Supporting Information

for

Chiral phosphoric acid-catalyzed Friedel-Crafts reaction of 2,5-disubstituted and 2-monosubstituted pyrroles with isoindolinone-derived ketimines

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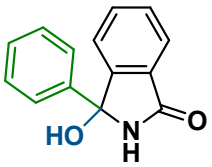
1. General Information

Chemicals and solvents were purchased from commercial suppliers and used as received. Flash column chromatography was carried out using silica gel (Merck, 40−63 μm particle size). Petroleum ether used are fractions collected at 40-60 °C. NMR spectra were recorded on Bruker Avance 600 and 300 MHz spectrometers, operating at 150.92 or 75.47 MHz for ^{13}C and 600.13 or 300.13 MHz for ^{1}H nuclei. Chemical shifts are quoted in ppm and are referenced to the residual nondeuterated solvent peak. Spectra were acquired at 298 K.

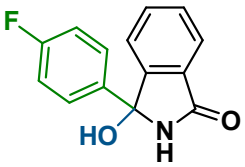
Infrared spectra were recorded on a Varian UV/Vis Cary 4000 spectrometer equipped with an attenuated total reflectance attachment with internal calibration. Mass spectrometry measurements were performed on an HPLC system coupled with a triple quadrupole mass spectrometer, operating in a positive electrospray ionization (ESI) mode. High resolution mass spectrometry (HRMS) was performed on MALDI-TOF Bruker Daltonik Microflex series. Melting points were determined using an Electrothermal 9100 apparatus in open capillaries and are uncorrected. Enantiomeric ratios were determined on a Shimadzu LC-40 HPLC system with PDA detector.

Substrates, 3-aryl 3-hydroxyisoindolinones **Iso-1**–**Iso-15** and **Iso-Me** were synthesized in high yields from readily available starting materials, by employing addition of a Grignard or an organolithium reagent to phthalimide.[1] Chiral phosphoric acid catalysts **CPA1-CPA9** were synthesized according to known procedures.[2] Racemic standards were obtained by employing phenylphosphonic or *p*-toluenesulfonic acid instead of the chiral catalyst.

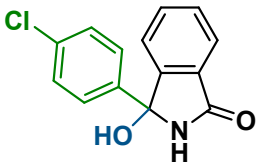
2. List of Starting Isoindolinone Alcohols



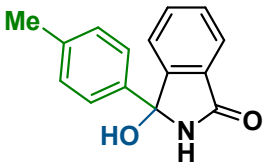
Iso-1



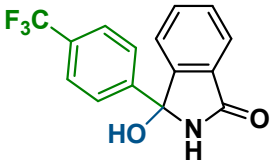
Iso-2



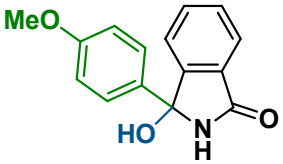
Iso-3



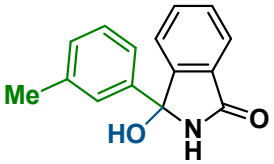
Iso-4



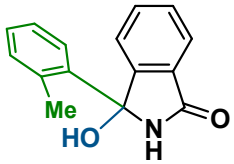
Iso-5



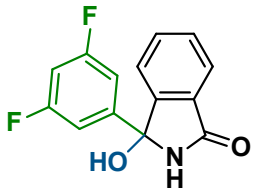
Iso-6



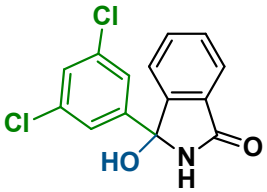
Iso-7



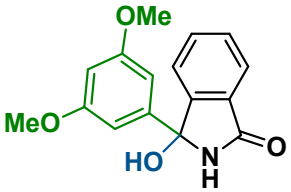
Iso-8



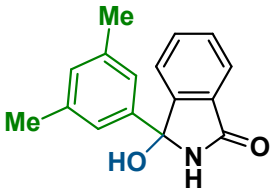
Iso-9



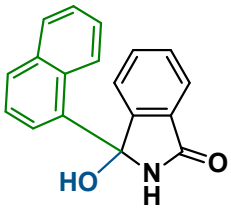
Iso-10



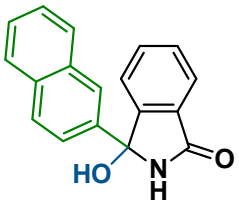
Iso-11



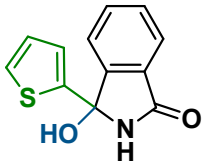
Iso-12



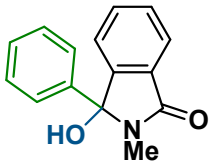
Iso-13



Iso-14



Iso-15



Iso-Me

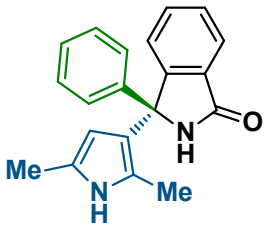
3. Experimental Procedures and Analytical Data

General procedure

Chiral phosphoric acid **CPA8** (0.005 mmol) was added to a suspension of isoindolinone alcohol (0.1 mmol) in toluene (2 mL) at room temperature. After stirring for 5 min, pyrrole derivative (0.11 mmol) was added, and the resulting reaction mixture was stirred in an oil bath at 80 °C until full consumption of the starting material (monitored by TLC). The reaction mixture was cooled to room temperature and directly purified by flash column chromatography on silica gel using ethyl acetate/petroleum ether as an eluent system. The solvent was evaporated, and the residue triturated with hexane to afford the corresponding product.

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-phenylisoindolinone (1)

Iso-1 (23 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **1** (29 mg, 96% yield) as a colorless solid. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Reaction time: 15 min. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **92:8 e.r.** t_{R1} = 9.1 min (major), t_{R2} = 14.3 min (minor).



^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.31 (s, 1H), 9.28 (s, 1H), 7.68 (d, *J* = 7.4 Hz, 1H), 7.64 – 7.52 (m, 2H), 7.52 – 7.43 (m, 3H), 7.40 – 7.24 (m, 3H), 5.20 (s, 1H), 2.07 (s, 3H), 1.65 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.8, 152.4, 144.7, 132.0, 131.3, 128.5, 128.3, 128.2, 127.4, 126.9, 126.7, 126.3, 124.8, 123.3, 123.3, 123.2, 119.8, 106.7, 66.9, 12.9, 12.6.

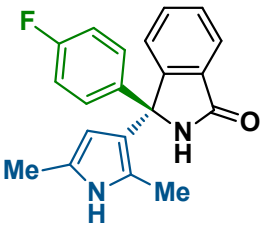
m.p. 270.1-271.3 °C

FT-IR: ν = 3249, 3182, 3041, 1662, 719 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{19}N_2O$: 303.1492; found: 303.1485

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(4-fluorophenyl)isoindolinone (2)

Iso-2 (24 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **2** (30 mg, 95% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3.



Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **92:8 e.r.** t_{R1} = 7.8 min (major), t_{R2} = 11.5 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.29 (s, 1H), 9.26 (s, 1H), 7.64 (d, *J* = 7.4 Hz, 1H), 7.61 – 7.52 (m, 1H), 7.53 – 7.39 (m, 4H), 7.13 (t, *J* = 8.9 Hz, 2H), 5.14 (s, 1H), 2.02 (s, 3H), 1.62 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d6) (δ/ppm): 168.3, 161.1 (d, $^{1}J_{C\text{-}F}$ = 242.2 Hz), 159.5, 151.8, 140.4, 131.7, 130.7, 128.3, 128.2, 127.8, 124.2, 122.9, 122.8, 122.7, 119.2, 114.9, 114.6, 106.2, 66.04, 12.4, 12.1.

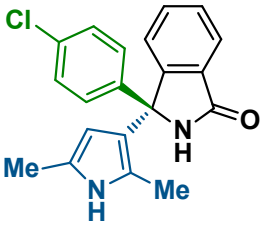
^{19}F NMR (282 MHz, DMSO) (δ/ppm): -114.8.

m.p. 205.3-206.0 °C

FT-IR: ν = 3355, 3174, 3047, 1681, 1218, 735 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{18}FN_2O$: 321.1398; found: 321.1396

(*S*)-3-(4-chlorophenyl)-3-(2,5-dimethyl-1H-pyrrol-3-yl)isoindolinone (3)



Iso-3 (26 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **3** (31 mg, 91% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **91:9 e.r.** t_{R1} = 7.6 min (major), t_{R2} = 12.0 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.31 (s, 1H), 9.27 (s, 1H), 7.64 (d, *J* = 7.4 Hz, 1H), 7.60 – 7.51 (m, 1H), 7.51 – 7.40 (m, 4H), 7.37 (d, *J* = 8.8 Hz, 2H), 5.14 (s, 1H), 2.02 (s, 3H), 1.63 (s, 3H).

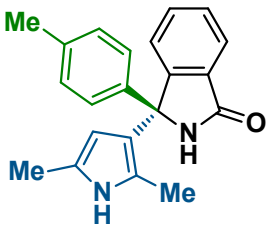
^{13}C NMR (75 MHz, DMSO-d6) (δ/ppm): 168.4, 151.5, 143.4, 131.7, 131.6, 130.7, 128.1, 128.0, 127.9, 124.2, 123.1, 122.9, 122.8, 118.9, 106.1, 66.1, 12.4, 12.2.

m.p. 230.9-231.7 °C

FT-IR: 3340, 3179, 3037, 1667, 754 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{18}ClN_2O$: 337.1102; found: 337.1097

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(*p*-tolyl)isoindolinone (4)



Iso-4 (24 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **4** (30 mg, 95% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **93:7** e.r. t_{R1} = 9.3 min (major), t_{R2} = 15.0 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.25 (s, 1H), 9.18 (s, 1H), 7.62 (d, *J* = 7.4 Hz, 1H), 7.59 – 7.50 (m, 1H), 7.50 – 7.38 (m, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.14 (s, 1H), 2.25 (s, 3H), 2.02 (s, 3H), 1.62 (s, 3H).

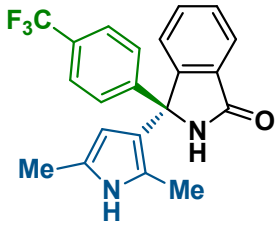
^{13}C NMR (75 MHz, DMSO-d6) (δ/ppm): 168.4, 152.1, 141.2, 135.9, 131.4, 130.8, 128.6, 127.6, 126.1, 124.2, 122.8, 122.6, 119.3, 106.3, 66.3, 20.5, 12.5, 12.2.

m.p. 241.6-242.3 °C

FT-IR: *v* = 3245, 3179, 3048, 1667, 739 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{21}H_{21}N_2O$: 317.1648; found: 317.1644

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(4-(trifluoromethyl)phenyl)isoindolinone (5)



Iso-5 (29 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **5** (32 mg, 86% yield) as a colorless solid. Reaction time: 10 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 15% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **94:6 e.r.** t_{R1} = 7.0 min (major), t_{R2} = 12.8 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.35 (s, 1H), 9.36 (s, 1H), 7.74 – 7.62 (m, 5H), 7.62 – 7.42 (m, 3H), 5.14 (s, 1H), 2.03 (s, 3H), 1.61 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d6) (δ/ppm): 168.4, 151.1, 149.1, 131.8, 130.8, 128.1, 126.9, 125.1 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 124.2, 123.2, 123.0, 122.9, 118.6, 106.1, 66.3, 12.4, 12.1.

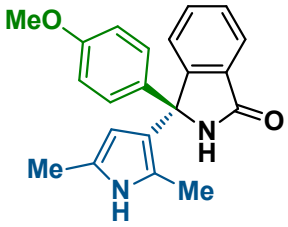
^{19}F NMR (282 MHz, DMSO) (δ/ppm): -59.5.

m.p. 230.4-230.8 °C

FT-IR: ν = 3355, 3169, 3053, 1677, 1328, 1118, 739 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{21}H_{18}F_3N_2O$: 371.1366; found: 371.1363

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(4-methoxyphenyl)isoindolinone (6)



Iso-6 (25 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **6** (30 mg, 91% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **88:12 e.r.** t_{R1} = 14.2 min (major), t_{R2} = 21.1 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.29 (s, 1H), 9.22 (s, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.49 (dd, *J* = 12.9, 6.9 Hz, 2H), 7.37 (d, *J* = 8.8 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 5.20 (s, 1H), 3.77 (s, 3H), 2.07 (s, 3H), 1.68 (s, 3H).

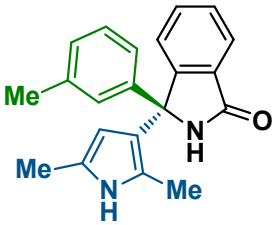
^{13}C NMR (75 MHz, DMSO-d6) (δ/ppm): 168.3, 158.1, 152.3, 136.1, 131.5, 130.8, 127.5, 127.37, 124.1, 122.8, 122.6, 119.5, 113.3, 106.3, 66.1, 54.9, 12.5, 12.2.

m.p. 228.5-229.5 °C

FT-IR: *v* = 3255, 3178, 3032, 1661, 1249, 755 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{21}H_{21}N_2O_2$: 333.1598; found: 333.1594

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(*m*-tolyl)isoindolinone (7)



Iso-7 (24 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **7** (30 mg, 95% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **67:33 e.r.** t_{R1} = 9.2 min (major), t_{R2} = 14.7 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.30 (s, 1H), 9.23 (s, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.64 – 7.54 (m, 1H), 7.49 (dd, *J* = 14.2, 7.1 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 5.19 (s, 1H), 2.31 (s, 3H), 2.07 (s, 3H), 1.67 (s, 3H).

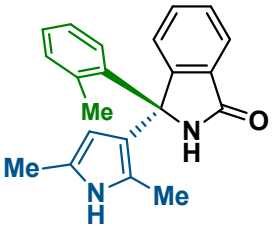
^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.9, 152.6, 141.8, 136.4, 131.9, 131.3, 129.1, 128.1, 126.6, 124.7, 123.3, 123.3, 123.1, 119.8, 106.8, 80.7, 66.8, 20.9, 12.9, 12.7.

m.p. 247.7-248.9 °C

FT-IR: *v* = 3255, 3178, 3037, 1667, 749 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{21}H_{21}N_2O$: 317.1648; found: 317.1645

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(*o*-tolyl)isoindolinone (8)



Iso-8 (24 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **8** (30 mg, 95% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **57:43 e.r.** t_{R1} = 8.8 min (major), t_{R2} = 10.2 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.23 (s, 1H), 9.08 (s, 1H), 7.71 (d, *J* = 7.4 Hz, 1H), 7.68 – 7.56 (m, 1H), 7.56 – 7.46 (m, 1H), 7.43 (d, *J* = 7.6 Hz, 1H), 7.24 – 7.07 (m, 4H), 5.31 (s, 1H), 2.13 (s, 3H), 2.08 (s, 3H), 1.83 (s, 3H).

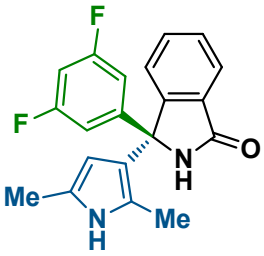
^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 169.2, 152.4, 141.2, 137.6, 132.9, 132.0, 131.4, 128.1, 127.9, 127.4, 125.9, 125.2, 124.1, 123.2, 121.7, 120.4, 105.3, 67.8, 21.5, 13.0, 12.7.

m.p. 207.7-208.7 °C

FT-IR: *v* = 3275, 2916, 2856, 1687, 704 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{21}H_{21}N_2O$: 317.1648; found: 317.1647

(*S*)-3-(3,5-difluorophenyl)-3-(2,5-dimethyl-1H-pyrrol-3-yl)isoindolinone (9)



Iso-9 (26 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **9** (27 mg, 80% yield) as a colorless solid. Reaction time: 1 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **98.5:1.5** e.r. t_{R1} = 5.6 min (major), t_{R2} = 6.5 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.36 (s, 1H), 9.31 (s, 1H), 7.71 – 7.54 (m, 3H), 7.53 – 7.43 (m, 1H), 7.21 – 7.03 (m, 3H), 5.13 (s, 1H), 2.03 (s, 3H), 1.63 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.3, 162.1 (d, $^1J_{C\text{-}F}$ = 247.6 Hz), 162.1 (d, $^1J_{C\text{-}F}$ = 246.1 Hz), 150.6, 149.2, 131.9, 130.7, 128.2, 124.3, 123.3, 123.0, 122.9, 118.3, 109.6, 109.4, 106.0, 102.6, 66.1, 12.4, 12.0.

^{19}F NMR (282 MHz, DMSO) (δ/ppm): -108.0.

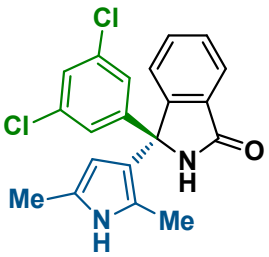
m.p. 243.7-244.4 °C

$[\alpha]_D$ = +104 ° (c 0.87, EtOAc) for 98.5:1.5 e.r.

FT-IR: ν = 3320, 3174, 3017, 1661, 1117, 755 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{17}F_2N_2O$: 339.1303; found: 339.1304

(*S*)-3-(3,5-dichlorophenyl)-3-(2,5-dimethyl-1H-pyrrol-3-yl)isoindolinone (10)



Iso-10 (29 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **10** (35 mg, 94% yield) as a colorless solid. Reaction time: 1 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3.. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 15% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **98:2 e.r.** t_{R1} = 6.8 min (major), t_{R2} = 8.5 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.39 (s, 1H), 9.34 (s, 1H), 7.73 – 7.44 (m, 5H), 7.40 (d, *J* = 1.9 Hz, 2H), 5.14 (s, 1H), 2.03 (s, 3H), 1.64 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.3, 150.4, 148.7, 133.9, 132.1, 130.6, 128.3, 126.8, 125.0, 124.3, 123.4, 122.9, 118.1, 106.0, 65.9, 12.4, 12.1.

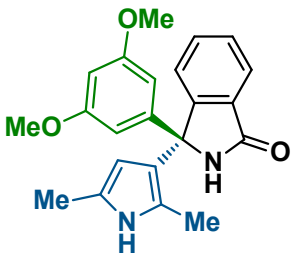
m.p. 248.8-249.5 °C

$[\alpha]_D$ = +90 ° (c 0.73, EtOAc) for 98:2 e.r.

FT-IR: *v* = 3345, 3174, 3047, 1672, 709 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{17}Cl_2N_2O$: 371.0712; found: 371.0710

(*S*)-3-(3,5-dimethoxyphenyl)-3-(2,5-dimethyl-1H-pyrrol-3-yl)isoindolinone (11)



Iso-11 (28 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **11** (30 mg, 83% yield) as a colorless solid. Reaction time: 1 h. Column chromatography eluent: petroleum ether/ethyl acetate = 1/2. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 30% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **96:4 e.r.** t_{R1} = 7.8 min (major), t_{R2} = 9.6 min (minor).

^{1}H NMR (600 MHz, DMSO-d6) (δ/ppm): 10.30 (d, *J* = 1.4 Hz, 1H), 9.23 (s, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.63 – 7.53 (m, 2H), 7.49 (t, *J* = 7.3 Hz, 1H), 6.61 (d, *J* = 2.2 Hz, 2H), 6.45 (t, *J* = 2.3 Hz, 1H), 5.19 (dd, *J* = 2.7, 0.7 Hz, 1H), 3.73 (s, 6H), 2.07 (s, 3H), 1.70 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d6) (δ/ppm): 168.4, 160.1, 151.6, 146.6, 131.5, 130.8, 127.7, 124.27, 122.9, 122.8, 122.7, 118.9, 106.2, 104.9, 98.1, 66.5, 55.1, 12.5, 12.1.

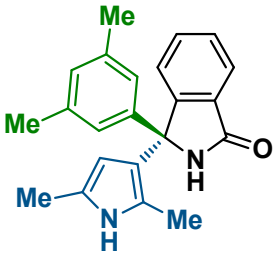
m.p. 249.9-250.5 °C

$[\alpha]_D$ = +90 ° (c 0.73, EtOAc) for 96:4 e.r.

FT-IR: *v* = 3345, 3174, 3047, 1672, 709 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{22}H_{23}N_2O_3$: 363.1703; found: 363.1699

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(3,5-dimethylphenyl)isoindolinone (12)



Iso-12 (25 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **12** (32 mg, 96% yield) as a colorless solid. Reaction time: 45 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **95:5 e.r.** t_{R1} = 7.8 min (major), t_{R2} = 11.0 min (minor).

^{1}H NMR (600 MHz, DMSO-d6) (δ/ppm): 10.28 (s, 1H), 9.18 (s, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.09 (s, 2H), 6.91 (s, 1H), 5.17 (d, *J* = 2.1 Hz, 1H), 2.27 (s, 6H), 2.07 (s, 3H), 1.66 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d6) (δ/ppm): 168.4, 152.0, 144.1, 136.9, 131.4, 130.8, 128.3, 127.58, 124.3, 123.9, 122.9, 122.7, 122.6, 119.3, 106.2, 66.4, 21.1, 12.5, 12.2.

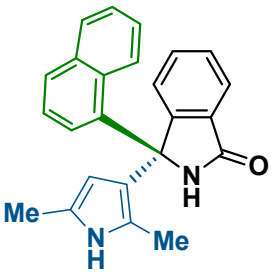
m.p. 238.1-238.7 °C

$[\alpha]_D$ = +115 ° (c 0.67, EtOAc) for 95:5 e.r.

FT-IR: *v* = 3285, 3189, 2927, 1667, 704 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{22}H_{23}N_2O$: 331.1805; found: 331.1803

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(naphthalen-1-yl)isoindolinone (13)



Iso-13 (28 mg) and 2,5-dimethylpyrrole (12 μL) afforded product **13** (34 mg, 96% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **88:12 e.r.** t_{R1} = 10.8 min (major), t_{R2} = 17.2 min (minor).

^{1}H NMR (600 MHz, DMSO-d6) (δ/ppm): 10.15 (s, 1H), 9.33 (d, *J* = 10.8 Hz, 1H), 8.17 (s, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.86 (s, 1H), 7.70 (s, 1H), 7.54 (s, 2H), 7.50 – 7.40 (m, 3H), 7.40 – 7.31 (m, 2H), 5.21 (s, 1H), 2.02 (s, 3H), 1.51 (s, 3H).

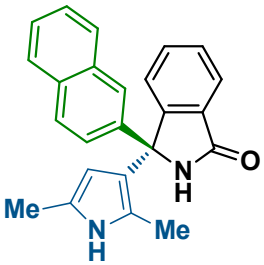
^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.5, 134.4, 131.5, 131.1, 130.7, 128.7, 128.5, 127.9, 126.8, 125.3, 125.1, 124.8, 124.6, 123.7, 123.1, 104.6, 67.1, 12.6, 11.8.

m.p. 246.6-247.7 °C

FT-IR: ν = 3279, 2927, 1692, 755 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{24}H_{21}N_2O$: 353.1648; found: 353.1645

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(naphthalen-2-yl)isoindolinone (14)



Iso-14 (28 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **14** (34 mg, 96% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **84:16 e.r.** t_{R1} = 10.8 min (major), t_{R2} = 17.3 min (minor).

^{1}H NMR (600 MHz, DMSO-d6) (δ/ppm): 10.20 (s, 1H), 9.39 (s, 1H), 8.24 (s, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 7.4 Hz, 1H), 7.59 (s, 2H), 7.56 – 7.45 (m, 3H), 7.43 – 7.37 (m, 2H), 5.27 (s, 1H), 2.07 (s, 3H), 1.57 (s, 3H).

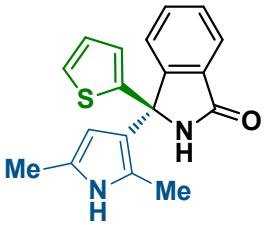
^{13}C NMR (75 MHz, DMSO-d6) (δ/ppm): 168.5, 134.4, 131.5, 131.1, 130.7, 128.7, 128.5, 127.9, 126.8, 125.3, 125.1, 124.8, 124.6, 123.7, 123.1, 104.6, 67.1, 12.6, 11.8.

m.p. 253.8-254.9 °C

FT-IR: ν = 3199, 3058, 1702, 785 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{24}H_{21}N_2O$: 353.1648; found: 353.1649

(*S*)-3-(2,5-dimethyl-1H-pyrrol-3-yl)-3-(thiophen-2-yl)isoindolinone (15)



Iso-15 (23 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **15** (25 mg, 82% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **90:10 e.r.** t_{R1} = 9.7 min (major), t_{R2} = 14.1 min (minor).

^{1}H NMR (600 MHz, DMSO-d6) (δ/ppm): 10.36 (s, 1H), 9.43 (s, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.42 (d, *J* = 5.1 Hz, 1H), 7.05 (d, *J* = 2.7 Hz, 1H), 7.03 – 6.96 (m, 1H), 5.29 (s, 1H), 2.08 (s, 3H), 1.76 (s, 3H).

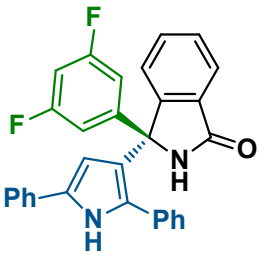
^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.1, 151.9, 149.2, 131.7, 130.4, 128.0, 126.8, 124.8, 123.9, 123.2, 122.9, 122.7, 118.8, 105.9, 64.1, 12.4, 12.1.

m.p. 257.0-257.5 °C

FT-IR: *v* = 3255, 3174, 3037, 1657, 704 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{18}H_{17}N_2OS$: 309.1056; found: 309.1054

(*S*)-3-(3,5-difluorophenyl)-3-(2,5-diphenyl-1H-pyrrol-3-yl)isoindolinone (16)



Iso-9 (26 mg) and 2,5-diphenylpyrrole (24 mg) afforded product **16** (34 mg, 73% yield) as a colorless solid. Reaction time: 8 h. Column chromatography eluent: petroleum ether/ethyl acetate = 1/1. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 25% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **71:29 e.r.** t_{R1} = 5.1 min (major), t_{R2} = 9.7 min (minor).

^{1}H NMR (600 MHz, DMSO-d6) (δ/ppm): 11.33 (s, 2H), 9.39 (s, 2H), 7.52 (d, *J* = 7.2 Hz, 7H), 7.49 – 7.41 (m, 3H), 7.40 – 7.30 (m, 5H), 7.22 (t, *J* = 7.6 Hz, 5H), 7.12 – 6.94 (m, 19H), 6.93 – 6.80 (m, 3H), 5.93 (s, 2H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 169.0, 162.4 (d, $^1J_{C\text{-}F}$ = 246.1 Hz), 162.3 (d, $^1J_{C\text{-}F}$ = 247.6 Hz), 151.2, 148.7, 134.8, 133.3, 132.5, 132.2, 131.1, 130.1, 129.9, 129.1, 128.8, 127.6, 127.2, 126.4, 124.9, 124.2, 123.4, 123.3, 122.3, 110.4, 110.2, 107.8, 102.8, 66.5.

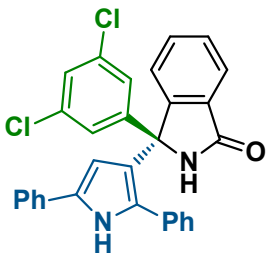
^{19}F NMR (282 MHz, DMSO) (δ/ppm): -108.4.

m.p. 185.7-186.8 °C

FT-IR: *v* = 3174, 3058, 3022, 1682, 1298, 740 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{30}H_{21}F_2N_2O$: 463.1616; found: 463.1619

(*S*)-3-(3,5-dichlorophenyl)-3-(2,5-diphenyl-1H-pyrrol-3-yl)isoindolinone (17)



Iso-10 (29 mg) and 2,5-diphenylpyrrole (24 mg) afforded product **17** (39 mg, 80% yield) as a colorless solid. Reaction time: 8 h. Column chromatography eluent: petroleum ether/ethyl acetate = 1/1. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 20% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **65:35 e.r.** t_{R1} = 5.7 min (major), t_{R2} = 12.3 min (minor).

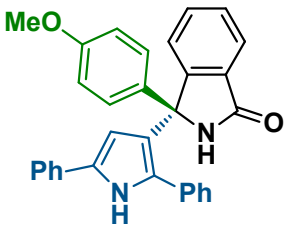
^{1}H NMR (600 MHz, DMSO) (δ/ppm): 11.48 (d, *J* = 2.4 Hz, 1H), 9.56 (s, 1H), 7.68 (d, *J* = 6.8 Hz, 1H), 7.65 (d, *J* = 7.4 Hz, 2H), 7.56 (d, *J* = 7.0 Hz, 1H), 7.53 – 7.45 (m, 2H), 7.42 (d, *J* = 1.9 Hz, 2H), 7.38 – 7.31 (m, 3H), 7.23 – 7.12 (m, 6H), 6.04 (d, *J* = 2.9 Hz, 1H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 167.9, 150.1, 146.9, 132.9, 132.2, 131.6, 131.3, 131.2, 123.0, 129.8, 128.9, 128.0, 127.8, 126.5, 126.2, 125.9, 125.3, 124.6, 123.7, 123.1, 122.3, 121.1, 106.5, 65.3.

m.p. 180.3-181.7 °C

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{30}H_{21}Cl_2N_2O$: 495.1026; found: 495.1025

(*S*)-3-(2,5-diphenyl-1H-pyrrol-3-yl)-3-(4-methoxyphenyl)isoindolinone (18)



Iso-6 (25 mg) and 2,5-diphenylpyrrole (24 mg) afforded product **18** (40 mg, 88% yield) as a colorless solid. Reaction time: 48 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 35% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **54:46 e.r.** t_{R1} = 7.6 min (major), t_{R2} = 16.3 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 11.31 (s, 1H), 9.25 (s, 1H), 7.67 – 7.46 (m, 3H), 7.39 – 7.20 (m, 7H), 7.19 – 7.00 (m, 4H), 6.95 (d, *J* = 6.6 Hz, 2H), 6.76 (d, *J* = 8.7 Hz, 2H), 6.10 (s, 1H), 3.67 (s, 3H).

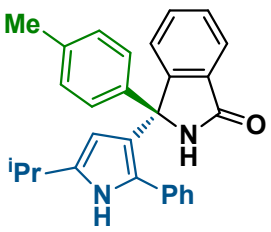
^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.8, 158.6, 152.3, 136.6, 133.6, 132.7, 131.1, 131.6, 131.4, 130.3, 129.9, 129.1, 128.0, 128.0, 127.6, 127.0, 126.2, 124.8, 124.1, 123.6, 123.1, 113.7, 108.4, 66.5, 55.5.

m.p. 265.1-265.5 °C

FT-IR: ν = 3300, 3204, 3048, 1667, 1249, 755 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{31}H_{25}N_2O$: 457.1911; found: 457.1908

(*S*)-3-(5-isopropyl-2-phenyl-1H-pyrrol-3-yl)-3-(*p*-tolyl)isoindolinone (19)



Iso-4 (24 mg) and 2-isopropyl-5-phenylpyrrole (21 mg) afforded product **19** (38 mg, 95% yield) as a colorless solid. Reaction time: 4 h. Column chromatography eluent: petroleum ether/ethyl acetate = 1/1. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 15% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **55:45 e.r.** t_{R1} = 5.9 min (major), t_{R2} = 8.3 min (minor).

^{1}H NMR (600 MHz, DMSO-d6) (δ/ppm): 10.69 (d, *J* = 2.4 Hz, 1H), 9.14 (s, 1H), 7.59 – 7.55 (m, 1H), 7.36 – 7.31 (m, 2H), 7.32 – 7.30 (m, 1H), 7.30 – 7.28 (m, 1H), 7.28 – 7.25 (m, 1H), 7.09 – 7.00 (m, 5H), 6.93 – 6.92 (m, 1H), 6.92 – 6.90 (m, 1H), 5.43 (d, *J* = 2.9 Hz, 1H), 2.89 – 2.83 (m, 1H), 2.23 (s, 3H), 1.20 (d, *J* = 1.5 Hz, 3H), 1.19 (d, *J* = 1.5 Hz, 3H).

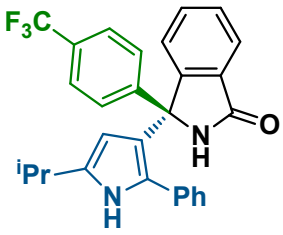
^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.4, 152.1, 141.6, 137.3, 135.8, 133.9, 131.3, 130.9, 128.9, 128.3, 127.9, 127.5, 127.1, 126.2, 125.9, 124.4, 122.5, 120.3, 105.0, 66.5, 26.5, 22.7, 20.5.

m.p. 225.6-226.4 °C

FT-IR: *v* = 3279, 2957, 2921, 1692, 1318, 759 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{28}H_{27}N_2O$: 407.2118; found: 407.2115

(*S*)-3-(5-isopropyl-2-phenyl-1H-pyrrol-3-yl)-3-(4-(trifluoromethyl)phenyl)isoindolinone (20)



Iso-5 (29 mg) and 2-isopropyl-5-phenylpyrrole (21 mg) afforded product **20** (44 mg, 95% yield) as a colorless solid. Reaction time: 12 h. Column chromatography eluent: petroleum ether/ethyl acetate = 1/1. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 15% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **51:49 e.r.** t_{R1} = 5.8 min (major), t_{R2} = 10.4 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.79 (s, 1H), 9.46 (s, 1H), 7.64 (d, *J* = 8.2 Hz, 3H), 7.54 – 7.33 (m, 5H), 7.10 – 6.93 (m, 5H), 5.32 (s, 1H), 2.97 – 2.75 (m, 1H), 1.19 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 169.0, 151.9, 148.9, 138.2, 133.9, 132.2, 131.2, 129.6, 129.0, 128.4, 127.5, 127.0, 126.4, 125.0 ($^3J_{C\text{-}F}$ = 3,8 Hz), 124.8, 123.2, 120.0, 104.9, 67.0, 26.9, 23.1, 22.9.

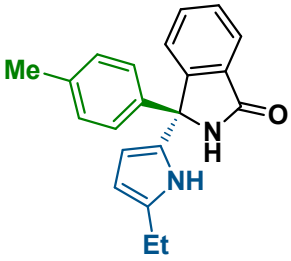
^{19}F NMR (282 MHz, DMSO) (δ/ppm): -59.6.

m.p. 181.9-182.6 °C

FT-IR: *v* = 3385, 3285, 3058, 1672, 1324, 1117, 749 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{28}H_{24}F_3N_2O$: 461.1835; found: 461.1834

(*S*)-3-(5-ethyl-1H-pyrrol-2-yl)-3-(*p*-tolyl)isoindolinone (21)



Iso-4 (24 mg) and 2-ethylpyrrole (11 μL) afforded product **21** (29 mg, 93% yield) as a colorless solid. Reaction time: 2 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 5% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **95.5:4.5 e.r.** t_{R1} = 8.4 min (minor), t_{R2} = 9.1 min (major).

^{1}H NMR (300 MHz, $(CD_3)_2CO$) (δ/ppm): 9.47 (s, 1H), 8.03 (s, 1H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.50 – 7.40 (m, 2H), 7.39 – 7.32 (m, 1H), 7.11 (d, *J* = 8.2 Hz, 2H), 6.99 (d, *J* = 8.1 Hz, 2H), 5.65 (s, 1H), 5.58 (s, 1H), 2.41 (q, *J* = 7.6 Hz, 2H), 2.16 (s, 3H), 1.01 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $(CD_3)_2CO$) (δ/ppm): 168.5, 150.6, 140.0, 137.2, 135.3, 131.7, 131.1, 130.5, 128.8, 128.1, 126.6, 124.2, 123.2, 107.7, 103.3, 66.3, 20.5, 20.0, 13.3.

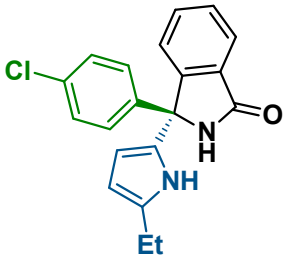
m.p. 223.6-224.9 °C

$[\alpha]_D$ = -82 ° (c 0.76, EtOAc) for 95.5:4.5 e.r.

FT-IR: *v* = 3386, 3174, 3053, 2972, 1672, 759 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{21}H_{21}N_2O$: 317.1648; found: 317.1645

(*S*)-3-(4-chlorophenyl)-3-(5-ethyl-1H-pyrrol-2-yl)isoindolinone (22)



Iso-3 (26 mg) and 2-ethylpyrrole (11 µL) afforded product **22** (31 mg, 92% yield) as a colorless solid. Reaction time: 2 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 10% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **96:4 e.r.** t_{R1} = 5.7 min (minor), t_{R2} = 6.9 min (major).

^{1}H NMR (300 MHz, $(CD_3)_2CO$) (δ/ppm): 9.56 (s, 1H), 8.21 (s, 1H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.54 – 7.42 (m, 2H), 7.42 – 7.32 (m, 1H), 7.29 – 7.18 (m, 4H), 5.66 (s, 1H), 5.59 (s, 1H), 2.41 (q, *J* = 7.5 Hz, 2H), 1.01 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $(CD_3)_2CO$) (δ/ppm): 168.6, 150.1, 142.0, 135.7, 133.1, 132.0, 131.0, 129.9, 128.5, 128.5, 128.3, 124.2, 123.4, 107.9, 103.5, 66.1, 20.5, 13.3.

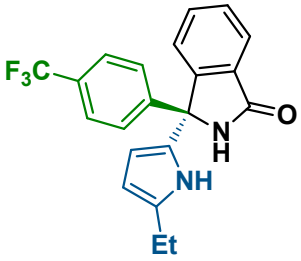
m.p. 228.1-228.9 °C

$[\alpha]_D$ = -90 ° (c 0.67, EtOAc) for 96:4 e.r.

FT-IR: *v* = 3275, 3164, 2967, 2931, 1651, 744 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{18}ClN_2O$: 337.1102; found: 337.1099

(*S*)-3-(5-ethyl-1H-pyrrol-2-yl)-3-(4-(trifluoromethyl)phenyl)isoindolinone (23)



Iso-5 (29 mg) and 2-ethylpyrrole (11 µL) afforded product **23** (19 mg, 51% yield) as a colorless solid. Reaction time: 10 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 5% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **96:4 e.r.** t_{R1} = 7.1 min (minor), t_{R2} = 10.5 min (major).

^{1}H NMR (300 MHz, $(CD_3)_2CO$) (δ/ppm): 9.59 (s, 1H), 8.26 (s, 1H), 7.65 – 7.45 (m, 7H), 7.44 – 7.35 (m, 1H), 5.67 (s, 1H), 5.61 (s, 1H), 2.41 (q, *J* = 7.6 Hz, 2H), 1.01 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $(CD_3)_2CO$) (δ/ppm): 168.6, 149.7, 147.7, 135.8, 132.1, 131.3, 129.6, 128.6, 127.5, 125.3 (q, $^3J_{C\text{-}F}$ = 3.1 Hz) , 124.2, 123.5, 108.2, 103.6, 66.3, 20.5, 13.3.

^{19}F NMR (282 MHz, $(CD_3)_2CO$) (δ/ppm): -61.6.

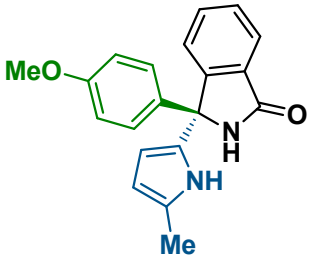
m.p. 197.4-198.2 °C

$[\alpha]_D$ = -18 ° (c 0.86, EtOAc) for 96:4 e.r.

FT-IR: *v* = 3290, 3164, 2962, 2917, 1646, 1102, 744 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{21}H_{18}F_3N_2O$: 371.1366; found: 371.1364

(*S*)-3-(4-methoxyphenyl)-3-(5-methyl-1H-pyrrol-2-yl)isoindolinone (24)



Iso-6 (25 mg) and 2-methylpyrrole (10 µL) afforded product **24** (30 mg, 95% yield) as a colorless solid. Reaction time: 1 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 10% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **93:7 e.r.** t_{R1} = 9.2 min (minor), t_{R2} = 10.0 min (major).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.29 (s, 1H), 9.19 (s, 1H), 7.68 (d, *J* = 7.4 Hz, 1H), 7.64 – 7.54 (m, 2H), 7.53 – 7.43 (m, 1H), 7.14 (d, *J* = 8.8 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 2H), 5.69 (s, 1H), 5.59 (s, 1H), 3.72 (s, 3H), 2.12 (s, 3H).

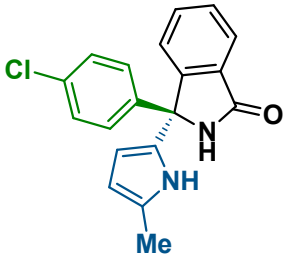
^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.7, 159.1, 150.8, 135.1, 132.3, 131.3, 130.7, 128.7, 128.6, 128.3, 124.6, 123.5, 114.0, 107.6, 105.0, 66.2, 55.6, 13.3.

m.p. 214.9-215.5 °C

FT-IR: *v* = 3300, 3239, 2921, 1642, 1238, 744 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{20}H_{19}N_2O_2$: 319.1441; found: 319.1439

(*S*)-3-(4-chlorophenyl)-3-(5-methyl-1H-pyrrol-2-yl)isoindolinone (25)



Iso-3 (26 mg) and 2-methylpyrrole (10 µL) afforded product **25** (31 mg, 96% yield) as a colorless solid. Reaction time: 1 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 5% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **97:3 e.r.** t_{R1} = 10.9 min (minor), t_{R2} = 12.6 min (major).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.34 (s, 1H), 9.30 (s, 1H), 7.69 (d, *J* = 7.4 Hz, 1H), 7.66 – 7.56 (m, 2H), 7.56 – 7.46 (m, 1H), 7.40 (d, *J* = 8.6 Hz, 2H), 7.26 (d, *J* = 8.6 Hz, 2H), 5.70 (s, 1H), 5.61 (s, 1H), 2.12 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.7, 150.1, 142.2, 132.8, 132.5, 131.3, 130.1, 129.1, 129.0, 128.9, 128.7, 124.5, 123.7, 107.8, 105.2, 66.2, 13.3.

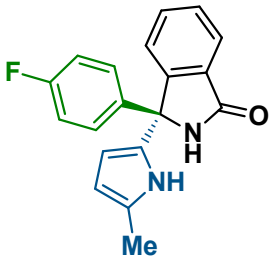
m.p. 272.2-272.8 °C

$[\alpha]_D$ = -104 ° (c 0.80, EtOAc) for 97:3 e.r.

FT-IR: *v* = 3315, 3264, 3159, 1652, 749 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{19}H_{16}ClN_2O$: 323.0946; found: 323.0944

(*S*)-3-(4-fluorophenyl)-3-(5-methyl-1H-pyrrol-2-yl)isoindolinone (26)



Iso-2 (24 mg) and 2-methylpyrrole (10 µL) afforded product **26** (30 mg, 96% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 5% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **95:5 e.r.** t_{R1} = 10.8 min (minor), t_{R2} = 11.5 min (major).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 10.33 (s, 1H), 9.27 (s, 1H), 7.79 – 7.45 (m, 4H), 7.35 – 7.07 (m, 4H), 5.68 (s, 1H), 5.60 (s, 1H), 2.11 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.7, 161.9 (d, $^1J_{C\text{-}F}$ = 244.6 Hz), 150.4, 139.3, 132.5, 131.3, 130.3, 129.2, 129.1, 128.9, 128.8, 124.6, 123.6, 115.5, 115.4, 107.8, 105.1, 66.1, 13.2.

^{19}F NMR (282 MHz, DMSO) (δ/ppm): -113.9.

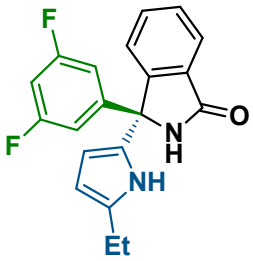
m.p. 263.4-265.2 °C

$[\alpha]_D$ = -72 ° (c 0.73, EtOAc) for 95:5 e.r.

FT-IR: ν = 3320, 3245, 2922, 1642, 1213, 744 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd for $C_{19}H_{16}FN_2O$: 307.1241; found: 307.1238

(*S*)-3-(3,5-difluorophenyl)-3-(5-ethyl-1H-pyrrol-2-yl)isoindolinone (27)



Iso-9 (26 mg) and 2-ethylpyrrole (11 µL) afforded product **27** (18 mg, 53% yield) as a colorless solid. Reaction time: 15 min. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IB N-3 (4.6 mm × 250 mm), 15% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **53:47 e.r.** t_{R1} = 4.4 min (major), t_{R2} = 4.8 min (minor).

^{1}H NMR (300 MHz, $(CD_3)_2CO$) (δ/ppm): 9.60 (s, 1H), 8.20 (s, 1H), 7.62 (d, *J* = 7.4 Hz, 1H), 7.58 – 7.47 (m, 2H), 7.46 – 7.36 (m, 1H), 6.97 – 6.75 (m, 3H), 5.68 (s, 1H), 5.61 (s, 1H), 2.41 (q, *J* = 7.5 Hz, 2H), 1.01 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $(CD_3)_2CO$) (δ/ppm): 169.3, 163.8 (d, $^1J_{C\text{-}F}$ = 247.6 Hz), 163.7 (d, $^1J_{C\text{-}F}$ = 247.6 Hz), 150.2, 148.8, 136.8, 135.1, 133.1, 131.8, 130.0, 129.7, 125.1, 124.4, 123.8, 110.9 (d, $^2J_{C\text{-}F}$ = 21.1 Hz), 110.8 (d, $^2J_{C\text{-}F}$ = 21.1 Hz), 109.1, 104.5, 103.8, 66.9, 21.4, 14.2.

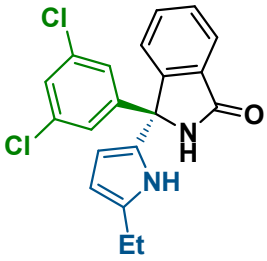
^{19}F NMR (282 MHz, $(CD_3)_2CO$) (δ/ppm): -109.2.

m.p. 244.2-245.7 °C

FT-IR: *v* = 3310, 3249, 3168, 2916, 1651,1122, 744 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{20}H_{17}F_2N_2O$: 339.1303; found: 339.1300

(*S*)-3-(3,5-dichlorophenyl)-3-(5-ethyl-1H-pyrrol-2-yl)isoindolinone (28)



Iso-10 (29 mg) and 2-ethylpyrrole (11 μL) afforded product **28** (19 mg, 52% yield) as a colorless solid. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Reaction time: 15 min. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 15% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **60:40 e.r.** t_{R1} = 4.0 min (minor), t_{R2} = 4.7 min (major).

^{1}H NMR (300 MHz, $(CD_3)_2CO$) (δ/ppm): 9.63 (s, 1H), 8.19 (s, 1H), 7.63 (d, *J* = 7.4 Hz, 1H), 7.58 – 7.50 (m, 2H), 7.43 (s, 1H), 7.29 (d, *J* = 1.8 Hz, 1H), 7.24 (d, *J* = 1.8 Hz, 2H), 5.68 (d, *J* = 2.9 Hz, 1H), 5.62 (s, 1H), 2.42 (q, *J* = 7.6 Hz, 2H), 1.02 (t, *J* = 7.6 Hz, 3H).

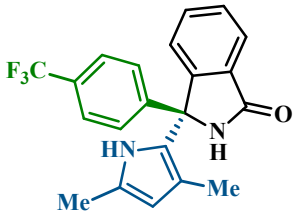
^{13}C NMR (75 MHz, $(CD_3)_2CO$) (δ/ppm): 167.8, 148.6, 146.9, 135.6, 134.1, 131.8, 130.5, 128.5, 128.3, 127.1, 125.0, 123.7, 123.1, 122.4, 121.8, 107.8, 103.2, 65.3, 19.9, 12.8.

m.p. 299.0-300.0 °C

FT-IR: *v* =3345, 3234, 2962, 2921, 1687, 724 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{20}H_{17}Cl_2N_2O$: 371.0712; found: 371.0710

(*S*)-3-(3,5-dimethyl-1H-pyrrol-2-yl)-3-(4-(trifluoromethyl)phenyl)isoindolinone (29)



Iso-5 (29 mg) and 2,4-dimethylpyrrole (12 μL) afforded product **29** (26 mg, 70% yield) as a colorless solid. Reaction time: 10 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 15% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **95:5 e.r.** t_{R1} = 5.8 min (major), t_{R2} = 7.2 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 9.82 (s, 1H), 9.50 (s, 1H), 7.76 (t, *J* = 7.8 Hz, 3H), 7.70 – 7.53 (m, 5H), 5.55 (s, 1H), 2.09 (s, 3H), 1.51 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 168.7, 149.9, 148.1, 132.8, 131.5, 129.0, 128.7, 128.5, 128.3, 127.9, 127.4, 126.4, 125.8, 125.8 (q, $^3J_{C\text{-}F}$ = 3.1 Hz), 125.6, 124.8, 124.1, 123.8, 123.6, 115.9, 109.9, 66.9, 13.0, 12.9.

^{19}F NMR (282 MHz, DMSO-d6) (δ/ppm): -69.83.

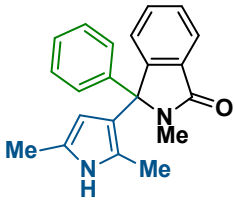
m.p. 178.6-179.7 °C

$[\alpha]_D$ = -36 ° (c 0.53, EtOAc) za 95:5 e.r.

FT-IR: *v* = 3280, 3184, 2927, 1672, 1314, 1057, 739 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{21}H_{18}F_3N_2O$: 371.1371; found: 371.1364

3-(2,5-dimethyl-1H-pyrrol-3-yl)-2-methyl-3-phenylisoindolin-1-one (rac-32)



Iso-Me (24 mg), *p*-toluenesulfonic acid (1,0 mg) and 2,5-dimethylpyrrole (12 µL) afforded product **rac-32** (27 mg, 85% yield) as a colorless solid. Reaction time: 2 h. Column chromatography eluent: petroleum ether/ethyl acetate = 2/3.

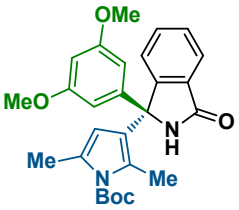
^{1}H NMR (600 MHz, DMSO-d6) (δ/ppm): 10.41 (s, 1H), 7.68 (d, *J* = 7.5 Hz, 1H), 7.50 (m, 1H), 7.45 – 7.38 (m, 2H), 7.37 – 7.32 (m, 2H), 7.32 – 7.25 (m, 3H), 5.16 (s, 1H), 2.75 (s, 3H), 2.05 (s, 3H), 1.49 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 166.7, 151.6, 141.4, 131.7, 129.9, 128.5, 127.7, 127.3, 126.5, 123.9, 123.7, 123.6, 122.5, 115.3, 106.9, 71.2, 25.3, 12.5, 12.4.

m.p. 196.3-197.8 °C

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{21}H_{21}N_2O$: 317.1648; found: 317.1645

(*S*)-*tert*-butyl 3-(1-(3,5-dimethoxyphenyl)-3-oxoisoindolin-1-yl)-2,5-dimethyl-1H-pyrrole-1-carboxylate (33)



Iso-11 (28 mg) and *N*-Boc-2,5-dimethylpyrrole (23 µL) afforded product **33** (8 mg, 16% yield) as a colorless solid. Reaction time: 7 days. Column chromatography eluent: petroleum ether/ethyl acetate = 1/2. Enantiomeric ratio determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 30% IPA in hexane, flow rate 1.0 mL/min, 230 nm), **77:23 e.r.** t_{R1} = 9.1 min (major), t_{R2} = 11.2 min (minor).

^{1}H NMR (300 MHz, DMSO-d6) (δ/ppm): 9.41 (s, 1H), 7.72 (d, *J* = 7.3 Hz, 1H), 7.69 – 7.50 (m, 3H), 6.54 (s, 2H), 6.49 (s, 1H), 5.44 (s, 1H), 3.75 (s, 6H), 2.27 (s, 3H), 1.94 (s, 3H), 1.58 (s, 9H).

^{13}C NMR (151 MHz, DMSO-d6) (δ/ppm): 169.0, 160.9, 151.1, 150.1, 146.4, 132.4, 131.1, 128.8, 128.6, 128.0, 124.8, 123.9, 123.5, 111.5, 104.9, 98.8, 84.3, 66.4, 55.6, 27.9, 16.1, 14.7.

m.p. 198.1-199.3 °C

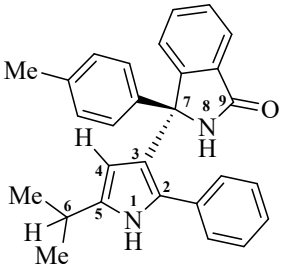
FT-IR: *v* = 3184, 2927, 1697, 1314, 1127, 728 cm^{-1}

HRMS (ESI): *m/z* $[M+H]^+$ calcd $C_{27}H_{31}N_2O_5$: 463.2227; found: 463.2226

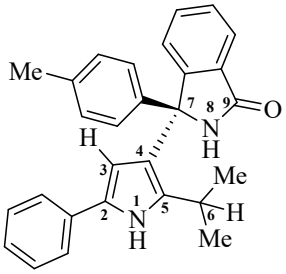
4. Structure Elucidation of Regioisiomers 19 and 27

(*S*)-3-(5-isopropyl-2-phenyl-1H-pyrrol-3-yl)-3-(*p*-tolyl)isoindolinone (19)

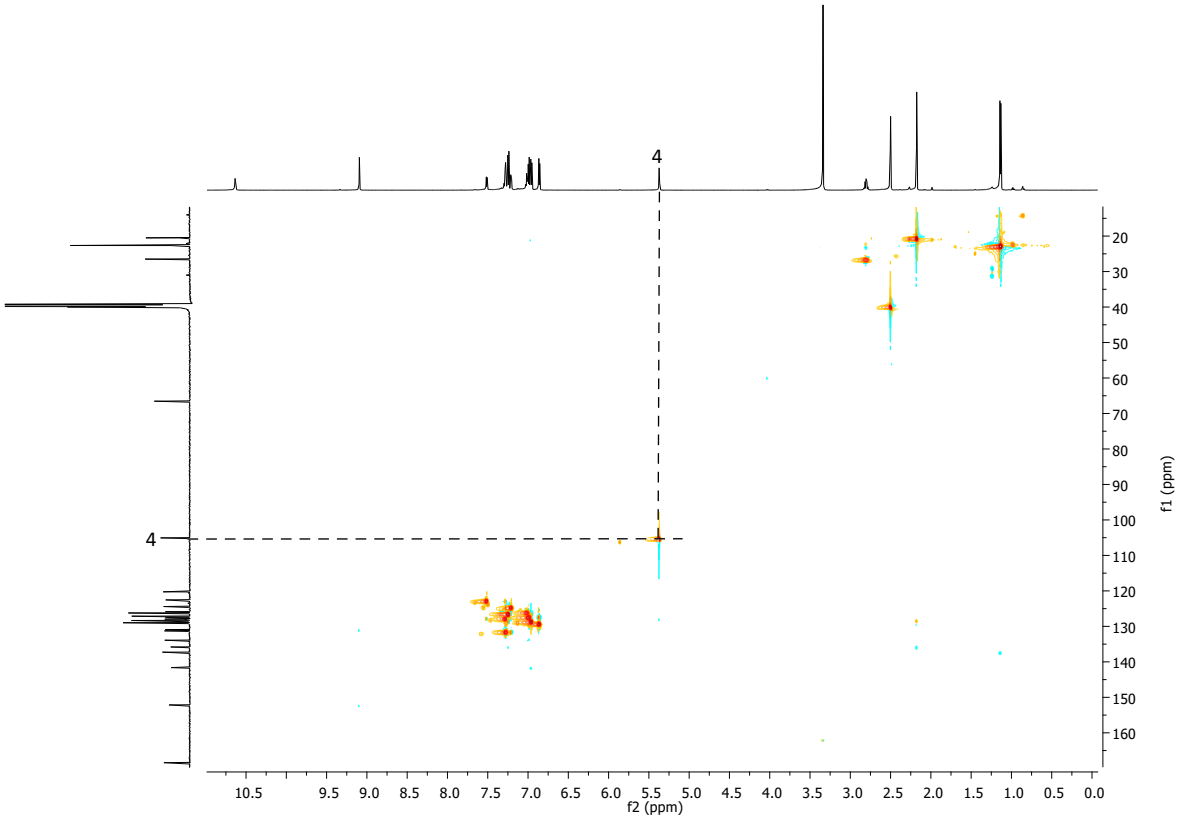
HSQC and HMBC NMR experiements were used to confirm the structure of the resulting regioisomer. Based on the HSQC spectrum, the pyrrole H4 proton and the corresponding C4 carbon were detected. In HMBC spectrum, a strong interaction between pyrrole C4 and the methine proton in the isopropyl group H6 is also observed, which strongly supports the formation of regioisomer **19a**. Weak interaction between the amide proton H8 and the pyrrole carbon C2 is observed, which would not be observable in regioisomer **19b**.



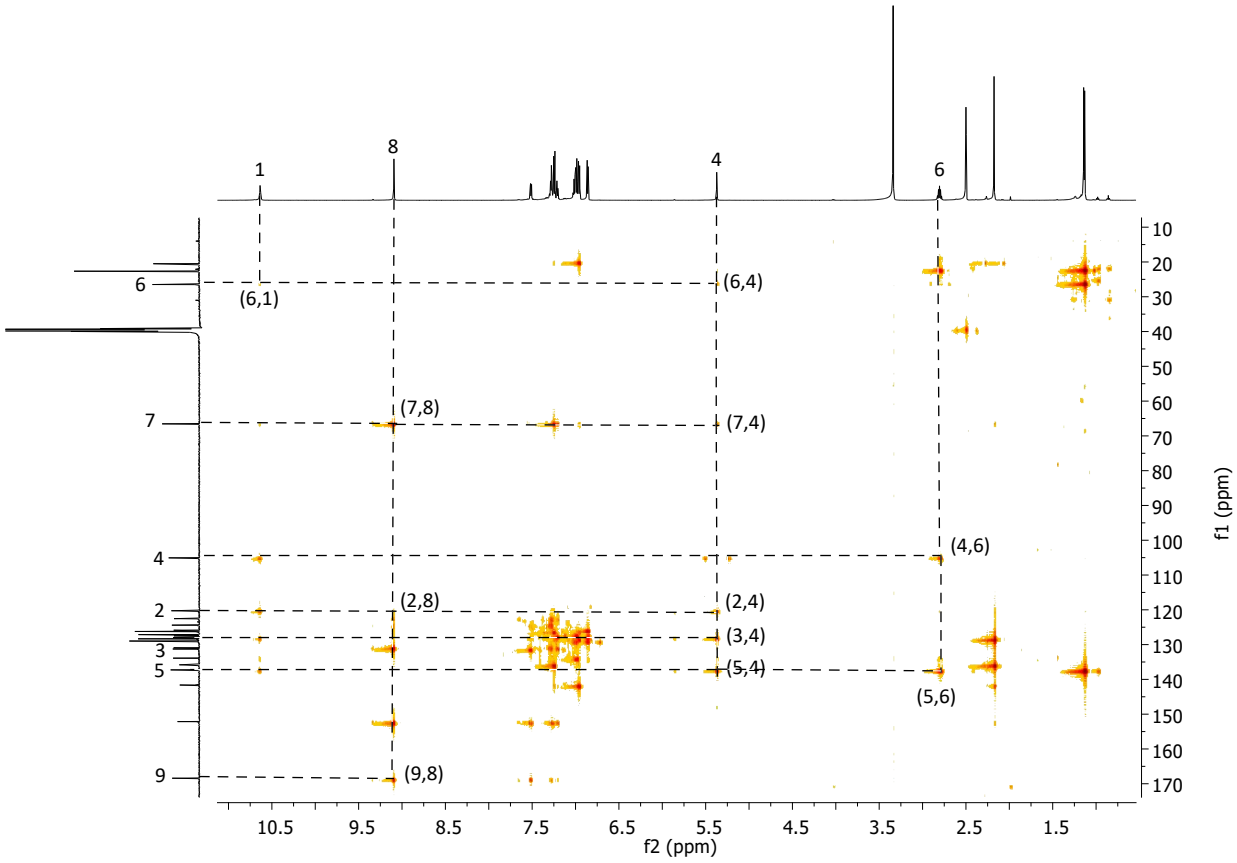
19a



19b



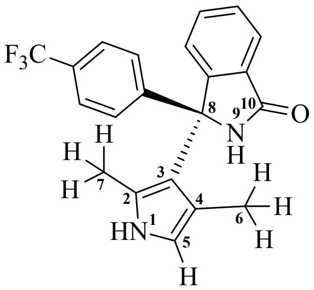
HSQC spectra of compound **19**.



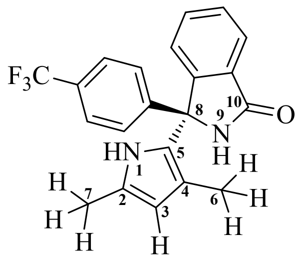
HMBC spectra of compound **19**.

(*S*)-3-(3,5-dimethyl-1H-pyrrol-2-yl)-3-(4-(trifluoromethyl)phenyl)isoindolinone (29)

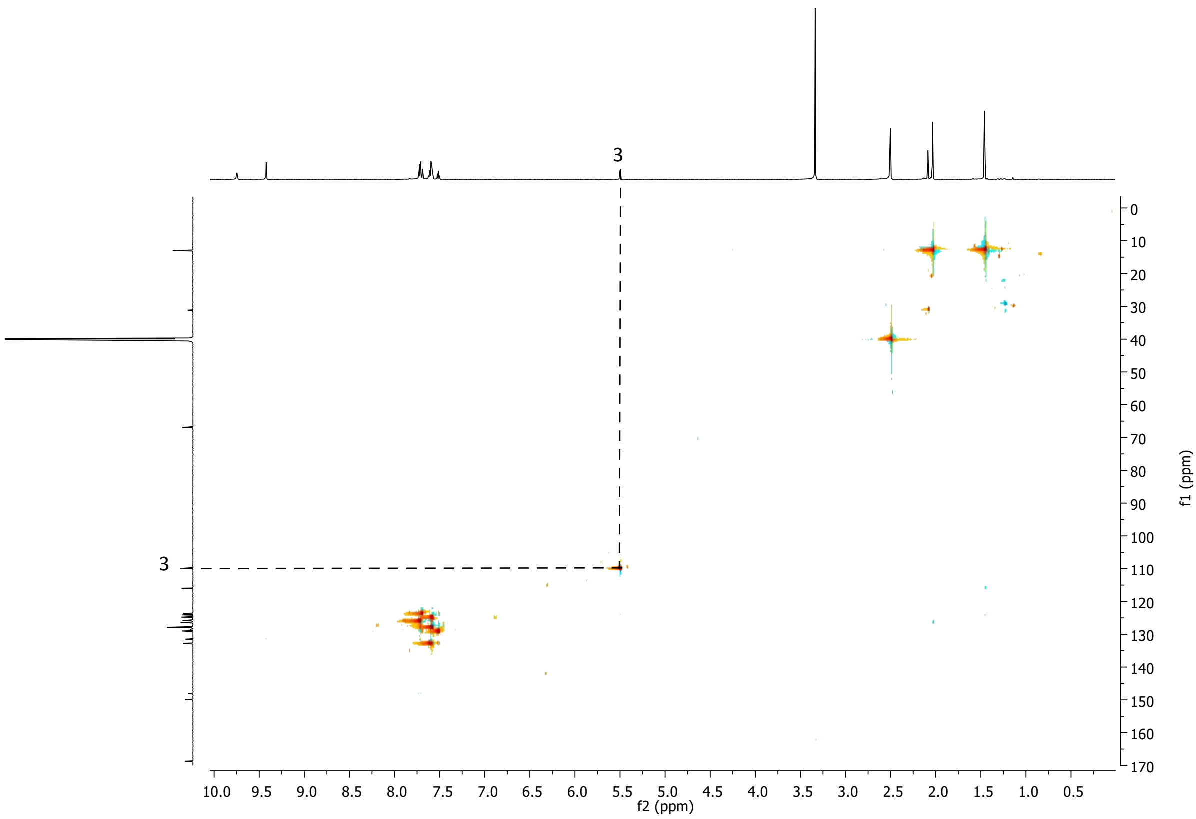
For compound **29**, the structure of regioisomer **29b** has been confirmed. From HMBC spectrum, the couplings of H3 proton to C6 and C7 methyl carbons are clearly visible in equal intensities, which is in favour of regioisomer **29b**. In case of structure **29a**, proton H5 would not interact with C7. The low interaction observed between quaternary carbon C8 and proton H1 also supports the formation of regioisomer **29b**.



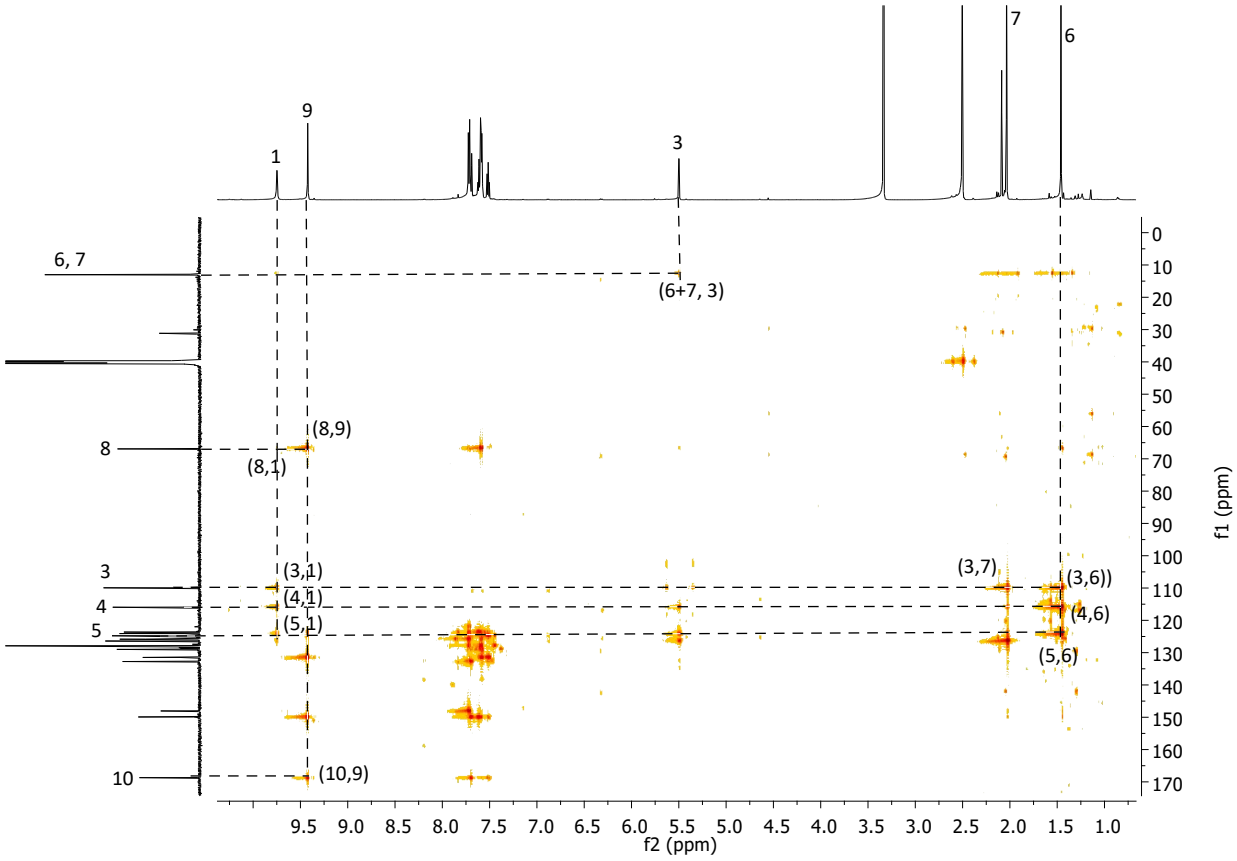
29a



29b



HSQC spectra of compound **29**.

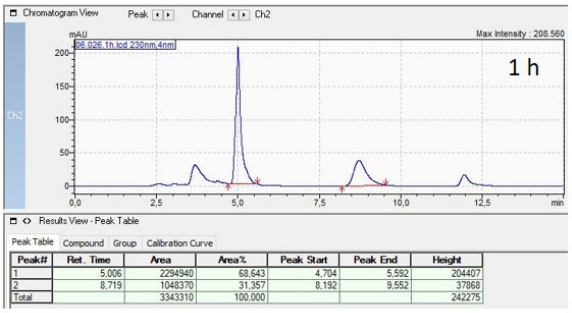


HMBC spectra of compound **29**.

6. Racemization test

Chiral phosphoric acid **CPA8** (7.2 mg, 0.0095 mmol) was added to a suspension of isoindolinone alcohol **Iso-9** (50 mg, 0.19 mmol) in toluene (4 mL) at room temperature. After stirring for 5 min, 2,5-diphenylpyrrole (46 mg, 0.21 mmol) was added, and the resulting reaction mixture was stirred in an oil bath at 80 °C. The product was first detected by TLC in the reaction mixture after 1 hour, and **Iso-9** was completely consumed after 8 hours (also detected by TLC). After 1, 2, 3, 4, 5, 6, 7, 8, 24, 72 and 168 hours, a 360 μL aliquot was taken from the reaction mixture, and filtered through a short column of silica gel using ethyl acetate-petroleum ether 1:1 as eluent. The enantiomeric ratio was determined by chiral HPLC (Daicel Chiralpack IC-3 (4.6 mm × 250 mm), 25% IPA in hexane, flow rate 1.0 mL/min, 230 nm).

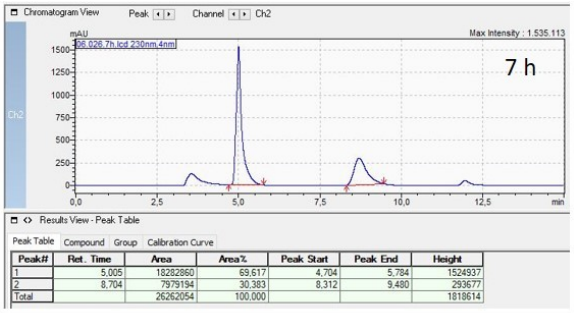
Entry	Time / h	e.r.
1	1	69:31
2	2	69:31
3	3	69:31
4	4	68:32
5	5	69:31
6	6	69:31
7	7	70:30
8	8	70:30
9	24	71:29
10	72	71:29
11	168	71:29



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

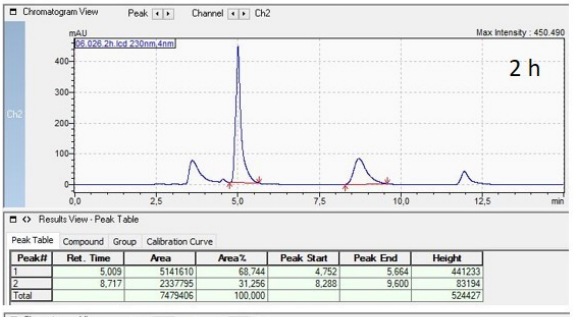
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,006	2294940	68,643	4,704	5,592	204407
2	8,719	1048370	31,357	8,192	9,552	37868
Total		3343310	100,000			242275



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

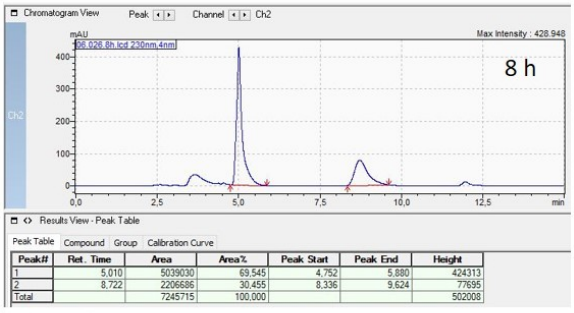
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,005	1828860	69,617	4,704	5,784	1524937
2	8,704	7979194	30,383	8,312	9,480	293677
Total		26262054	100,000			1818614



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

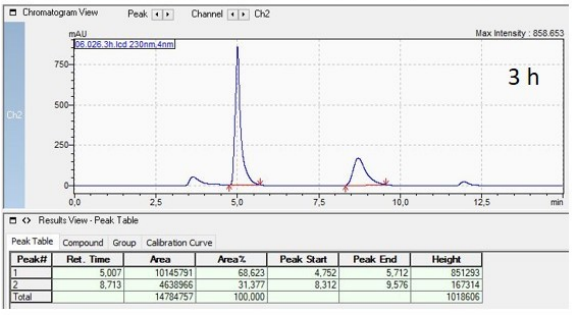
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,009	5141610	68,744	4,752	5,664	441233
2	8,717	2337795	31,256	8,288	9,600	83194
Total		7479406	100,000			524427



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

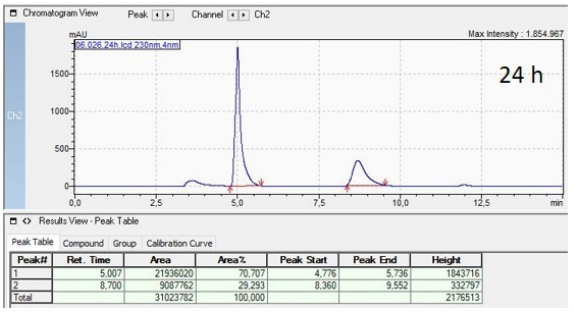
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,010	5039030	69,545	4,752	5,880	424313
2	8,722	2206686	30,455	8,336	9,624	77695
Total		7245715	100,000			502008



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

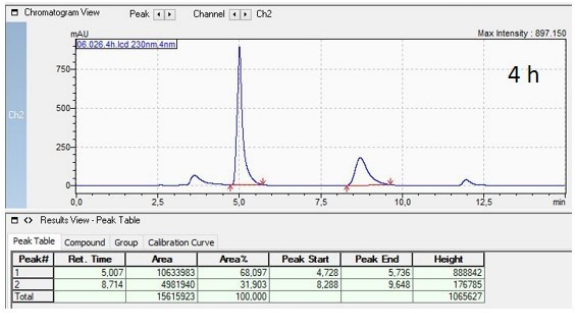
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,007	10145791	68,623	4,752	5,712	851293
2	8,713	4638966	31,377	8,312	9,576	167314
Total		14784757	100,000			1018606



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

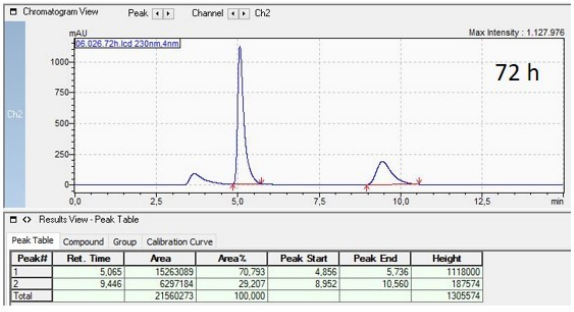
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,007	21936020	70,707	4,776	5,736	1843716
2	8,700	9087762	29,293	8,360	9,552	332797
Total		31023782	100,000			2176513



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

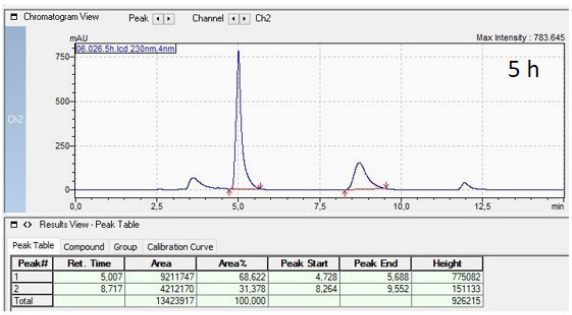
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,007	10633883	68,097	4,728	5,736	888842
2	8,714	4981940	31,903	8,288	9,648	176785
Total		15615923	100,000			1065627



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

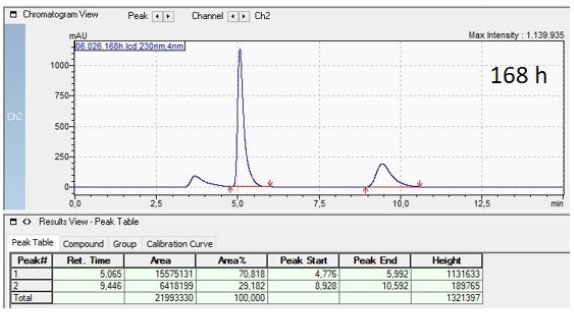
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,065	15263089	70,793	4,856	5,736	1118000
2	9,446	6297184	29,207	8,952	10,560	187574
Total		21560273	100,000			1305574



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,007	9211747	68,622	4,728	5,688	775082
2	8,717	4212170	31,378	8,264	9,552	151133
Total		13423917	100,000			926215



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
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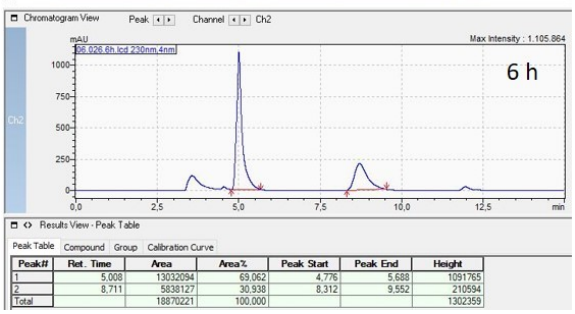
2	9,446	6418199	29,182	8,928	10,592	189765
Total		21993330	100,000			1321397



Results View - Peak Table

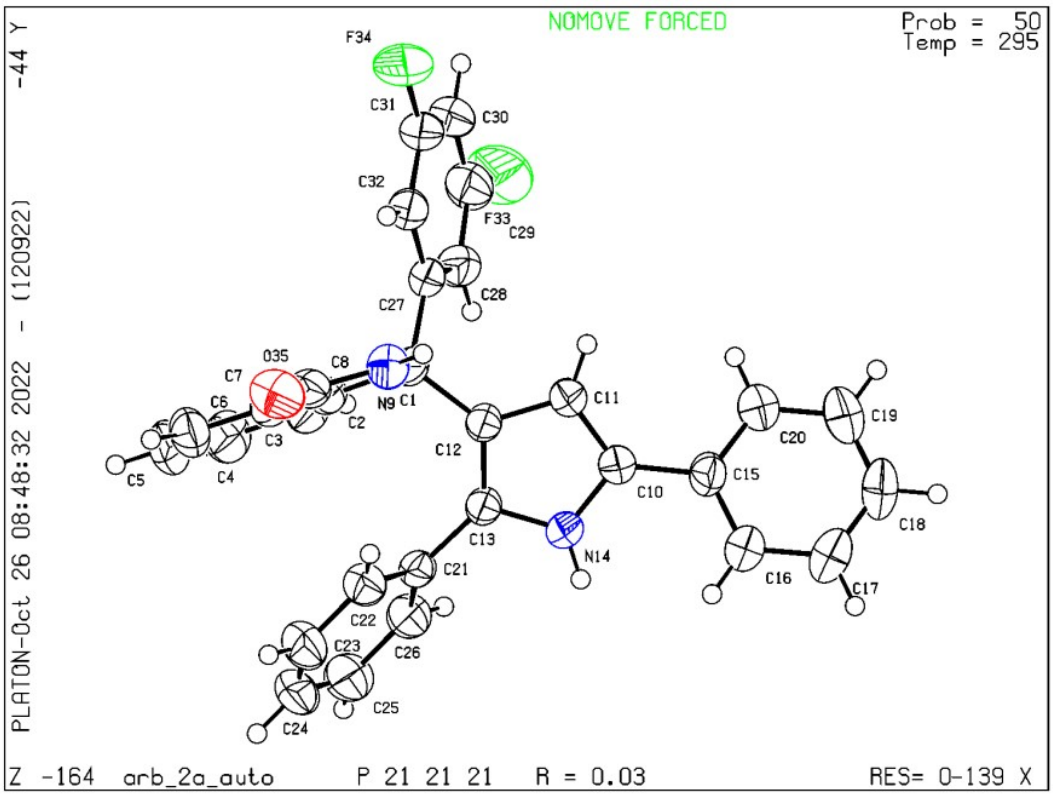
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,008	13032094	69,062	4,776	5,688	1091765
2	8,711	5838127	30,938	8,312	9,552	210594
Total		18870221	100,000			1302359

5. X-ray Crystallography

Single crystal measurement was performed on an Rigaku XtaLAB Synergy S (microfocus Cu tube) at room temperature [293(2) K]. Friedel pairs were measured to unambiguously establish absolute configuration of the stereogenic centre. Program package CrysAlis PRO [CrysAlis] was used for data reduction and multi-scan absorption correction. The crystal structure was solved by direct methods using SHELXT.[3] Non-hydrogen atoms were refined isotropically followed by anisotropic refinement by full matrix least-squares calculations based on F2 using SHELXL.[4] Hydrogen atoms were first located in the Fourier difference map, then positioned geometrically and allowed to ride on their respective parent atoms. Diagrams and publication materials were generated using OLEX2[5] and Mercury®.

Absolute configuration of the product **ent-16** was determined by solving its crystal structure. Flack parameter[6] x = 0.044 (0.087) calculated using 1644 Parsons' quotients [(I+)-(I-)]/[(I+)+(I-)][7] confirms assigned absolute configuration. Colourless crystals of **ent-16** suitable for crystallographic analysis were obtained by evaporation method from hexane-2-propanol 9:1. The crystal structure has been deposited at the Cambridge Crystallographic Centre (deposition number: CCDC 2215386). The data can be obtained free of charge at www.ccdc.cam.ac.uk/getstructures



6. References

1. Glavač, D.; Dokli, I.; Gredičak, M. Synthesis of 3–Aryl 3–Hydroxyisoindolinones by the Addition of Grignard and Organolithium Reagents to Phthalimides. *Curr. Org. Chem.* **2017**, *21*, 1335–1340.

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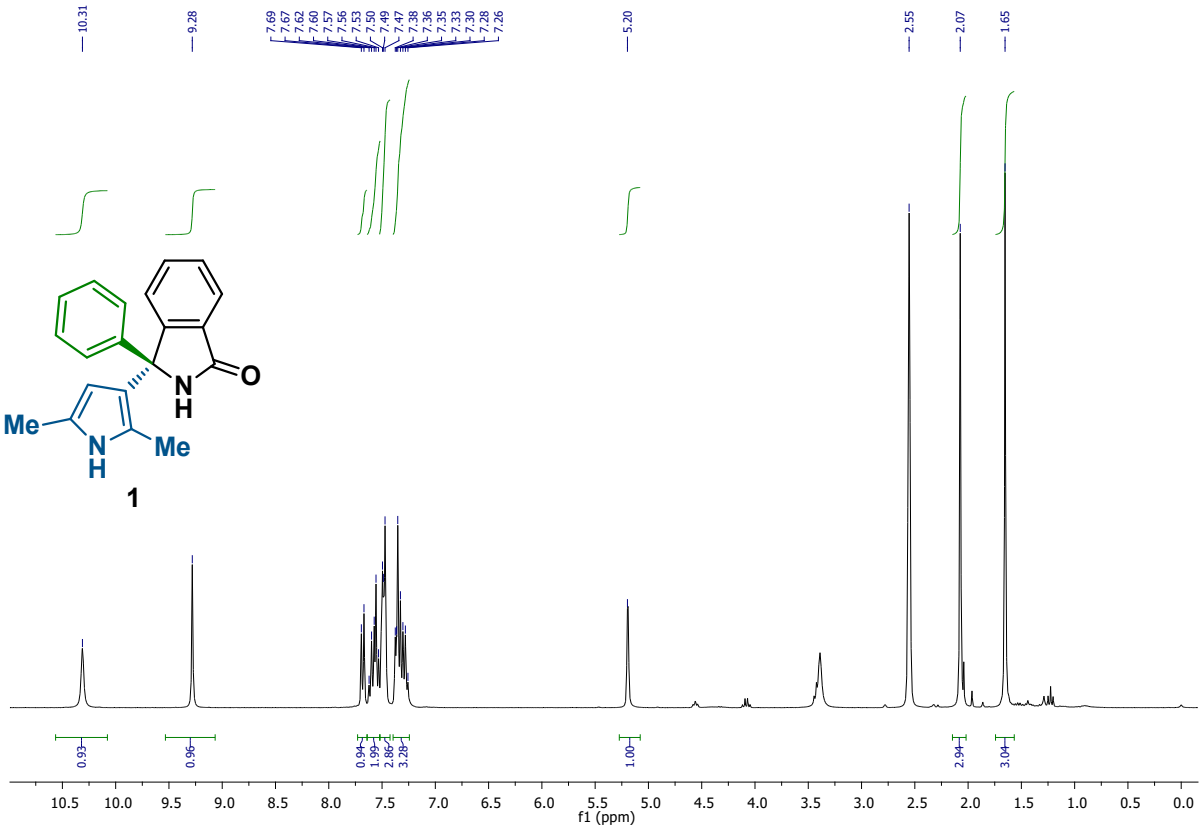
4. Sheldrick, G.M. Crystal structure refinement with SHELXL. *Acta Cryst.* **2015**, C71, 3-8.

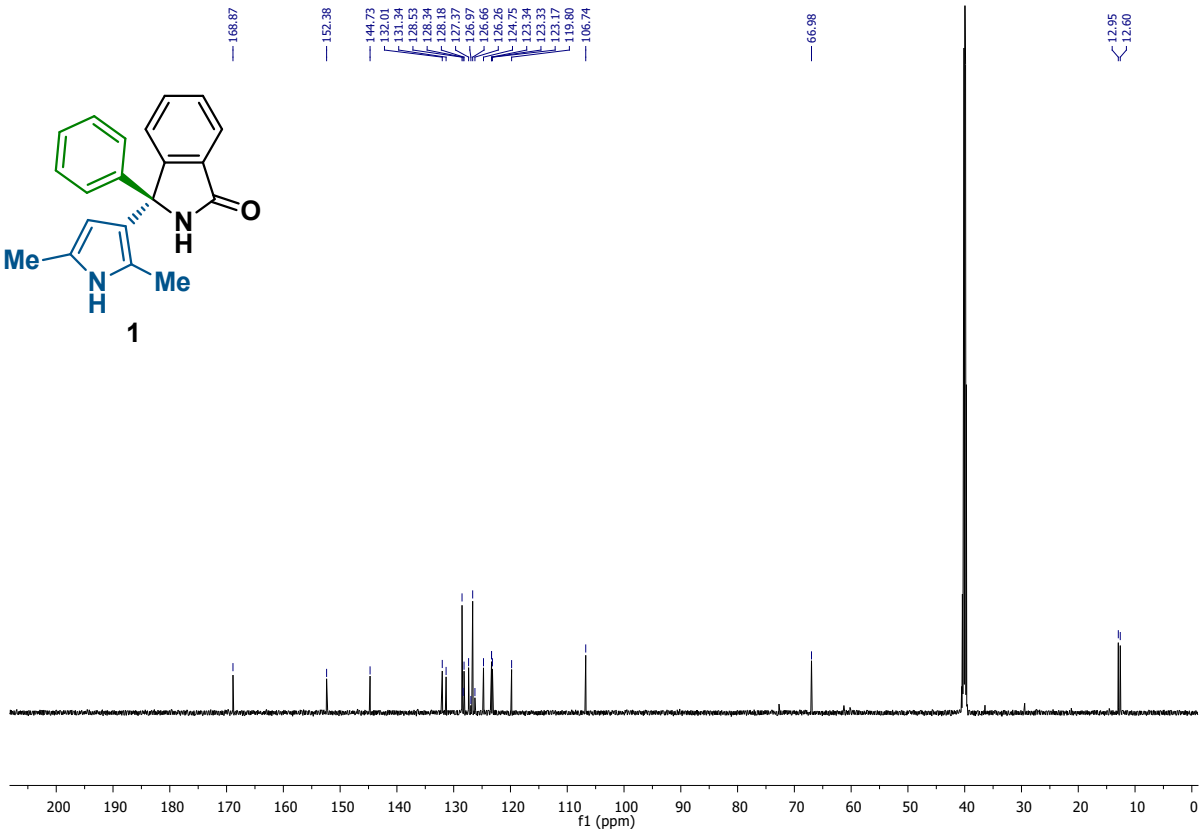
5. Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009**, *42*, 339-341.

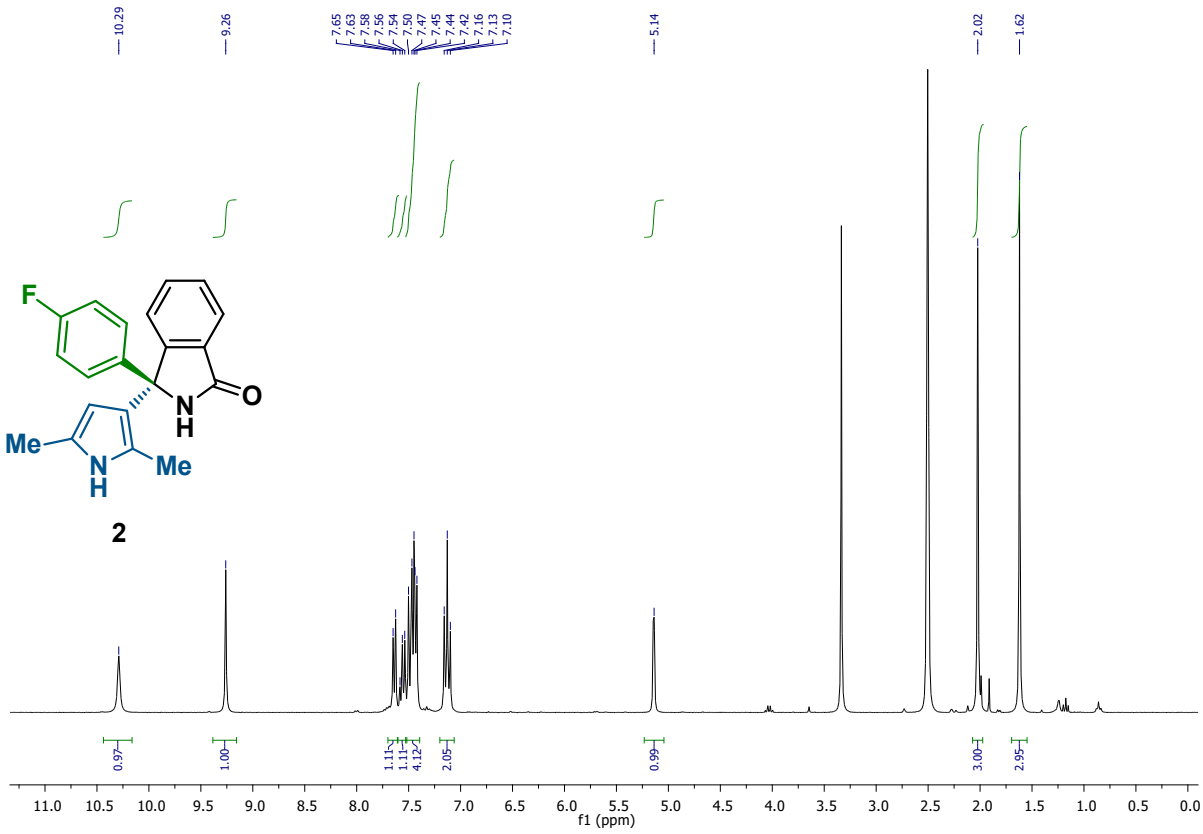
6. Flack, H. D. On enantiomorph-polarity estimation, *Acta Cryst.* **1983**, A39, 876-881.

7. Parsons, S.; Flack, H. D.; Wagner, T. Use of intensity quotients and differences in absolute structure refinement, *Acta Cryst.* **2013**, B69, 249-259.

7. NMR Spectra



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7.16
7.13
7.10
5.14
2.02
1.62
F
O
N
H
Me
N
H
Me
2
0.97
1.00
1.11
1.11
4.12
2.05
0.99
3.00
2.95
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
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1.0
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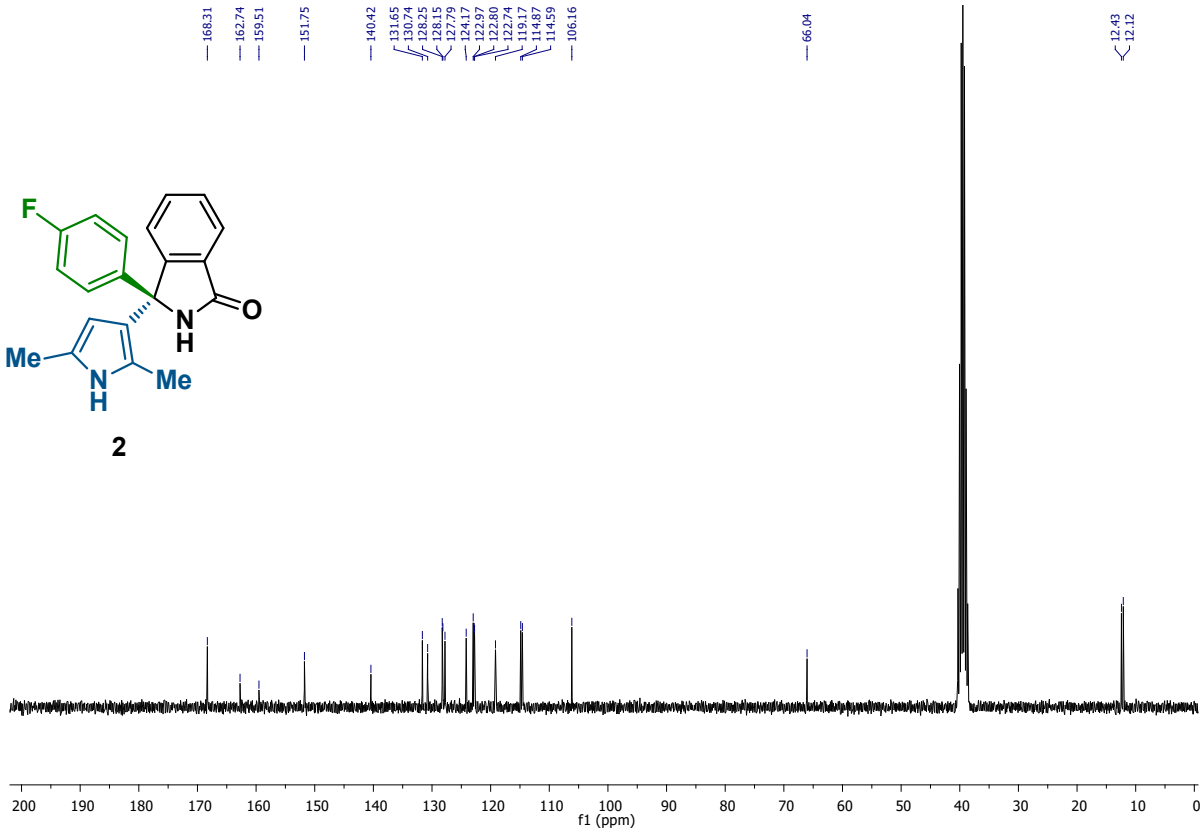
0.0
f1 (ppm)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151.75
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131.65
130.74
128.25
128.15
127.79
124.17
122.97
122.80
122.74
119.17
114.87
114.59
106.16
66.04
12.43
12.12
F
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H
Me
N
H
Me
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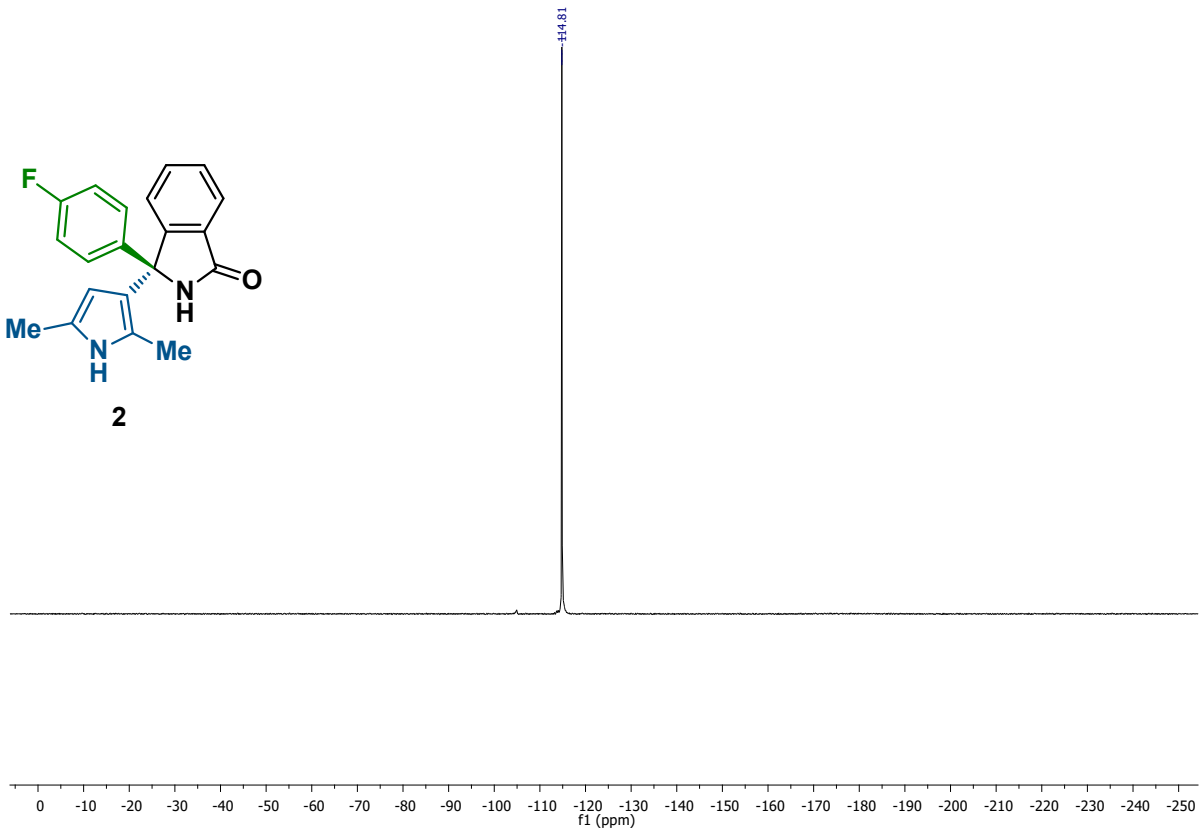
f1 (ppm)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N
H
Me
2
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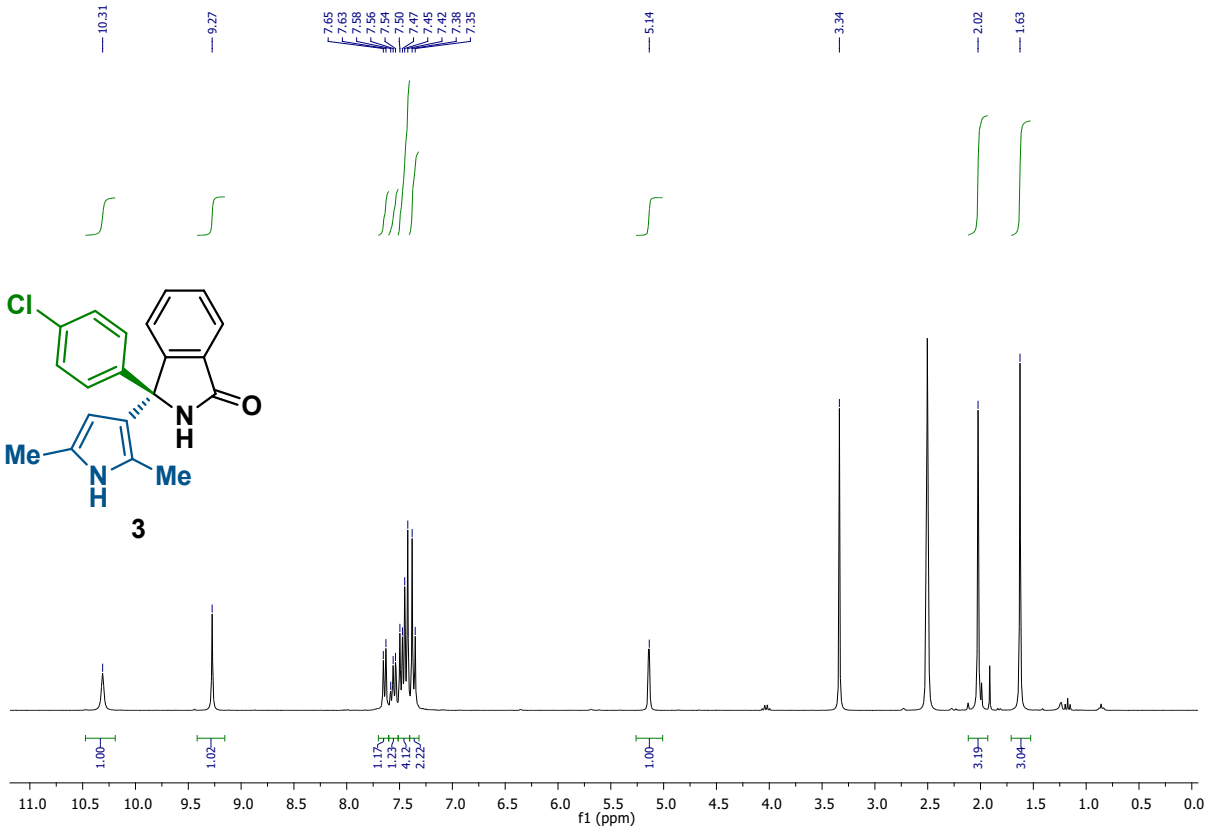
f1 (ppm)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7.42
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7.35
5.14
3.34
2.02
1.63
Cl
O
N
H
Me
N
H
Me
1.00
1.02
1.17
1.23
4.12
2.22
1.00
3.19
3.04
11.0
10.5
10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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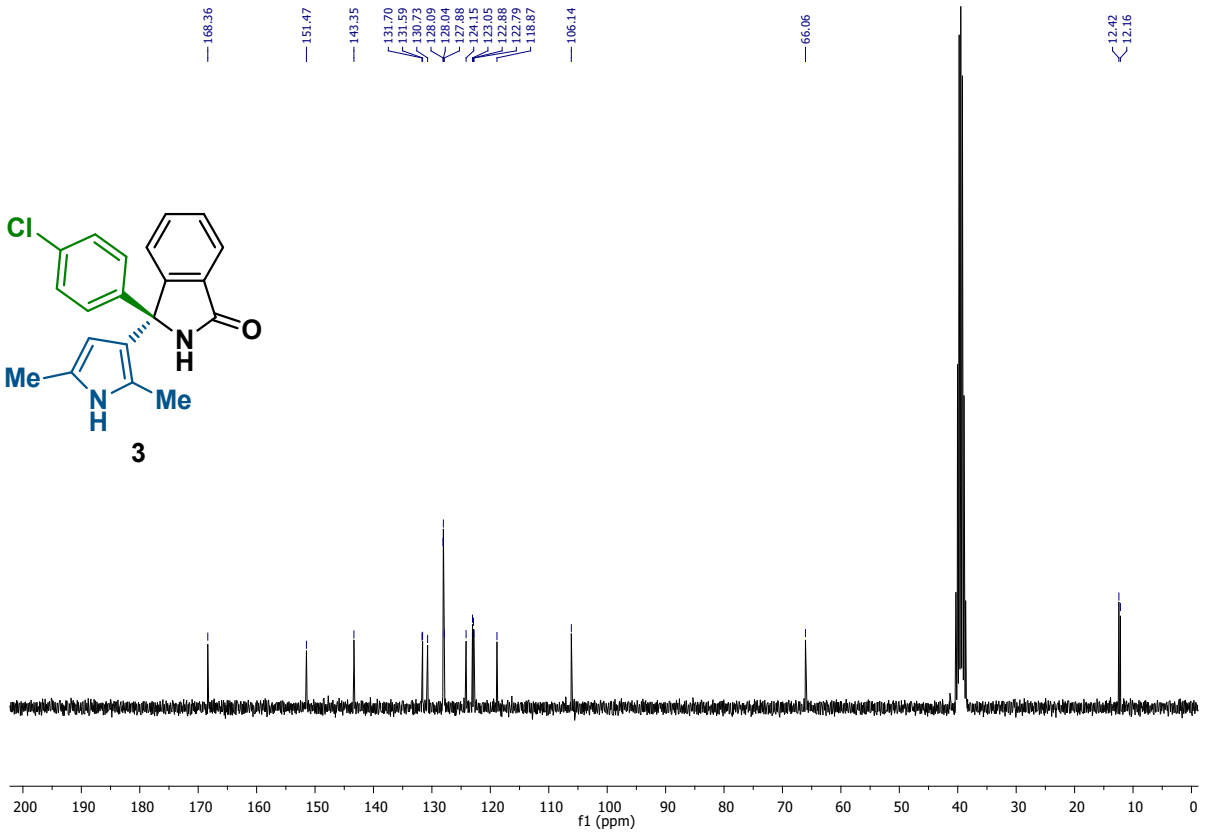
0.0
f1 (ppm)

3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106.14
66.06
12.42
12.16
Cl
O
N
H
Me
N
H
Me
200
190
180
170
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150
140
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120
110
100
90
80
70
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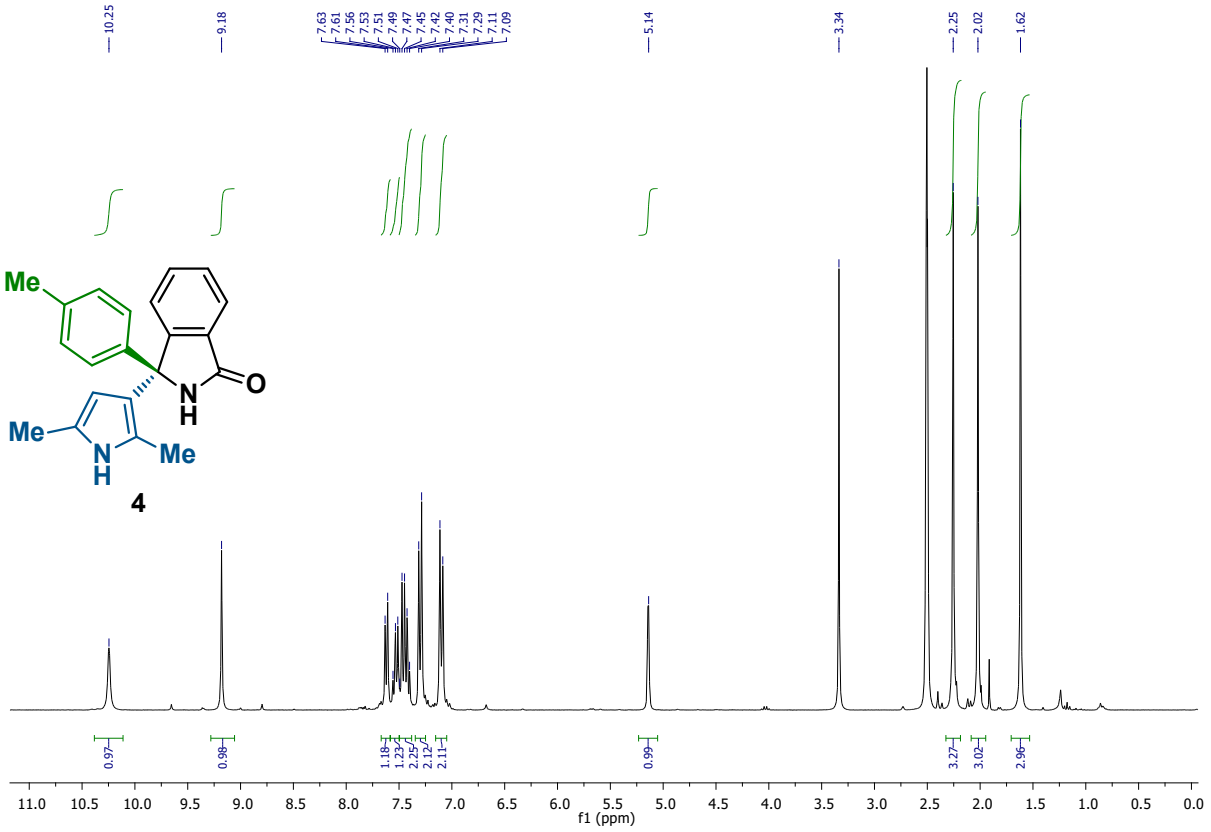
50
40
30
20
10
0
f1 (ppm)

3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7.09
5.14
3.34
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2.02
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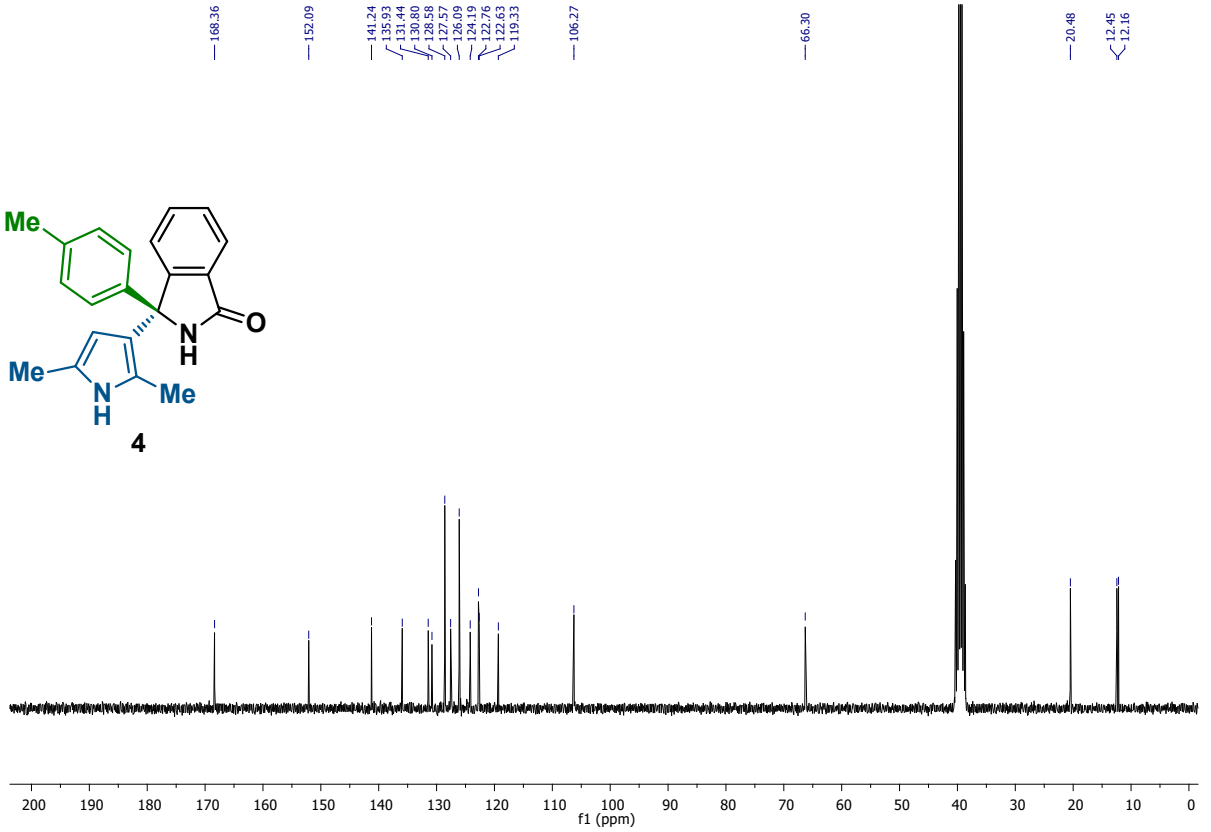
Me
N
H
O
Me
N
H
Me
4
0.97
0.98
1.18
1.23
2.25
2.12
2.11
0.99
3.27
3.02
2.96
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.19
122.76
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119.33
106.27
66.30
20.48
12.45
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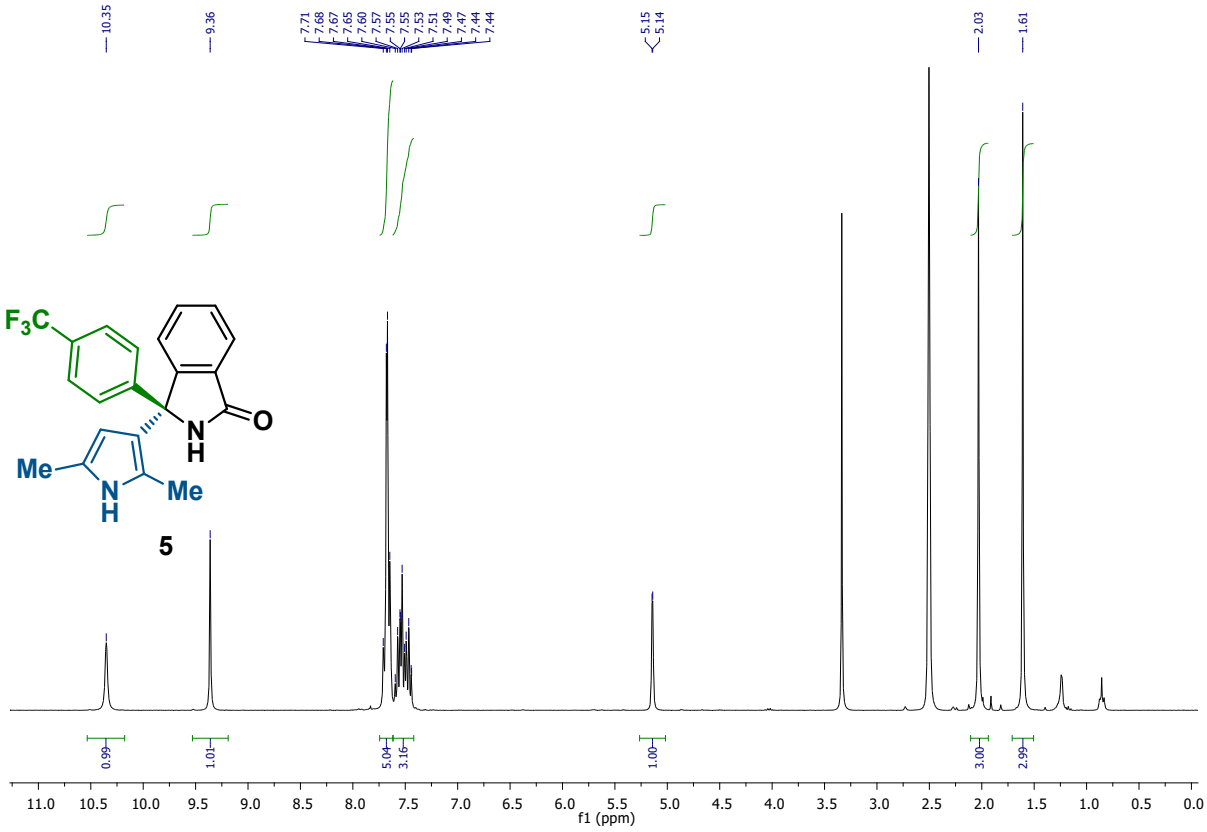
H
O
Me
N
H
Me
4
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.53
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7.44
7.44
5.15
5.14
2.03
1.61
F3C
N
H
O
Me
N
H
Me
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5.04
3.16
1.00
3.00
2.99
11.0
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10.0
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9.0
8.5
8.0
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6.0
5.5
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3.5
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2.0
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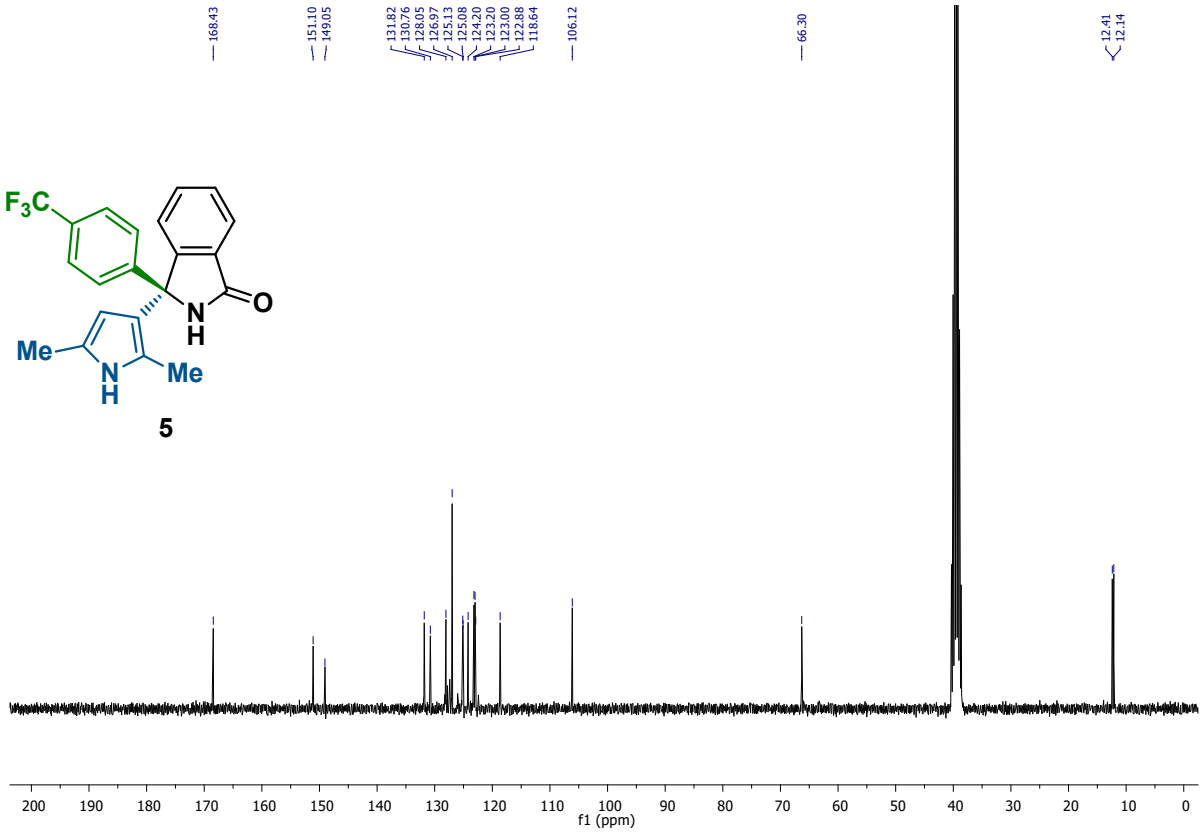
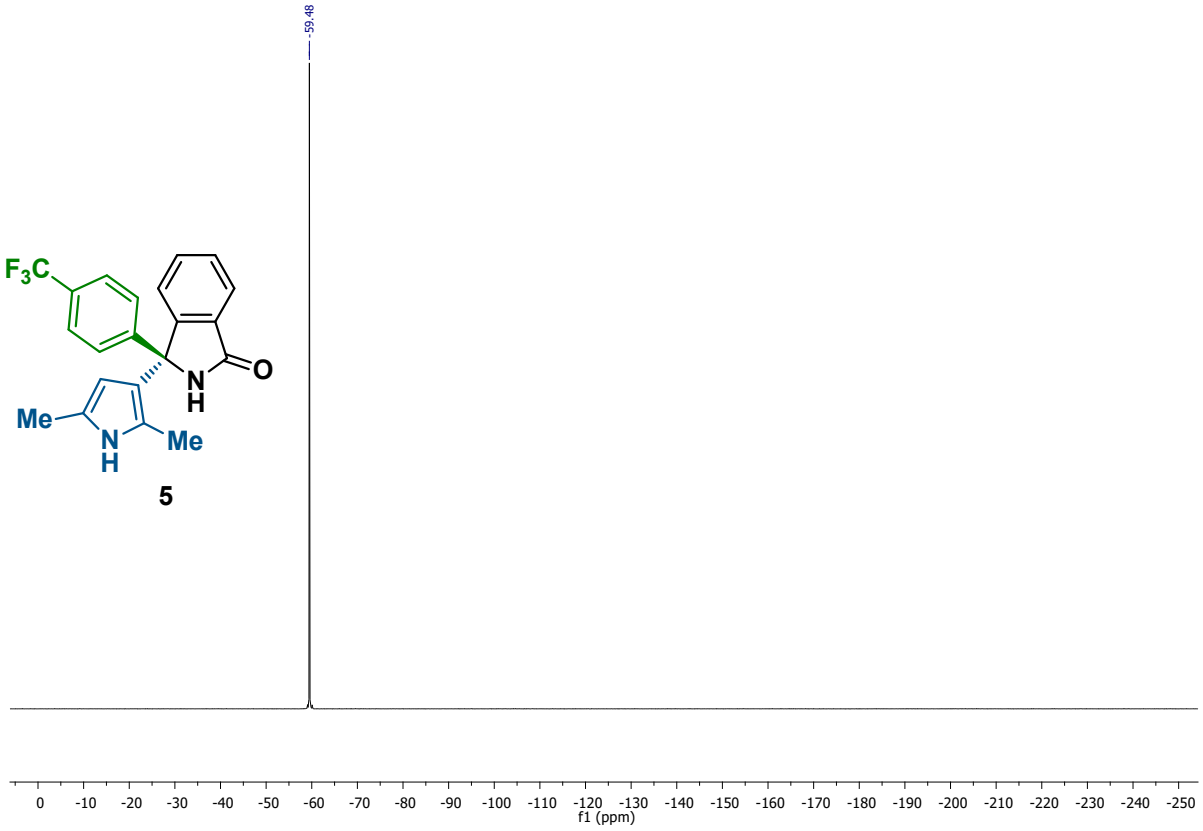
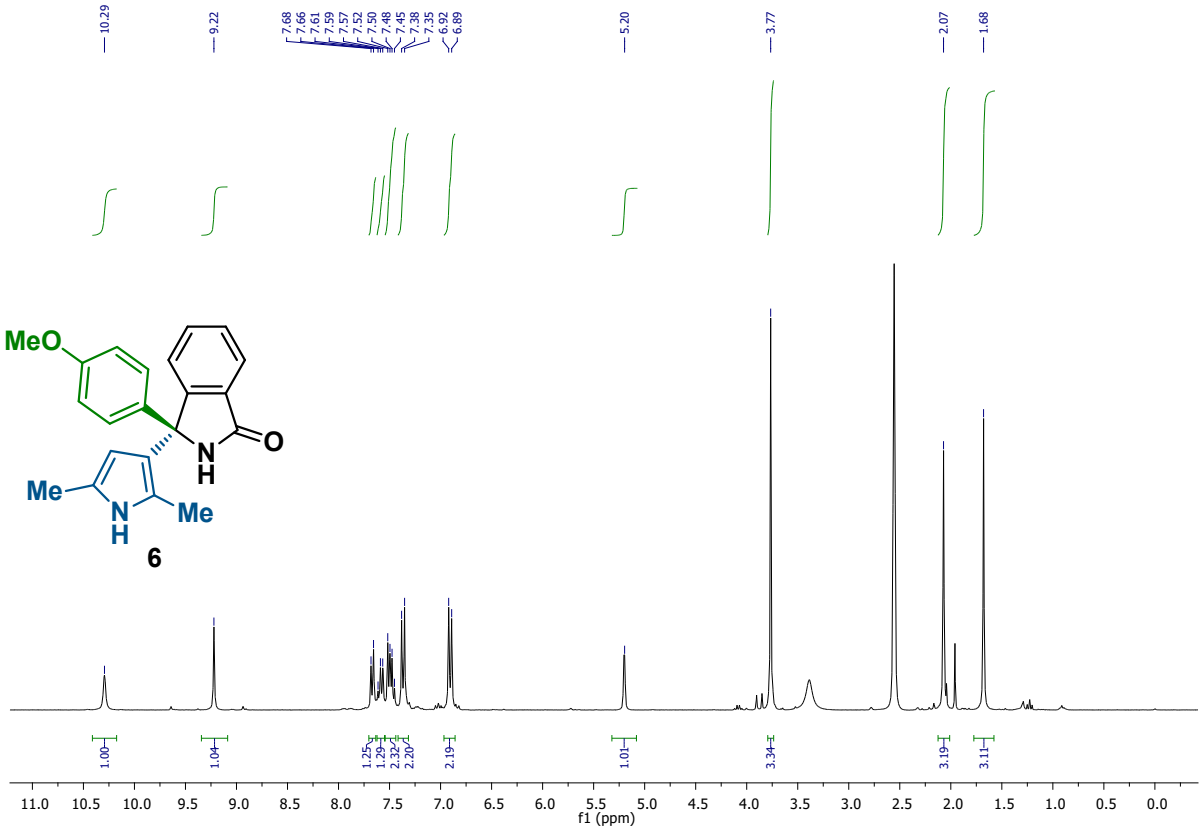
0.5
0.0
f1 (ppm)


168.43
151.10
149.05
131.82
130.76
128.05
126.97
125.13
125.08
124.20
123.20
123.00
122.88
118.64
106.12
66.30
12.41
12.14
F3C
O
N
H
Me
N
H
Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

5


-59.48
F3C
O
N
H
Me
N
H
Me
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250
f1 (ppm)

5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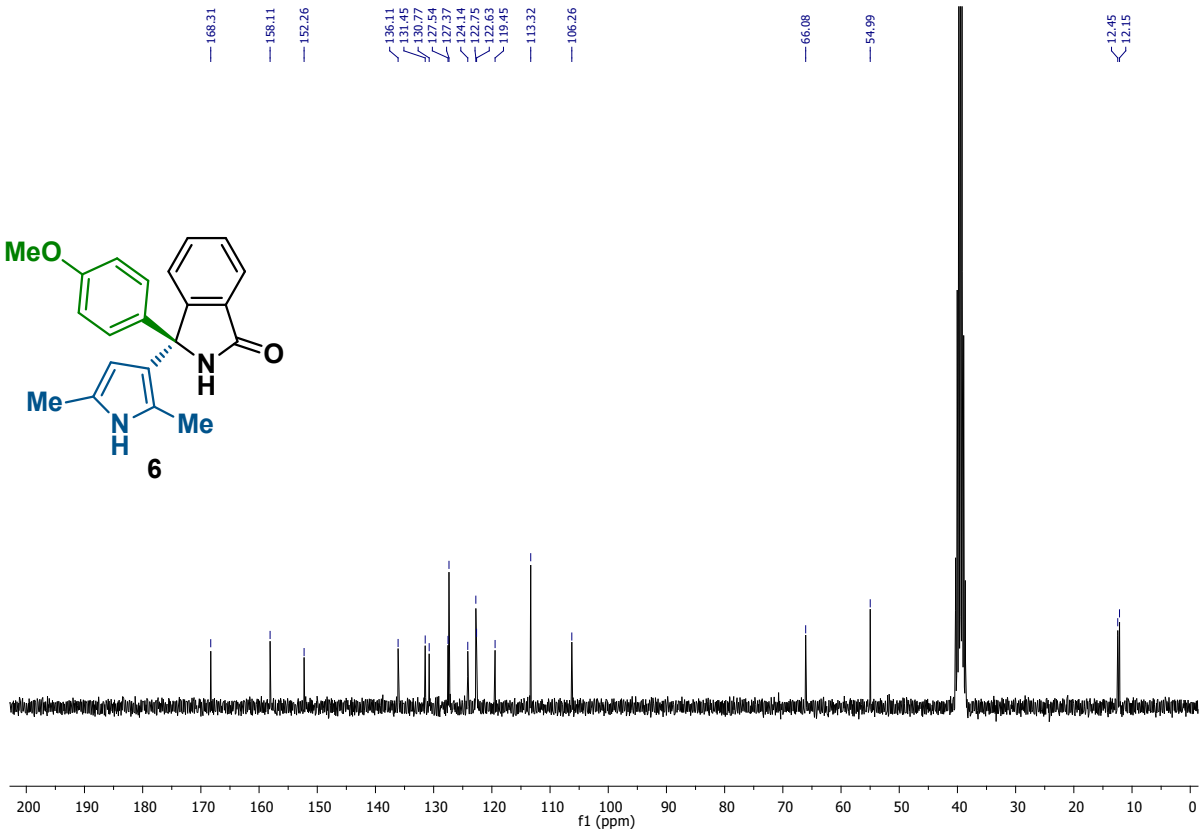
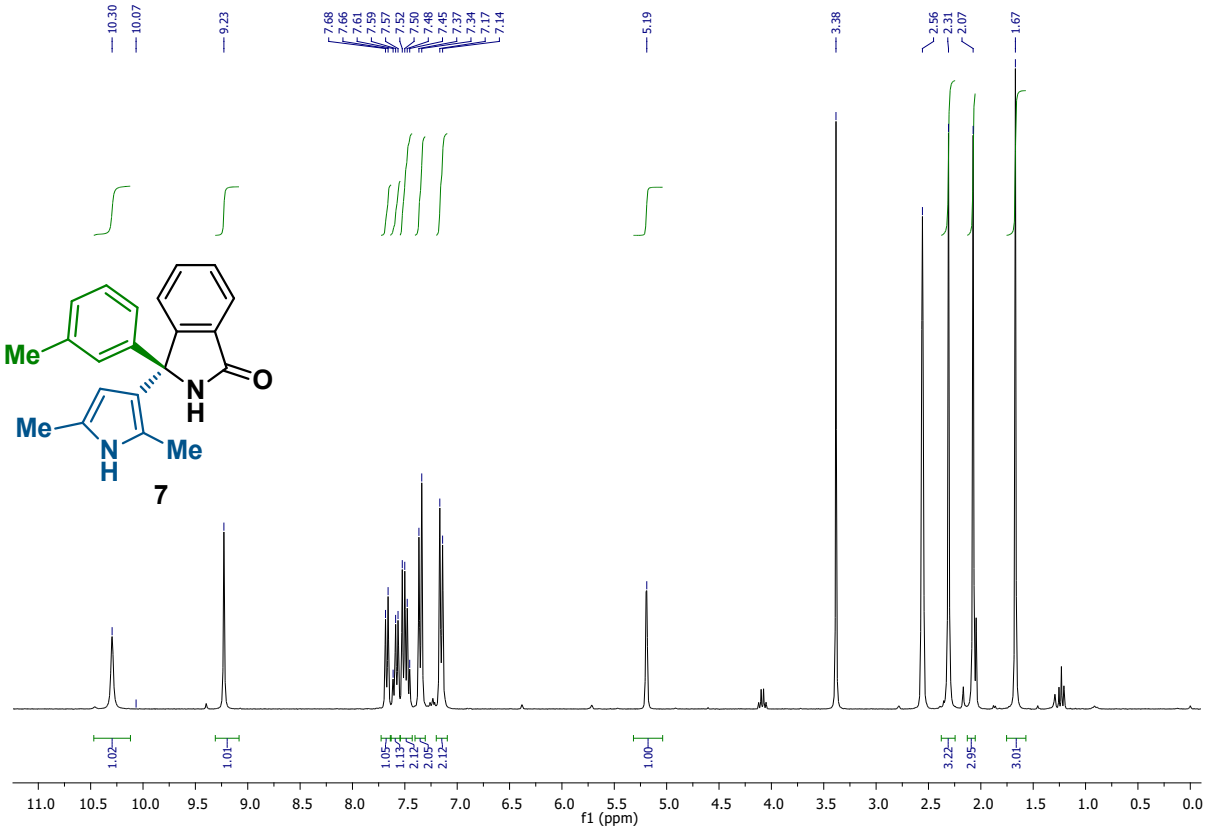
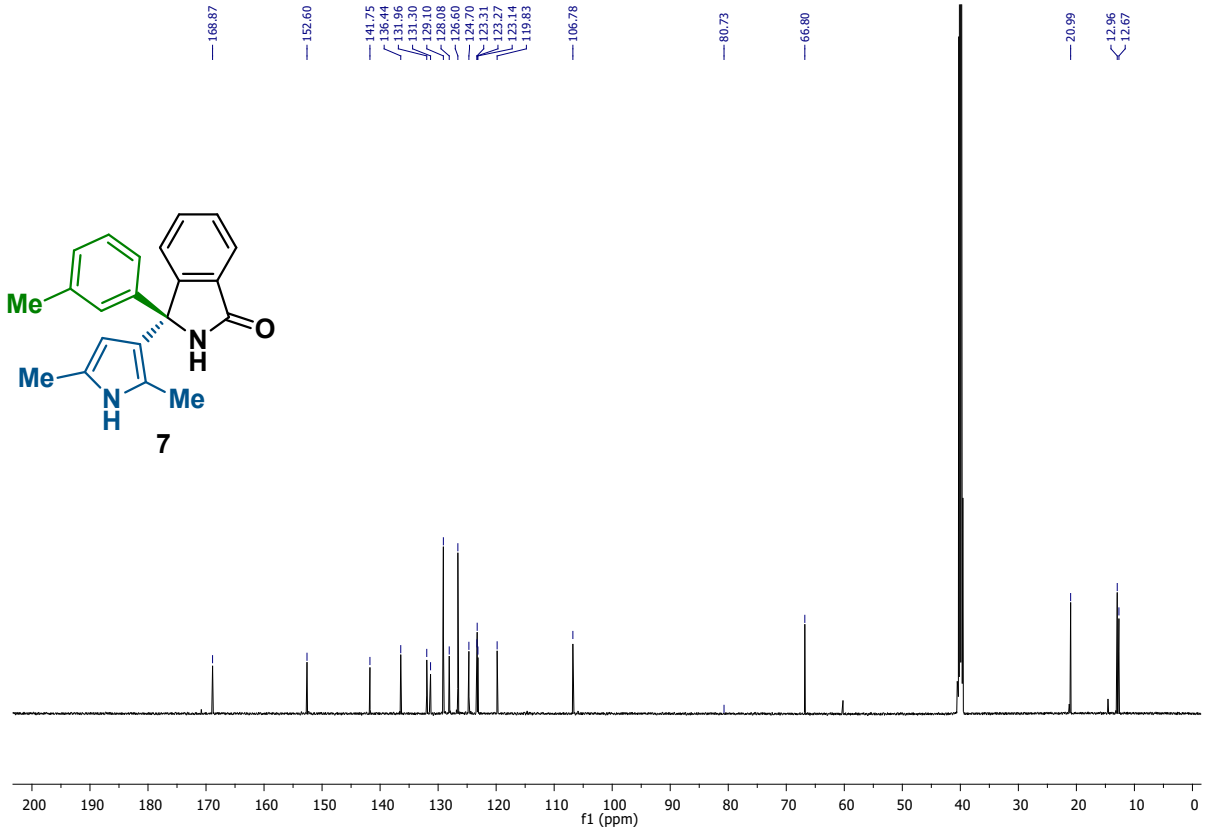
9.22
7.68
7.66
7.61
7.59
7.57
7.52
7.50
7.48
7.45
7.38
7.35
6.92
6.89
5.20
3.77
2.07
1.68
MeO
O
N
H
Me
N
H
Me
6
1.00
1.04
1.25
1.29
2.32
2.20
2.19
1.01
3.34
3.19
3.11
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.31
158.11
152.26
136.11
131.45
130.77
127.54
127.37
124.14
122.75
122.63
119.45
113.32
106.26
66.08
54.99
12.45
12.15
MeO
O
N
H
Me
N
H
Me
6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


10.30
10.07
9.23
7.68
7.66
7.61
7.59
7.57
7.52
7.50
7.48
7.45
7.37
7.34
7.17
7.14
5.19
3.38
2.56
2.31
2.07
1.67
Me
N
H
O
Me
N
H
Me
7
1.02
1.01
1.05
1.13
2.12
2.05
2.12
1.00
3.22
2.95
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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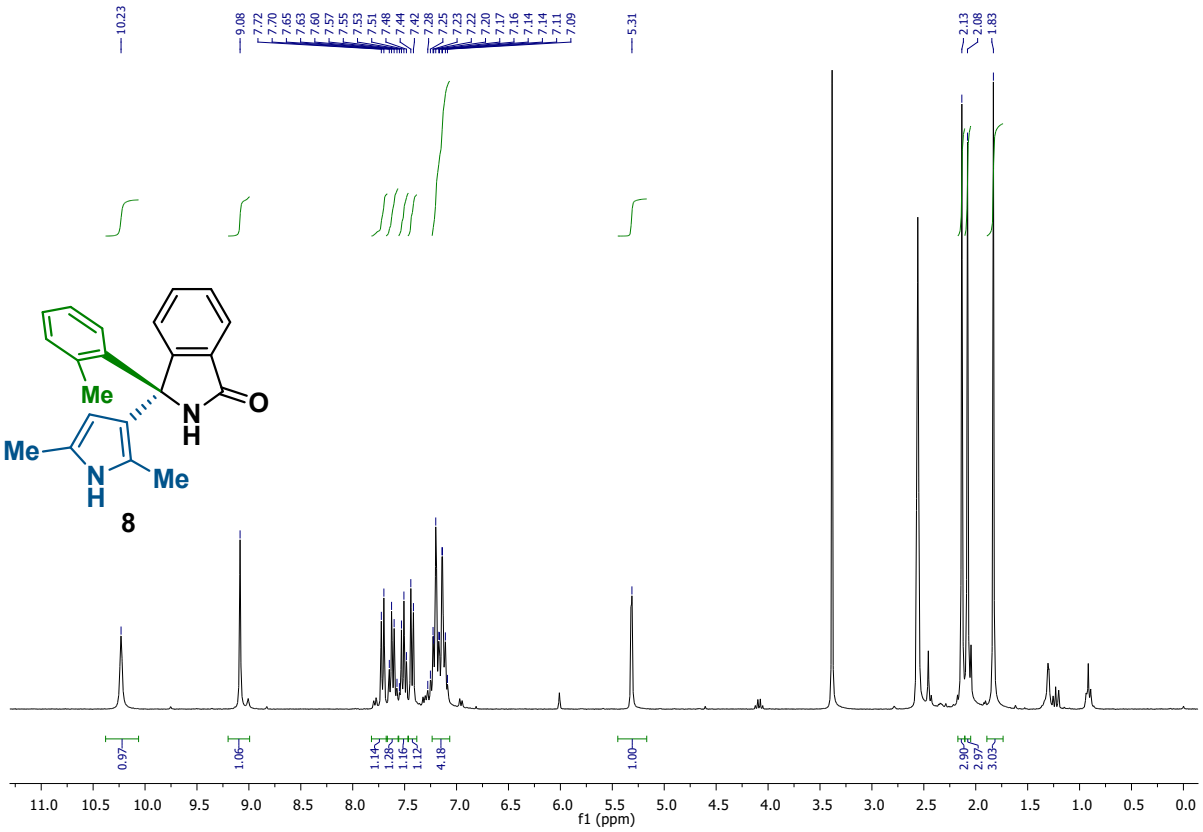
152.60
141.75
136.44
131.96
131.30
129.10
128.08
126.60
124.70
123.31
123.27
123.14
119.83
106.78
80.73
66.80
20.99
12.96
12.67
Me
N
H
O
Me
N
H
Me
7
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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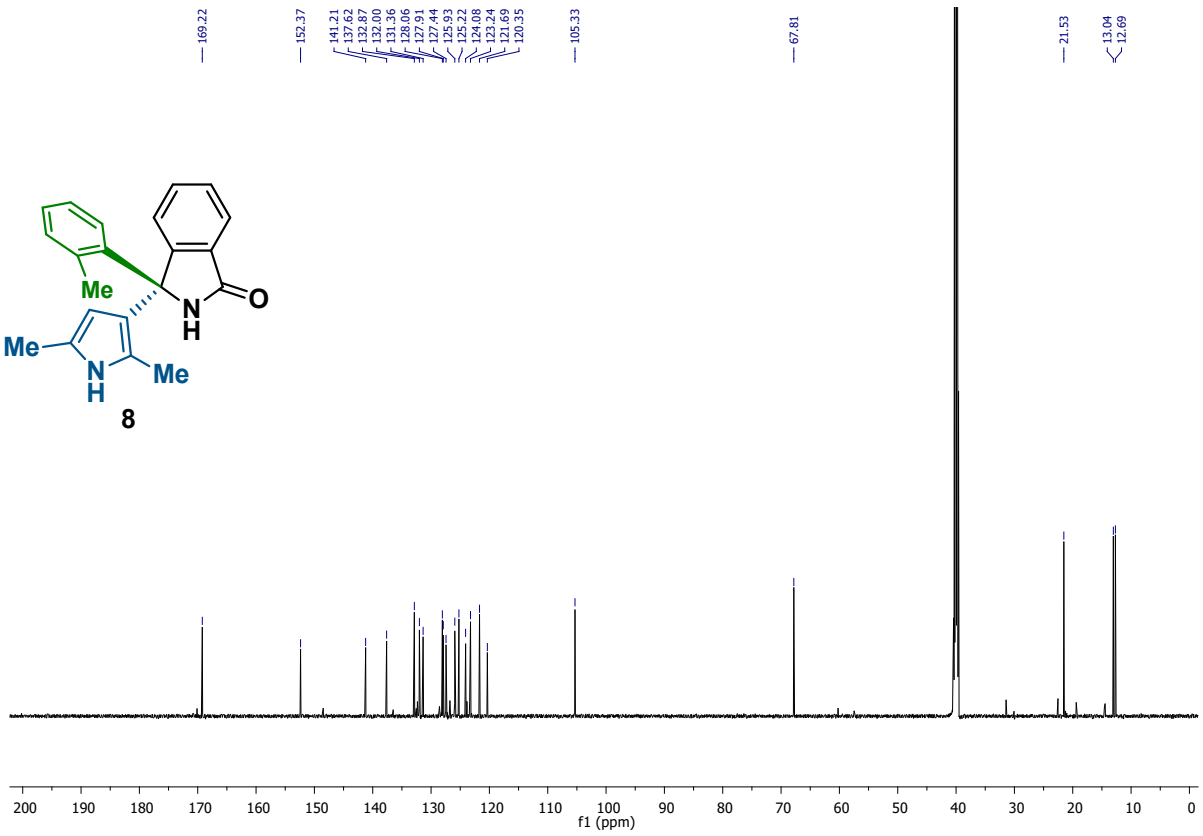
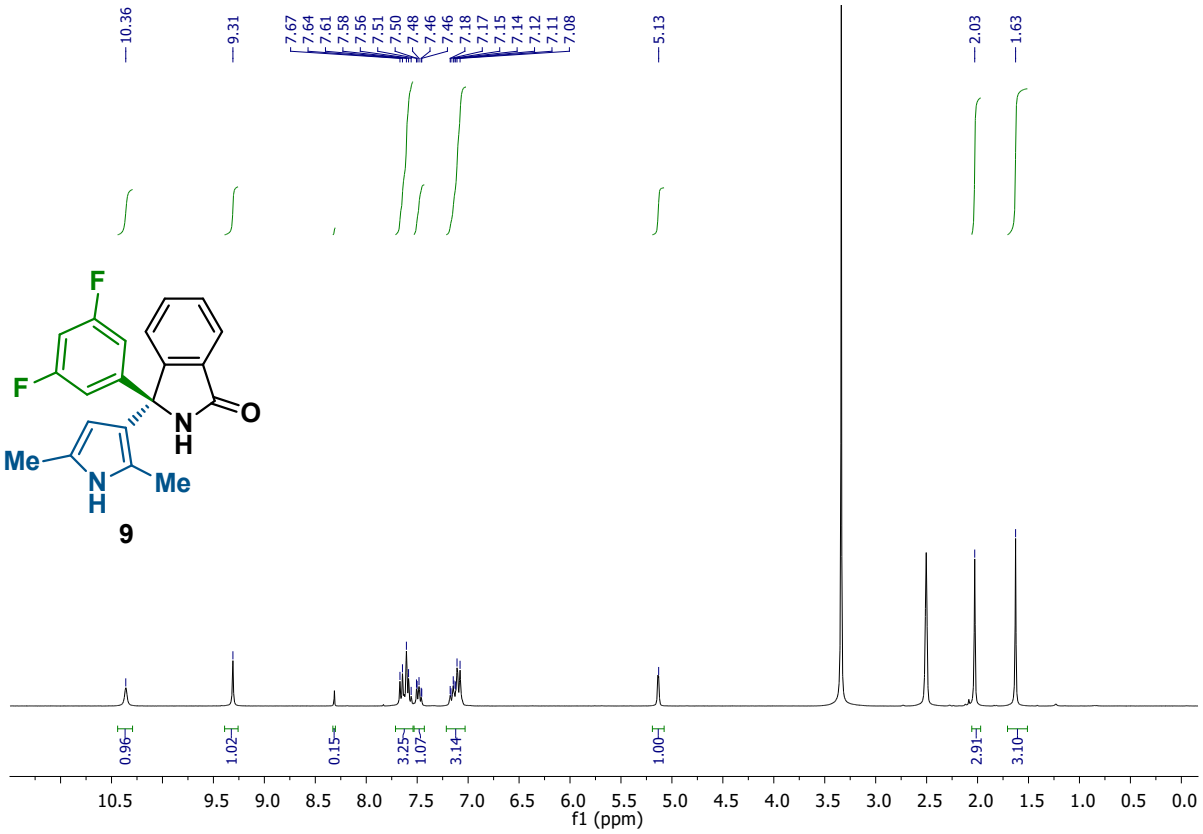
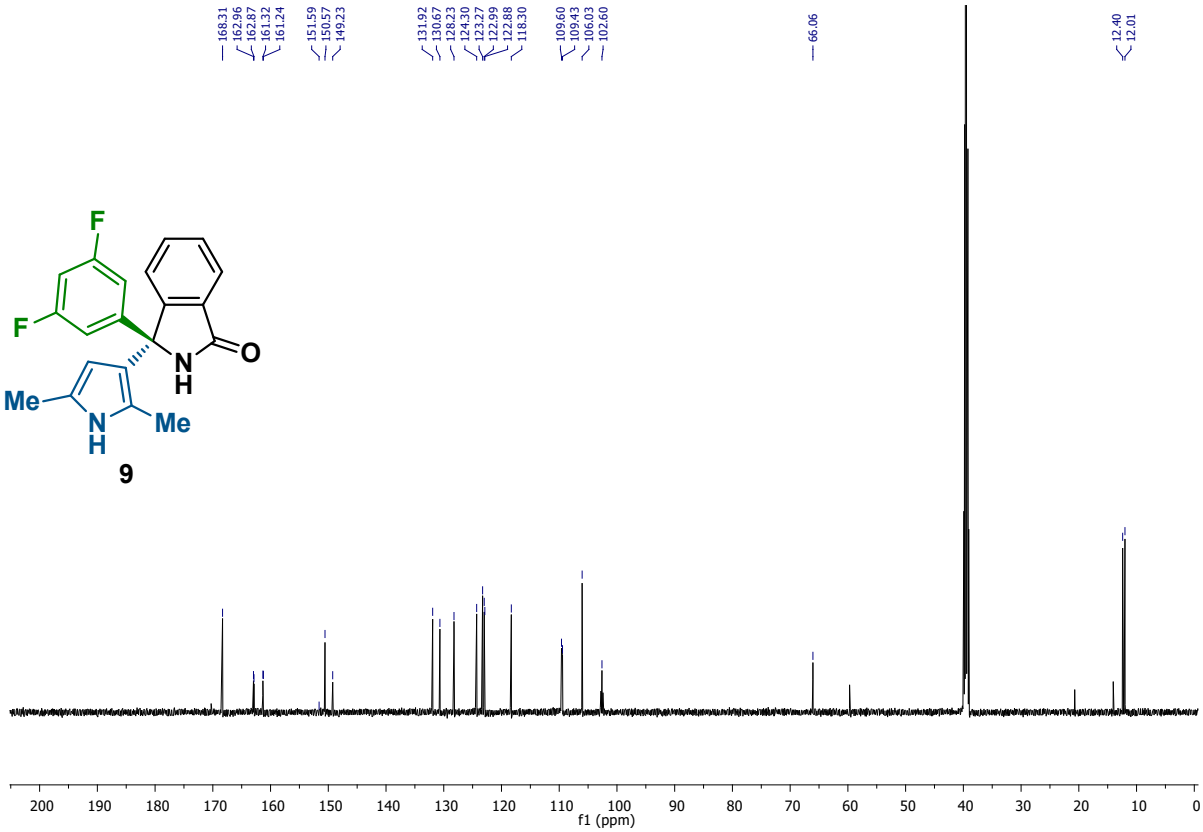
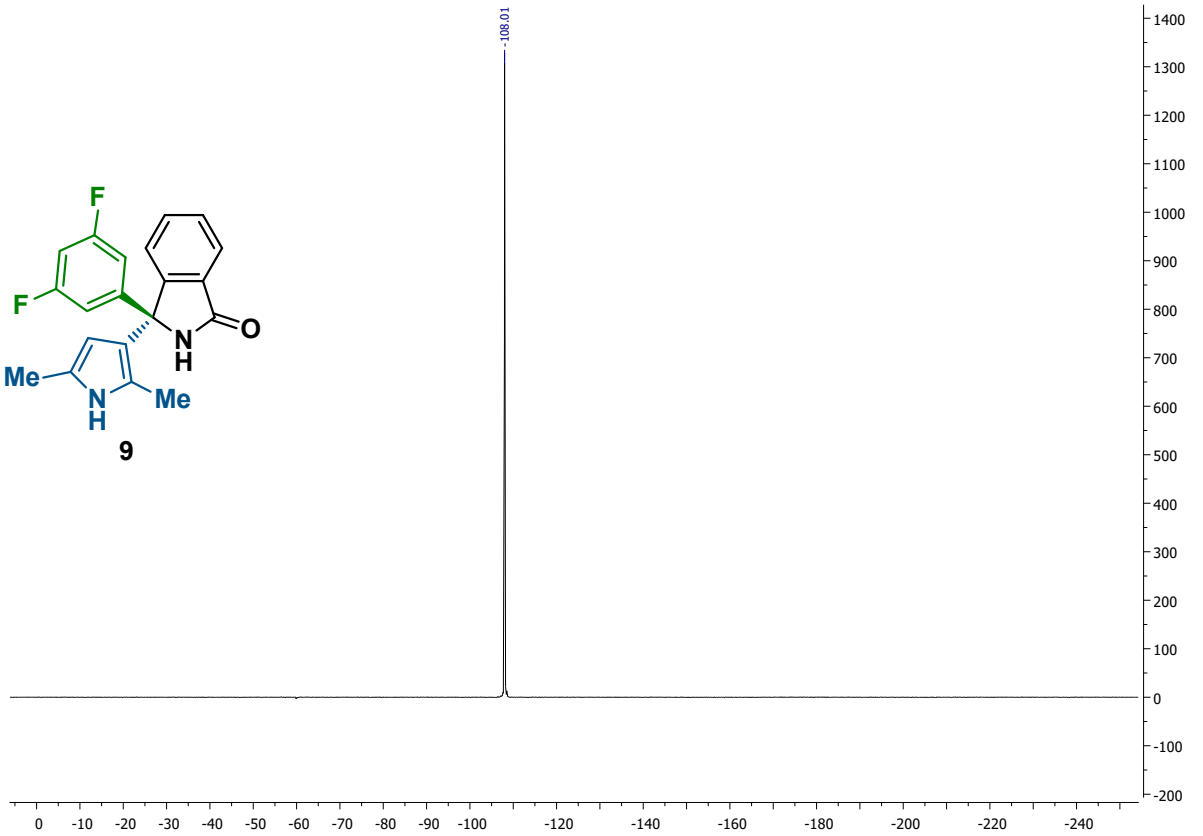
9.08
7.72
7.70
7.65
7.63
7.60
7.57
7.55
7.53
7.51
7.48
7.44
7.42
7.28
7.25
7.23
7.22
7.20
7.17
7.16
7.14
7.14
7.11
7.09
5.31
2.13
2.08
1.83
Me
N
H
O
Me
N
H
Me
8
0.97
1.06
1.14
1.28
1.16
1.12
4.18
1.00
2.90
2.97
3.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

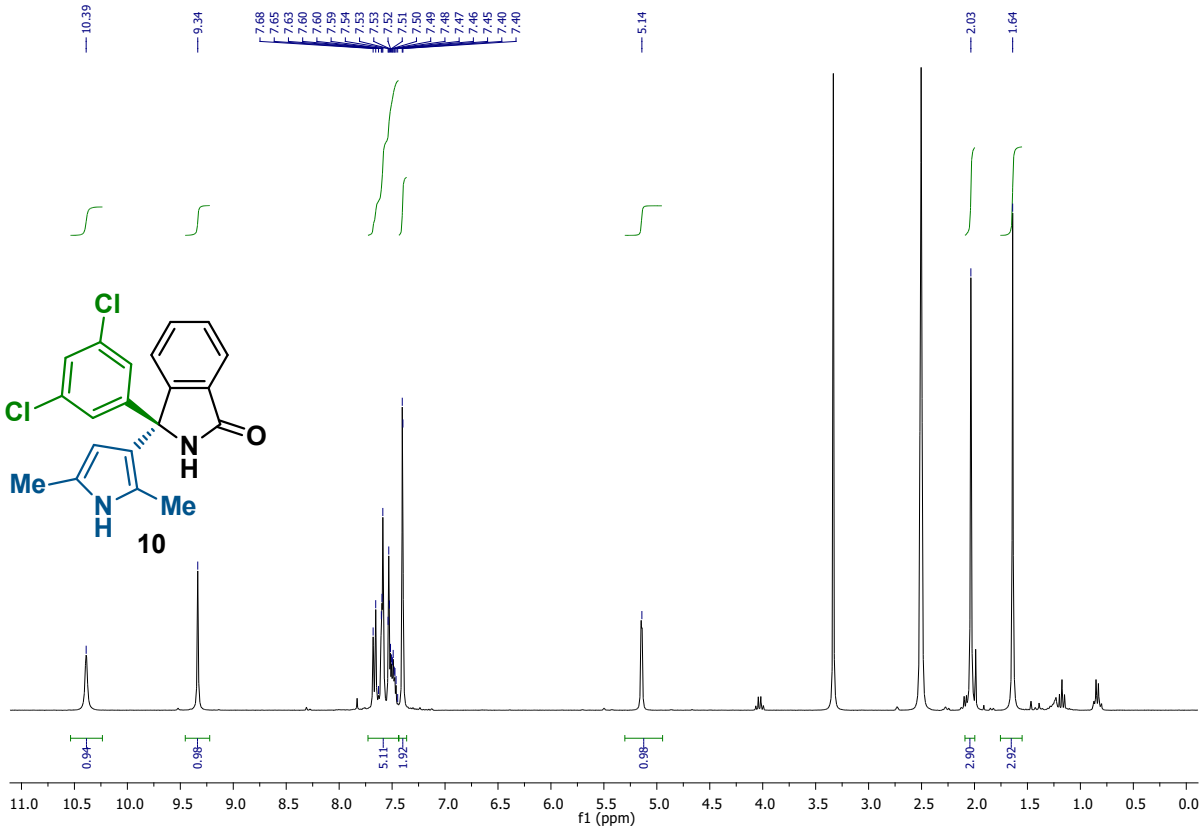

169.22
152.37
141.21
137.62
132.87
132.00
131.36
128.06
127.91
127.44
125.93
125.22
124.08
123.24
121.69
120.35
105.33
67.81
21.53
13.04
12.69
Me
N
H
O
Me
N
H
Me
8
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

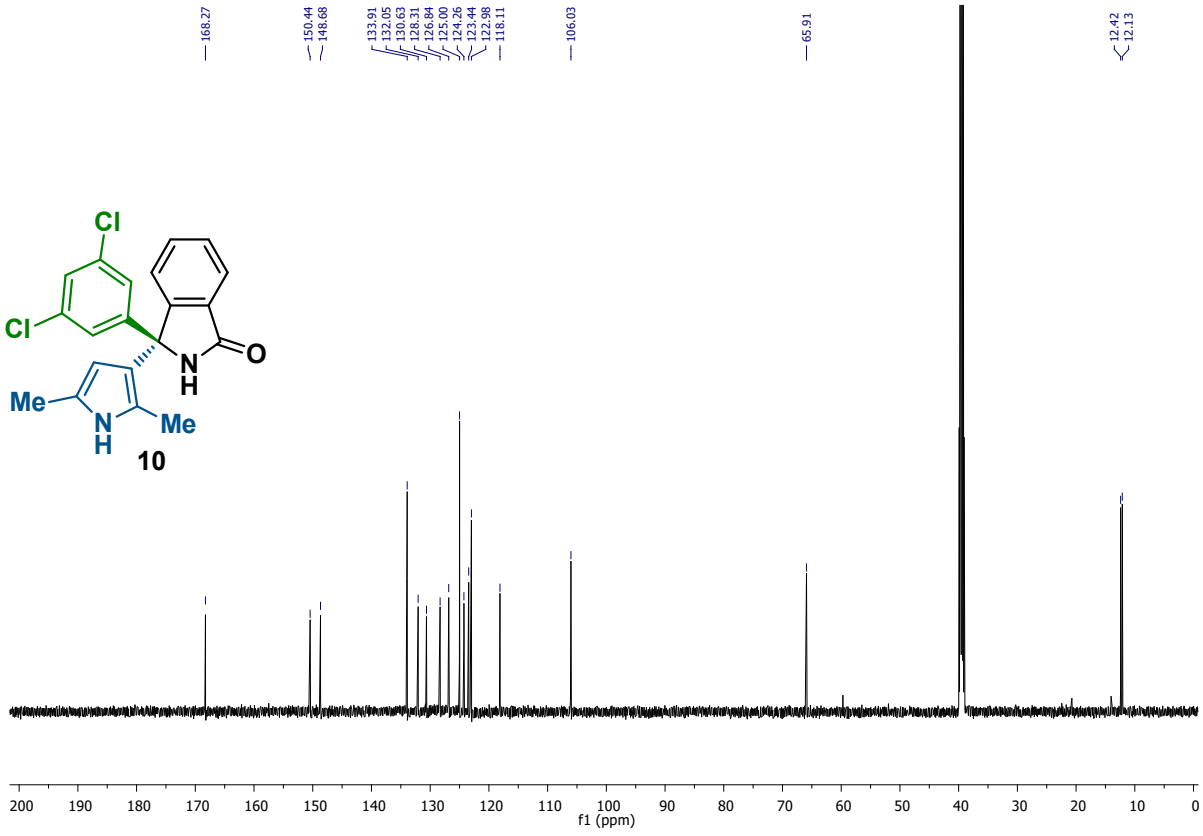

10.36
9.31
7.67
7.64
7.61
7.58
7.56
7.51
7.50
7.48
7.46
7.46
7.18
7.17
7.15
7.14
7.12
7.11
7.08
5.13
2.03
1.63
F
F
N
H
O
Me
N
H
Me
0.96
1.02
0.15
3.25
1.07
3.14
1.00
2.91
3.10
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

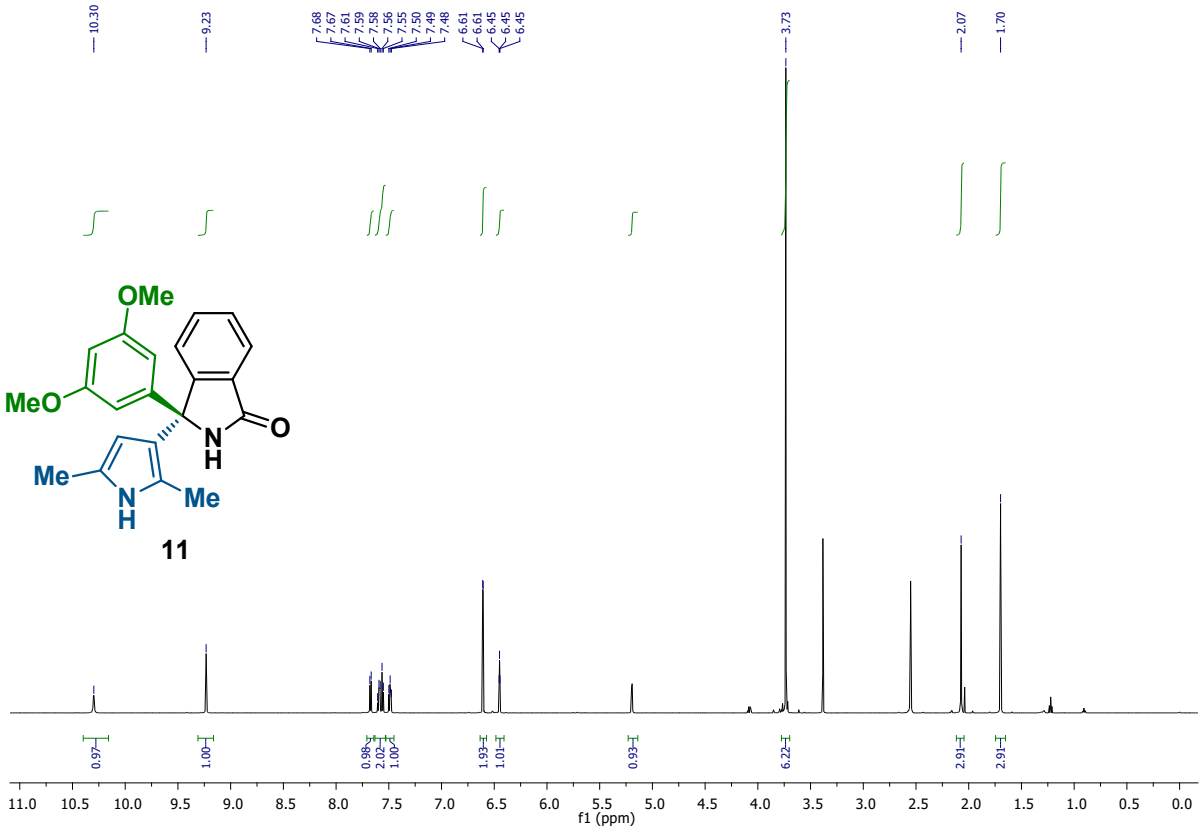
9

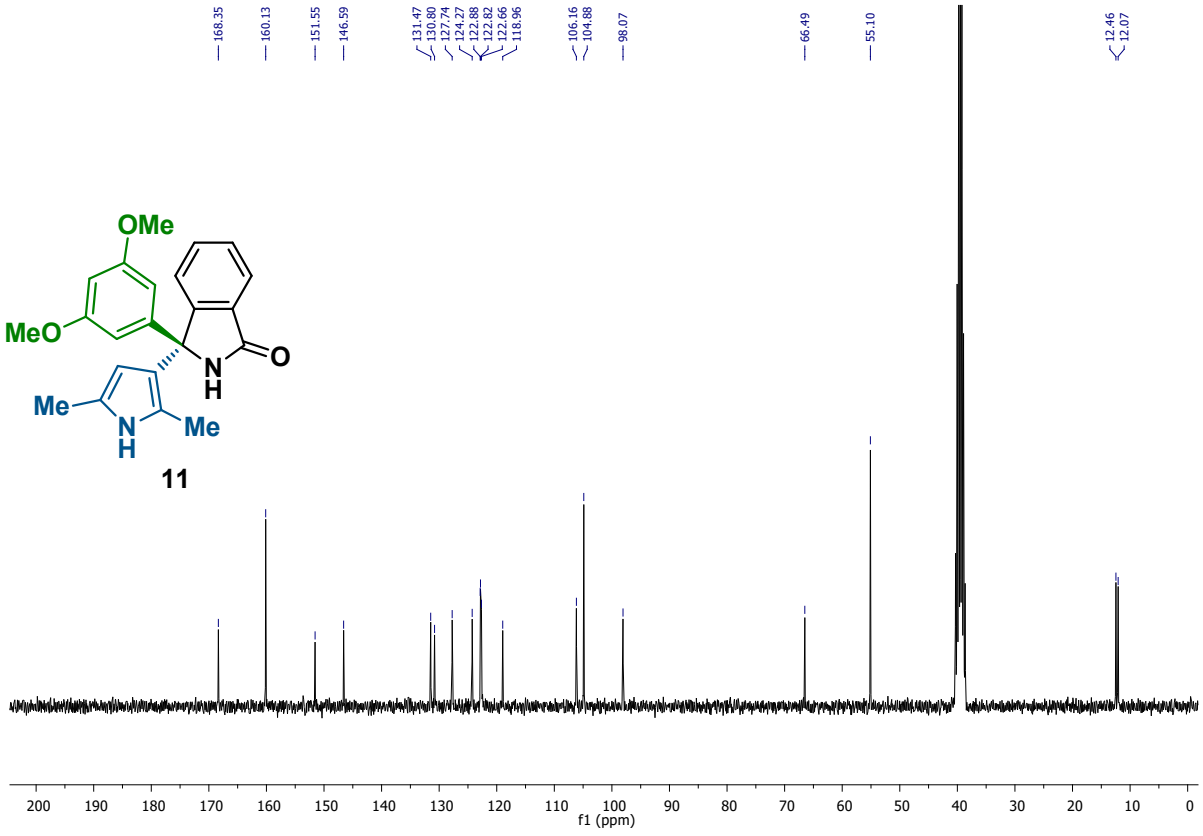

168.31
162.96
162.87
161.32
161.24
151.59
150.57
149.23
131.92
130.67
128.23
124.30
123.27
122.99
122.88
118.30
109.60
109.43
106.03
102.60
66.06
12.40
12.01
F
F
N
H
O
Me
N
H
Me
9
f1 (ppm)


-108.01
F
F
N
H
O
Me
N
H
Me
9

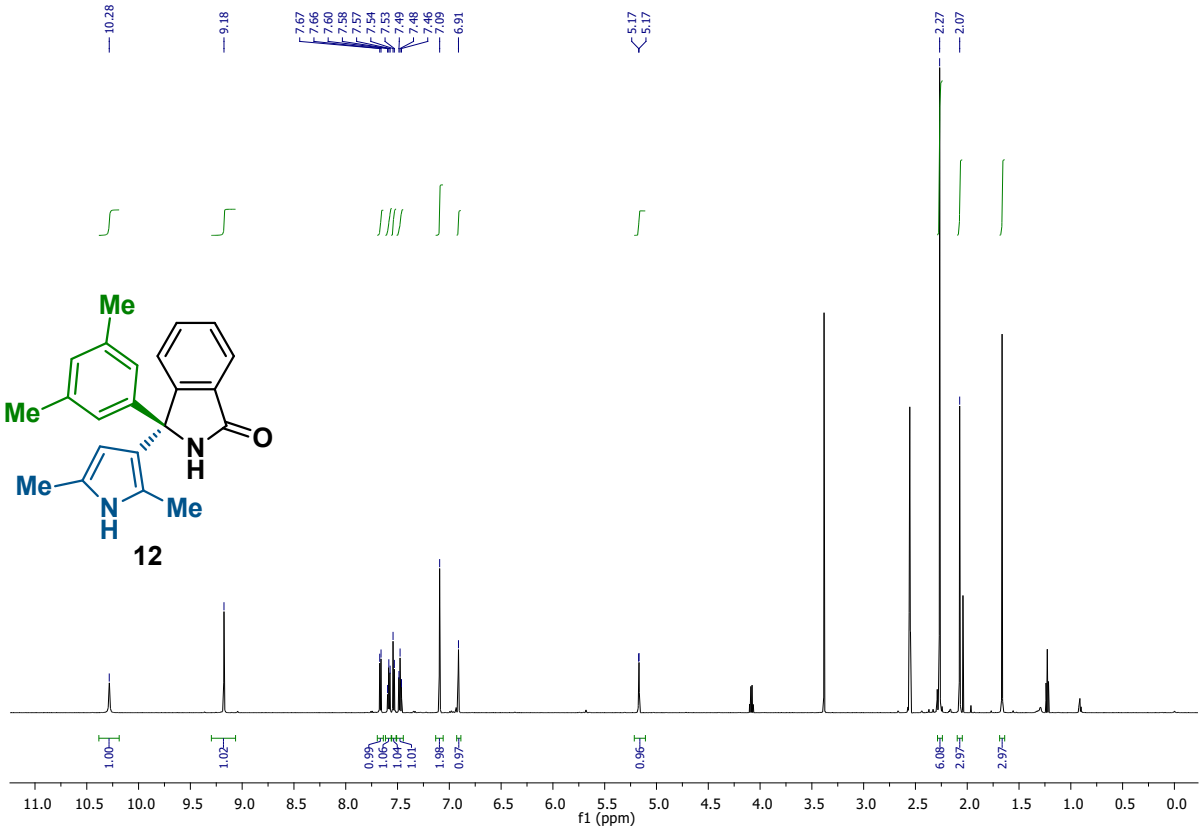

10.39
9.34
7.68
7.65
7.63
7.60
7.60
7.59
7.54
7.53
7.53
7.52
7.51
7.50
7.49
7.48
7.47
7.46
7.45
7.40
7.40
5.14
2.03
1.64
Cl
Cl
N
H
O
Me
N
H
Me
10
0.94
0.98
5.11
1.92
0.98
2.90
2.92
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

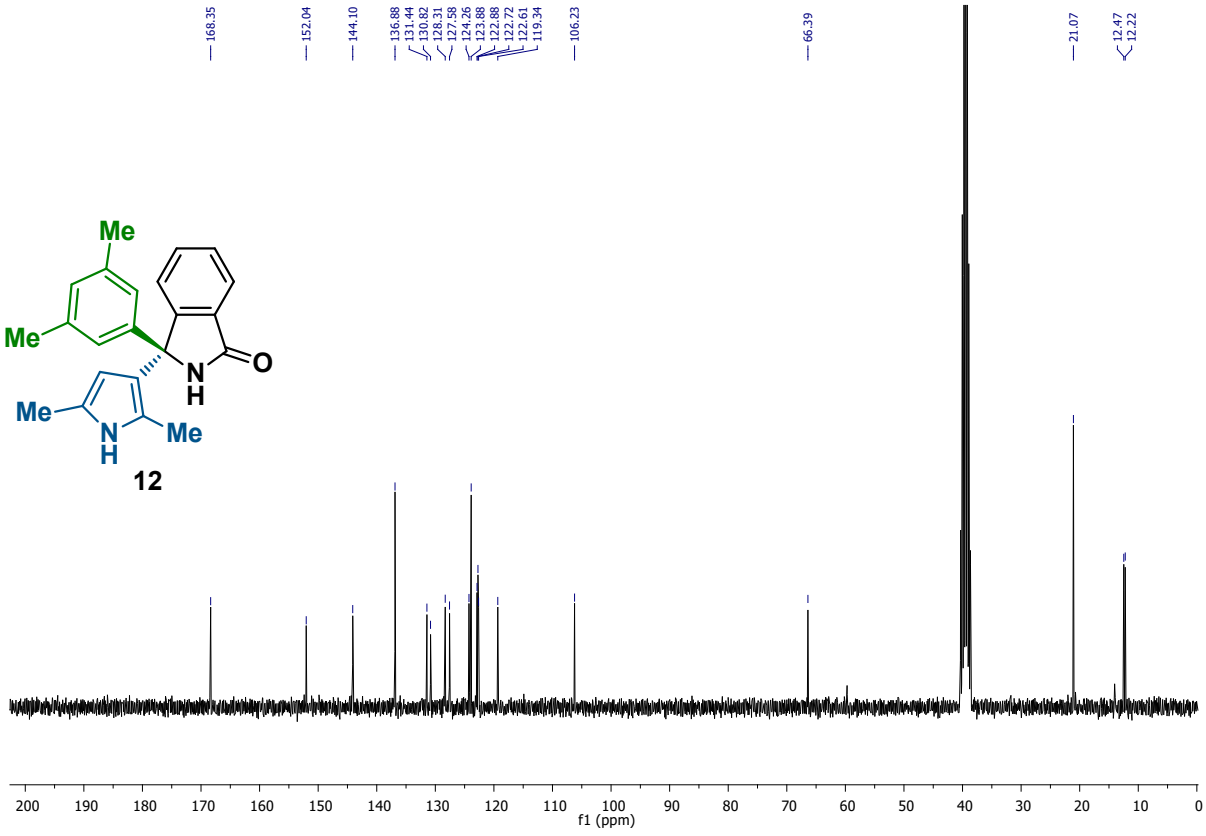

168.27
150.44
148.68
133.91
132.05
130.63
128.31
126.84
125.00
124.26
123.44
122.98
118.11
106.03
65.91
12.42
12.13
Cl
Cl
N
H
O
Me
N
H
Me
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.30
9.23
7.68
7.67
7.61
7.59
7.58
7.56
7.55
7.50
7.49
7.48
6.61
6.61
6.45
6.45
6.45
3.73
2.07
1.70
OMe
MeO
N
H
O
Me
N
H
Me
11
0.97
1.00
0.98
2.02
1.00
1.93
1.01
0.93
6.22
2.91
2.91
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

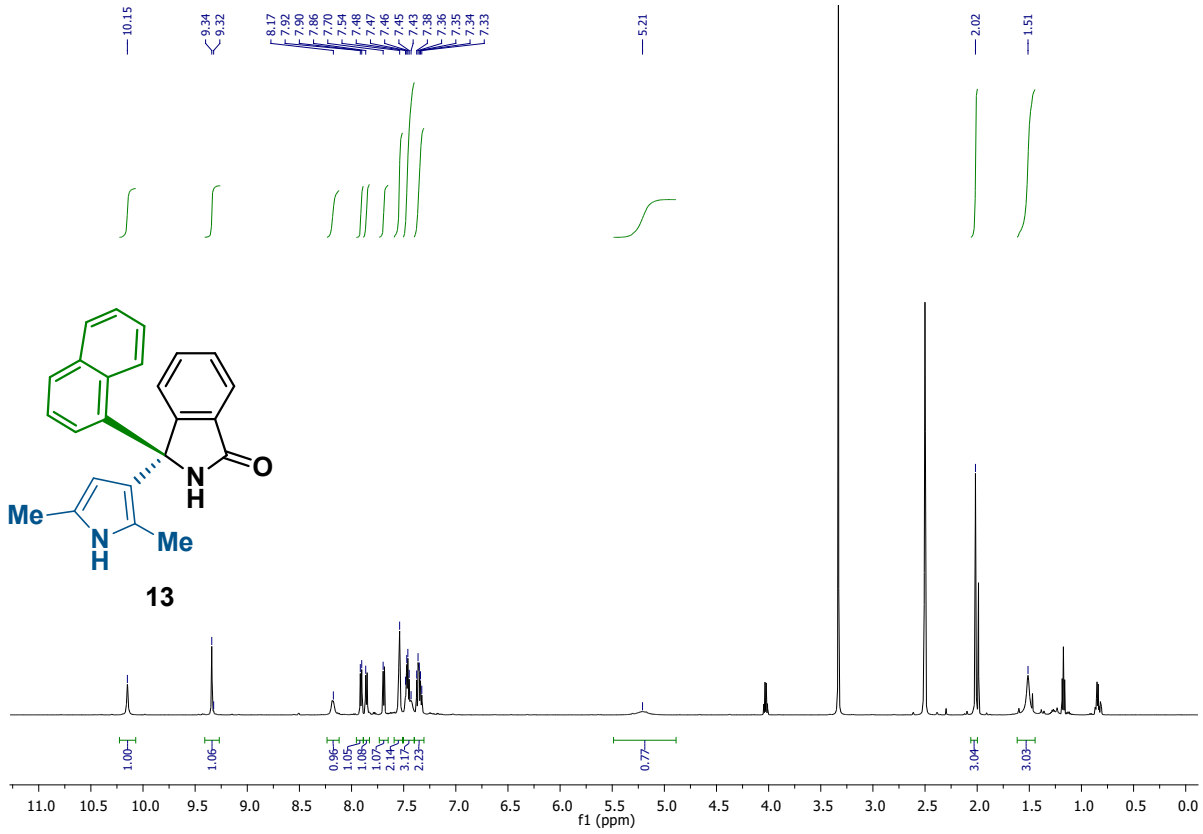

168.35
160.13
151.55
146.59
131.47
130.80
127.74
124.27
122.88
122.82
122.66
118.96
106.16
104.88
98.07
66.49
55.10
12.46
12.07
OMe
MeO
N
H
O
Me
N
H
Me
11
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

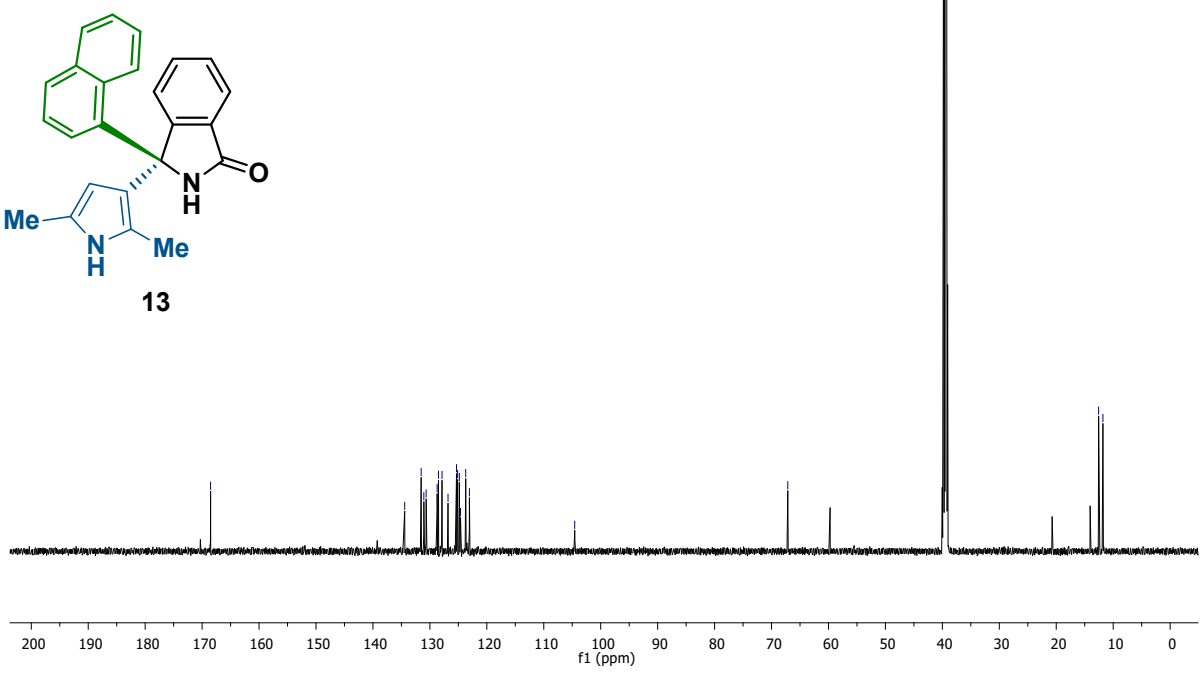
Traces of ethyl acetate observable in spectra.

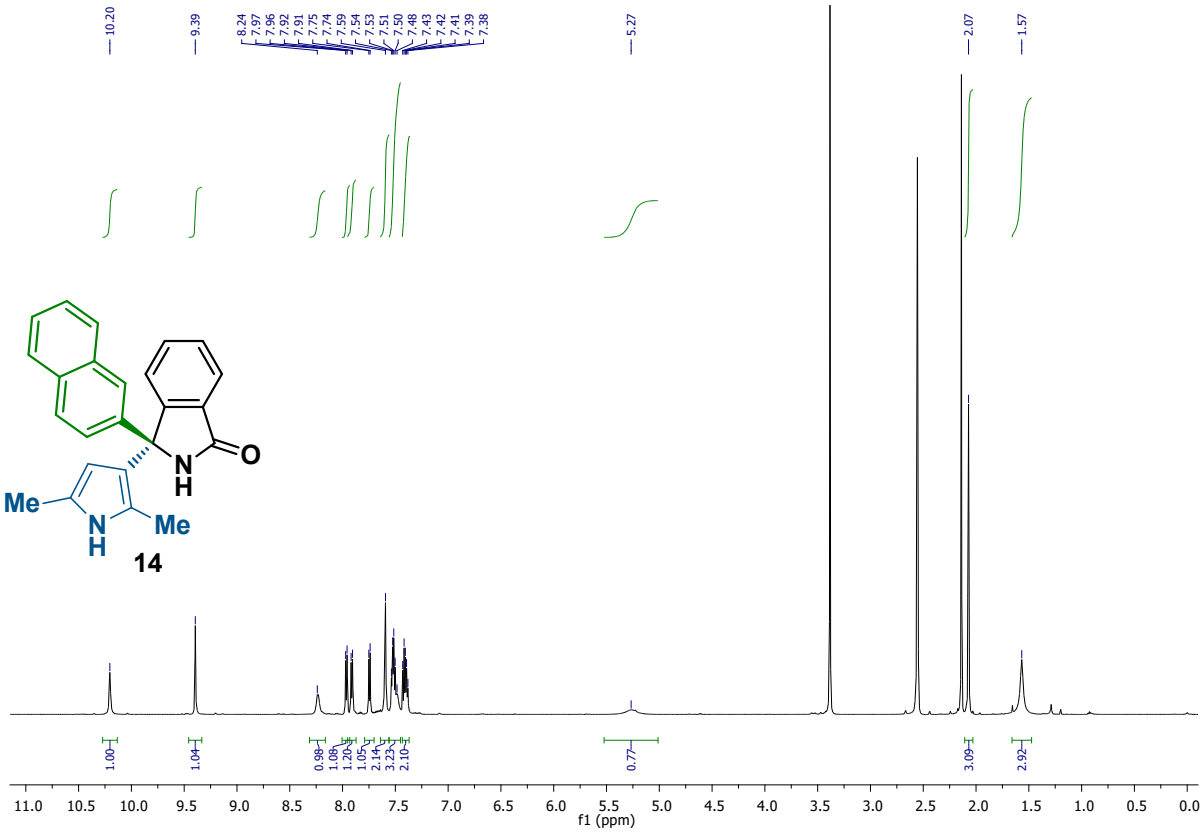


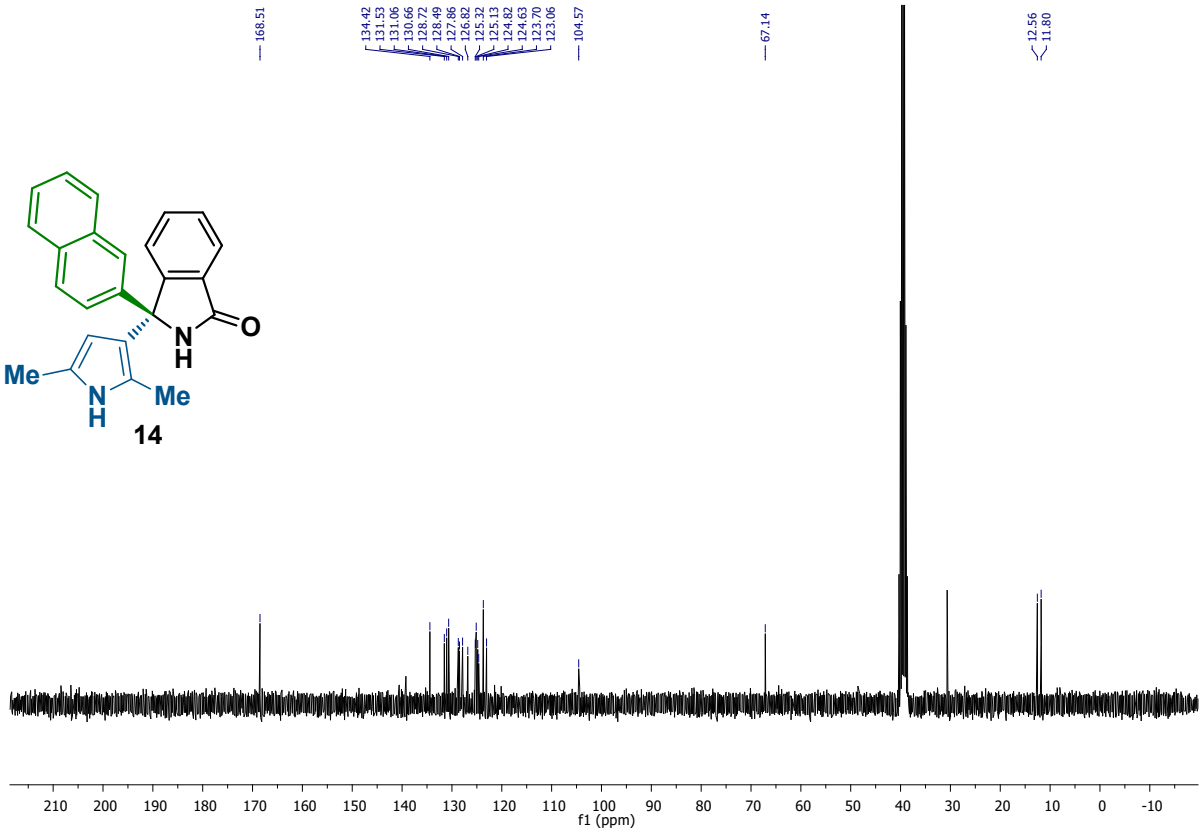


Traces of ethyl acetate observable in spectra.

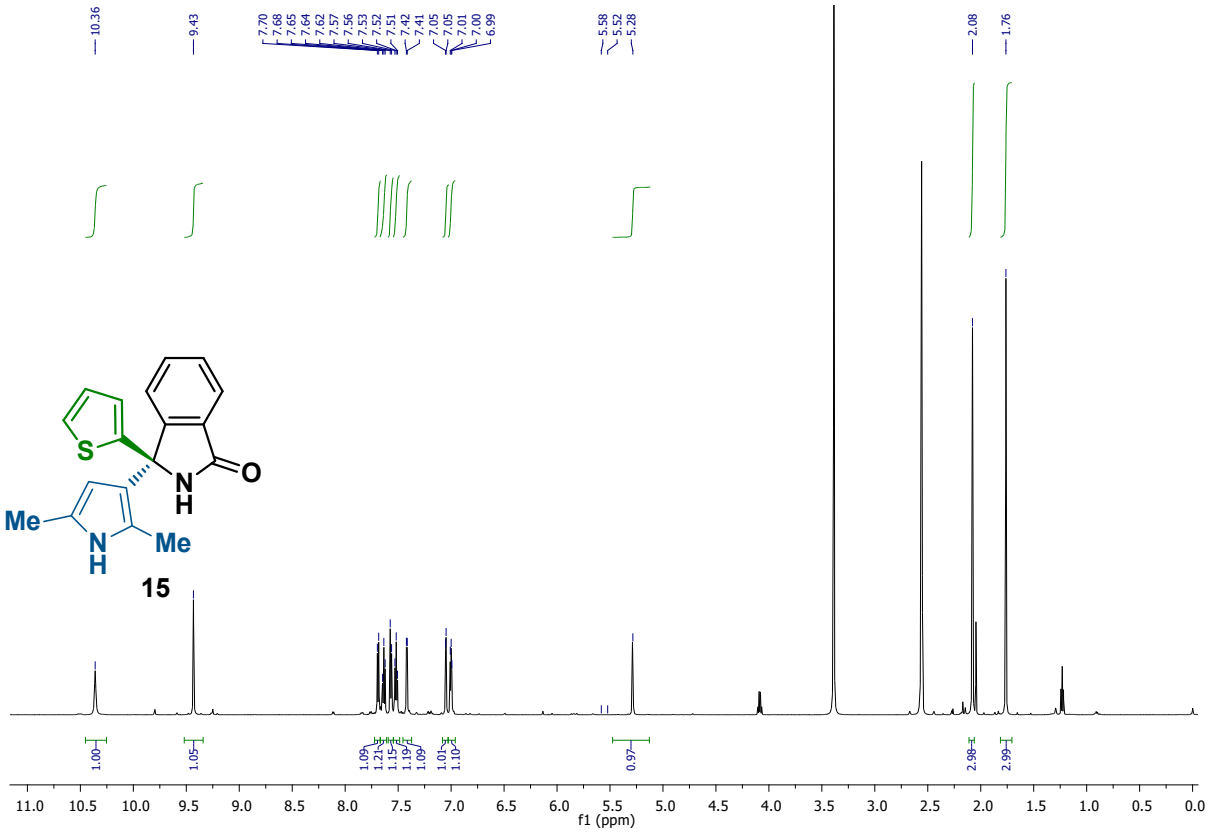


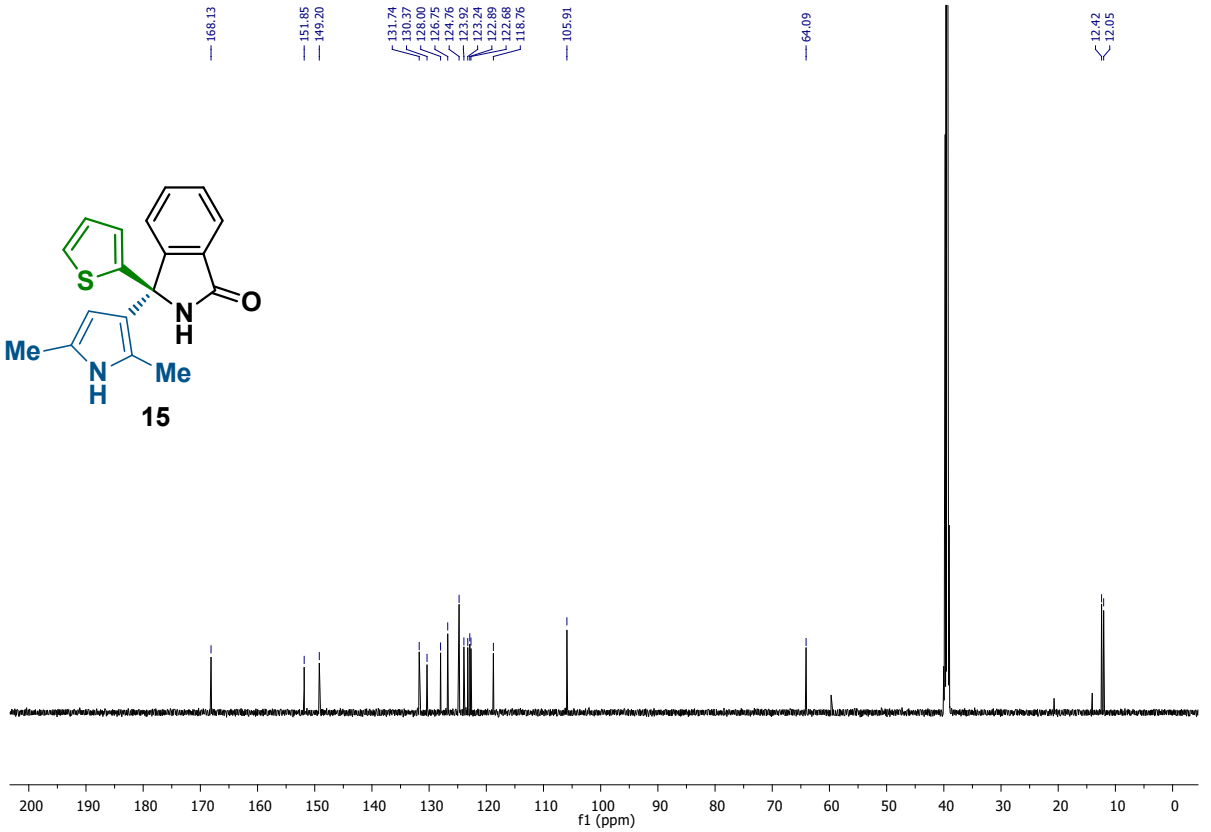



10.20
9.39
8.24
7.97
7.96
7.92
7.91
7.75
7.74
7.59
7.54
7.53
7.51
7.50
7.48
7.43
7.42
7.41
7.39
7.38
5.27
2.07
1.57
Me
N
H
Me
N
H
O
14
1.00
1.04
0.98
1.08
1.20
1.05
2.14
3.23
2.10
0.77
3.09
2.92
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

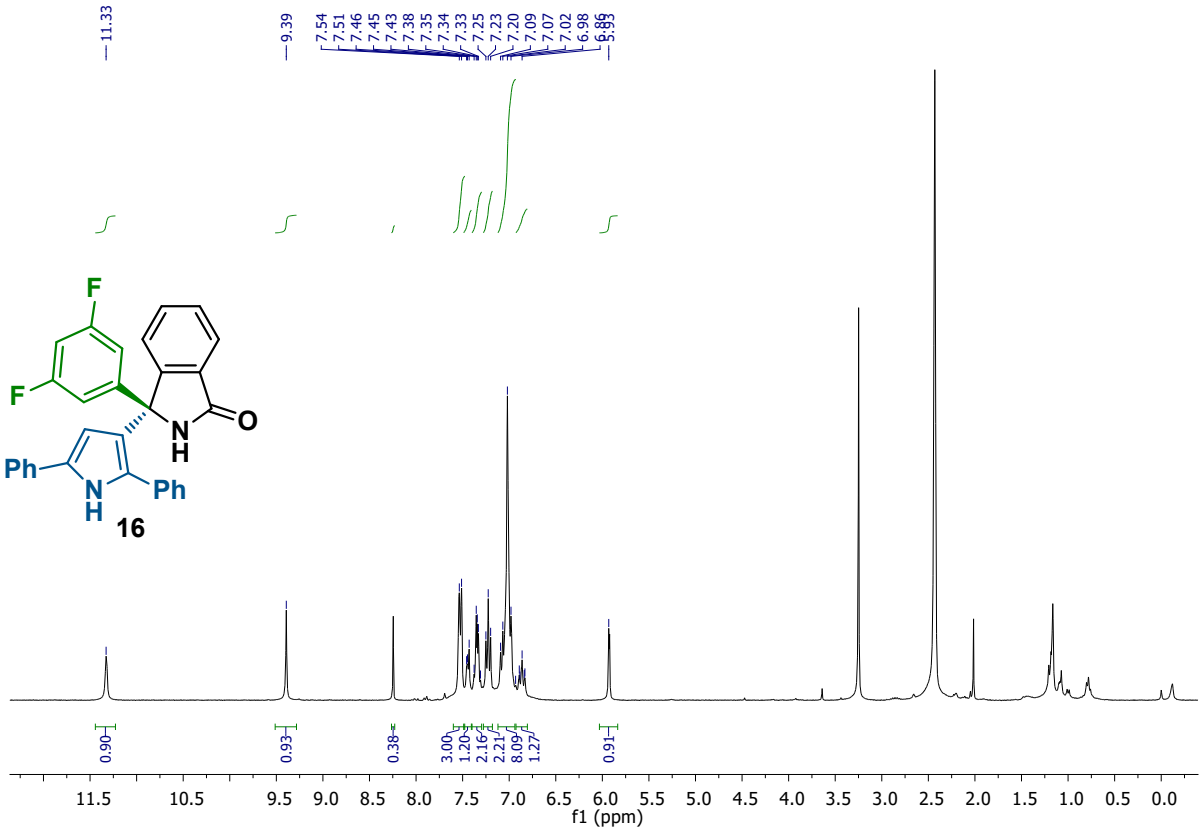

168.51
134.42
131.53
131.06
130.66
128.72
128.49
127.86
126.82
125.32
125.13
124.82
124.63
123.70
123.06
104.57
67.14
12.56
11.80
Me
N
H
Me
N
H
O
14
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

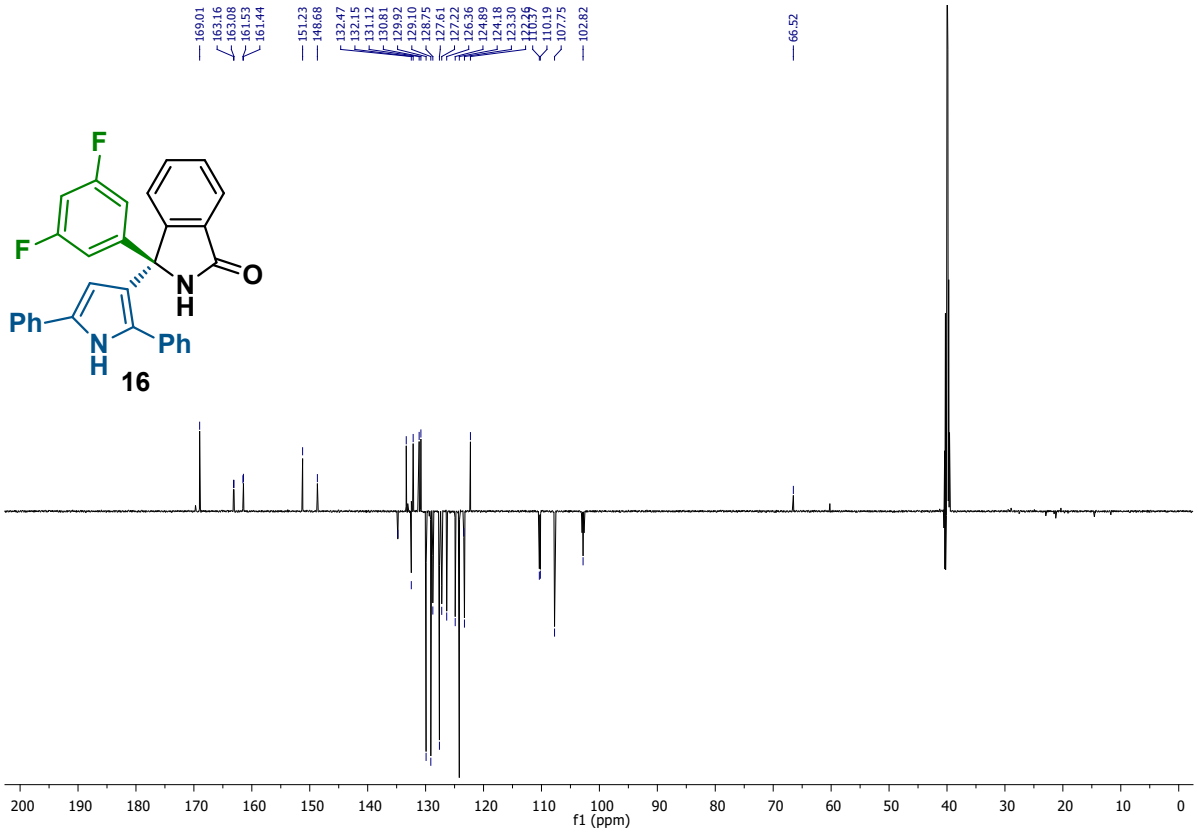
Traces of ethyl acetate observable in spectra.

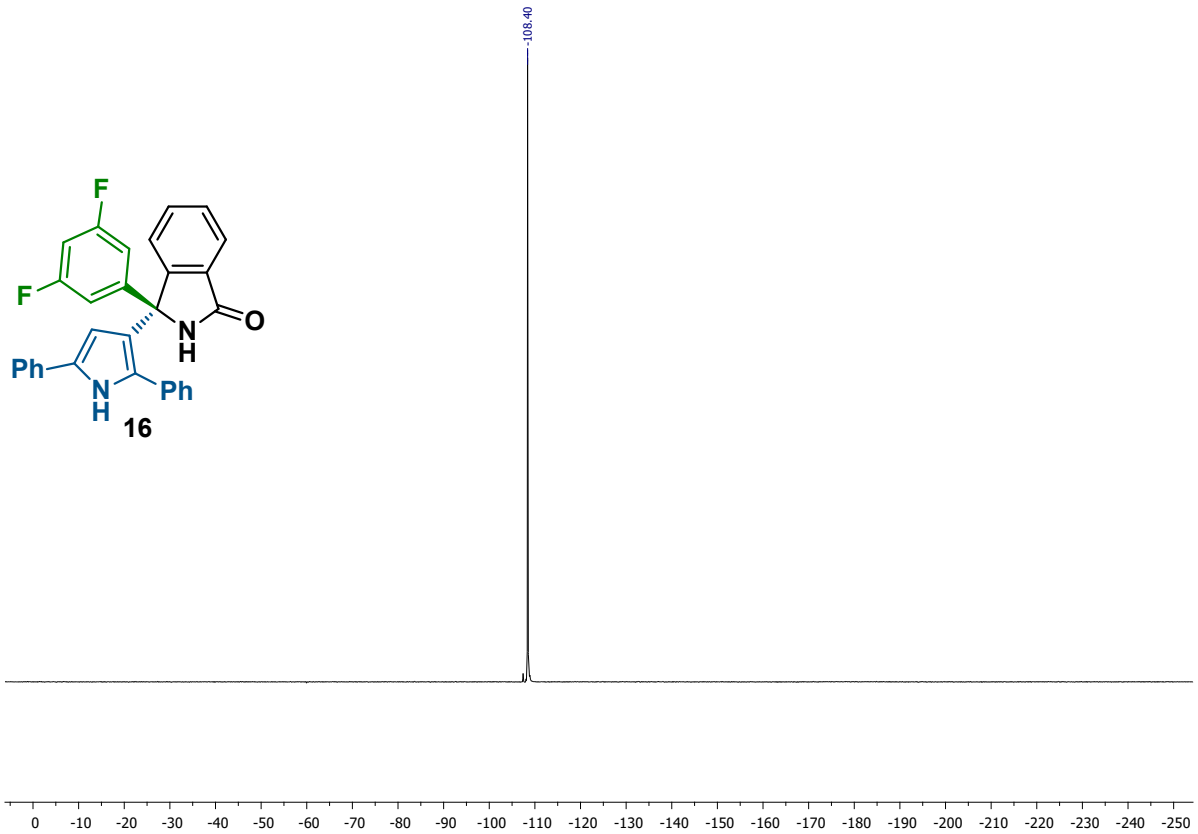




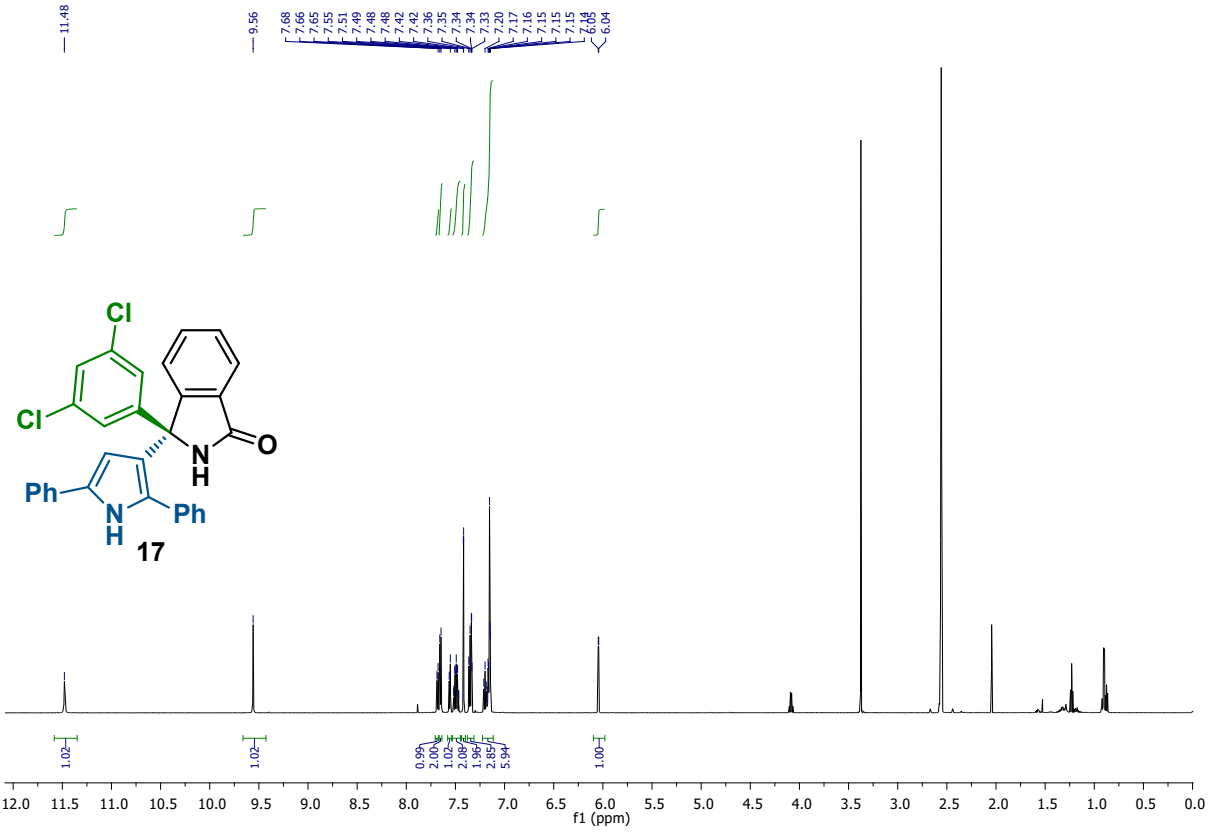
Traces of grease observable in spectra.

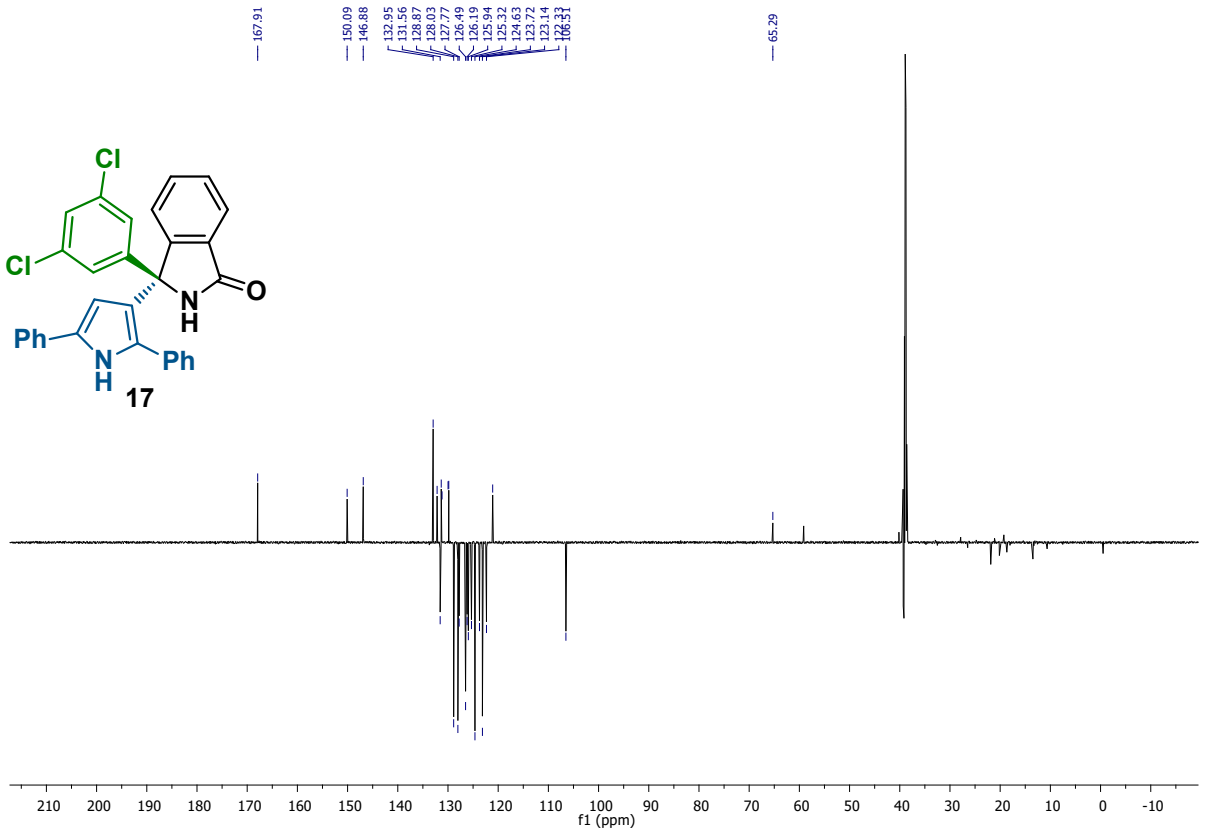



169.01
163.16
163.08
161.53
161.44
151.23
148.68
132.47
132.15
131.12
130.81
129.92
129.10
128.75
127.61
127.22
126.36
124.89
124.18
123.30
110.19
107.75
102.82
66.52
F
F
N
H
O
Ph
N
H
Ph
16
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

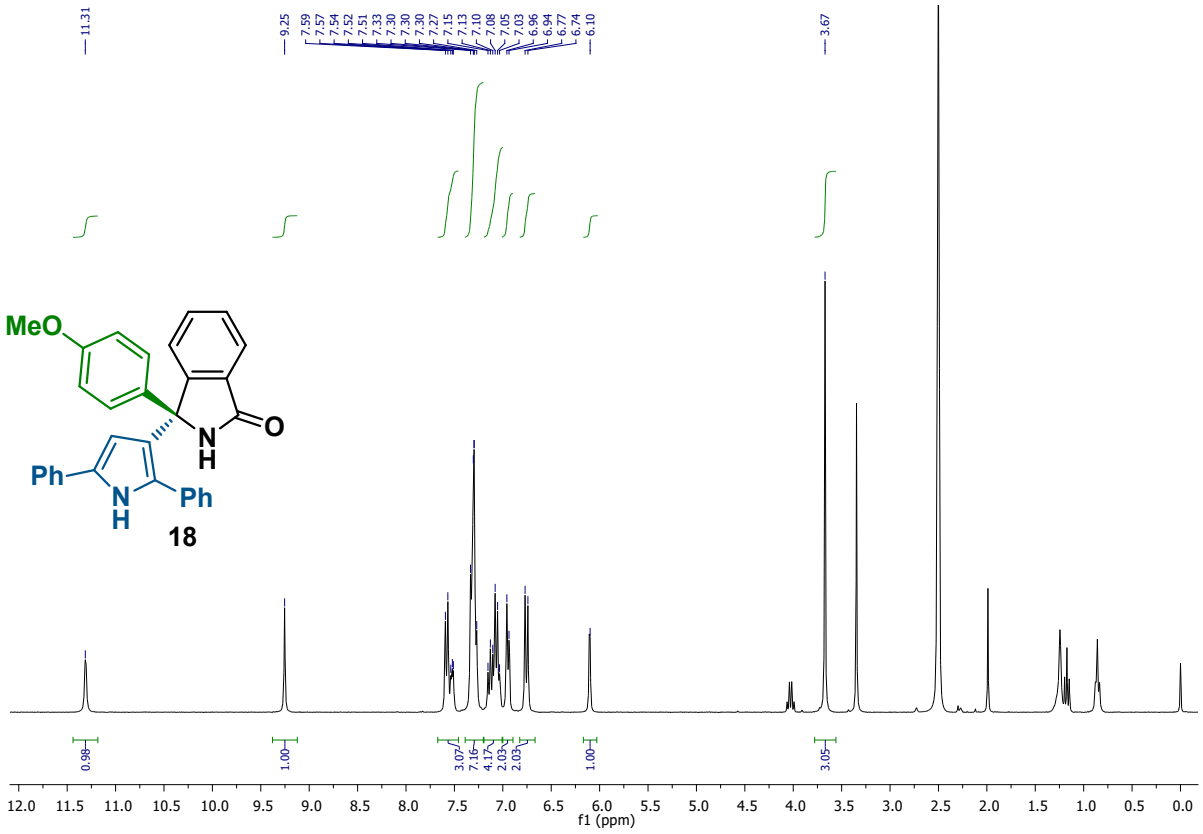

-108.40
F
F
N
H
O
Ph
N
H
Ph
16
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
-230
-240
-250

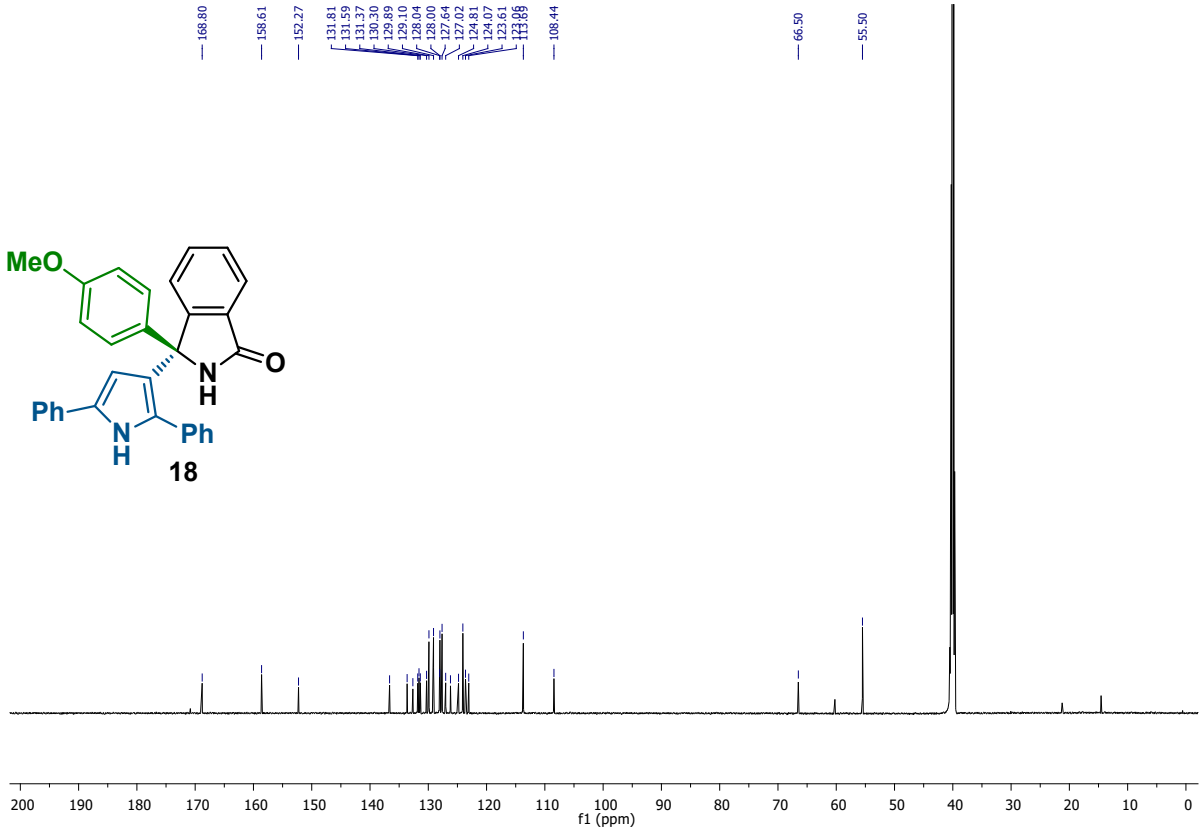
Traces of ethyl acetate observable in spectra.

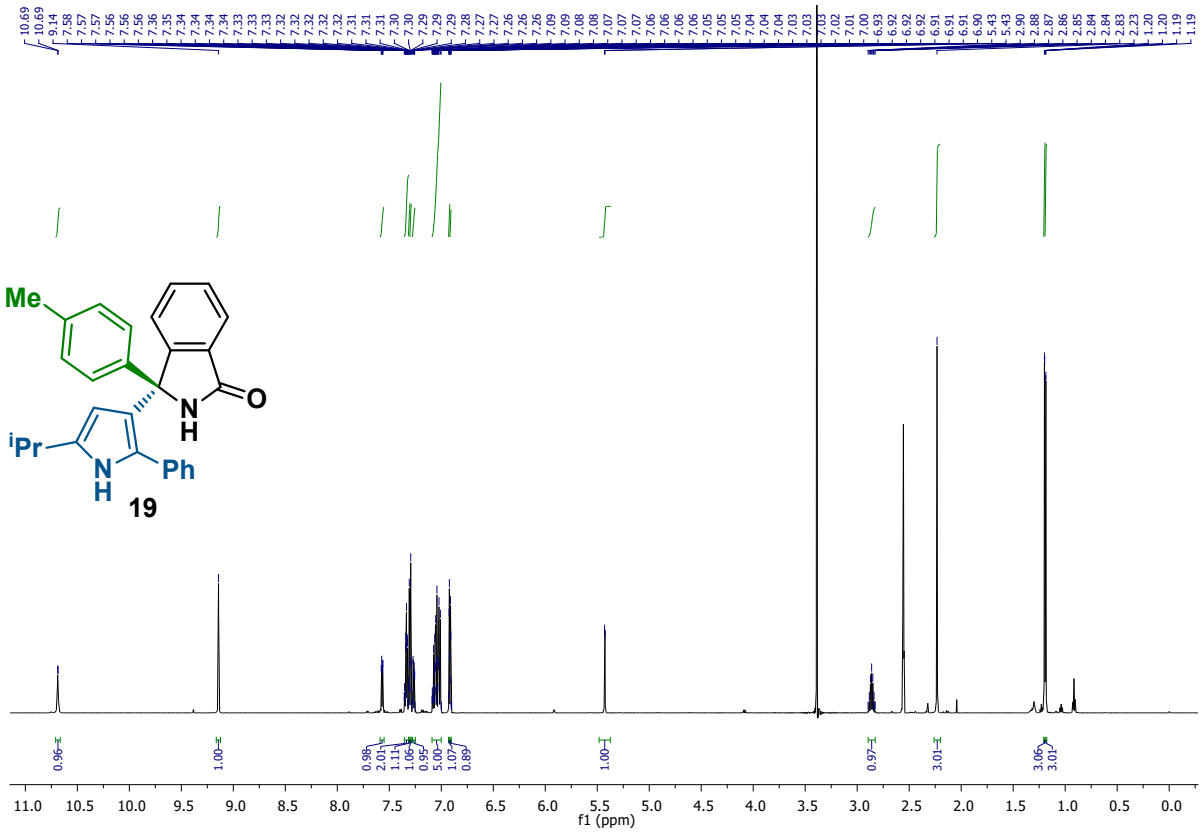


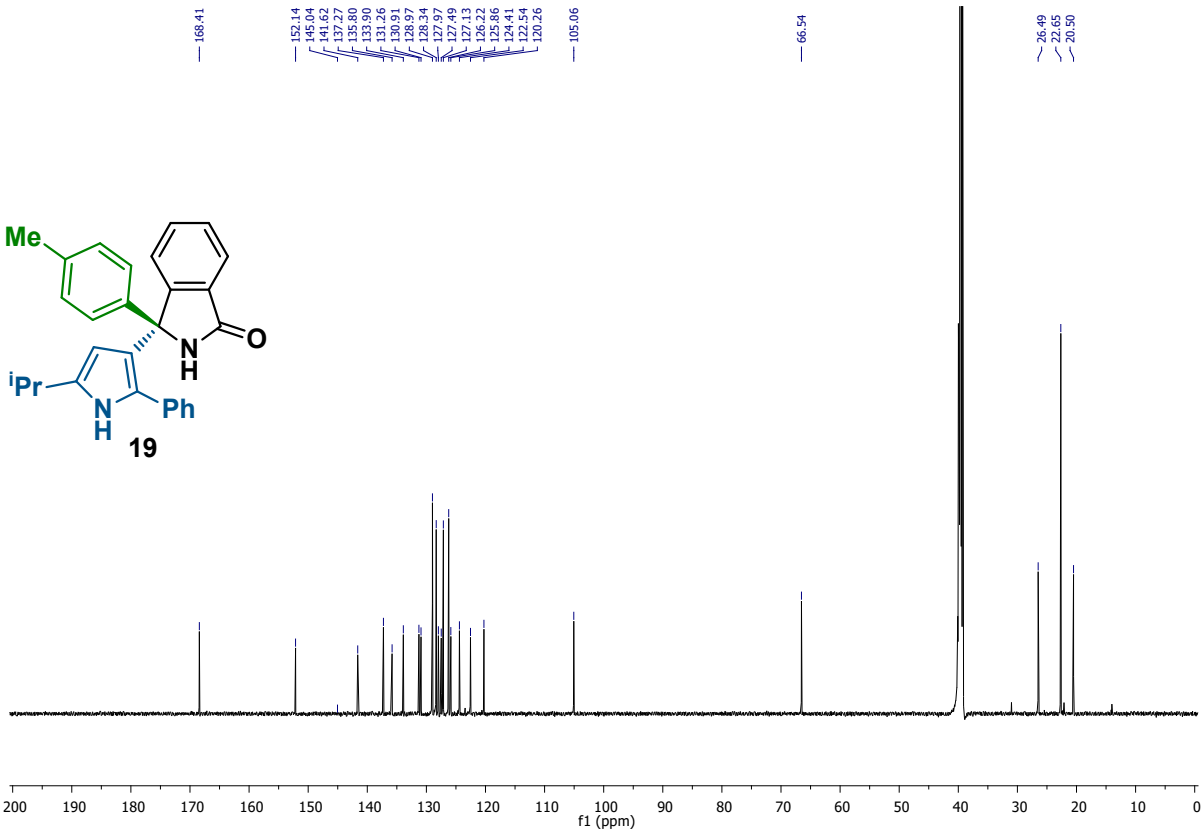


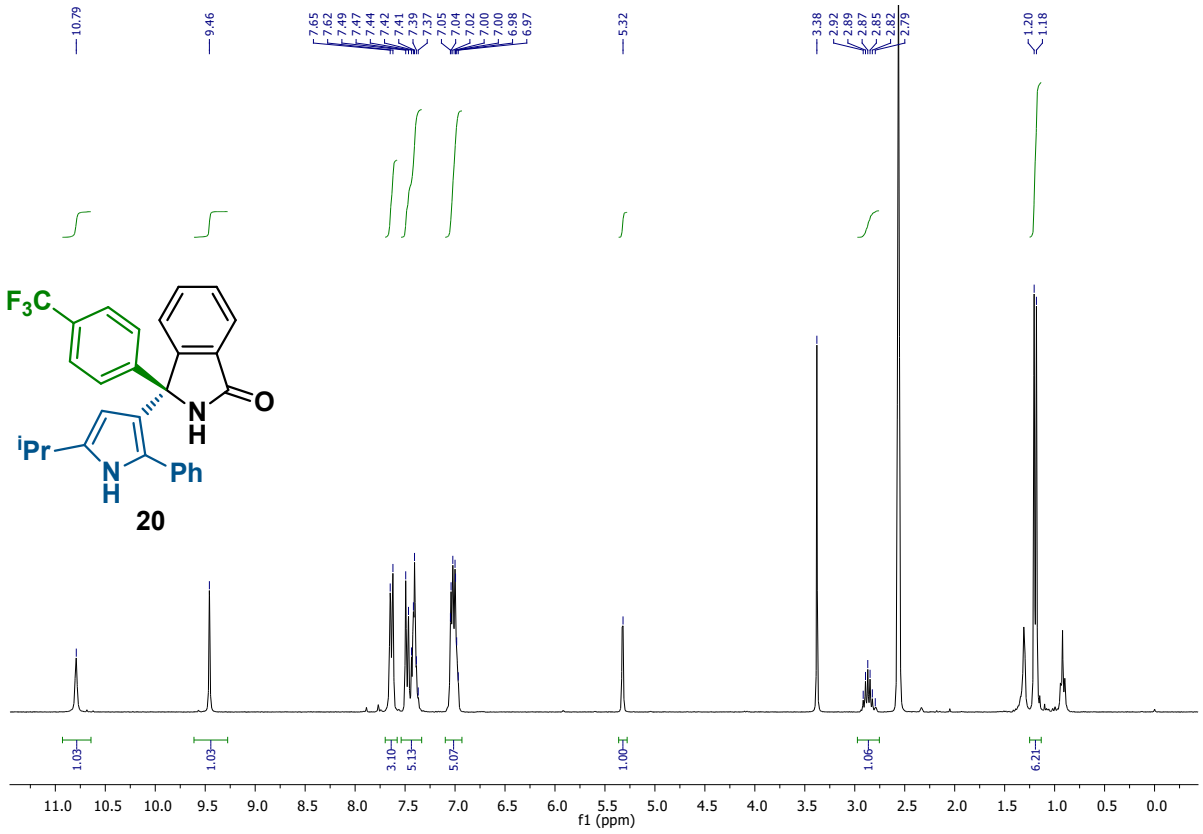
Traces of ethyl acetate observable in spectra.

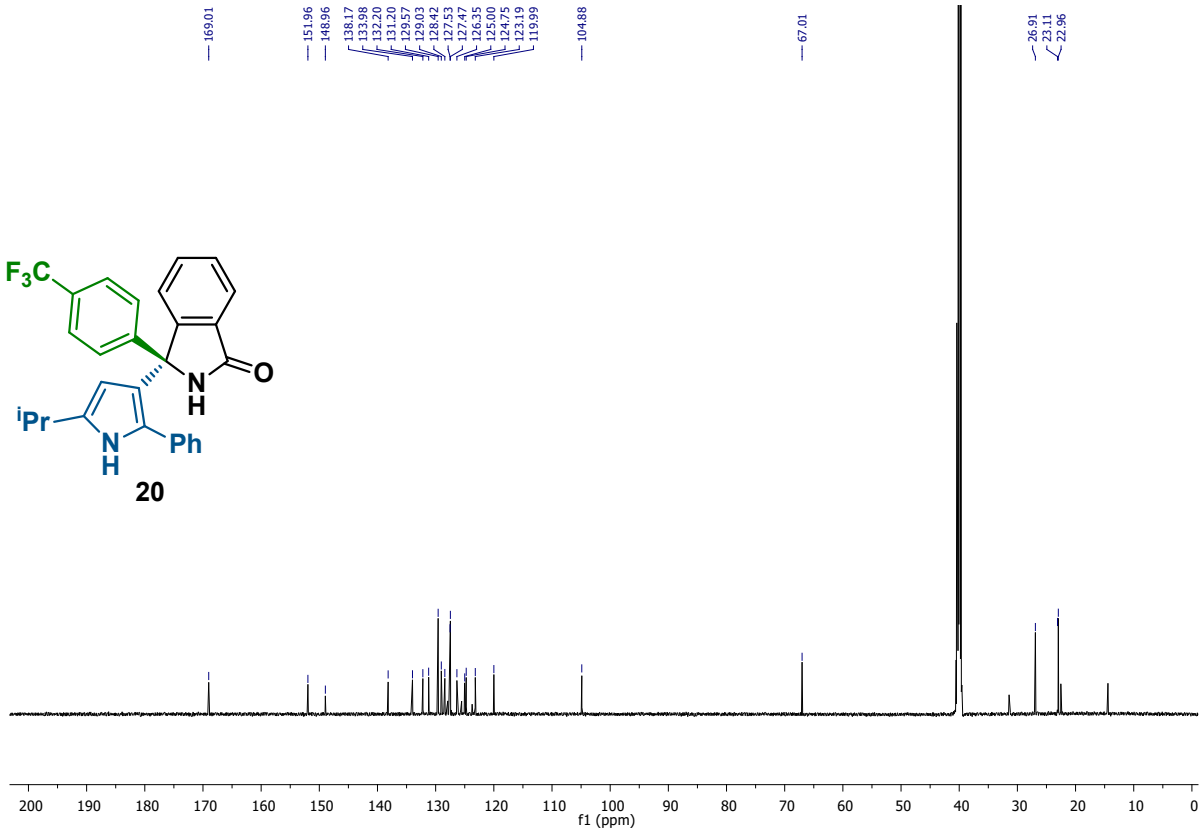


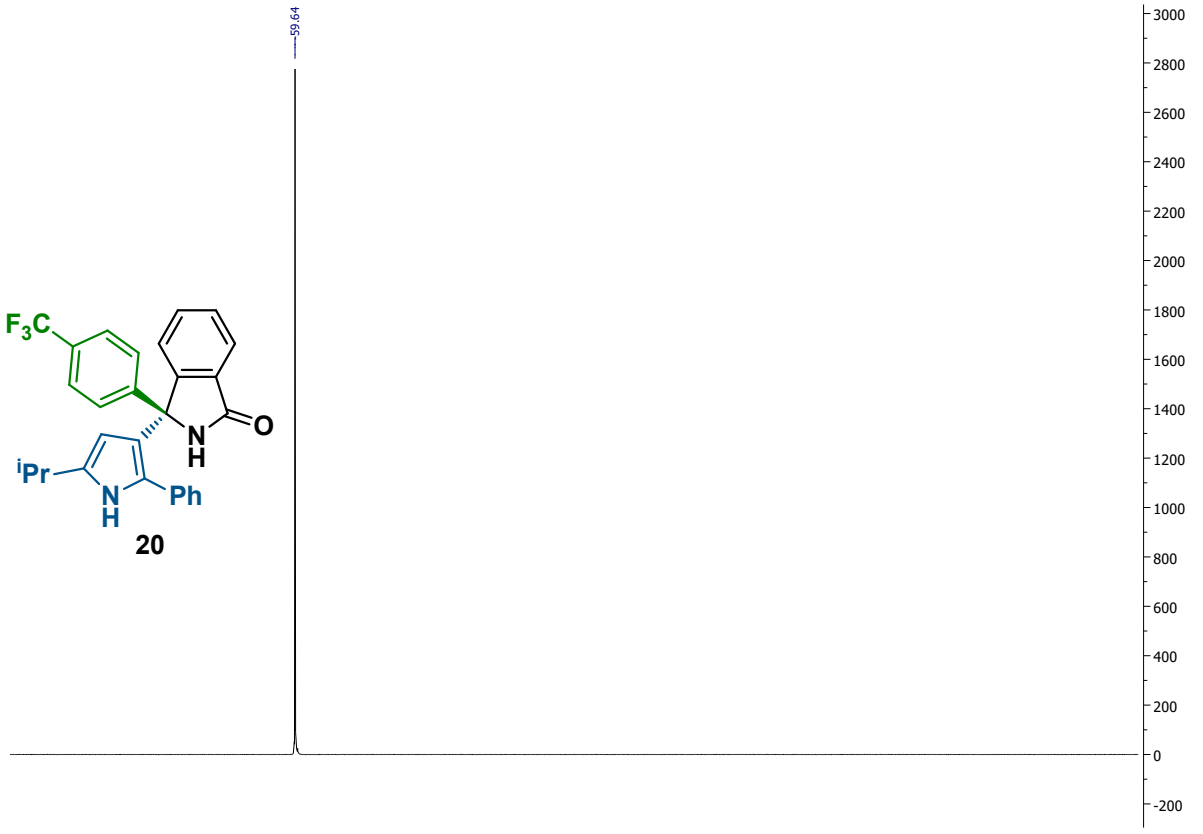


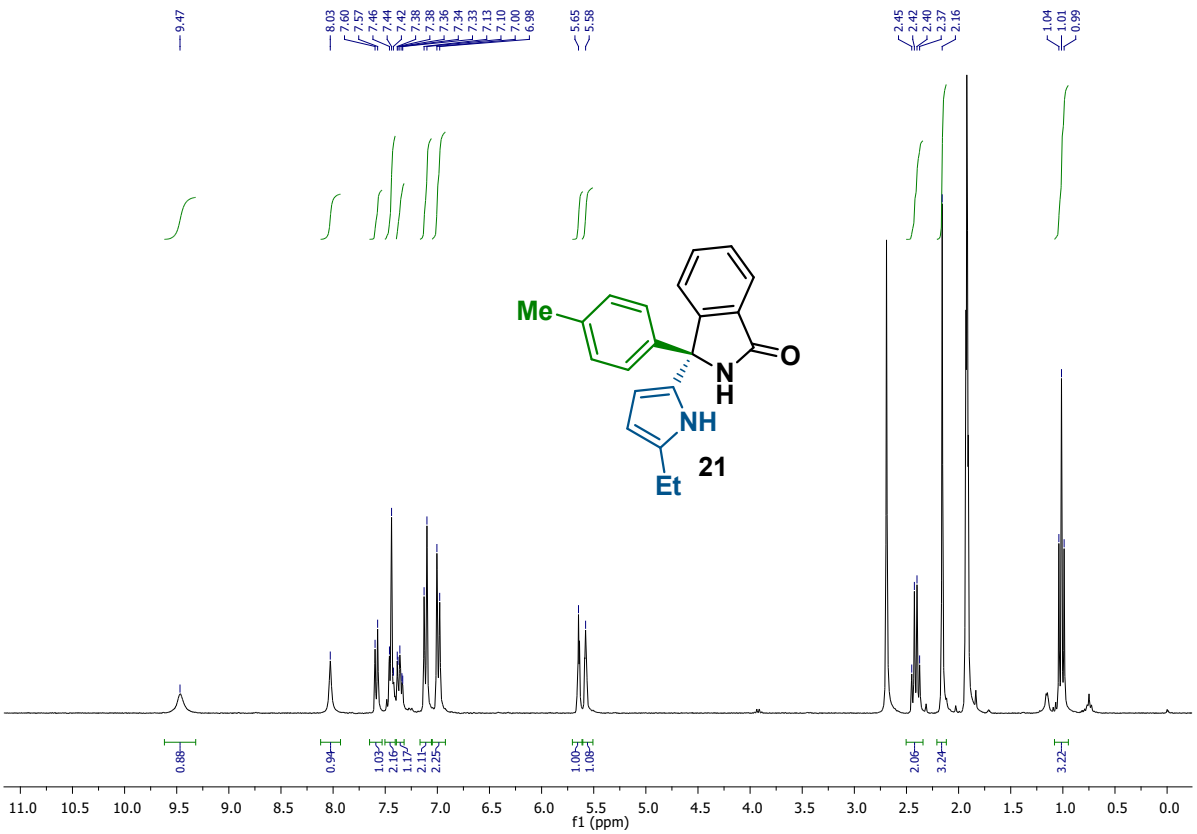

Me
iPr
N
H
Ph
N
H
O
19
f1 (ppm)

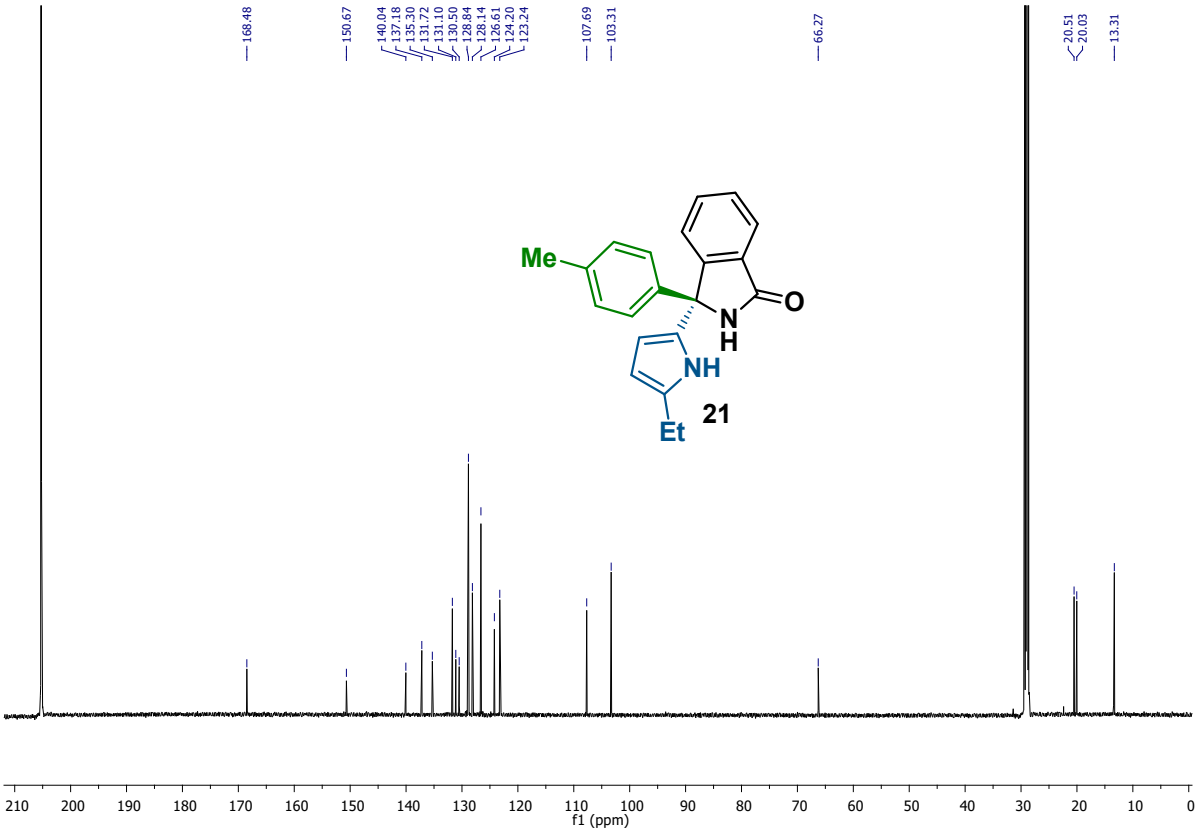

Me
iPr
N
H
Ph
N
H
O
19
f1 (ppm)

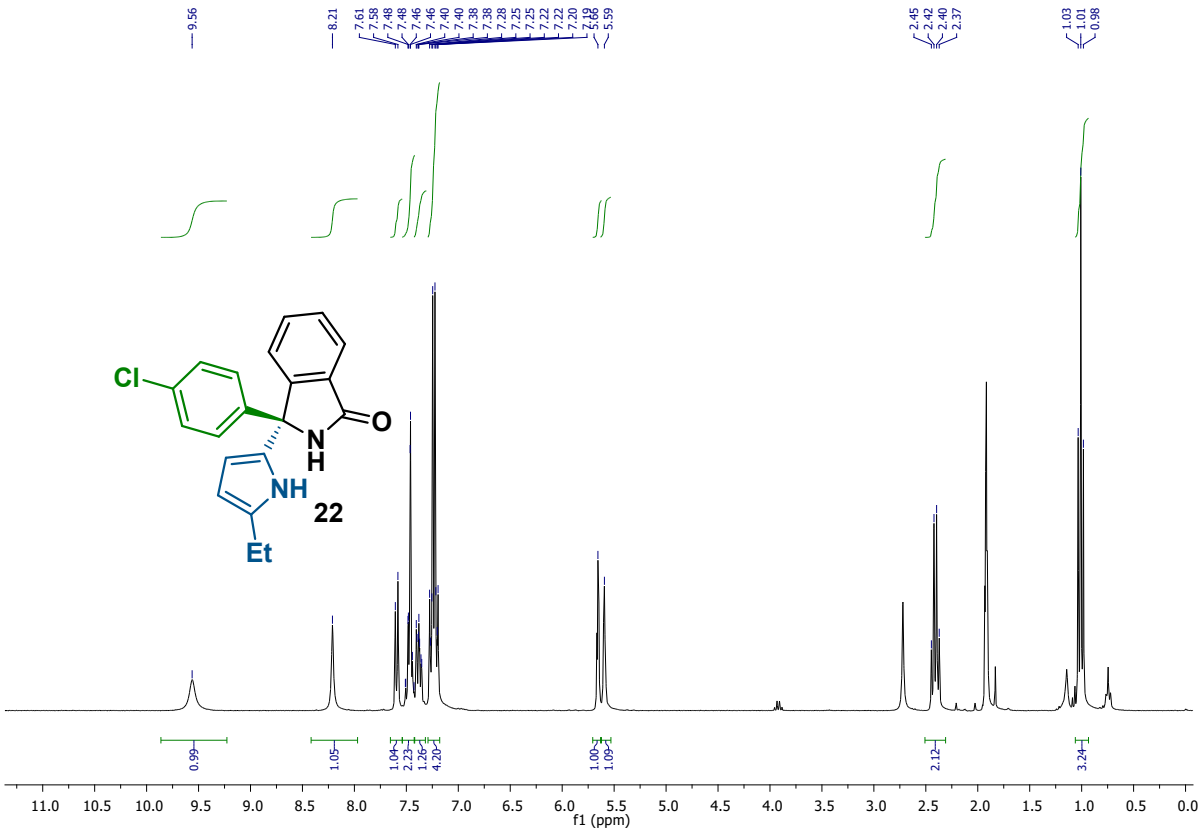

10.79
9.46
7.65
7.62
7.49
7.47
7.44
7.42
7.41
7.39
7.37
7.05
7.04
7.02
7.00
7.00
6.98
6.97
5.32
3.38
2.92
2.89
2.87
2.85
2.82
2.79
1.20
1.18
F3C
O
N
H
iPr
N
H
Ph
20
1.03
1.03
3.10
5.13
5.07
1.00
1.06
6.21
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

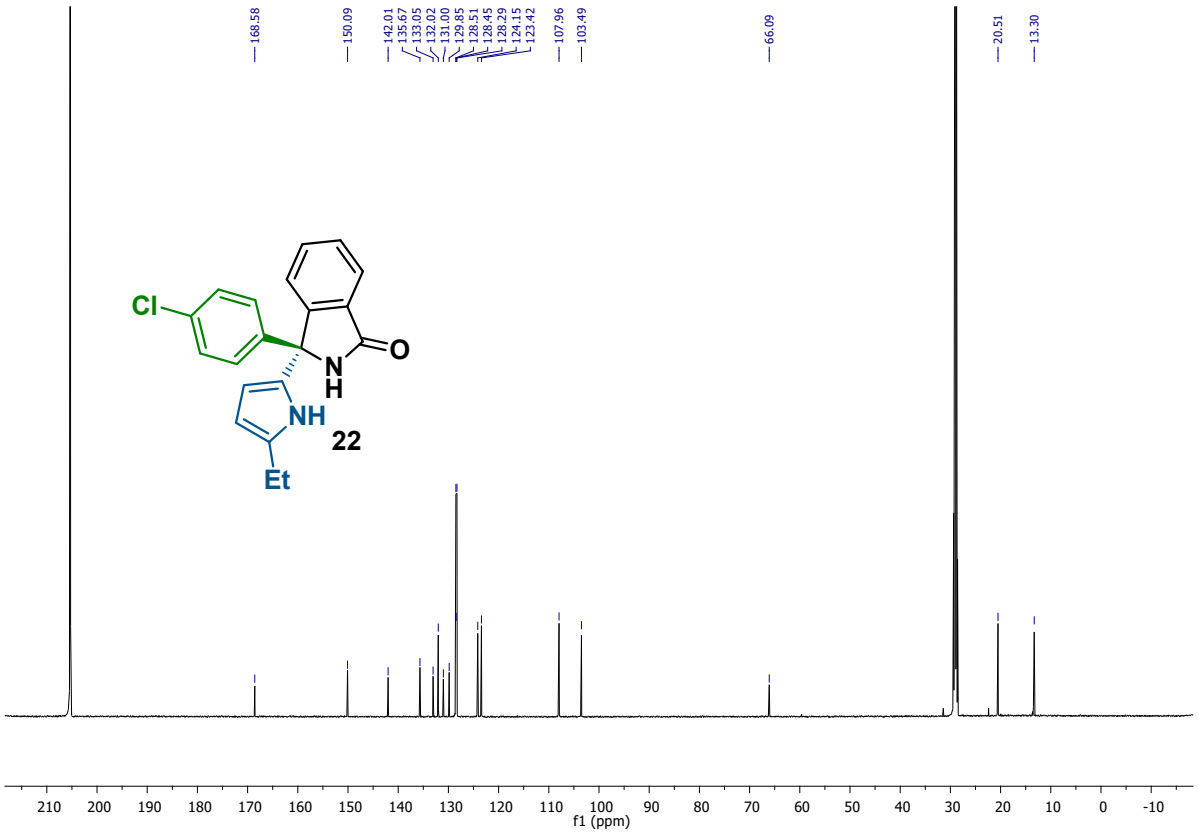

169.01
151.96
148.96
138.17
133.98
132.20
131.20
129.57
129.03
128.42
127.53
127.47
126.35
125.00
124.75
123.19
119.99
104.88
67.01
26.91
23.11
22.96
F3C
O
N
H
iPr
N
H
Ph
20
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

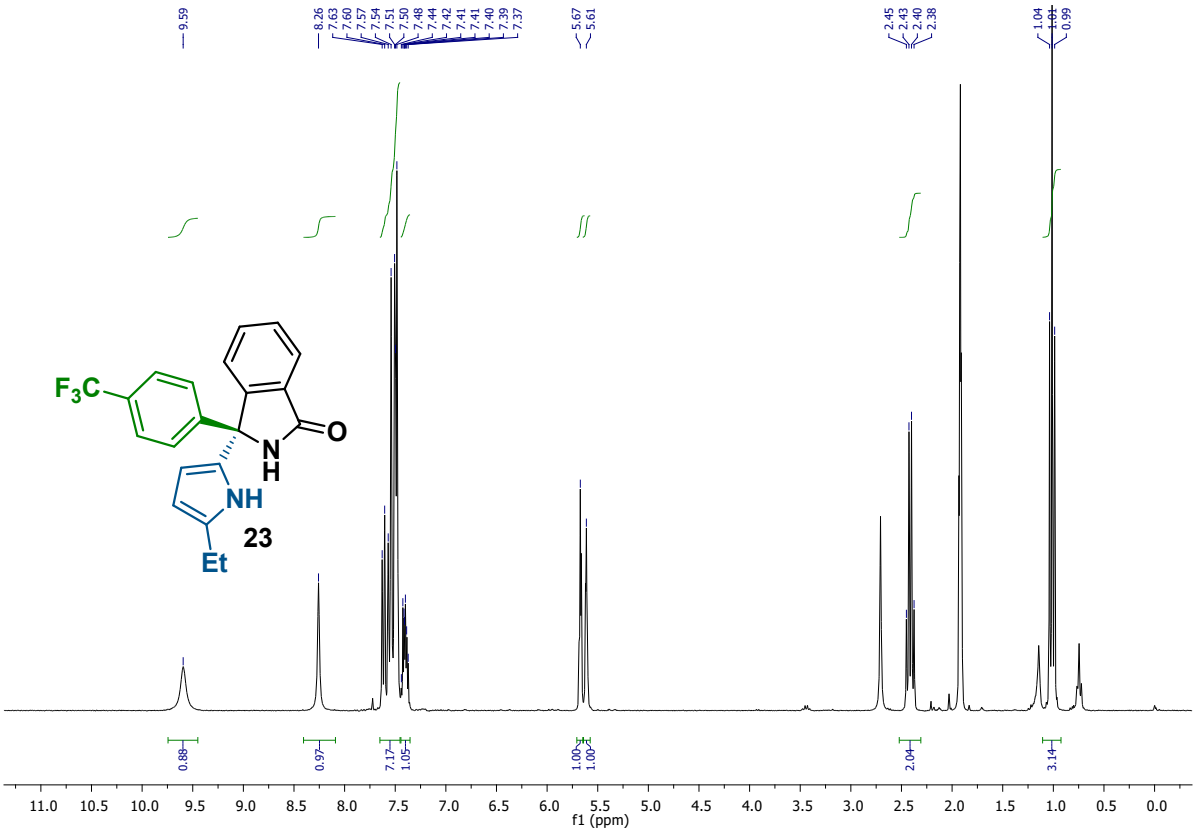

59.64
F3C
O
N
H
iPr
N
H
Ph
20
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200

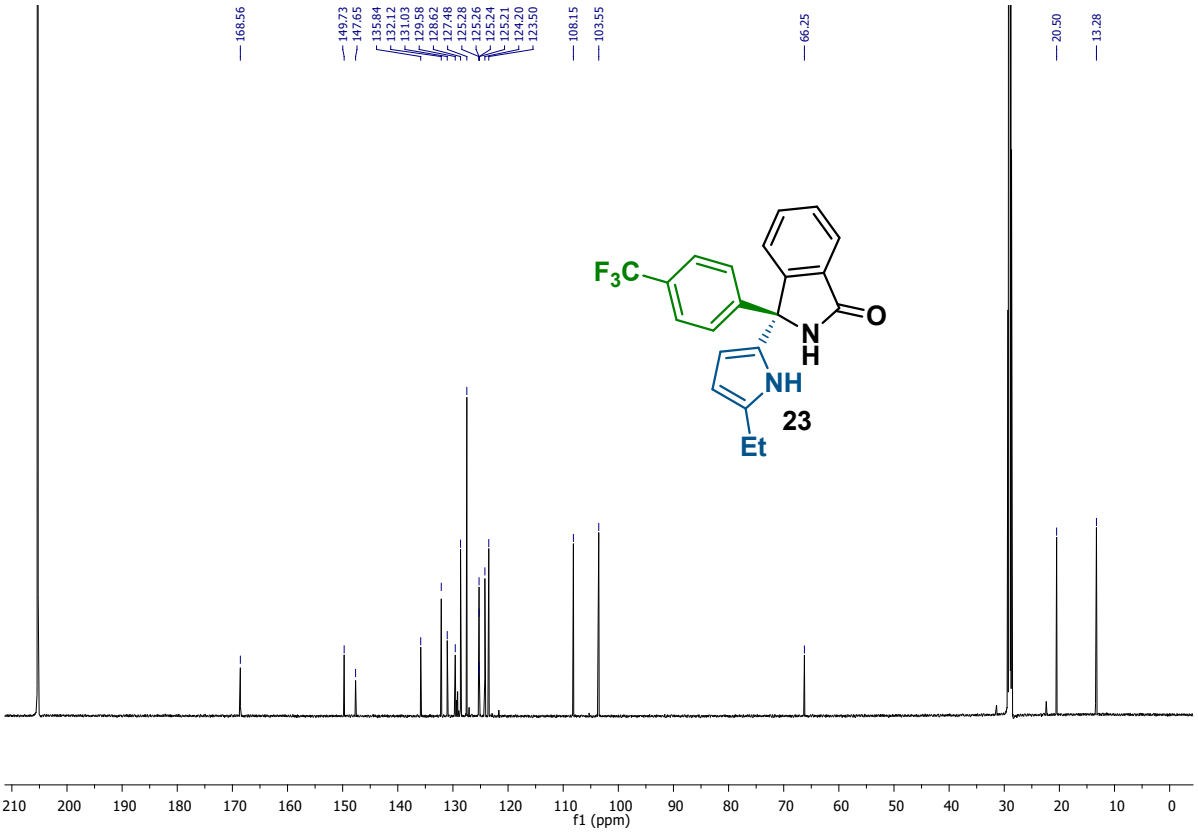

9.47
8.03
7.60
7.57
7.46
7.44
7.42
7.38
7.38
7.36
7.34
7.33
7.13
7.10
7.00
6.98
5.65
5.58
2.45
2.42
2.40
2.37
2.16
1.04
1.01
0.99
Me
O
N
H
NH
Et
21
0.88
0.94
1.03
2.16
1.17
2.11
2.25
1.00
1.08
2.06
3.24
3.22
f1 (ppm)

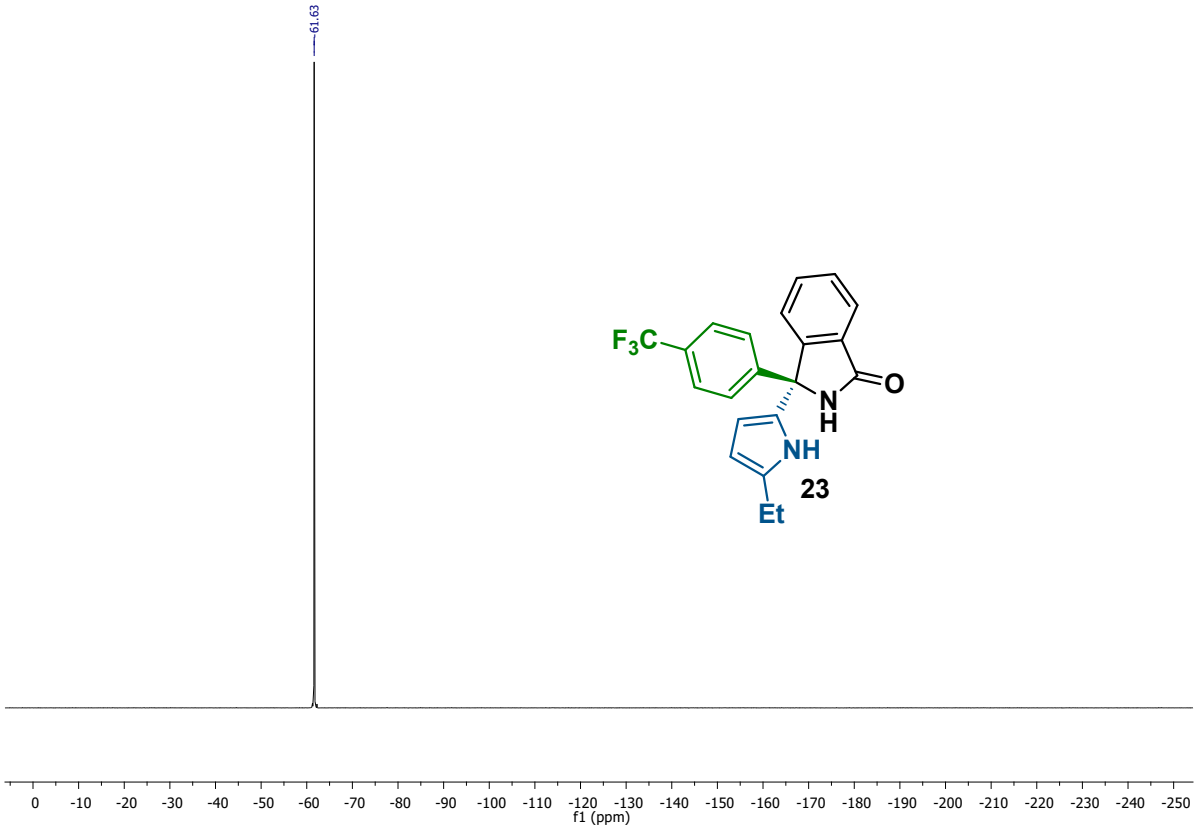

168.48
150.67
140.04
137.18
135.30
131.72
131.10
130.50
128.84
128.14
126.61
124.20
123.24
107.69
103.31
66.27
20.51
20.03
13.31
Me
O
N
H
NH
Et
21
f1 (ppm)

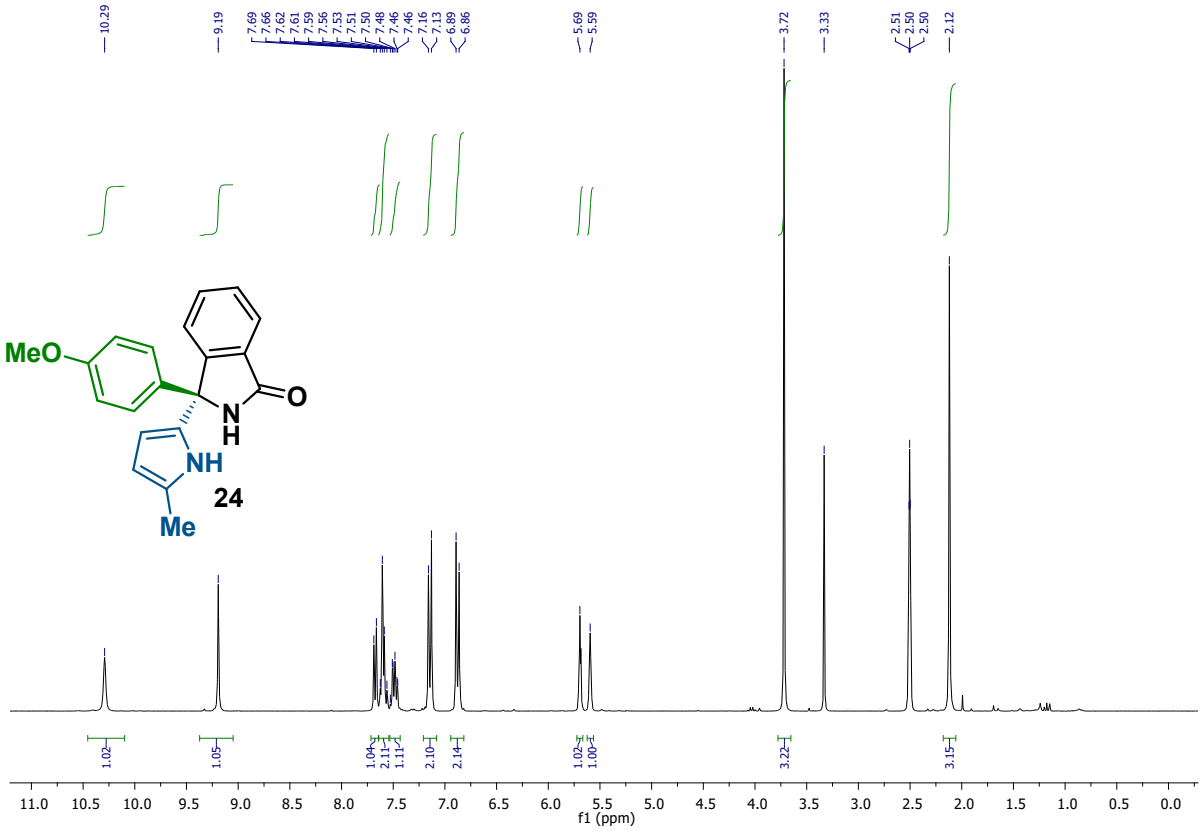

9.56
8.21
7.61
7.58
7.48
7.48
7.46
7.46
7.40
7.40
7.38
7.38
7.28
7.25
7.25
7.22
7.22
7.20
5.60
5.59
2.45
2.42
2.40
2.37
1.03
1.01
0.98
Cl
O
N
H
NH
22
Et
0.99
1.05
1.04
2.23
1.26
4.20
1.00
1.09
2.12
3.24
f1 (ppm)

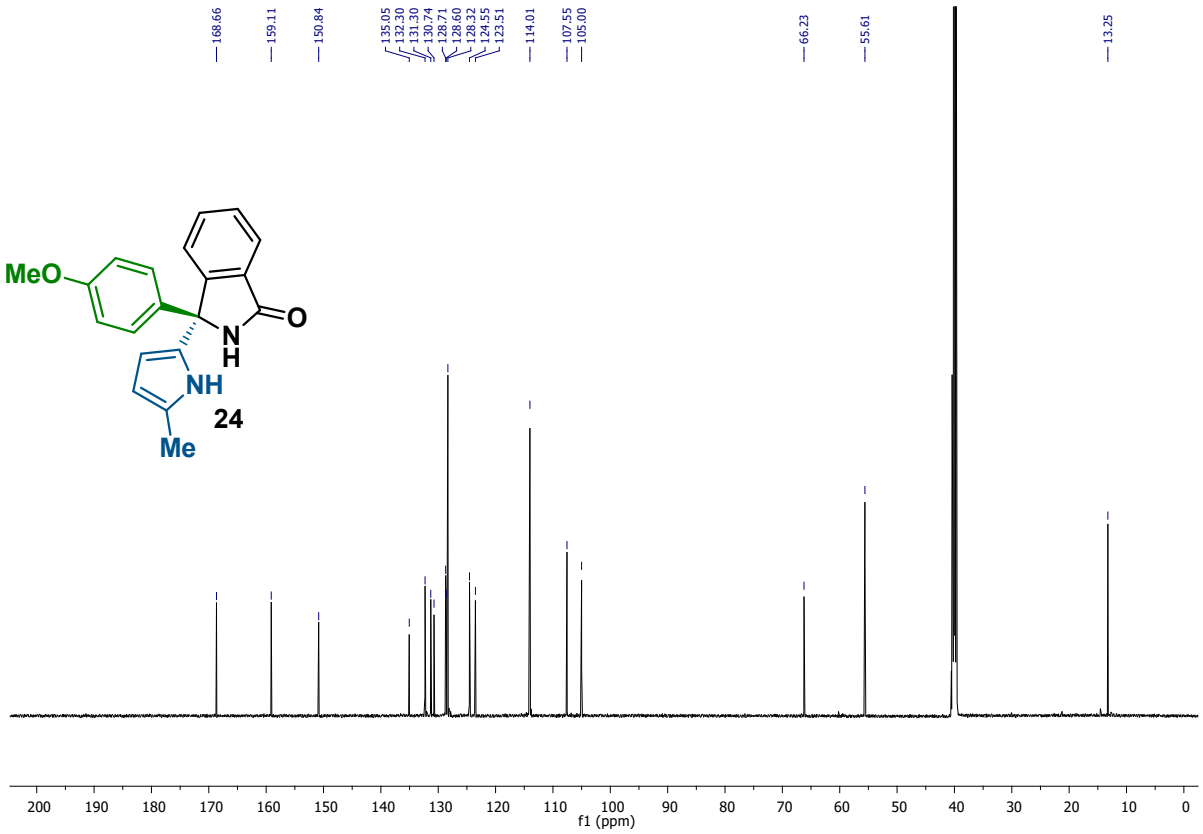

168.58
150.09
142.01
135.67
133.05
132.02
131.00
129.85
128.51
128.45
128.29
124.15
123.42
107.96
103.49
66.09
20.51
13.30
Cl
O
N
H
NH
22
Et
f1 (ppm)

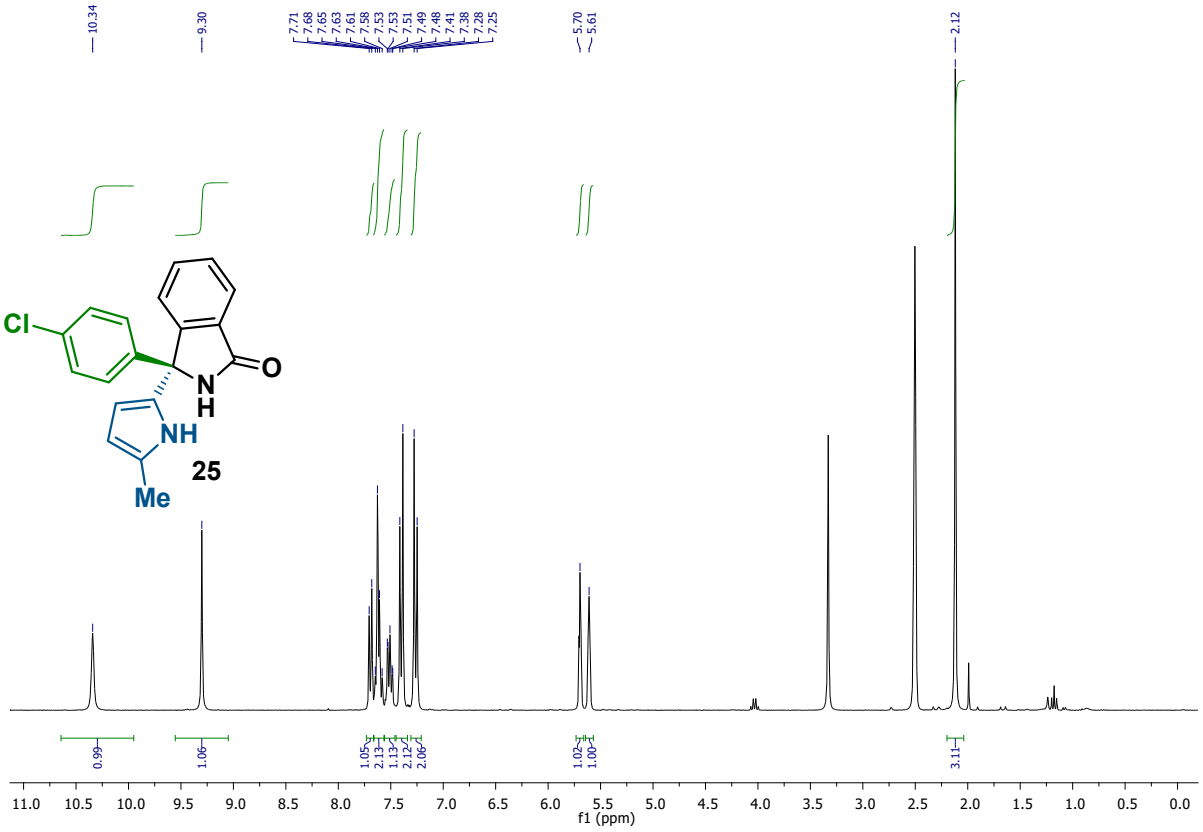

9.59
8.26
7.63
7.60
7.57
7.54
7.51
7.50
7.48
7.44
7.42
7.41
7.41
7.40
7.39
7.37
5.67
5.61
2.45
2.43
2.40
2.38
1.04
1.01
0.99
F3C
O
N
H
NH
Et
23
0.88
0.97
7.17
1.05
1.00
1.00
2.04
3.14
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

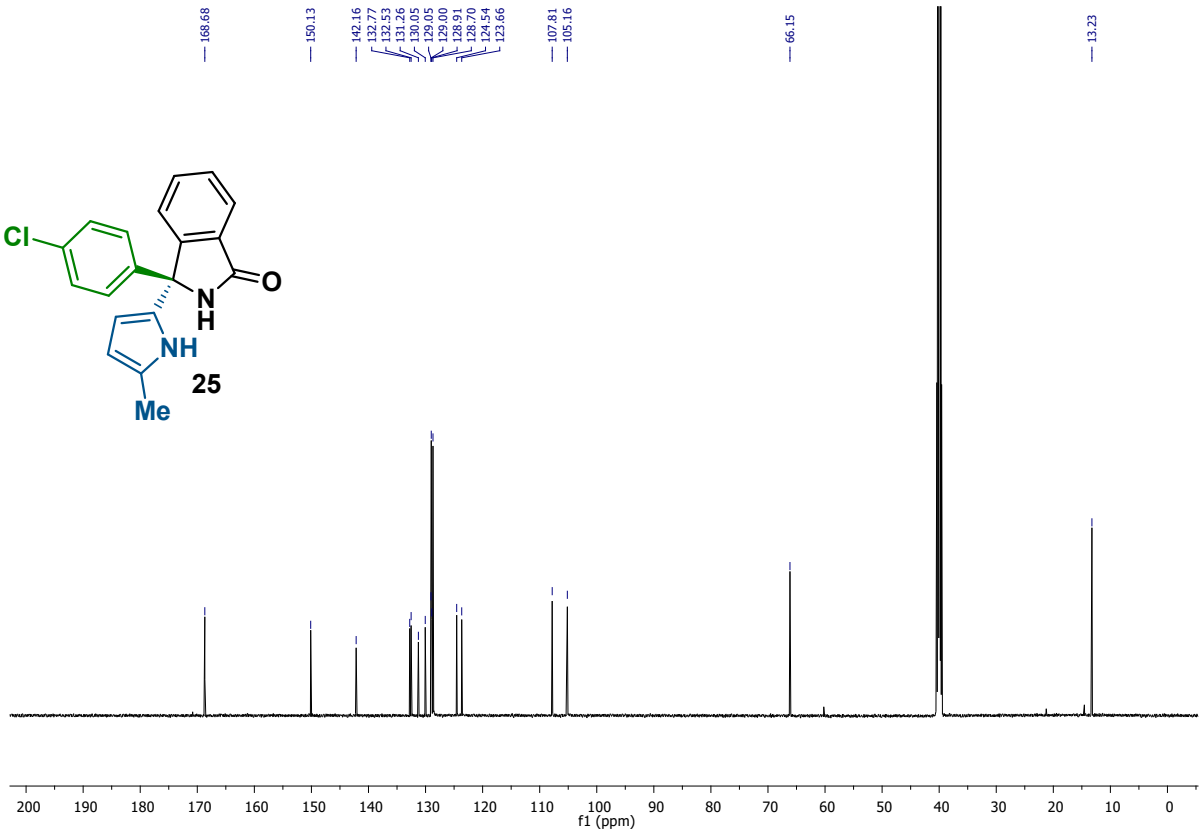

168.56
149.73
147.65
135.84
132.12
131.03
129.58
128.62
127.48
125.28
125.26
125.24
125.21
124.20
123.50
108.15
103.55
66.25
20.50
13.28
F3C
O
N
H
NH
Et
23
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

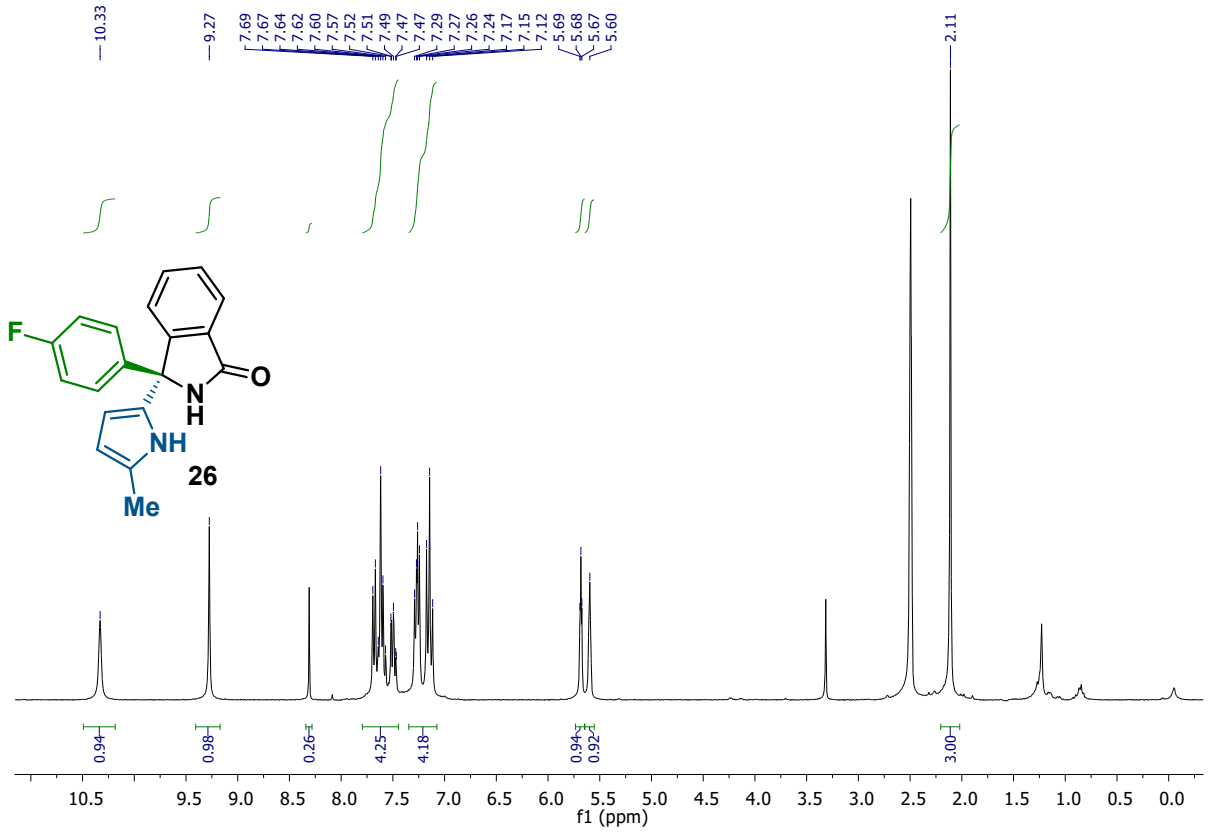

61.63
F3C
O
N
H
NH
Et
23
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250
f1 (ppm)

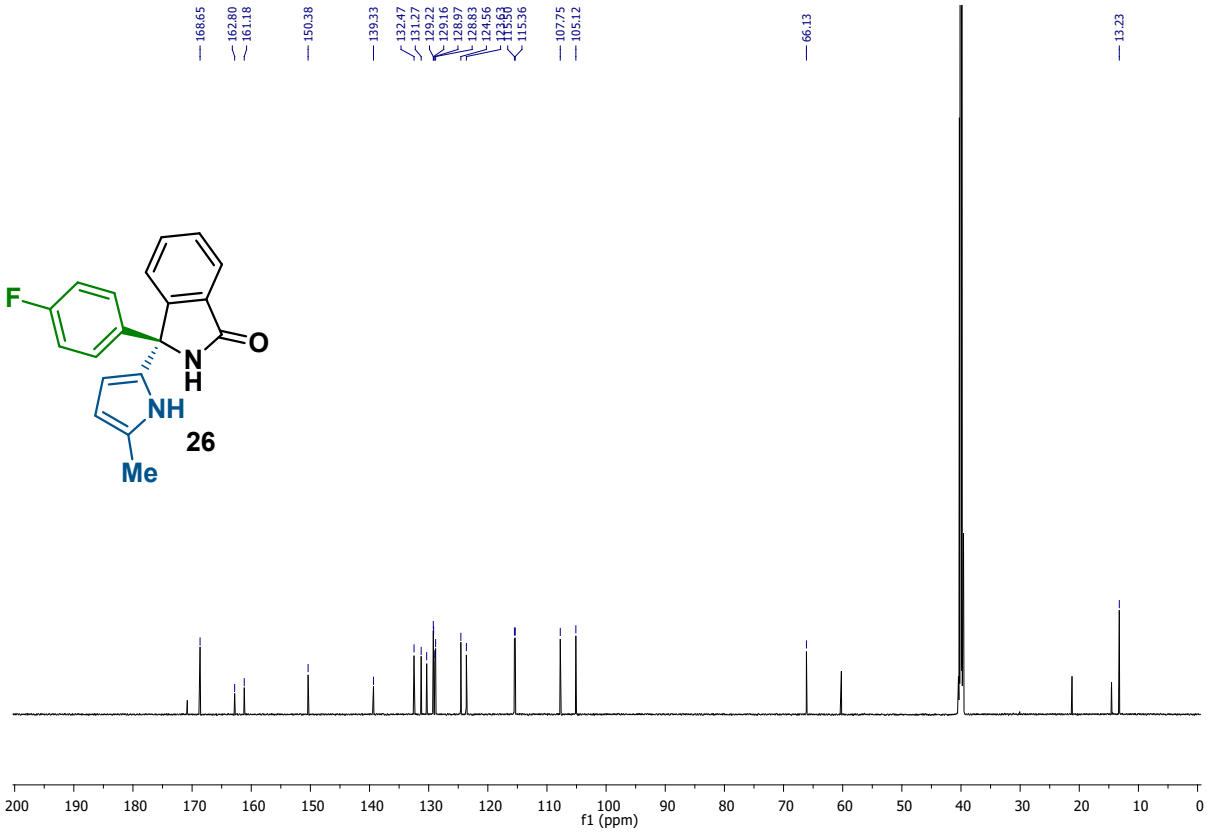

10.29
9.19
7.69
7.66
7.62
7.61
7.59
7.56
7.53
7.51
7.50
7.48
7.46
7.46
7.16
7.13
6.89
6.86
5.69
5.59
3.72
3.33
2.51
2.50
2.50
2.12
MeO
O
N
H
NH
Me
24
1.02
1.05
1.04
2.11
1.11
2.10
2.14
1.02
1.00
3.22
3.15
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

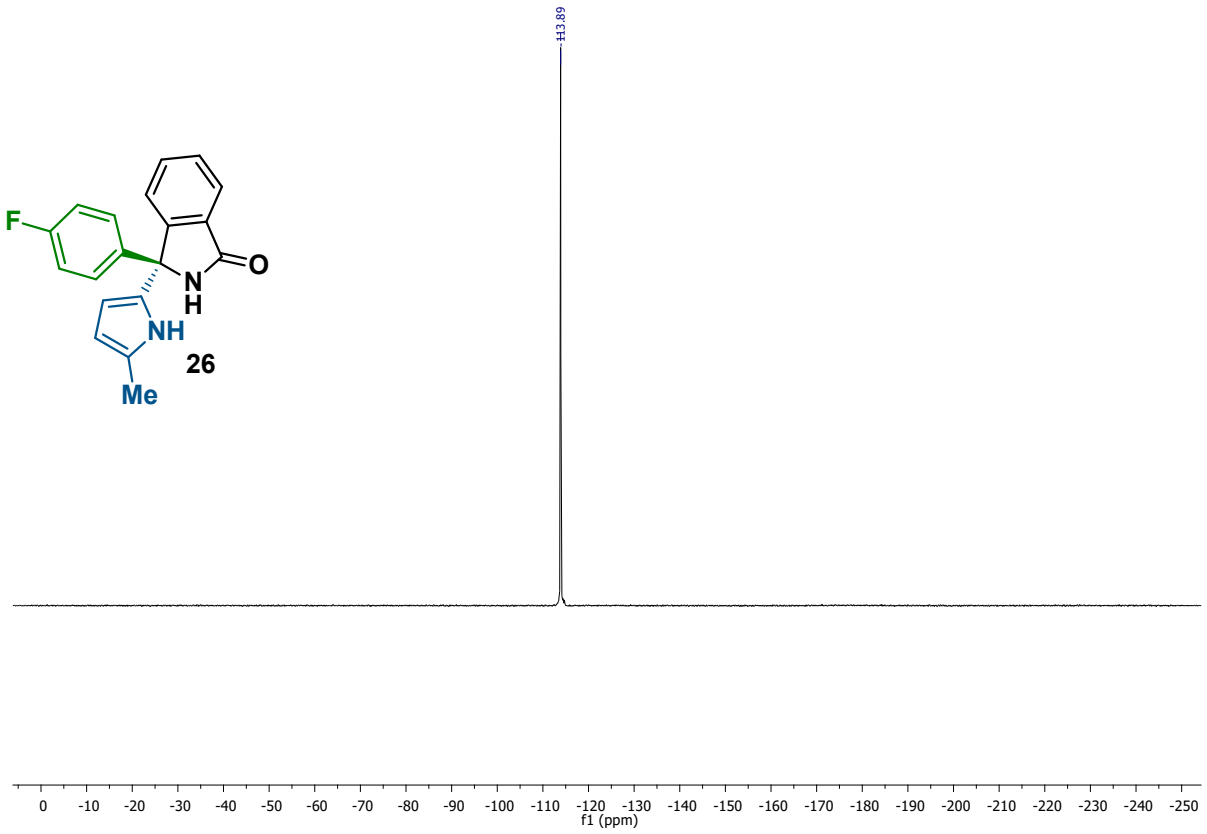

168.66
159.11
150.84
135.05
132.30
131.30
130.74
128.71
128.60
128.32
124.55
123.51
114.01
107.55
105.00
66.23
55.61
13.25
MeO
O
N
H
NH
Me
24
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

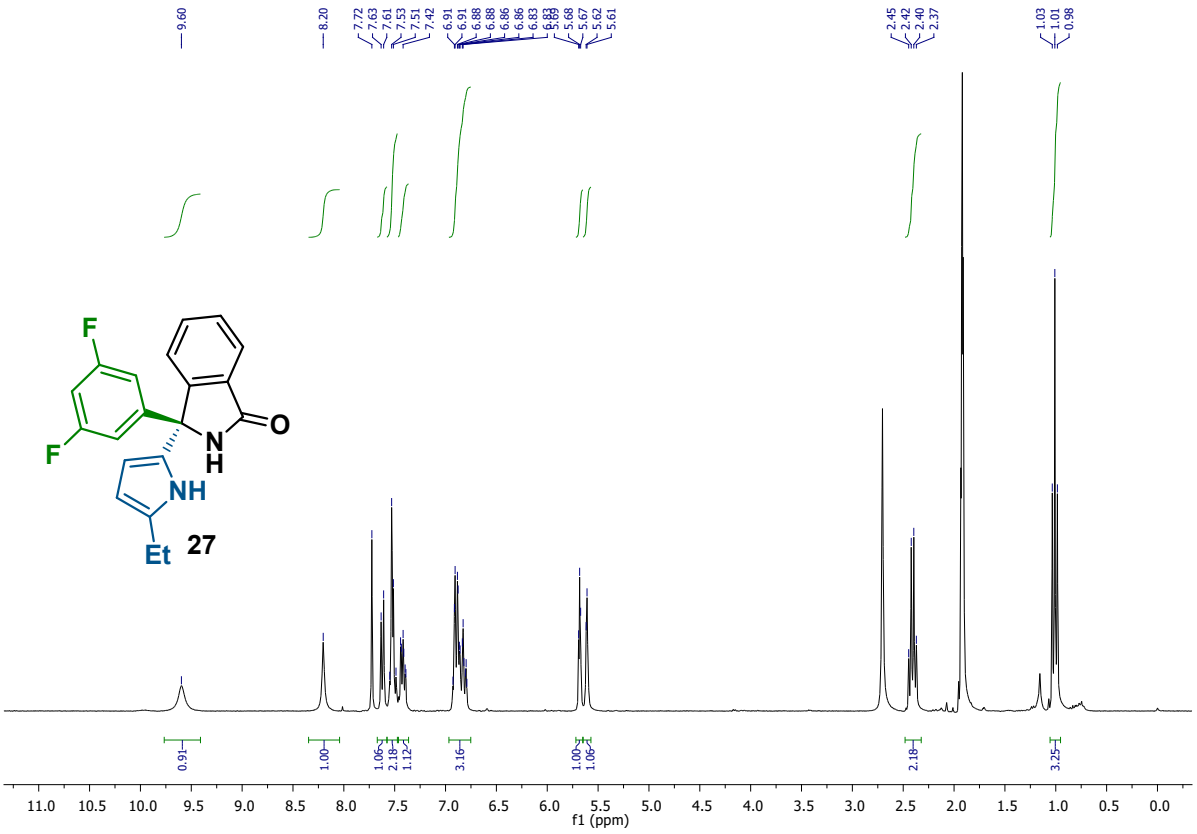

10.34
9.30
7.71
7.68
7.65
7.63
7.61
7.58
7.53
7.53
7.51
7.49
7.48
7.41
7.38
7.28
7.25
5.70
5.61
2.12
Cl
O
N
H
NH
Me
25
0.99
1.06
1.05
2.13
1.13
2.12
2.06
1.02
1.00
3.11
f1 (ppm)


168.68
150.13
142.16
132.77
132.53
131.26
130.05
129.05
129.00
128.91
128.70
124.54
123.66
107.81
105.16
66.15
13.23
Cl
O
N
H
NH
Me
25
f1 (ppm)


10.33
9.27
7.69
7.67
7.64
7.62
7.60
7.57
7.52
7.51
7.49
7.47
7.47
7.29
7.27
7.26
7.24
7.17
7.15
7.12
5.69
5.68
5.67
5.60
2.11
F
O
N
H
NH
Me
26
0.94
0.98
0.26
4.25
4.18
0.94
0.92
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


168.65
162.80
161.18
150.38
139.33
132.47
131.27
129.22
129.16
128.97
128.83
124.56
115.36
107.75
105.12
66.13
13.23
F
O
N
H
NH
26
Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


13.89
F
O
N
H
NH
26
Me
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250
f1 (ppm)


9.60
8.20
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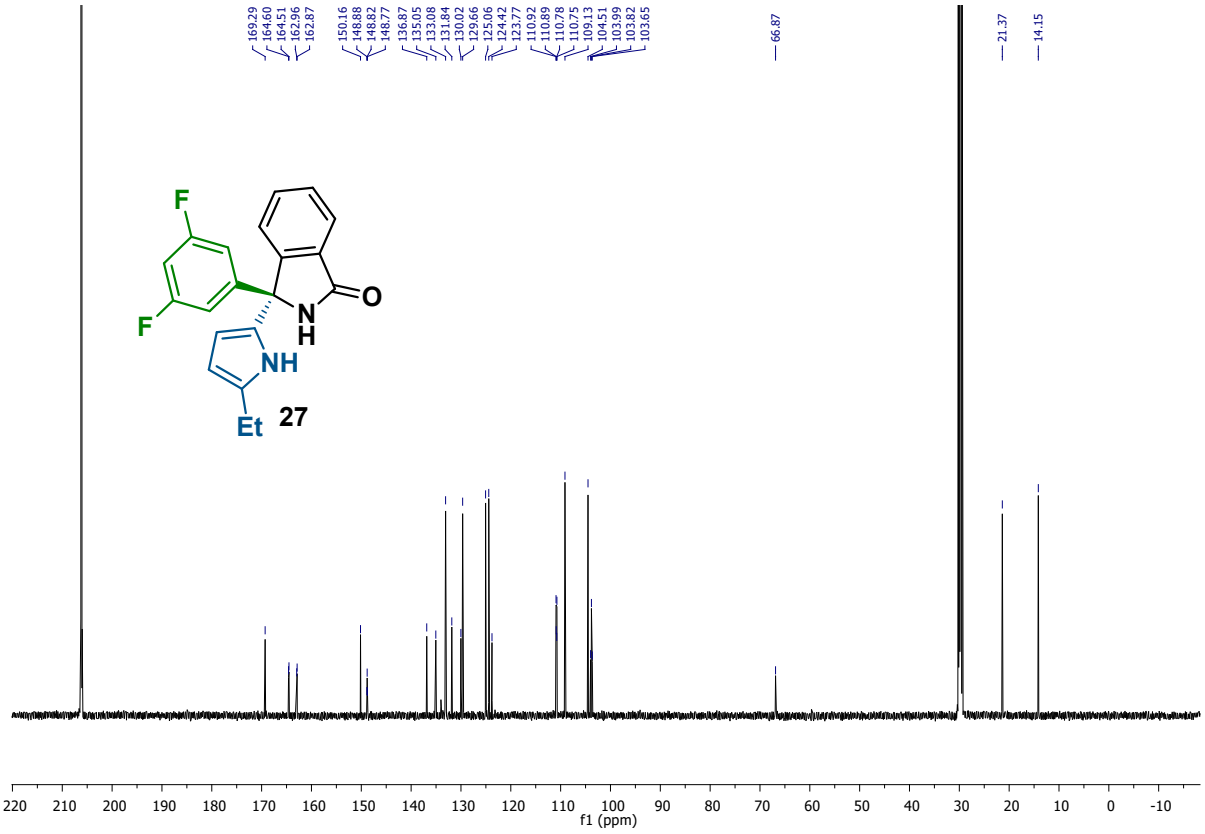
7.63
7.61
7.53
7.51
7.42
6.91
6.91
6.88
6.88
6.86
6.86
6.83
5.68
5.67
5.62
5.61
2.45
2.42
2.40
2.37
1.03
1.01
0.98
F
F
O
N
H
NH
Et
27
0.91
1.00
1.06
2.18
1.12
3.16
1.00
1.06
2.18
3.25
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


169.29
164.60
164.51
162.96
162.87
150.16
148.88
148.82
148.77
136.87
135.05
133.08
131.84
130.02
129.66
125.06
124.42
123.77
110.92
110.89
110.78
110.75
109.13
104.51
103.99
103.82
103.65
66.87
21.37
14.15
F
F
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N
H
NH
Et
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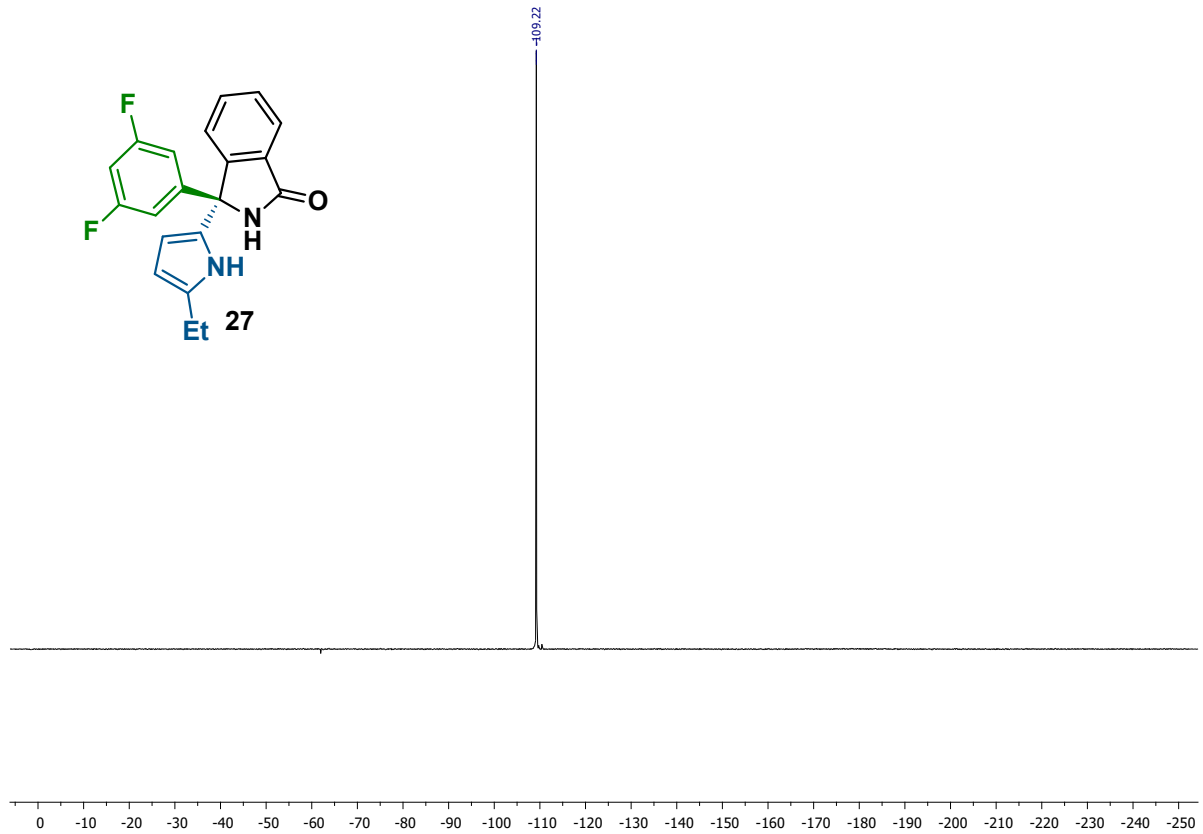
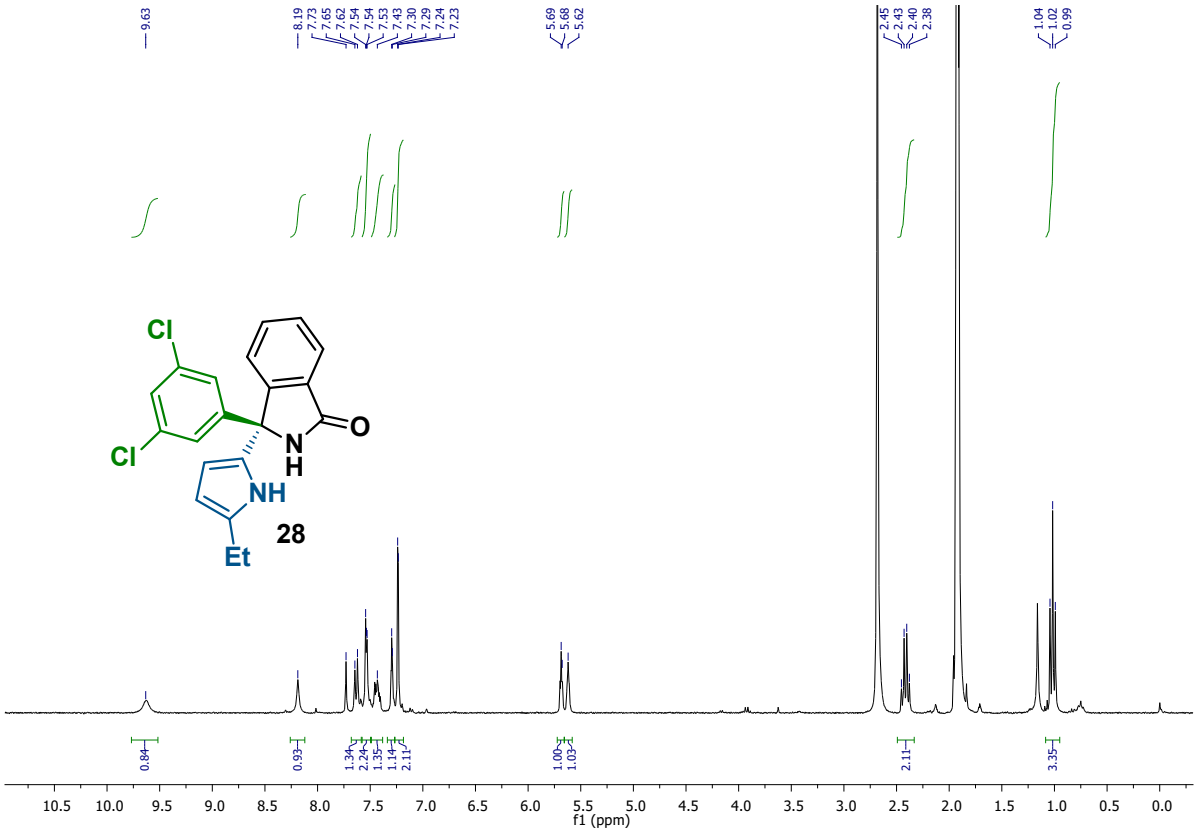
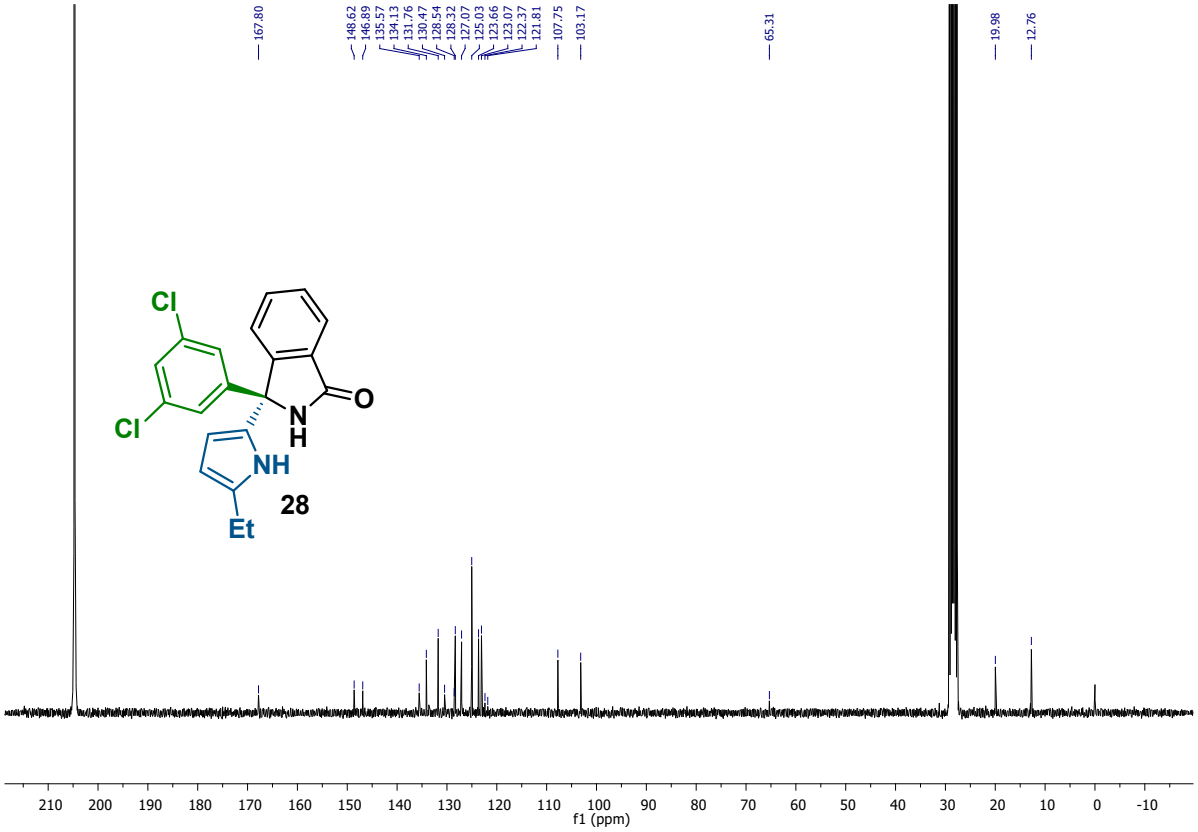
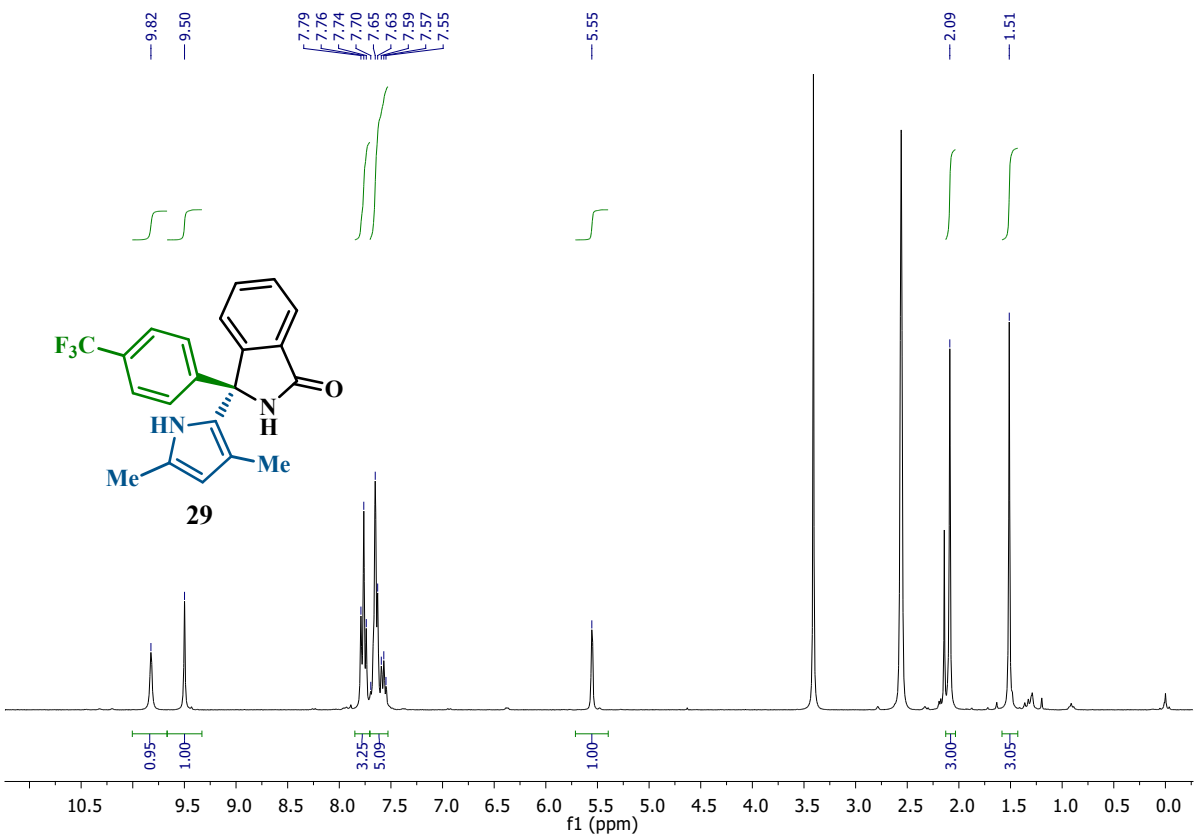
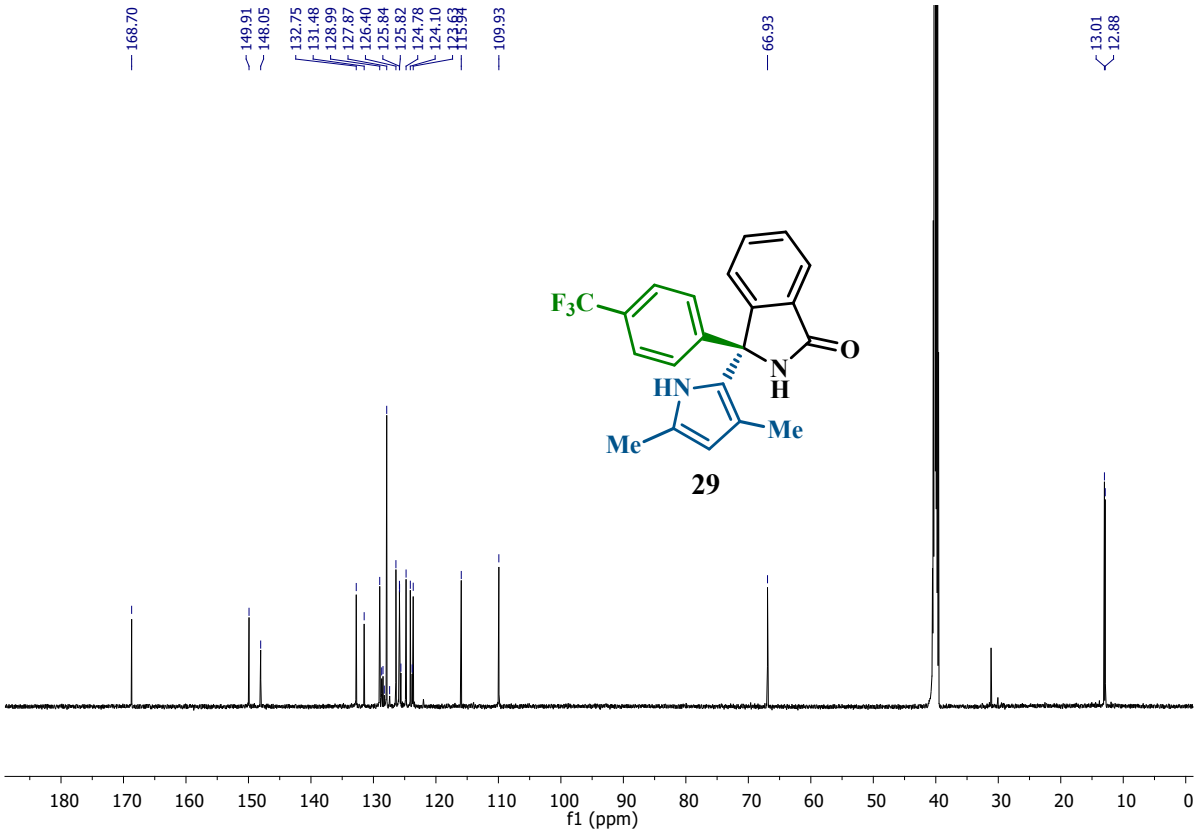
f1 (ppm)

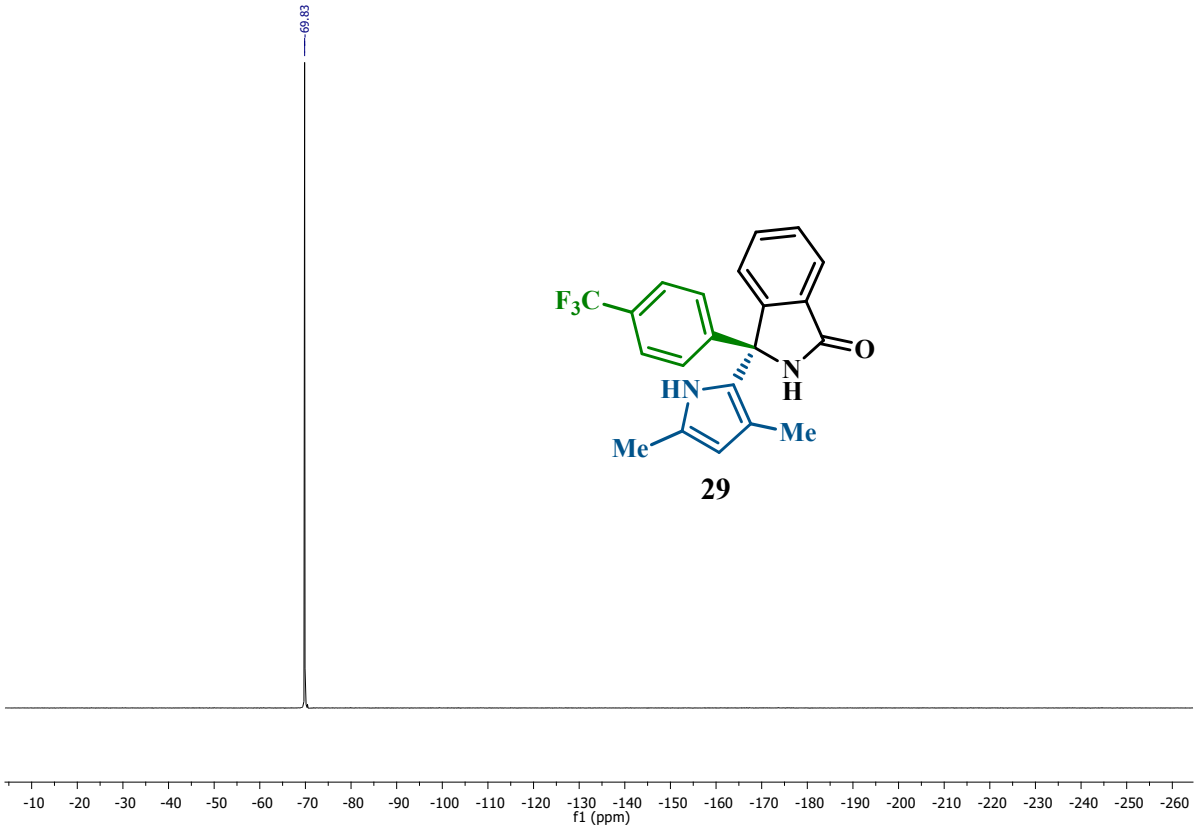

-109.22
F
F
O
N
H
NH
Et
27
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250

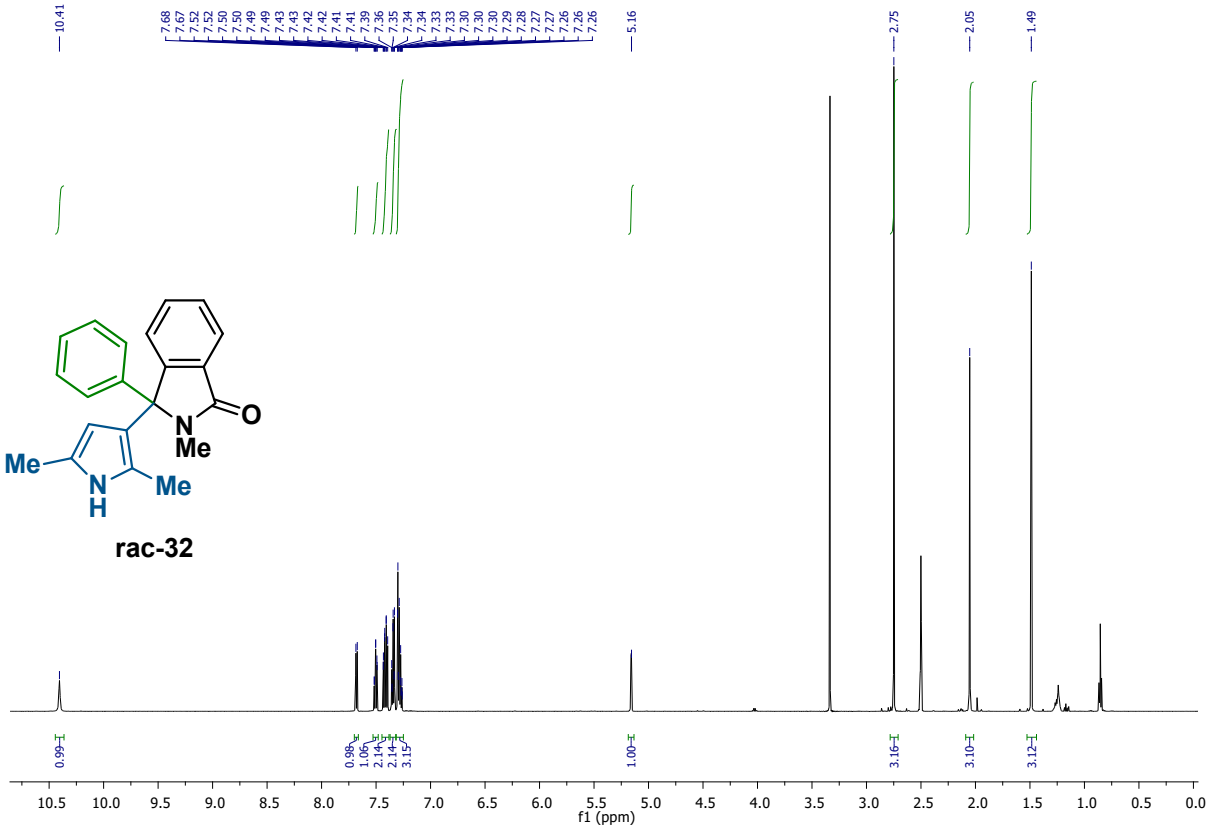

9.63
8.19
7.73
7.65
7.62
7.54
7.54
7.53
7.43
7.30
7.29
7.24
7.23
5.69
5.68
5.62
2.45
2.43
2.40
2.38
1.04
1.02
0.99
Cl
Cl
N
H
O
NH
Et
28
0.84
0.93
1.34
2.24
1.35
1.14
2.11
1.00
1.03
2.11
3.35
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.80
148.62
146.89
135.57
134.13
131.76
130.47
128.54
128.32
127.07
125.03
123.66
123.07
122.37
121.81
107.75
103.17
65.31
19.98
12.76
Cl
Cl
N
H
O
NH
Et
28
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


9.82
9.50
7.79
7.76
7.74
7.70
7.65
7.63
7.59
7.57
7.55
5.55
2.09
1.51
F3C
O
N
H
HN
Me
Me
29
0.95
1.00
3.25
5.09
1.00
3.00
3.05
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


168.70
149.91
148.05
132.75
131.48
128.99
127.87
126.40
125.84
125.82
124.78
124.10
109.93
66.93
13.01
12.88
F3C
O
N
H
HN
Me
Me
29
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


69.83
F3C
O
N
H
HN
Me
Me
29
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260
f1 (ppm)


10.41
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7.67
7.52
7.52
7.50
7.50
7.49
7.49
7.43
7.42
7.42
7.41
7.41
7.39
7.36
7.35
7.34
7.34
7.33
7.33
7.30
7.30
7.30
7.29
7.28
7.27
7.27
7.26
7.26
7.26
5.16
2.75
2.05
1.49
0.99
0.98
1.06
2.14
2.14
3.15
1.00
3.16
3.10
3.12
10.5
10.0
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O
N
Me
Me
N
H
Me

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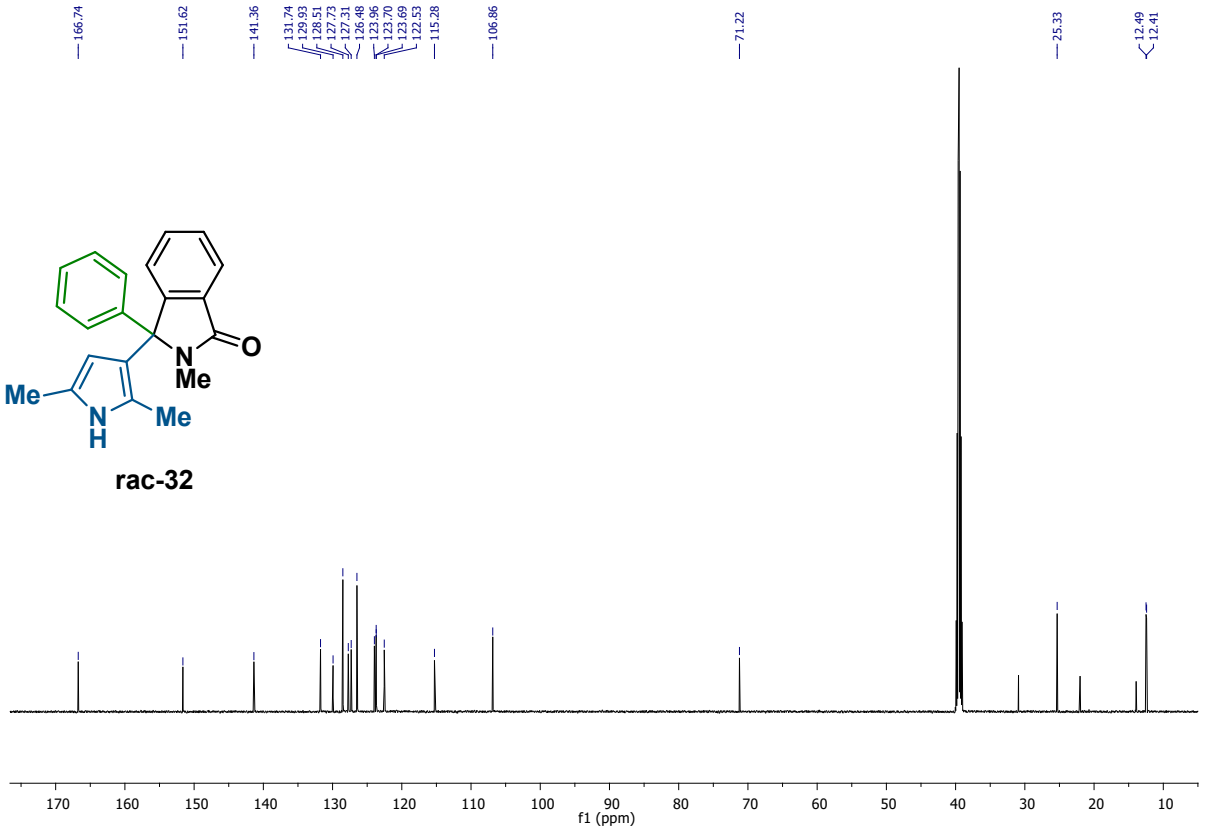
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106.86
71.22
25.33
12.49
12.41
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160
150
140
130
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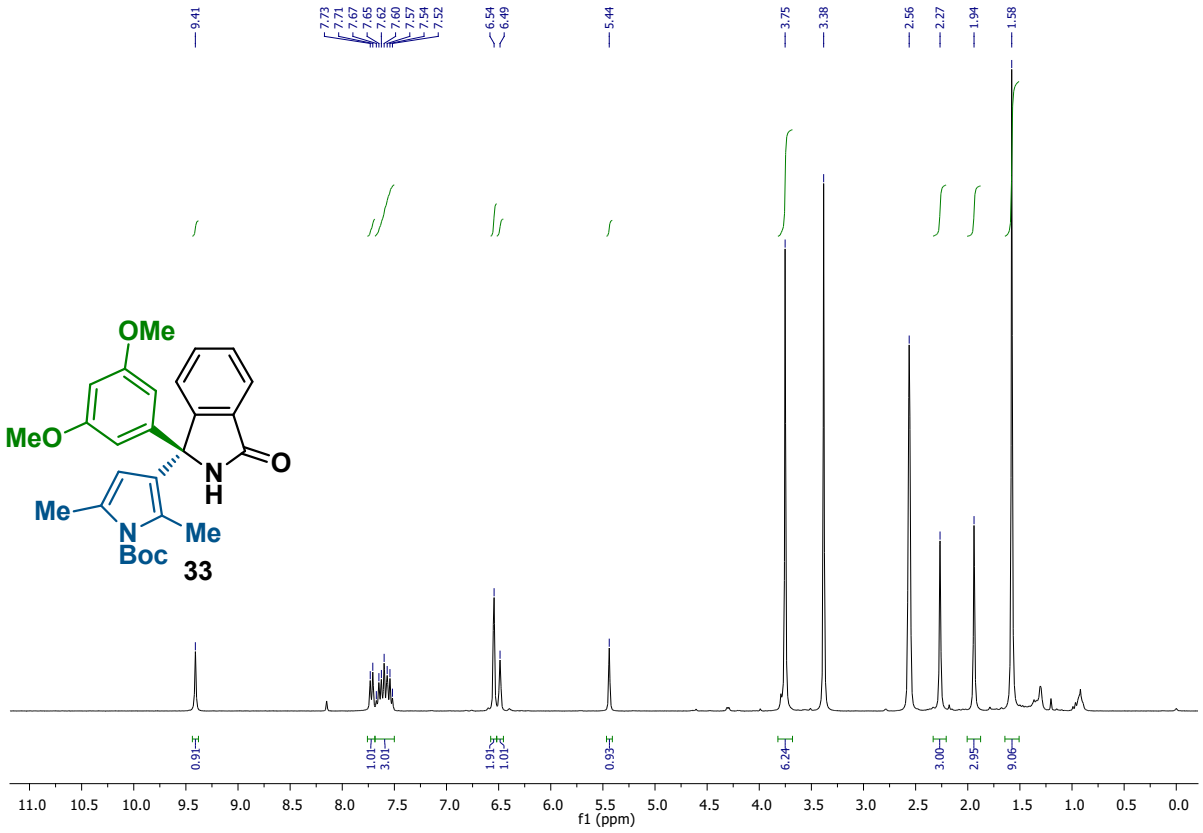
f1 (ppm)
O
N
Me
Me
N
H
Me

rac-32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3.38
2.56
2.27
1.94
1.58
OMe
MeO
N
H
O
Me
N
Boc
Me
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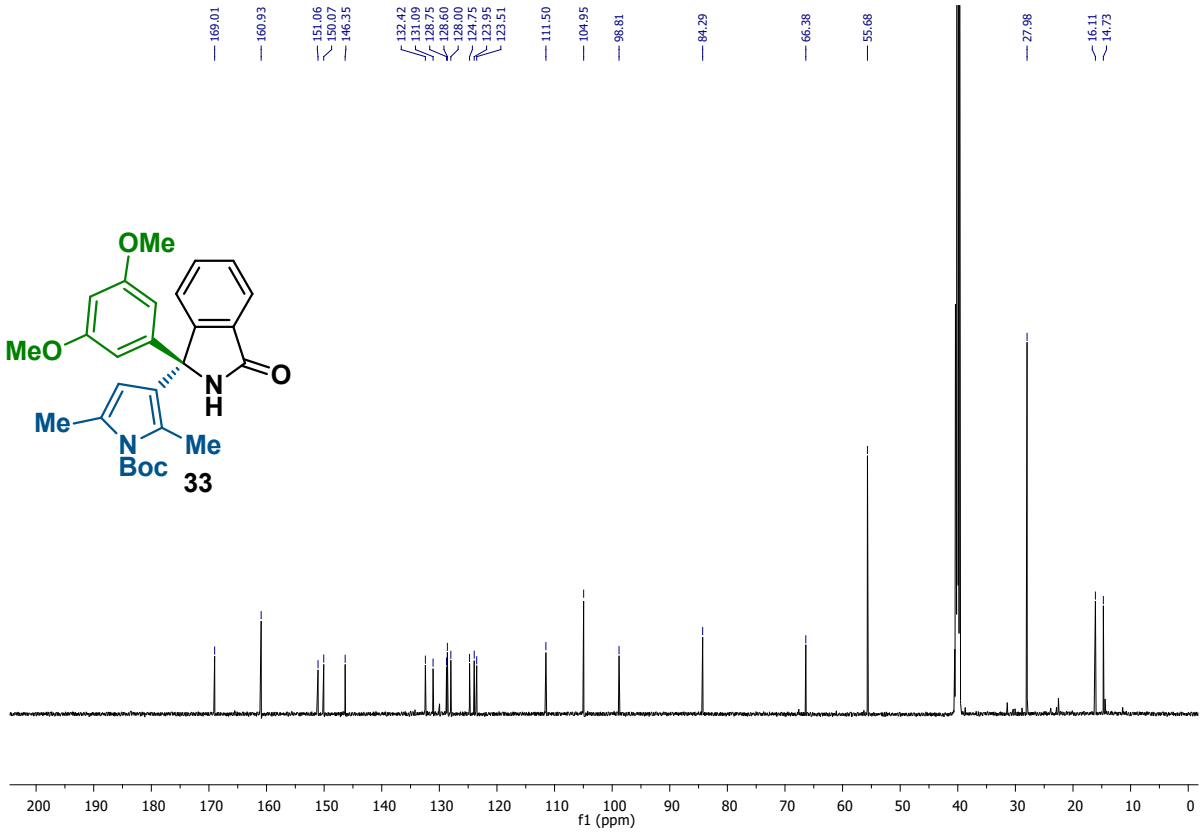
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84.29
66.38
55.68
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MeO
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H
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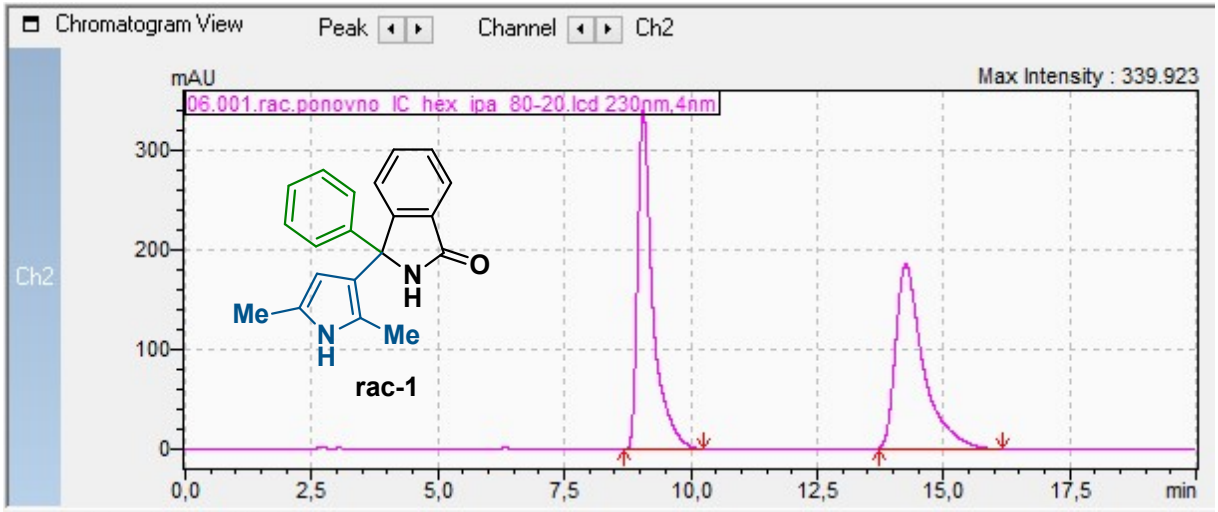
Boc
Me
33
f1 (ppm)

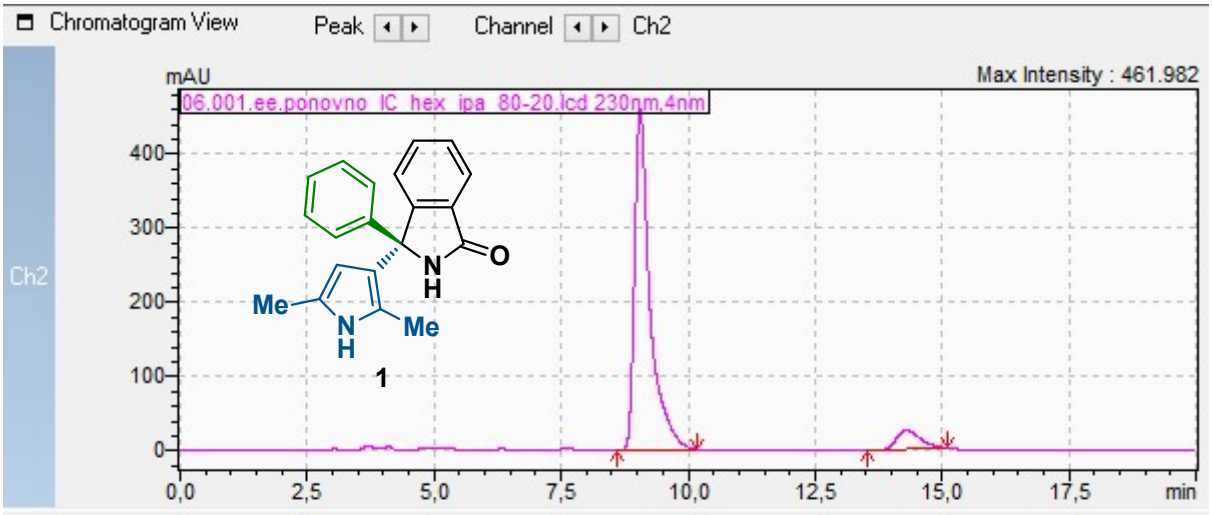
8. HPLC Traces



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

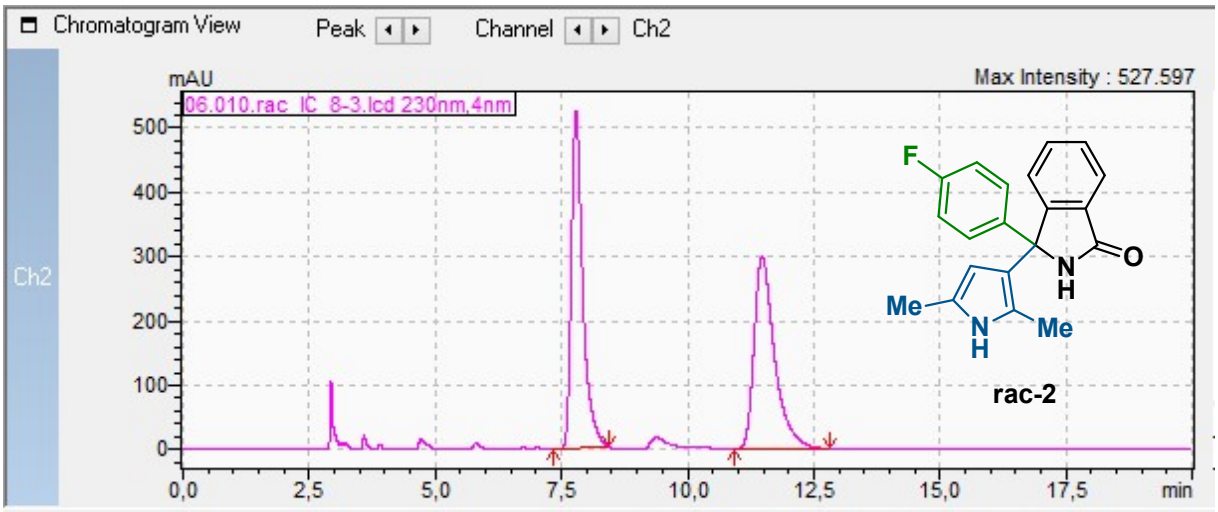
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,061	7127443	50,341	8,664	10,256	339410
2	14,256	7030803	49,659	13,728	16,160	183863
Total		14158246	100,000			523273



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

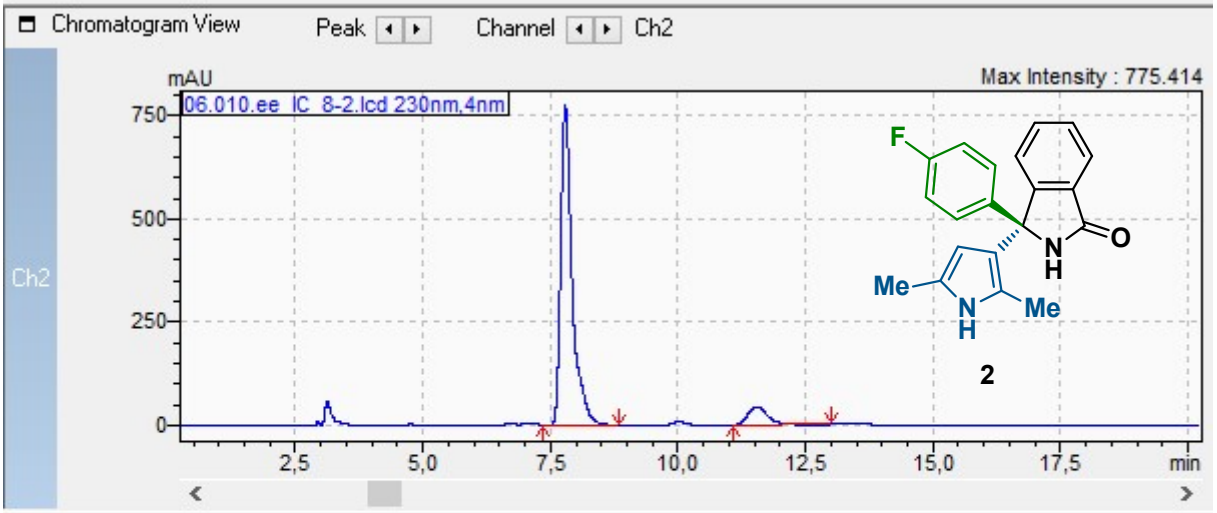
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,057	9673325	91,877	8,616	10,160	460313
2	14,311	855228	8,123	13,536	15,128	25494
Total		10528553	100,000			485807



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

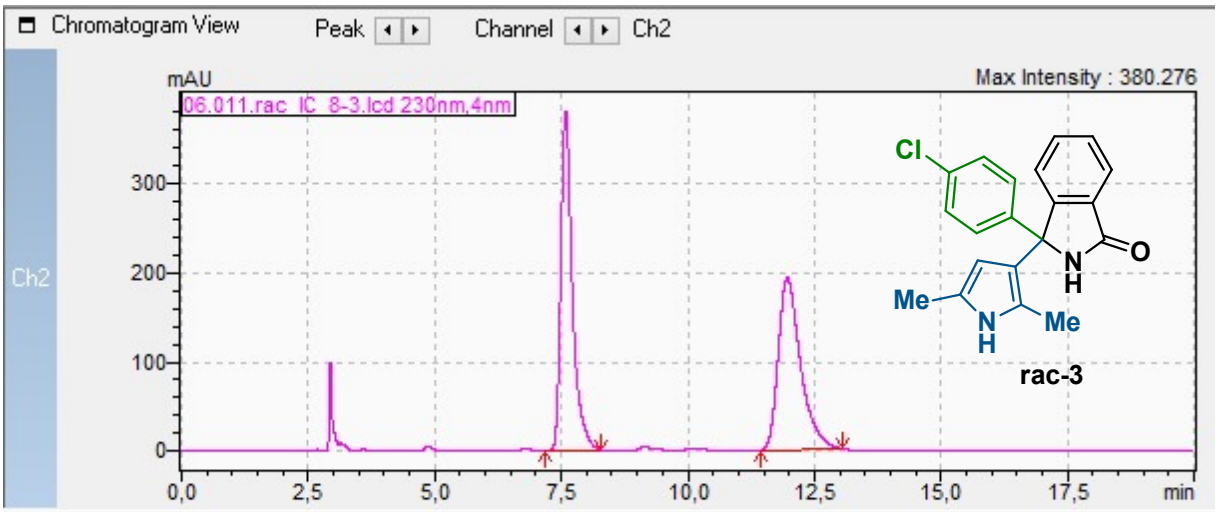
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,789	8292079	49,454	7,352	8,432	525424
2	11,479	8475253	50,546	10,912	12,832	299295
Total		16767332	100,000			824719



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

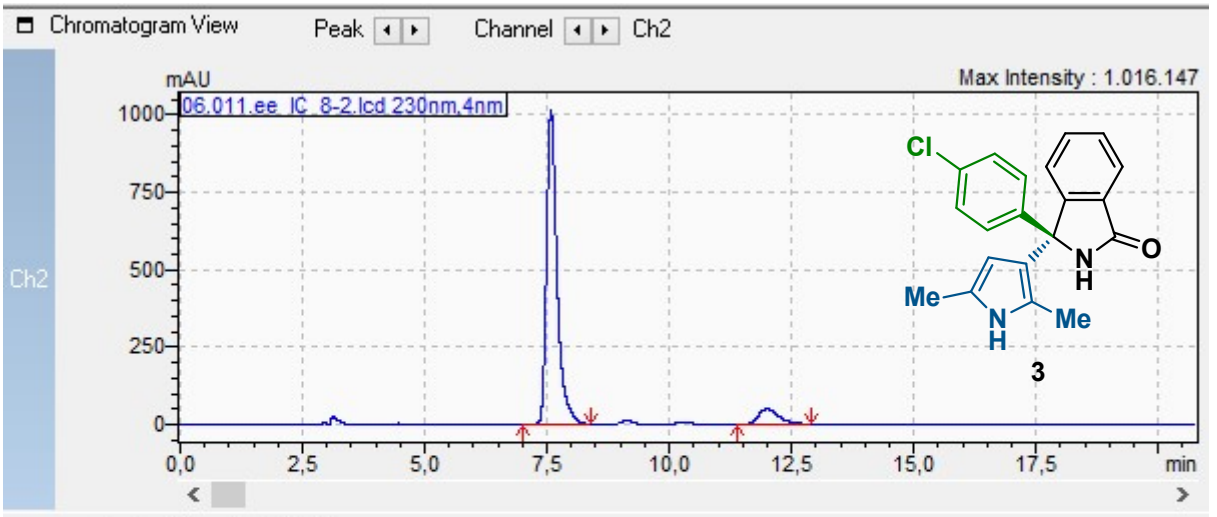
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,791	12056285	91,252	7,336	8,848	773682
2	11,534	1155832	8,748	11,064	13,008	44507
Total		13212117	100,000			818190



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

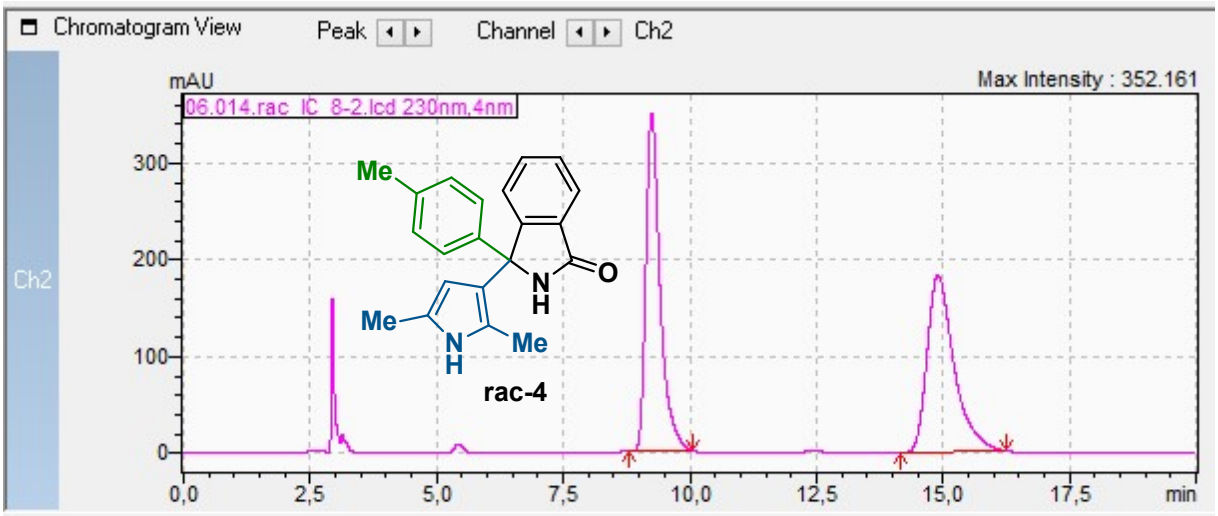
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,585	6008322	50,350	7,168	8,288	378489
2	11,967	5924827	49,650	11,432	13,072	192314
Total		11933149	100,000			570803



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

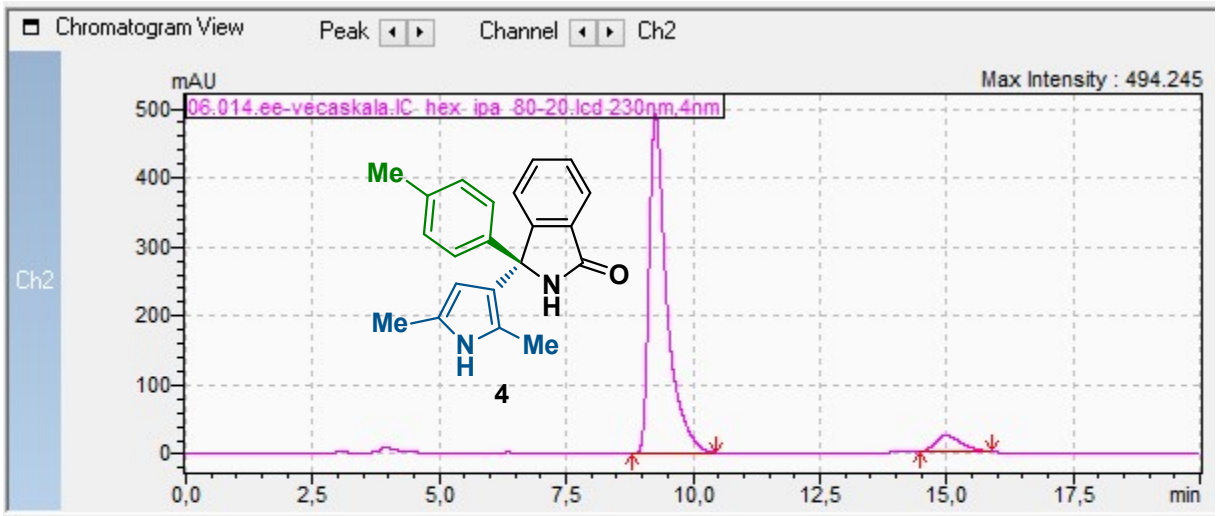
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,581	15120367	90,890	7,016	8,416	1013600
2	11,999	1515578	9,110	11,384	12,896	50761
Total		16635944	100,000			1064361



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

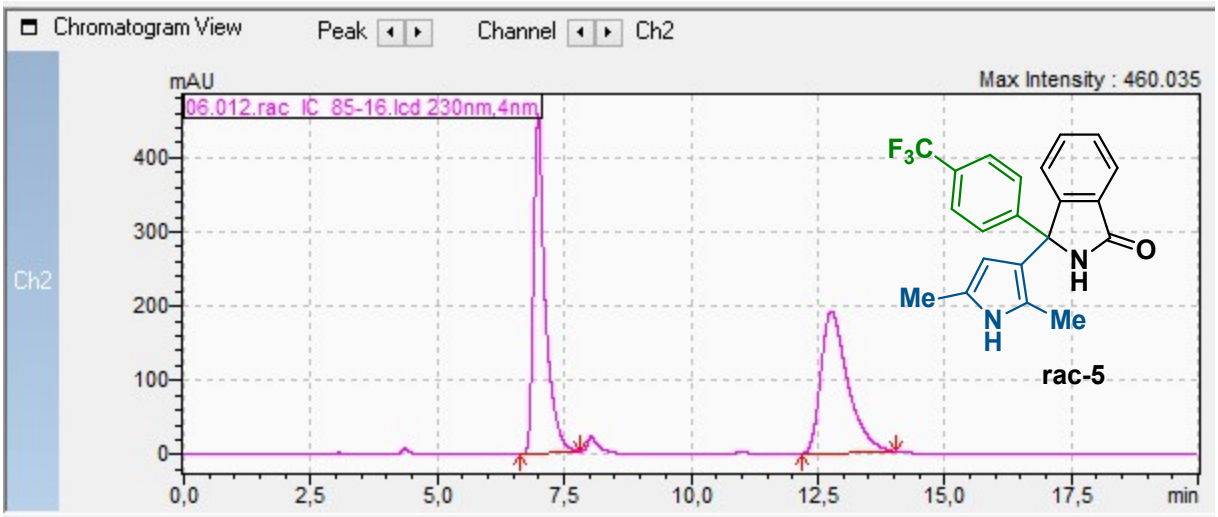
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,249	6823493	50,040	8,808	10,072	349264
2	14,903	6812470	49,960	14,144	16,256	183342
Total		13635964	100,000			532606



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

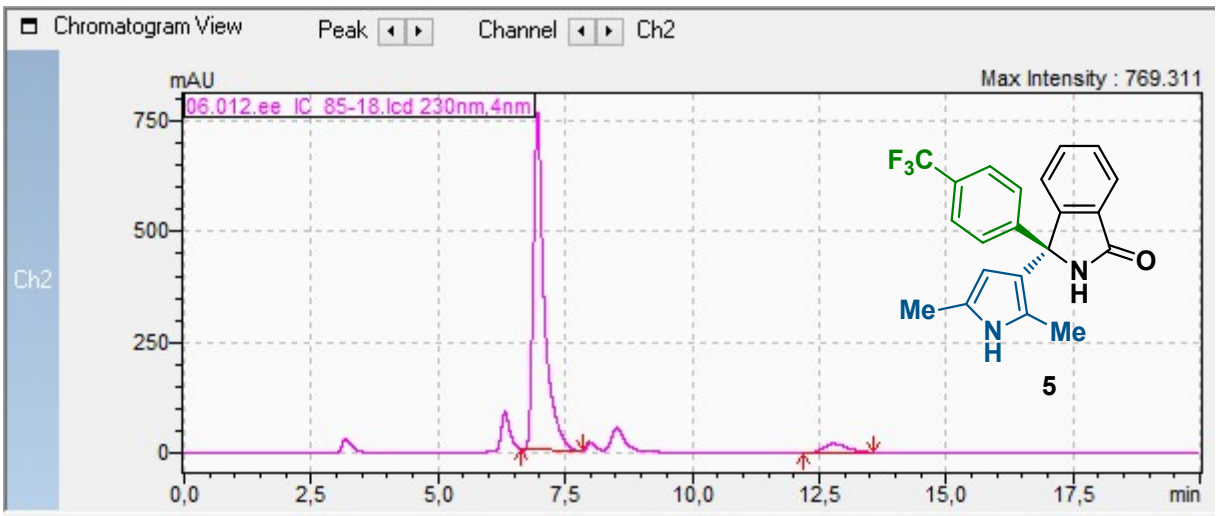
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,262	11925835	93,154	8,808	10,440	492835
2	15,000	876392	6,846	14,496	15,896	23533
Total		12802227	100,000			516368



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

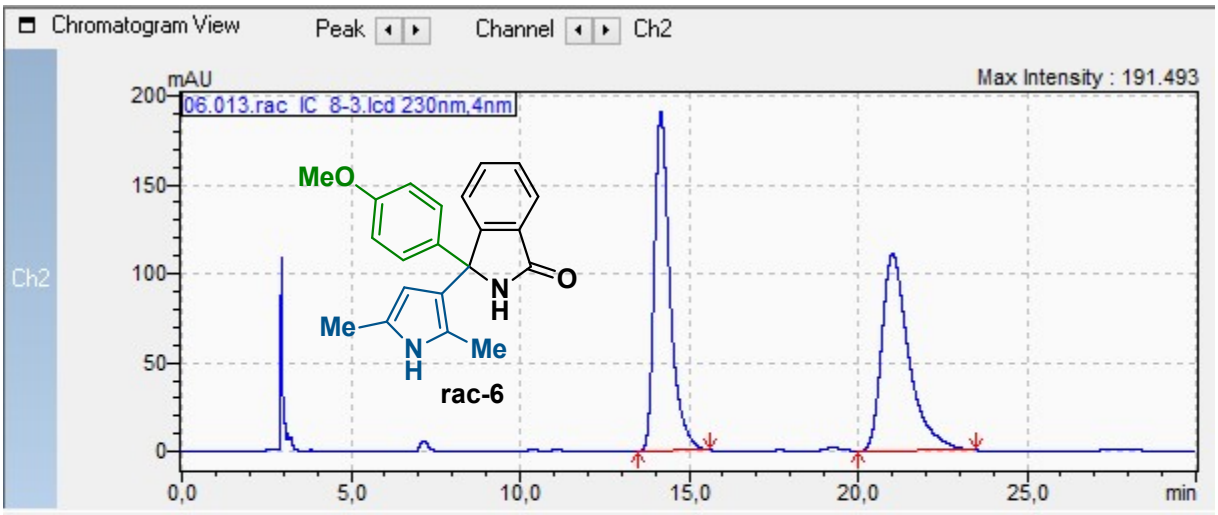
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	6,988	7306409	50,792	6,608	7,824	457703
2	12,768	7078535	49,208	12,176	14,056	190734
Total		14384944	100,000			648437



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

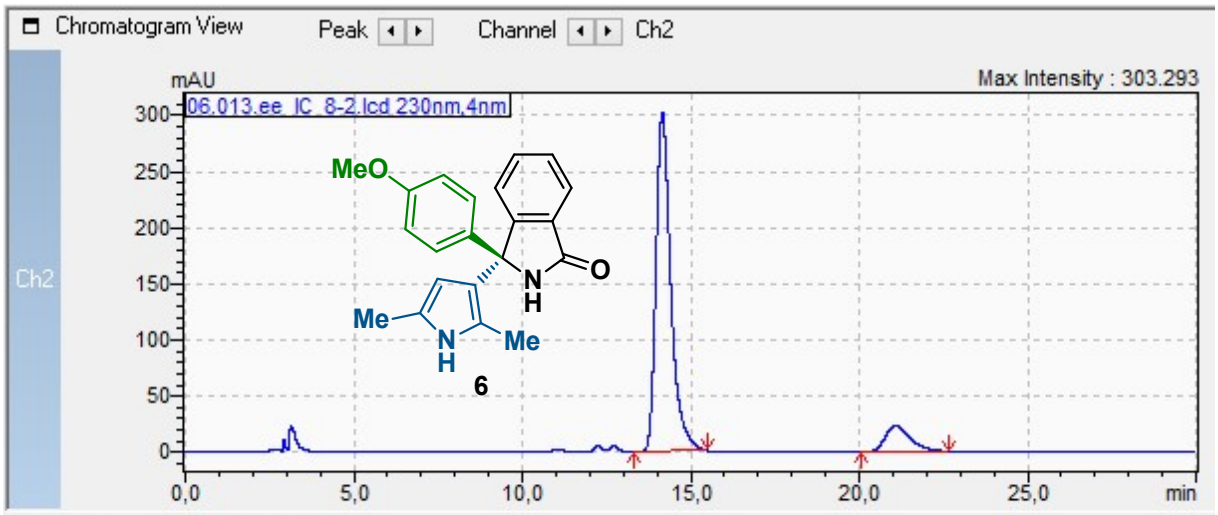
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	6,960	11418317	94,134	6,616	7,840	758646
2	12,798	711499	5,866	12,192	13,560	20935
Total		12129816	100,000			779581



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

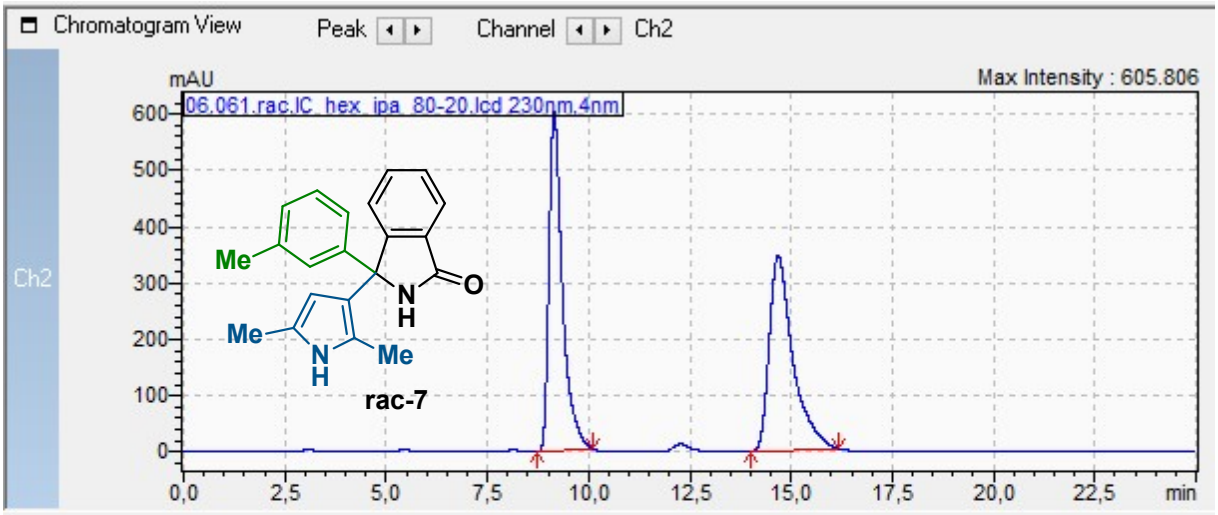
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	14,168	6158818	49,910	13,488	15,600	191219
2	21,022	6181001	50,090	20,024	23,464	110491
Total		12339819	100,000			301709



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

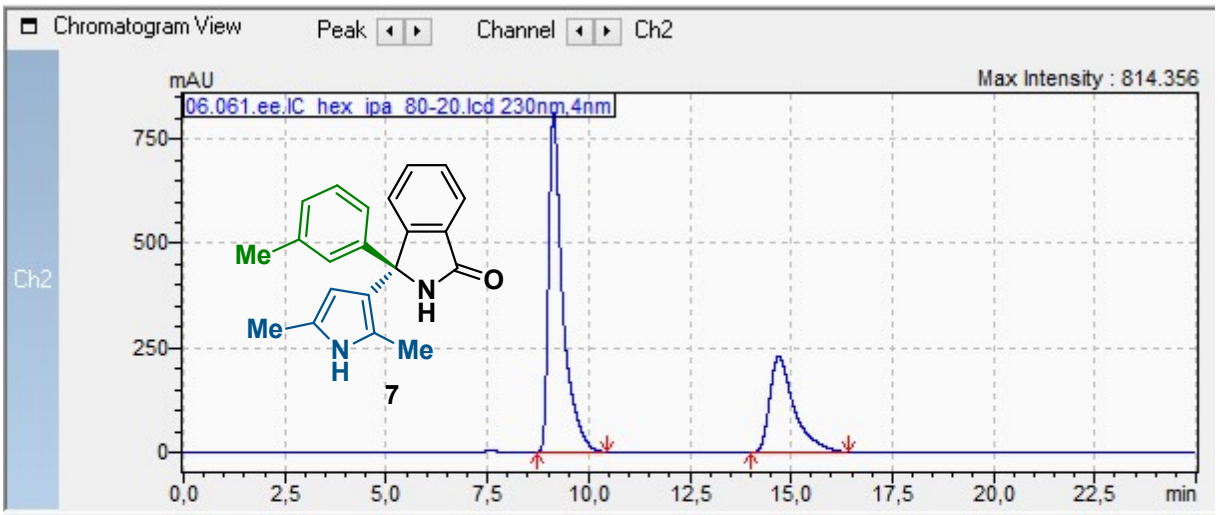
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	14,158	9246277	88,184	13,328	15,488	302621
2	21,098	1238973	11,816	20,072	22,664	23254
Total		10485249	100,000			325875



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

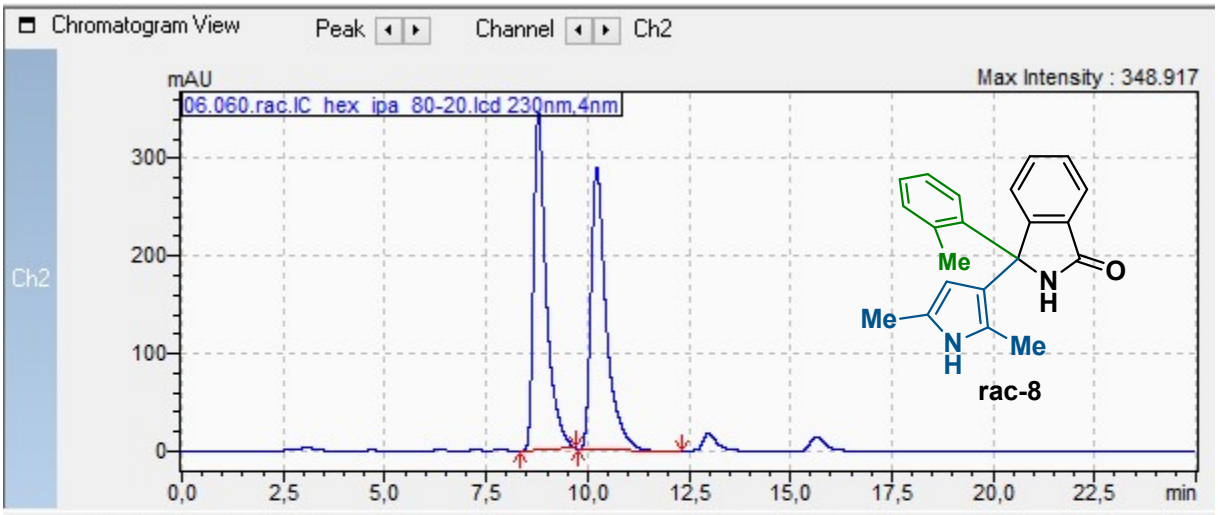
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,149	13951650	49,749	8,752	10,128	603664
2	14,682	14092422	50,251	14,024	16,176	346434
Total		28044072	100,000			950098



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

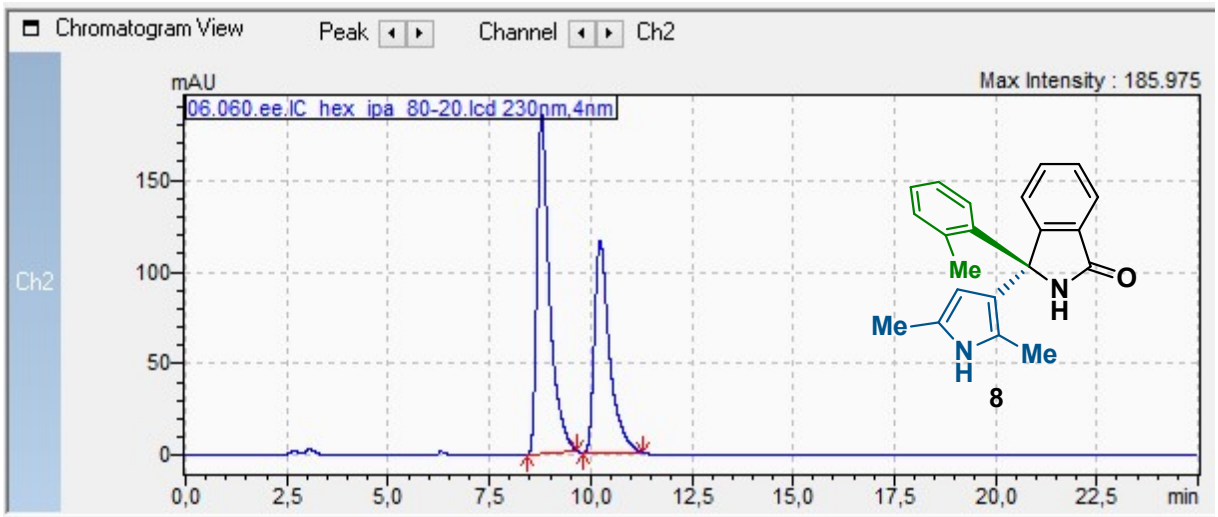
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,135	19702865	67,034	8,720	10,464	812034
2	14,697	9689461	32,966	14,024	16,432	229055
Total		29392326	100,000			1041089



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

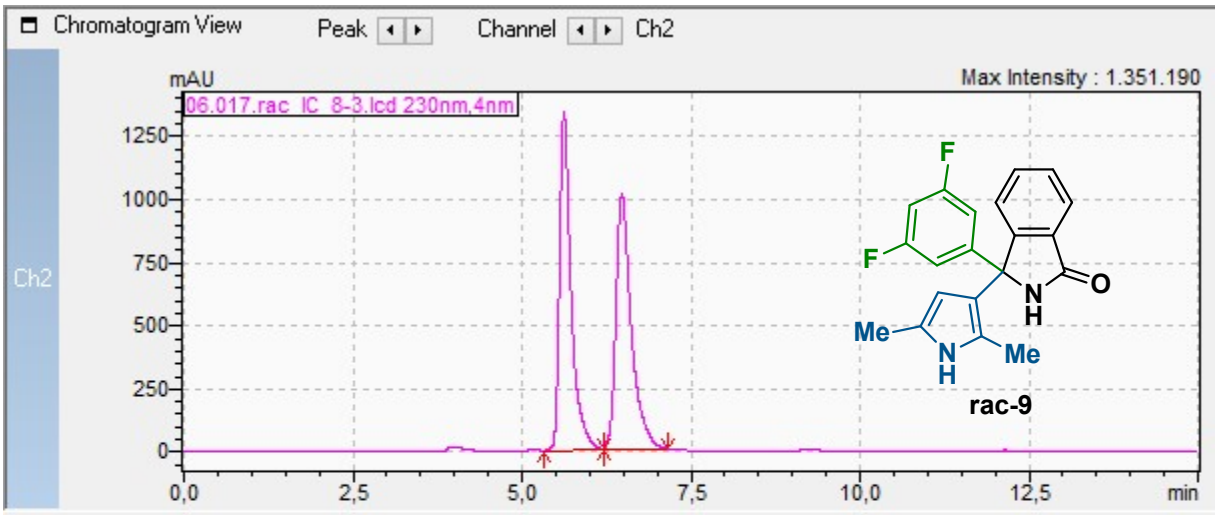
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	8,786	7579892	50,100	8,312	9,720	347442
2	10,227	7549649	49,900	9,752	12,312	289040
Total		15129541	100,000			636482



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

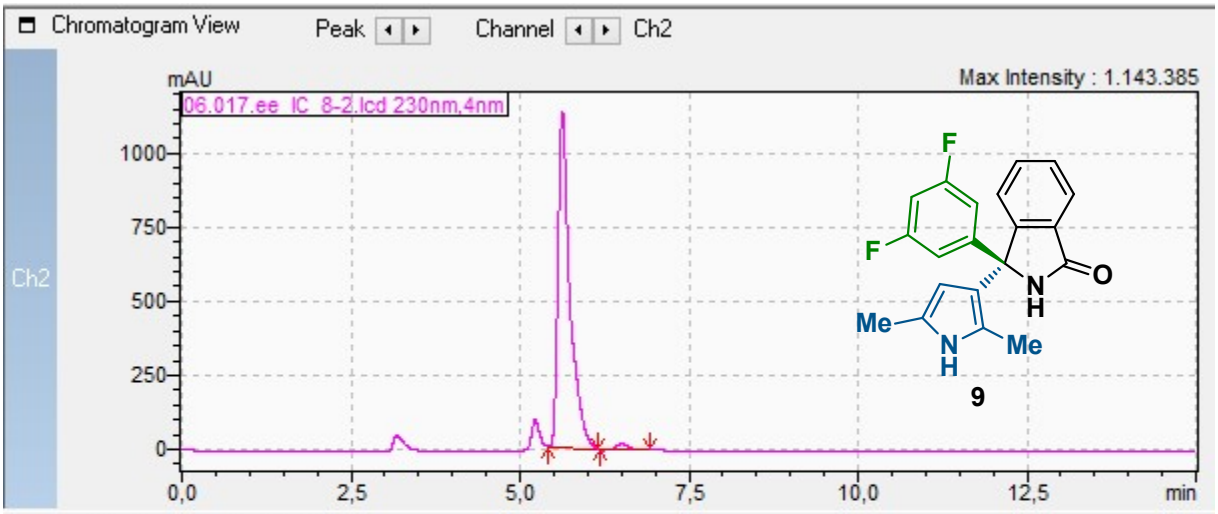
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	8,790	4000213	56,876	8,456	9,648	184532
2	10,237	3032986	43,124	9,792	11,312	116040
Total		7033200	100,000			300572



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

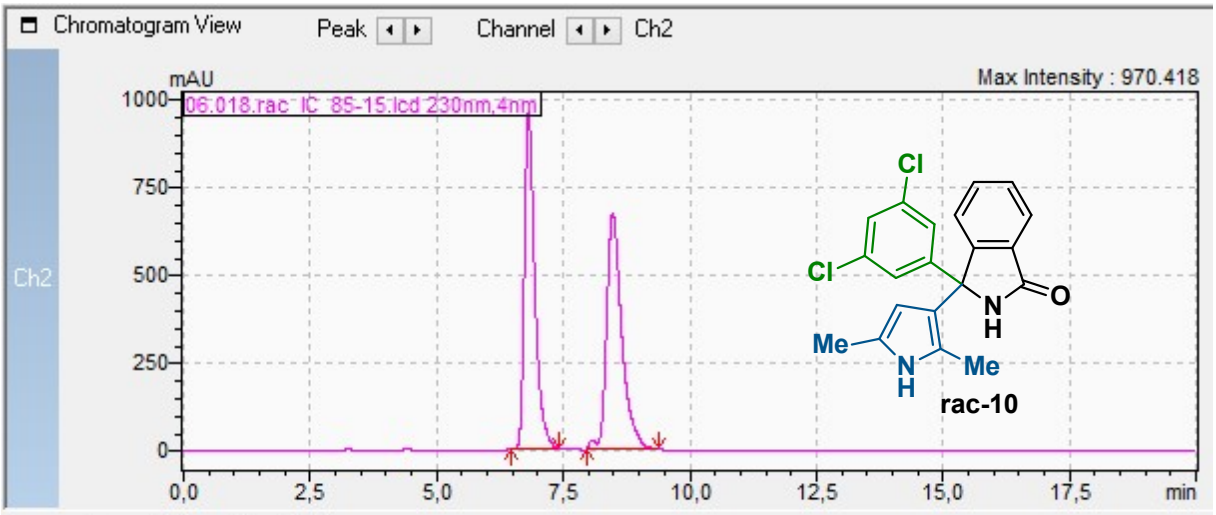
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,622	15841025	49,970	5,312	6,208	1341105
2	6,478	15859875	50,030	6,208	7,152	1005696
Total		31700900	100,000			2346801



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

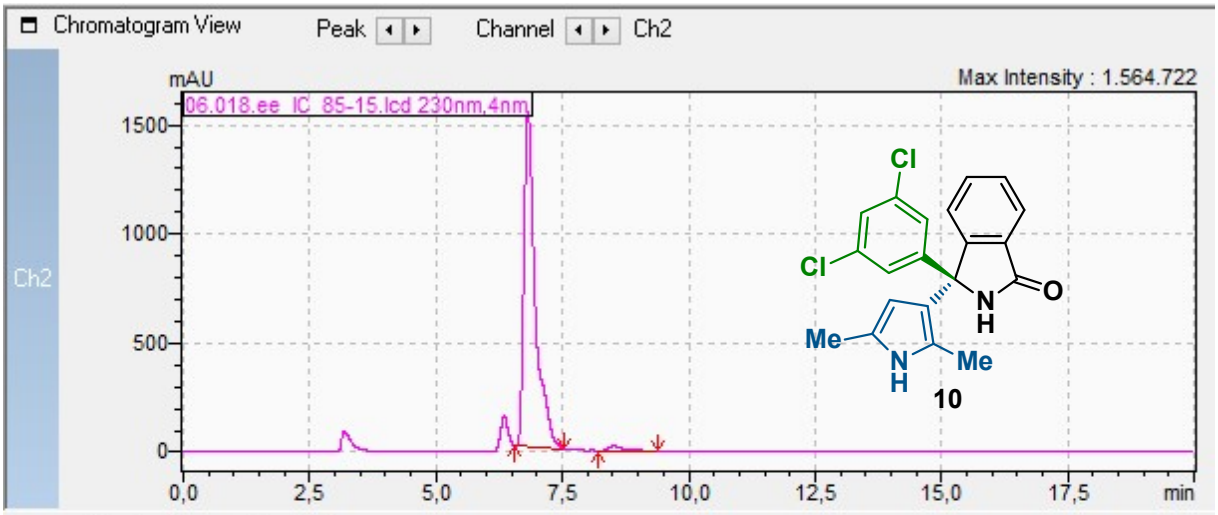
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,627	13876306	98,544	5,424	6,152	1136005
2	6,509	204964	1,456	6,176	6,936	19117
Total		14081270	100,000			1155122



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

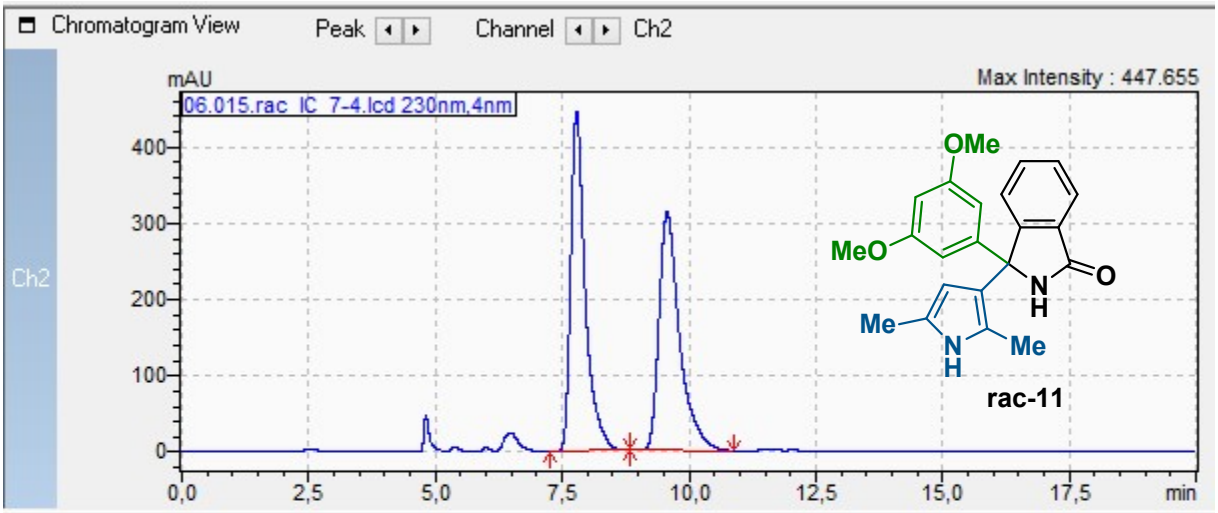
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	6,814	13762112	49,562	6,472	7,408	962903
2	8,479	14005432	50,438	7,968	9,392	670877
Total		27767544	100,000			1633780



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

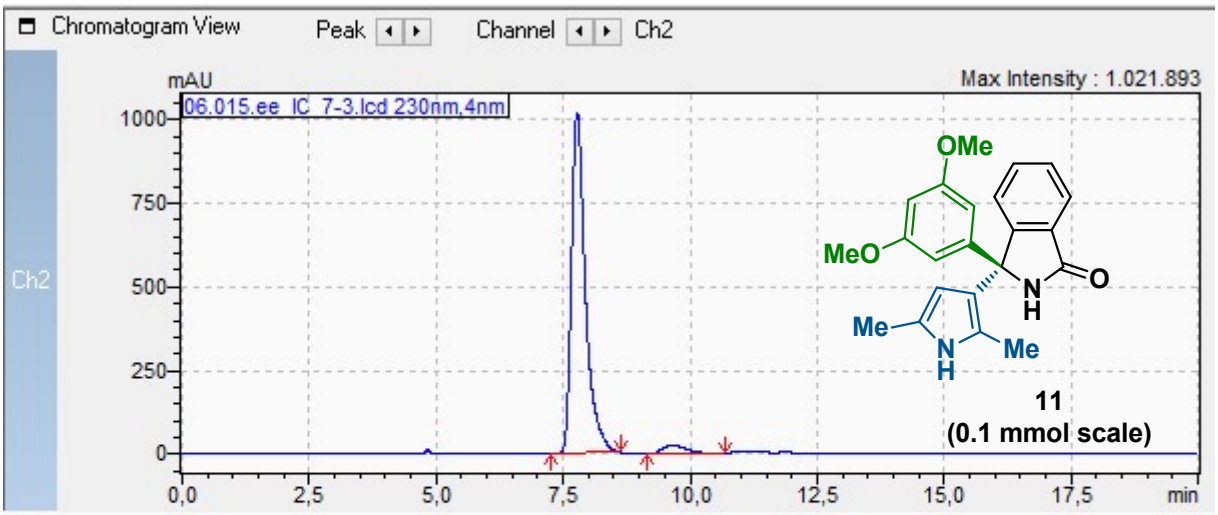
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	6,821	24106201	98,002	6,560	7,520	1539788
2	8,526	491526	1,998	8,216	9,408	22037
Total		24597727	100,000			1561825



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

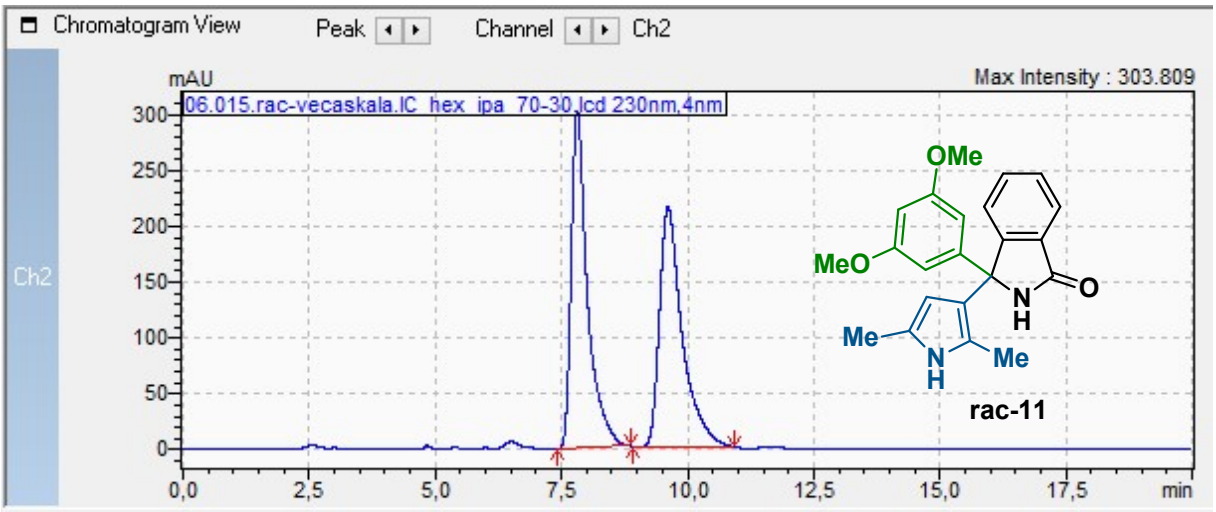
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,783	8822689	50,203	7,264	8,848	445669
2	9,570	8751406	49,797	8,848	10,896	311311
Total		17574094	100,000			756980



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

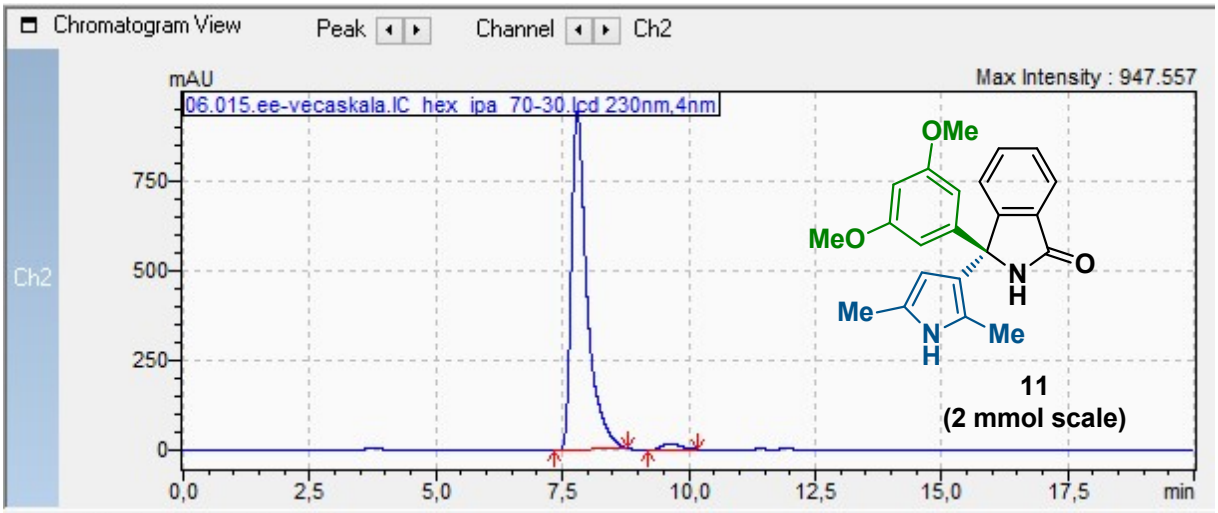
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,776	19518033	95,908	7,264	8,632	1018988
2	9,642	832697	4,092	9,136	10,680	26468
Total		20350730	100,000			1045456



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

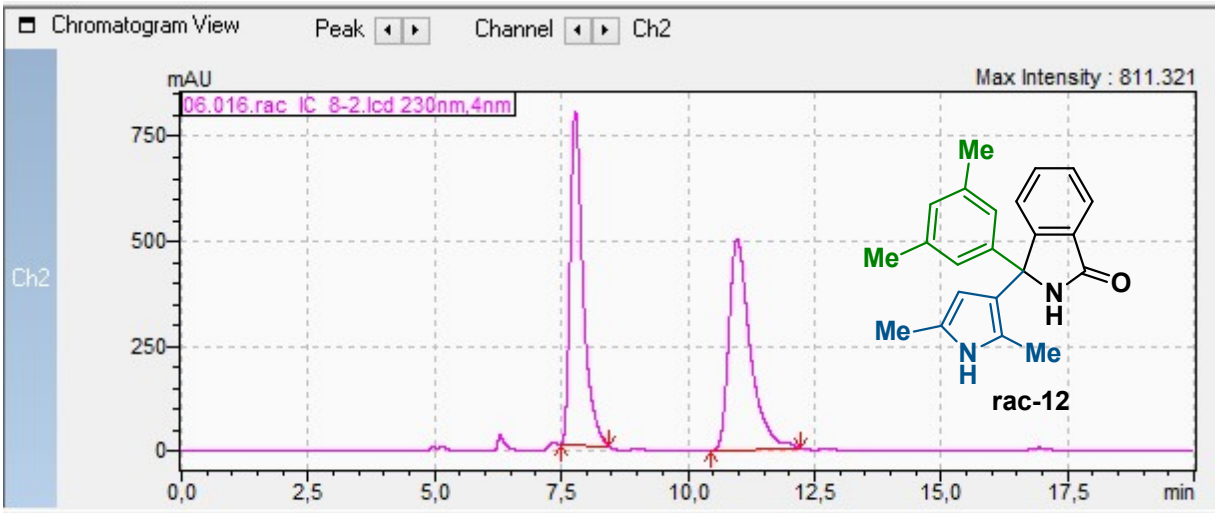
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,814	6778241	50,338	7,416	8,880	302413
2	9,614	6687188	49,662	8,912	10,928	214251
Total		13465429	100,000			516663



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

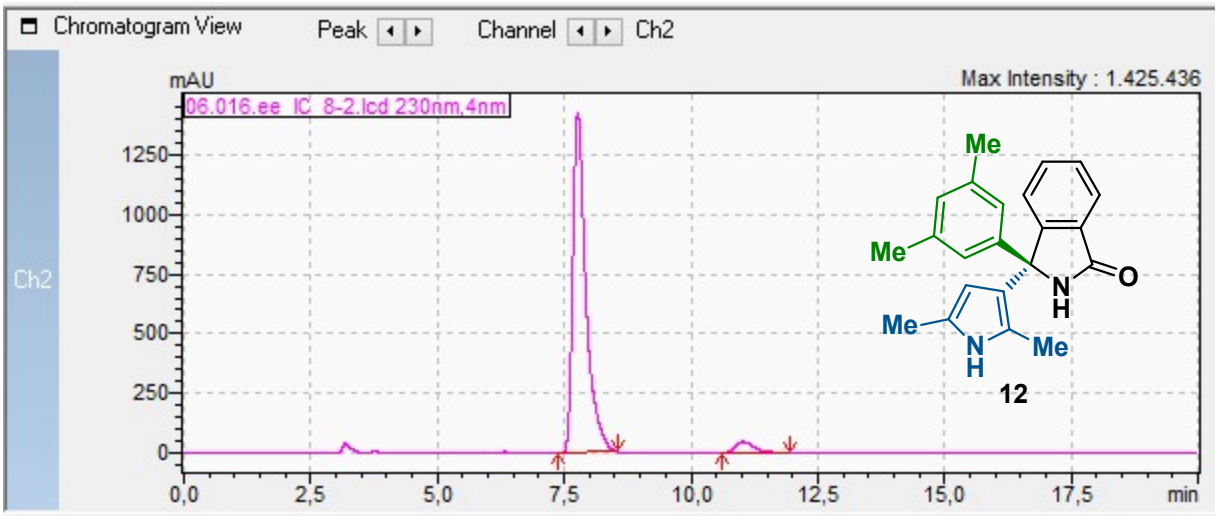
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,796	20414695	97,811	7,320	8,808	944193
2	9,629	456936	2,189	9,184	10,160	17905
Total		20871631	100,000			962097



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

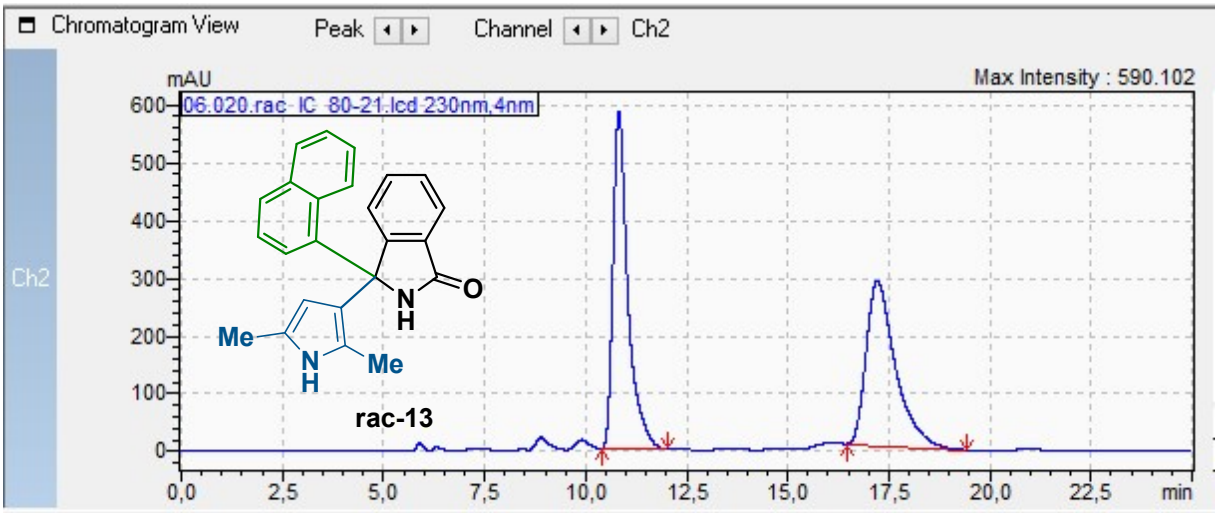
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,776	14155184	48,745	7,480	8,456	795919
2	10,976	14884107	51,255	10,472	12,232	503431
Total		29039291	100,000			1299350



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

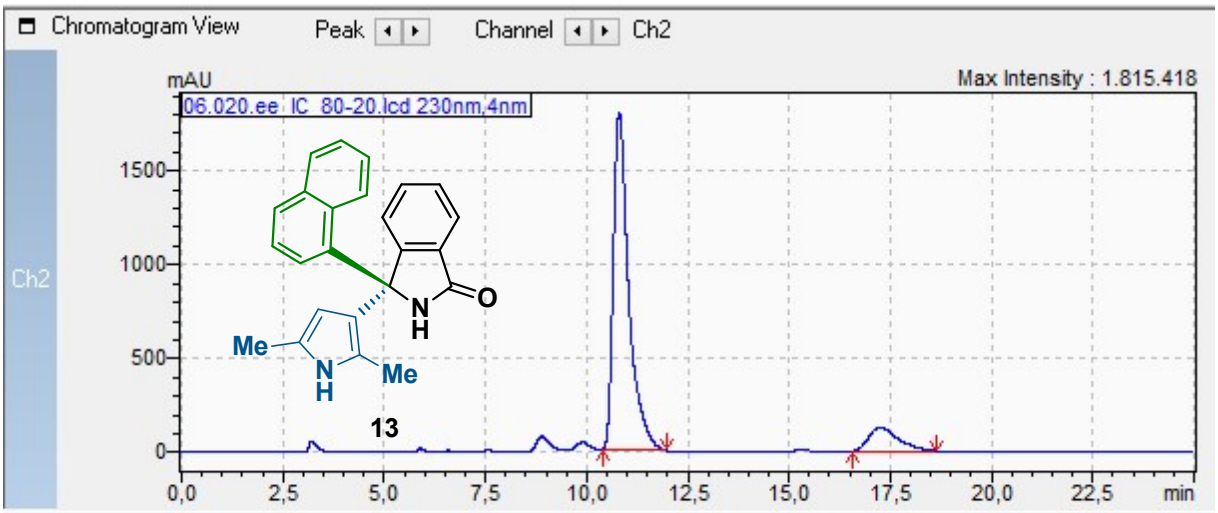
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,769	25425832	94,828	7,376	8,560	1418096
2	11,029	1386613	5,172	10,616	11,944	47878
Total		26812445	100,000			1465974



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

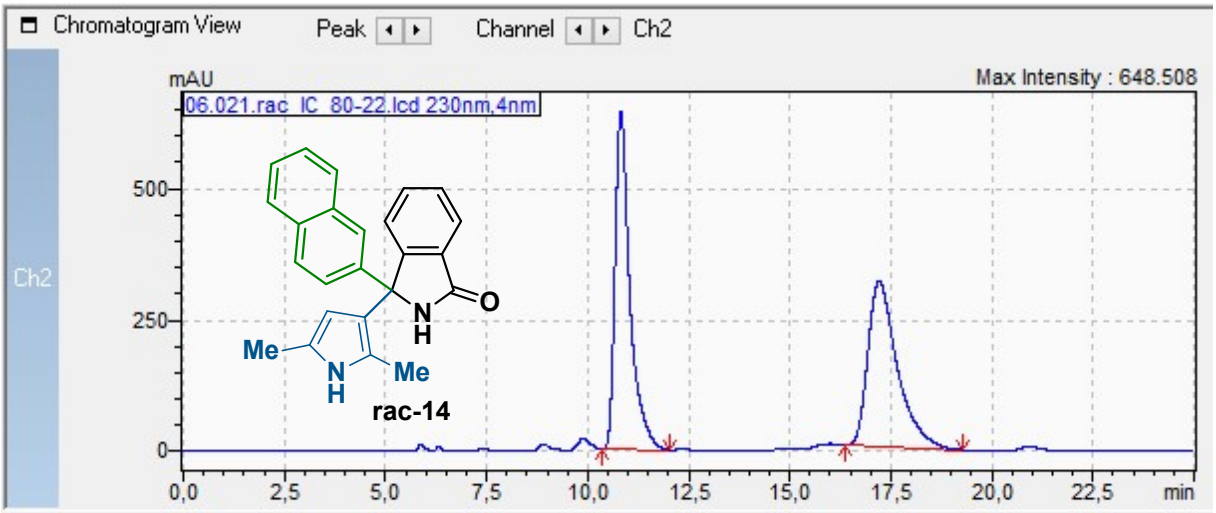
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	10,823	15012269	51,177	10,384	12,008	585517
2	17,219	14321498	48,823	16,456	19,424	284744
Total		29333767	100,000			870261



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

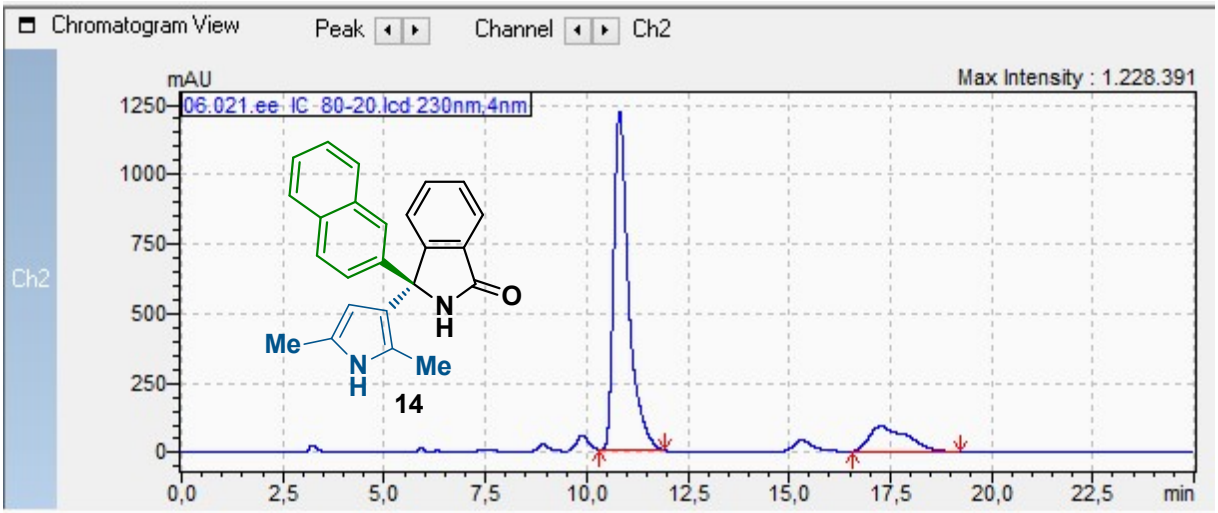
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	10,806	47761756	87,982	10,384	11,960	1802061
2	17,247	6524183	12,018	16,544	18,616	128963
Total		54285939	100,000			1931024



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

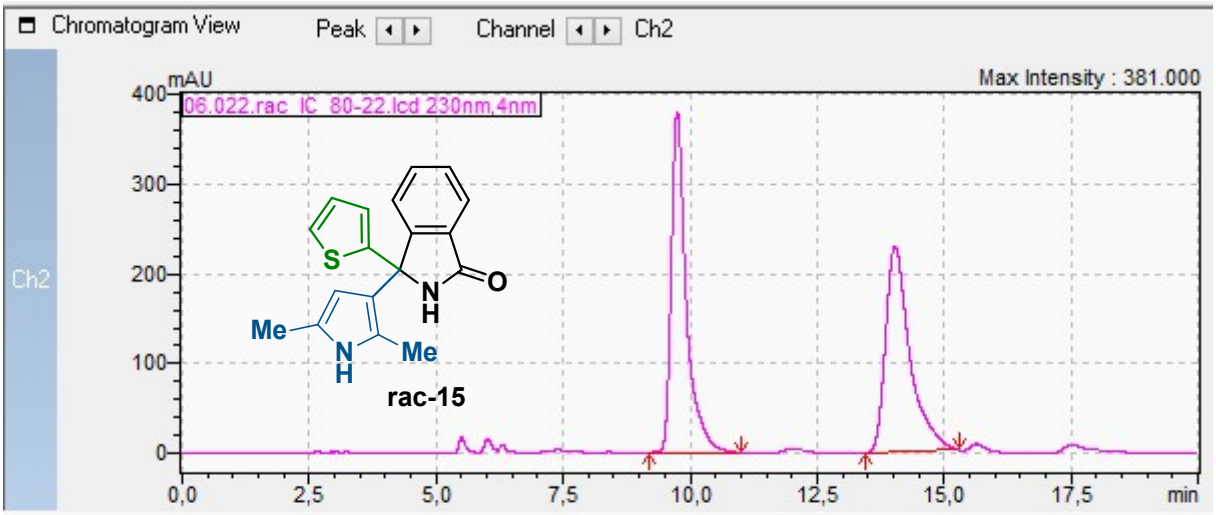
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	10,823	16474520	50,874	10,344	12,008	644527
2	17,213	15908650	49,126	16,368	19,288	315542
Total		32383170	100,000			960069



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

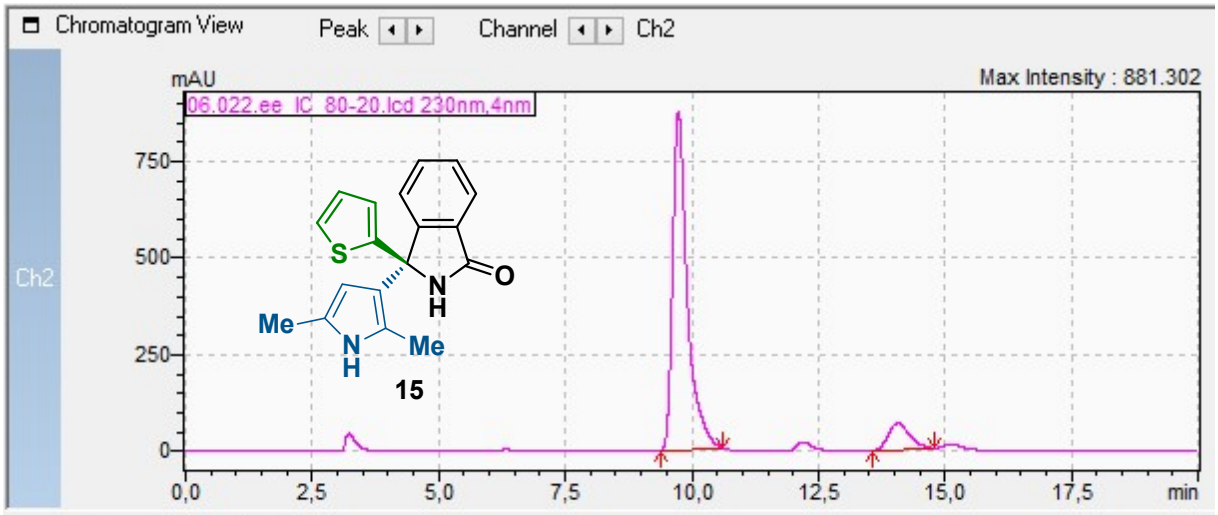
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	10,813	31087662	83,853	10,296	11,912	1216468
2	17,260	5986304	16,147	16,544	19,248	90968
Total		37073967	100,000			1307436



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

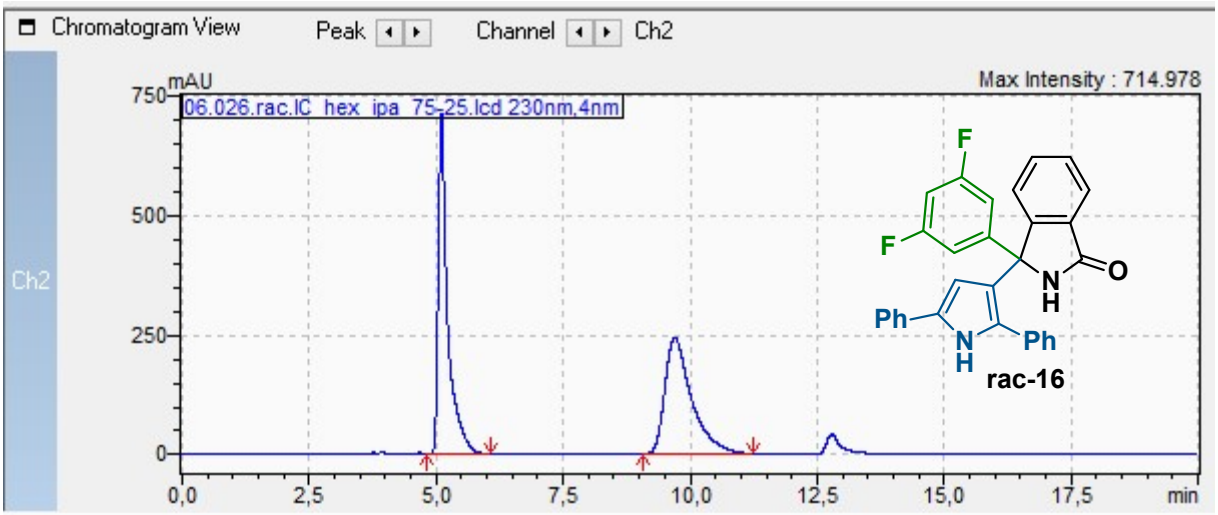
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,747	7843451	50,556	9,208	11,008	380030
2	14,036	7671051	49,444	13,456	15,288	229513
Total		15514502	100,000			609543



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

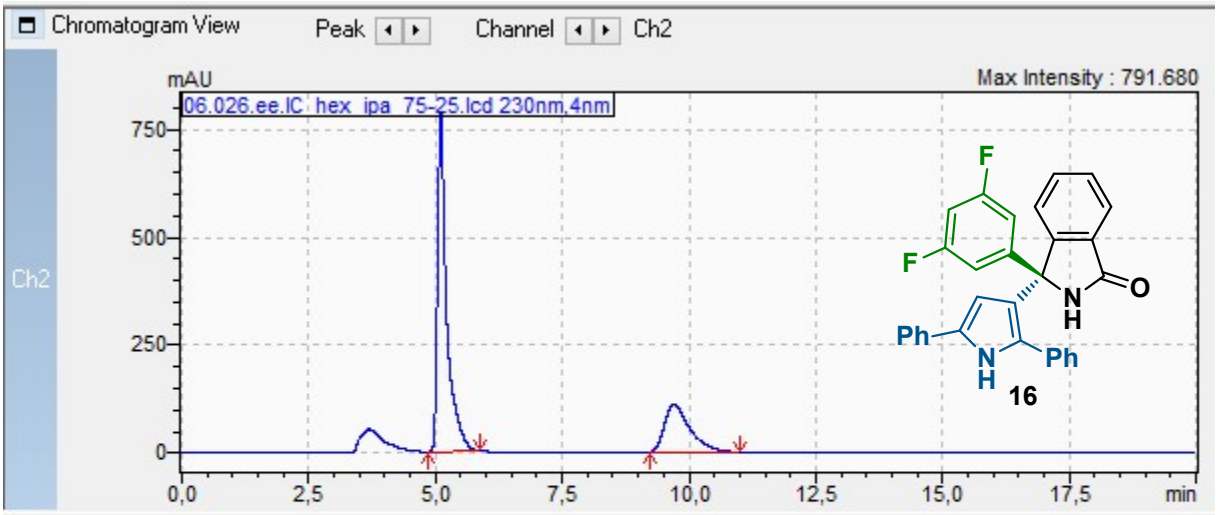
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,737	17644350	89,858	9,392	10,616	876465
2	14,067	1991534	10,142	13,560	14,784	68036
Total		19635884	100,000			944501



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

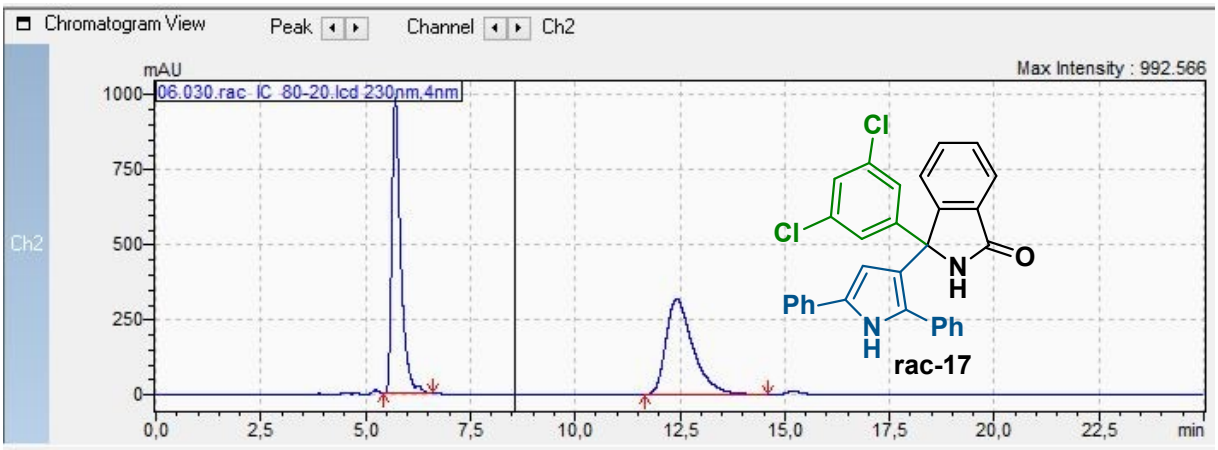
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,104	9124820	50,751	4,800	6,064	711416
2	9,696	8854856	49,249	9,088	11,232	242814
Total		17979677	100,000			954230



Results View - Peak Table

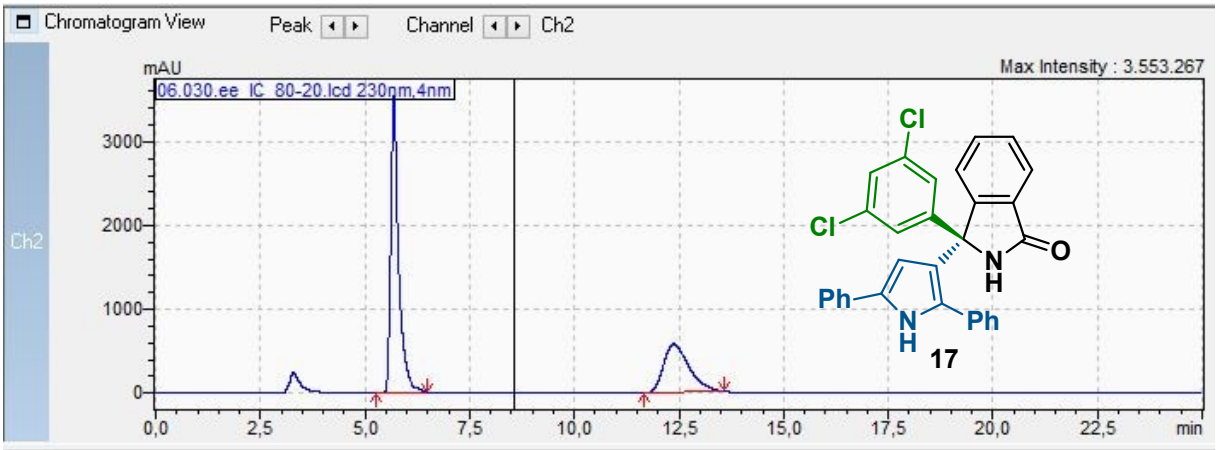
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,103	9866841	71,342	4,848	5,872	786506
2	9,709	3963489	28,658	9,232	11,000	111436
Total		13830330	100,000			897942



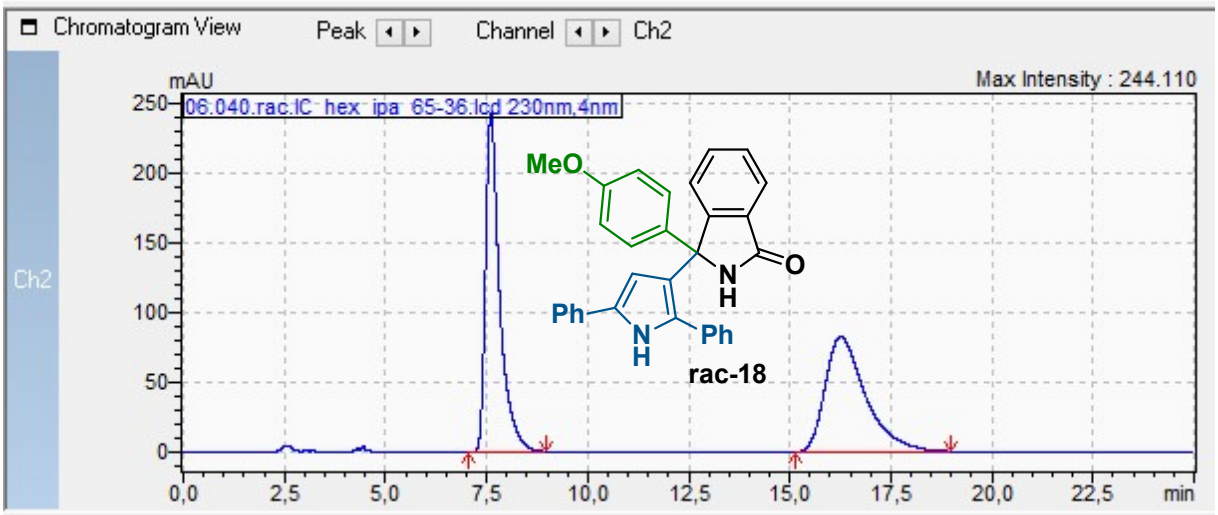
Results View - Peak Table

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,710	14567858	50,436	5,408	6,616	985996
2	12,421	14316252	49,564	11,680	14,616	318645
Total		28884110	100,000			1304642



Results View - Peak Table

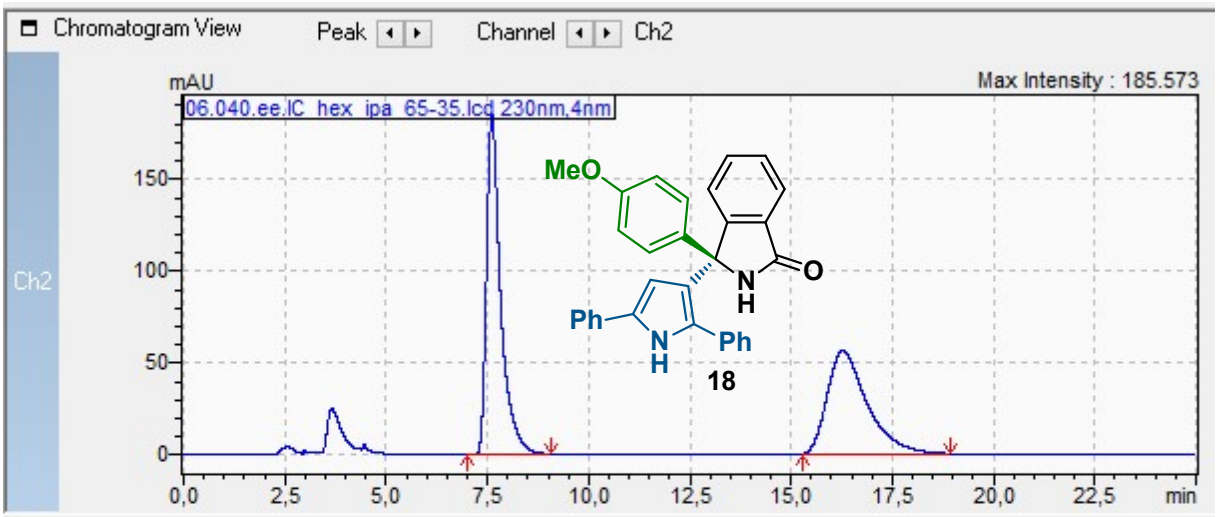
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,691	45816772	65,080	5,280	6,488	3541005
2	12,376	24584390	34,920	11,680	13,584	576864
Total		70401163	100,000			4117870



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

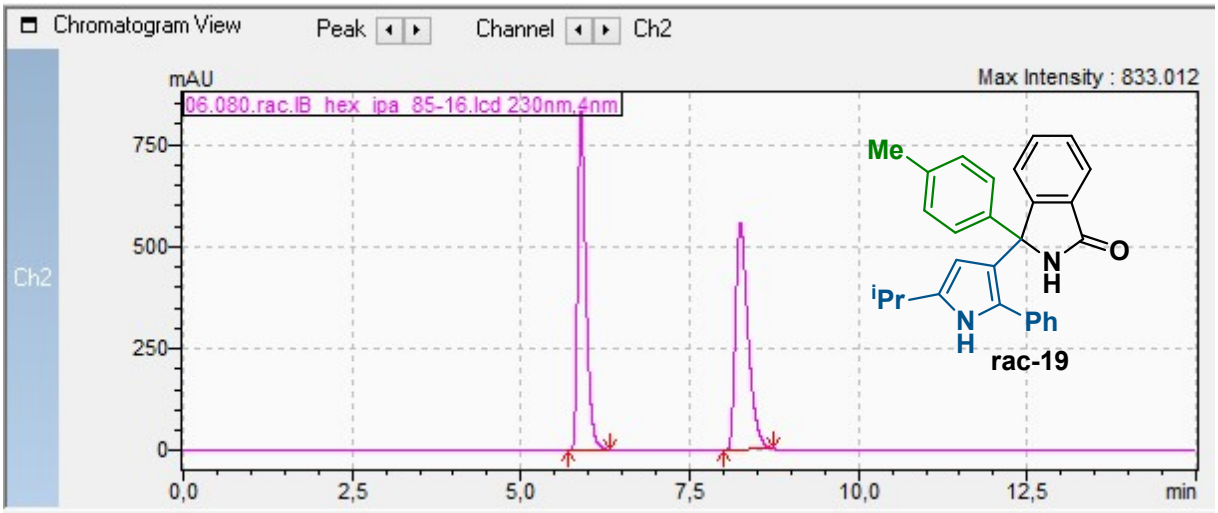
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,606	5949852	50,704	7,048	8,976	243278
2	16,263	5784601	49,296	15,152	19,000	83094
Total		11734452	100,000			326372



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

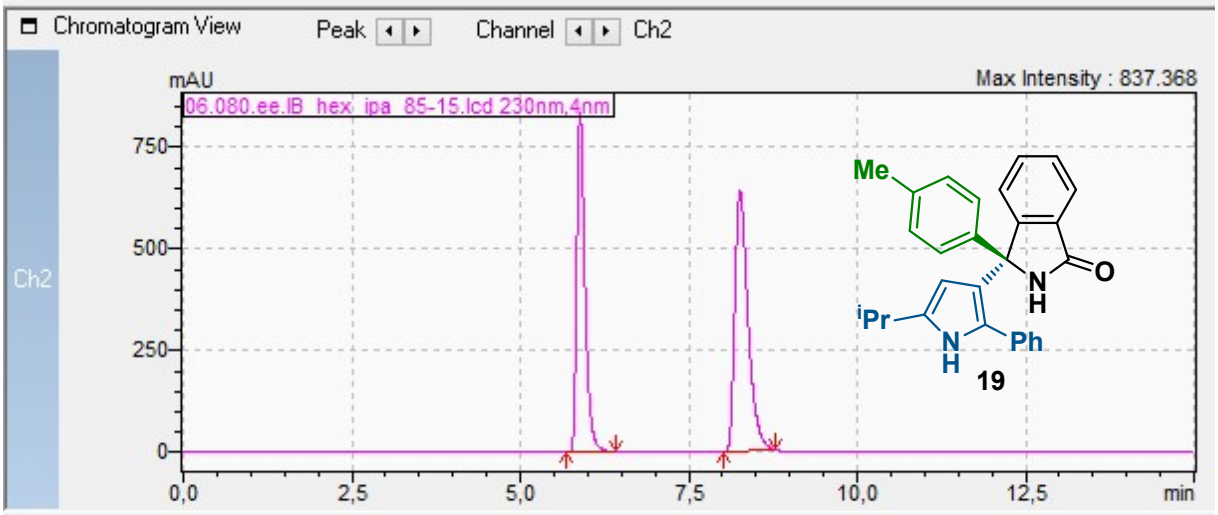
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,611	4494934	53,804	6,992	9,088	184990
2	16,281	3859418	46,196	15,272	18,936	56048
Total		8354352	100,000			241038



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

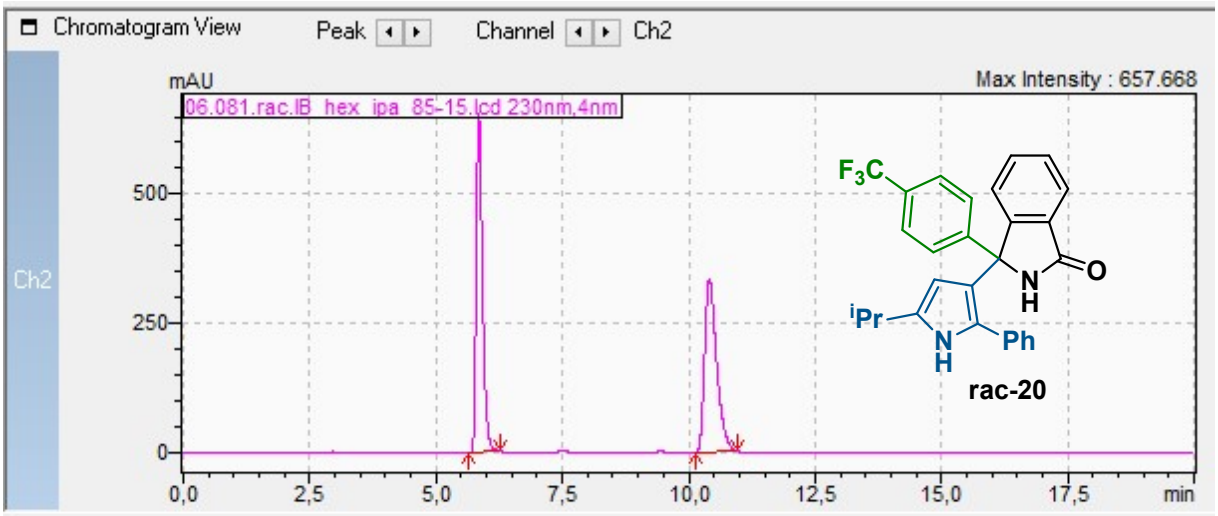
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,890	7134204	49,548	5,696	6,320	830378
2	8,251	7264299	50,452	8,000	8,744	555357
Total		14398504	100,000			1385735



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

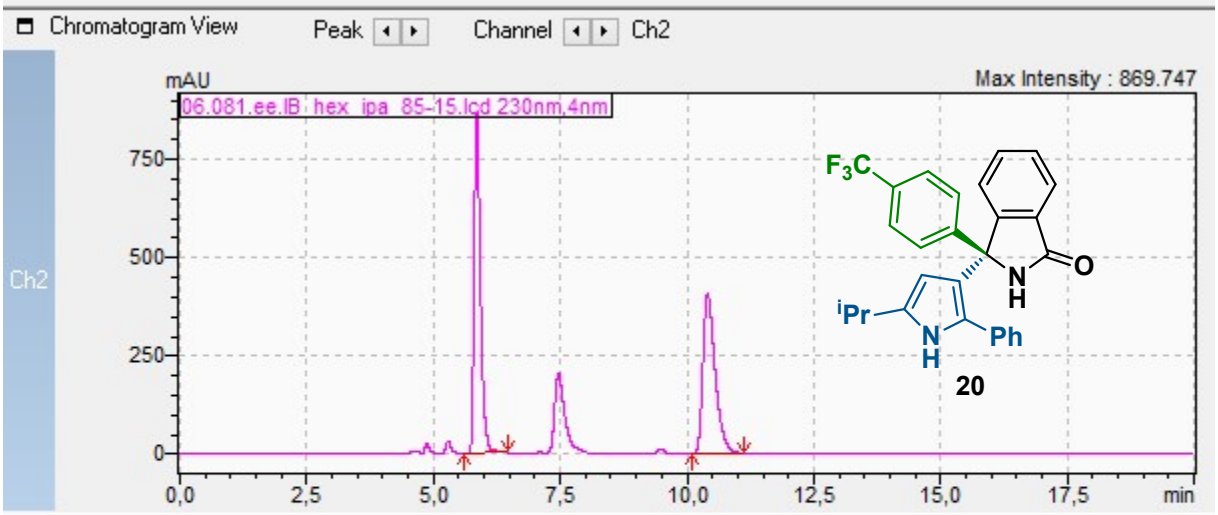
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,887	7132825	44,996	5,688	6,432	834767
2	8,263	8719238	55,004	8,008	8,784	639587
Total		15852063	100,000			1474354



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

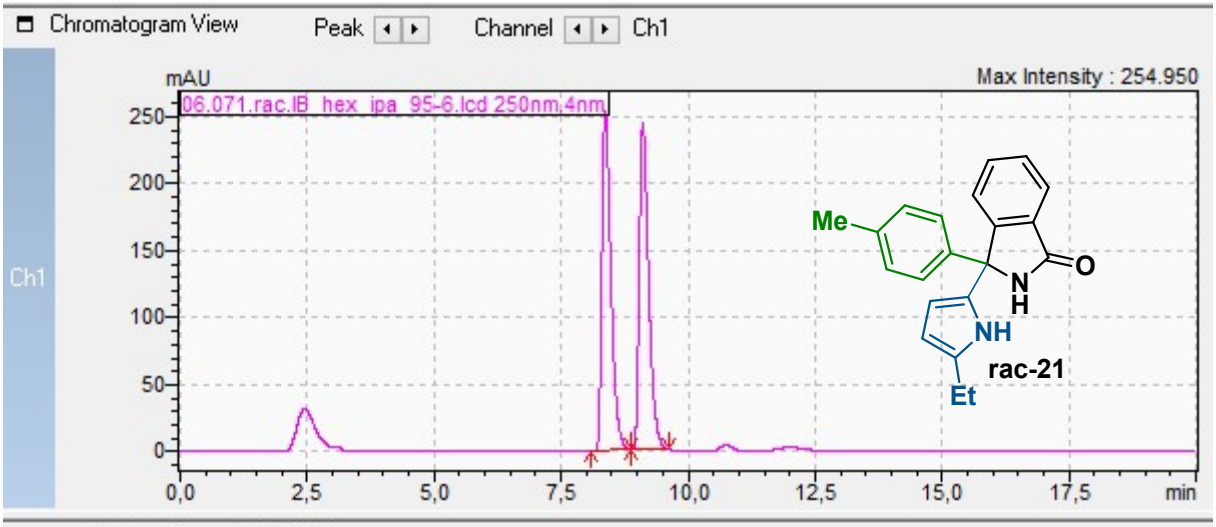
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,846	5668104	50,365	5,624	6,280	656344
2	10,410	5585885	49,635	10,120	10,960	335639
Total		11253989	100,000			991983



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

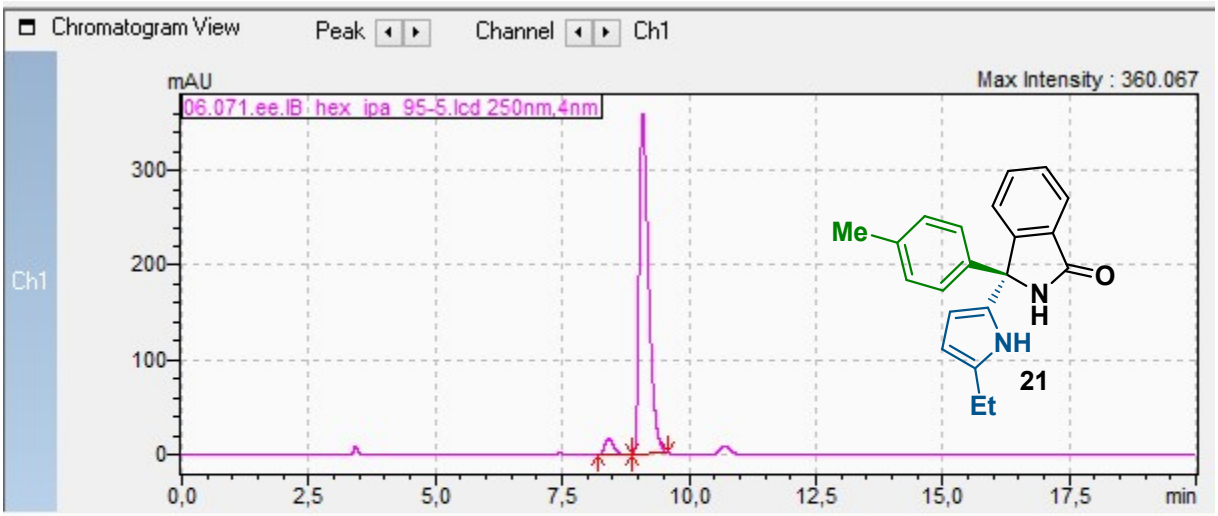
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,853	7494091	52,324	5,616	6,456	864706
2	10,409	6828383	47,676	10,080	11,128	404990
Total		14322474	100,000			1269696



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

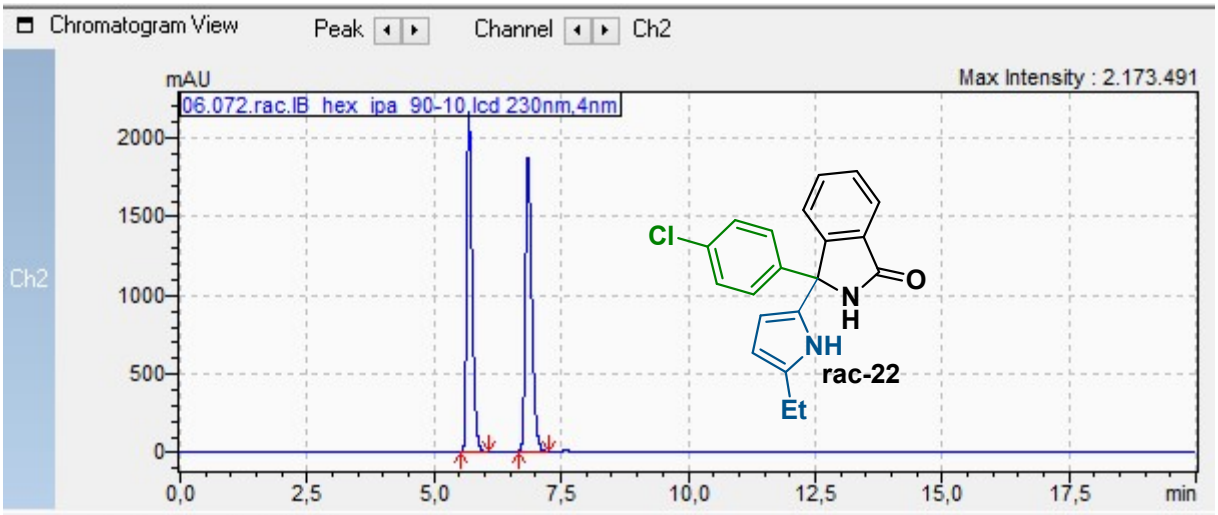
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	8,369	3131406	50,060	8,088	8,880	253774
2	9,109	3123938	49,940	8,880	9,624	242833
Total		6255344	100,000			496606



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

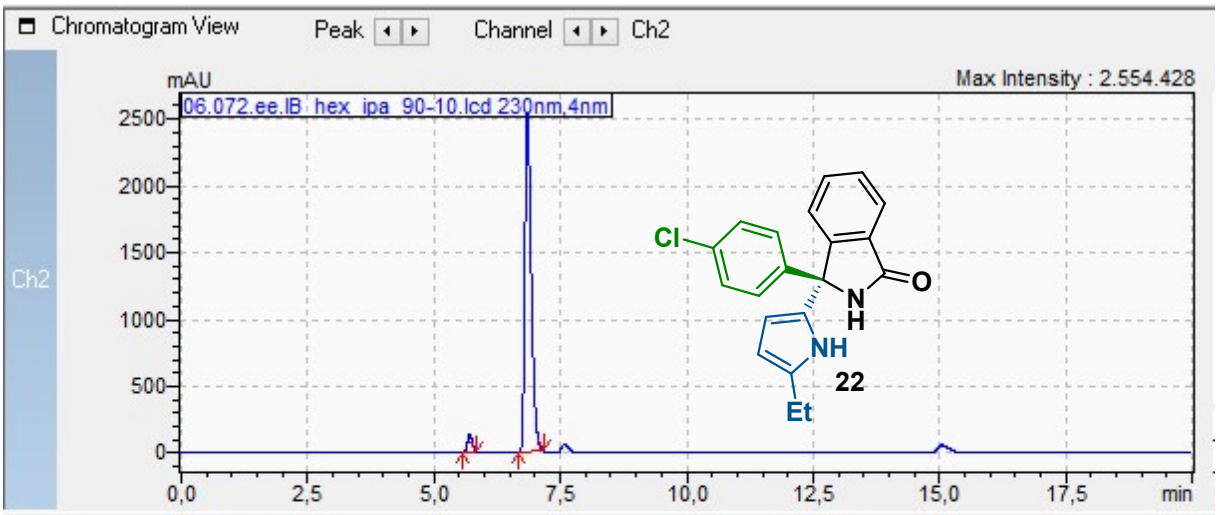
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	8,414	209460	4,327	8,208	8,880	17716
2	9,086	4631496	95,673	8,880	9,584	358729
Total		4840955	100,000			376445



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

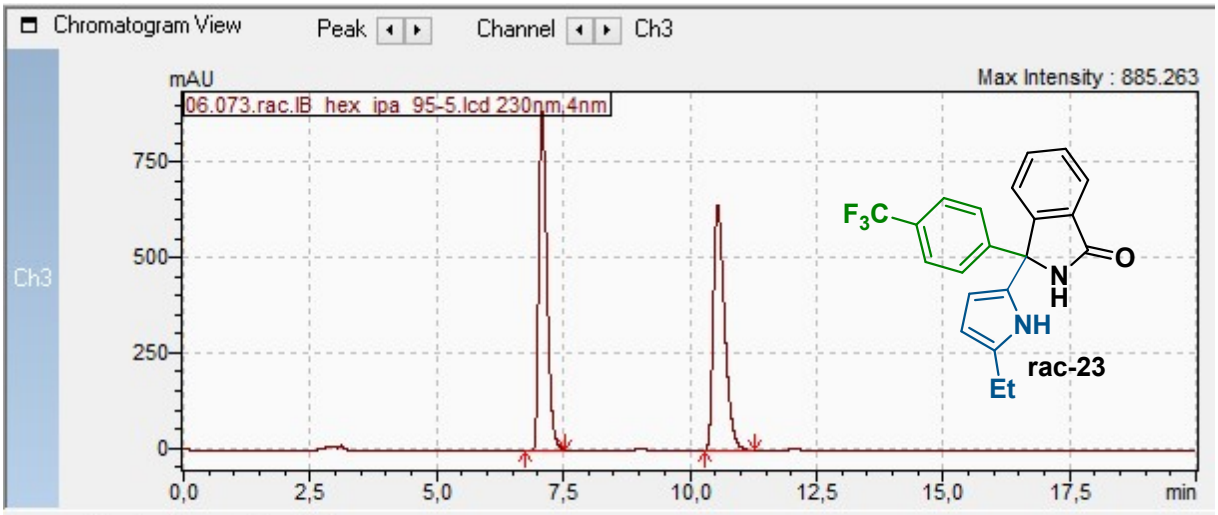
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,683	16441164	49,716	5,528	6,088	2166037
2	6,849	16629248	50,284	6,648	7,264	1868423
Total		33070412	100,000			4034460



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

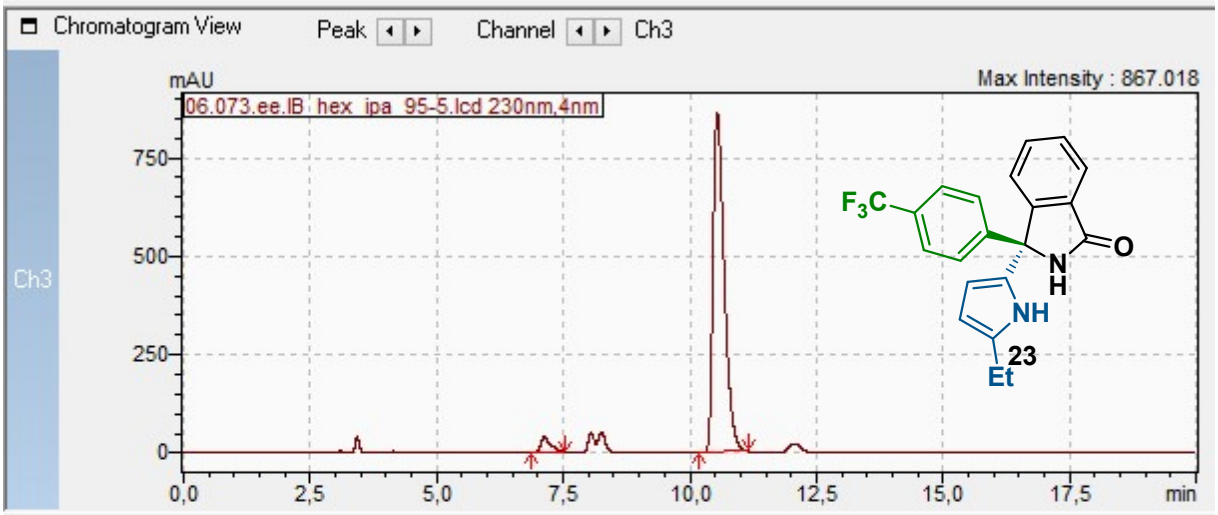
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,704	926302	3,957	5,552	5,856	133077
2	6,848	22482651	96,043	6,680	7,168	2538574
Total		23408953	100,000			2671651



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

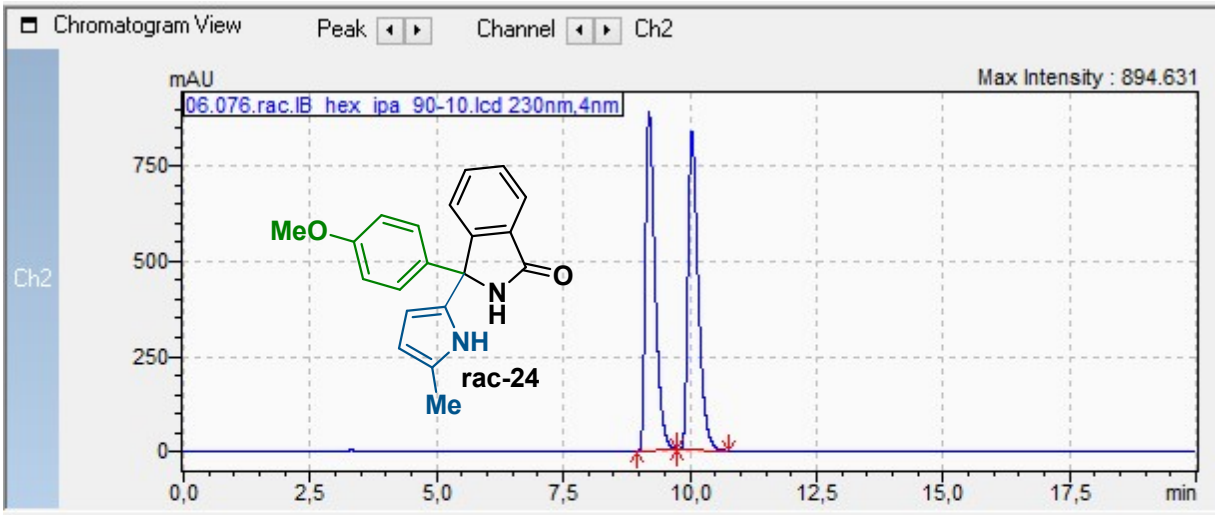
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,080	10085478	49,894	6,744	7,536	890895
2	10,552	10128513	50,106	10,296	11,280	644650
Total		20213991	100,000			1535544



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

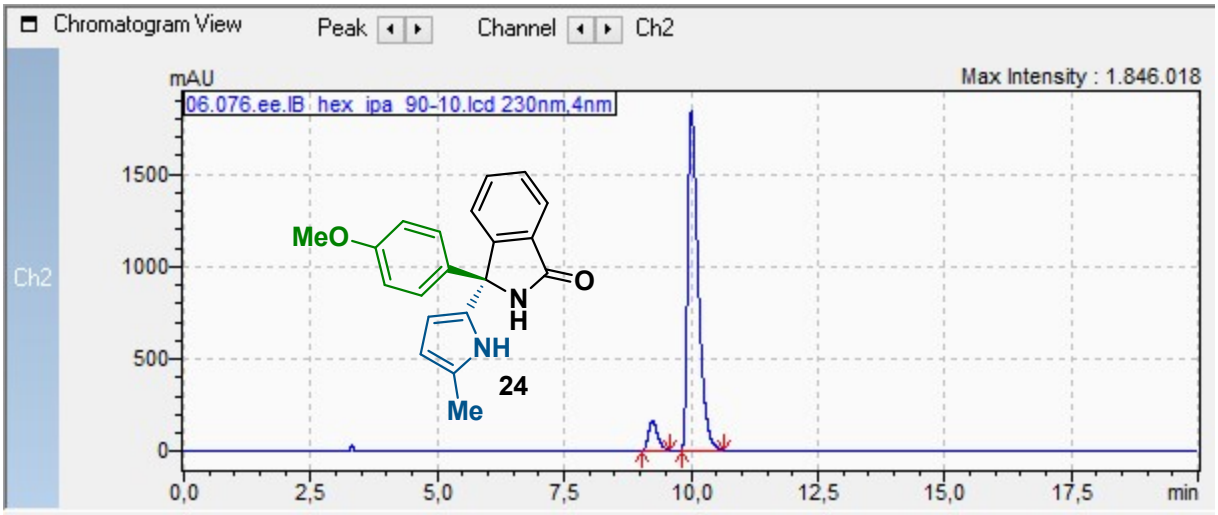
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	7,123	564629	4,084	6,856	7,552	41701
2	10,542	13261483	95,916	10,160	11,144	864342
Total		13826111	100,000			906043



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

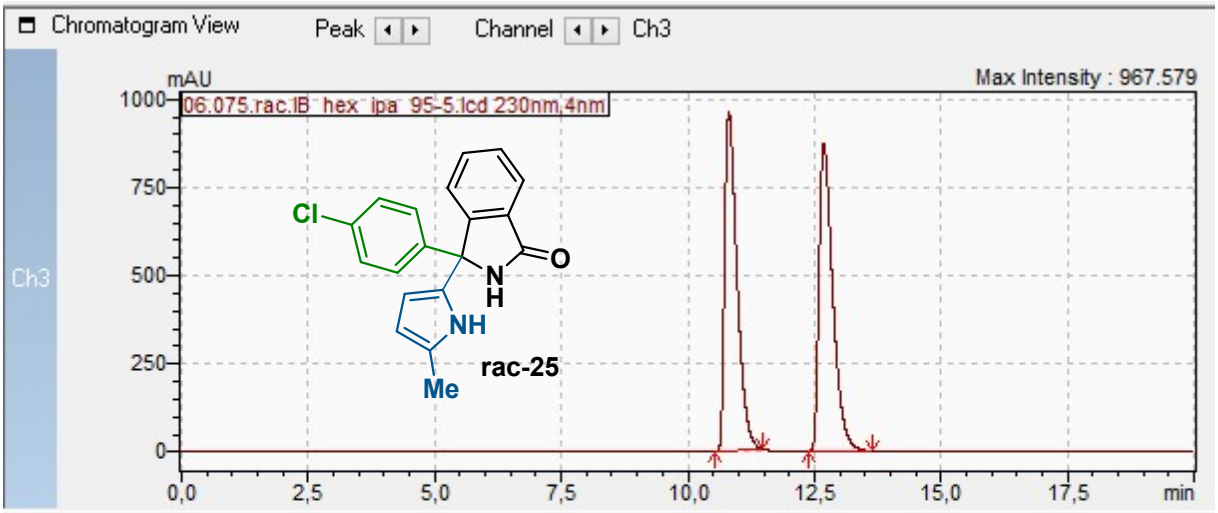
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,196	11848162	49,998	8,944	9,728	891742
2	10,043	11849063	50,002	9,760	10,752	832701
Total		23697225	100,000			1724444



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

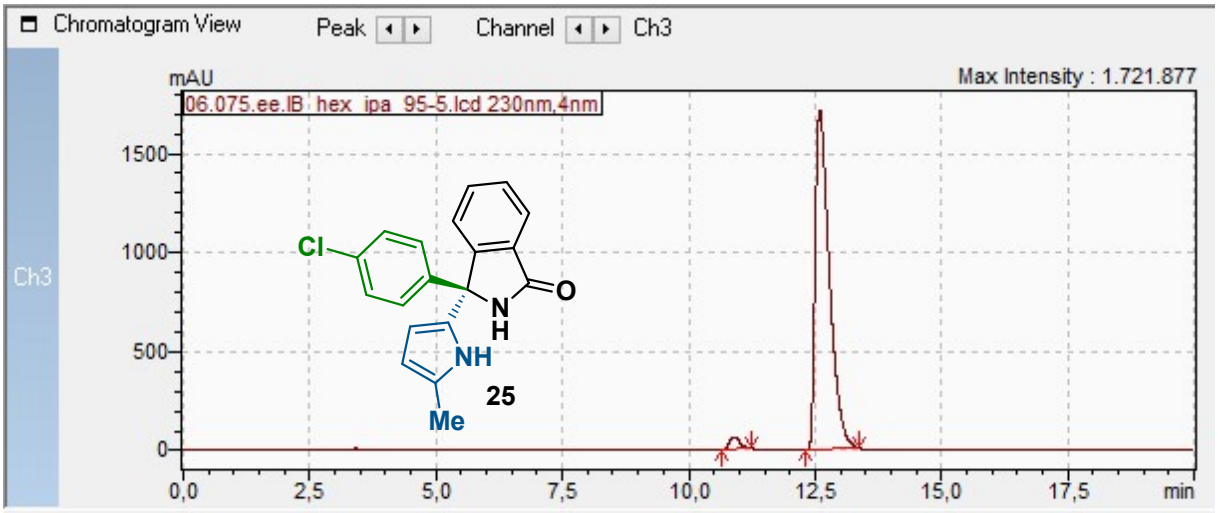
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,237	2119869	7,420	9,032	9,600	163694
2	10,011	26450625	92,580	9,816	10,648	1837128
Total		28570494	100,000			2000821



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

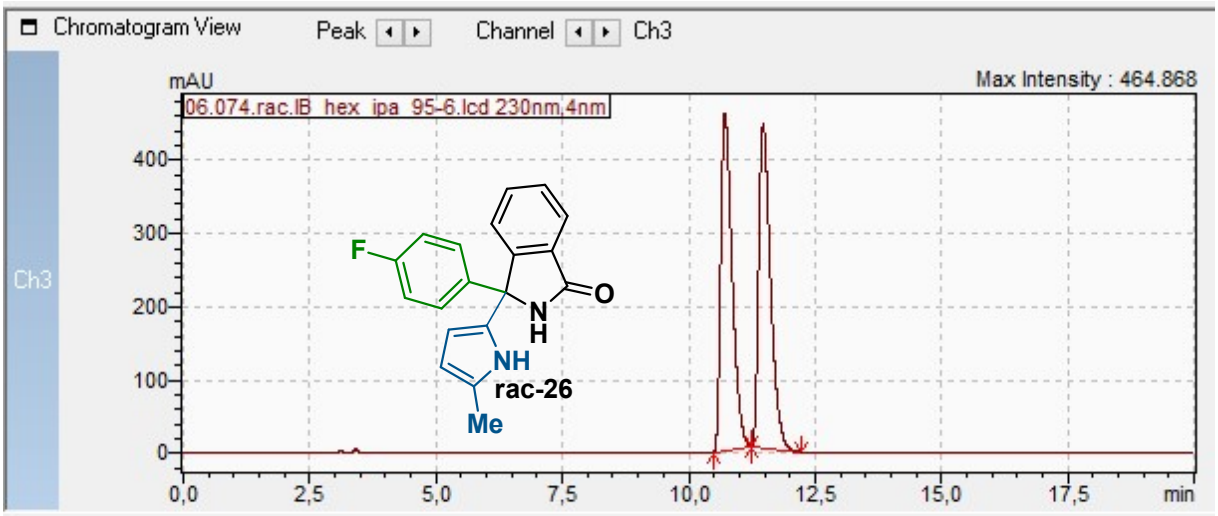
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	10,811	16376860	49,660	10,536	11,472	964173
2	12,689	16600827	50,340	12,368	13,632	871759
Total		32977687	100,000			1835932



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

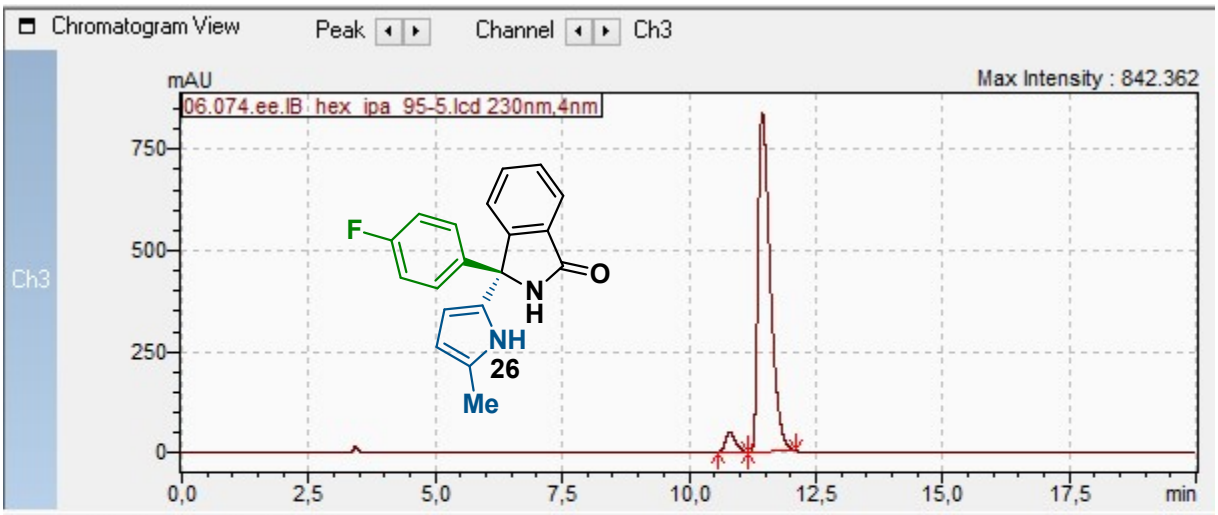
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	10,896	935366	2,707	10,632	11,232	63788
2	12,594	33619413	97,293	12,312	13,384	1717205
Total		34554779	100,000			1780993



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

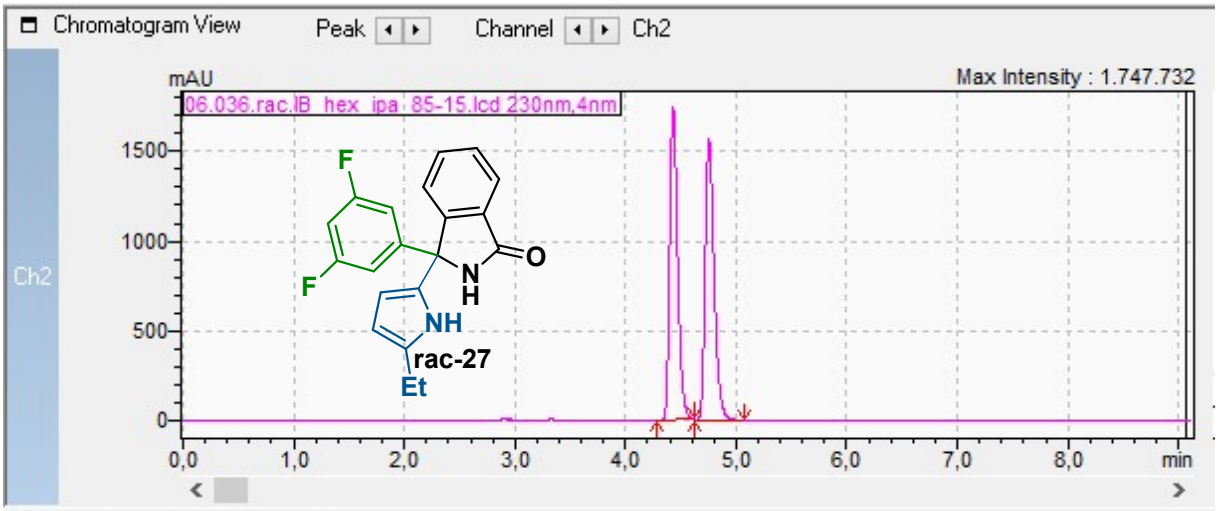
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	10,719	7220247	49,936	10,488	11,232	461269
2	11,473	7238720	50,064	11,232	12,216	442794
Total		14458967	100,000			904063



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

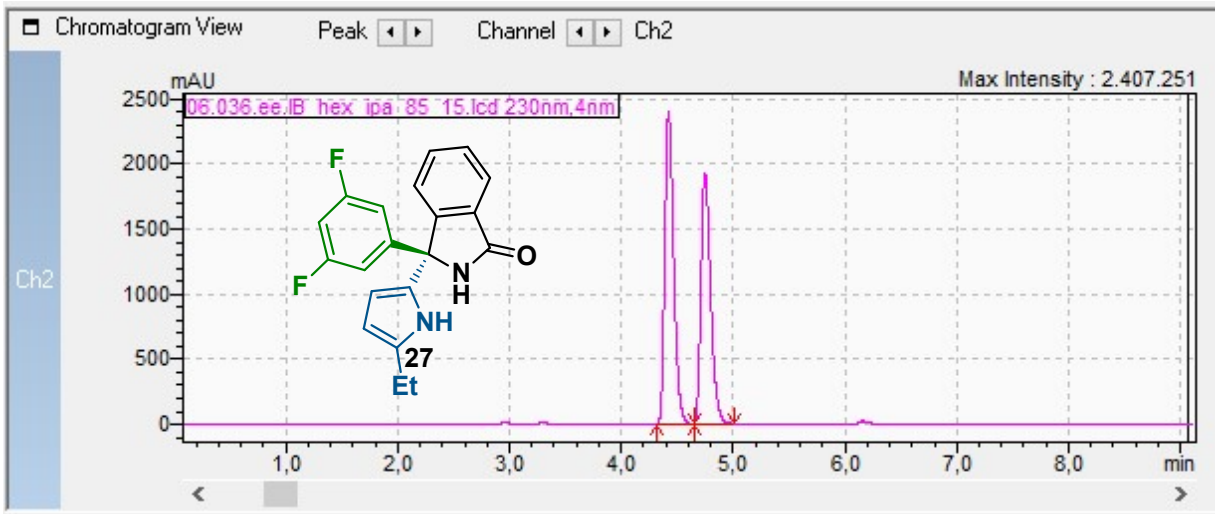
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	10,806	729167	4,946	10,560	11,176	49931
2	11,447	14012699	95,054	11,176	12,120	839198
Total		14741866	100,000			889130



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

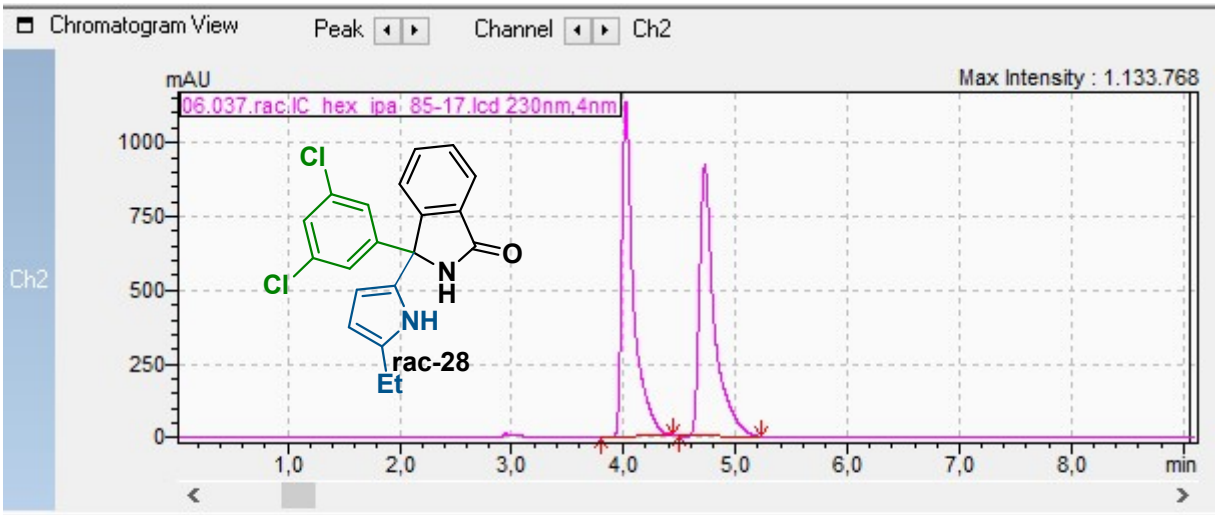
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	4,431	8728581	49,851	4,288	4,616	1737876
2	4,755	8780849	50,149	4,632	5,080	1560899
Total		17509429	100,000			3298775



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

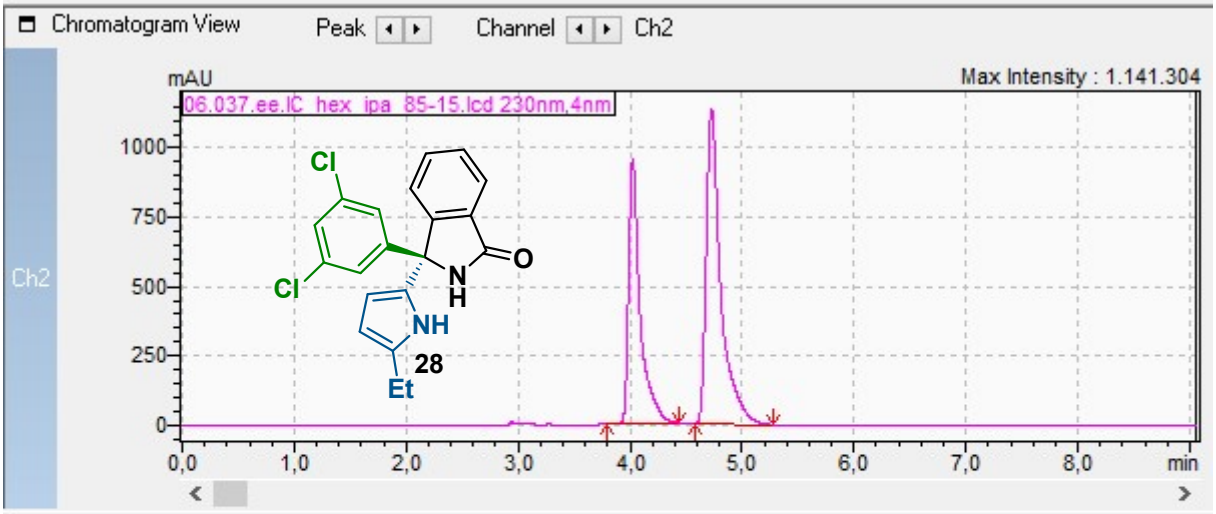
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	4,423	13218039	53,241	4,312	4,648	2391928
2	4,749	11608891	46,759	4,648	5,008	1914590
Total		24826930	100,000			4306518



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

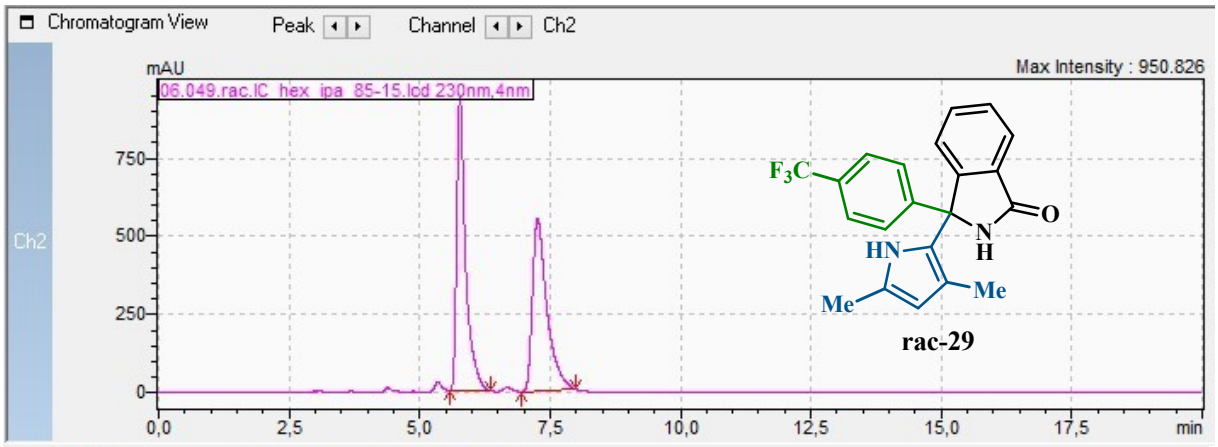
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	4,021	8270701	49,473	3,800	4,440	1126375
2	4,725	8446822	50,527	4,488	5,232	914445
Total		16717524	100,000			2040820



Results View - Peak Table

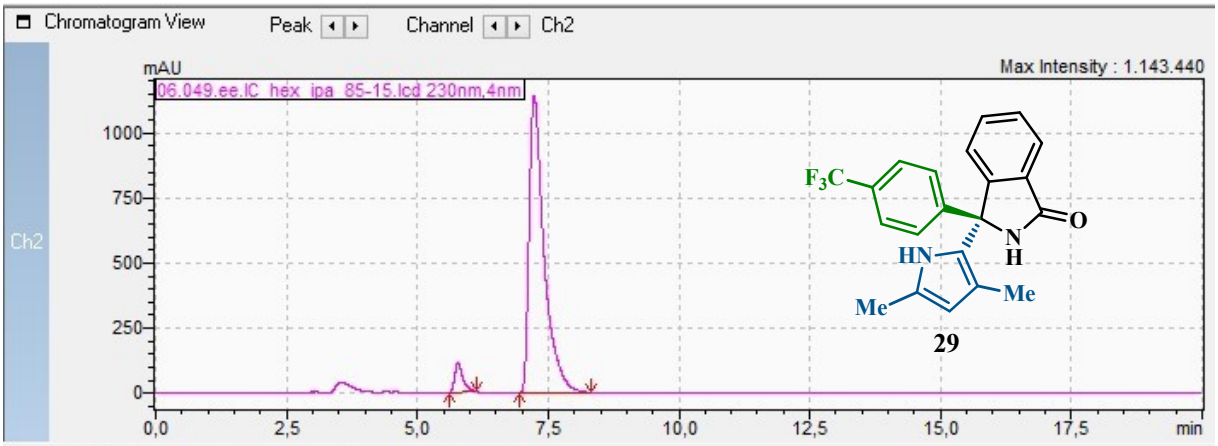
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	4,024	6801505	39,724	3,800	4,440	951483
2	4,728	10320439	60,276	4,584	5,280	1134580
Total		17121945	100,000			2086063



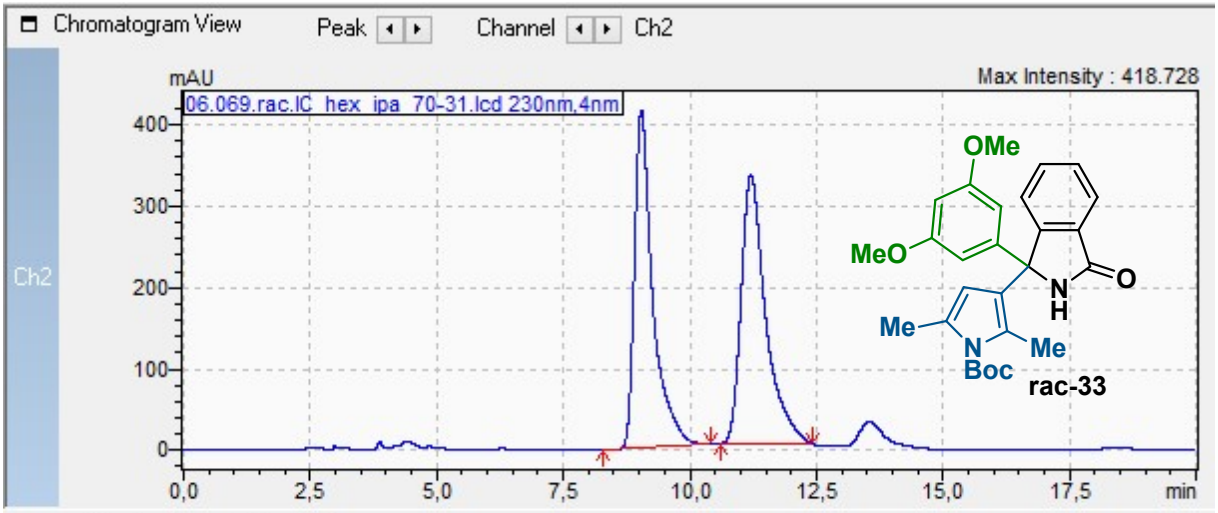
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,774	11192015	51,221	5,576	6,368	943691
2	7,264	10658429	48,779	6,936	8,008	552592
Total		21850444	100,000			1496283



Peak Table | Compound | Group | Calibration Curve

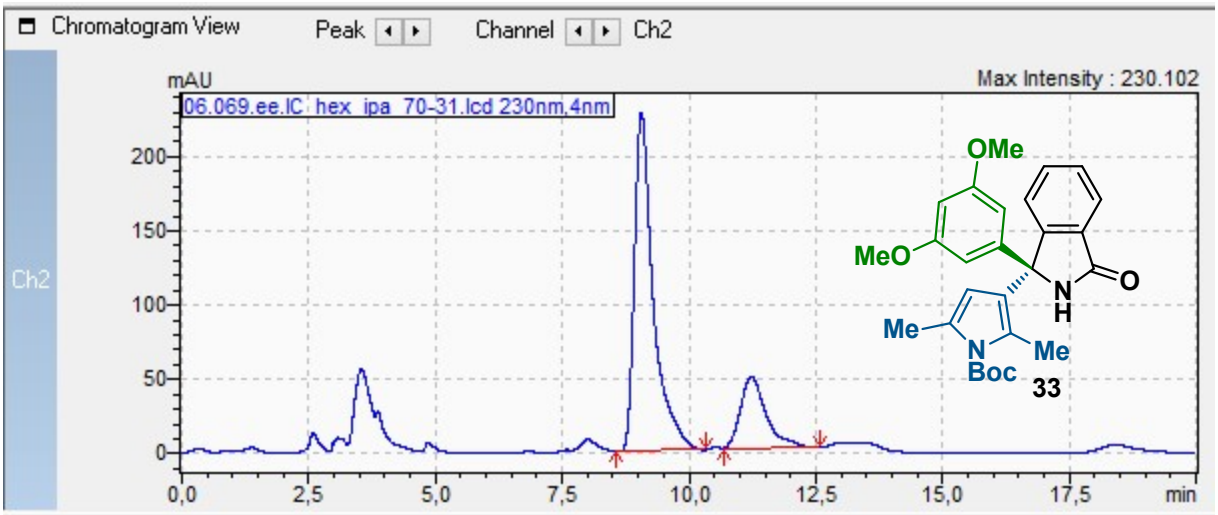
Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	5,778	1258222	5,278	5,608	6,144	113498
2	7,235	22580302	94,722	6,944	8,336	1141551
Total		23838524	100,000			1255049



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,042	10435617	48,263	8,272	10,424	415062
2	11,209	11186686	51,737	10,608	12,432	330576
Total		21622303	100,000			745638



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Area	Area%	Peak Start	Peak End	Height
1	9,064	5926283	77,692	8,576	10,352	228269
2	11,230	1701649	22,308	10,672	12,584	47938
Total		7627931	100,000			276207