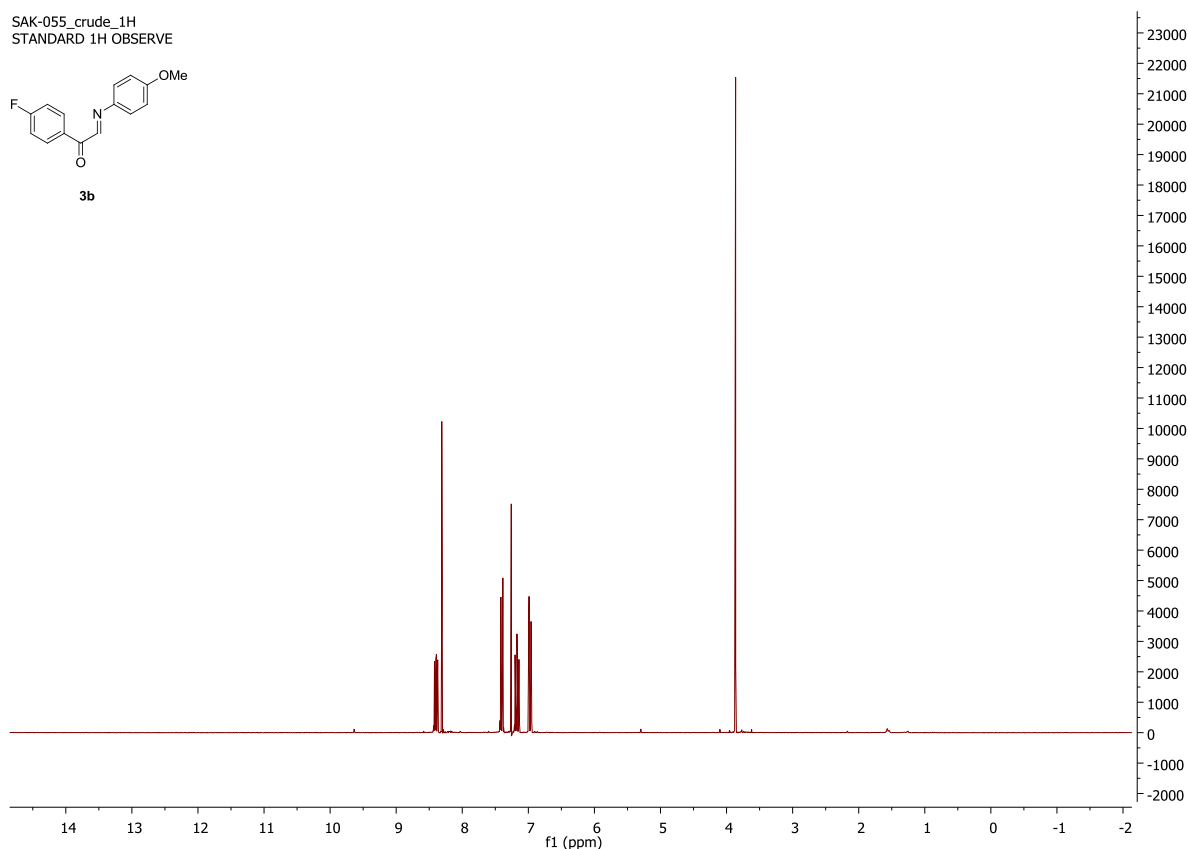
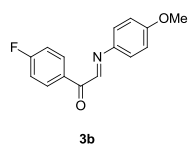
IR (neat): 3196, 1684, 1596, 1132 cm⁻¹.

References:

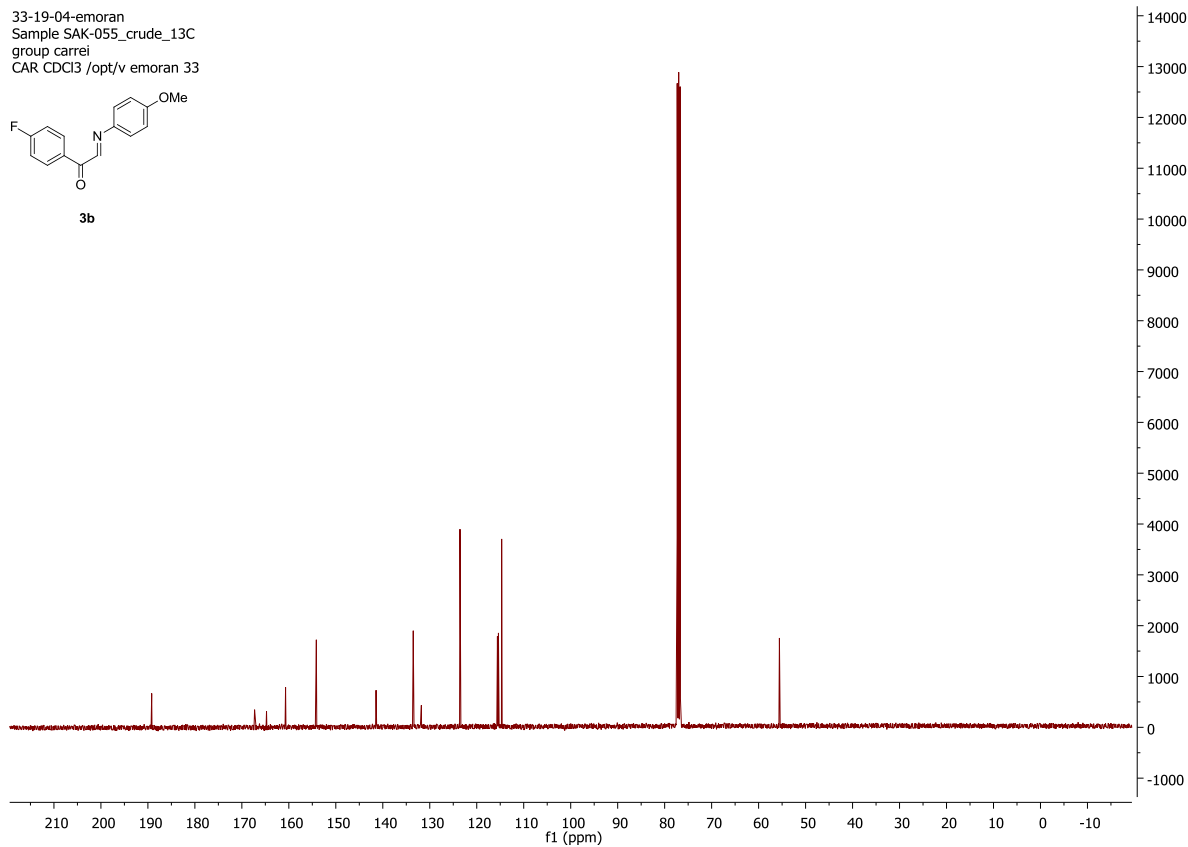
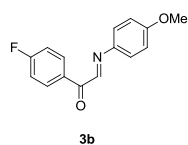
- ¹ Floyd, M. B.; Du, M. T.; Fabio, P. F.; Jacob, L. A.; Johnson, B. D. *J. Org. Chem.* **1985**, *50*, 5022.
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- ⁶ Spannedra, M. V.; Crousse, B.; Narizuka, S.; Bonnet-Delpon, D.; Bégué, J.-P. *Collect. Czech. Chem. Commun.* **2002**, *67*, 1359.



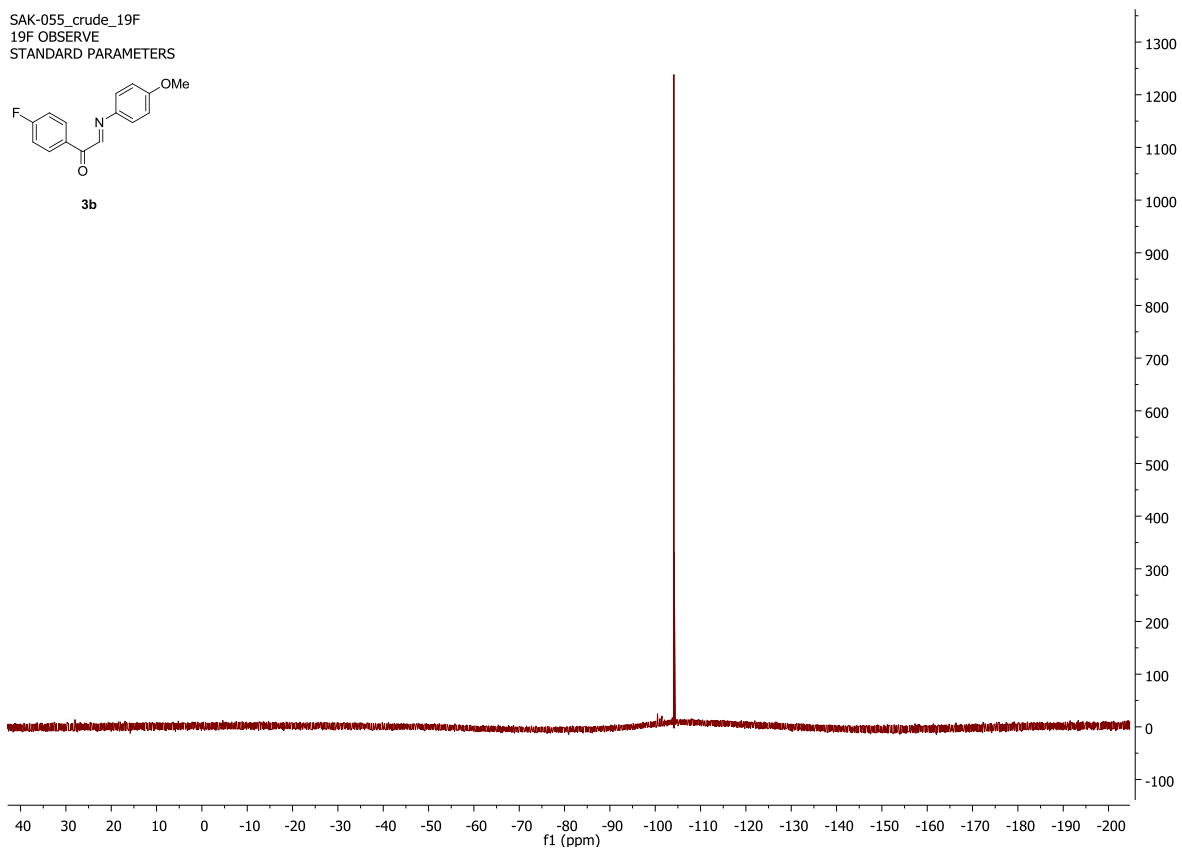
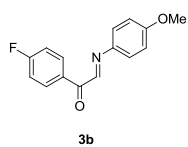
SAK-055_crude_1H
STANDARD 1H OBSERVE



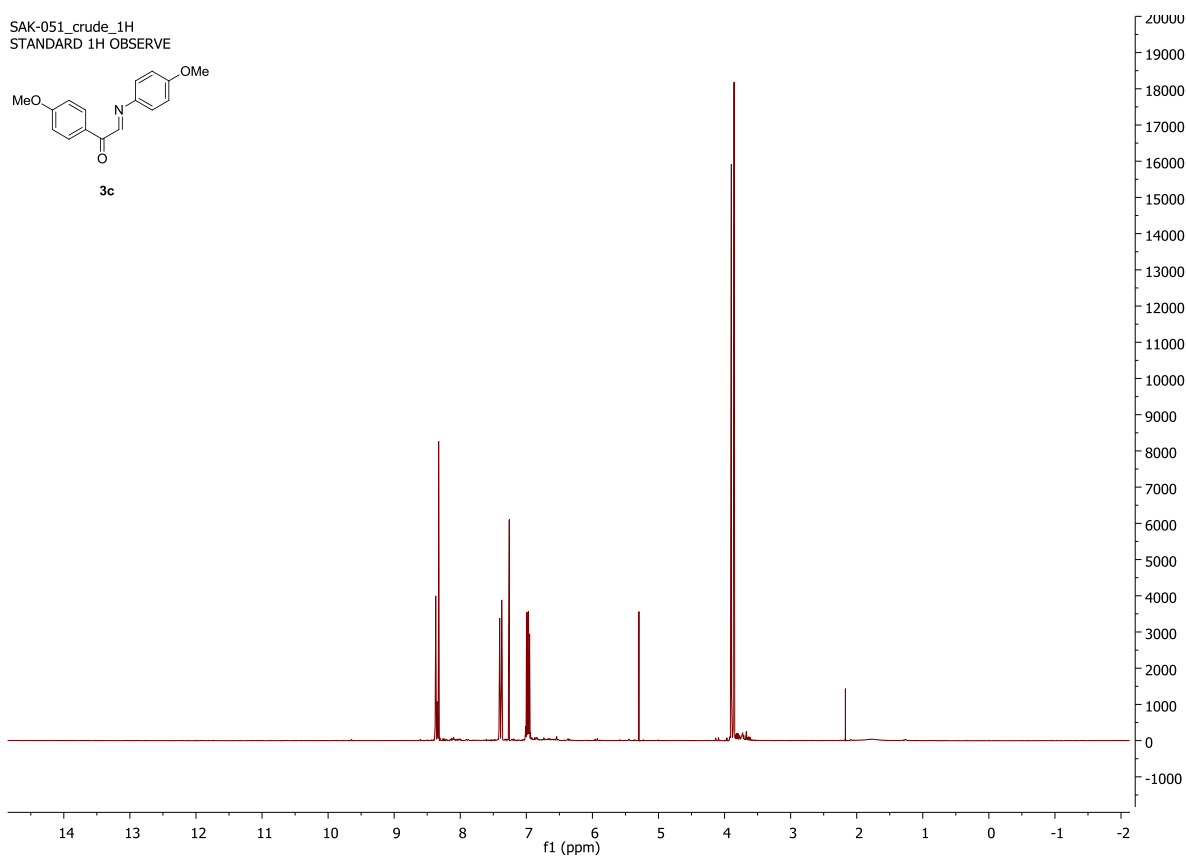
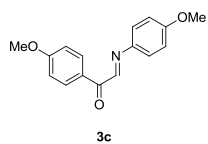
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group carrei
CAR CDCl3 /opt/v emoran 33



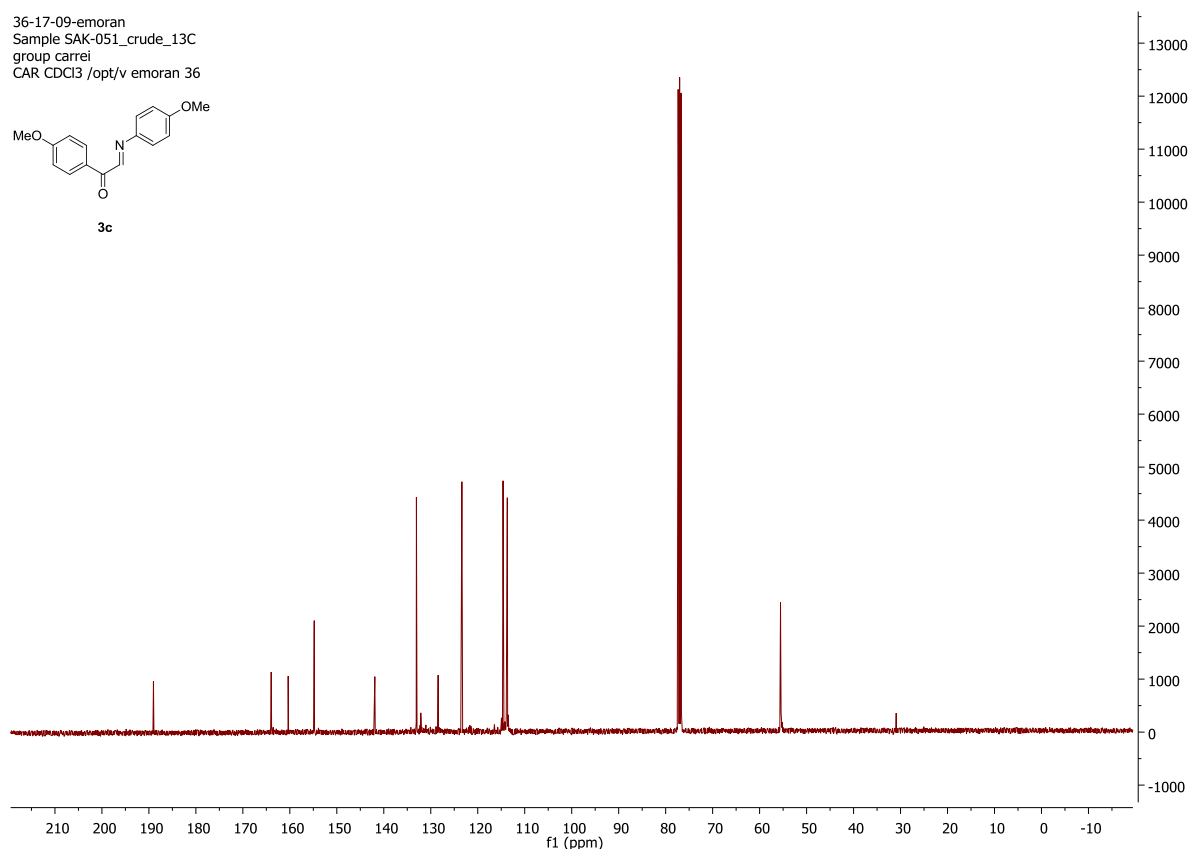
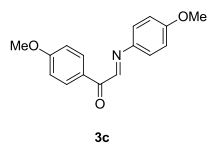
SAK-055_crude_19F
19F OBSERVE
STANDARD PARAMETERS



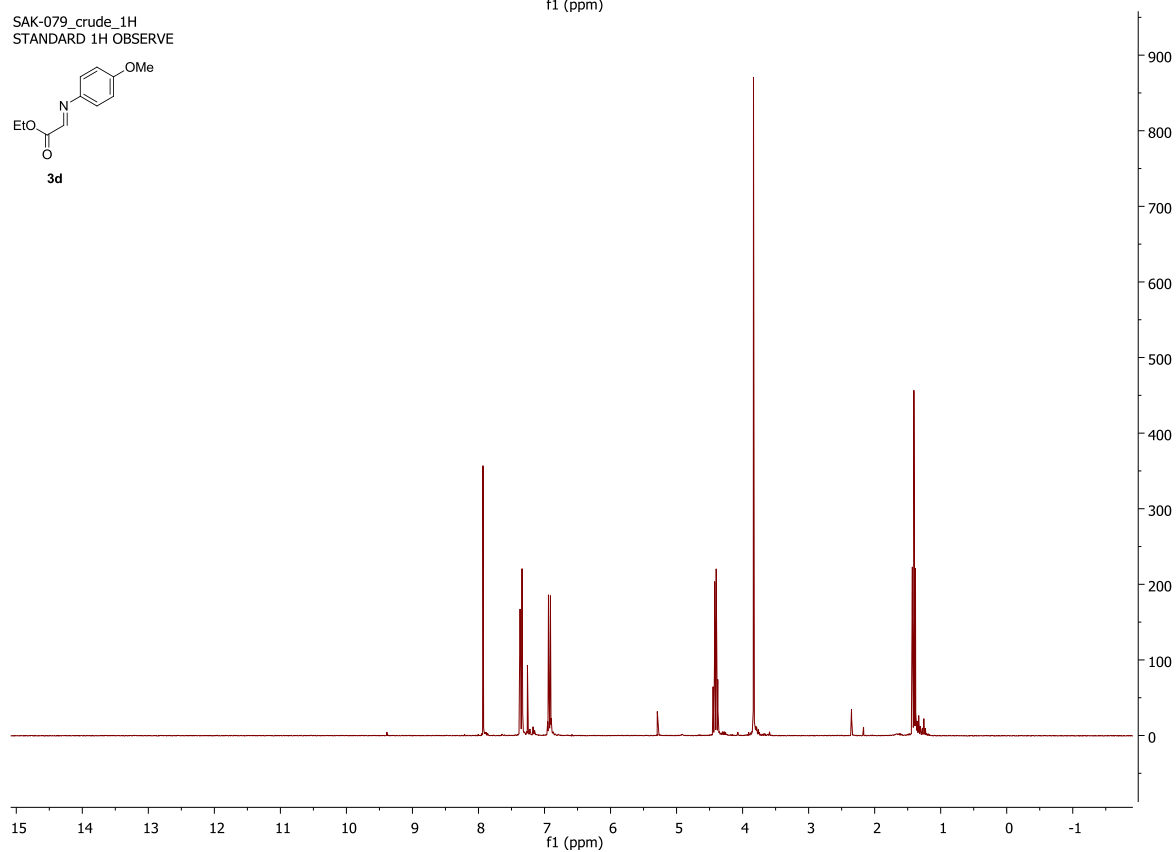
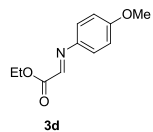
SAK-051_crude_1H
STANDARD 1H OBSERVE



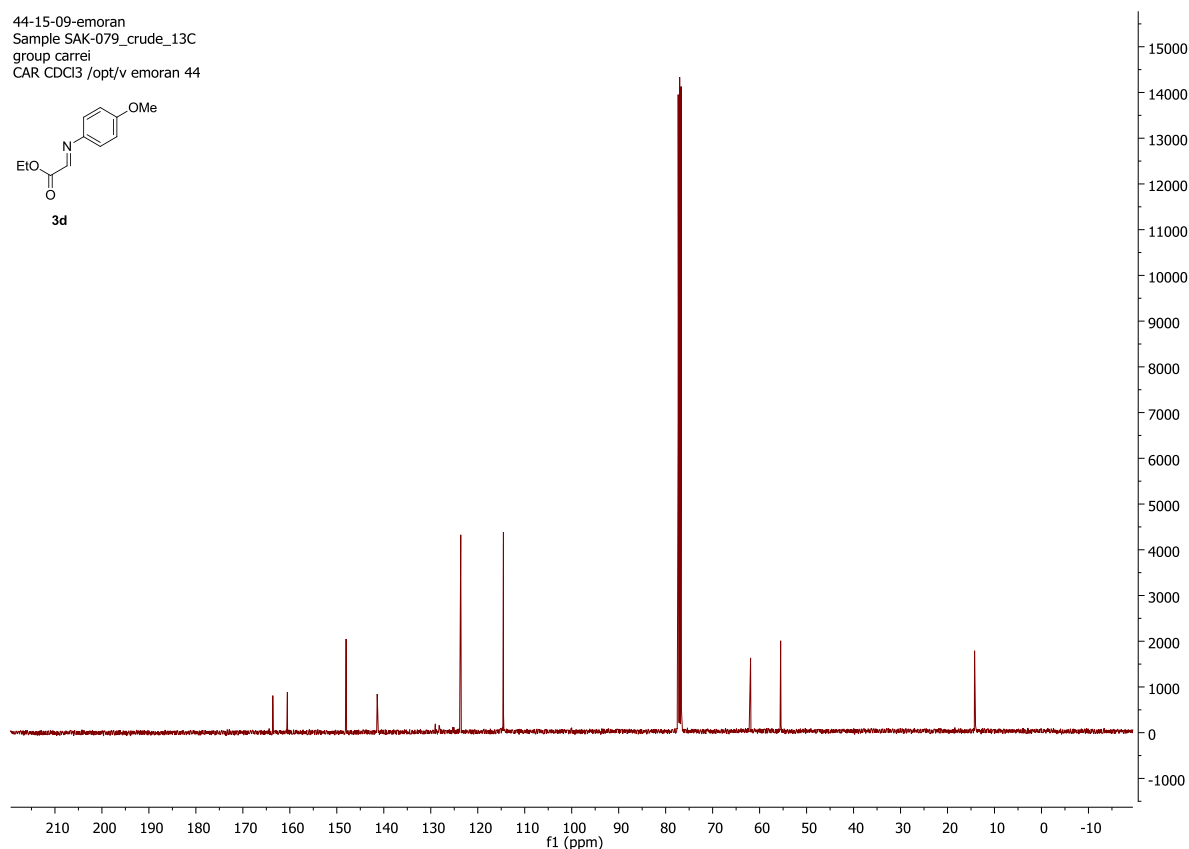
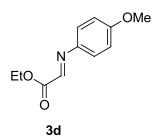
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 group carrei
 CAR CDCl3 /opt/v emoran 36



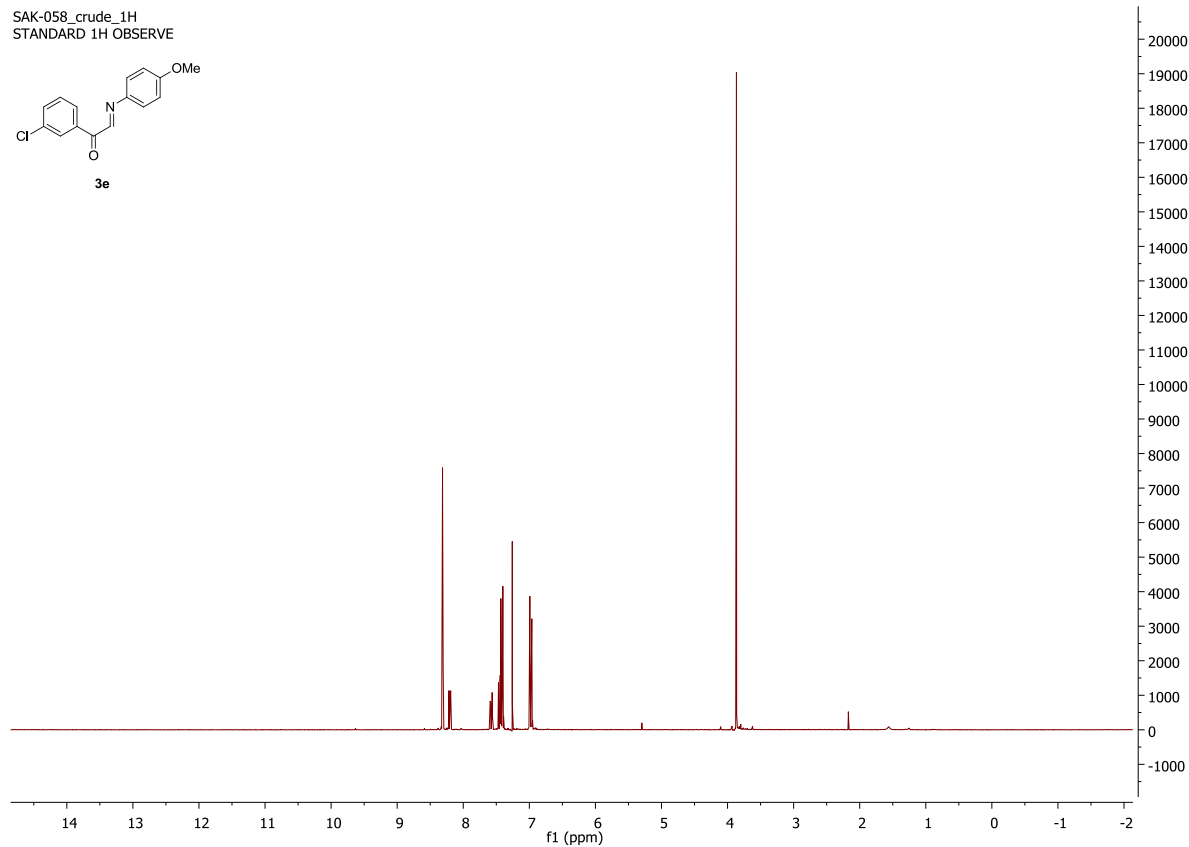
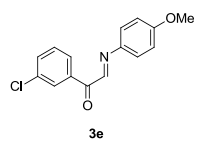
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 STANDARD 1H OBSERVE



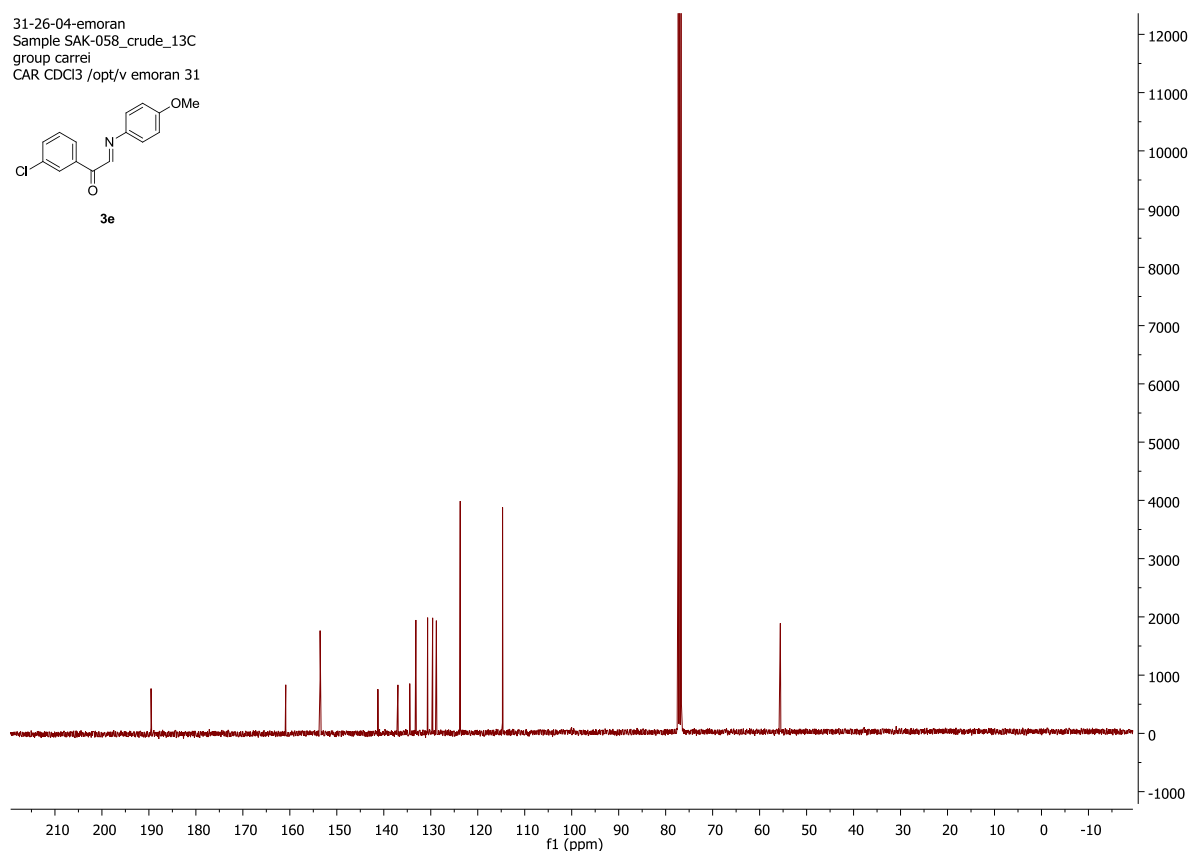
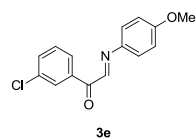
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 group carrei
 CAR CDCl3 /opt/v emoran 44



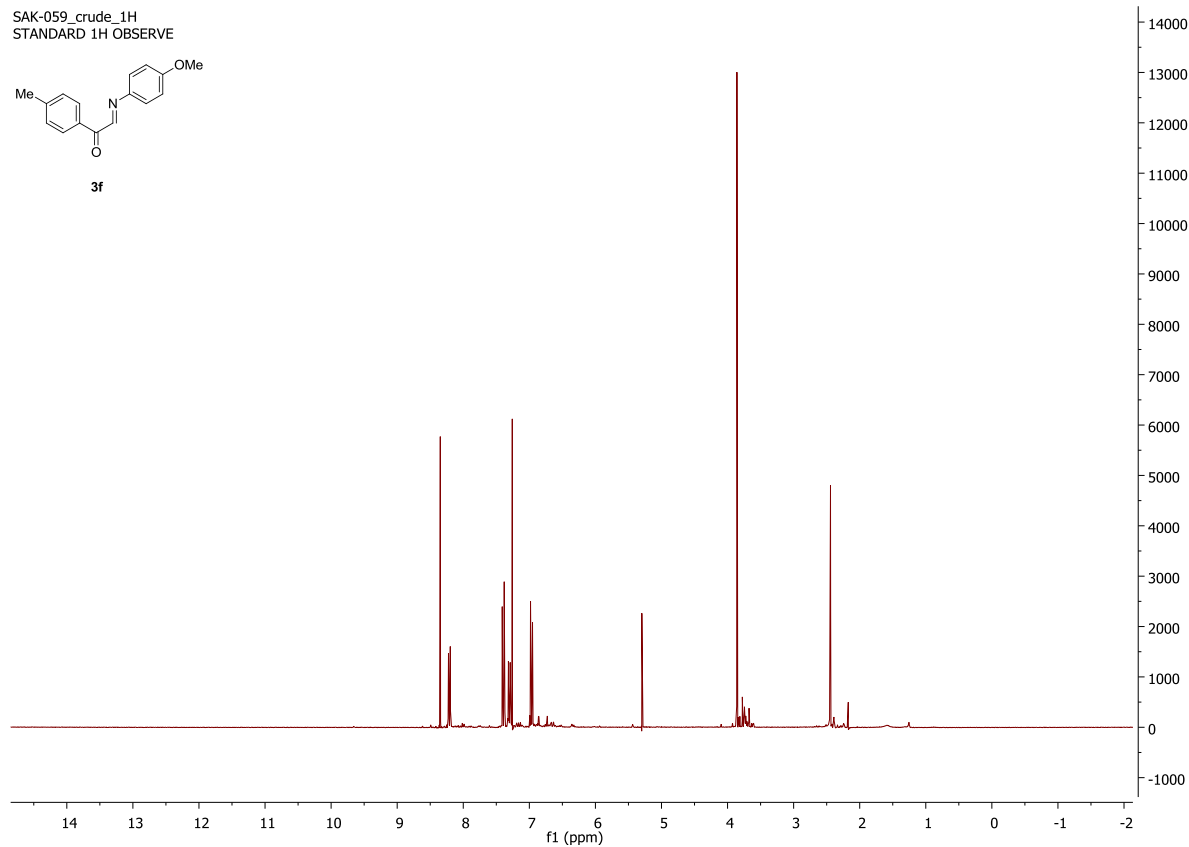
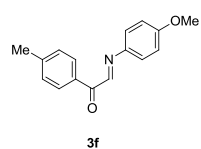
SAK-058_crude_1H
 STANDARD 1H OBSERVE

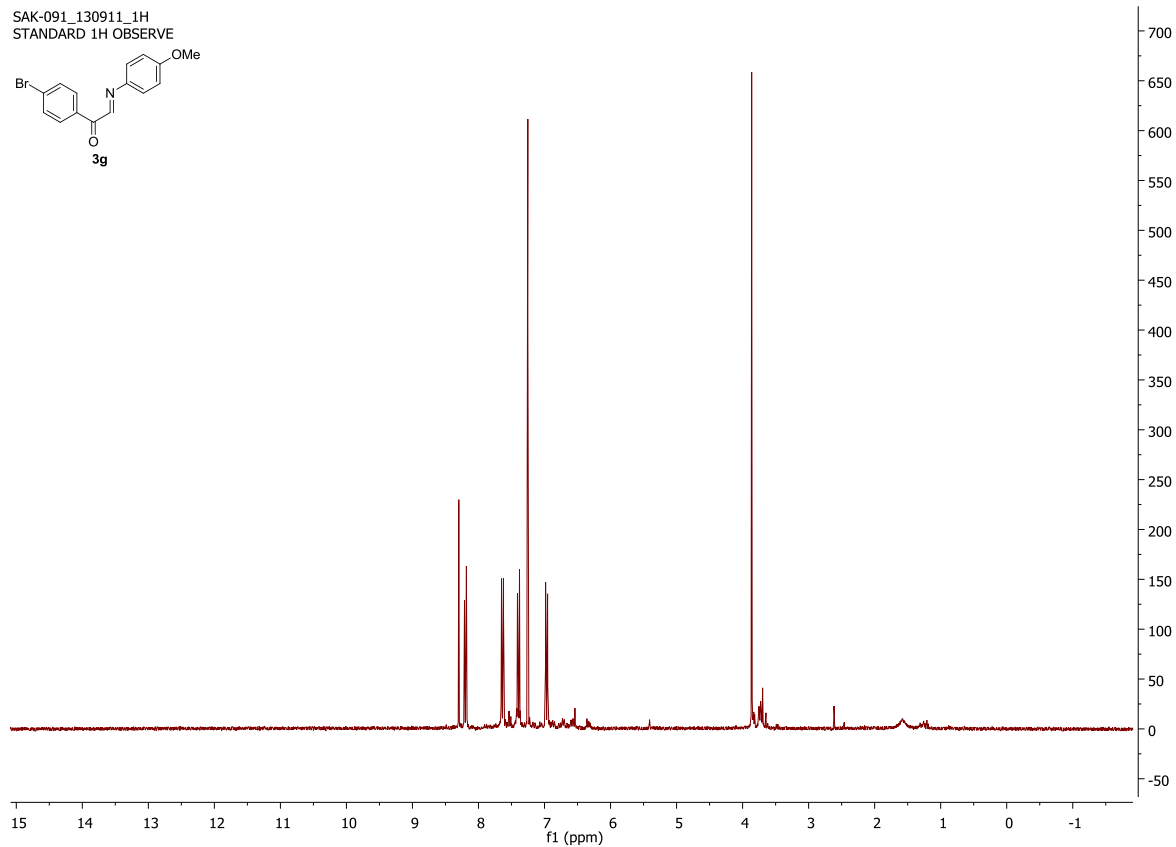
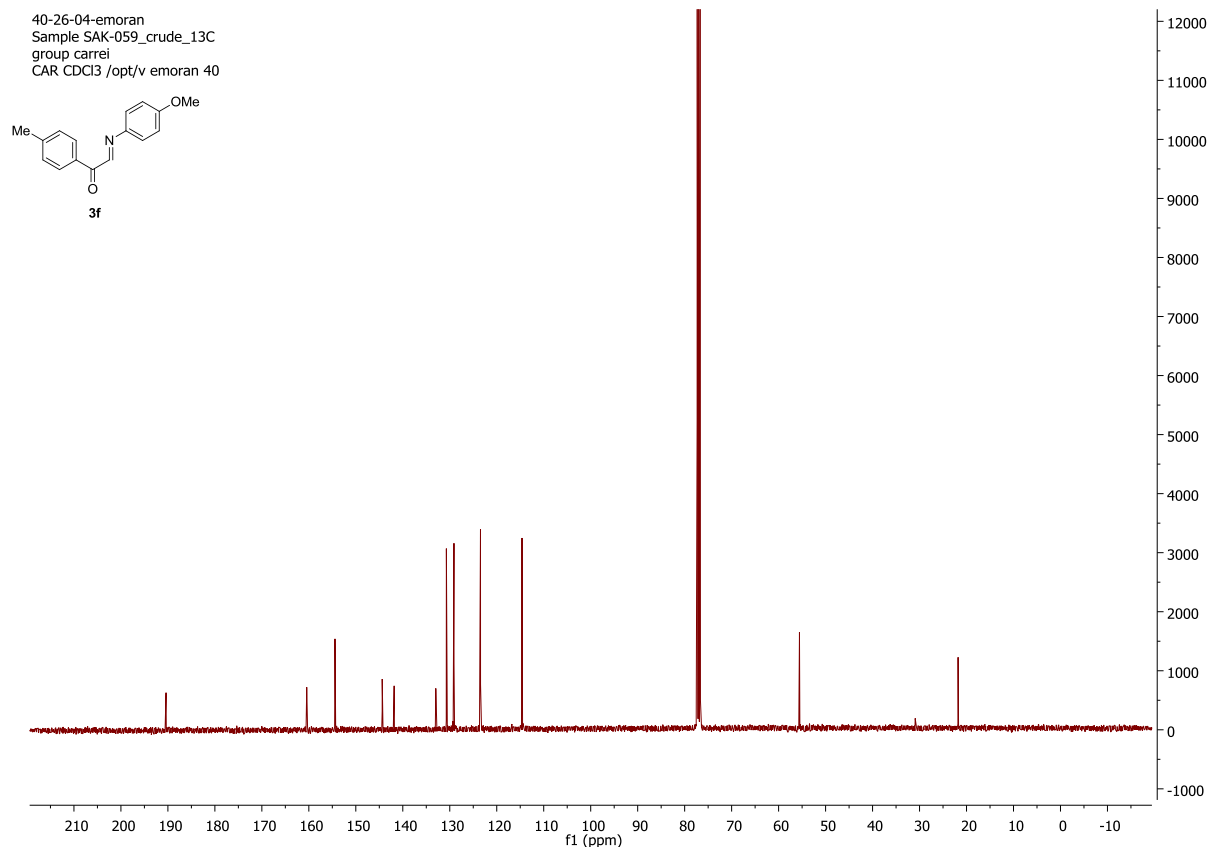


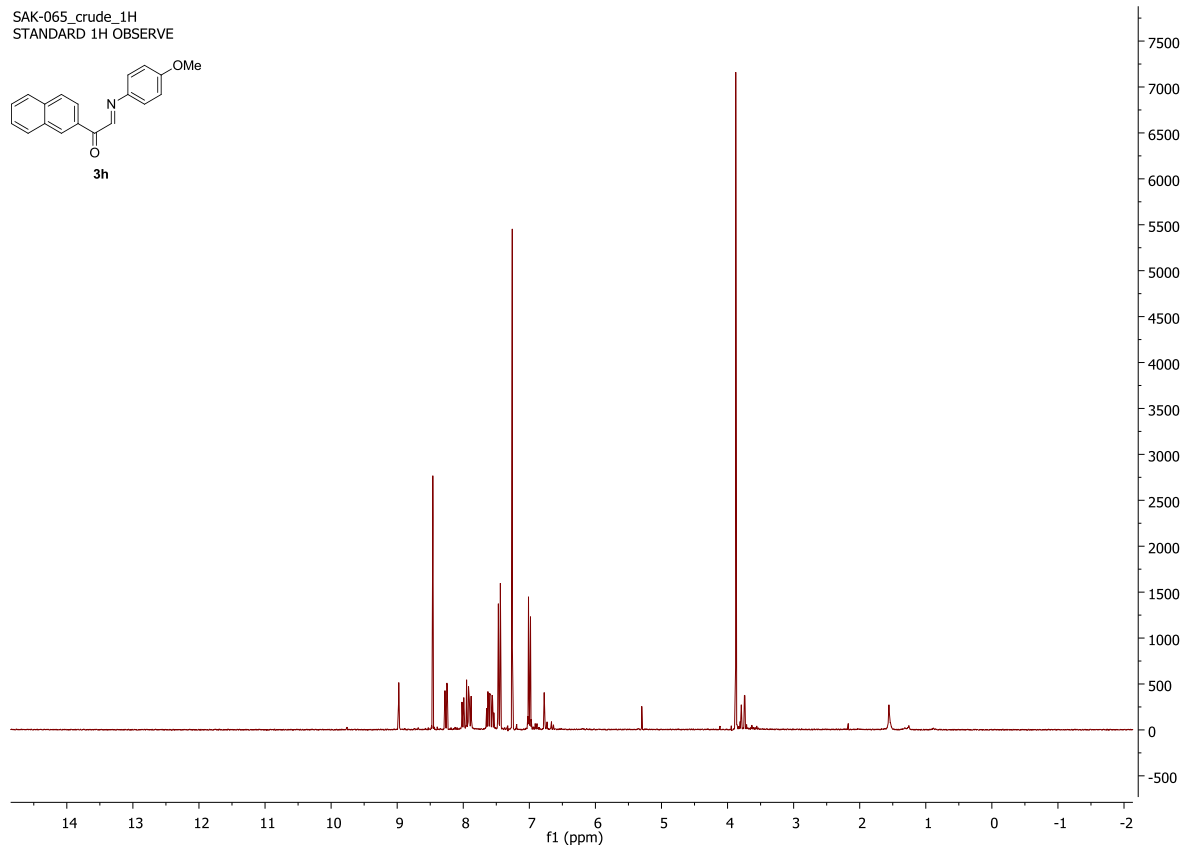
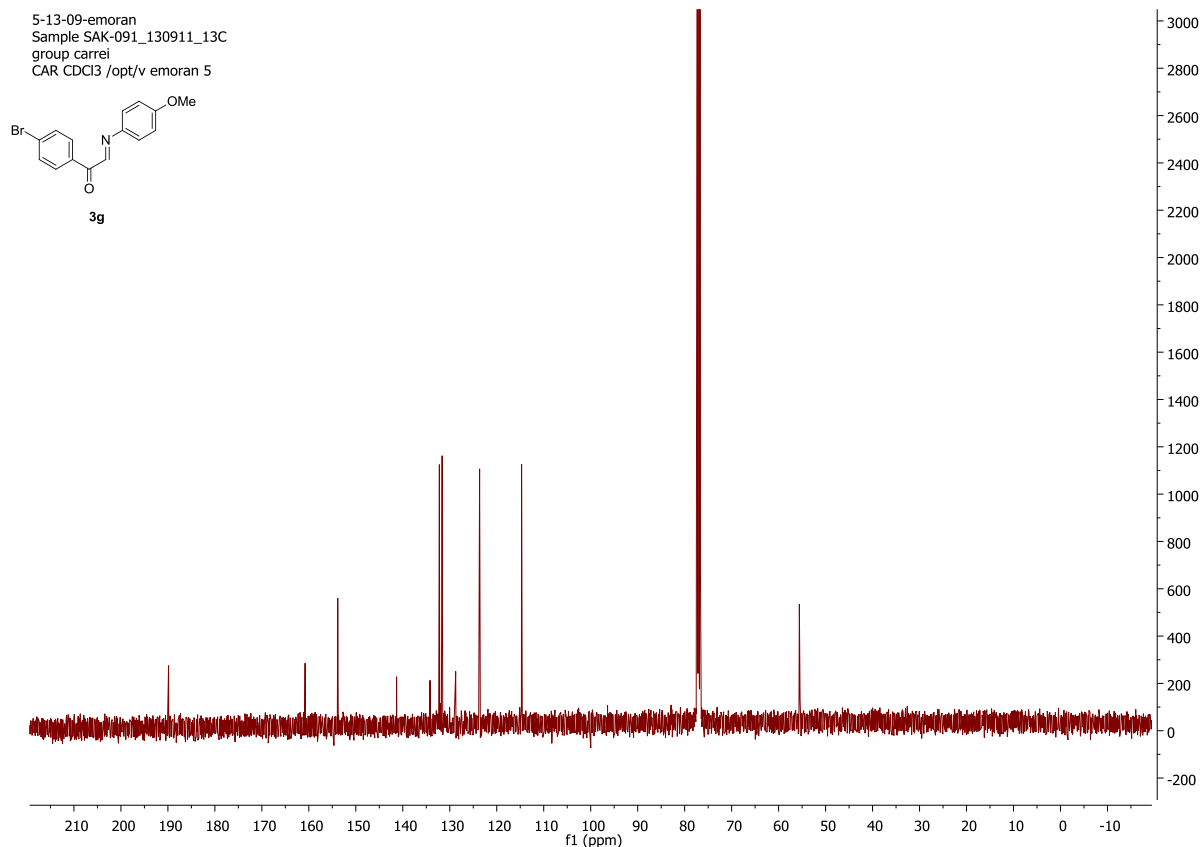
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 group carrei
 CAR CDCl3 /opt/v emoran 31



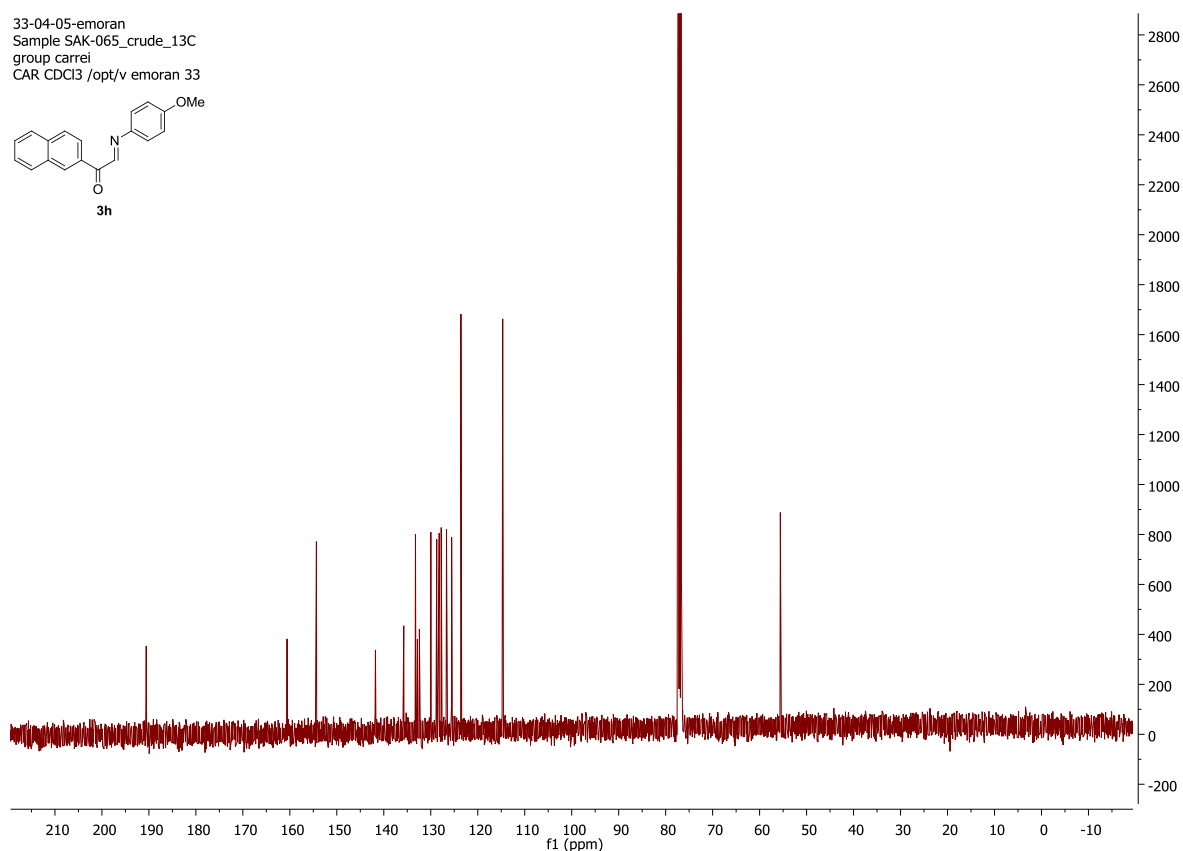
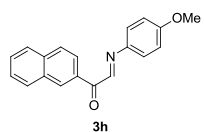
SAK-059_crude_1H
 STANDARD 1H OBSERVE



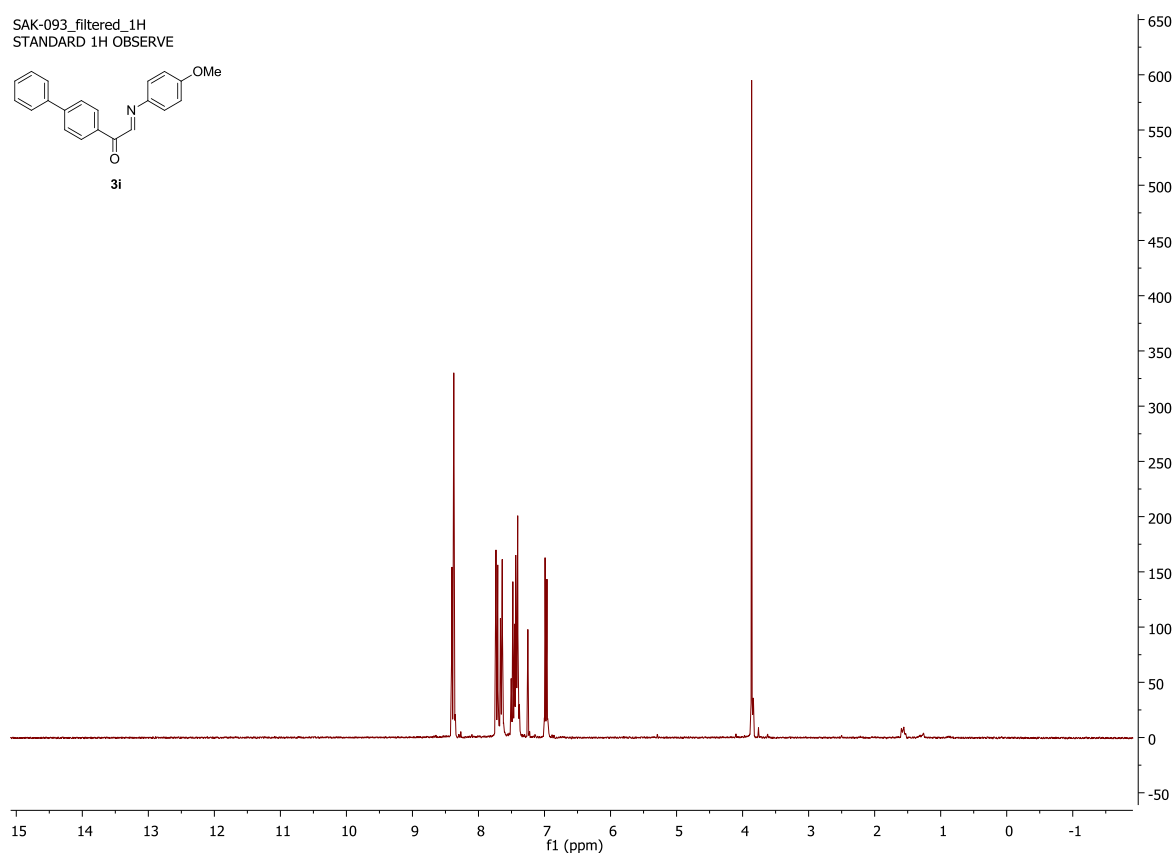
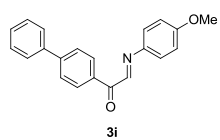


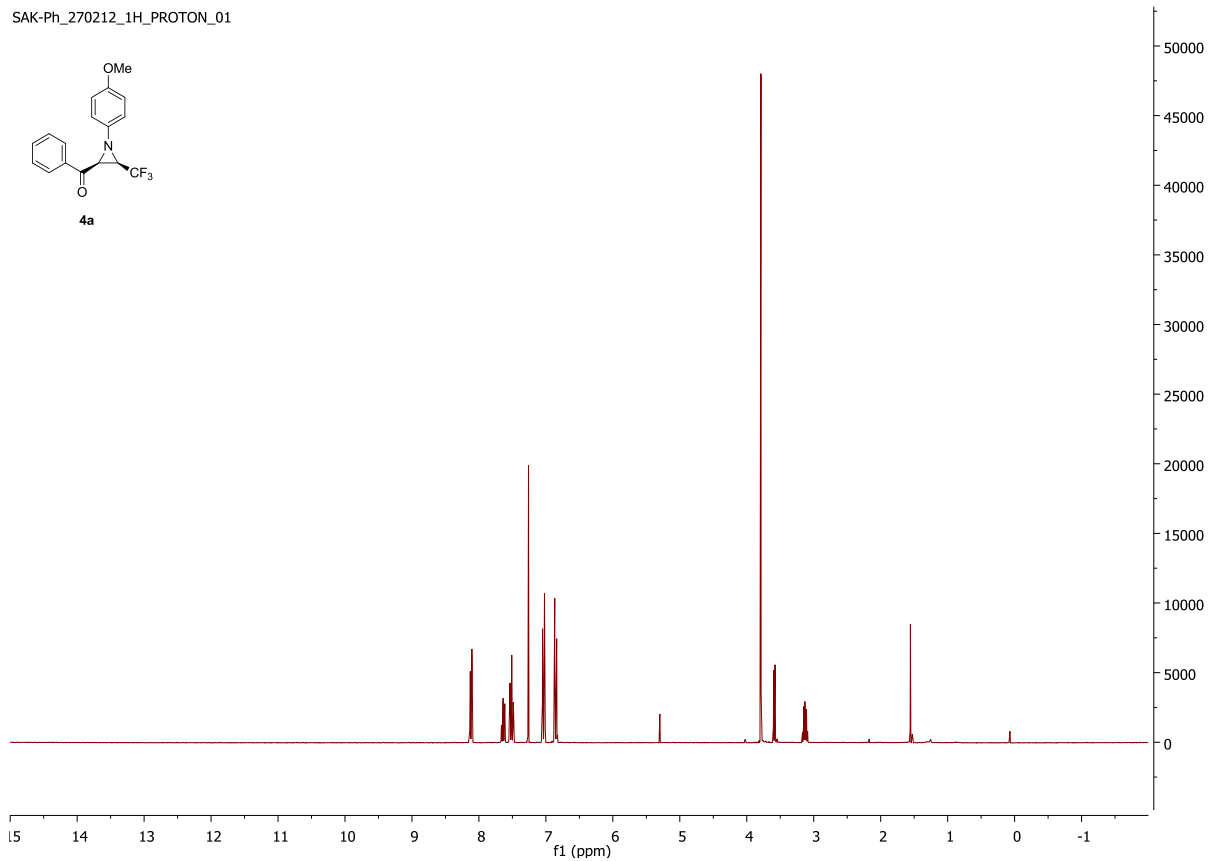
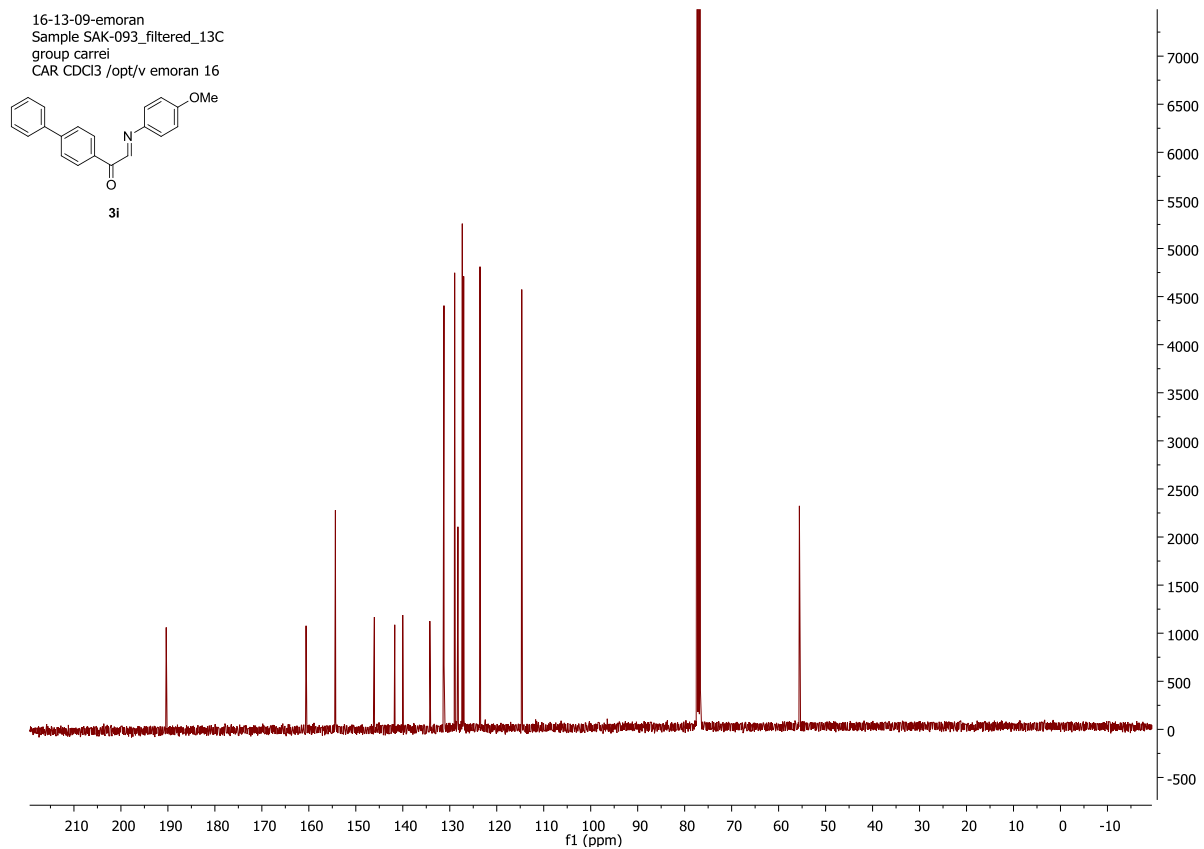


33-04-05-emoran
Sample SAK-065_crude_13C
group carrei
CAR CDCl3 /opt/v emoran 33

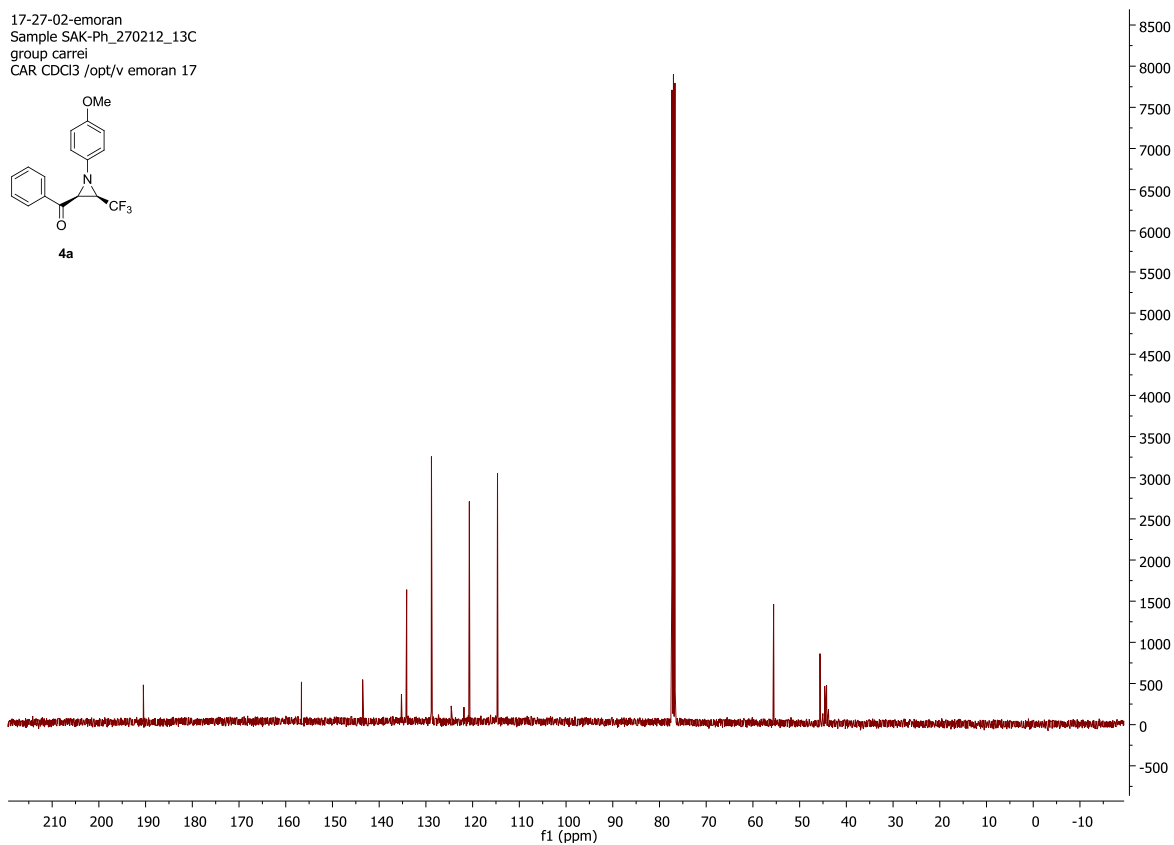
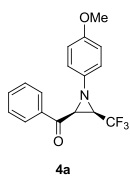


SAK-093_filtered_1H
STANDARD 1H OBSERVE

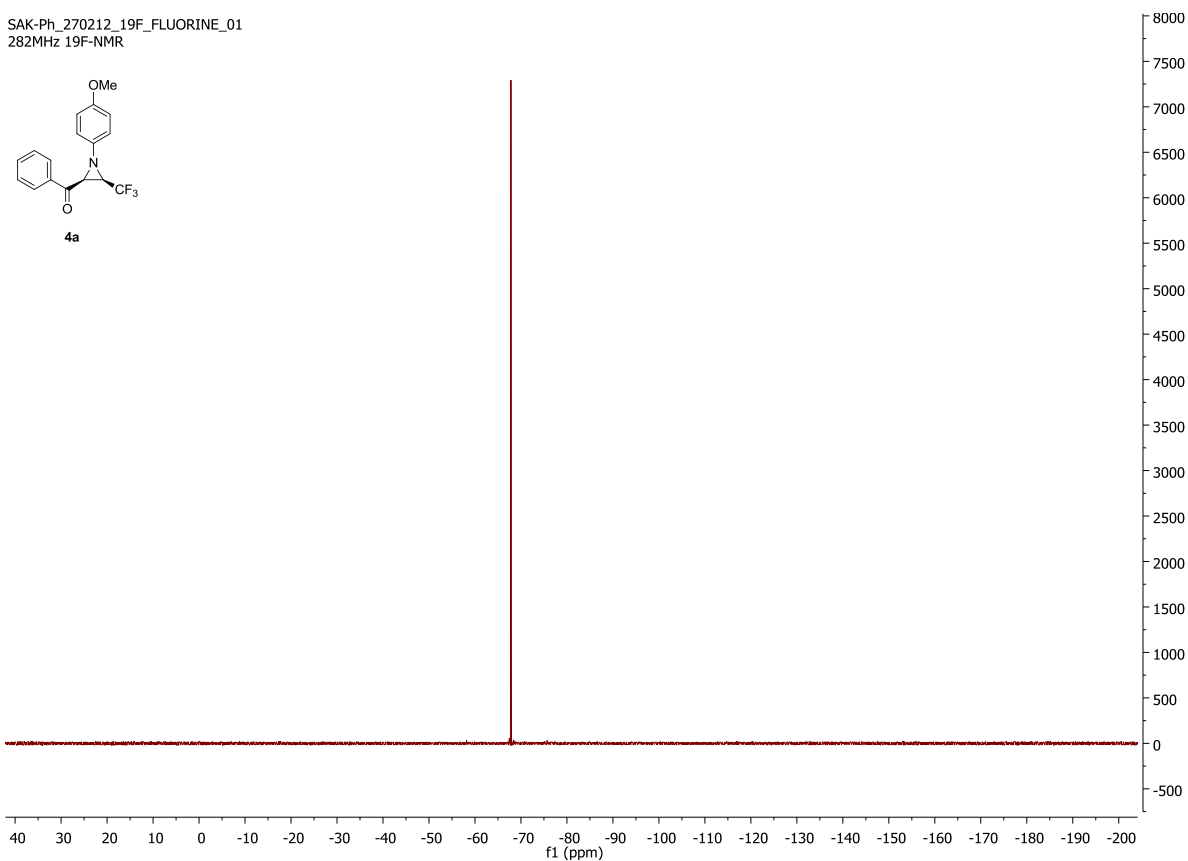
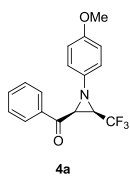


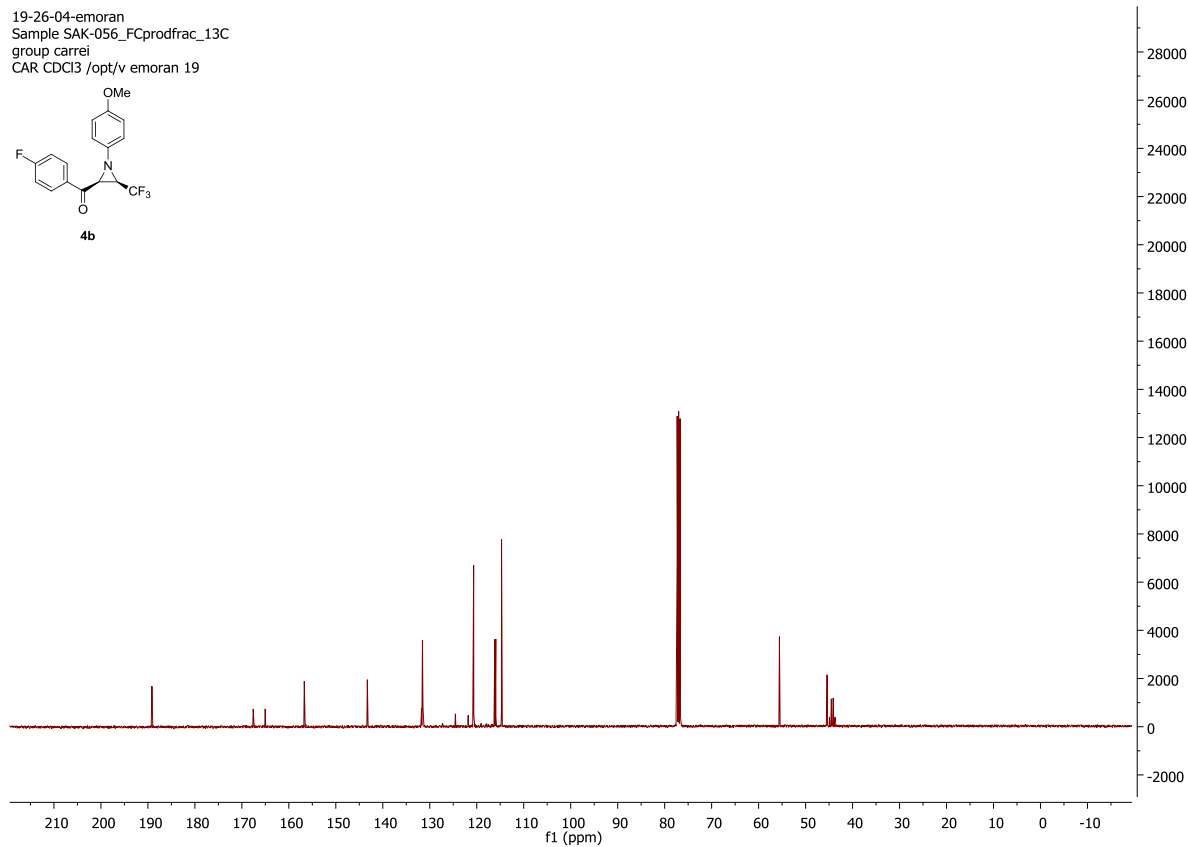
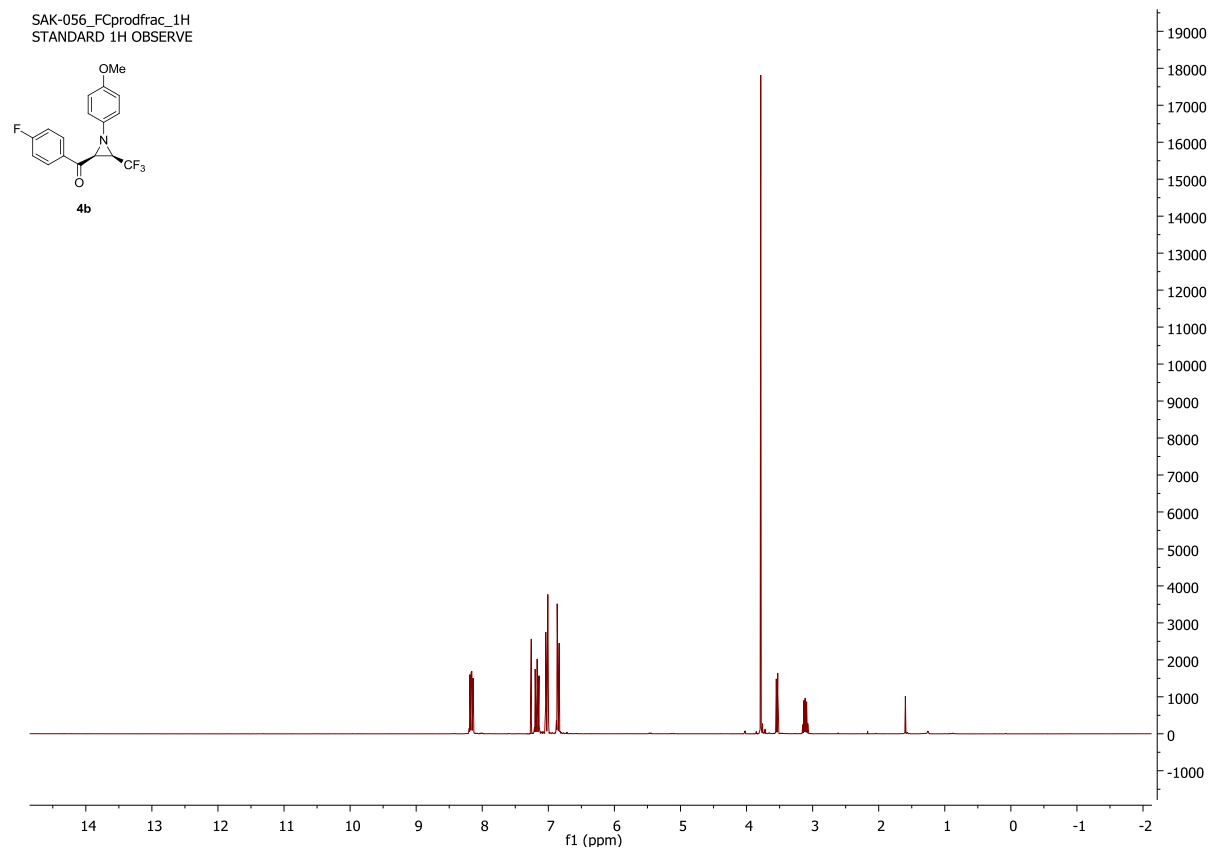


17-27-02-emoran
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group carrei
CAR CDCl3 /opt/v emoran 17

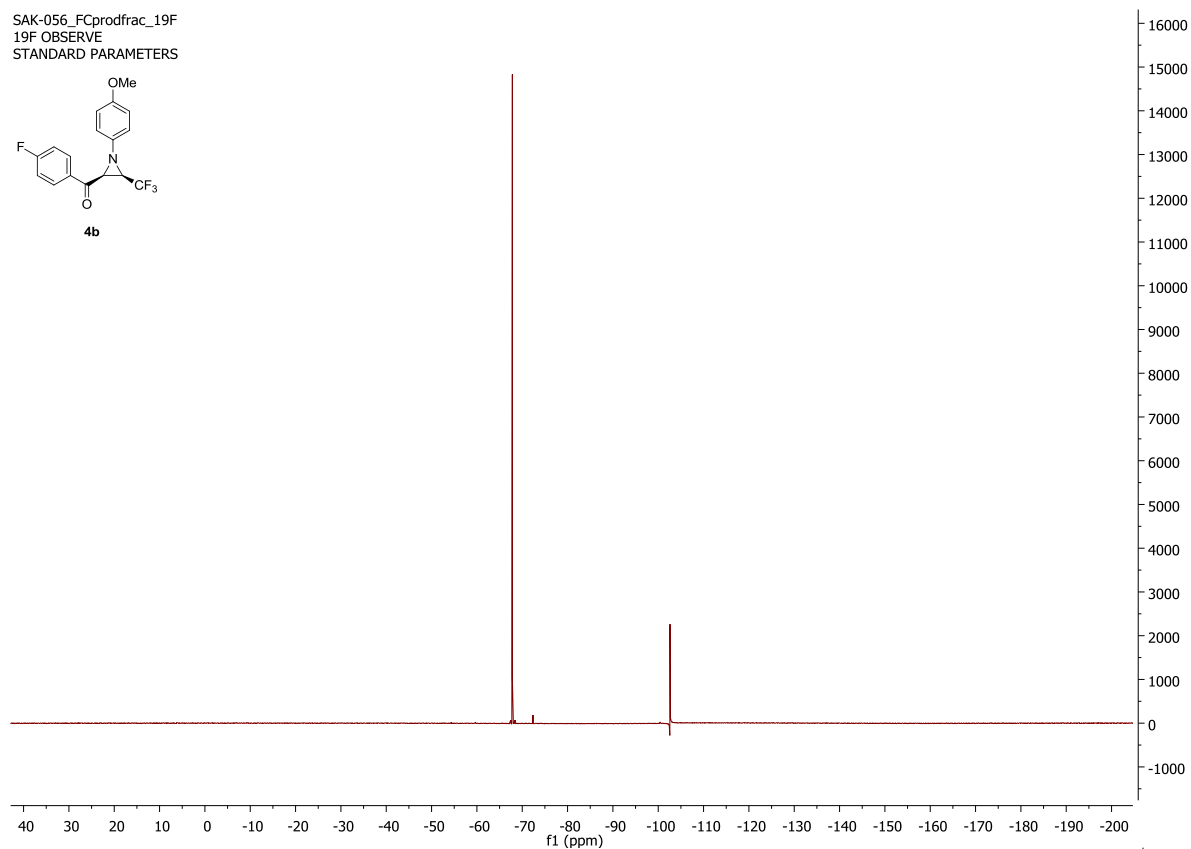
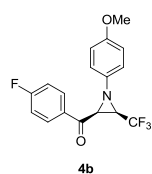


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282MHz 19F-NMR

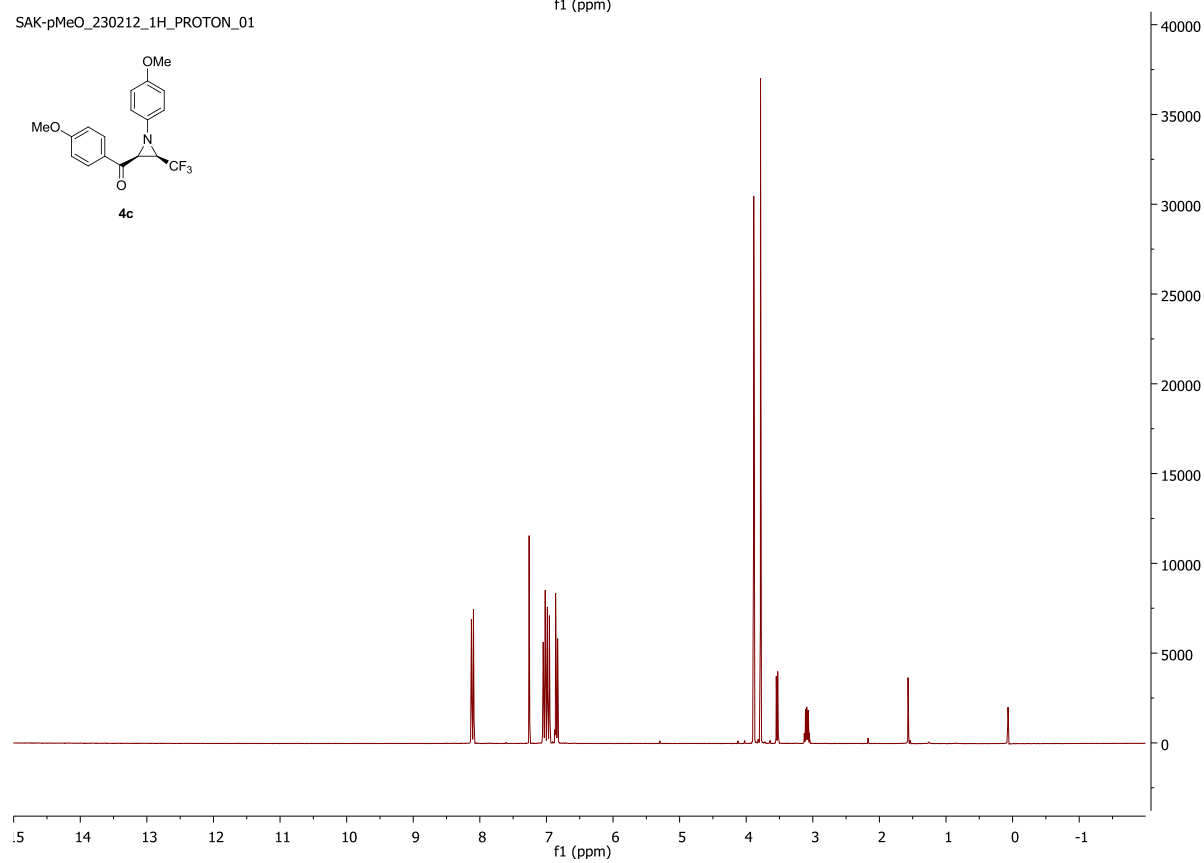
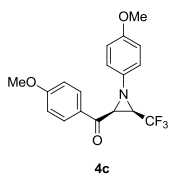




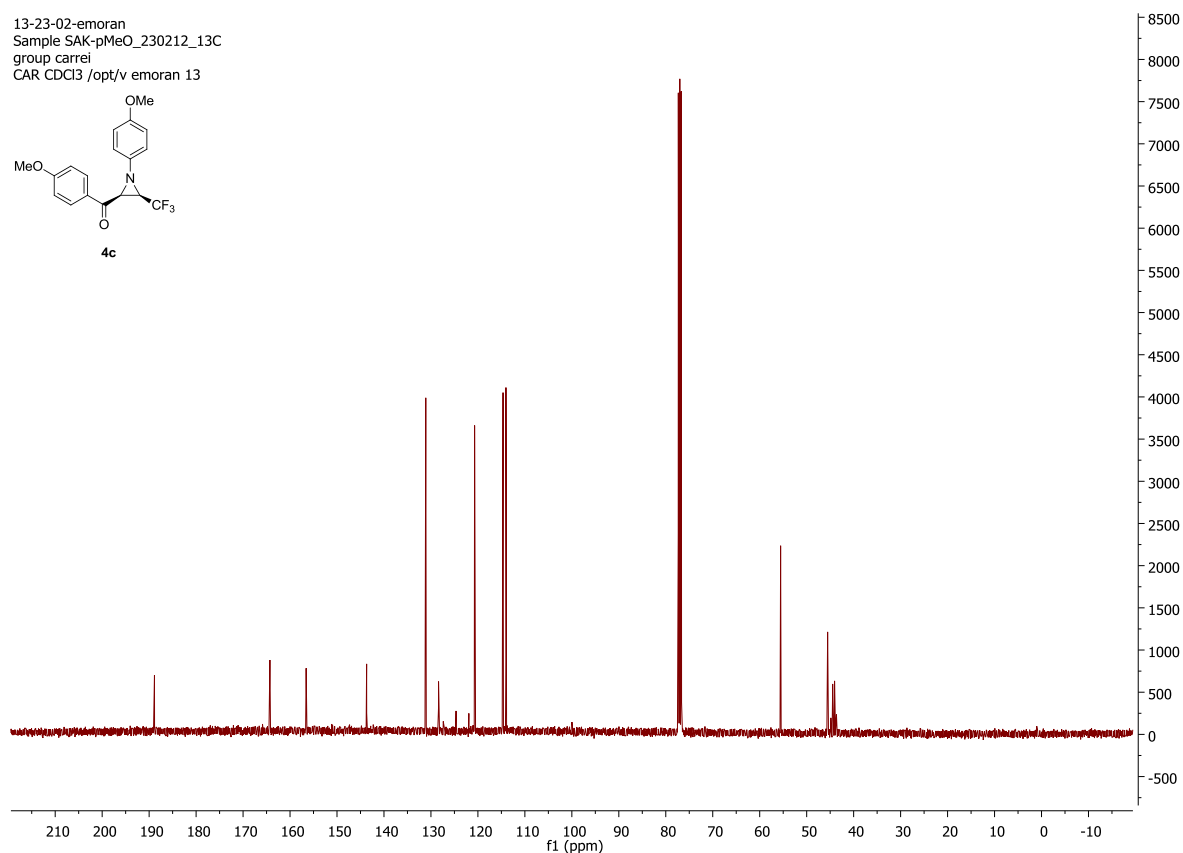
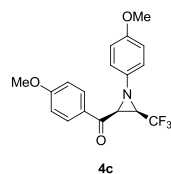
SAK-056_FCprodfrac_19F
19F OBSERVE
STANDARD PARAMETERS



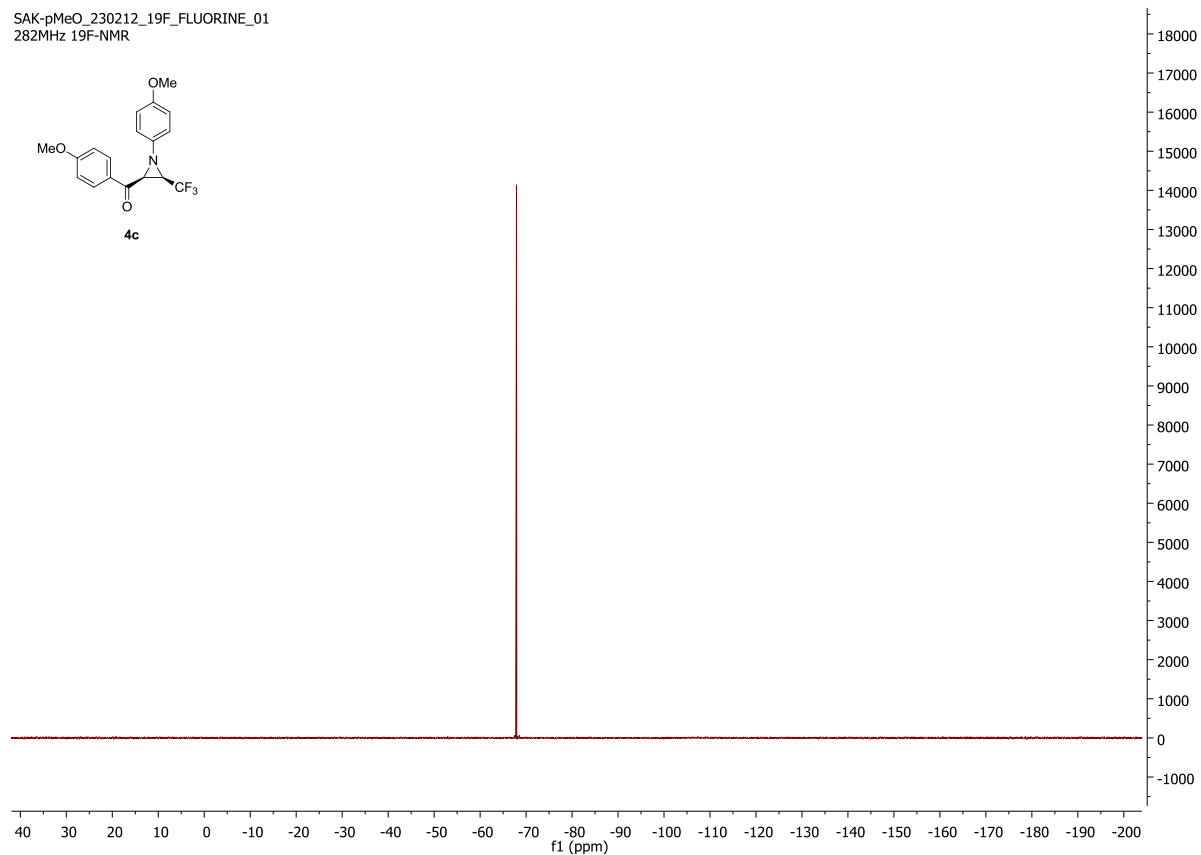
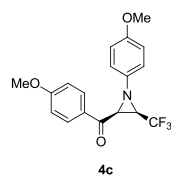
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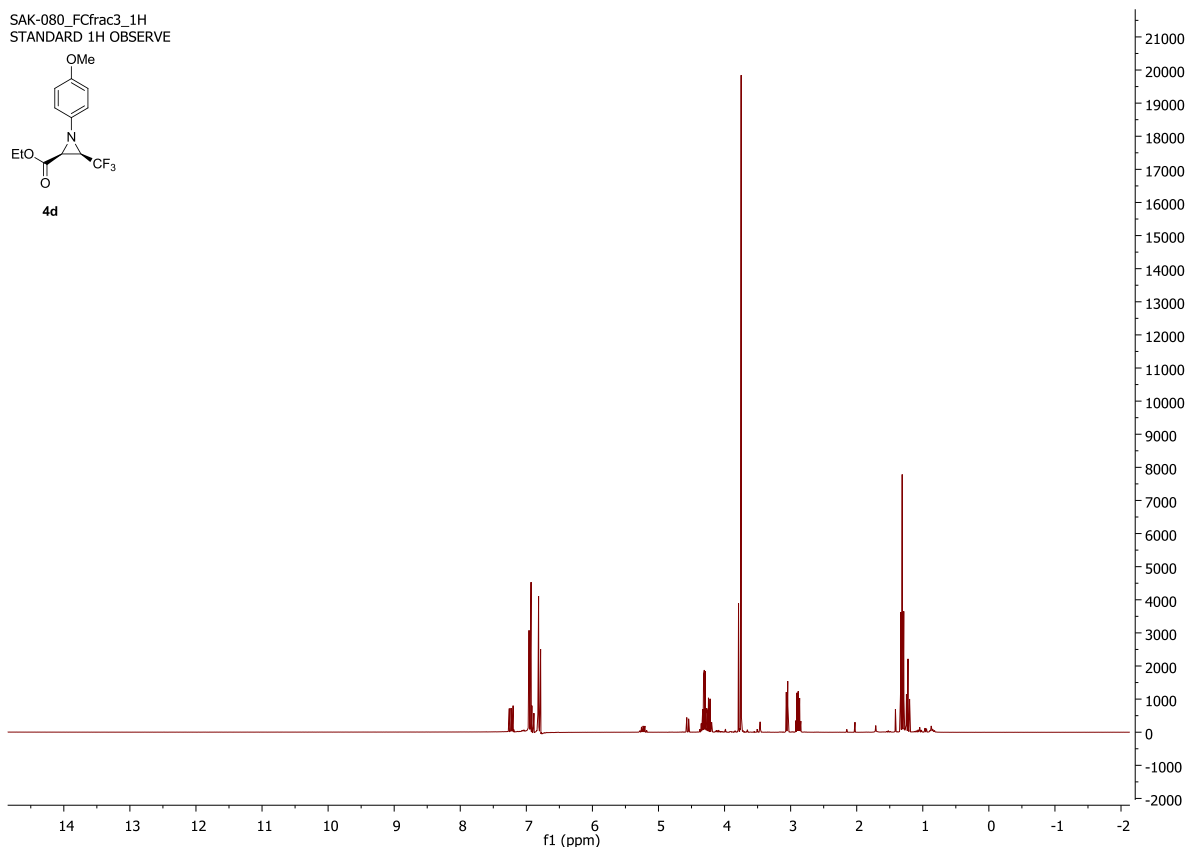
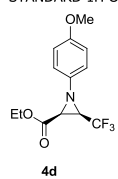
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 group carrei
 CAR CDCl3 /opt/v emoran 13



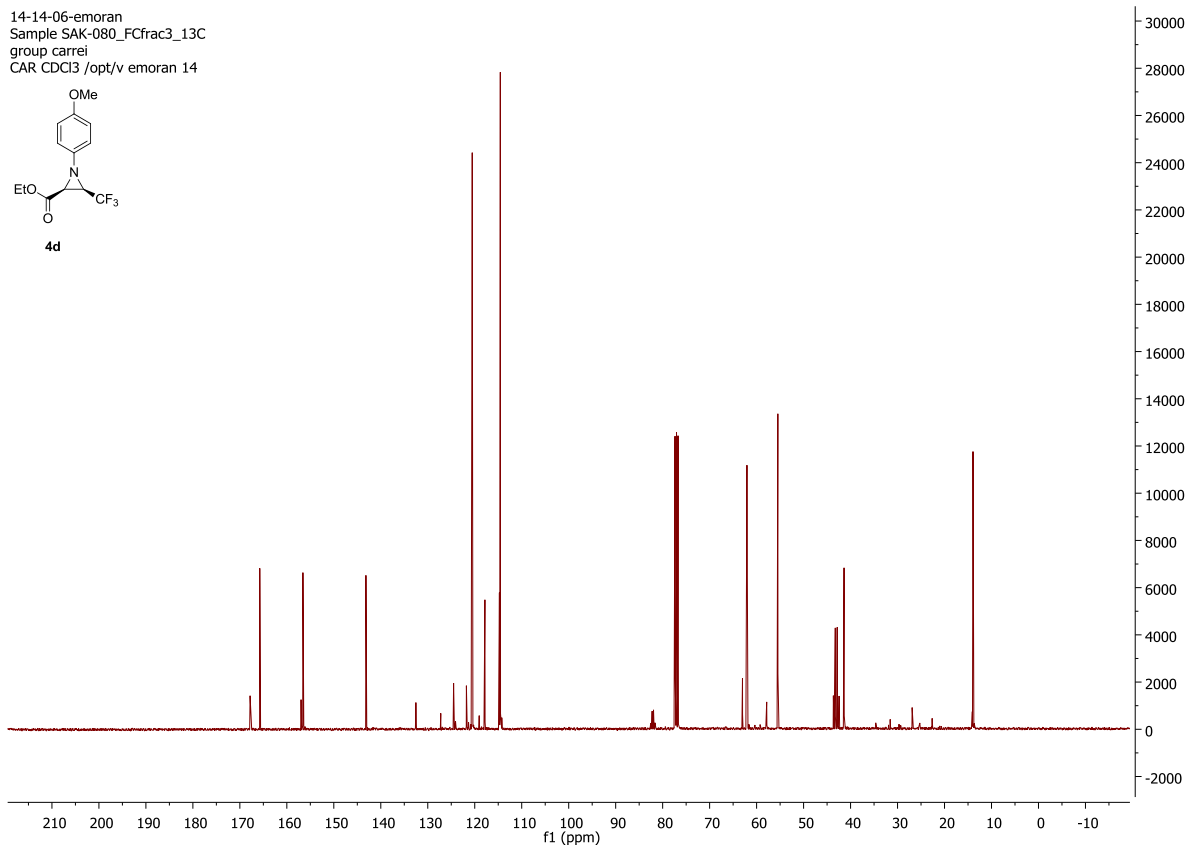
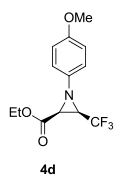
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 282MHz 19F-NMR



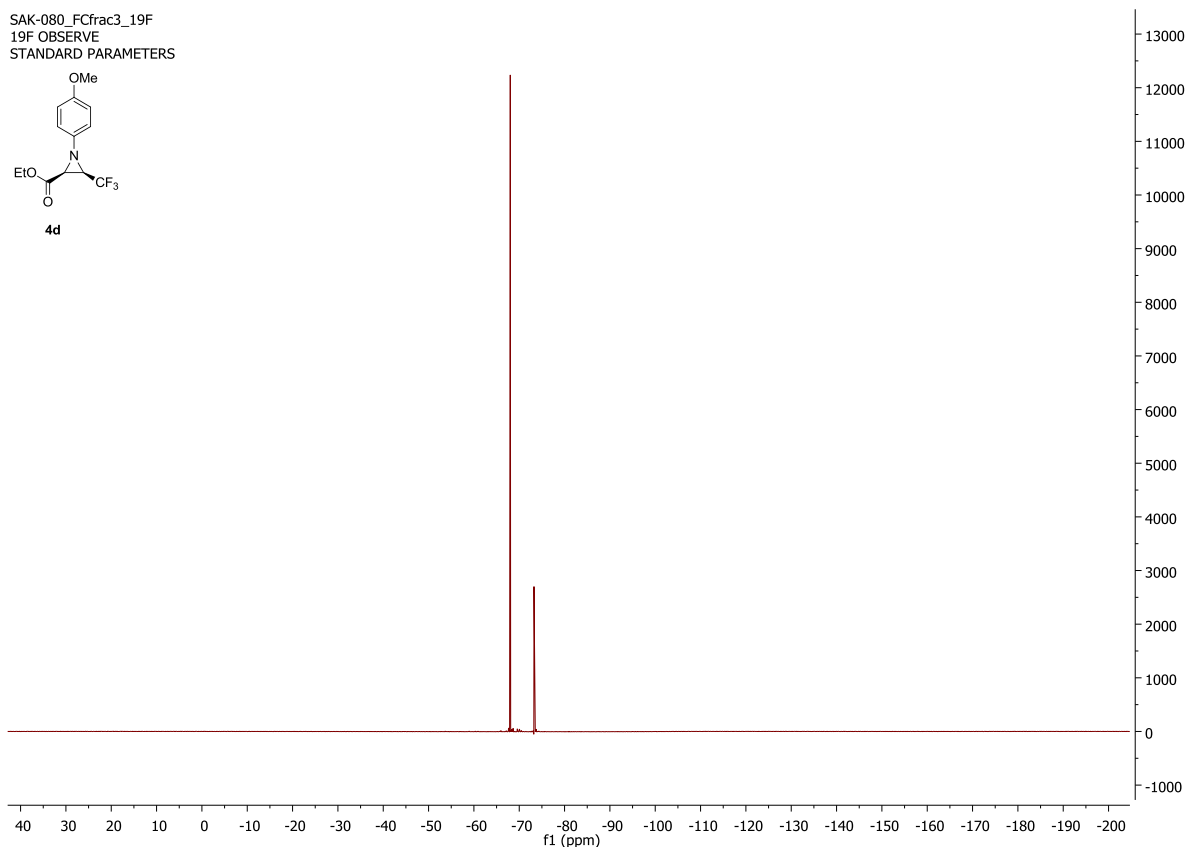
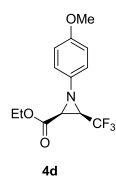
SAK-080_FCfrac3_1H
STANDARD 1H OBSERVE



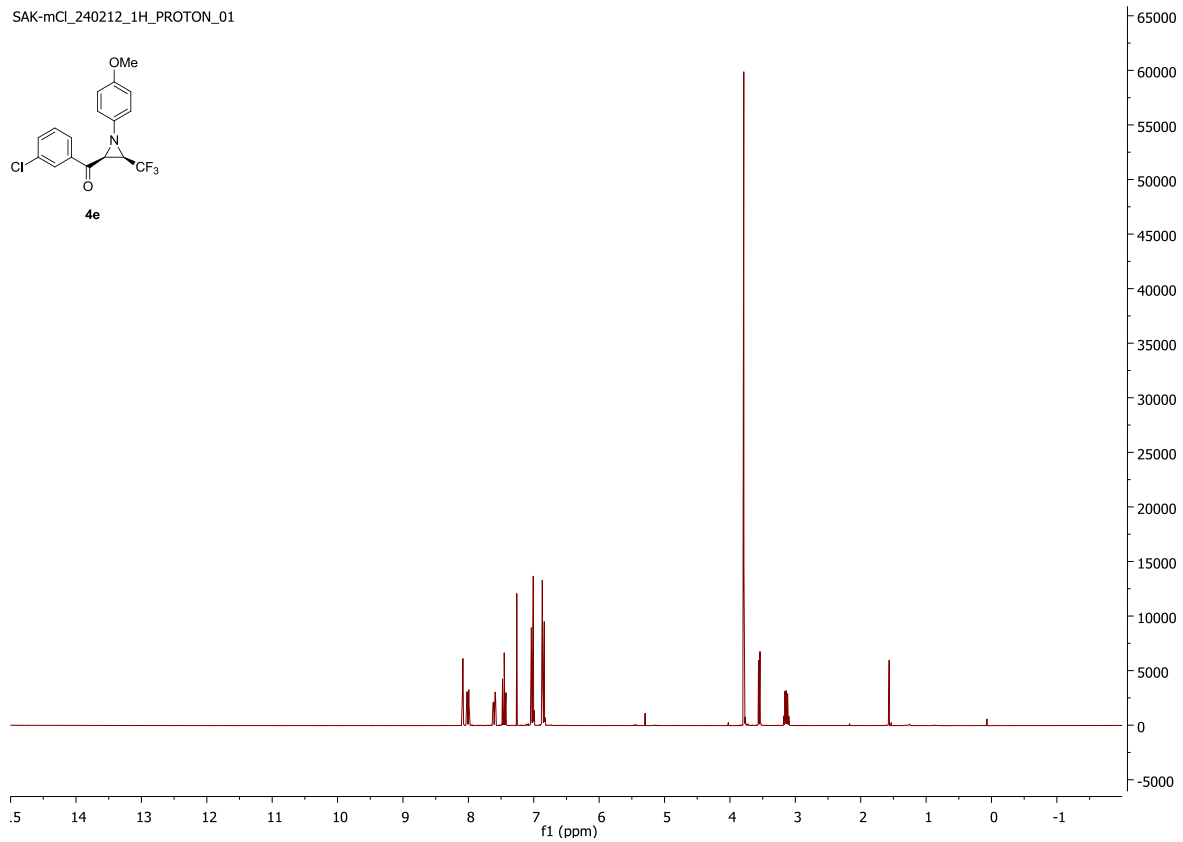
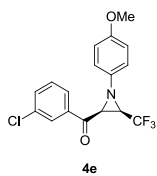
14-14-06-emoran
Sample SAK-080_FCfrac3_13C
group carrei
CAR CDCl3 /opt/v emoran 14



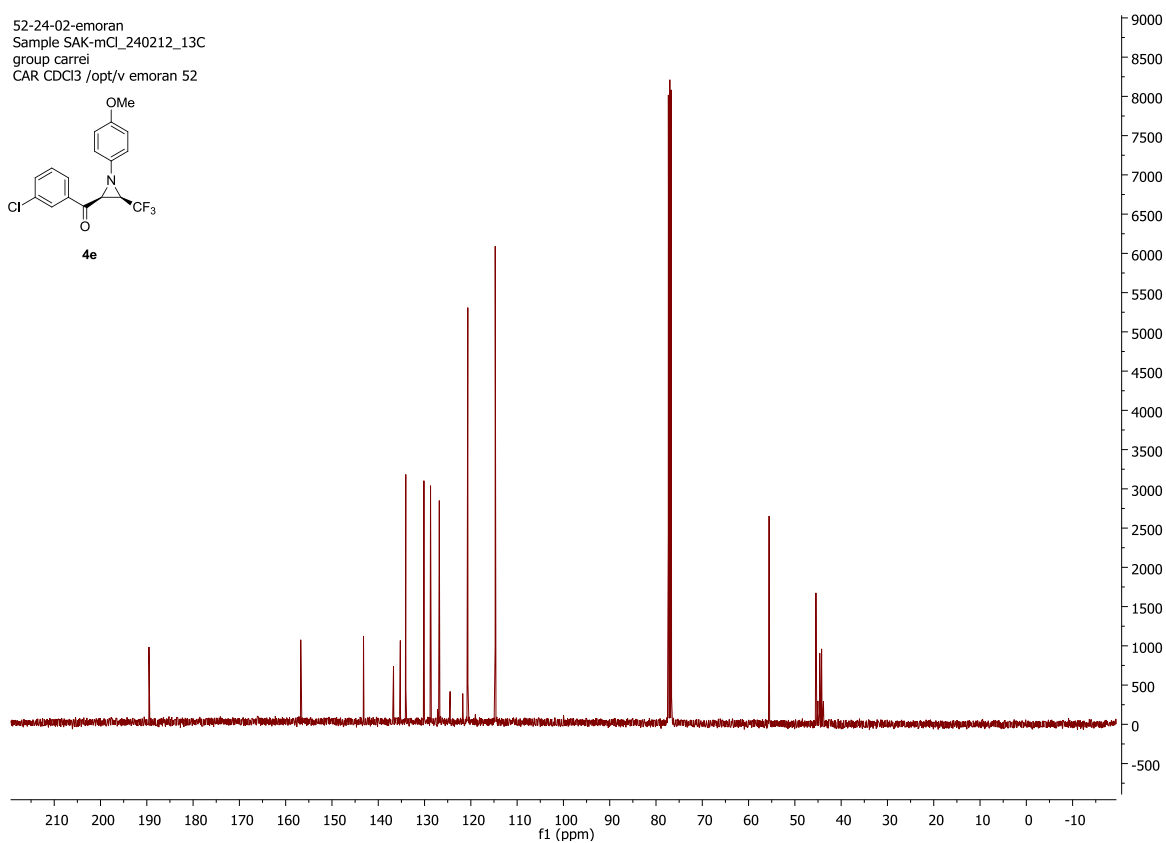
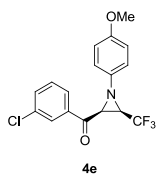
SAK-080_FCfrac3_19F
19F OBSERVE
STANDARD PARAMETERS



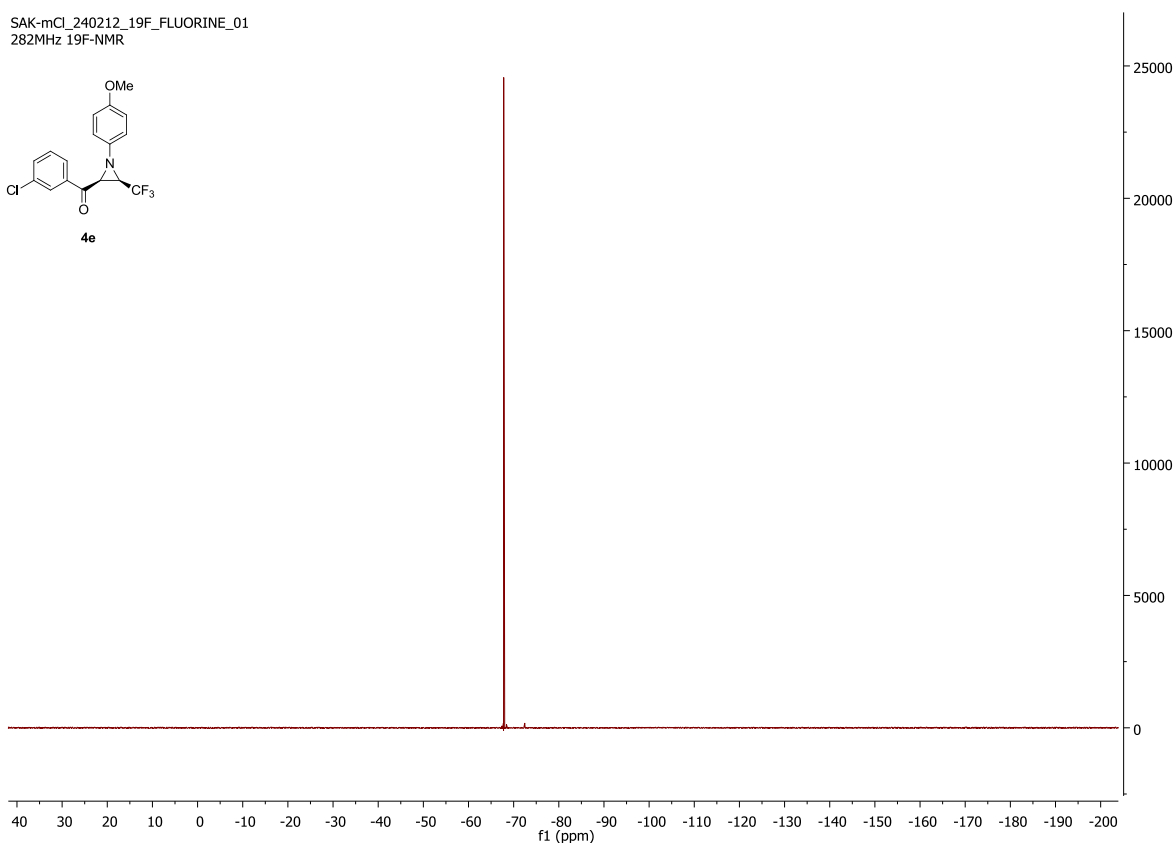
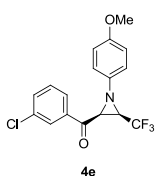
SAK-mCl_240212_1H_PROTON_01



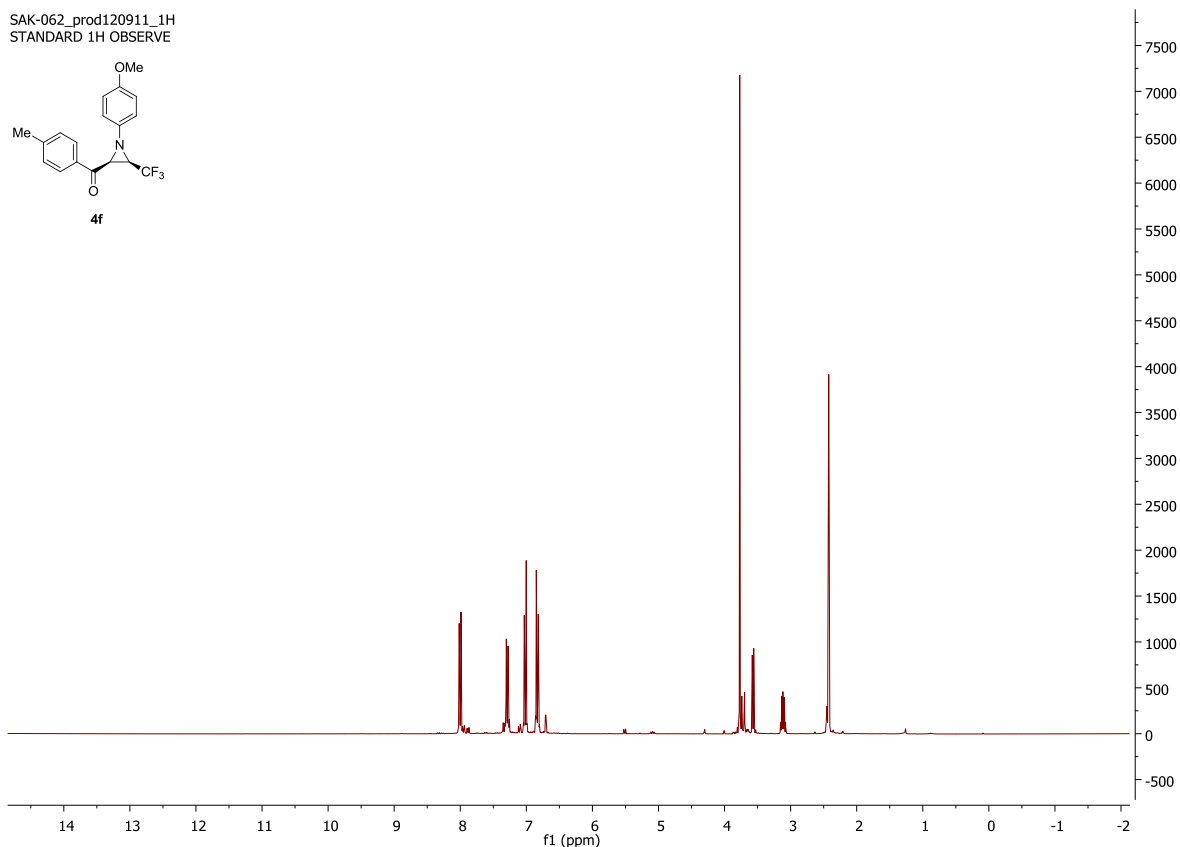
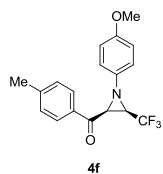
52-24-02-emoran
 Sample SAK-mCl_240212_13C
 group carrei
 CAR CDCl3 /opt/v emoran 52



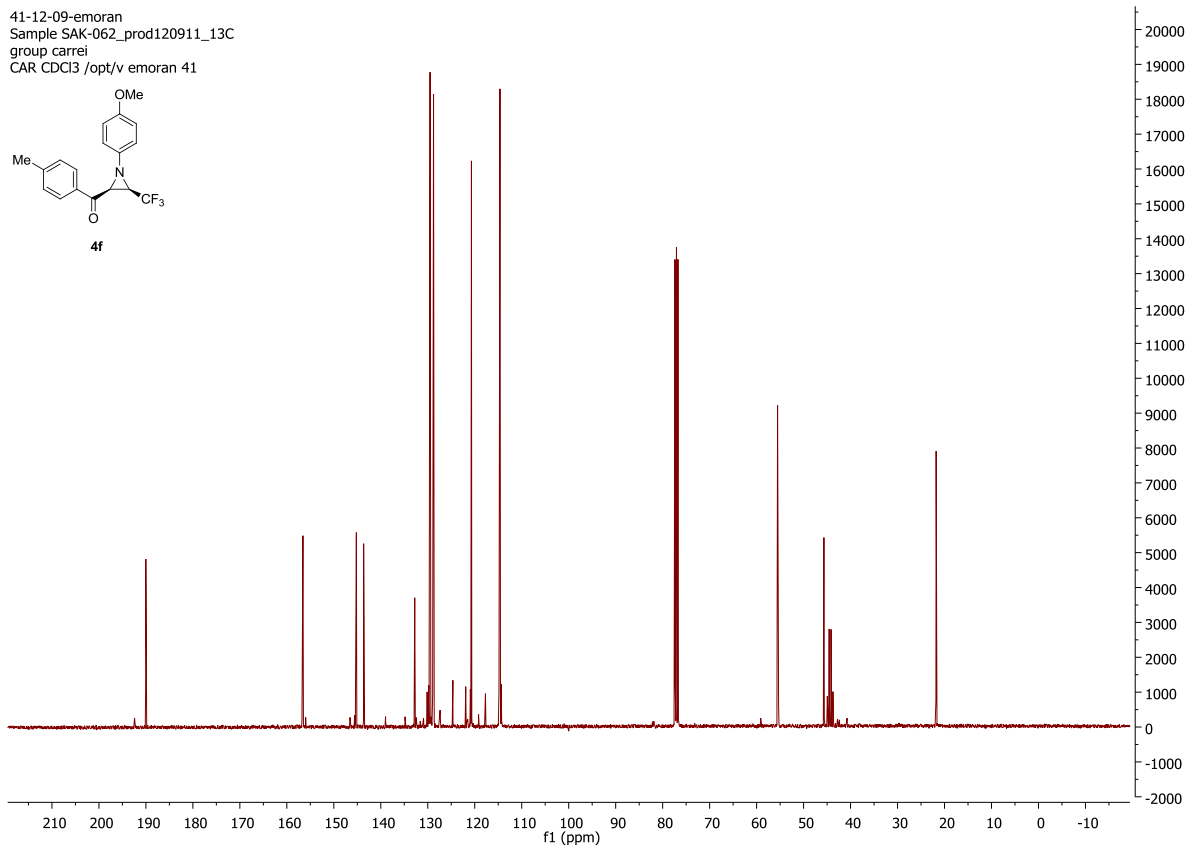
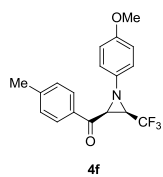
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 282MHz 19F-NMR



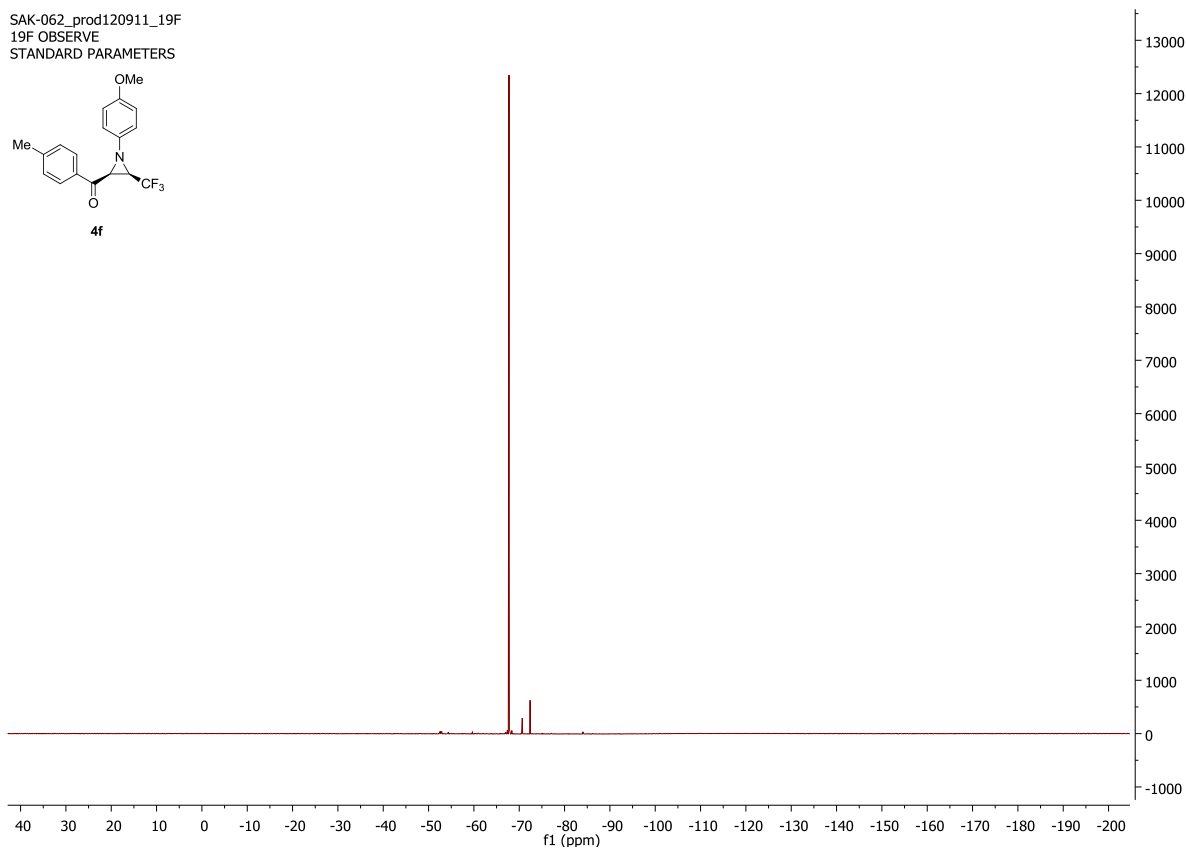
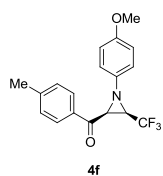
SAK-062_prod120911_1H
STANDARD 1H OBSERVE



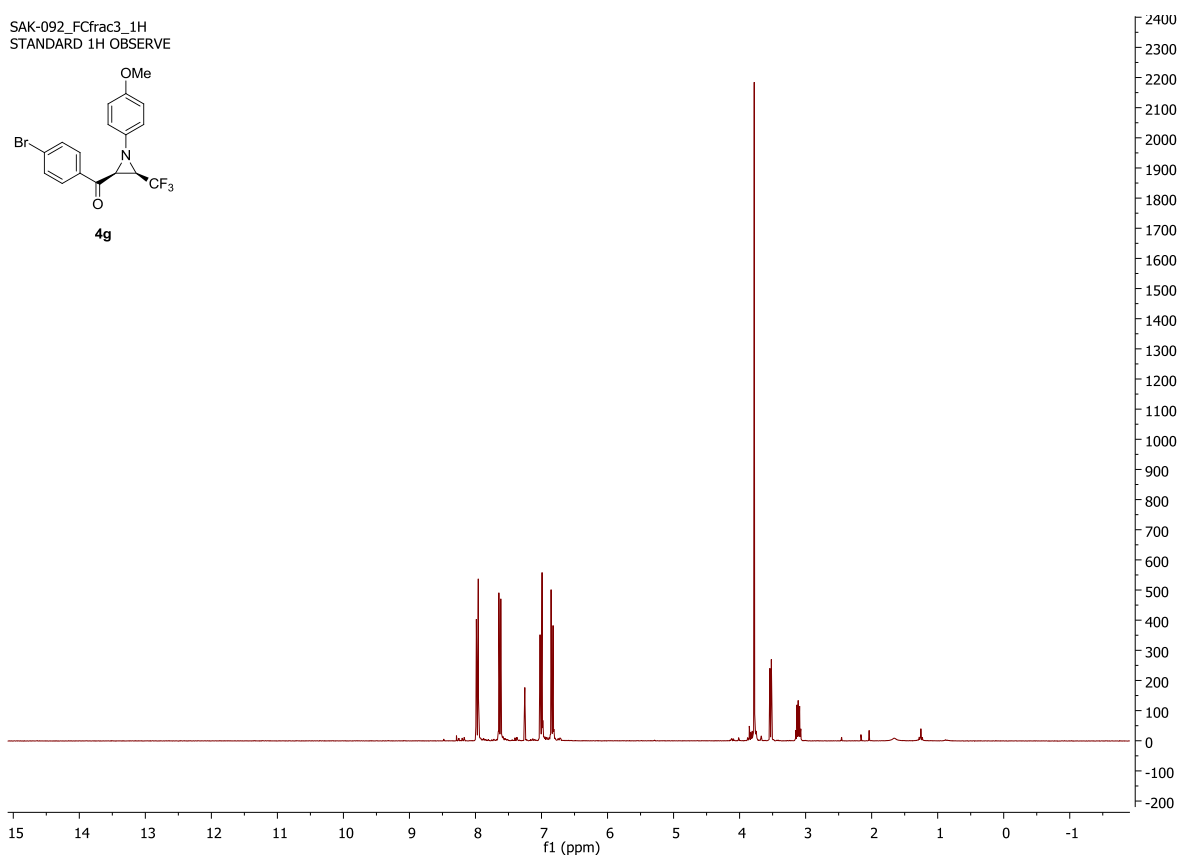
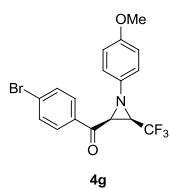
41-12-09-emoran
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group carrei
CAR CDCl3 /opt/v emoran 41



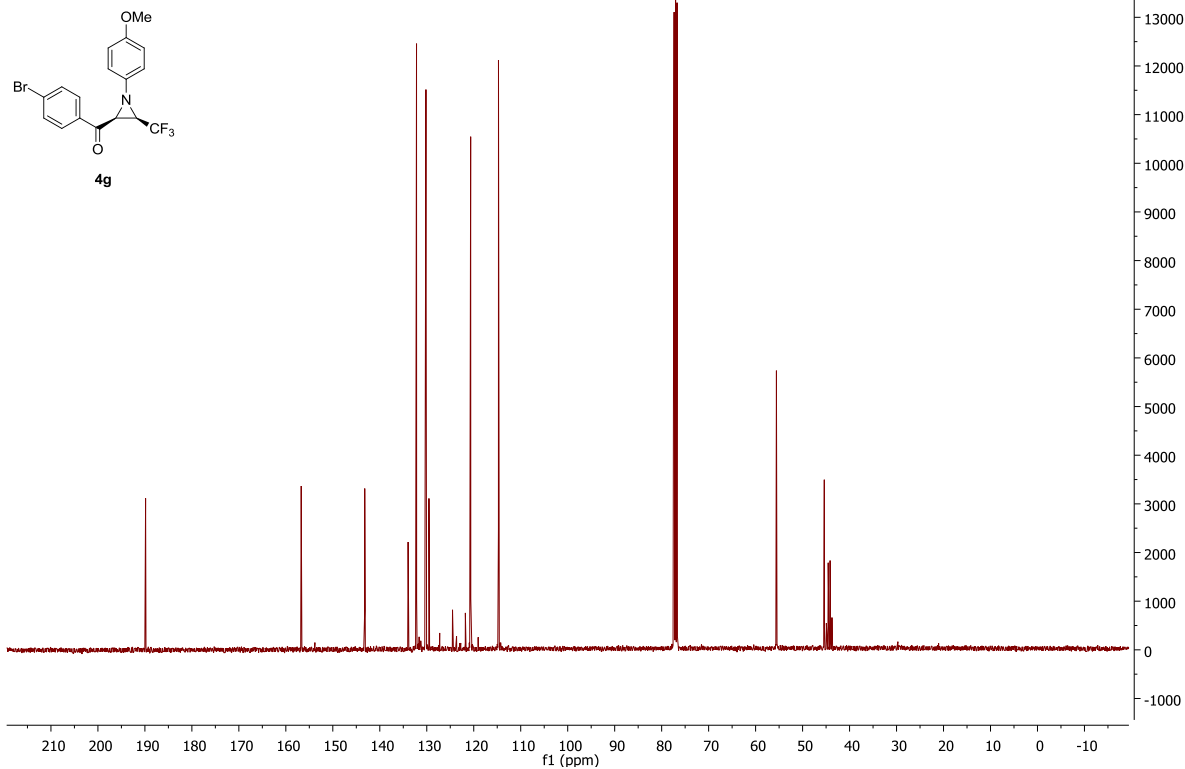
SAK-062_prod120911_19F
19F OBSERVE
STANDARD PARAMETERS



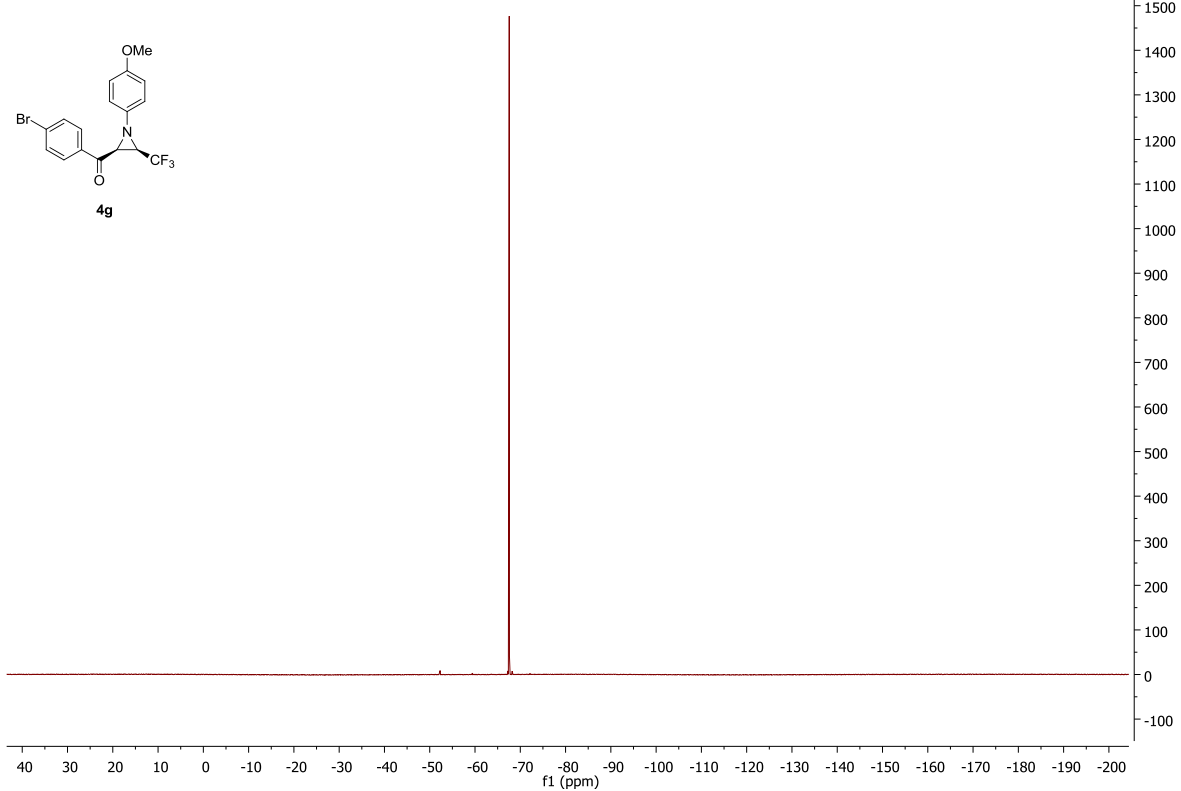
SAK-092_FCfrac3_1H
STANDARD 1H OBSERVE



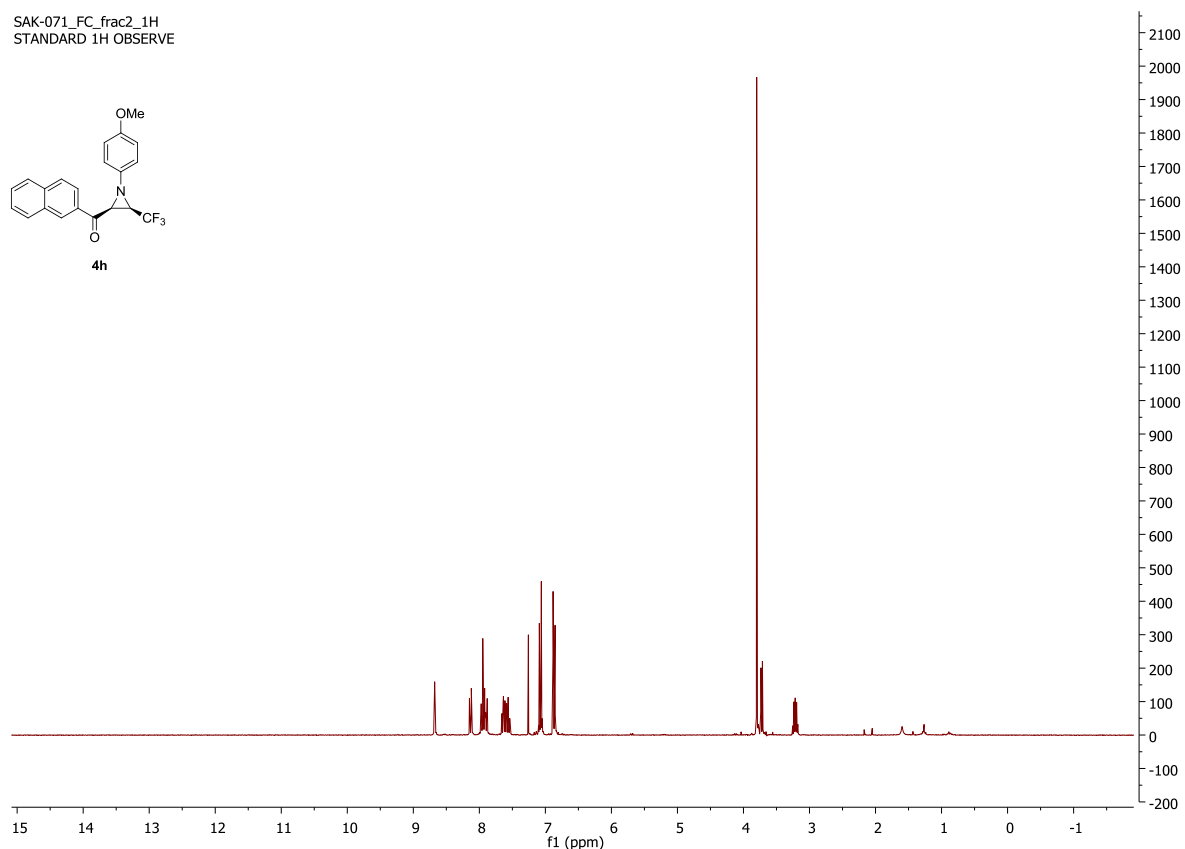
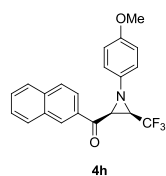
7-13-09-emoran
 Sample SAK-092_FCfrac3_13C
 group carrei
 CAR CDCl3 /opt/v emoran 7



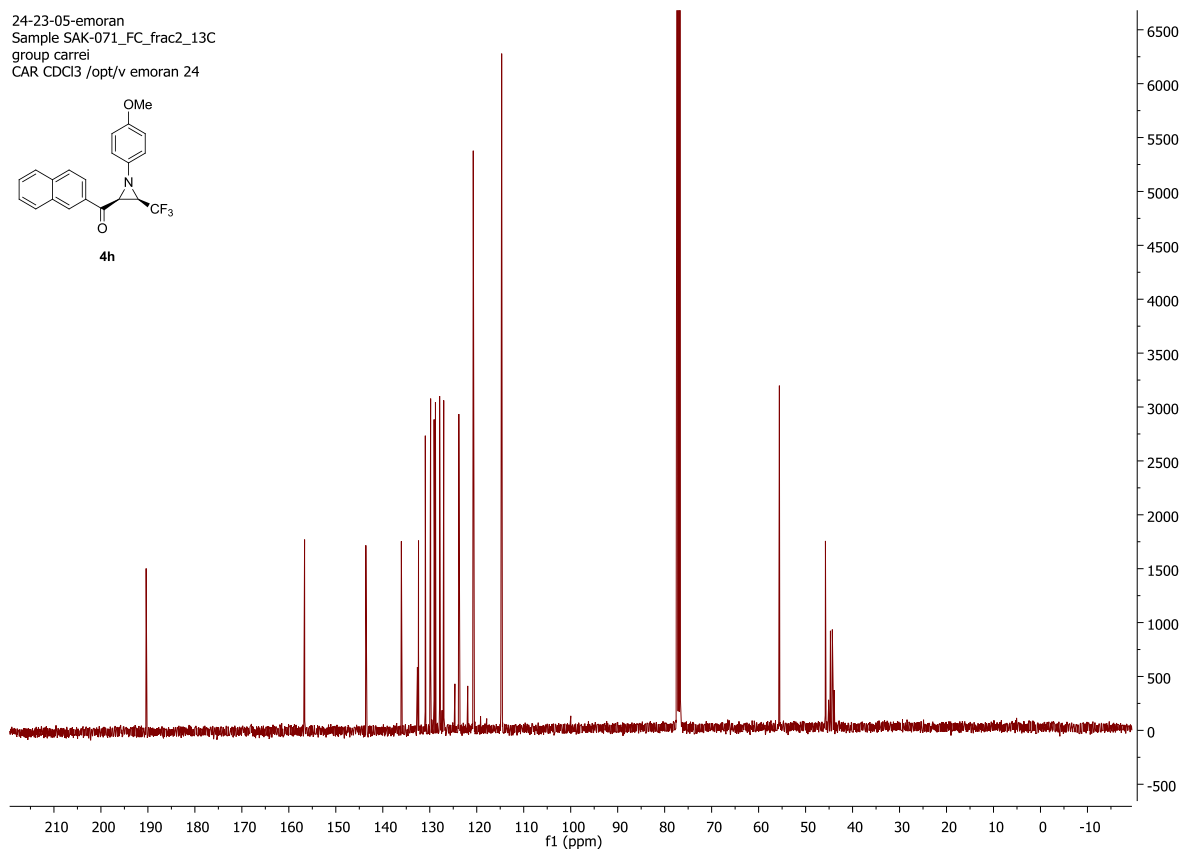
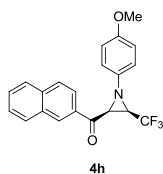
SAK-092_FCfrac3_19F
 19F OBSERVE
 STANDARD PARAMETERS



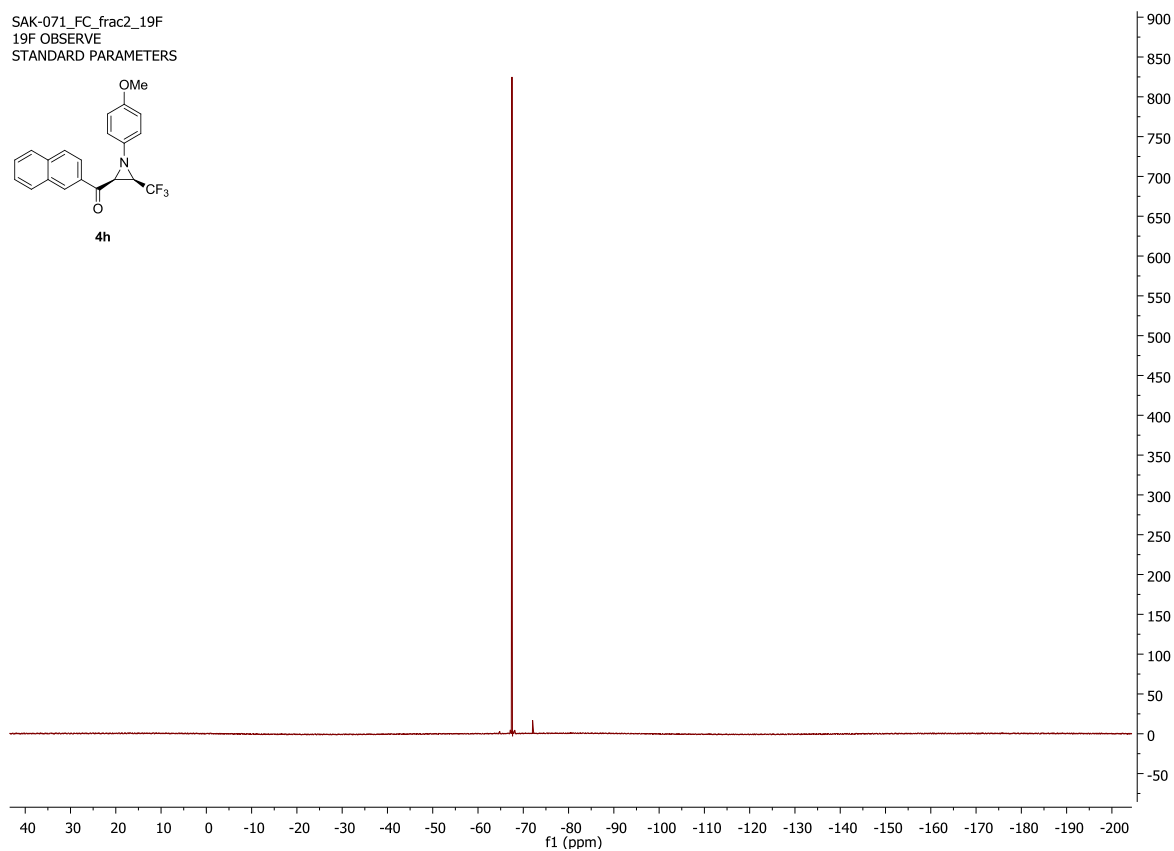
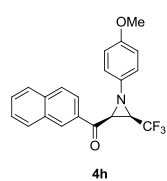
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STANDARD 1H OBSERVE



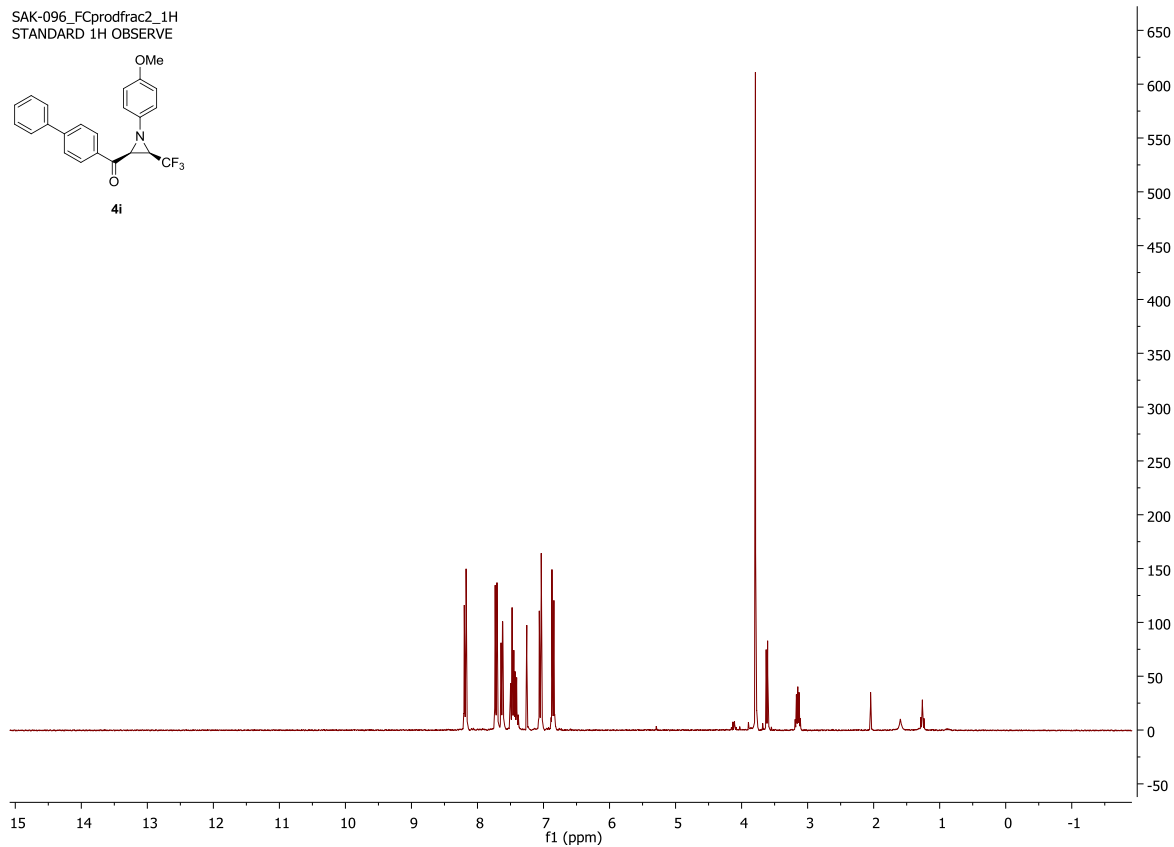
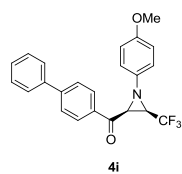
24-23-05-emoran
Sample SAK-071_FC_frac2_13C
group carrei
CAR CDCl₃ /opt/v emoran 24



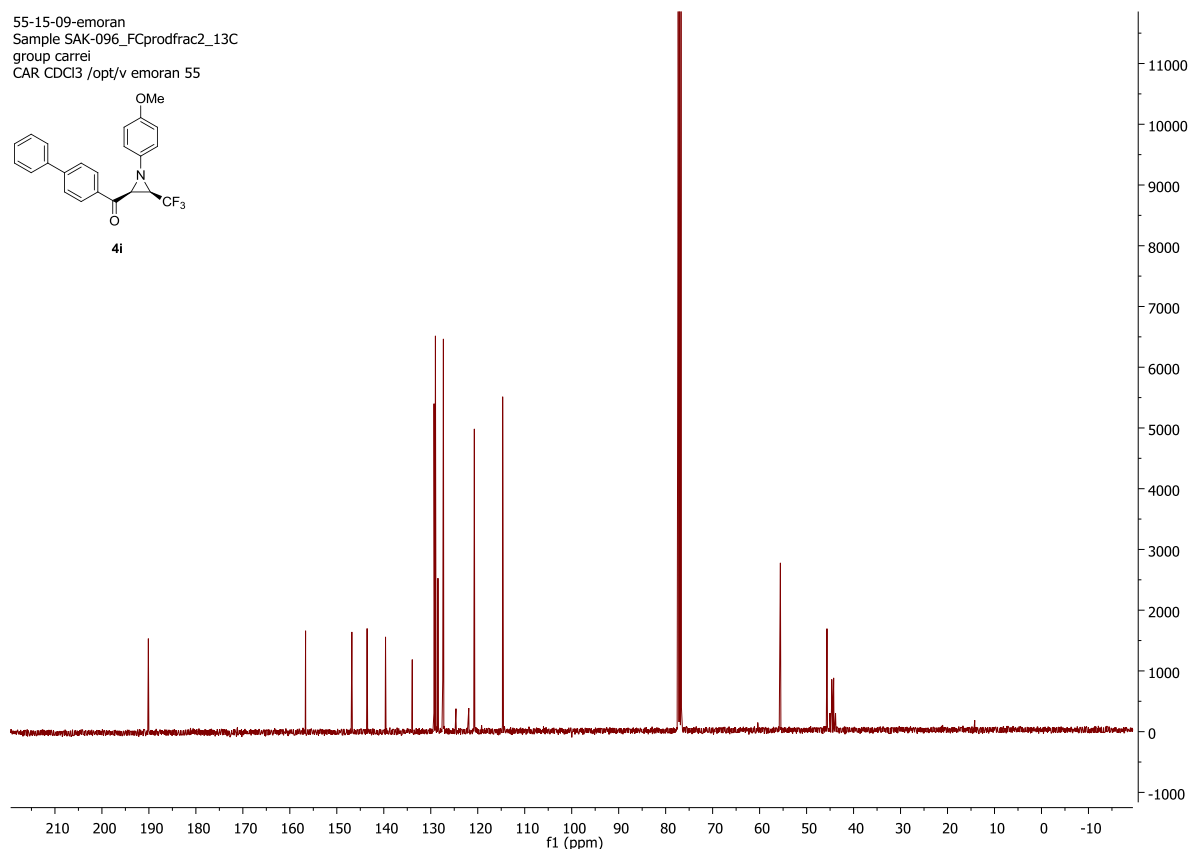
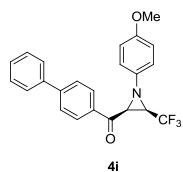
SAK-071_FC_frac2_19F
19F OBSERVE
STANDARD PARAMETERS



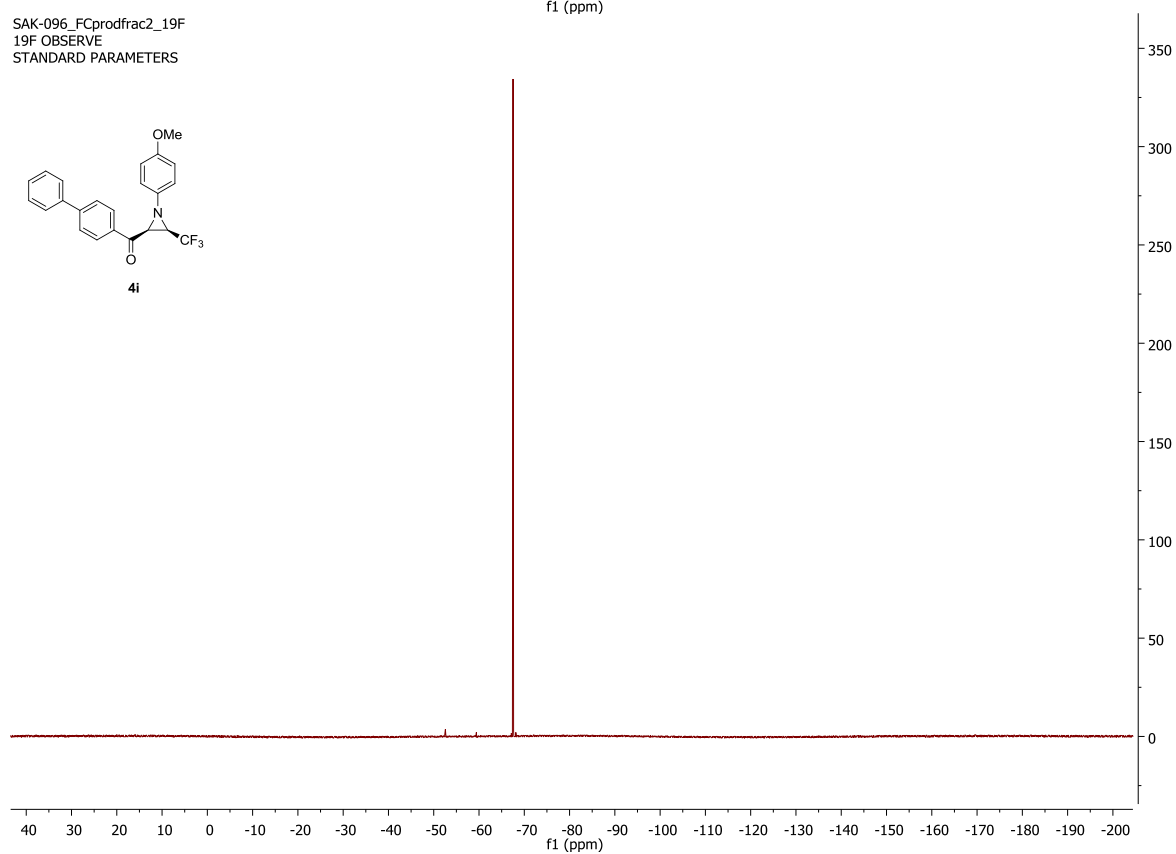
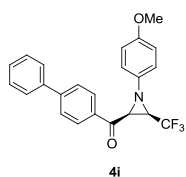
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STANDARD 1H OBSERVE



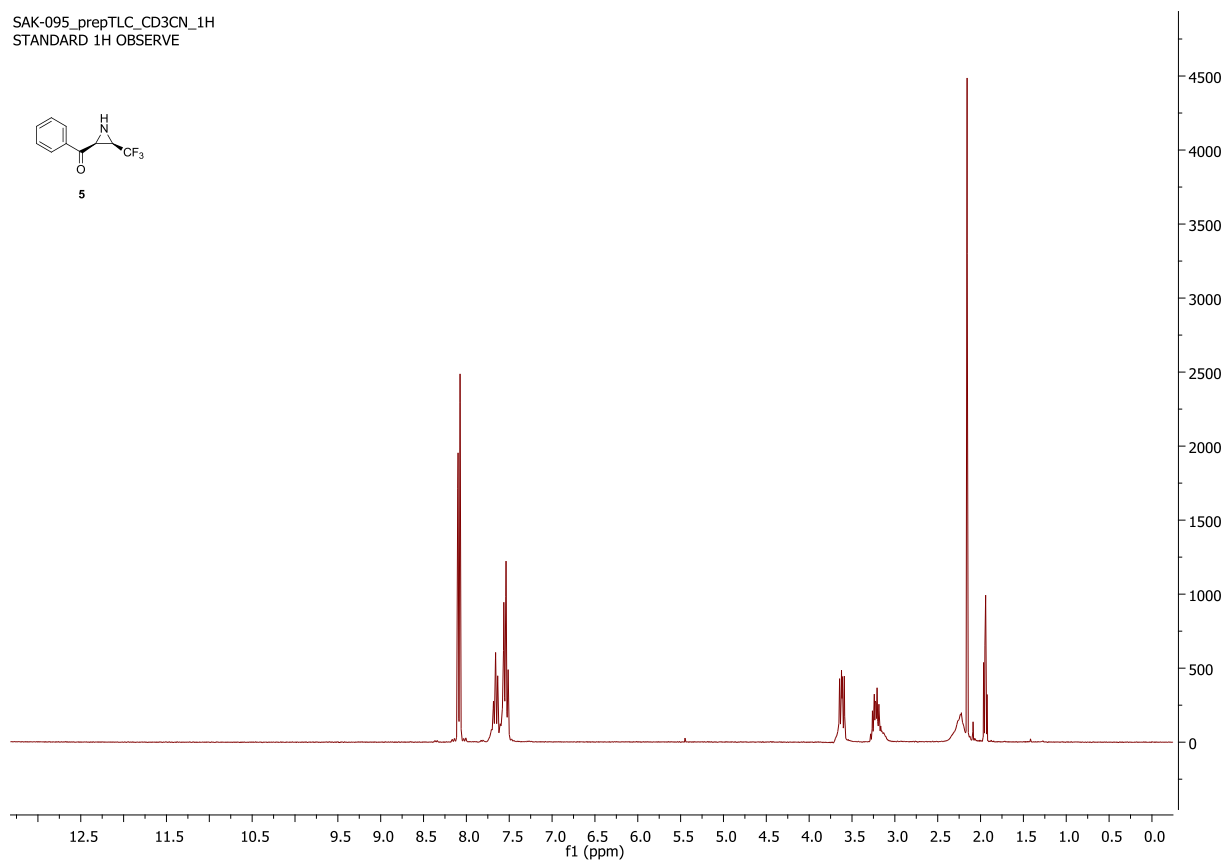
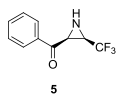
55-15-09-emoran
 Sample SAK-096_FCprodfrac2_13C
 group carrei
 CAR CDCl3 /opt/v emoran 55



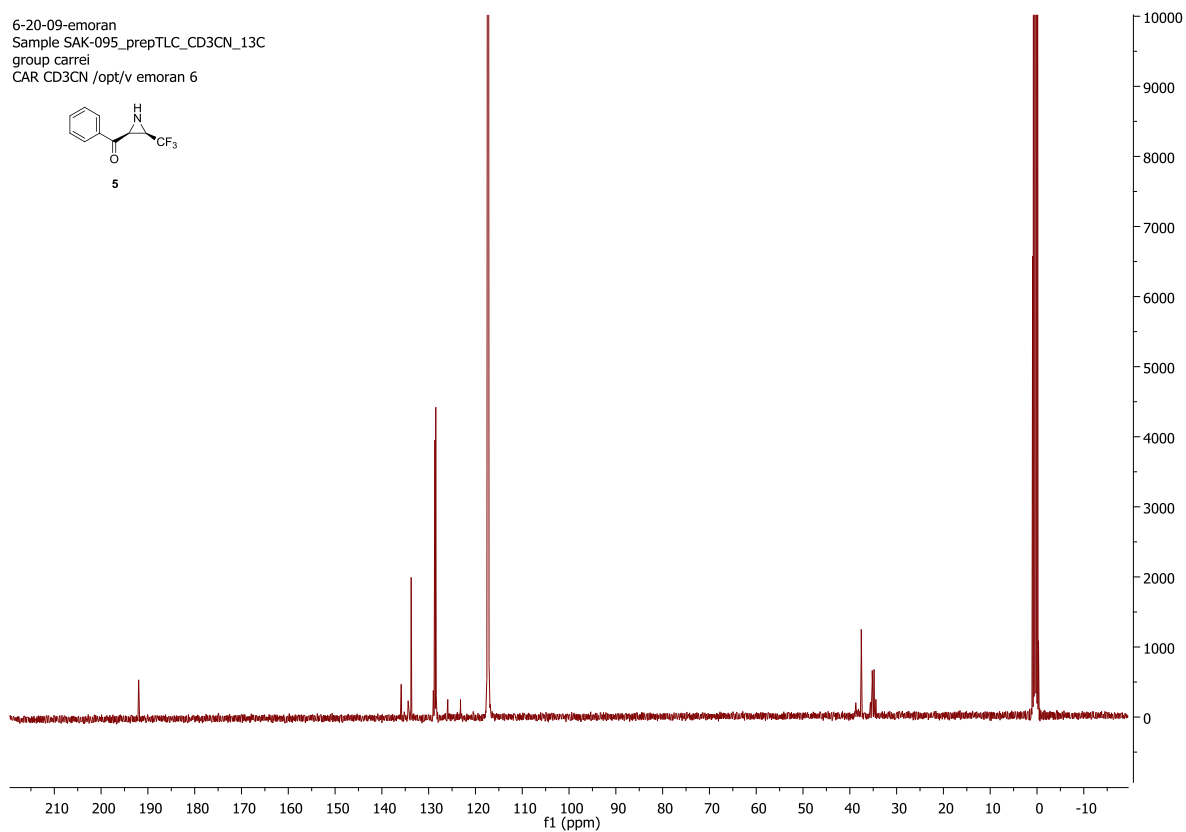
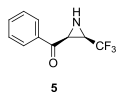
SAK-096_FCprodfrac2_19F
 19F OBSERVE
 STANDARD PARAMETERS



SAK-095_prepTLC_CD3CN_1H
STANDARD 1H OBSERVE



6-20-09-emoran
Sample SAK-095_prepTLC_CD3CN_13C
group carrel
CAR CD3CN /opt/v emoran 6



SAK-095_prepTLC_CD3CN_19F
19F OBSERVE
STANDARD PARAMETERS

