Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

for

Enantioselective construction of a congested quaternary stereogenic center in isoindolinones bearing three aryl groups *via* an organocatalytic formal Betti reaction

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1. General Information

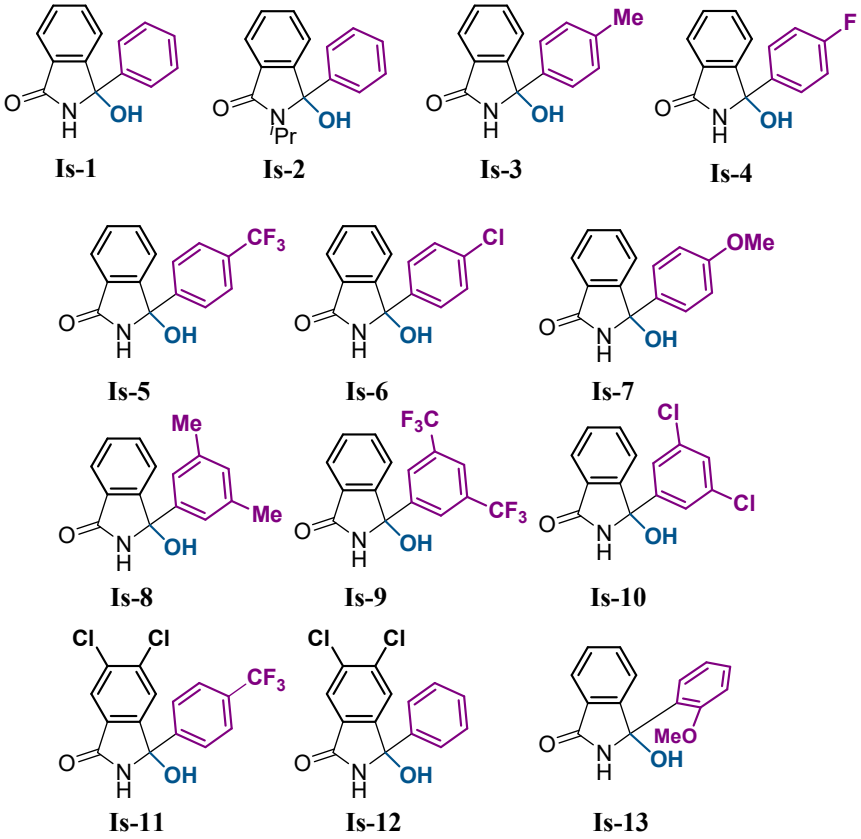
Unless otherwise indicated, solvents were used as supplied (analytical or HPLC grade) without further purification. Reagents were used directly as supplied by major chemical suppliers. Flash column chromatography was carried out using silica gel (Merck, 40−63 μm particle size). Analytical thin-layer chromatography was carried out on Merck Kieselgel 60 F254 0.25 mm precoated aluminium plates. Visualization was carried out under ultra-violet irradiation (254 nm) and by appropriate heating with ammonium molybdate solution. Ammonium molybdate solution was prepared by dissolving ammonium molybdate (5 g) and ceric sulfate (200 mg) in 5% aqueous sulfuric acid (100 mL).

All NMR spectra were acquired on Bruker Avance 600 MHz and 300 MHz spectrometers. ^{1}H NMR chemical shifts were recorded relative to $SiMe_4$ (δ = 0.00 ppm) or residual protiated solvents (DMSO: δ = 2.50 ppm, $(CD_3)_2CO$: δ = 2.05 ppm). Multiplicities were given as: *s* (singlet), *d* (doublet), *dd* (doublet of doublets), *t* (triplet), *q* (quartet) and *m* (multiplet). Coupling constants were reported as a *J* value in Hz. ^{13}C NMR chemical shifts were recorded relative to solvent resonance (DMSO: δ = 39.52 ± 0.06 ppm, $(CD_3)_2CO$: δ = 29.84 ± 0.01 ppm, 206.26 ± 0.13 ppm).

Infrared spectra were recorded on a Bruker Tensor 27 FTIR spectrometer equipped with an attenuated total reflectance attachment with internal calibration. Absorbtion maxima (ν_{max}) are reported in wavenumbers (cm^{-1}). High resolution mass spectrometry (HRMS) was performed on a 4800 Plus MALDI TOF/TOF Analyzer. Melting points were determined using an Electrothermal 9100 apparatus in open capillaries and are uncorrected. Optical rotations were measured on an Autopol IV instrument (Rudolf Research Analytical, Flanders, USA).

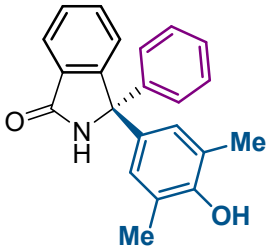
Where given, systematic compound names are those generated by ChemBioDraw Ultra 12.0 following IUPAC conventions. The starting isoindolinone alcohols (**Is-1** – **Is-13**)[1] and chiral phosphoric acids (**BA1-BA5**)[2] and (**BA6-BA7**)[3] have been synthesized according to the known procedures. Racemic standards were obtained by employing *p*-toluenesulfonic or phenylphosphonic acid (10 mol%) instead of the chiral catalyst. Enantiomeric ratios were determined using a normal phase chiral high performance liquid chromatography with PDA detector.

2. List of starting isoindolinone alcohols



3. Experimental Procedures and Analytical Data

(*R*)-3-(4-hydroxy-3,5-dimethylphenyl)-3-phenylisoindolin-1-one (1)



BA2 (7.7 mg, 0.011 mmol) was added to a suspension of **Is-1** (25 mg, 0.11 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (67 mg, 0.55 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 2 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **1** as a colorless solid. Yield: 35 mg (96%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 96.5:4.5 e.r. t_{R1} = 8.1 min (major), t_{R2} = 9.2 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.52 (s, 1H), 8.27 (s, 1H), 7.65 (d, *J* = 7.4 Hz, 1H), 7.58 (d, *J* = 3.7 Hz, 2H), 7.54 – 7.43 (m, *J* = 8.3, 7.8, 4.1 Hz, 1H), 7.36 – 7.14 (m, 5H), 6.76 (s, 2H), 2.06 (s, 6H), 2.06 (s, 6H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.7, 153.0, 150.8, 144.2, 133.9, 132.3, 131.5, 128.7, 127.8, 127.3, 127.2, 125.3, 124.3, 123.6, 70.2, 17.3.

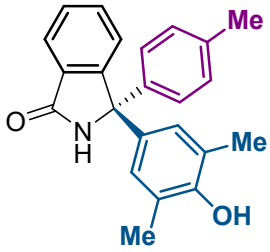
m.p. 238.2–239.4 °C

$[\alpha]_D$ = +17 ° (c 0.5, THF) for 96.5:4.5 e.r.

IR: ν = 3178, 3051, 1672, 1488, 1200, 1143, 713, 642 cm^{-1}

HRMS (ESI): found 330.1508; $C_{22}H_{20}NO_2$ $[M+H]^+$ requires 330.1494

(*R*)-3-(4-hydroxy-3,5-dimethylphenyl)-3-(*p*-tolyl)isoindolin-1-one (2)



BA2 (7.4 mg, 0.010 mmol) was added to a suspension of **Is-3** (25 mg, 0.10 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (64 mg, 0.50 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 2 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **2** as a colorless solid. Yield: 33 mg (96%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 92:8 e.r. t_{R1} = 8.2 min (major), t_{R2} = 10.5 min (minor).

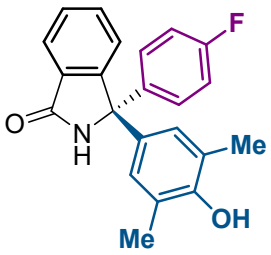
^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.50 (s, 1H), 8.28 (s, 1H), 7.67 (d, J = 7.4 Hz, 1H), 7.64 – 7.54 (m, 2H), 7.53 – 7.44 (m, 1H), 7.12 (s, 3H), 6.78 (s, 2H), 2.26 (s, 3H), 2.08 (s, 6H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.7, 153.0, 150.9, 141.3, 136.9, 134.0, 132.2, 131.53, 129.2, 128.6, 127.3, 125.3, 124.3, 123.6, 70.0, 21.0, 17.3.

m.p. 262.4–263.1 °C

IR: ν = 3201, 3069, 1677, 1488, 1181, 1135, 763, 704 cm^{-1}

HRMS (ESI): found 344.1650; $C_{23}H_{22}NO_2$ $[M+H]^+$ requires 344.1651



(*R*)-3-(4-fluorophenyl)-3-(4-hydroxy-3,5-dimethylphenyl)isoindolin-1-one (3)

BA2 (7.4 mg, 0.010 mmol) was added to a suspension of **Is-4** (25 mg, 0.10 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (64 mg, 0.50 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 2 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **3** as a colorless solid. Yield: 32 mg (91%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 96:4 e.r. t_{R1} = 11.3 min (minor), t_{R2} = 22.9 min (major).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.57 (s, 1H), 8.32 (s, 1H), 7.69 (d, J = 7.4 Hz, 1H), 7.61 (d, J = 3.3 Hz, 2H), 7.56 – 7.46 (m, 1H), 7.35 – 7.21 (m, 2H), 7.15 (t, J = 8.8 Hz, 2H), 6.79 (s, 2H), 2.09 (s, 6H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.7, 161.8 (d, $J_{C\text{-}F}$ = 244.6 Hz), 153.1, 150.70, 140.5, 140.4, 133.7, 132.4, 131.5, 129.5, 129.4, 128.8, 127.2, 125.2, 124.4, 123.7, 115.5, 115.4, 69.7, 17.3.

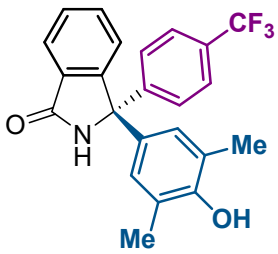
m.p. 264.7–266.2 °C

$[\alpha]_D$ = +16 ° (c 0.5, THF) for 96:4 e.r.

IR: ν = 3187, 3067, 1677, 1484, 1356, 1180, 1139, 762, 731 cm^{-1}

HRMS (ESI): found 348.1413; $C_{22}H_{19}FNO_2$ $[M+H]^+$ requires 348.1400

(*R*)-3-(4-hydroxy-3,5-dimethylphenyl)-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (4)



BA2 (6.0 mg, 0.0085 mmol) was added to a suspension of **Is-5** (25 mg, 0.085 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (52 mg, 0.43 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **4** as a colorless solid. Yield: 30 mg (88%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 15 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 97.5:2.5 e.r. t_{R1} = 6.5 min (major), t_{R2} = 9.5 min (minor).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.66 (s, 1H), 8.37 (s, 1H), 7.70 (t, J = 7.4 Hz, 3H), 7.66 – 7.61 (m, 2H), 7.55 – 7.50 (m, J = 7.9, 6.1, 2.2 Hz, 1H), 7.47 (d, J = 8.3 Hz, 2H), 6.80 (s, 2H), 2.09 (s, 6H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.8, 153.3, 150.0, 149.0, 133.1, 132.6, 131.5, 129.0, 128.5, 128.3, 128.1, 127.3, 125.8 (q, $^3J_{C\text{-}CF3}$ = 3.8 Hz), 125.5, 125.2, 124.6, 123.8, 123.7, 70.0, 17.3.

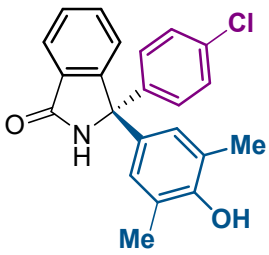
m.p. 238.9–240.6 °C

$[\alpha]_D$ = +120 ° (c 1.4, THF) for 97.5:2.5 e.r.

IR: ν = 3169, 3050, 1677, 1488, 1323, 1112, 1161, 749, 695 cm^{-1}

HRMS (ESI): found 398.1366; $C_{23}H_{19}F_3NO_2$ $[M+H]^+$ requires 398.1368

(*R*)-3-(4-chlorophenyl)-3-(4-hydroxy-3,5-dimethylphenyl)isoindolin-1-one (5)



BA2 (7.4 mg, 0.010 mmol) was added to a suspension of **Is-6** (25 mg, 0.10 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (64 mg, 0.55 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **5** as a colorless solid. Yield: 13 mg (35%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 92:8 e.r. t_{R1} = 6.9 min (major), t_{R2} = 8.6 min (minor).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.58 (s, 1H), 8.33 (s, 1H), 7.69 (d, J = 7.5 Hz, 1H), 7.64 – 7.58 (m, 2H), 7.54 – 7.47 (m, J = 7.8, 6.3, 2.0 Hz, 1H), 7.41 – 7.35 (m, 2H), 7.25 (d, J = 8.7 Hz, 2H), 6.78 (s, 2H), 2.08 (s, 6H).

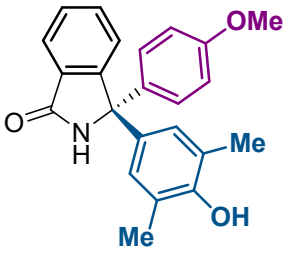
^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.7, 153.1, 150.4, 143.3, 133.4, 132.5, 132.5, 131.4, 129.3, 128.9, 128.7, 127.2, 125.2, 124.5, 123.7, 69.8, 17.3.

m.p. 222.2–223.6 °C

IR: ν = 3164, 3036, 1668, 1488, 1186, 1135, 749, 694 cm^{-1}

HRMS (ESI): found 364.1094; $C_{22}H_{19}ClNO_2$ $[M+H]^+$ requires 364.1104

(*R*)-3-(4-hydroxy-3,5-dimethylphenyl)-3-(4-methoxyphenyl)isoindolin-1-one (6)



BA2 (7.4 mg, 0.010 mmol) was added to a suspension of **Is-7** (25 mg, 0.10 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (64 mg, 0.50 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **6** as a colorless solid. Yield: 33 mg (96%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 84:16 e.r. t_{R1} = 12.8 min (major), t_{R2} = 14.9 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.48 (s, 1H), 8.27 (s, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 2H), 7.48 (t, *J* = 6.2 Hz, 1H), 7.14 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 6.79 (s, 2H), 3.69 (d, *J* = 19.7 Hz, 3H), 2.08 (s, 6H).

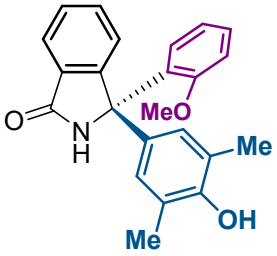
^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.7, 158.8, 152.9, 151.2, 136.1, 134.1, 132.2, 131.49, 128.6, 127.2, 125.1, 124.2, 123.5, 114.0, 69.8, 55.5, 17.3.

m.p. 229.9–230.9 °C

IR: ν = 3169, 3040, 1668, 1488, 1245, 1171, 754, 726 cm^{-1}

HRMS (ESI): found 360.1586; $C_{23}H_{22}NO_3$ $[M+H]^+$ requires 360.1600

(*R*)-3-(4-hydroxy-3,5-dimethylphenyl)-3-(2-methoxyphenyl)isoindolin-1-one (7)



BA2 (7.4 mg, 0.010 mmol) was added to a suspension of **Is-13** (25 mg, 0.10 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (64 mg, 0.50 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **7** as a colorless solid. Yield: 8 mg (23%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 66:34 e.r. t_{R1} = 11.9 min (major), t_{R2} = 14.5 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 8.94 (s, 1H), 8.11 (s, 1H), 7.69 (d, J = 7.4 Hz, 1H), 7.63 – 7.53 (m, 2H), 7.55 – 7.42 (m, 1H), 7.40 – 7.25 (m, 1H), 7.18 (dd, J = 7.7, 1.5 Hz, 1H), 7.04 (d, J = 7.6 Hz, 1H), 6.89 (t, J = 7.1 Hz, 1H), 6.70 (s, 2H), 3.53 (s, 3H), 2.06 (s, 6H).

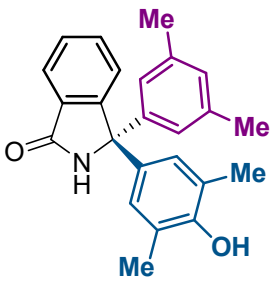
^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.8, 157.9, 152.4, 150.7, 134.4, 132.0, 131.4, 130.65, 129.9, 128.5, 127.7, 125.9, 125.2, 124.2, 123.6, 120.3, 113.1, 69.0, 56.0, 17.3.

m.p. 235.5–237.4 °C

IR: ν = 3247, 3049, 1677, 1479, 1186, 1139, 749, 694 cm^{-1}

HRMS (ESI): found 360.1596; $C_{23}H_{22}NO_3$ $[M+H]^+$ requires 360.1600

(*R*)-3-(3,5-dimethylphenyl)-3-(4-hydroxy-3,5-dimethylphenyl)isoindolin-1-one (8)



BA2 (7.4 mg, 0.010 mmol) was added to a suspension of **Is-8** (25 mg, 0.10 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (64 mg, 0.50 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **8** as a colorless solid. Yield: 34 mg (94%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 90:10 e.r. t_{R1} = 7.0 min (major), t_{R2} = 8.2 min (minor).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.45 (s, 1H), 8.28 (s, 1H), 7.66 (d, J = 7.5 Hz, 1H), 7.60 (d, J = 3.8 Hz, 2H), 7.53 – 7.43 (m, 1H), 6.89 (s, 1H), 6.86 (s, 2H), 6.77 (s, 2H), 2.19 (s, 6H), 2.08 (s, 6H).

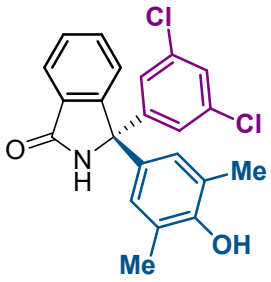
^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.7, 152.9, 150.7, 144.2, 137.6, 134.1, 132.2, 131.5, 129.2, 128.6, 127.3, 125.3, 125.0, 124.3, 123.6, 70.2, 21.5, 17.3.

m.p. 285.4–286.3 °C

IR: ν = 3178, 3040, 1668, 1493, 1195, 1135, 722, 607 cm^{-1}

HRMS (ESI): found 358.1802; $C_{24}H_{24}NO_2$ $[M+H]^+$ requires 358.1807

(*S*)-3-(3,5-dichlorophenyl)-3-(4-hydroxy-3,5-dimethylphenyl)isoindolin-1-one (9)



BA2 (6.0 mg, 0.0085 mmol) was added to a suspension of **Is-10** (25 mg, 0.085 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (52 mg, 0.43 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 5 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **9** as a colorless solid. Yield: 28 mg (84%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 96:4 e.r. t_{R1} = 7.3 min (minor), t_{R2} = 10.5 min (major).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.63 (s, 1H), 8.39 (s, 1H), 7.74 (d, J = 7.7 Hz, 1H), 7.71 (d, J = 7.5 Hz, 1H), 7.66 (t, J = 7.0 Hz, 1H), 7.57 (t, J = 1.8 Hz, 1H), 7.54 (t, J = 7.4 Hz, 1H), 7.24 (d, J = 1.9 Hz, 2H), 6.79 (s, 2H), 2.10 (s, 6H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.6, 153.4, 149.3, 148.5, 134.5, 132.8, 132.6, 131.4, 129.3, 127.8, 127.1, 126.1, 125.3, 124.7, 123.9, 69.6, 17.3.

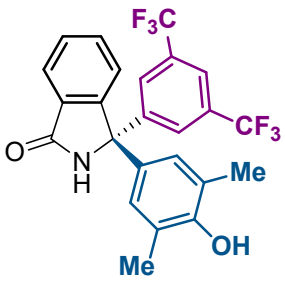
m.p. 312.6–313.2 °C

$[\alpha]_D$ = +24 ° (c 0.5, THF) for 96:4 e.r.

IR: ν = 3178, 3082, 1668, 1488, 1195, 1016, 791, 704 cm^{-1}

HRMS (ESI): found 398.0720; $C_{22}H_{18}Cl_2NO_2$ $[M+H]^+$ requires 398.0715

(*S*)-3-(3,5-bis(trifluoromethyl)phenyl)-3-(4-hydroxy-3,5-dimethylphenyl)isoindolin-1-one (10)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (43 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **10** as a colorless solid. Yield: 24 mg (75%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 10 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 98:2 e.r. t_{R1} = 5.7 min (major), t_{R2} = 8.4 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.76 (s, 1H), 8.44 (s, 1H), 8.12 (s, 1H), 7.85 (d, J = 9.1 Hz, 2H), 7.82 – 7.63 (m, 3H), 7.56 (t, J = 7.0 Hz, 1H), 6.79 (s, 2H), 2.10 (s, J = 3.1 Hz, 6H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.6, 153.5, 149.2, 147.5, 133.0, 132.5, 131.3, 131.0, 130.6, 129.4, 127.8 (q, $^3J_{C\text{-}CF3}$ = 3.8 Hz), 127.1, 125.4, 125.1, 124.9, 124.0, 121.8, 69.7, 17.2.

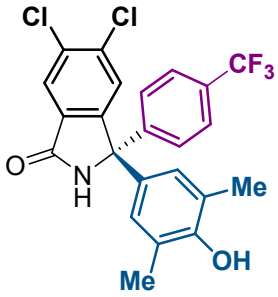
m.p. 279.3–280.4 °C

$[\alpha]_D$ = +51 ° (c 1.1, THF) for 98:2 e.r.

IR: ν = 3187, 3049, 1681, 1484, 1369, 1278, 1171, 1121, 1016, 704, 676 cm^{-1}

HRMS (ESI): found 466.1244; $C_{24}H_{18}F_6NO_2$ $[M+H]^+$ requires 466.1242

(*R*)-5,6-dichloro-3-(4-hydroxy-3,5-dimethylphenyl)-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (11)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-11** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (43 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 5 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **11** as a colorless solid. Yield: 31 mg (94%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack OD, 10 % IPA in hexane, flow rate 1.0 mL/min, 230 nm), 92:8 e.r. t_{R1} = 6.6 min (major), t_{R2} = 12.2 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.91 (s, 1H), 8.42 (s, 1H), 8.04 (s, 1H), 7.92 (s, 1H), 7.72 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.2 Hz, 2H), 6.82 (s, 2H), 2.11 (s, 6H).

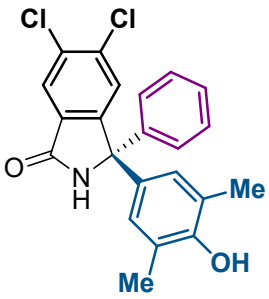
^{13}C NMR (75 MHz, DMSO) (δ/ppm): 166.4, 153.5, 150.0, 147.8, 135.6, 132.6, 132.1, 132.0, 128.9, 128.5, 128.4, 127.4, 127.3, 125.9 (q, $^3J_{C\text{-}CF3}$ = 3.8 Hz), 125.7, 124.7, 69.9, 17.2.

m.p. 287.0–287.7 °C

IR: ν = 3205, 3004, 1681, 1484, 1319, 1278, 1126, 1076, 851, 704 cm^{-1}

HRMS (ESI): found 466.0568; $C_{23}H_{17}Cl_2F_3NO_2$ $[M+H]^+$ requires 466.0588

(*R*)-5,6-dichloro-3-(4-hydroxy-3,5-dimethylphenyl)-3-phenylisoindolin-1-one (12)



BA2 (6.0 mg, 0.0085 mmol) was added to a suspension of **Is-12** (25 mg, 0.085 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (52 mg, 0.45 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 3 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **12** as a colorless solid. Yield: 25 mg (73%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 25 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 95:5 e.r. t_{R1} = 6.7 min (minor), t_{R2} = 11.5 min (major).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.81 (s, 1H), 8.37 (s, 1H), 7.95 (s, 1H), 7.88 (s, 1H), 7.36 – 7.25 (m, 5H), 6.79 (s, 2H), 2.09 (s, 6H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 166.5, 153.3, 150.8, 143.1, 135.4, 132.8, 132.3, 132.1, 128.9, 128.1, 127.4, 127.3, 125.5, 124.5, 70.1, 17.2.

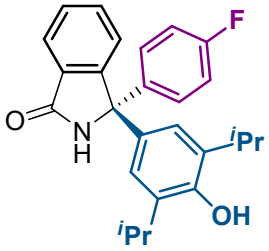
m.p. 264.6–266.1 °C

$[\alpha]_D$ = +23 ° (c 1.1, THF) for 95:5 e.r.

IR: ν = 3182, 3059, 1673, 1484, 1190, 1153, 607 cm^{-1}

HRMS (ESI): found 398.0724; $C_{22}H_{18}Cl_2NO_2$ $[M+H]^+$ requires 398.0715

(*R*)-3-(4-fluorophenyl)-3-(4-hydroxy-3,5-diisopropylphenyl)isoindolin-1-one (13)



BA2 (7.4 mg, 0.010 mmol) was added to a suspension of **Is-4** (25 mg, 0.10 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-diisopropylphenol (94 µL, 0.50 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **13** as a colorless solid. Yield: 36 mg (85%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 97:3 e.r. t_{R1} = 6.3 min (minor), t_{R2} = 13.0 min (major).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.66 (s, 1H), 8.16 (s, 1H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.62 (t, *J* = 8.8, 4.4 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.51 (t, *J* = 7.4, 3.8 Hz, 1H), 7.28 – 7.21 (m, *J* = 15.7, 7.9, 4.7 Hz, 2H), 7.18 – 7.11 (m, 2H), 6.87 (s, 2H), 3.29 – 3.18 (m, *J* = 6.9 Hz, 2H), 1.04 (t, *J* = 7.3 Hz, 12H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.8, 161.7 (d, $J_{C\text{-}F}$ = 243.1 Hz), 150.8, 150.6, 140.6, 135.3, 134.0, 132.3, 131.5, 129.4, 129.3, 128.8, 125.1, 123.7, 122.4, 115.5, 115.3, 70.1, 26.7, 23.3, 23.3.

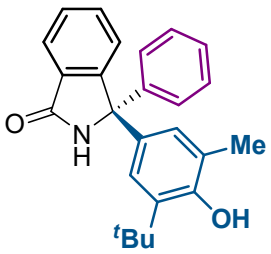
m.p. 211.9–212.4 °C

$[\alpha]_D$ = +67 ° (c 1.7, THF) for 97:3 e.r.

IR: *v* = 3178, 2957, 1673, 1466, 1341, 1204, 1153, 731, 704 cm^{-1}

HRMS (ESI): found 404.2014; $C_{26}H_{27}FNO_2$ $[M+H]^+$ requires 404.2026

(*R*)-3-(3-(*tert*-butyl)-4-hydroxy-5-methylphenyl)-3-phenylisoindolin-1-one (14)



BA2 (7.7 mg, 0.011 mmol) was added to a suspension of **Is-1** (25 mg, 0.11 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-(*tert*-butyl)-6-methylphenol (90 mg, 0.55 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 6 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **14** as a colorless solid. Yield: 38 mg (92%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 95:5 e.r. t_{R1} = 9.7 min (minor), t_{R2} = 16.9 min (major).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.59 (s, 1H), 8.17 (s, 1H), 7.69 (d, J = 7.5 Hz, 1H), 7.65 – 7.54 (m, 2H), 7.50 (t, J = 7.3 Hz, 1H), 7.36 – 7.28 (m, 2H), 7.29 – 7.24 (m, 3H), 6.93 (s, 1H), 6.80 (s, 1H), 2.10 (s, 3H), 1.26 (s, 9H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.8, 153.4, 150.9, 144.3, 136.5, 133.6, 132.3, 131.6, 128.7, 127.7, 127.6, 127.3, 125.2, 125.2, 123.6, 123.6, 70.5, 35.0, 30.0, 17.7.

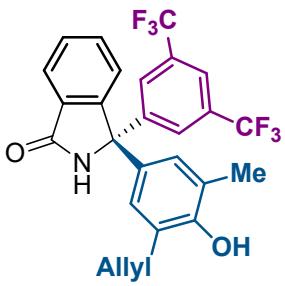
m.p. 276.1–277.8 °C

$[\alpha]_D$ = +77 ° (c 1.8, THF) for 95:5 e.r.

IR: ν = 3201, 2953, 1673, 1470, 1158, 1135, 740, 694 cm^{-1}

HRMS (ESI): found 371.1950; $C_{25}H_{26}NO_2$ $[M+H]^+$ requires 371.1964

(*S*)-3-(3-allyl-4-hydroxy-5-methylphenyl)-3-(3,5-bis(trifluoromethyl)phenyl)isoindolin-1-one (15)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-allyl-6-methylphenol (50 µL, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **15** as a colorless solid. Yield: 29 mg (85%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 5 % IPA in hexane, flow rate 1.0 mL/min, 220 nm), 98:2 e.r. t_{R1} = 8.1 min (major), t_{R2} = 13.2 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.76 (s, 1H), 8.50 (s, 1H), 8.12 (s, 1H), 7.84 (s, 2H), 7.79 – 7.64 (m, 3H), 7.56 (t, J = 6.5 Hz, 1H), 6.81 (s, J = 2.1 Hz, 1H), 6.78 (s, J = 2.3 Hz, 1H), 6.05 – 5.68 (m, 1H), 5.04 – 4.78 (m, 2H), 3.28 (d, J = 5.4 Hz, 2H), 2.11 (s, 3H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.6, 153.0, 149.3, 147.5, 137.3, 133.0, 132.6, 131.3, 130.8 (q, $^2J_{C\text{-}CF3}$ = 33.2 Hz), 129.5, 127.9 (q, $^3J_{C\text{-}CF3}$ = 3.8 Hz), 127.5, 127.1, 126.7, 125.2, 125.1, 124.5, 124.1, 122.7, 122.3, 115.7, 69.7, 34.5, 17.3.

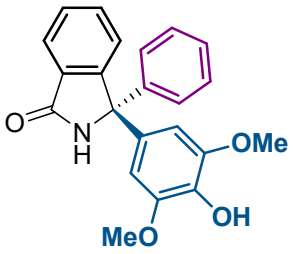
m.p. 249.6–250.3 °C

$[\alpha]_D$ = +36 ° (c 1.3, THF) for 98:2 e.r.

IR: ν = 3233, 3054, 1677, 1475, 1365, 1278, 1176, 1121, 892, 699, 630 cm^{-1}

HRMS (ESI): found 492.1401; $C_{26}H_{20}F_6NO_2$ $[M+H]^+$ requires 492.1398

(*R*)-3-(4-hydroxy-3,5-dimethoxyphenyl)-3-phenylisoindolin-1-one (16)



BA2 (7.7 mg, 0.011 mmol) was added to a suspension of **Is-1** (25 mg, 0.11 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethoxylphenol (85 mg, 0.55 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 5 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **16** as a colorless solid. Yield: 33 mg (84%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 40 % IPA in hexane, flow rate 1.0 mL/min, 230 nm), 89:11 e.r. t_{R1} = 18.1 min (major), t_{R2} = 36.5 min (minor).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.70 (s, 1H), 8.53 (s, 1H), 7.75 (dd, *J* = 13.6, 7.6 Hz, 2H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.32 (t, *J* = 7.1 Hz, 1H), 7.29 (d, *J* = 7.5 Hz, 2H), 6.58 (s, 2H), 3.69 (s, 6H).

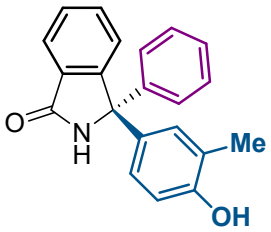
^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.9, 150.3, 148.0, 144.2, 135.7, 133.2, 132.3, 131.50, 128.9, 128.8, 127.9, 127.2, 125.3, 123.8, 105.7, 70.6, 56.5.

m.p. 265.3–266.9 °C

IR: ν = 3067, 2962, 1691, 1461, 1103, 1021, 800, 731 cm^{-1}

HRMS (ESI): found 362.1382; $C_{22}H_{20}NO_4$ $[M+H]^+$ requires 362.1392

(*R*)-3-(4-hydroxy-3-methylphenyl)-3-phenylisoindolin-1-one (17)



BA2 (7.7 mg, 0.011 mmol) was added to a suspension of **Is-1** (25 mg, 0.11 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-methylphenol (55 mg, 0.55 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 2 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **17** as a colorless solid. Yield: 34 mg (98%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 40 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 88:12 e.r. t_{R1} = 7.7 min (major), t_{R2} = 11.8 min (minor).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.56 (s, 1H), 9.36 (s, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.64 – 7.56 (m, J = 14.5, 4.4 Hz, 2H), 7.54 – 7.47 (m, 1H), 7.32 (t, J = 7.3 Hz, 2H), 7.30 – 7.24 (m, J = 6.7, 1.3 Hz, 3H), 6.93 (d, J = 2.1 Hz, 1H), 6.84 (dd, J = 8.4, 2.4 Hz, 1H), 6.70 (d, J = 8.4 Hz, 1H), 2.04 (s, 3H).

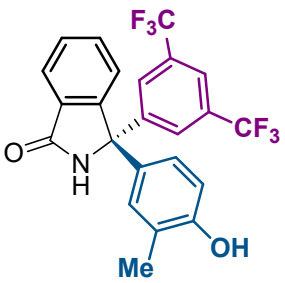
^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.8, 155.2, 150.8, 144.2, 133.6, 132.3, 131.5, 129.7, 128.7, 128.7, 127.8, 127.3, 125.9, 125.2, 124.1, 123.6, 114.4, 70.2, 16.6.

m.p. 240.3–240.9 °C

IR: ν = 3174, 3040, 1663, 1488, 1273, 1112, 754, 694 cm^{-1}

HRMS (ESI): found 316.1342; $C_{21}H_{18}NO_2$ $[M+H]^+$ requires 316.1338

(*S*)-3-(3,5-bis(trifluoromethyl)phenyl)-3-(4-hydroxy-3-methylphenyl)isoindolin-1-one (18)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-methylphenol (36 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 1 day at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **18** as a colorless solid. Yield: 28 mg (87%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 10 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 99:1 e.r. t_{R1} = 5.3 min (major), t_{R2} = 9.8 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.79 (s, 1H), 9.52 (s, 1H), 8.12 (s, 1H), 7.89 (s, 2H), 7.81 – 7.71 (m, 2H), 7.69 (t, J = 7.4 Hz, 1H), 7.57 (t, J = 7.1 Hz, 1H), 6.94 (d, J = 2.0 Hz, 1H), 6.85 (d, J = 6.0 Hz, 1H), 6.75 (d, J = 8.4 Hz, 1H), 2.06 (s, 3H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.6, 155.7, 149.2, 147.5, 133.0, 132.3, 131.4, 131.0, 130.6, 129.4, 127.8 (q, $^3J_{C\text{-}CF3}$ = 3.2 Hz), 126.0, 125.1, 124.6, 124.1, 115.0, 69.7, 16.5.

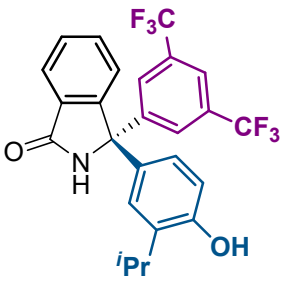
m.p. 221.6–222.1 °C

$[\alpha]_D$ = +66 ° (c 1.25, THF) for 99:1 e.r.

IR: ν = 3182, 3045, 1668, 1461, 1365, 1282, 1176, 1116, 906, 699, 671 cm^{-1}

HRMS (ESI): found 452.1093; $C_{23}H_{16}F_6NO_2$ $[M+H]^+$ requires 42.1085

(*S*)-3-(3,5-bis(trifluoromethyl)phenyl)-3-(4-hydroxy-3-isopropylphenyl)isoindolin-1-one (19)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-isopropylphenol (48 µL, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 3 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **19** as a colorless solid. Yield: 30 mg (90%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack OD, 8 % IPA in hexane, flow rate 1.0 mL/min, 220 nm), 98.5:1.5 e.r. t_{R1} = 6.3 min (major), t_{R2} = 9.9 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.80 (s, 1H), 9.56 (s, 1H), 8.12 (s, 1H), 7.84 (s, 2H), 7.81 – 7.64 (m, 3H), 7.62 – 7.51 (m, 1H), 6.96 (d, J = 2.3 Hz, 1H), 6.83 (dd, J = 8.4, 2.4 Hz, 1H), 6.75 (d, J = 8.4 Hz, 1H), 3.24 – 3.07 (m, 1H), 1.05 (d, J = 6.9 Hz, 6H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.7, 154.7, 149.4, 147.7, 134.9, 133.0, 132.2, 131.4, 130.8 (q, $^2J_{C\text{-}CF3}$ = 33.2 Hz), 129.5, 127.9 (q, $^3J_{C\text{-}CF3}$ = 3.2 Hz), 125.5, 125.1, 124.5, 124.1, 122.7, 122.2, 115.3, 69.9, 26.9, 22.7, 22.7.

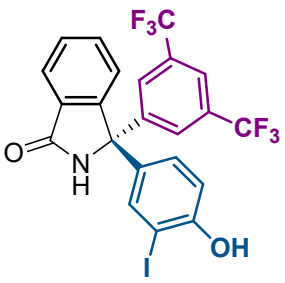
m.p. 233.9–235.0 °C

$[\alpha]_D$ = +72 ° (c 1.5, THF) for 98.5:1.5 e.r.

IR: ν = 3237, 3047, 1673, 1466, 1365, 1282, 1167, 1126, 901, 704, 681 cm^{-1}

HRMS (ESI): found 480.1404; $C_{25}H_{20}F_6NO_2$ $[M+H]^+$ requires 480.1398

(*R*)-3-(3,5-bis(trifluoromethyl)phenyl)-3-(4-hydroxy-3-iodophenyl)isoindolin-1-one (20)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-iodophenol (77 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **20** as a colorless solid. Yield: 11 mg (27%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 10 % IPA in hexane, flow rate 1.0 mL/min, 220 nm), 91:9 e.r. t_{R1} = 6.2 min (major), t_{R2} = 11.1 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 10.58 (s, 1H), 9.83 (s, 1H), 8.14 (s, 1H), 7.89 (s, 2H), 7.83 – 7.66 (m, 3H), 7.58 (t, *J* = 7.1 Hz, 1H), 7.48 (d, *J* = 2.3 Hz, 1H), 7.05 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.86 (d, *J* = 8.5 Hz, 1H).

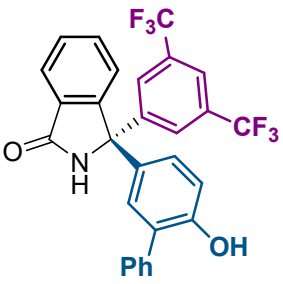
^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.6, 157.1, 148.8, 146.9, 137.1, 134.7, 133.2, 131.2, 131.0, 130.8, 129.7, 129.1, 127.8 (q, $^{3}J_{C\text{-}CF3}$ = 3.2 Hz**)**, 125.1, 124.4, 124.2, 122.6, 122.5, 115.4, 85.2, 69.1.

m.p. 251.8–252.5 °C

IR: *v* = 3247, 3054, 1668, 1493, 1374, 1273, 1176, 1116, 892, 749, 689 cm^{-1}

HRMS (ESI): found 563.9913; $C_{22}H_{13}F_6INO_2$ $[M+H]^+$ requires 563.9895

(*S*)-3-(3,5-bis(trifluoromethyl)phenyl)-3-(6-hydroxy-[1,1'-biphenyl]-3-yl)isoindolin-1-one (21)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-phenylphenol (60 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **21** as a colorless solid. Yield: 21 mg (58%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack OD, 7 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 94:6 e.r. t_{R1} = 12.9 min (major), t_{R2} = 17.5 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.85 (s, 2H), 8.13 (s, 1H), 7.95 (s, 2H), 7.85 (d, J = 7.7 Hz, 1H), 7.76 (d, J = 7.4 Hz, 1H), 7.70 (t, J = 7.1 Hz, 1H), 7.58 (t, J = 7.2 Hz, 1H), 7.45 (d, J = 7.1 Hz, 2H), 7.37 (t, J = 7.4 Hz, 2H), 7.28 (t, J = 7.1 Hz, 1H), 7.08 (d, J = 2.3 Hz, 1H), 7.02 (dd, J = 8.5, 2.4 Hz, 1H), 6.94 (d, J = 8.5 Hz, 1H).

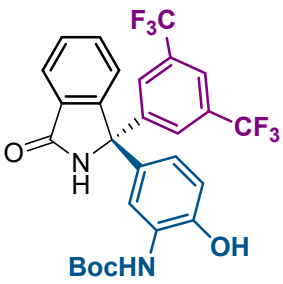
^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.7, 154.6, 149.1, 147.5, 138.5, 133.0, 133.0, 131.4, 130.8 (q, $^2J_{C\text{-}CF3}$ = 33.2 Hz), 129.6, 129.4, 128.5, 128.2, 127.8 (q, $^3J_{C\text{-}CF3}$ = 3.2 Hz), 127.7, 127.3, 125.2, 124.5, 124.1, 122.7, 116.7, 69.7.

m.p. 296.8–297.7 °C

IR: ν = 3169, 3054, 1673, 1466, 1365, 1278, 1176, 1116, 892, 749, 694 cm^{-1}

HRMS (ESI): found 514.1229; $C_{28}H_{18}F_6NO_2$ $[M+H]^+$ requires 514.1242

(*R*)-tert-butyl-(5-(1-(3,5-bis(trifluoromethyl)phenyl)-3-oxoisoindolin-1-yl)-2-hydroxyphenyl)carbamate (22)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, *tert*-butyl (2-hydroxyphenyl)carbamate (73 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **22** as a orange solid. Yield: 14 mg (38%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 6 % IPA in hexane, flow rate 1.0 mL/min, 220 nm), 90:10 e.r. t_{R1} = 7.4 min (major), t_{R2} = 11.8 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 10.00 (s, 1H), 9.84 (s, 1H), 8.13 (s, 1H), 7.89 (s, 2H), 7.81 (s, 1H), 7.75 (d, J = 7.4 Hz, 1H), 7.69 (d, J = 3.8 Hz, 2H), 7.64 – 7.51 (m, 2H), 6.80 (d, J = 8.4 Hz, 1H), 6.68 (dd, J = 8.4, 2.4 Hz, 1H), 1.37 (s, 9H).

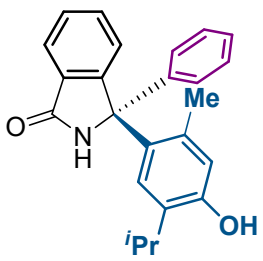
^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.6, 153.2, 149.2, 147.5, 147.2, 133.0, 132.8, 131.4, 130.8 (q, $^2J_{C\text{-}CF3}$ = 33.2 Hz), 130.5, 129.5, 127.9 (q, $^3J_{C\text{-}CF3}$ = 3.2 Hz), 126.8, 126.3, 125.0, 124.5, 124.3, 122.9, 122.7, 122.3, 115.6, 79.9, 69.8, 28.4.

m.p. 216.6–217.9 °C

IR: ν = 3242, 3114, 2980, 1723, 1681, 1438, 1374, 1273, 1181, 1131, 892, 740, 704 cm^{-1}

HRMS (ESI): found 575.1380; $C_{27}H_{22}F_6N_2O_4Na$ $[M+Na]^+$ requires 575.1381

(*R*)-3-(4-hydroxy-5-isopropyl-2-methylphenyl)-3-phenylisoindolin-1-one (23)



BA2 (7.7 mg, 0.011 mmol) was added to a suspension of **Is-1** (25 mg, 0.11 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, thymol (83 mg, 0.55 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 4 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **23** as a colorless solid. Yield: 35 mg (89%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 15 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 52:48 e.r. t_{R1} = 7.7 min (major), t_{R2} = 9.7 min (minor).

^{1}H NMR (600 MHz, DMSO) (δ/ppm): 9.35 (s, 1H), 9.26 (s, 1H), 7.71 (d, J = 7.5 Hz, 1H), 7.61 (t, J = 8.1 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.45 (d, J = 7.7 Hz, 1H), 7.32 (d, J = 4.3 Hz, 4H), 7.28 – 7.22 (m, 1H), 6.69 (s, 1H), 6.57 (s, 1H), 3.11 – 2.92 (m, 1H), 1.72 (s, 3H), 0.99 (d, J = 6.9 Hz, 3H), 0.90 (d, J = 6.9 Hz, 3H).

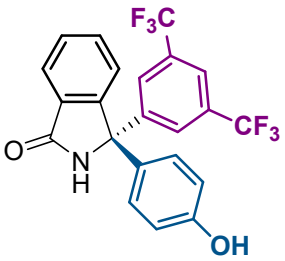
^{13}C NMR (151 MHz, DMSO) (δ/ppm): 169.6, 154.3, 151.4, 145.1, 135.5, 132.1, 131.2, 131.0, 130.8, 129.0, 128.6, 127.5, 126.5, 125.8, 125.7, 123.7, 119.5, 71.1, 26.7, 22.8, 22.7, 21.3.

m.p. 287.6–288.5 °C

IR: ν = 3054, 2967, 1677, 1415, 1273, 1039, 754, 694 cm^{-1}

HRMS (ESI): found 358.1808; $C_{24}H_{24}NO_2$ $[M+H]^+$ requires 358.1807

(*S*)-3-(3,5-bis(trifluoromethyl)phenyl)-3-(4-hydroxyphenyl)isoindolin-1-one (24)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, phenol (33 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **24** as a colorless solid. Yield: 15 mg (49%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 10 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 94:6 e.r. t_{R1} = 6.6 min (major), t_{R2} = 11.1 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.83 (s, 1H), 9.63 (s, 1H), 8.13 (s, 1H), 7.90 (s, 2H), 7.83 – 7.63 (m, 3H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.03 (d, *J* = 8.7 Hz, 2H), 6.75 (d, *J* = 8.7 Hz, 2H).

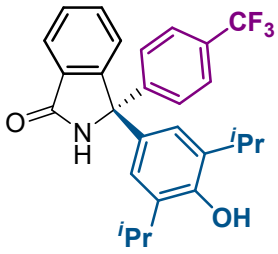
^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.6, 157.6, 149.2, 147.5, 133.0, 132.5, 131.4, 130.8 (q, $^{2}J_{C\text{-}CF3}$ = 33.2 Hz), 129.5, 128.6, 127.8 (q, $^{3}J_{C\text{-}CF3}$ = 3.2 Hz), 125.1, 124.5, 124.1, 122.7, 122.3, 115.9, 69.7.

m.p. 269.2–270.5 °C

IR: ν = 3252, 3036, 1667, 1466, 1374, 1273, 1163, 1126, 892, 749, 699 cm^{-1}

HRMS (ESI): found 438.0936 ; $C_{22}H_{14}F_6NO_2$ $[M+H]^+$ requires 438.0929

(*R*)-3-(4-hydroxy-3,5-diisopropylphenyl)-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (25)



BA2 (6.0 mg, 0.0085 mmol) was added to a suspension of **Is-5** (25 mg, 0.085 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-diisopropylphenol (76 µL, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **25** as a colorless solid. Yield: 31 mg (95%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 20 % IPA in hexane, flow rate 1.0 mL/min, 220 nm), 96.5:3.5 e.r. t_{R1} = 5.9 min (minor), t_{R2} = 11.7 min (major).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.77 (s, 1H), 8.22 (s, 1H), 7.71 (t, J = 8.3 Hz, 3H), 7.66 – 7.48 (m, 3H), 7.45 (d, J = 8.2 Hz, 2H), 6.88 (s, 2H), 3.25 (m, 2H), 1.04 (dd, J = 8.4, 7.0 Hz, 12H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 169.3, 168.8, 150.7, 146.2, 138.0, 135.4, 133.5, 131.8, 130.6, 130.5, 128.5, 128.0, 127.1, 126.9, 125.9 (q, $^3J_{C\text{-}CF3}$ = 3.8 Hz) , 125.7, 125.6, 125.1, 123.9, 123.6, 123.2, 122.5, 70.6, 50.4, 26.7, 23.3, 21.1

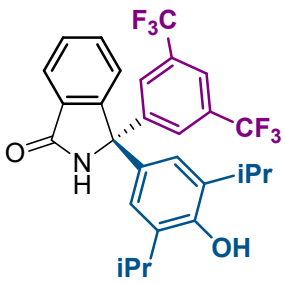
m.p. 208.5–210.3 °C

$[\alpha]_D$ = +75 ° (c 1.5, THF) for 96.5:2.5 e.r.

IR: ν = 3178, 2957, 1677, 1466, 1323, 1112, 1066, 741, 708 cm^{-1}

HRMS (ESI): found 454.1976; $C_{27}H_{27}F_3NO_2$ $[M+H]^+$ requires 454.1994

(*S*)-3-(3,5-bis(trifluoromethyl)phenyl)-3-(4-hydroxy-3,5-diisopropylphenyl)isoindolin-1-one (26)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-9** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-diisopropylphenol (63 µL, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **26** as a colorless solid. Yield: 30 mg (81%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 5 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 99.5:0.5 e.r. t_{R1} = 5.6 min (major), t_{R2} = 11.2 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.80 (s, 1H), 8.32 (s, 1H), 8.11 (s, 1H), 7.77 (t, J = 7.4 Hz, 3H), 7.67 (d, J = 3.8 Hz, 2H), 7.62 – 7.53 (m, 1H), 6.81 (s, 2H), 3.31 – 3.17 (m, J = 13.6, 6.8 Hz, 2H), 1.03 (d, J = 6.8 Hz, 12H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.8, 151.0, 149.6, 147.7, 135.7, 133.0, 132.6, 131.3, 130.8 (q, $^2J_{C\text{-}CF3}$ = 33.2 Hz), 129.5, 127.9 (q, $^3J_{C\text{-}CF3}$ = 3.8 Hz), 126.3, 125.0, 124.5, 124.1, 122.7, 122.5, 122.2, 70.0, 23.2, 23.1.

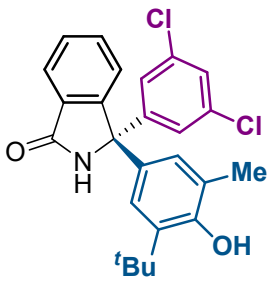
m.p. 217.2–218.3 °C

$[\alpha]_D$ = +43 ° (c 1.4, THF) for 99.5:0.5 e.r.

IR: ν = 3205, 2967, 1668, 1466, 1365, 1273, 1181, 1131, 901, 713, 676 cm^{-1}

HRMS (ESI): found 522.1855; $C_{28}H_{26}F_6NO_2$ $[M+H]^+$ requires 522.1868

(*S*)-3-(3-(*tert*-butyl)-4-hydroxy-5-methylphenyl)-3-(3,5-dichlorophenyl)isoindolin-1-one (27)



BA2 (6.0 mg, 0.0085 mmol) was added to a suspension of **Is-10** (25 mg, 0.085 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-(*tert*-butyl)-6-methylphenol (52 mg, 0.43 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **27** as a colorless solid. Yield: 26 mg (71%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack OD, 8 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 98.5:1.5 e.r. t_{R1} = 8.1 min (minor), t_{R2} = 10.2 min (major).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.67 (s, 1H), 8.30 (s, 1H), 7.77 – 7.62 (m, 3H), 7.61 – 7.51 (m, 2H), 7.26 (d, J = 1.9 Hz, 2H), 6.90 (s, 1H), 6.80 (s, 1H), 2.12 (s, 3H), 1.27 (s, 9H).

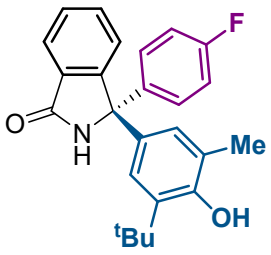
^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.6, 153.8, 149.4, 148.6, 136.8, 134.5, 132.7, 132.33, 131.4, 129.3, 127.7, 127.6, 126.1, 125.6, 125.2, 123.9, 123.4, 69.9, 35.0, 29.9, 17.7.

m.p. 237.7–238.5 °C

$[\alpha]_D$ = +83 ° (c 1.2, THF) for 98.5:1.5 e.r.

IR: ν = 3197, 2949, 1677, 1470, 1195, 1163, 791, 717 cm^{-1}

HRMS (ESI): found 440.1200; $C_{25}H_{24}Cl_2NO_2$ $[M+H]^+$ requires 440.1184



(*R*)-3-(3-(*tert*-butyl)-4-hydroxy-5-methylphenyl)-3-(4-fluorophenyl)isoindolin-1-one (28)

BA2 (7.4 mg, 0.010 mmol) was added to a suspension of **Is-4** (25 mg, 0.10 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-(tert-butyl)-6-methylphenol (64 mg, 0.50 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **28** as a colorless solid. Yield: 34 mg (83%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 97:3 e.r. t_{R1} = 7.1 min (minor), t_{R2} = 9.7 min (major).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.52 (s, 1H), 8.11 (s, 1H), 7.60 (d, J = 7.4 Hz, 1H), 7.50 (t, J = 8.6 Hz, 2H), 7.41 (t, J = 7.1 Hz, 1H), 7.26 – 7.12 (m, 2H), 7.06 (t, J = 8.9 Hz, 2H), 6.83 (s, 1H), 6.71 (s, 1H), 2.02 (s, J = 6.2 Hz, 3H), 1.17 (s, 9H).

^{13}C NMR (151 MHz, DMSO) (δ/ppm): 168.7, 161.8 (d, $J_{C\text{-}F}$ = 243.1 Hz), 153.4, 150.8, 140.5, 136.5, 133.4, 132.4, 131.5, 129.4, 129.4, 128.8, 127.6, 125.3, 125.1, 123.7, 123.5, 115.5, 115.3, 70.0, 35.0, 30.0, 17.7.

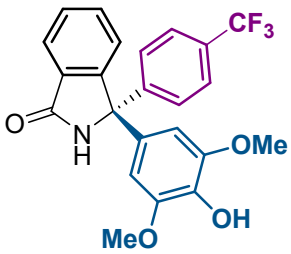
m.p. 208.2–208.7 °C

$[\alpha]_D$ = +65 ° (c 1.6, THF) for 97:3 e.r.

IR: ν = 3192, 2939, 1677, 1475, 1365, 1158, 1139, 804, 749 cm^{-1}

HRMS (ESI): found 390.1853; $C_{25}H_{25}FNO_2$ $[M+H]^+$ requires 390.1869

(*R*)-3-(4-hydroxy-3,5-dimethoxyphenyl)-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (29)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-5** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (43 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **29** as a colorless solid. Yield: 15 mg (48%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack IC-3, 40 % IPA in hexane, flow rate 1.0 mL/min, 230 nm), 94:6 e.r. t_{R1} = 9.6 min (major), t_{R2} = 28.2 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.74 (s, 1H), 8.54 (s, 1H), 8.01 – 7.26 (m, 8H), 6.52 (s, 2H), 3.63 (s, 6H).

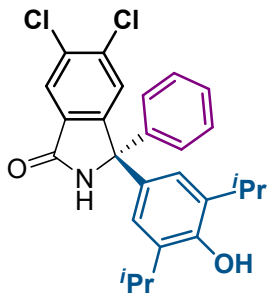
^{13}C NMR (75 MHz, DMSO) (δ/ppm): 168.8, 149.6, 149.0, 148.2, 135.9, 132.6, 132.3, 131.5, 129.2, 128.0, 125.8 (q, $^{3}J_{C\text{-}CF3}$ = 3.8 Hz), 125.3, 123.9, 105.7, 70.3, 56.6.

m.p. 210.7–211.6 °C

IR: ν = 3182, 2953, 1681, 1461, 1319, 1108, 1066, 740, 726 cm^{-1}

HRMS (ESI): found 430.1266; $C_{23}H_{19}F_3NO_4$ $[M+H]^+$ requires 430.1266

(*R*)-5,6-dichloro-3-(4-hydroxy-3,5-diisopropylphenyl)-3-phenylisoindolin-1-one (30)



BA2 (6.0 mg, 0.0085 mmol) was added to a suspension of **Is-12** (25 mg, 0.085 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2,6-diisopropylphenol (76 µL, 0.45 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 40 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **30** as a colorless solid. Yield: 18 mg (47%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 20 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 98:2 e.r. t_{R1} = 5.3 min (minor), t_{R2} = 7.5 min (major).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.98 (s, 1H), 8.27 (s, 1H), 7.96 (d, J = 5.1 Hz, 2H), 7.50 – 7.24 (m, 5H), 6.91 (s, 2H), 3.36 – 3.20 (m, 2H), 1.11 (d, J = 4.7 Hz, 12H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 166.5, 150.8, 143.2, 135.4, 135.2, 133.1, 132.2, 128.83, 127.3, 125.6, 122.5, 70.5, 26.8, 23.3, 23.2.

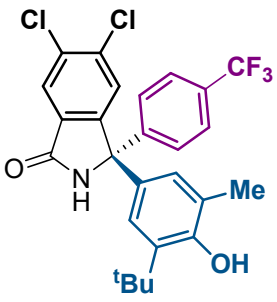
m.p. 202.8–203.5 °C

$[\alpha]_D$ = +13 ° (c 0.8, THF) for 98:22 e.r.

IR: ν = 3178, 2953, 1677, 1461, 1204, 1149, 699 cm^{-1}

HRMS (ESI): found 454.1339; $C_{26}H_{26}Cl_2NO_2$ $[M+H]^+$ requires 454.1341

(*R*)-3-(3-(tert-butyl)-4-hydroxy-5-methylphenyl)-5,6-dichloro-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (31)



BA2 (4.9 mg, 0.007 mmol) was added to a suspension of **Is-11** (25 mg, 0.07 mmol) in toluene (0.5 mL) at 25 °C. After stirring for 10 min, 2-(*tert*-butyl)-6-methylphenol (58 mg, 0.35 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 5:1) to afford product **31** as a colorless solid. Yield: 19 mg (54%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack OD, 10 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 96.5:3.5 e.r. t_{R1} = 5.1 min (major), t_{R2} = 9.3 min (minor).

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 9.98 (s, 1H), 8.31 (s, 1H), 8.03 (s, 1H), 7.93 (s, 1H), 7.72 (d, J = 8.4 Hz, 2H), 7.52 (d, J = 8.2 Hz, 2H), 6.91 (s, 1H), 6.84 (s, 1H), 2.13 (s, 3H), 1.26 (s, 9H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 166.5, 153.9, 150.0, 147.9, 136.7, 135.6, 132.6, 132.07, 131.8, 128.3, 127.8, 127.3, 125.8 (q, $^3J_{C\text{-}CF3}$ = 3.8 Hz), 125.7, 123.3, 70.1, 35.0, 29.9, 17.6.

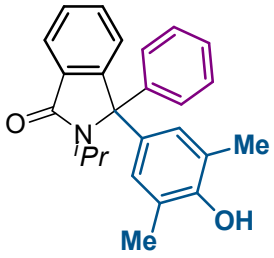
m.p. 276.3–277.1 °C

$[\alpha]_D$ = +41 ° (c 0.9, THF) for 96.5:3.5 e.r.

IR: ν = 3329, 2953, 1663, 1479, 1319, 1176, 1112, 1061, 846, 699 cm^{-1}

HRMS (ESI): found 508.1066; $C_{26}H_{23}Cl_2F_3NO_2$ $[M+H]^+$ requires 508.1058

3-(4-hydroxy-3,5-dimethylphenyl)-2-isopropyl-3-phenylisoindolin-1-one (32)

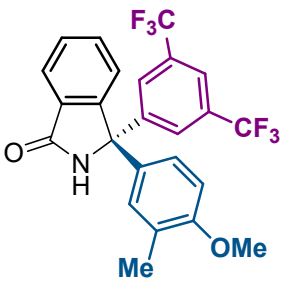


p-Toluenesulfonic acid monohydrate (3.6 mg, 0.019 mmol) was added to a suspension of **Is-2** (50 mg, 0.19 mmol) in toluene (1 mL) at 25 °C. After stirring for 10 min, 2,6-dimethylphenol (114 mg, 0.94 mmol) was added, and the resulting reaction mixture was stirred in an oil bath for 7 days at 50 °C. Then, the solvent was evaporated, and the residue was purified by flash coloumn chromatography on silica gel (dichloromethane/acetone 10:1) to afford product **32** as a colorless solid. Yield: 64 mg (90%)

^{1}H NMR (300 MHz, DMSO) (δ/ppm): 8.40 (s, 1H), 7.65 (d, *J* = 6.7 Hz, 1H), 7.56 – 7.36 (m, 2H), 7.24 (d, *J* = 7.3 Hz, 1H), 7.17 (d, *J* = 8.3 Hz, 2H), 7.11 (d, *J* = 8.3 Hz, 2H), 6.75 (s, 2H), 3.54 – 3.36 (m, *J* = 13.6, 7.0 Hz, 1H), 2.29 (s, 3H), 2.09 (s, 6H), 1.11 (d, *J* = 6.6 Hz, 3H), 1.06 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (75 MHz, DMSO) (δ/ppm): 167.81, 153.49, 151.54, 138.20, 137.68, 132.55, 131.74, 130.67, 129.55, 128.47, 128.35, 128.28, 124.58, 124.07, 122.79, 76.16, 46.18, 21.00, 20.06, 19.95, 17.32.

(*S*)-3-(3,5-bis(trifluoromethyl)phenyl)-3-(4-methoxy-3-methylphenyl)isoindolin-1-one (34)



To a solution of **18** (20 mg, 0.04 mmol) in acetone (2.0 mL) were added K_2CO_3 (28 mg, 0.2 mmol) and MeI (1.6 µL, 0.05 mmol), and the resulting mixture was refluxed for 24 h in an oil bath. Then, the solvent was evaporated, and column chromatography of the residue on silica gel (dichloromethane/acetone 10:1) to afford product **34** as a colorless solid. Yield: 10 mg (63%)

Enantiomeric ratio determined by HPLC (Daicel Chiralpack AD, 10 % IPA in hexane, flow rate 1.0 mL/min, 254 nm), 98:2 e.r. t_{R1} = 4.0 min (major), t_{R2} = 7.0 min (minor).

^{1}H NMR (300 MHz, $(CD_3)_2CO$) (δ/ppm): 8.76 (s, 1H), 8.02 (d, J = 6.5 Hz, 3H), 7.82 (d, J = 7.4 Hz, 1H), 7.79 – 7.66 (m, 2H), 7.60 (t, J = 7.3 Hz, 1H), 7.13 (dd, J = 8.2, 1.5 Hz, 2H), 6.96 – 6.86 (m, 1H), 3.83 (s, 3H), 2.11 (s, 3H).

^{13}C NMR (151 MHz, $(CD_3)_2CO$) (δ/ppm): 168.3, 157.7, 149.1, 147.6, 133.6, 132.4, 131.6, 131.5 (q, $^2J_{C\text{-}CF3}$ = 33.2 Hz), 131.3, 129.2, 129.0, 127.6 (q, $^3J_{C\text{-}CF3}$ = 3.2 Hz), 127.6, 126.7, 126.1, 125.8, 124.7, 124.3, 123.9, 122.5, 109.9, 69.7, 54.9, 15.5.

m.p. 201.0–201.4 °C

$[\alpha]_D$ = +16 ° (c 0.4 THF) for 98:2 e.r.

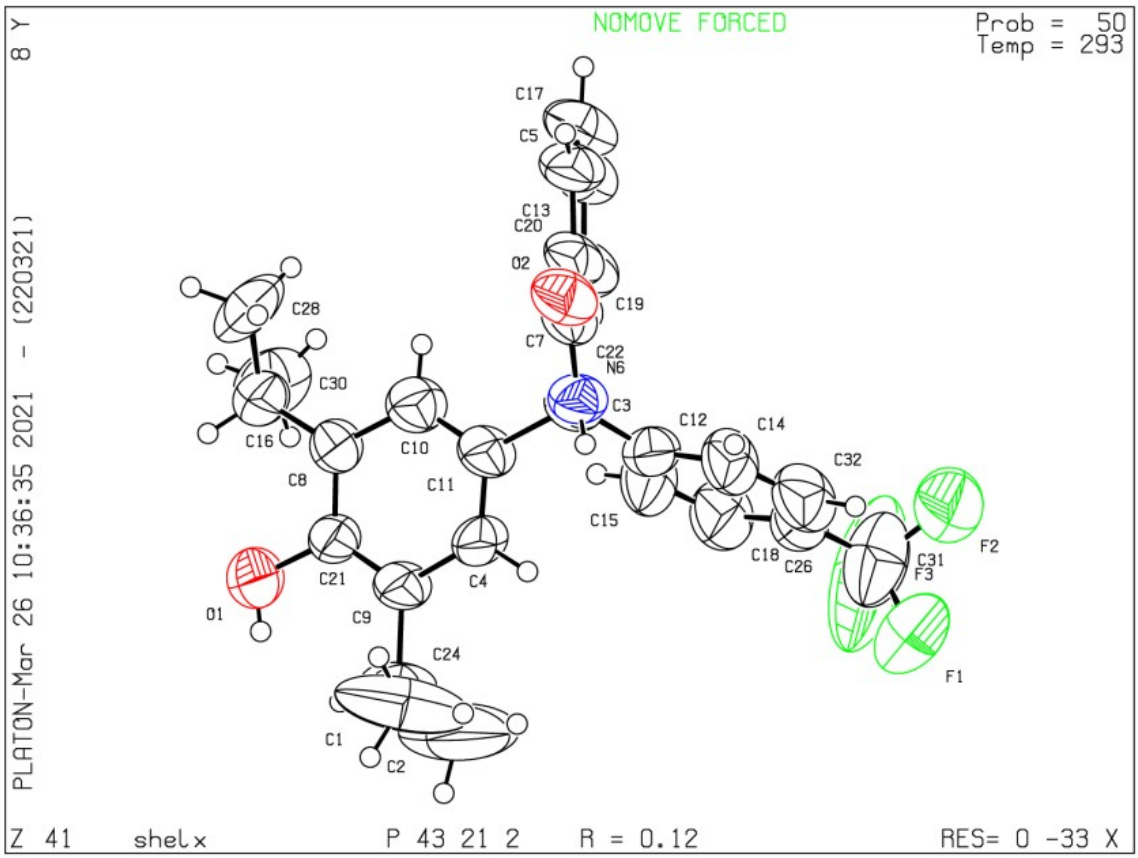
IR: ν = 2921, 1695, 1466, 1365, 1273, 1167, 1131, 892, 731, 676 cm^{-1}

HRMS (ESI): found 466.1226; $C_{24}H_{18}F_6NO_2$ $[M+H]^+$ requires 466.1242

4. X-ray Crystallography

Single crystal measurement was performed on an Oxford Diffraction Xcalibur Nova R (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 SIR-92. Non-hydrogen atoms were refined isotropically followed by anisotropic refinement by full matrix least-squares calculations based on F_2 using SIR-92.[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 ORTEP3,[5] PLATON[6] and Mercury®. Absolute configuration of the product **ent-25** was determined by solving its crystal structure. Absolute configuration of other products was assigned by analogy. The crystal structure has been deposited at the Cambridge Crystallographic Centre (deposition number: CCDC 2073369). The data can be obtained free of charge at www.ccdc.cam.ac.uk/getstructures.

Datablock shelx - ellipsoid plot



5. DFT Calculations

Computational Methods

The computational studies were performed with Gaussian 16[7] package. Density functional theory (DFT) calculations were carried out using the B3LYP functional[8] including the D3 version of Grimme's empirical dispersion correction with Becke−Johnson damping.[9] The def2-SVP basis sets[10] were applied for all atoms. Optimizations were conducted without any constraint in the gas phase. Frequency analyses were carried out to confirm each structure being a minimum (no imaginary frequency) or a transition state (only one imaginary frequency). Single point calculations were performed at B3LYP-D3(BJ)/def2-TZVPP level of theory in toluene (SMD model,[11] ε = 2.3741). The relative Gibbs free energies (Δ*G*) are discussed in kcal/mol. The optimized structures are visualized by VMD.[12]

Derailed Results for the Stereochemical Model

According to the controlled experiments, chiral phosphoric acid works as a bifunctional catalyst. Hydrogen-bonding interactions can be established between the catalyst and each substrate. Thus, a total of four different transition states can be located for the key nucleophilic attack event (Figure S1), two for the formation of (*R*)-**1** (**TS-*Re***, 0.0 kcal/mol and **TS-*Re′***, 2.7 kcal/mol) and two for (*S*)-**1** (**TS-*Si***, 2.4 kcal/mol and **TS-*Si′***, 2.7 kcal/mol). The structural variation in each series is the different alignment of the O•••H•••O hydrogen bonds. The energetically more favorable transition states (**TS-*Re*** and **TS-*Si***) are discussed in the main text.

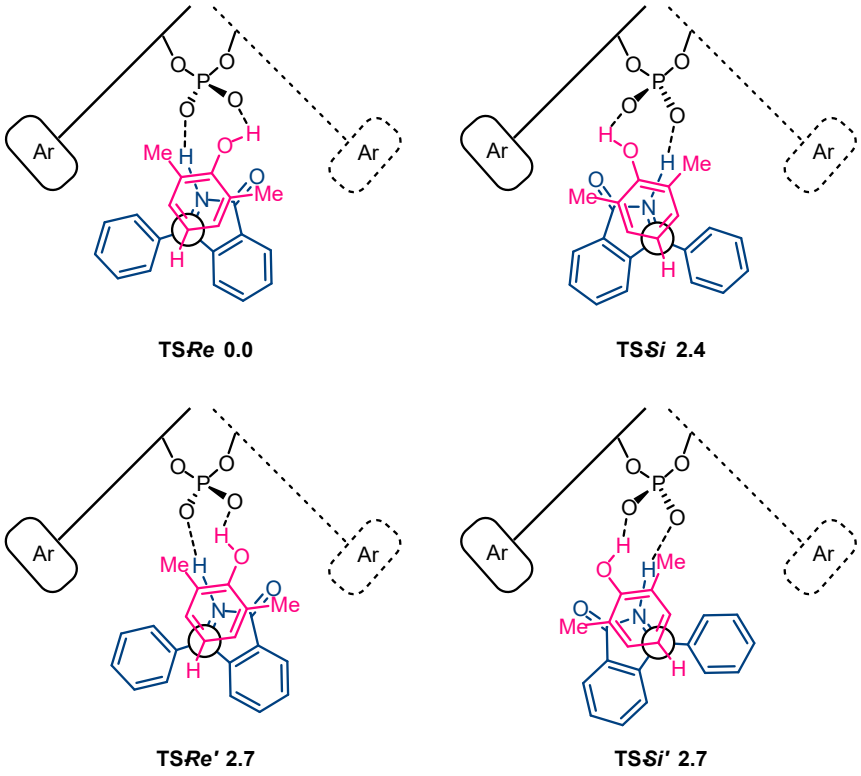


Figure S1. The schematic description and calculated relative Gibbs free energies (in kcal/mol) of all possible transition states.

Cartesian Coordinates and Energies of the Optimized Structures

TS-*Re*

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase

SCF Done: E(B3LYP) = -3541.98700429 a.u.

Zero-point correction = 0.990258 Hartree/Particle

Sum of electronic and thermal Free Energies = -3541.092151 a.u.

Imaginary frequency = -363.7498 cm^{-1}

Sp @ B3LYP-D3(BJ)/def2-TZVPP in toluene (SMD model)

SCF Done: E(B3LYP) = -3545.65808272 a.u.

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H,0,2.8234544234,2.8325072758,-3.5597702575

H,0,-0.4576143924,1.9958896153,-1.2800241047

TS-*Re'*

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase

SCF Done: E(B3LYP) = -3541.98651956 a.u.

Zero-point correction = 0.989809 Hartree/Particle

Sum of electronic and thermal Free Energies = -3541.092679 a.u.

Imaginary frequency = -383.6498 cm^{-1}

Sp @ B3LYP-D3(BJ)/def2-TZVPP in toluene (SMD model)

SCF Done: E(B3LYP) = -3545.65276606 a.u.

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C,0,-0.1336024083,3.4143760077,-4.0890123537
C,0,-0.4263978888,3.9121936117,-2.8442188608
C,0,0.1282000166,5.150455475,-2.4086985307
C,0,0.9639054126,5.8575434942,-3.2349022763
H,0,-0.5637795682,2.4655969323,-4.4113183734
H,0,-1.0894132358,3.3558342074,-2.1775260709
H,0,-0.1180342718,5.5323361309,-1.4149931529
H,0,1.390368472,6.8114265082,-2.9136969425
C,0,5.0825113216,5.4179290214,-4.1176711365
C,0,6.0960321941,5.7315488711,-5.0396003014
C,0,6.776879701,6.9437600867,-4.9109525643
C,0,6.4041205165,7.8201923518,-3.8820423066
C,0,5.3881200737,7.4930812476,-2.9733228965
C,0,4.719759047,6.269740548,-3.0823358262
C,0,4.5541108305,4.0660913741,-4.4359859406
C,0,6.296574384,4.5251262983,-5.9250239203
H,0,7.6024926017,7.2203160854,-5.5649925281
H,0,6.9272990349,8.7742184059,-3.7825677902
H,0,5.1270978708,8.194058932,-2.1773265301
H,0,3.9283865425,5.9737333696,-2.3909122152
O,0,3.6919425742,3.4184296055,-3.8789849123
N,0,5.2741014029,3.6615046473,-5.5515784038
H,0,4.9851075339,2.7962257798,-6.0359284883
C,0,6.623788084,4.5876841309,-7.3827517542

C,0,7.3416852107,5.6585945631,-7.9368590657

C,0,6.2411791105,3.5324272264,-8.2304103775

C,0,7.6592569472,5.6846808597,-9.2960792794

H,0,7.6516540061,6.4938851437,-7.314266216

C,0,6.5696530814,3.5548676156,-9.5851768408

H,0,5.6628540841,2.6910238458,-7.8512071503

C,0,7.2761444591,4.6308438448,-10.1287301634

H,0,8.2098324352,6.5357483468,-9.7038022547

H,0,6.2543786897,2.7255536076,-10.222480848

H,0,7.5259941734,4.6484328973,-11.1920832475

C,0,7.967718481,3.7371394356,-5.1594548036

C,0,7.9552870199,2.4121676361,-5.7540838065

C,0,7.2780696601,1.3840554907,-5.1747192534

C,0,6.6351920359,1.625098474,-3.8736646406

C,0,6.9999809534,2.8273344698,-3.1107859893

C,0,7.7000140569,3.8099367686,-3.7386033752

H,0,8.6973345488,4.4455468468,-5.5619481433

H,0,8.4111694082,2.2759708276,-6.7375512671

H,0,7.9307288923,4.7355798844,-3.2067184878

O,0,5.8147329876,0.8218376392,-3.3785617486

C,0,7.1231599553,0.0290587857,-5.8021595086

H,0,7.1427699095,-0.7654551949,-5.0440340776

H,0,6.1612502517,-0.0498805605,-6.3309843864

H,0,7.9177762409,-0.1572671655,-6.538839734

C,0,6.4599088116,2.9357806579,-1.7186474476

H,0,5.3574692673,2.9492861625,-1.7593326057

H,0,6.7374730381,2.0613437519,-1.1097392747

H,0,6.8118169306,3.8523208586,-1.22435112

H,0,4.71430871,0.2156343823,-4.0942025974

TS-*Si*

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase

SCF Done: E(B3LYP) = -3541.97873802 a.u.

Zero-point correction = 0.989828 Hartree/Particle

Sum of electronic and thermal Free Energies = -3541.083977 a.u.

Imaginary frequency = -193.1767 cm^{-1}

Sp @ B3LYP-D3(BJ)/def2-TZVPP in toluene (SMD model)

SCF Done: E(B3LYP) = -3545.65413249 a.u.

C,0,-6.929336822,-2.5448200898,0.3236938302

C,0,-5.8835985903,-1.7146747284,-0.0206125535

C,0,-4.5493964588,-2.2055115696,-0.0912732515

C,0,-4.3148869458,-3.5786828761,0.2482454558

C,0,-5.4174130267,-4.412243189,0.5848638842

C,0,-6.7000218788,-3.9112977498,0.6170705119

H,0,-7.9438175006,-2.1426929378,0.3761049013

H,0,-6.0755203736,-0.6638156267,-0.2333073498

C,0,-3.4307664039,-1.3750648086,-0.4429614009

C,0,-2.9862183056,-4.0753472471,0.2660296598

H,0,-5.22252259,-5.4593630068,0.8297796338

H,0,-7.5384766636,-4.559582764,0.8818273617

C,0,-1.8995888547,-3.2646875025,0.0042549392

C,0,-2.1516362627,-1.9075022443,-0.3366676653

H,0,-2.8158857797,-5.1242162984,0.5186598312

C,0,-3.6093543961,0.0423007086,-0.8591826628

C,0,-4.4344964707,0.4156174698,-1.9738272868

C,0,-2.9397115837,1.0438690638,-0.1690048994

C,0,-5.0440993296,-0.5389629978,-2.8353188003

C,0,-4.6279929141,1.8081943402,-2.25923148

C,0,-3.1014081803,2.4277423369,-0.4514095298

C,0,-5.8329503295,-0.1397902612,-3.8934546435

H,0,-4.8750159578,-1.5999957274,-2.6549813362

C,0,-5.4599761733,2.1860793888,-3.3496556376

C,0,-3.9636584294,2.7828326164,-1.4697206245

C,0,-6.0560831221,1.2354523645,-4.1486636577

H,0,-6.2862004733,-0.891549645,-4.5438468547

H,0,-5.6071036965,3.2507973812,-3.5478263638

H,0,-4.1133363084,3.8406526904,-1.6969761323

H,0,-6.6890304575,1.5379694568,-4.9860652385

C,0,-0.5157935642,-3.8192659779,0.0617072628

C,0,0.0771004908,-4.0961729034,1.3132688694

C,0,0.1683952293,-4.1153243498,-1.1377636649

C,0,-0.5436341217,-3.7421523317,2.5542265043

C,0,1.3697828675,-4.7406490937,1.3605299644

C,0,1.4586956889,-4.7614990426,-1.0804092228

C,0,0.0635364656,-4.011471397,3.7545035053

H,0,-1.499901583,-3.2214773726,2.5322056075

C,0,1.963107835,-5.0141234652,2.6333202851

C,0,2.0127016792,-5.0772120758,0.1650772248

C,0,1.3317958141,-4.6610288033,3.7979891265

H,0,-0.4218542653,-3.7154174674,4.6873087778

H,0,2.9401220906,-5.5040807013,2.6554174193

H,0,2.9775020469,-5.5910046919,0.2075398166

H,0,1.8005929376,-4.8668894223,4.763249807

C,0,-2.3371704916,3.4499533294,0.3167814382

C,0,-2.6543478819,3.7080522111,1.6697618743

C,0,-1.2976930242,4.1615460447,-0.3243628808

C,0,-3.6880376895,3.0024525842,2.3645667223

C,0,-1.9221255206,4.7237116419,2.3910415842

C,0,-0.5896467285,5.1934210617,0.3983818516

C,0,-3.9642418884,3.2641576757,3.6825792522

H,0,-4.2576701908,2.2414871705,1.8308273645

C,0,-2.2425726868,4.9669805187,3.7641776462

C,0,-0.922012598,5.4487680984,1.73272454

C,0,-3.2307382494,4.2568278772,4.3956618693

H,0,-4.7525750754,2.7069096926,4.193986753

H,0,-1.6775616131,5.7338803042,4.300163575

H,0,-0.3761701422,6.2217635276,2.2801635714

H,0,-3.4624748347,4.4491936466,5.4458641736

C,0,-0.8933251185,3.8854022124,-1.6704145748

C,0,0.1093874326,4.6022383256,-2.2704882055

C,0,0.793090196,5.633885329,-1.5625988334

C,0,0.453670964,5.9143418239,-0.2647664334

H,0,-1.3889064146,3.0822133219,-2.2142539277

H,0,0.3900096017,4.3750123279,-3.3015295839

H,0,1.5952366031,6.1889203787,-2.053904262

H,0,0.9795027119,6.6938900056,0.2925190191

C,0,-0.3719958369,-3.8053508073,-2.4258245253

C,0,0.319786403,-4.0924460295,-3.575832548

C,0,1.5947431522,-4.726187315,-3.516048552

C,0,2.1408215652,-5.0567728184,-2.3021898502

H,0,-1.3478173144,-3.3227514817,-2.4857066121

H,0,-0.1081933565,-3.8348118713,-4.5475288631

H,0,2.1316006355,-4.9493627813,-4.4411685339

H,0,3.1164081314,-5.5472233573,-2.2475493673

O,0,-1.0580530775,-1.0943552411,-0.5833664768

O,0,-2.0873674921,0.69623023,0.8571295792

P,0,-0.6281364464,0.0289798309,0.5138075964

O,0,0.3458983592,1.0059137395,-0.045769222

O,0,-0.3212325727,-0.745589285,1.8369734634

C,0,4.2842405419,-1.5566722733,-0.6664675965

C,0,5.0820580259,-0.4278148675,-0.9141457688

C,0,6.4257910013,-0.587777363,-1.2508668602

C,0,6.9450120712,-1.8882781963,-1.3107435307

C,0,6.1452147913,-3.0079735834,-1.0412432291

C,0,4.7931190215,-2.8485971899,-0.7184451174

C,0,2.9048762103,-1.0941578211,-0.3660773539

C,0,4.2329259747,0.7868520827,-0.6963894034

H,0,7.0694024466,0.2638880349,-1.4692669309

H,0,7.995627587,-2.0300938788,-1.5751850877

H,0,6.5809326752,-4.0081853753,-1.0937191364

H,0,4.1393079918,-3.6958706496,-0.5156854684
O,0,1.9199501521,-1.7394580504,-0.0777281397
N,0,2.9565835181,0.2974131507,-0.4933474855
H,0,2.0876841501,0.8316391987,-0.3304345701
C,0,4.4079925306,2.0312784633,-1.4912128884
C,0,5.6648152816,2.6549838168,-1.6028199526
C,0,3.3148433353,2.5997002655,-2.1662438207
C,0,5.8295905221,3.8000389251,-2.3789958624
H,0,6.5221537355,2.2572821226,-1.0602598395
C,0,3.4864395407,3.7432266211,-2.9492538832
H,0,2.3261836513,2.1451581798,-2.0891871372
C,0,4.7393216903,4.3472119066,-3.0626145901
H,0,6.8138405972,4.2689242557,-2.4487959426
H,0,2.6296190277,4.160677737,-3.4782564617
H,0,4.8666740273,5.2415152395,-3.6768351166
C,0,4.8926074318,1.3537245205,1.2263942568
C,0,3.9580370388,2.4334653032,1.4439518525
C,0,2.7606408807,2.2264765518,2.0601538789
C,0,2.4546376724,0.8895561859,2.5754069763
C,0,3.4804505328,-0.1622404865,2.5138536105
C,0,4.6864005327,0.1255060561,1.9407266423
H,0,5.9182765157,1.6171816018,0.9603363977
H,0,4.1820301556,3.4107237174,1.0090597747
H,0,5.4647153034,-0.6405546787,1.9066408858
O,0,1.3284143929,0.6606423099,3.0723788181
C,0,1.685302389,3.262180987,2.1682186718
H,0,1.3222601891,3.3591997516,3.2026638118
H,0,0.8199251388,2.957237199,1.5603309932
H,0,2.0326389651,4.2396813805,1.8072614197
C,0,3.1123833022,-1.5070304642,3.0579329297
H,0,2.3361407408,-1.9653677752,2.4213153124
H,0,2.6822220432,-1.4313295609,4.0678494319
H,0,3.9769355312,-2.1850811814,3.0770971079

H,0,0.3605483022,-0.2788265424,2.4415818572

TS-*Si'*

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase

SCF Done: E(B3LYP) = -3541.97714414 a.u.

Zero-point correction = 0.990051 Hartree/Particle

Sum of electronic and thermal Free Energies = -3541.082654 a.u.

Imaginary frequency = -347.8479 cm^{-1}

Sp @ B3LYP-D3(BJ)/def2-TZVPP in toluene (SMD model)

SCF Done: E(B3LYP) = -3545.65337879 a.u.

C,0,-5.6060160295,-0.9152422514,-3.9971361103

C,0,-4.7677733087,-1.2014674209,-2.9404552028

C,0,-4.3640151058,-0.1854622773,-2.0299638714

C,0,-4.8186674792,1.1537573537,-2.2623816196

C,0,-5.6977970669,1.41273672,-3.3509618961

C,0,-6.0891303485,0.4010225261,-4.1996052601

H,0,-5.8969320024,-1.7105299847,-4.6873308135

H,0,-4.3991748088,-2.2169660153,-2.7995371299

C,0,-3.5049676662,-0.4422934867,-0.9080351011

C,0,-4.3636121243,2.1992823851,-1.42032489

H,0,-6.0458372642,2.4368492648,-3.5076991355

H,0,-6.7593220095,0.6119604647,-5.0360757921

C,0,-3.4459874277,1.9814697119,-0.408355735

C,0,-3.0283548986,0.6387899201,-0.177274271

H,0,-4.7262425607,3.2134869246,-1.5989519202

C,0,-3.1260397854,-1.8267505181,-0.5164290265

C,0,-4.1256255295,-2.8184346186,-0.2261729205

C,0,-1.7876013629,-2.1717223995,-0.3732864027

C,0,-5.5187088455,-2.5274798367,-0.1882422084

C,0,-3.7066093592,-4.153783186,0.0840135984

C,0,-1.3543717193,-3.4854855865,-0.0465771919

C,0,-6.4433890761,-3.5104306735,0.0945485717
H,0,-5.8557099594,-1.5091417032,-0.3761797803
C,0,-4.6865938433,-5.1486948654,0.355803935
C,0,-2.3219224851,-4.4521097322,0.1458526425
C,0,-6.0285279072,-4.8392333189,0.3554760735
H,0,-7.5063765196,-3.2596769294,0.1230255541
H,0,-4.3491938965,-6.1640581974,0.5784335014
H,0,-2.0100248614,-5.4706141628,0.3870732531
H,0,-6.772300022,-5.6098626929,0.5706328189
C,0,-2.9197553152,3.1182302884,0.3971959307
C,0,-2.2593560419,4.1874387381,-0.2612853066
C,0,-3.1297727552,3.165747474,1.7979260755
C,0,-1.9799473655,4.1869905737,-1.6683766841
C,0,-1.8450034534,5.3459989976,0.499390382
C,0,-2.6343015482,4.2920159413,2.5563692204
C,0,-1.4334647286,5.2818601947,-2.2901529091
H,0,-2.2063086533,3.2950949181,-2.2509134131
C,0,-1.2796670461,6.468137335,-0.1867697076
C,0,-2.0182491385,5.3555404798,1.8872590204
C,0,-1.1020959098,6.4517757825,-1.5459323398
H,0,-1.2360488216,5.2528988935,-3.3641480043
H,0,-0.99653106,7.3442941629,0.4020854883
H,0,-1.6813118669,6.2230887132,2.4610367572
H,0,-0.6795484006,7.3188049465,-2.0590106789
C,0,0.0865451302,-3.8421426479,0.1013770831
C,0,0.895553033,-4.0143830701,-1.0421360097
C,0,0.6062549494,-4.0856690621,1.393740468
C,0,0.4310189656,-3.7222903304,-2.3628511448
C,0,2.246646452,-4.4998687569,-0.8894334276
C,0,1.9550944202,-4.5827869352,1.5338456594
C,0,1.2481821669,-3.8754520696,-3.453828042
H,0,-0.5876032376,-3.3562818497,-2.4944672221
C,0,3.0605463959,-4.664206659,-2.053489709

C,0,2.7312021462,-4.7936265547,0.388761035

C,0,2.5819262726,-4.3542439307,-3.300473855

H,0,0.8764219569,-3.6302517355,-4.4515442788

H,0,4.0790930143,-5.0404672611,-1.9237264809

H,0,3.7500526455,-5.1751238475,0.4985457882

H,0,3.2164569793,-4.4761399203,-4.181882853

C,0,-0.1488036019,-3.8438144419,2.5866378937

C,0,0.3885351929,-4.0796543308,3.8263061978

C,0,1.7130636305,-4.587976193,3.9602443155

C,0,2.4697303543,-4.8343312054,2.8442266306

H,0,-1.1540136423,-3.4339093547,2.4986649947

H,0,-0.199855944,-3.8679233641,4.7221704327

H,0,2.1225923893,-4.7735741259,4.9561286924

H,0,3.4895281739,-5.2171291251,2.9350836939

C,0,-3.8473233958,2.1505379535,2.5089857619

C,0,-4.0139151608,2.2137457037,3.868979918

C,0,-3.4823009546,3.3031433297,4.6181755382

C,0,-2.8192626639,4.3157332042,3.9754835453

H,0,-4.2685224191,1.3122886715,1.9562529127

H,0,-4.5604595825,1.4211556496,4.3851430401

H,0,-3.6174370808,3.3318736209,5.7019196771

H,0,-2.4247593309,5.1680538963,4.5345464535

O,0,-0.8190807188,-1.198695768,-0.5568675636

O,0,-2.1510709655,0.4112108783,0.862892771

P,0,-0.6137538186,-0.06289243,0.5959207422

O,0,0.2866974261,1.0190478836,0.1085456674

O,0,-0.3094956426,-0.7578103947,1.957041792

C,0,4.5528966907,-0.4396801127,-1.5957457935

C,0,5.033290097,0.8711523776,-1.4360762331

C,0,6.2946432775,1.2053872217,-1.9270662143

C,0,7.0484033629,0.2081813176,-2.5626602552

C,0,6.5615162146,-1.098459817,-2.7069741192

C,0,5.2926558856,-1.4351674113,-2.2221969186

C,0,3.1910396337,-0.5155076804,-1.0042957869

C,0,4.006223791,1.6428874247,-0.6514153331

H,0,6.7041686132,2.2103647187,-1.8316110312

H,0,8.0366854073,0.4589055337,-2.9555416076

H,0,7.1746623131,-1.8510729498,-3.2077470353

H,0,4.8721829716,-2.4370336561,-2.3303033107

O,0,2.4306050858,-1.4551383123,-0.9237178583

N,0,2.9335837347,0.7723003134,-0.5416982791

H,0,1.990664035,0.9912044589,-0.1821203872

C,0,3.7020191425,3.0837207383,-0.8883424049

C,0,4.7262209682,4.043041511,-0.9795714732

C,0,2.3676896295,3.5167171202,-0.9725977775

C,0,4.4281582634,5.3935658819,-1.1569126563

H,0,5.769578683,3.7427418708,-0.8864534712

C,0,2.072335007,4.8704784978,-1.138359311

H,0,1.5438713923,2.806347264,-0.9007518504

C,0,3.097012886,5.813803239,-1.2341099195

H,0,5.2404959008,6.1211026779,-1.2252770524

H,0,1.0309819369,5.1838016631,-1.1906422802

H,0,2.8591321702,6.8723930827,-1.3631832532

C,0,4.841978304,1.6881602322,1.2028714526

C,0,3.7047599476,2.1597395349,1.9651882628

C,0,2.7735042558,1.2974217606,2.4592471761

C,0,2.995560614,-0.1438183475,2.2691221874

C,0,4.3237078608,-0.6062521205,1.8386531296

C,0,5.2212118192,0.3082517592,1.3796083199

H,0,5.6445207356,2.4057172095,1.0173653797

H,0,3.5418166143,3.2375085114,2.0454050259

H,0,6.1910563092,-0.0250493764,1.0030120598

O,0,2.1047996012,-0.9963267007,2.4885329883

C,0,1.5147510772,1.7610817023,3.1364964222

H,0,1.2035365963,1.0632919879,3.9270609516

H,0,0.6895411619,1.8296978706,2.4119326525

H,0,1.6549449014,2.7596368014,3.5750963171

C,0,4.5567970621,-2.0825096332,1.826749887

H,0,3.8707369487,-2.5505825402,1.103199115

H,0,4.3216371363,-2.5359836644,2.8012454083

H,0,5.592738082,-2.3206775113,1.5463508308

H,0,0.6953837217,-0.8345107292,2.2328024279

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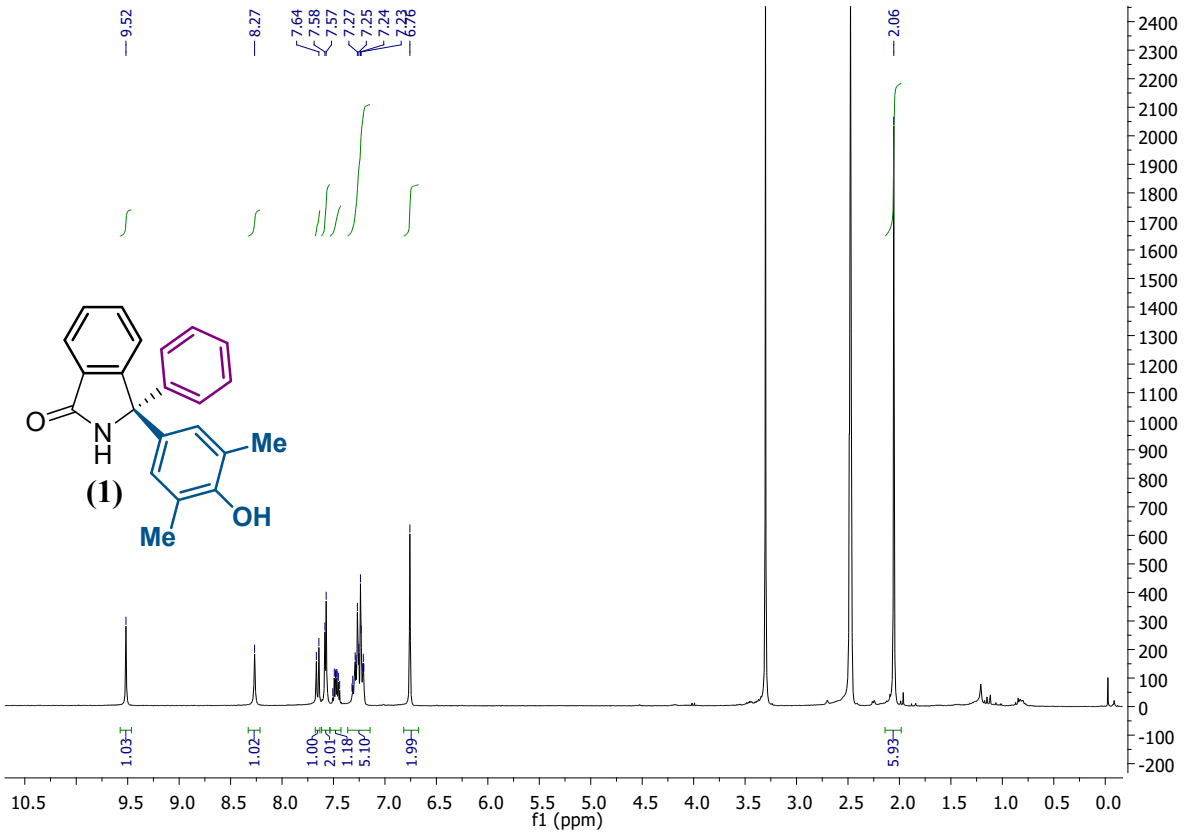
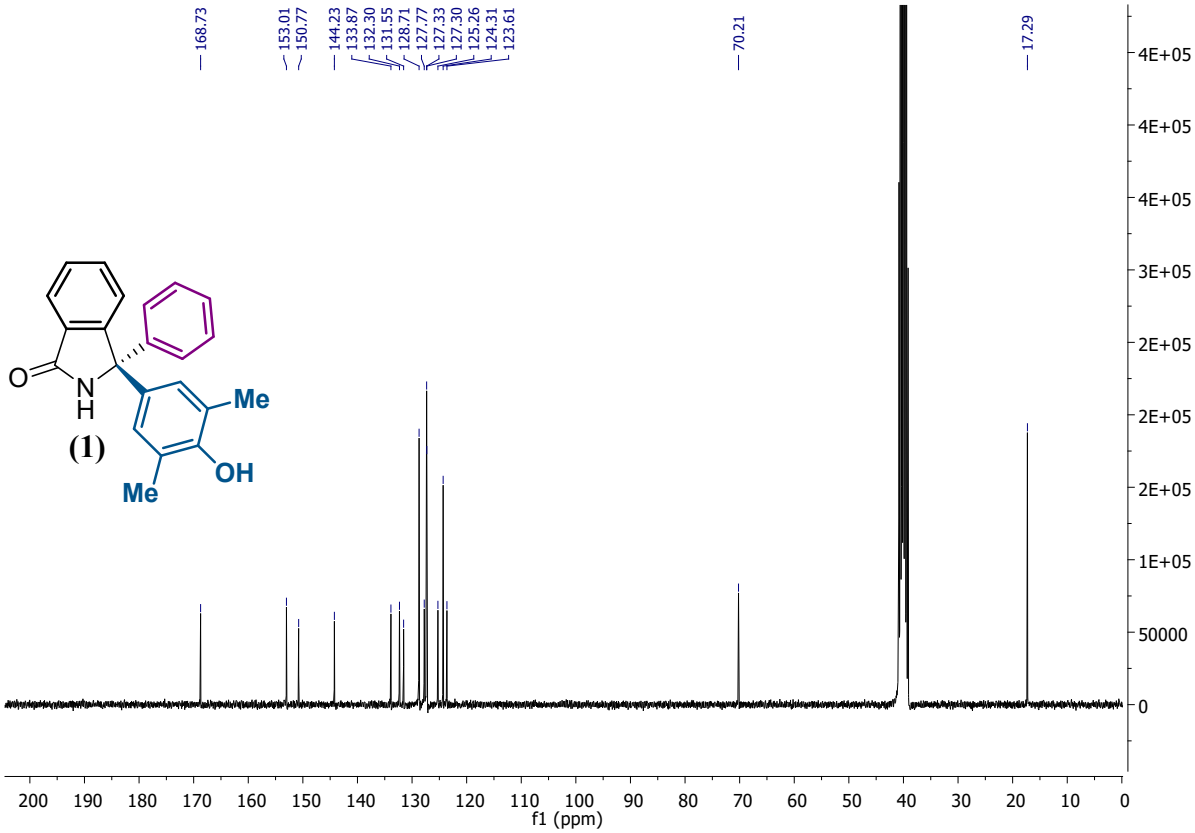
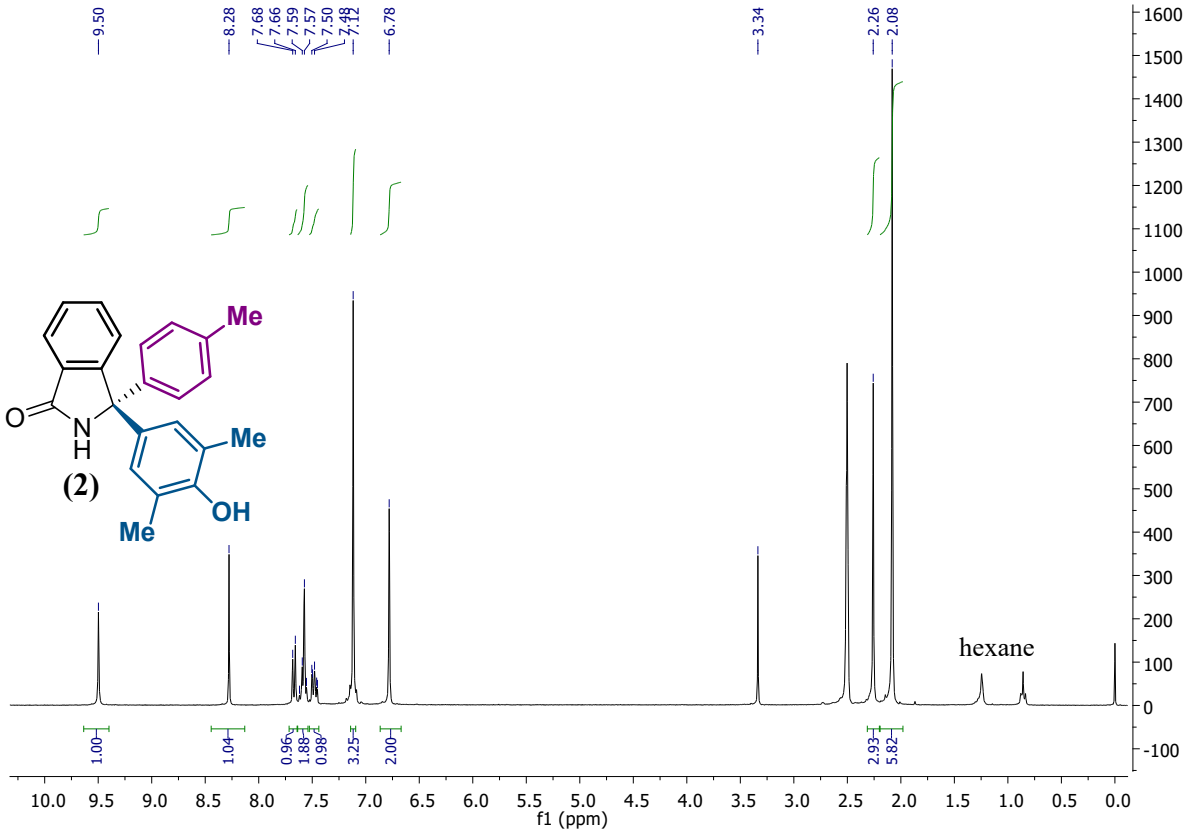
7. NMR Spectra



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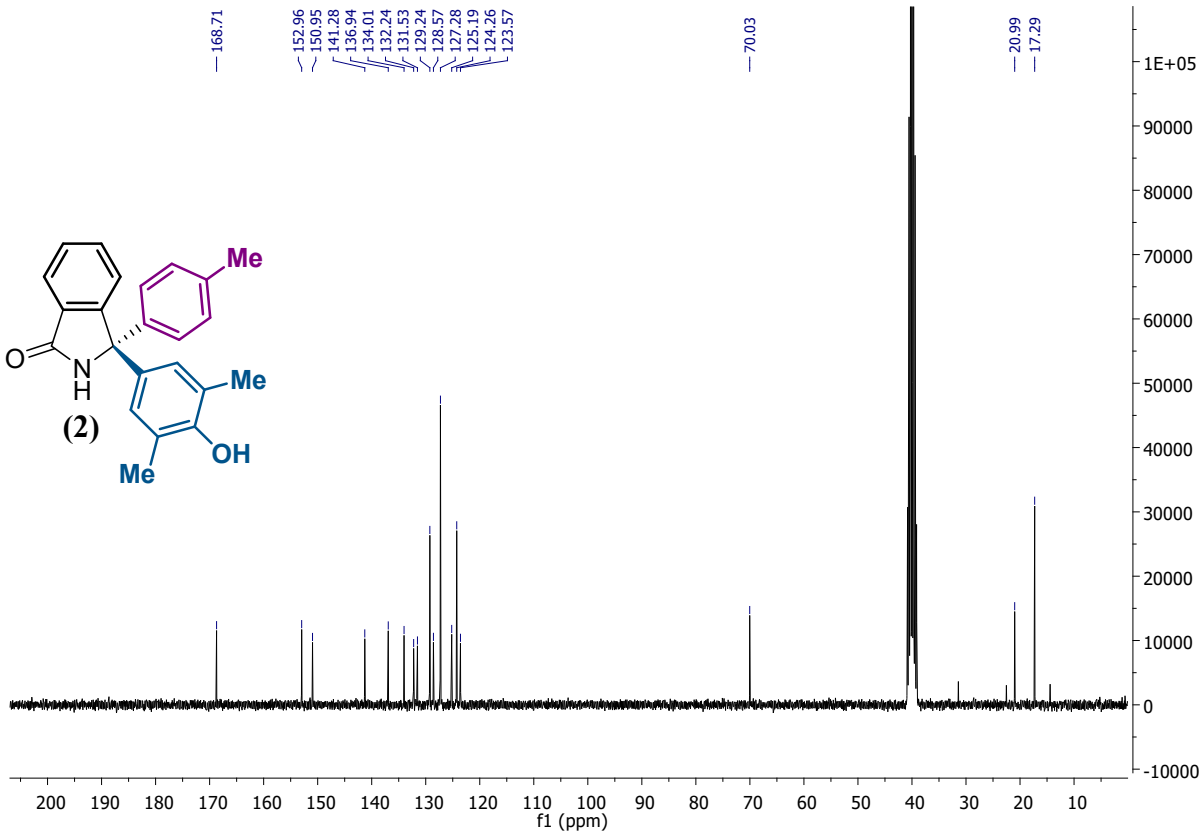
7.66
7.59
7.57
7.50
7.48
7.12
6.78
3.34
2.26
2.08
Me
Me
OH
Me
O
N
H
(2)
hexane
1.00
1.04
0.96
1.88
0.98
3.25
2.00
2.93
5.82
f1 (ppm)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150.95
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136.94
134.01
132.24
131.53
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128.57
127.28
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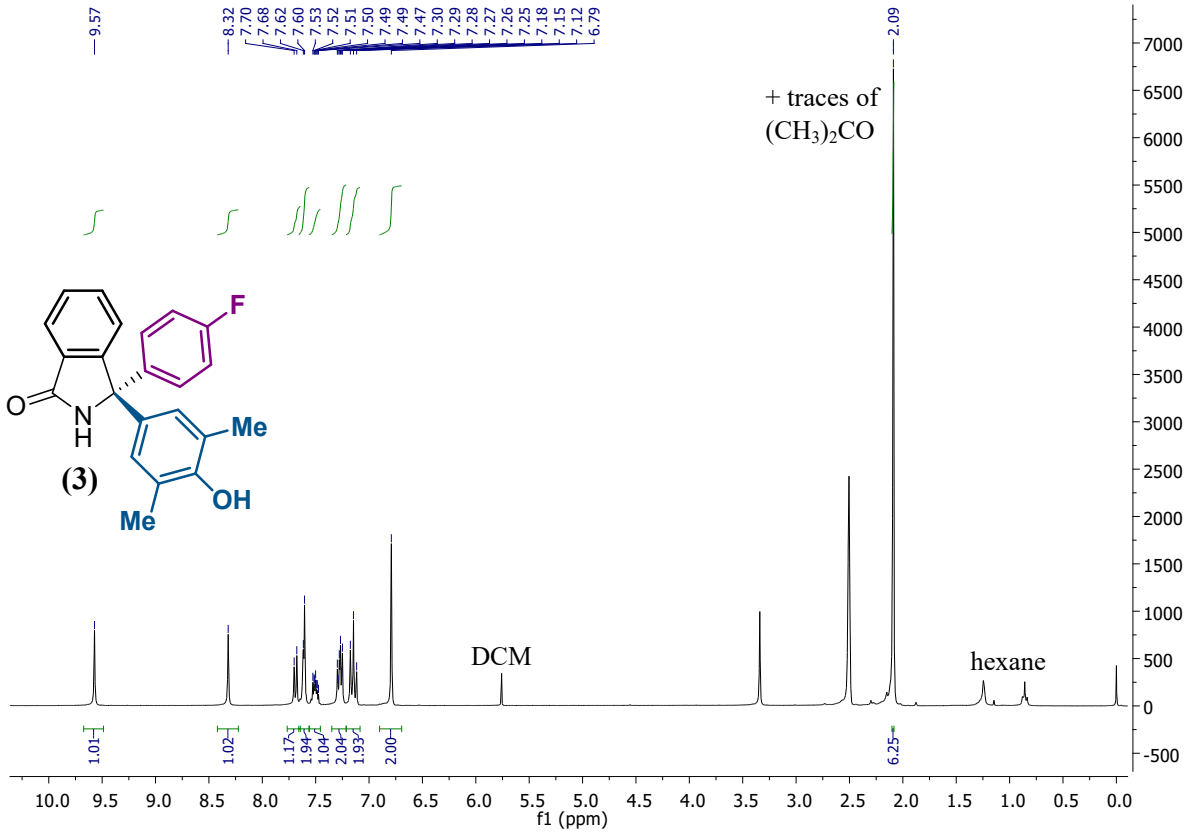
124.26
123.57
70.03
20.99
17.29
Me
Me
OH
Me
O
N
H
(2)
f1 (ppm)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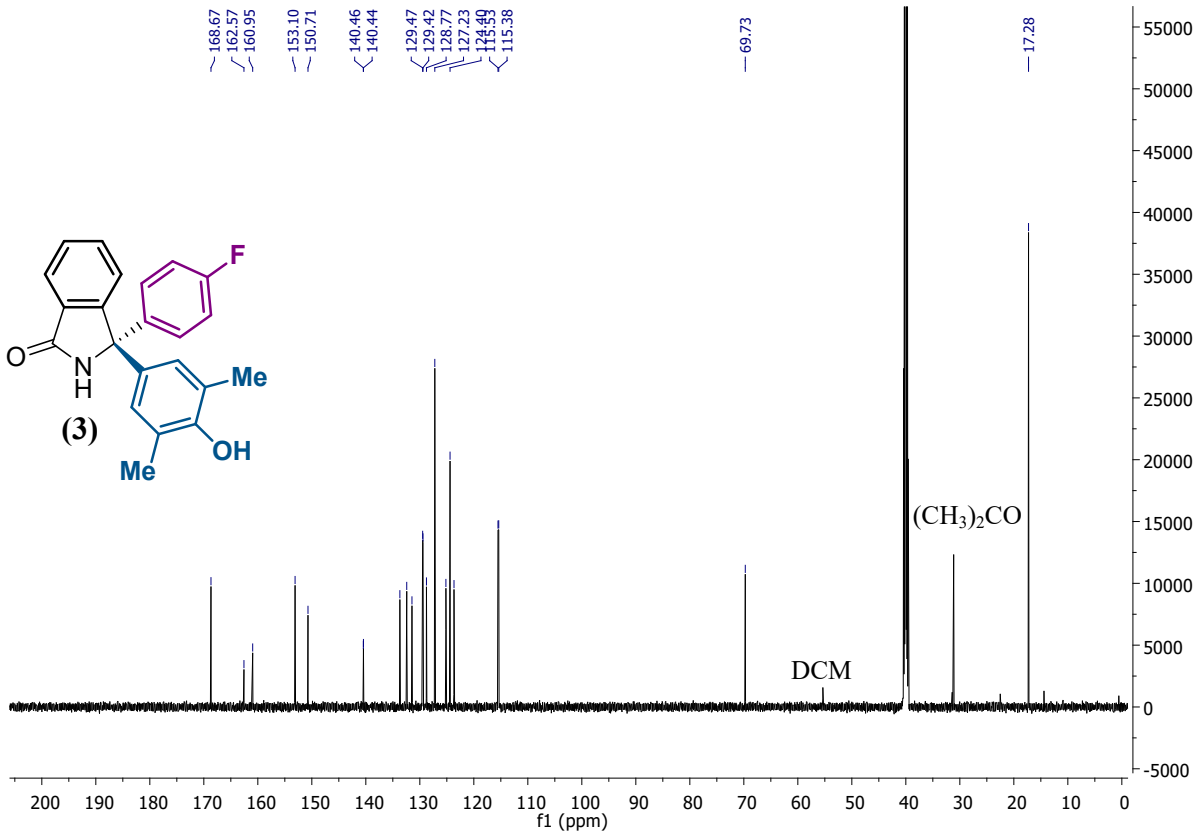
8.32
7.70
7.68
7.62
7.60
7.53
7.52
7.51
7.50
7.49
7.49
7.47
7.30
7.29
7.28
7.27
7.26
7.25
7.18
7.15
7.12
6.79
2.09
+ traces of
(CH3)2CO
F
O
N
H
Me
OH
Me
(3)
DCM
hexane
1.01
1.02
1.17
1.94
1.04
2.04
1.93
2.00
6.25
f1 (ppm)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150.71
140.46
140.44
129.47
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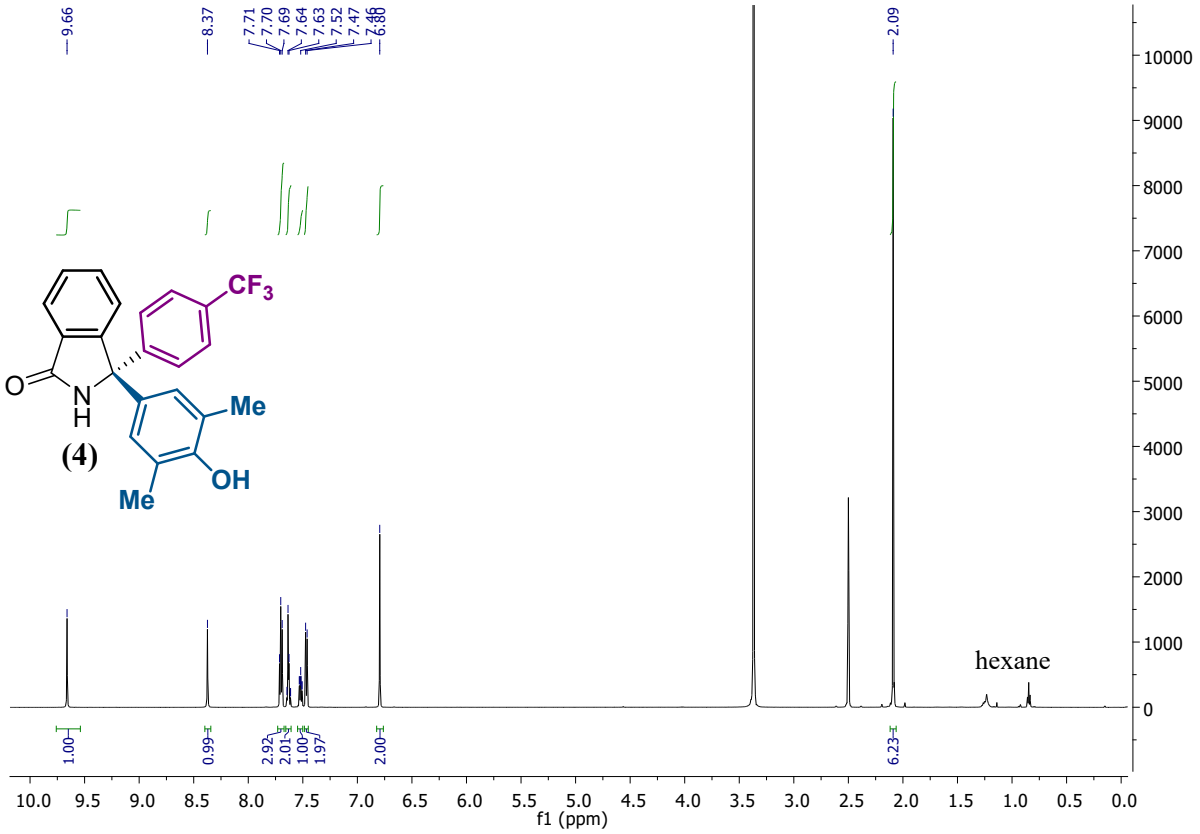
128.77
127.23
124.40
115.53
115.38
69.73
17.28
F
O
N
H
Me
OH
Me
(3)
(CH3)2CO
DCM
f1 (ppm)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7.64
7.63
7.52
7.47
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CF3
O
N
H
Me
OH
Me
(4)
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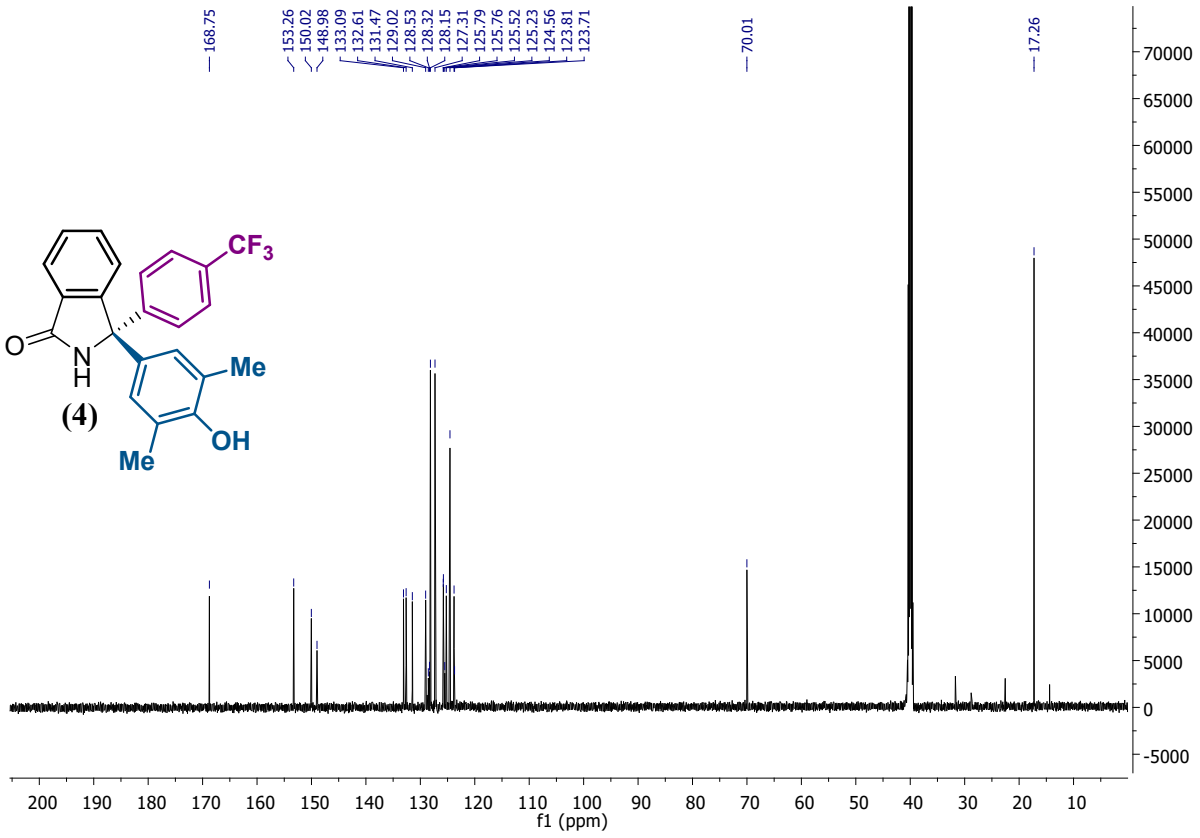
0.99
2.92
2.01
1.00
1.97
2.00
6.23
f1 (ppm)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125.79
125.76
125.52
125.23
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123.71
70.01
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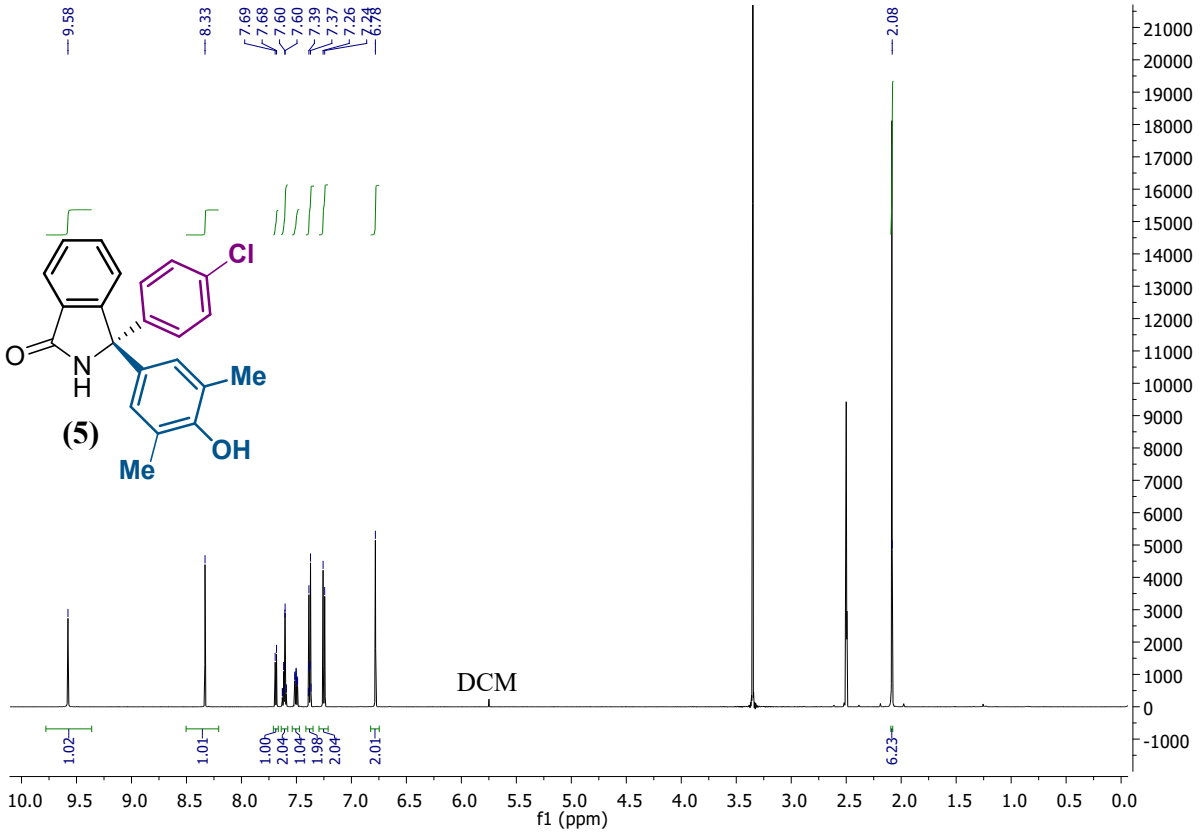
O
N
H
Me
OH
Me
(4)
f1 (ppm)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7.60
7.60
7.39
7.37
7.26
6.78
2.08
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O
N
H
Me
OH
Me
(5)
DCM
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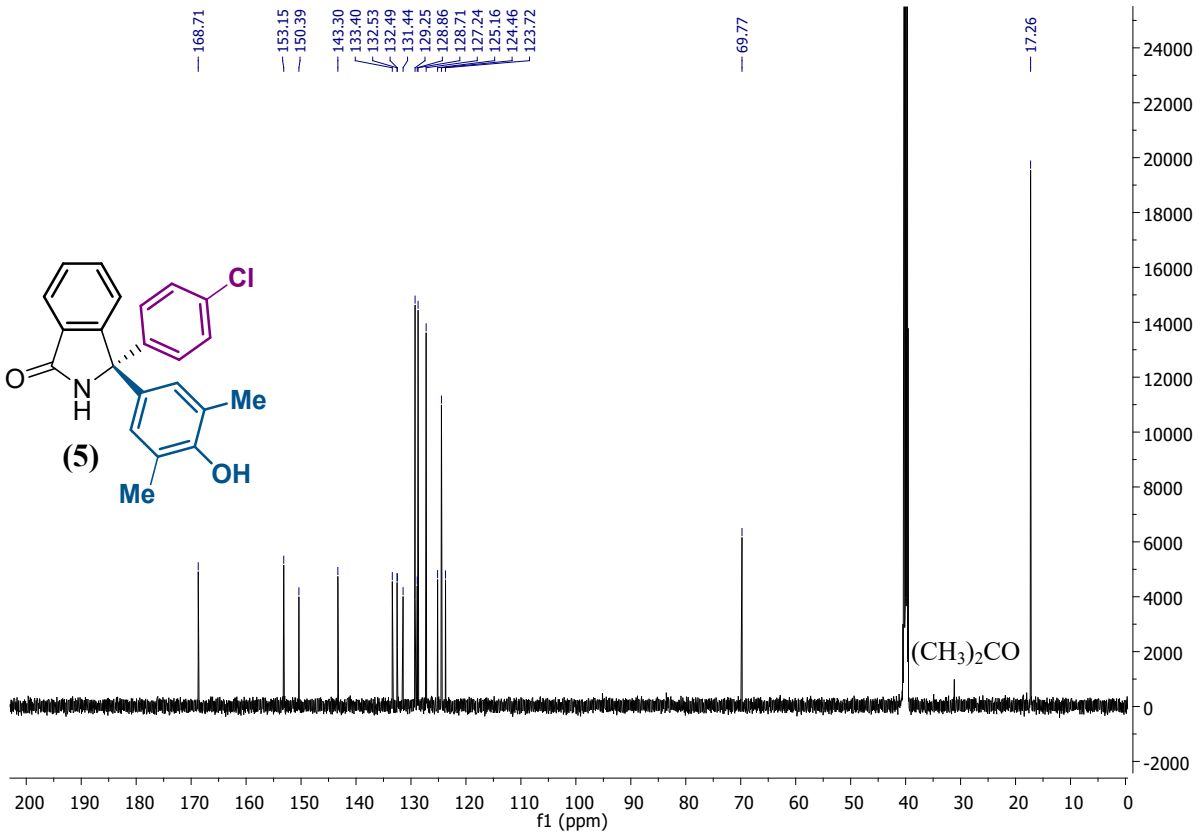
1.01
1.00
2.04
1.04
1.98
2.04
2.01
6.23
f1 (ppm)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132.49
131.44
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128.71
127.24
125.16
124.46
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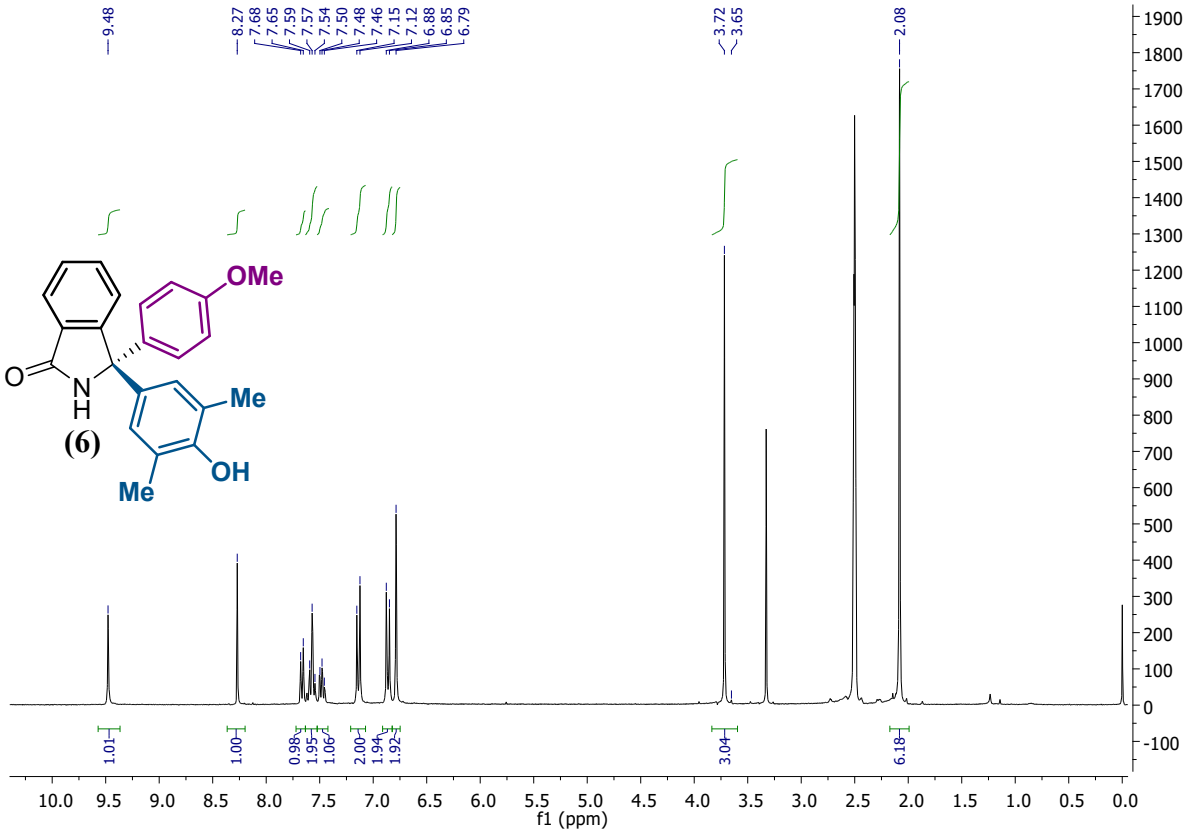
69.77
17.26
Cl
O
N
H
Me
OH
Me
(5)
(CH3)2CO
f1 (ppm)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7.46
7.15
7.12
6.88
6.85
6.79
3.72
3.65
2.08
OMe
Me
OH
Me
O
N
H
(6)
1.01
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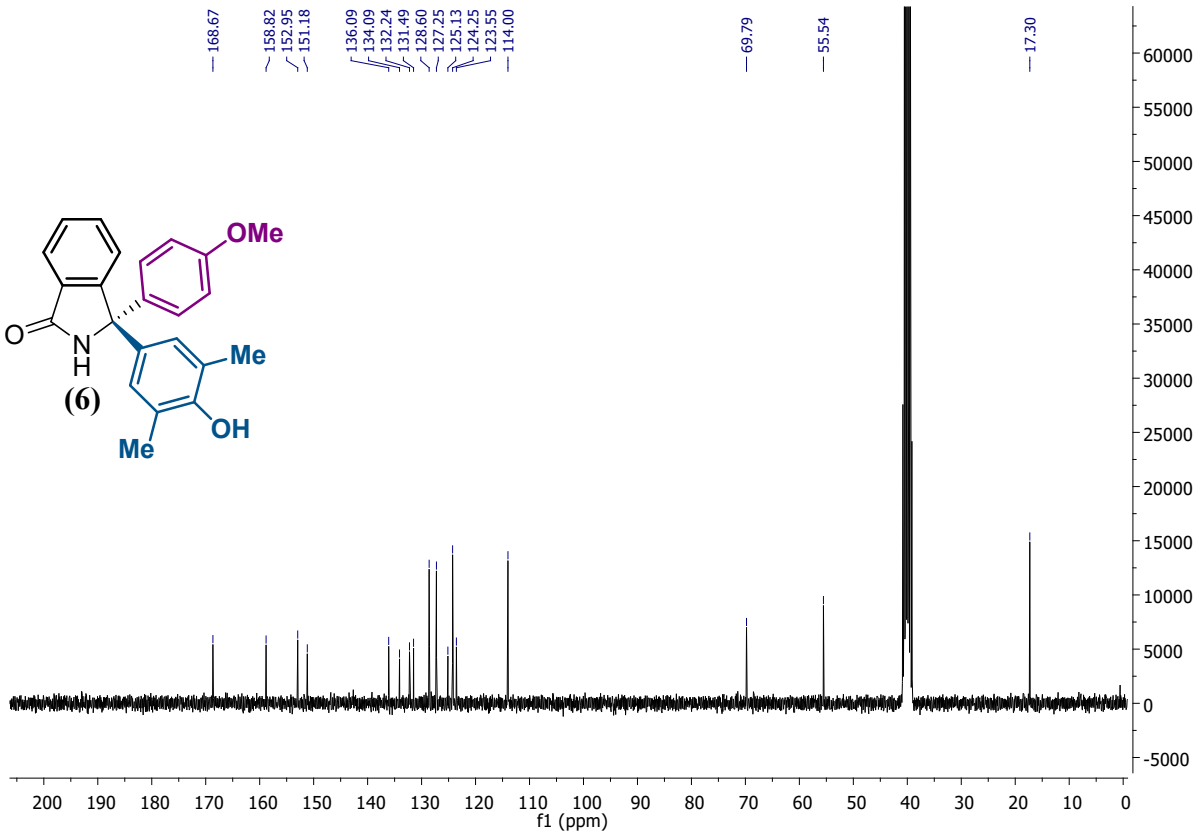
0.98
1.95
1.06
2.00
1.94
1.92
3.04
6.18
f1 (ppm)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127.25
125.13
124.25
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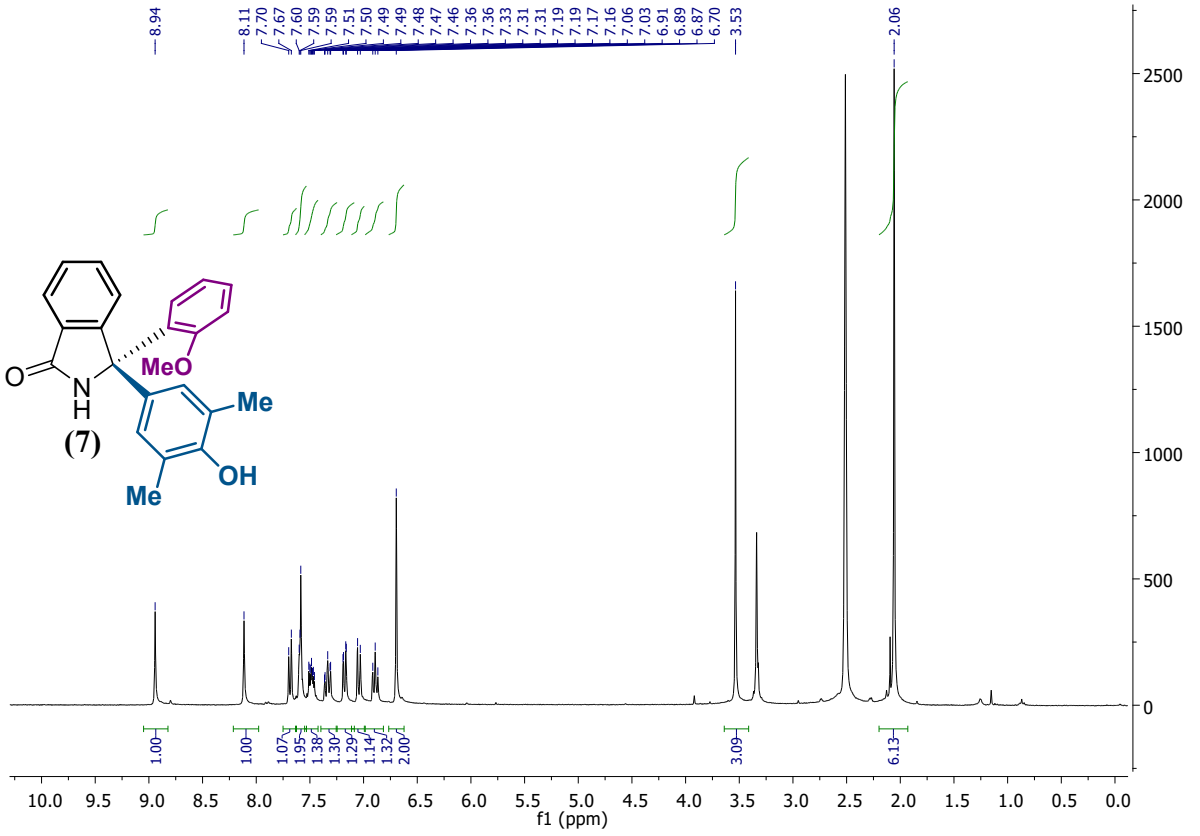
69.79
55.54
17.30
OMe
Me
OH
Me
O
N
H
(6)
f1 (ppm)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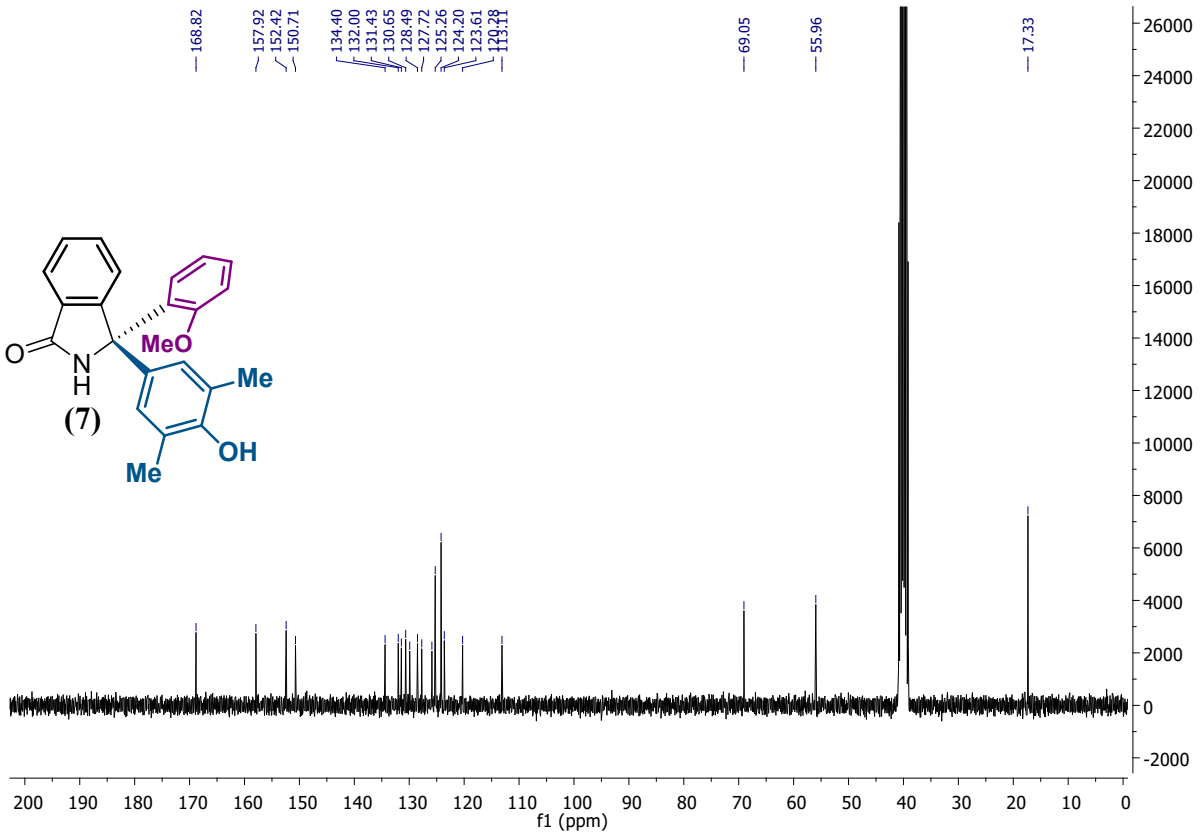
7.50
7.49
7.49
7.48
7.47
7.46
7.36
7.36
7.33
7.31
7.31
7.19
7.19
7.17
7.16
7.06
7.03
6.91
6.89
6.87
6.70
3.53
2.06
MeO
Me
OH
Me
O
N
H
(7)
1.00
1.00
1.07
1.95
1.38
1.30
1.29
1.14
1.32
2.00
3.09
6.13
f1 (ppm)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130.65
128.49
127.72
125.26
124.20
123.61
120.28
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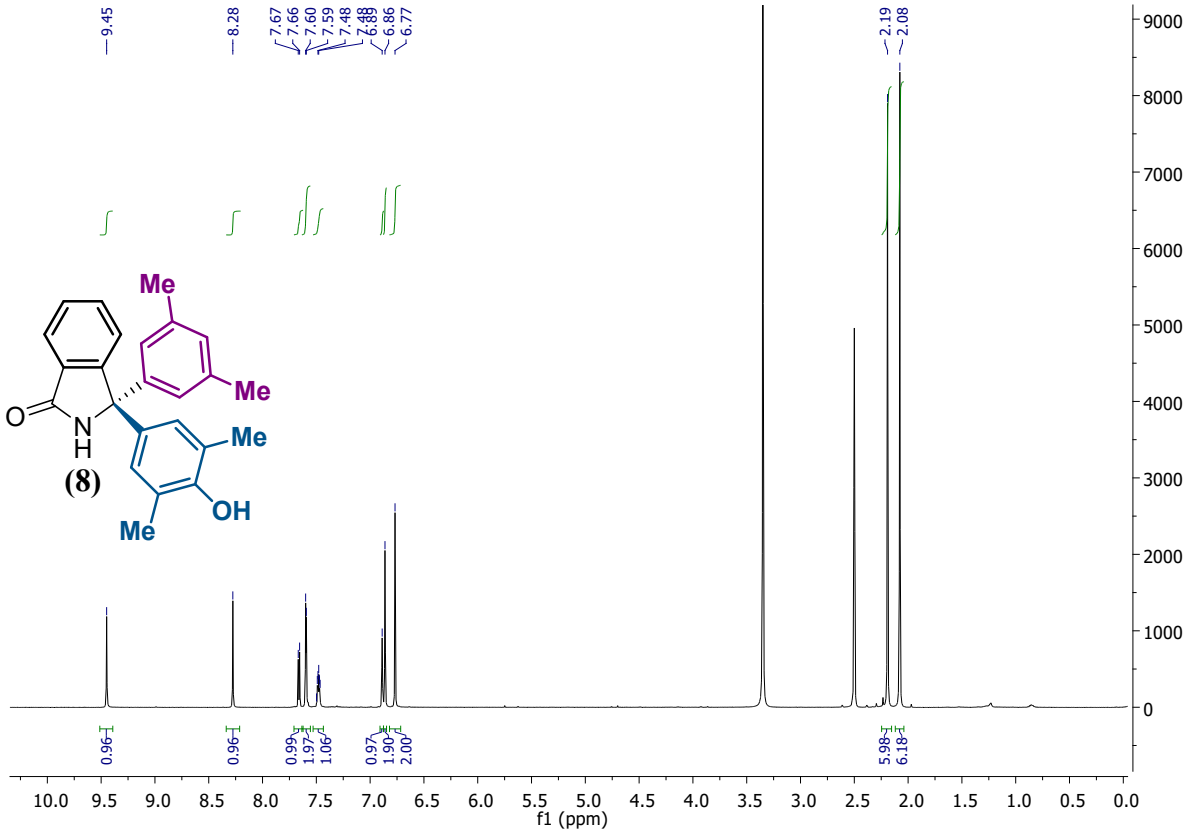
69.05
55.96
17.33
MeO
Me
OH
Me
O
N
H
(7)
f1 (ppm)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2.19
2.08
Me
Me
Me
Me
OH
O
N
H
(8)
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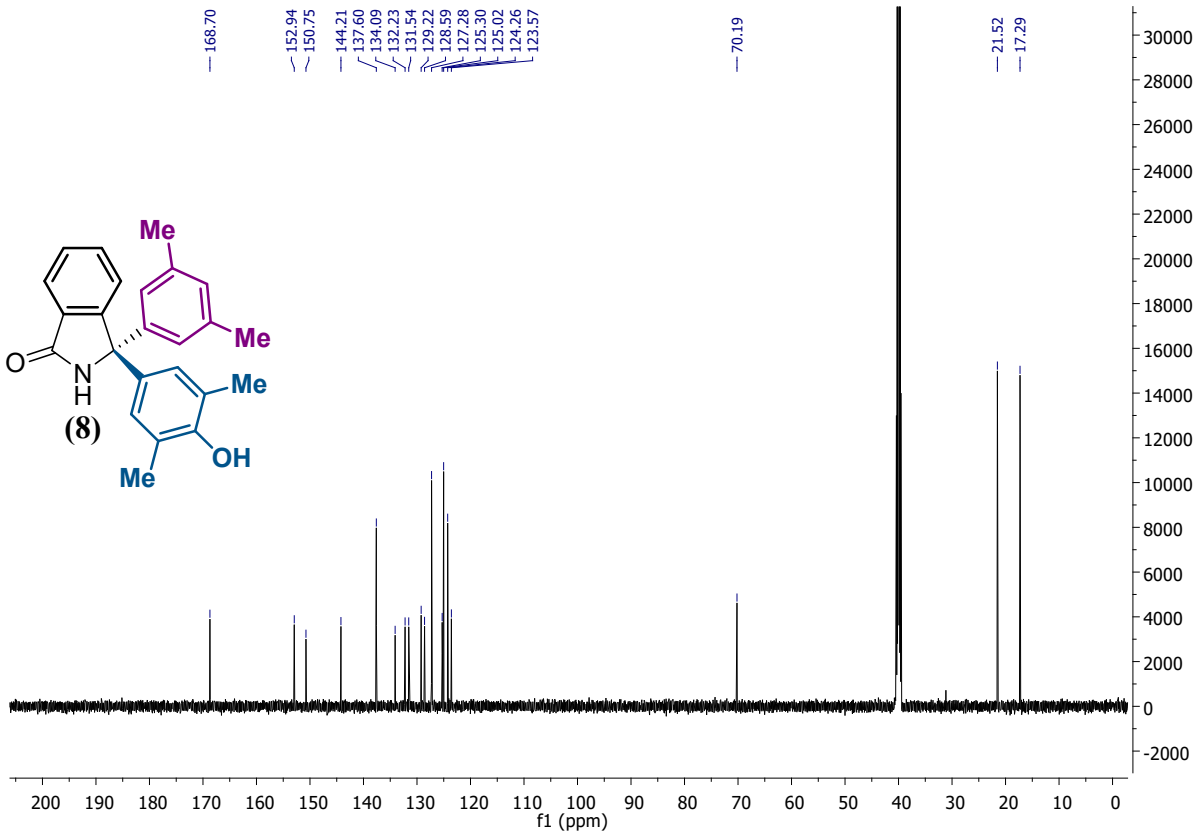
0.99
1.97
1.06
0.97
1.90
2.00
5.98
6.18
f1 (ppm)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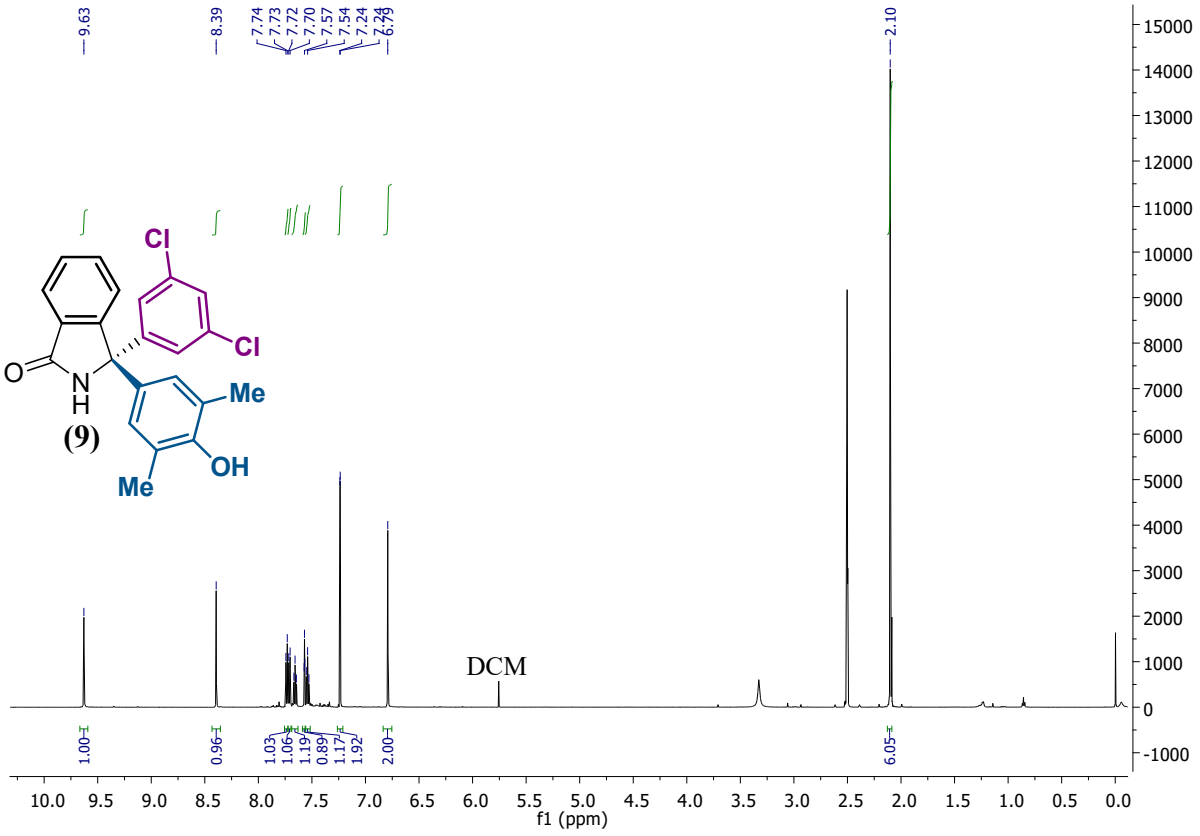
Me
Me
OH
O
N
H
(8)
f1 (ppm)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7.54
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6.79
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Cl
O
N
H
(9)
Me
OH
Me
DCM
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0.89
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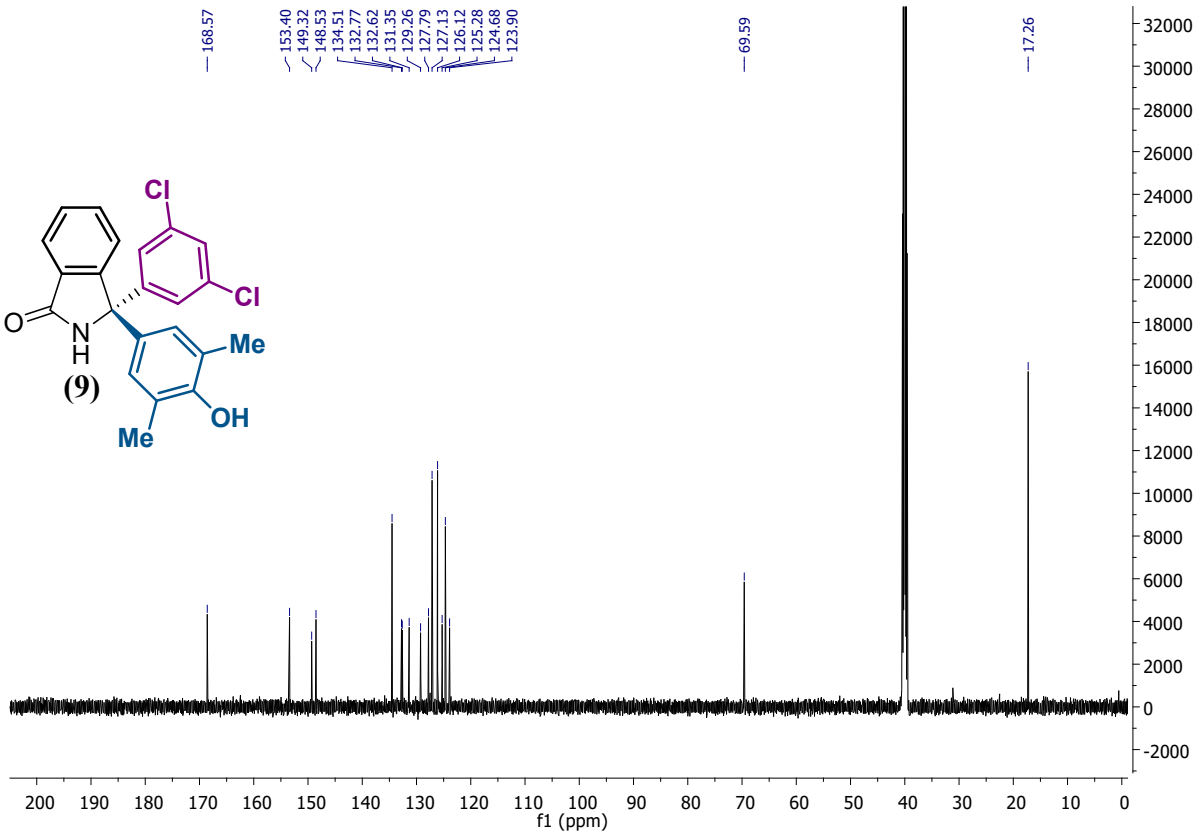
1.92
2.00
6.05
f1 (ppm)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69.59
17.26
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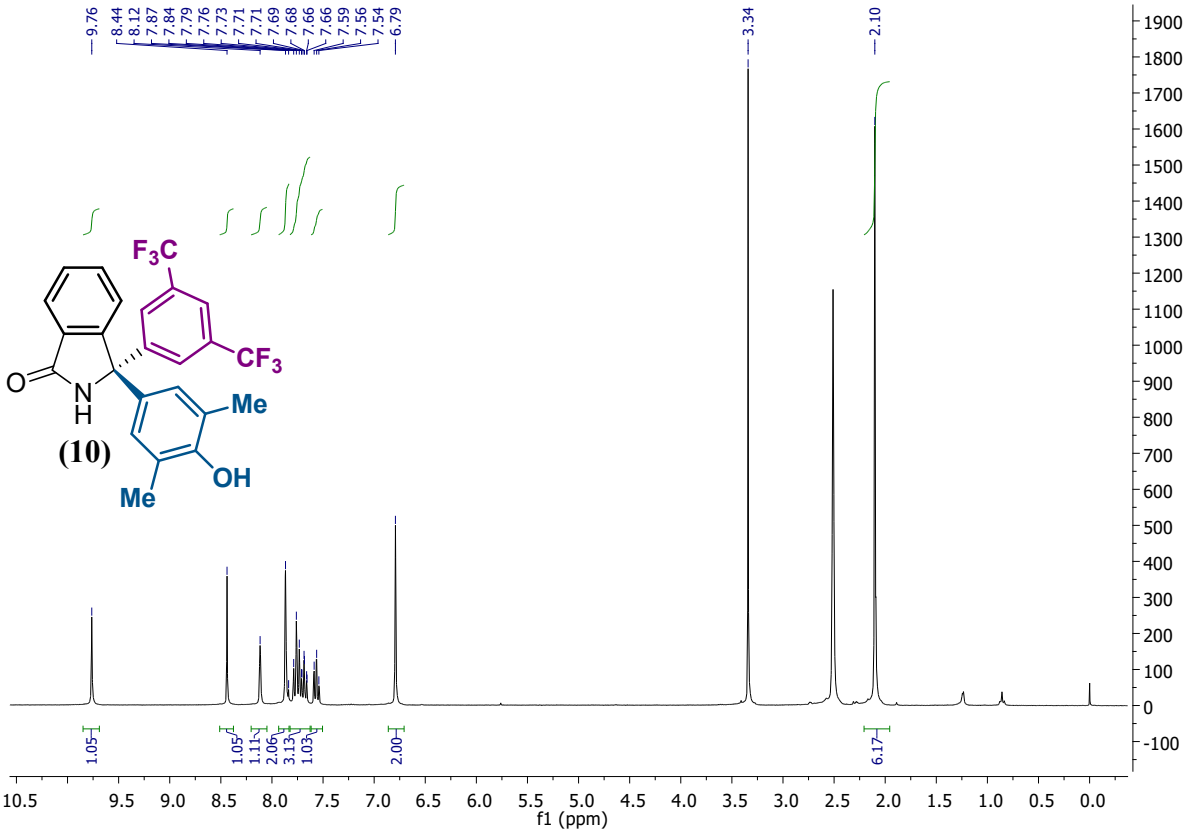
O
N
H
(9)
Me
OH
Me
f1 (ppm)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7.71
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7.68
7.66
7.66
7.59
7.56
7.54
6.79
3.34
2.10
F3C
CF3
O
N
H
Me
OH
Me
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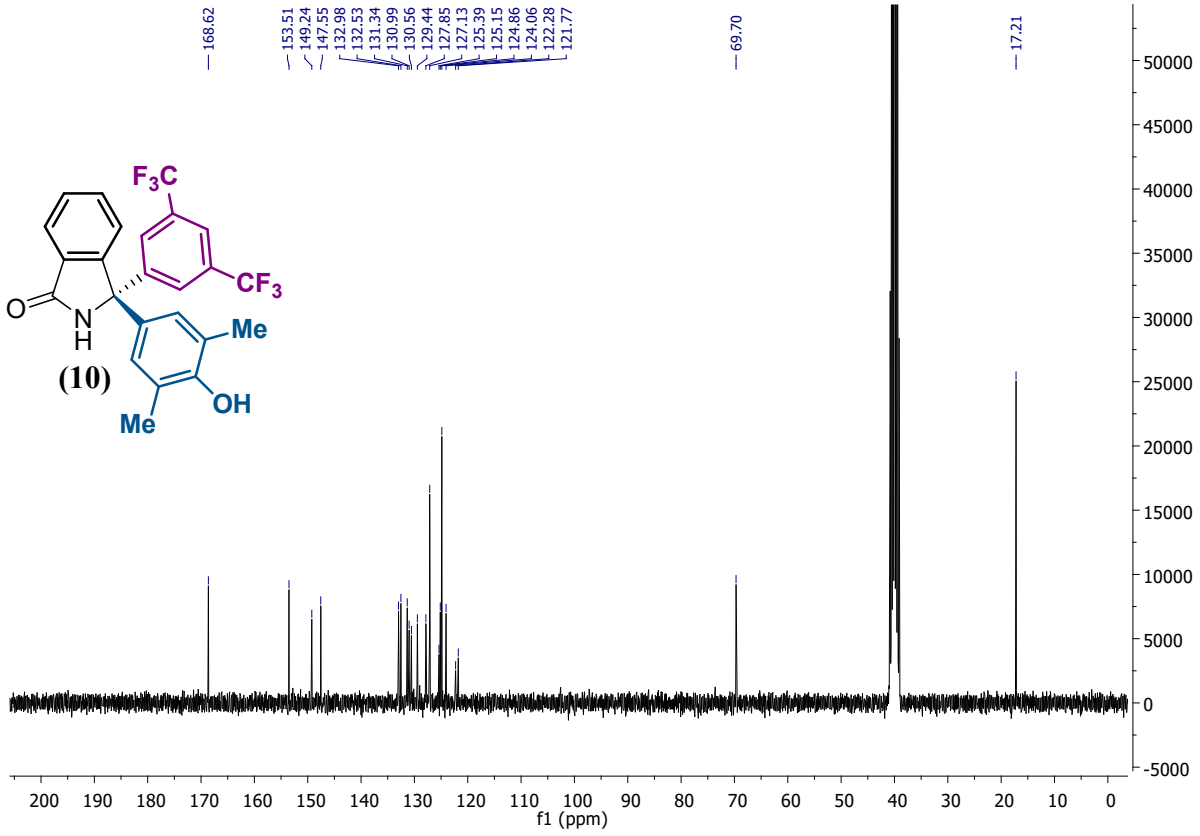
1.05
1.05
1.11
2.06
3.13
1.03
2.00
6.17
f1 (ppm)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125.39
125.15
124.86
124.06
122.28
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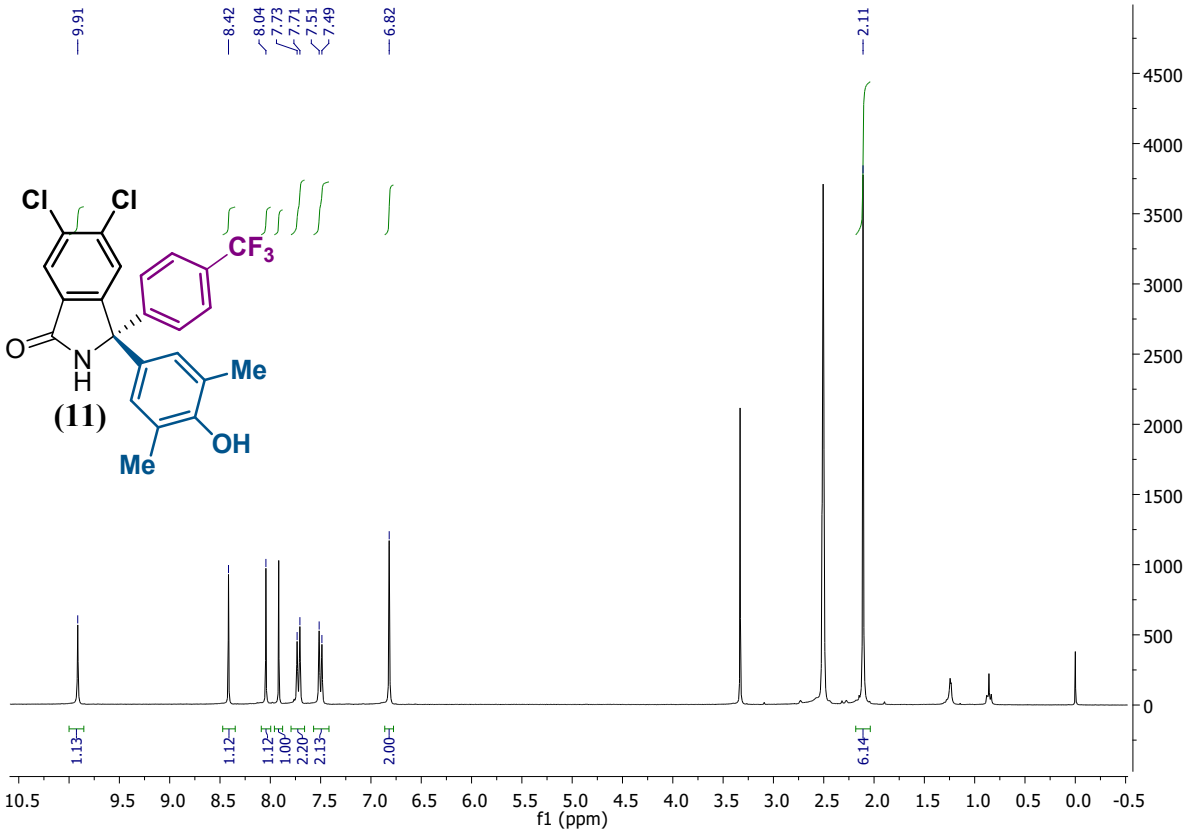
69.70
17.21
F3C
CF3
O
N
H
Me
OH
Me
(10)
f1 (ppm)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Cl
Cl
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O
N
H
Me
OH
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2.13
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6.14
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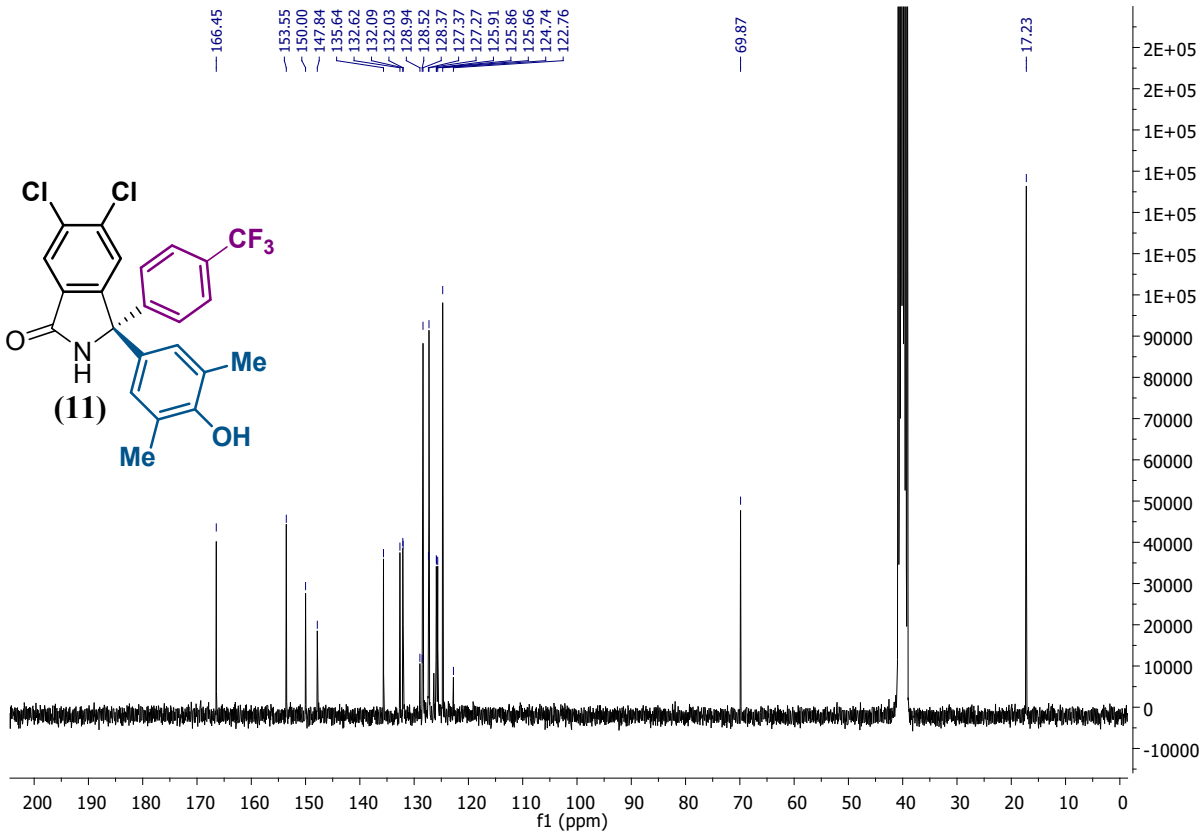
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127.27
125.91
125.86
125.66
124.74
122.76
69.87
17.23
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Cl
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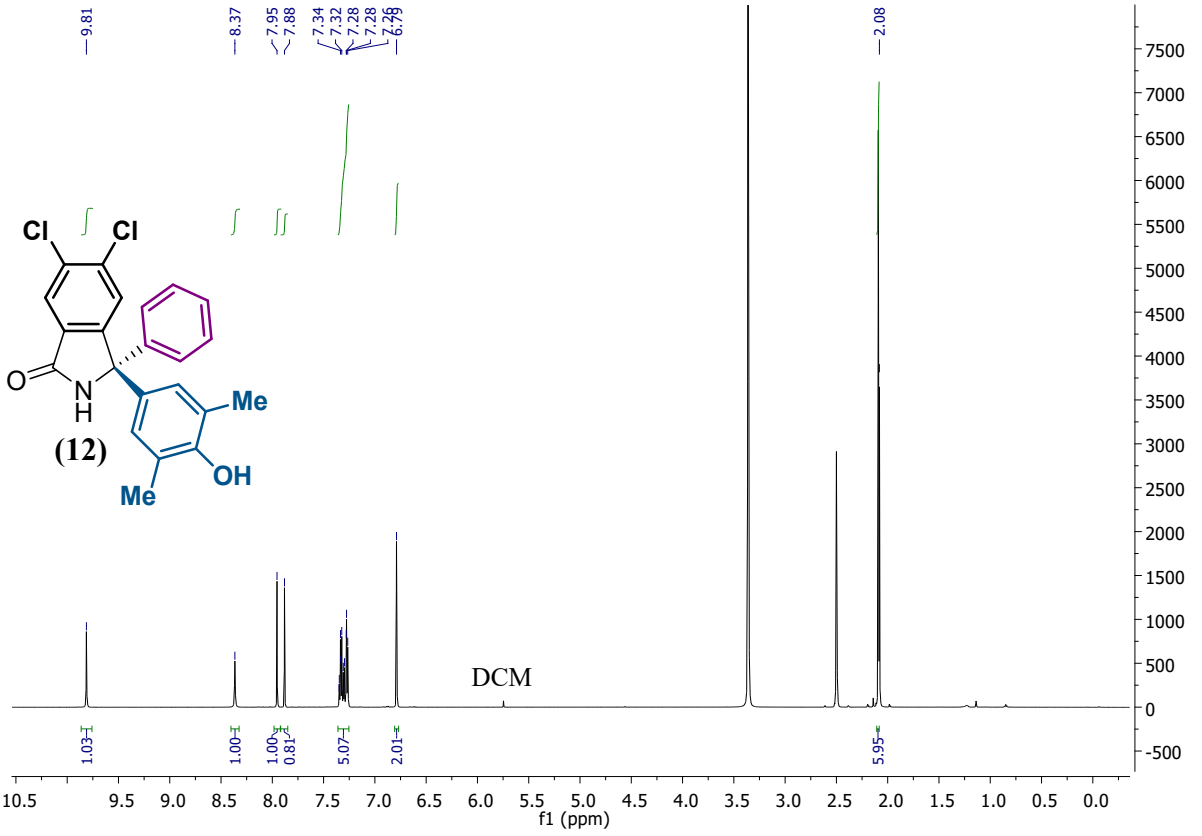
O
N
H
Me
OH
Me
(11)
f1 (ppm)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2.08
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Cl
O
N
H
Me
OH
Me
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1.00
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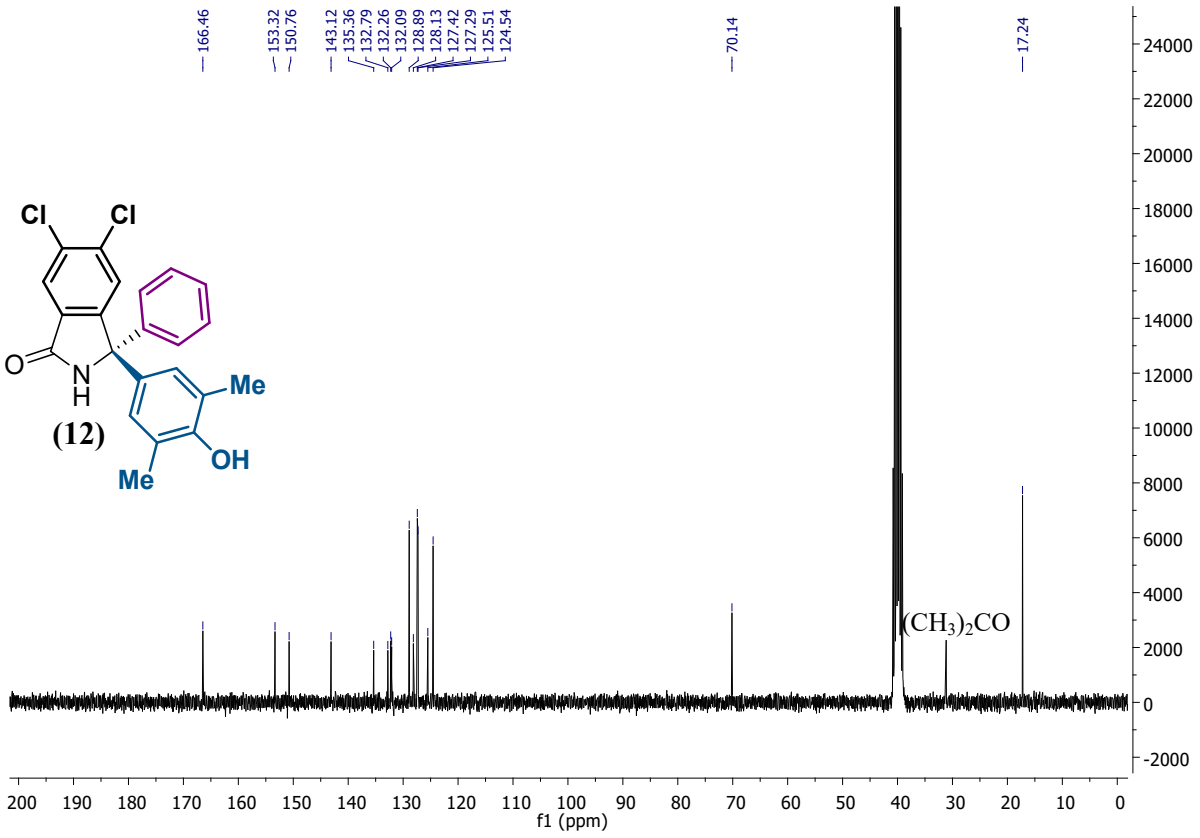
5.07
2.01
5.95
f1 (ppm)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125.51
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17.24
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N
H
Me
OH
Me
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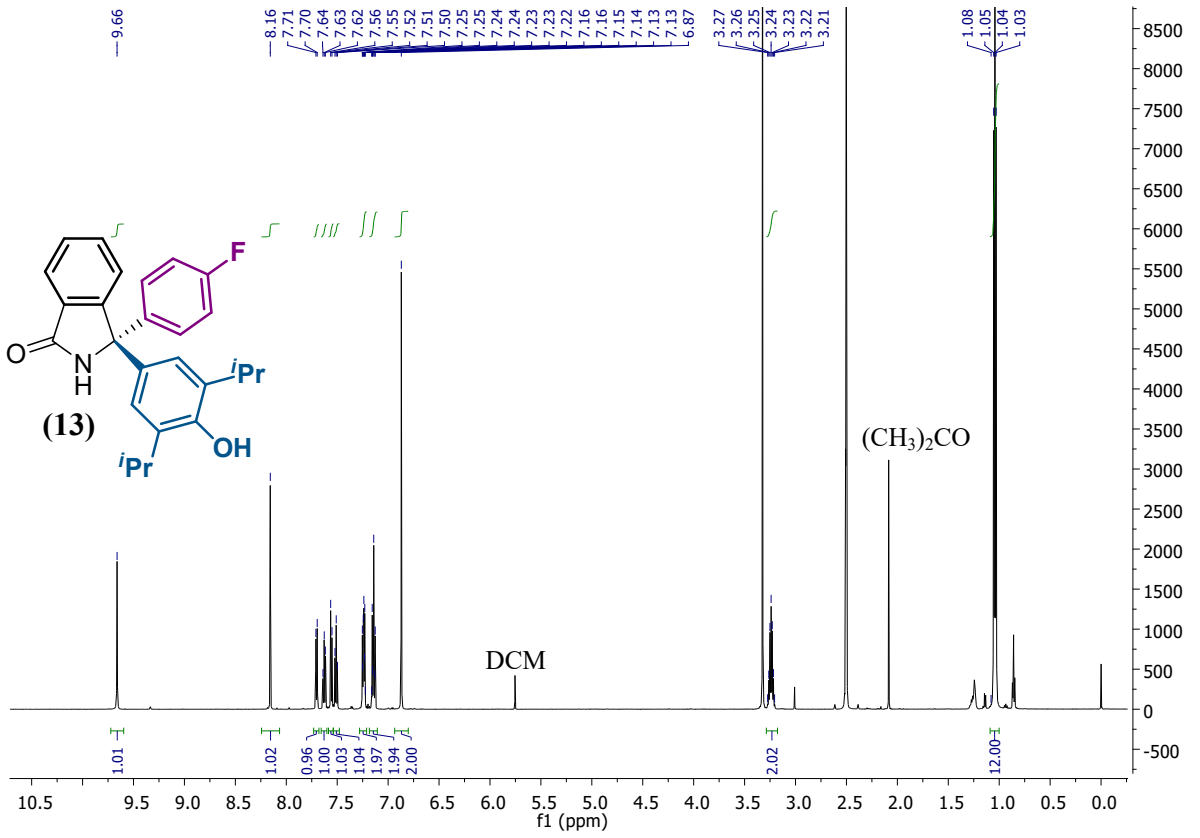
(CH3)2CO
f1 (ppm)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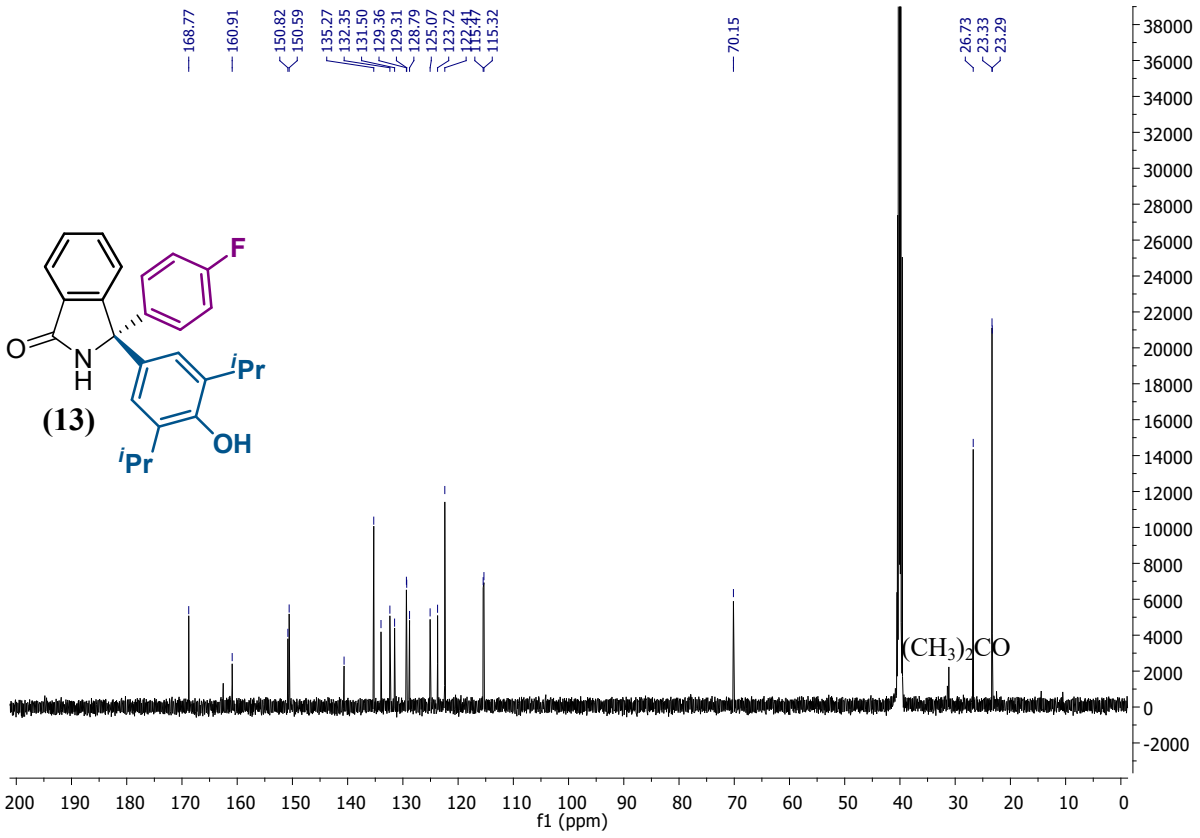
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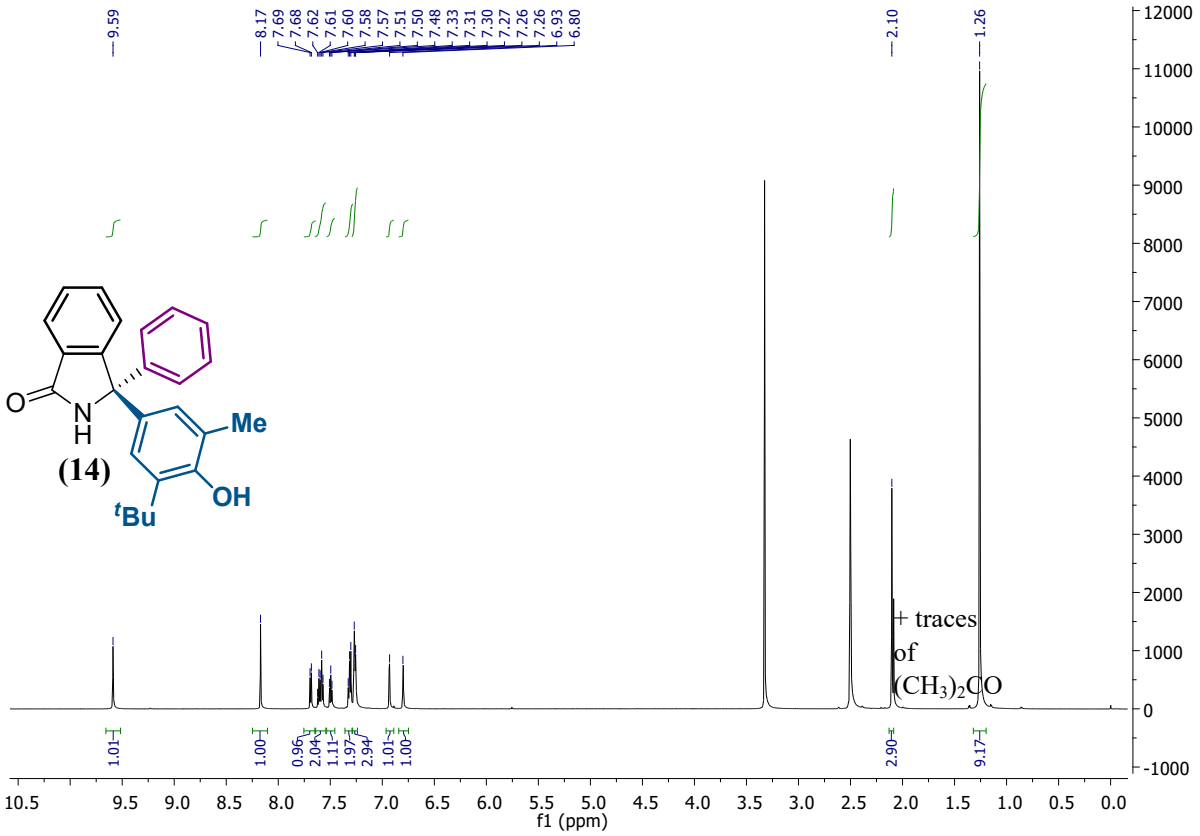
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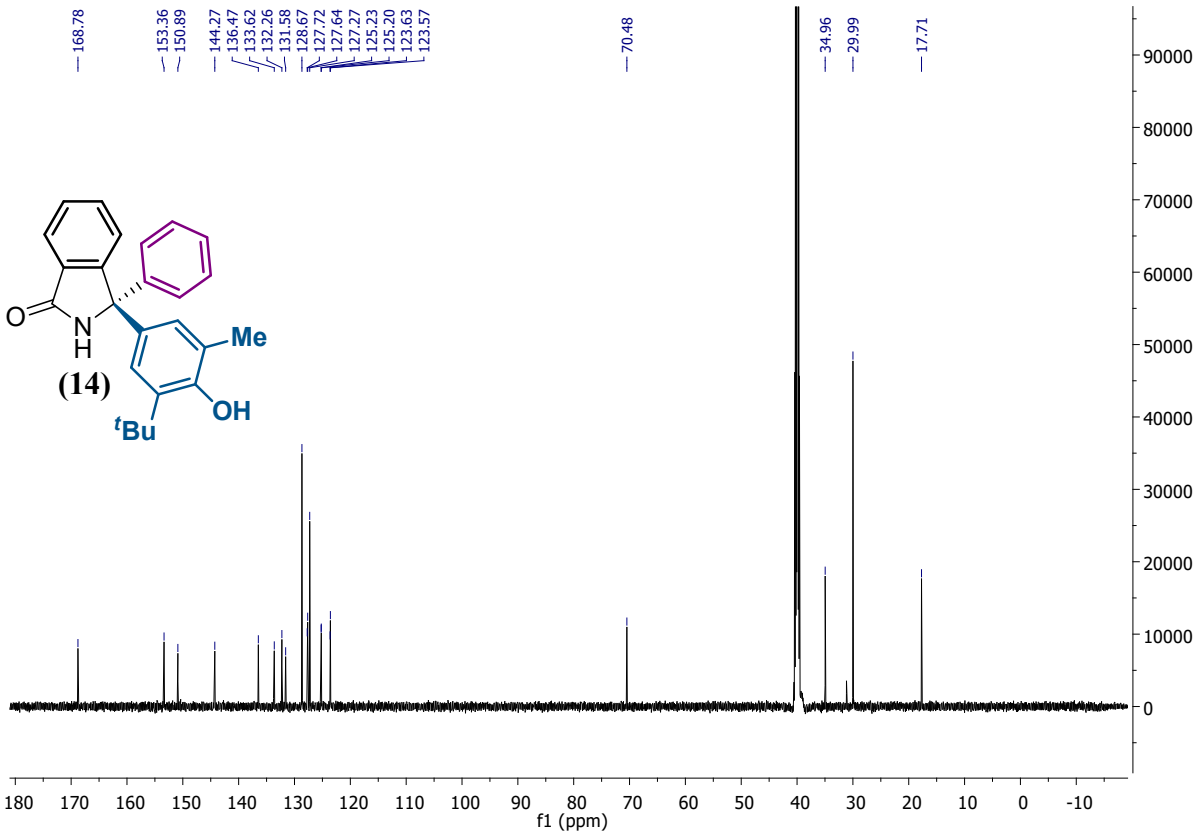
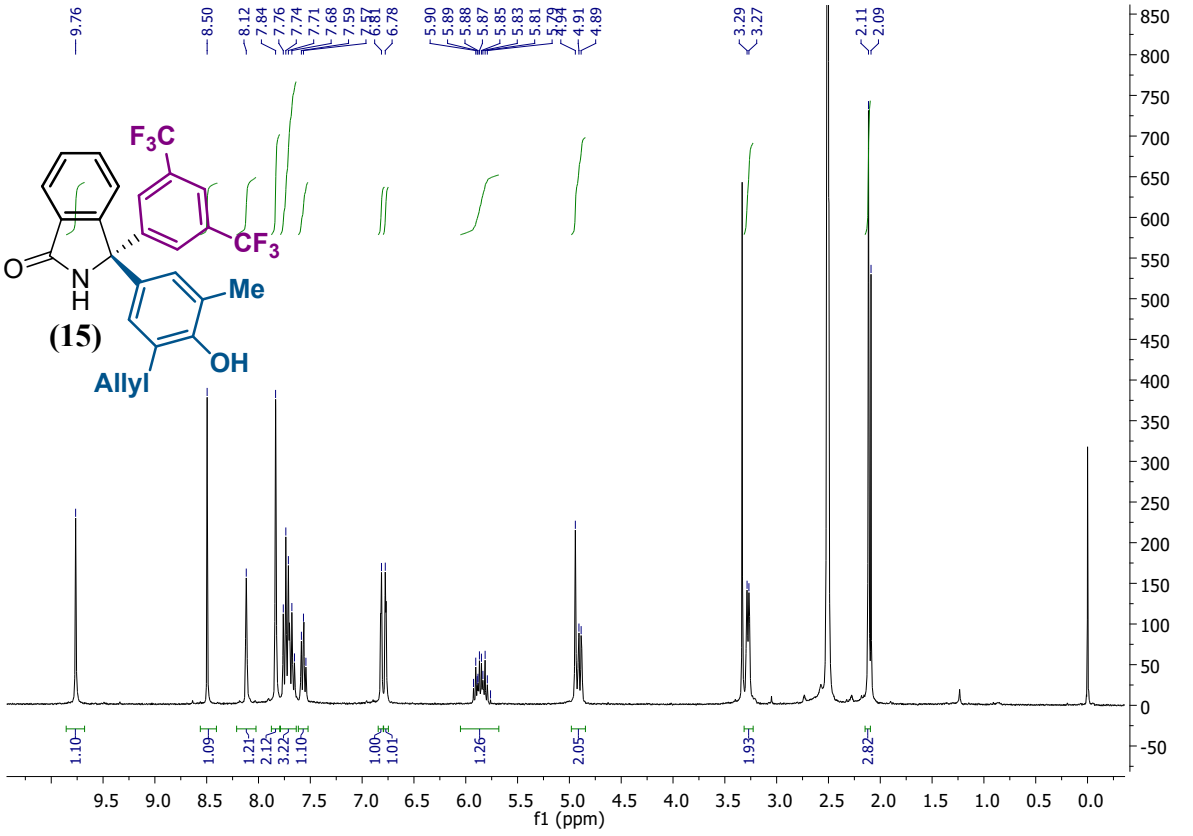
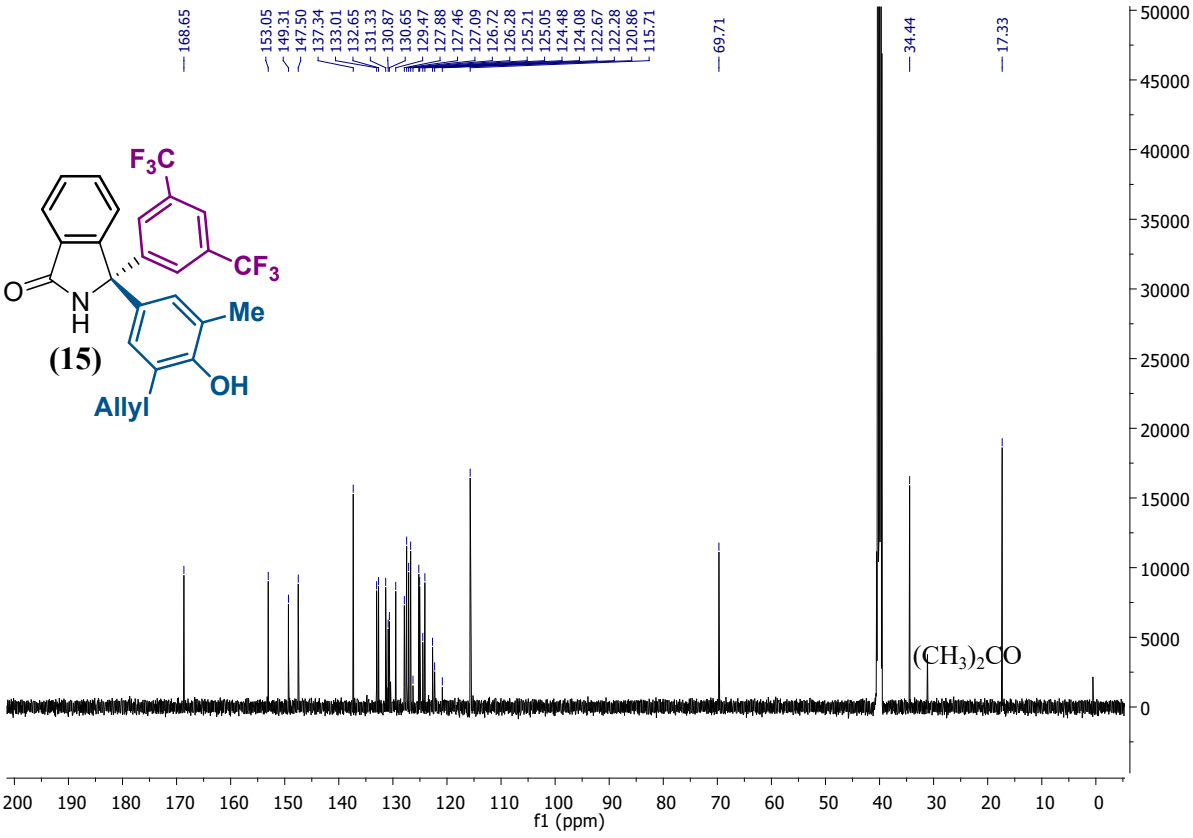
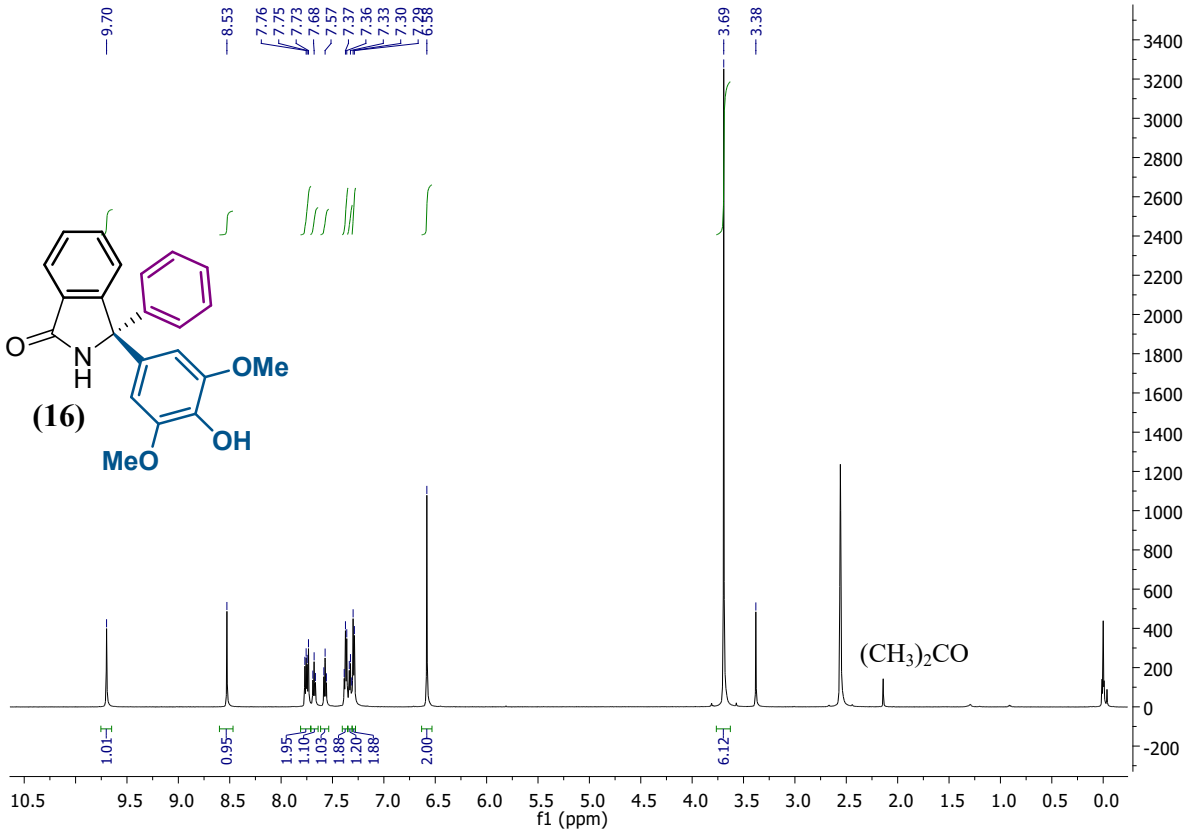
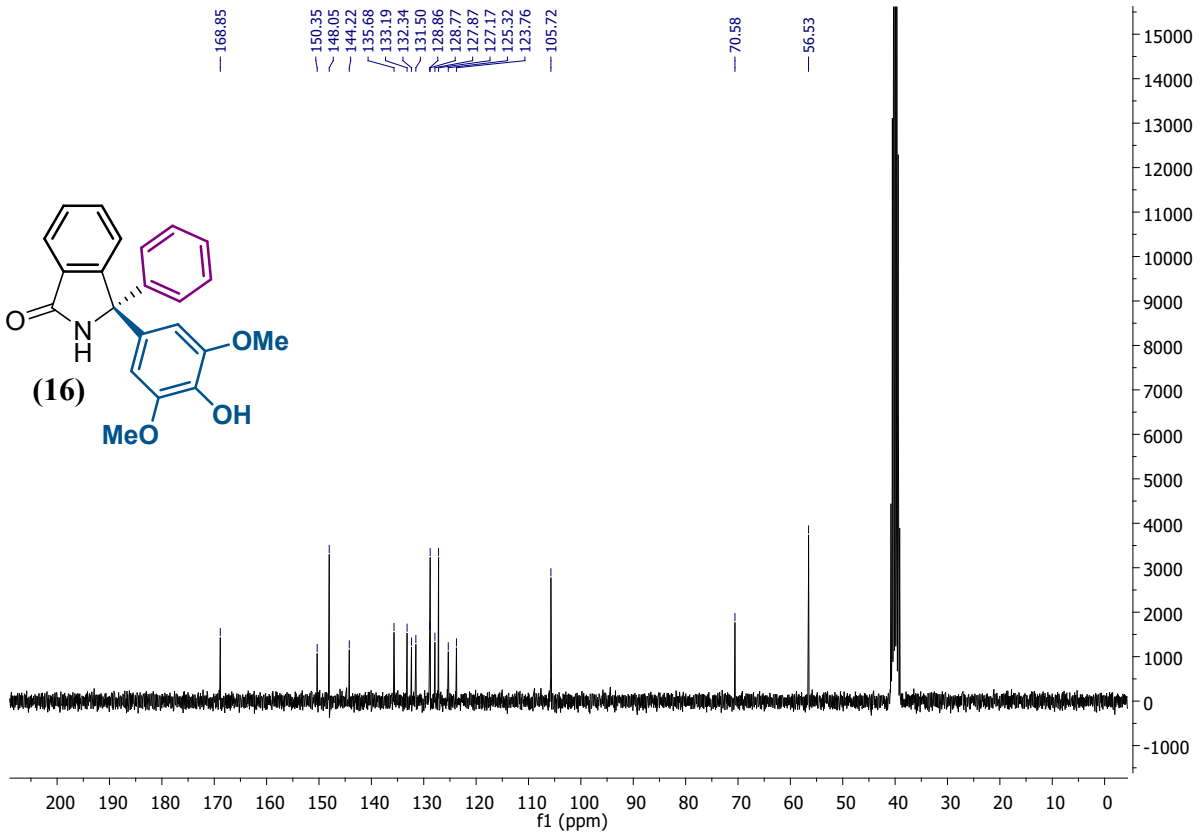
7.68
7.62
7.61
7.60
7.58
7.57
7.51
7.50
7.48
7.33
7.31
7.30
7.27
7.26
6.93
6.80
2.10
1.26
(14)
Me
OH
tBu
+ traces
of
(CH3)2CO
1.01
1.00
0.96
2.04
1.11
1.97
2.94
1.01
1.00
2.90
9.17
f1 (ppm)


168.78
153.36
150.89
144.27
136.47
133.62
132.26
131.58
128.67
127.72
127.64
127.27
125.23
125.20
123.63
123.57
70.48
34.96
29.99
17.71
(14)
Me
OH
tBu
f1 (ppm)


F3C
CF3
O
N
H
Me
OH
Allyl
(15)
f1 (ppm)


F3C
CF3
O
N
H
Me
OH
Allyl
(15)
(CH3)2CO
f1 (ppm)


9.70
8.53
7.76
7.75
7.73
7.68
7.57
7.37
7.36
7.33
7.30
6.58
3.69
3.38
OMe
OH
MeO
(16)
(CH3)2CO
1.01
0.95
1.95
1.10
1.03
1.88
1.20
1.88
2.00
6.12
f1 (ppm)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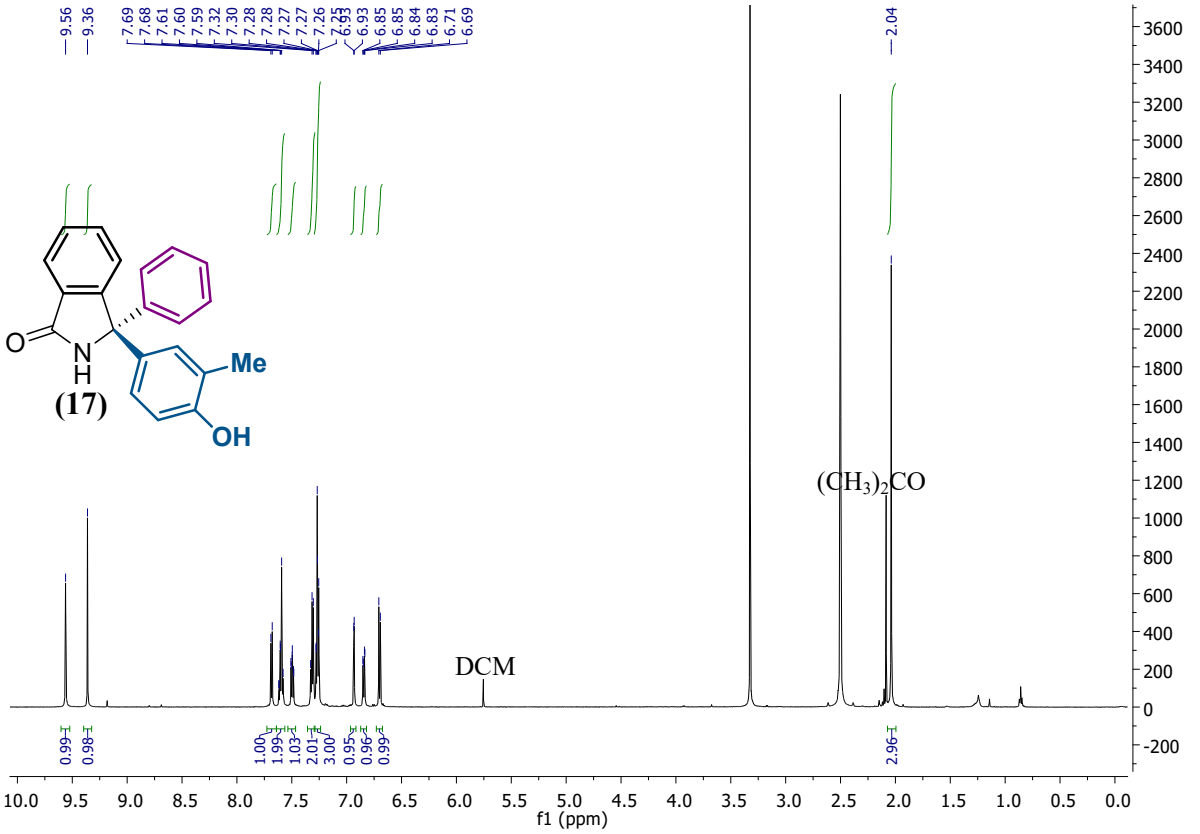
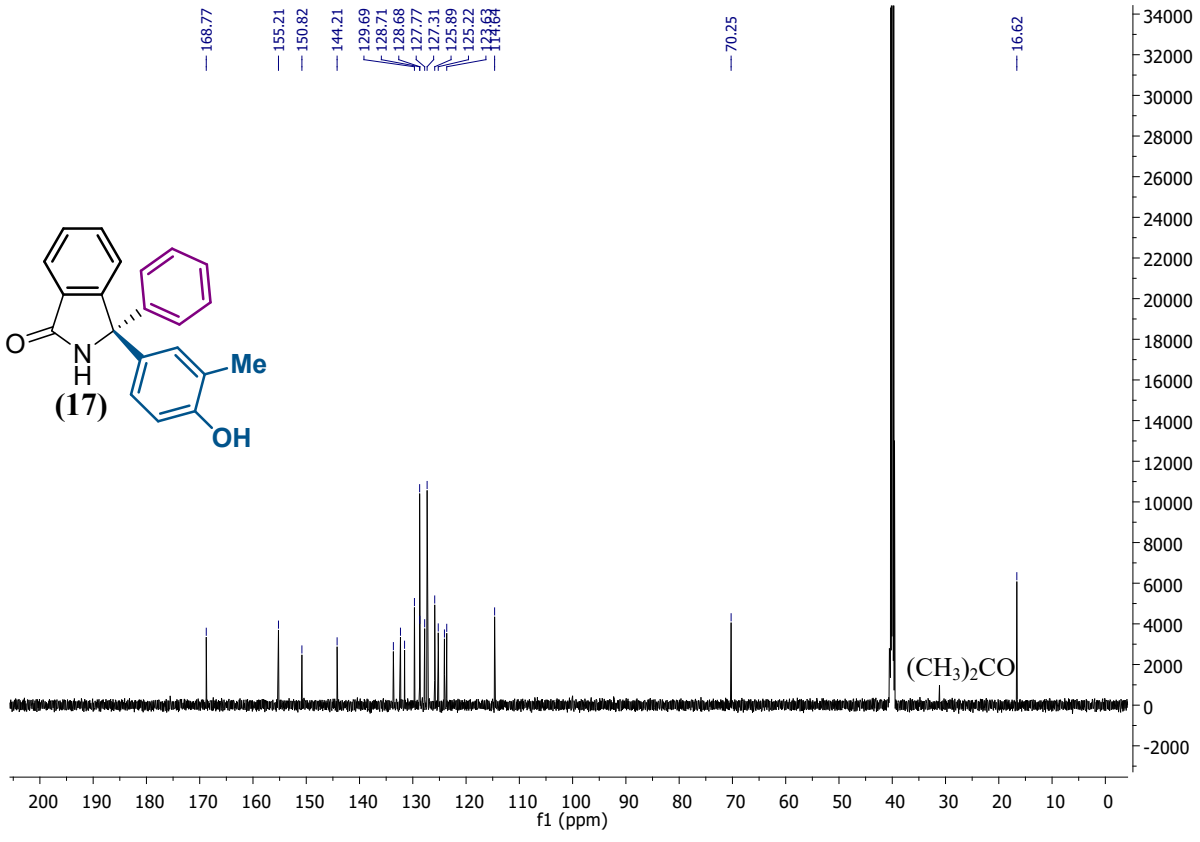
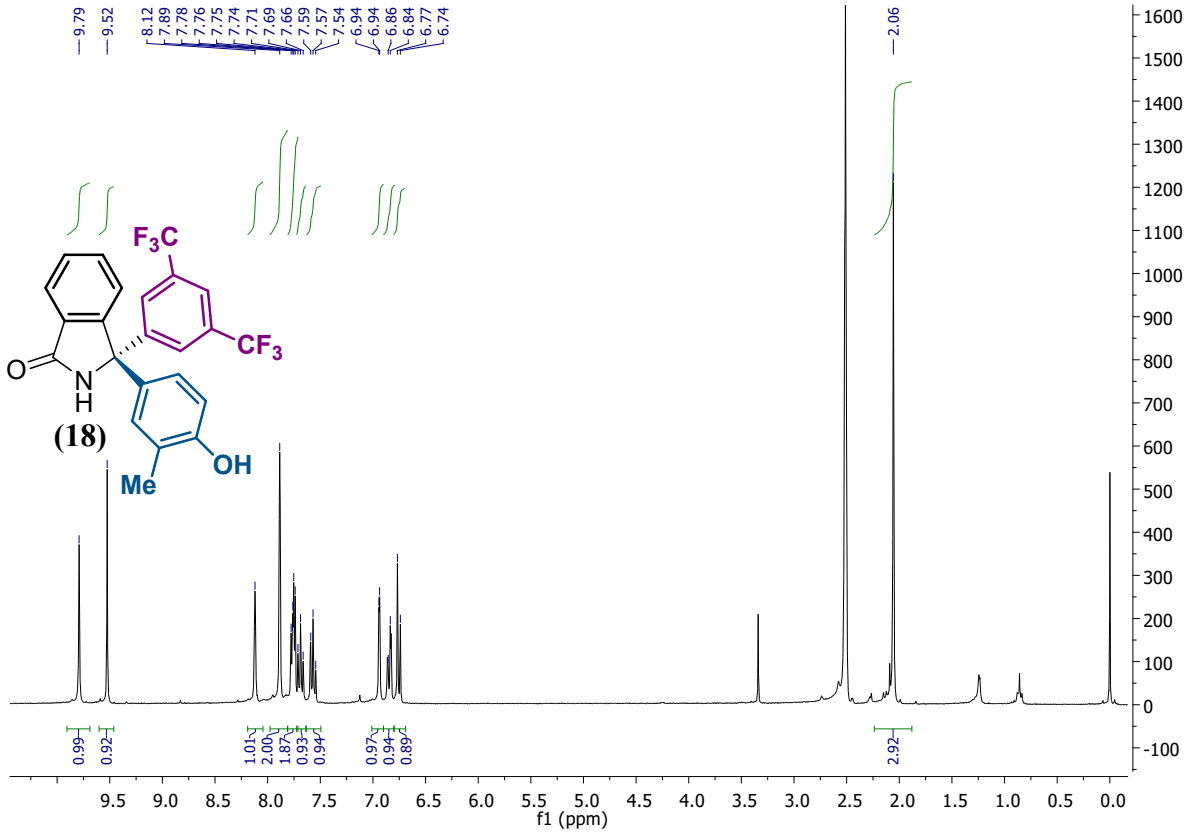
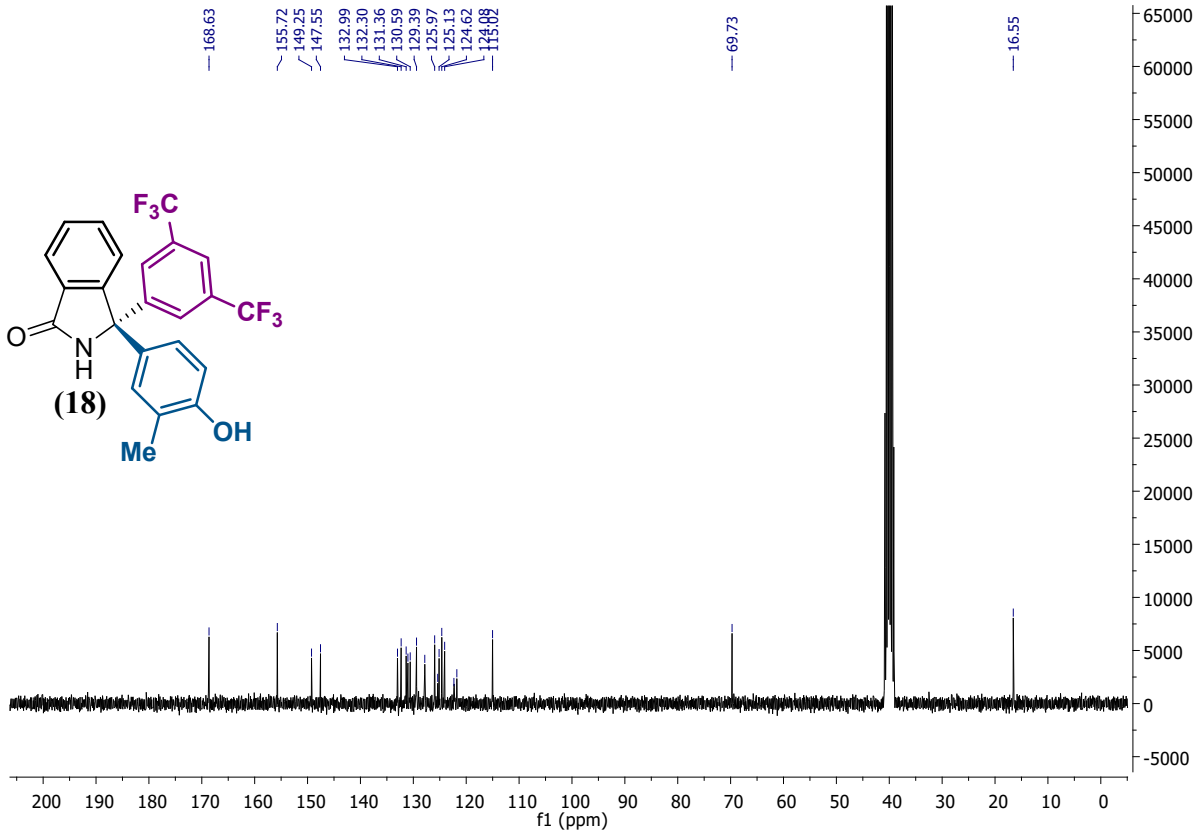
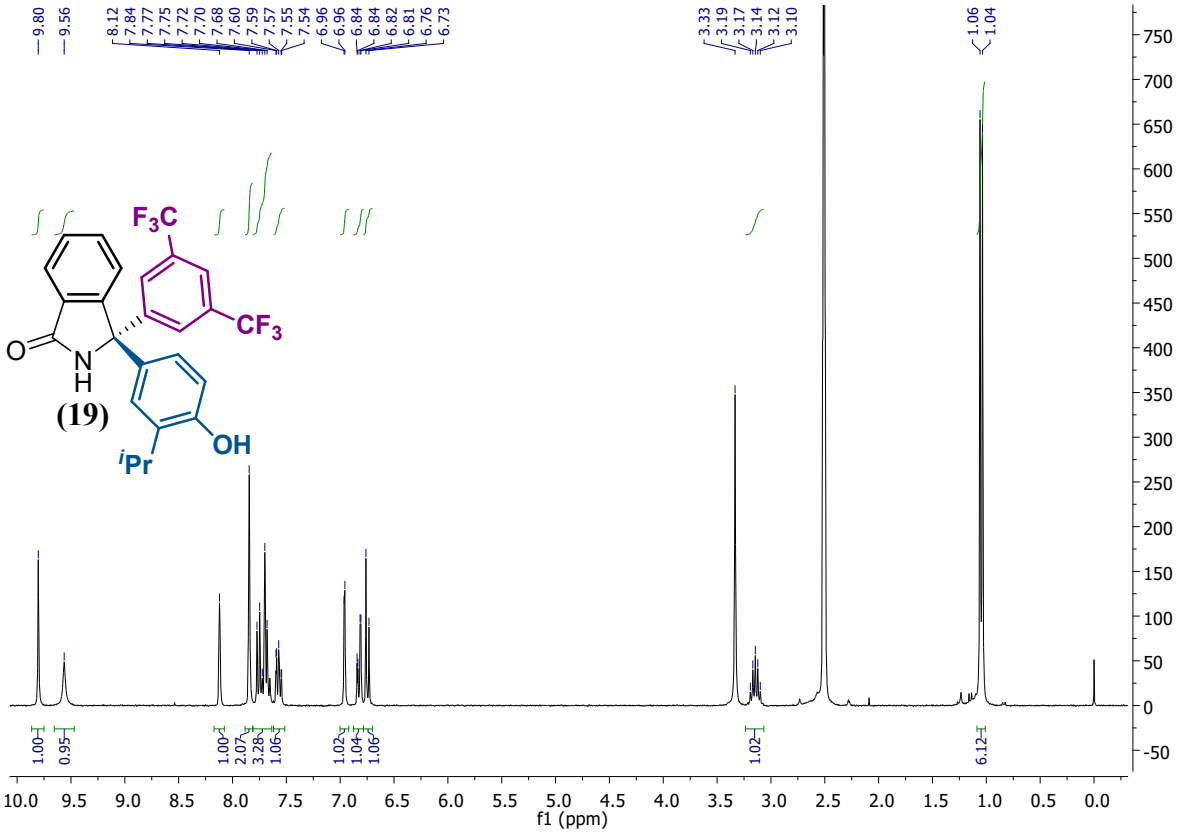
150.35
148.05
144.22
135.68
133.19
132.34
131.50
128.86
128.77
127.87
127.17
125.32
123.76
105.72
70.58
56.53
OMe
OH
MeO
(16)
f1 (ppm)


9.56
9.36
7.69
7.68
7.61
7.60
7.59
7.32
7.30
7.28
7.28
7.27
7.27
7.26
6.93
6.85
6.85
6.84
6.83
6.71
6.69
2.04
O
N
H
Me
OH
(17)
(CH3)2CO
DCM
0.99
0.98
1.00
1.99
1.03
2.01
3.00
0.95
0.96
0.99
2.96
f1 (ppm)


168.77
155.21
150.82
144.21
129.69
128.71
128.68
127.77
127.31
125.89
125.22
70.25
16.62
O
N
H
Me
OH
(17)
(CH3)2CO
f1 (ppm)


9.79
9.52
8.12
7.89
7.78
7.76
7.75
7.74
7.71
7.69
7.66
7.59
7.57
7.54
6.94
6.94
6.86
6.84
6.77
6.74
2.06
F3C
CF3
O
N
H
(18)
OH
Me
0.99
0.92
1.01
2.00
1.87
0.93
0.94
0.97
0.94
0.89
2.92
f1 (ppm)


168.63
155.72
149.25
147.55
132.99
132.30
131.36
130.59
129.39
125.97
125.13
124.62
69.73
16.55
F3C
CF3
O
N
H
(18)
OH
Me
f1 (ppm)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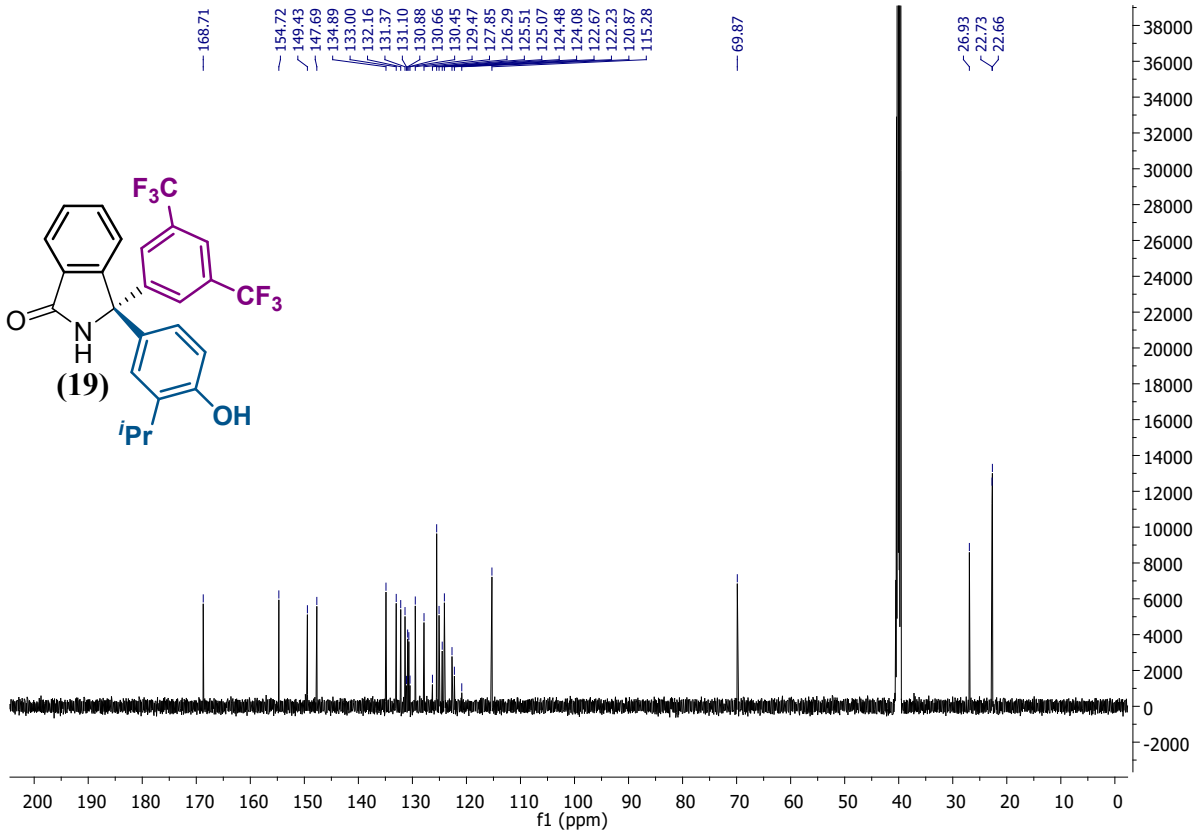
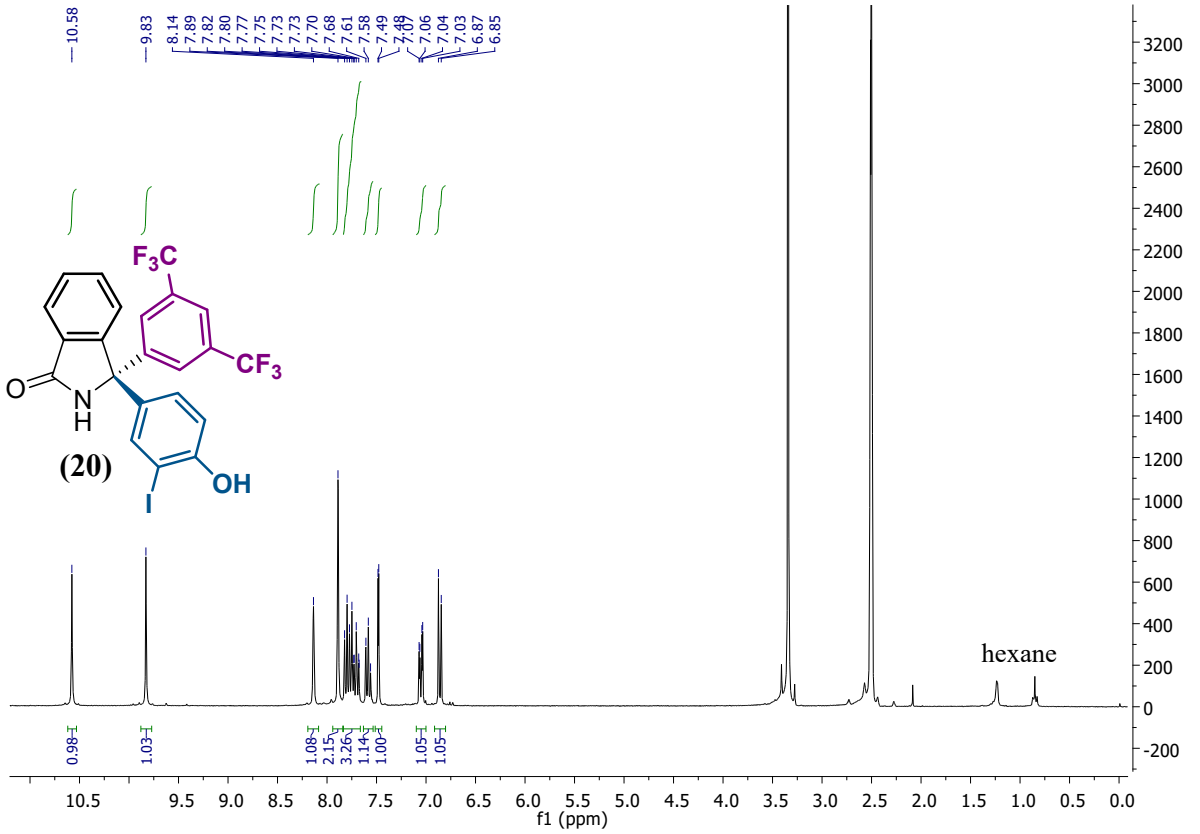
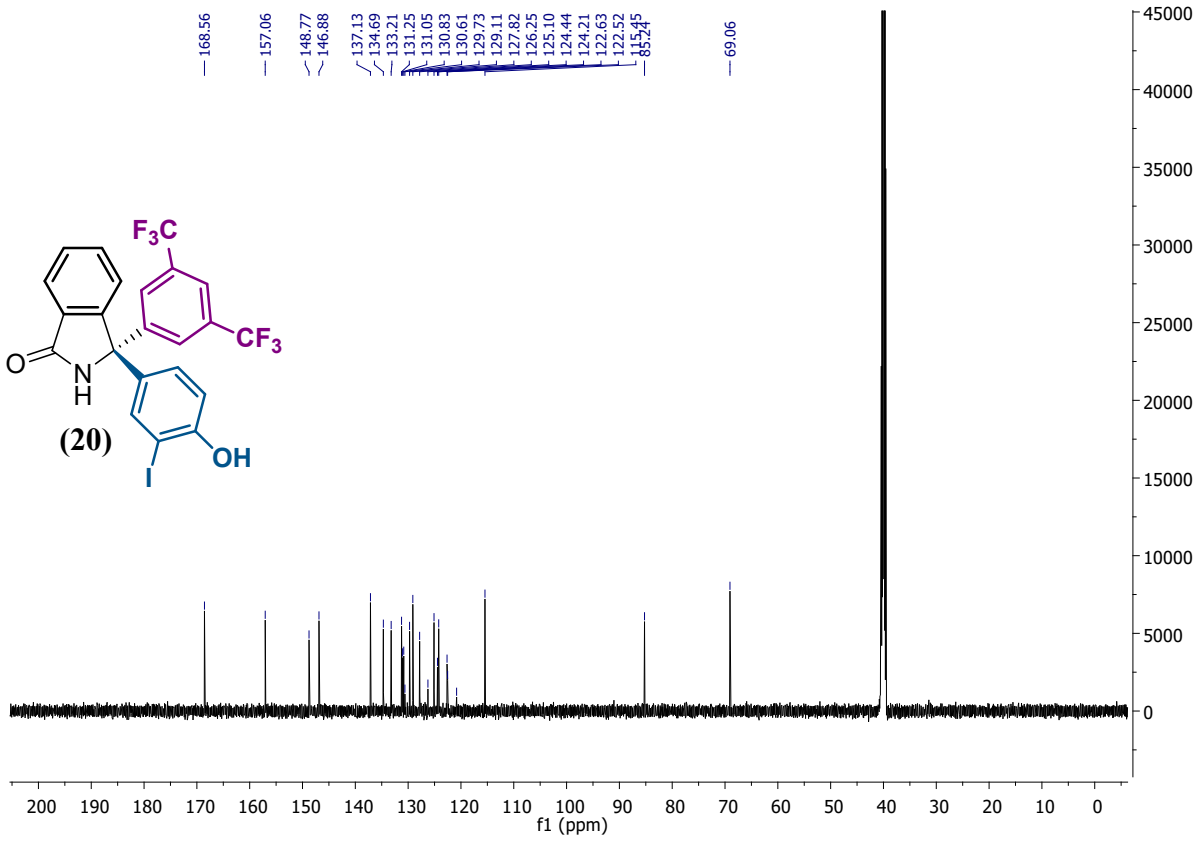
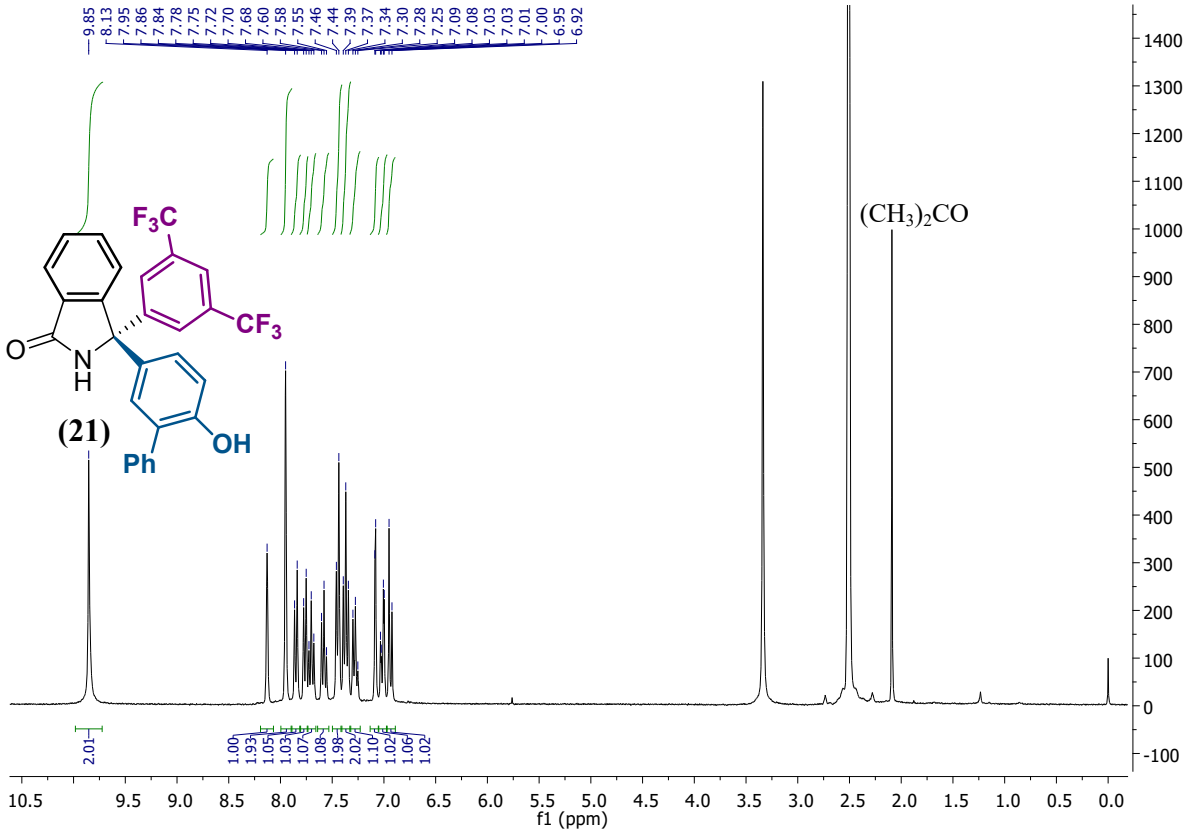
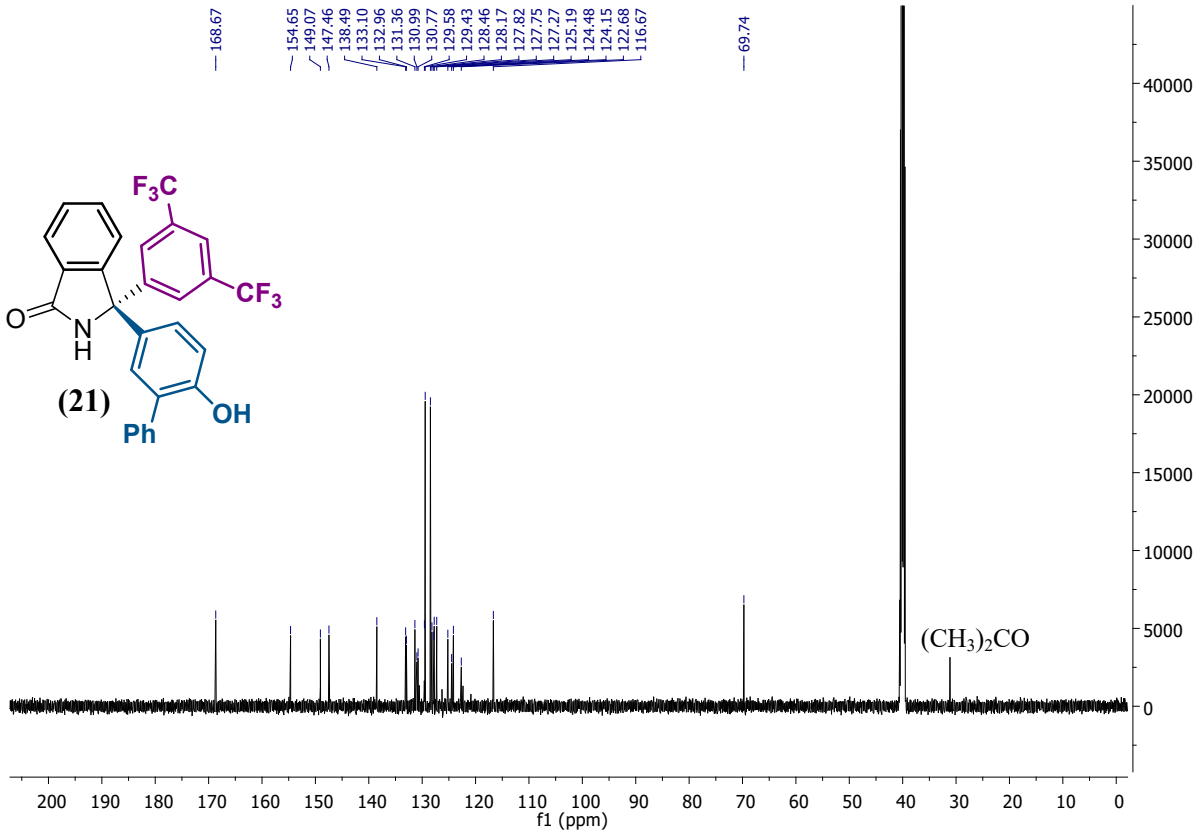
9.56
8.12
7.84
7.77
7.75
7.72
7.70
7.68
7.60
7.59
7.57
7.55
7.54
6.96
6.96
6.84
6.84
6.82
6.81
6.76
6.73
3.33
3.19
3.17
3.14
3.12
3.10
1.06
1.04
F3C
CF3
O
N
H
(19)
OH
iPr
1.00
0.95
1.00
2.07
3.28
1.06
1.02
1.04
1.06
1.02
6.12
f1 (ppm)


168.71
154.72
149.43
147.69
134.89
133.00
132.16
131.37
131.10
130.88
130.66
130.45
129.47
127.85
126.29
125.51
125.07
124.48
124.08
122.67
122.23
120.87
115.28
69.87
26.93
22.73
22.66
F3C
CF3
O
N
H
(19)
OH
iPr
f1 (ppm)


10.58
9.83
8.14
7.89
7.82
7.80
7.77
7.75
7.73
7.73
7.70
7.68
7.61
7.58
7.49
7.06
7.04
7.03
6.87
6.85
F3C
CF3
O
N
H
(20)
OH
I
hexane
0.98
1.03
1.08
2.15
3.26
1.14
1.00
1.05
1.05
f1 (ppm)


168.56
157.06
148.77
146.88
137.13
134.69
133.21
131.25
131.05
130.83
130.61
129.73
129.11
127.82
126.25
125.10
124.44
124.21
122.63
122.52
115.45
85.24
69.06
F3C
CF3
O
N
H
(20)
OH
I
f1 (ppm)


9.85
8.13
7.95
7.86
7.84
7.78
7.75
7.72
7.70
7.68
7.60
7.58
7.55
7.46
7.44
7.39
7.37
7.34
7.30
7.28
7.25
7.09
7.08
7.03
7.03
7.01
7.00
6.95
6.92
F3C
CF3
O
N
H
(21)
OH
Ph
(CH3)2CO
2.01
1.00
1.93
1.05
1.03
1.07
1.08
1.98
2.02
1.10
1.02
1.06
1.02
f1 (ppm)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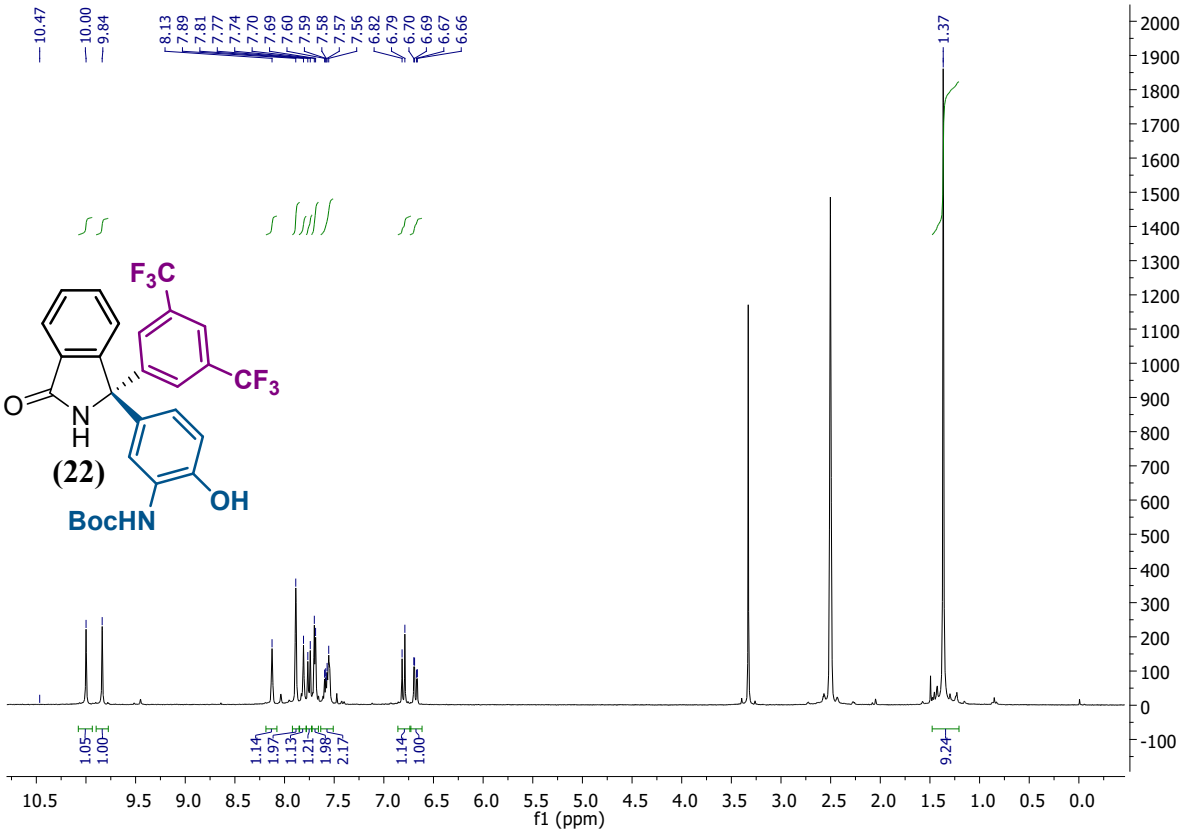
154.65
149.07
147.46
138.49
133.10
132.96
131.36
130.99
130.77
129.58
129.43
128.46
128.17
127.82
127.75
127.27
125.19
124.48
124.15
122.68
116.67
69.74
F3C
CF3
O
N
H
(21)
OH
Ph
(CH3)2CO
f1 (ppm)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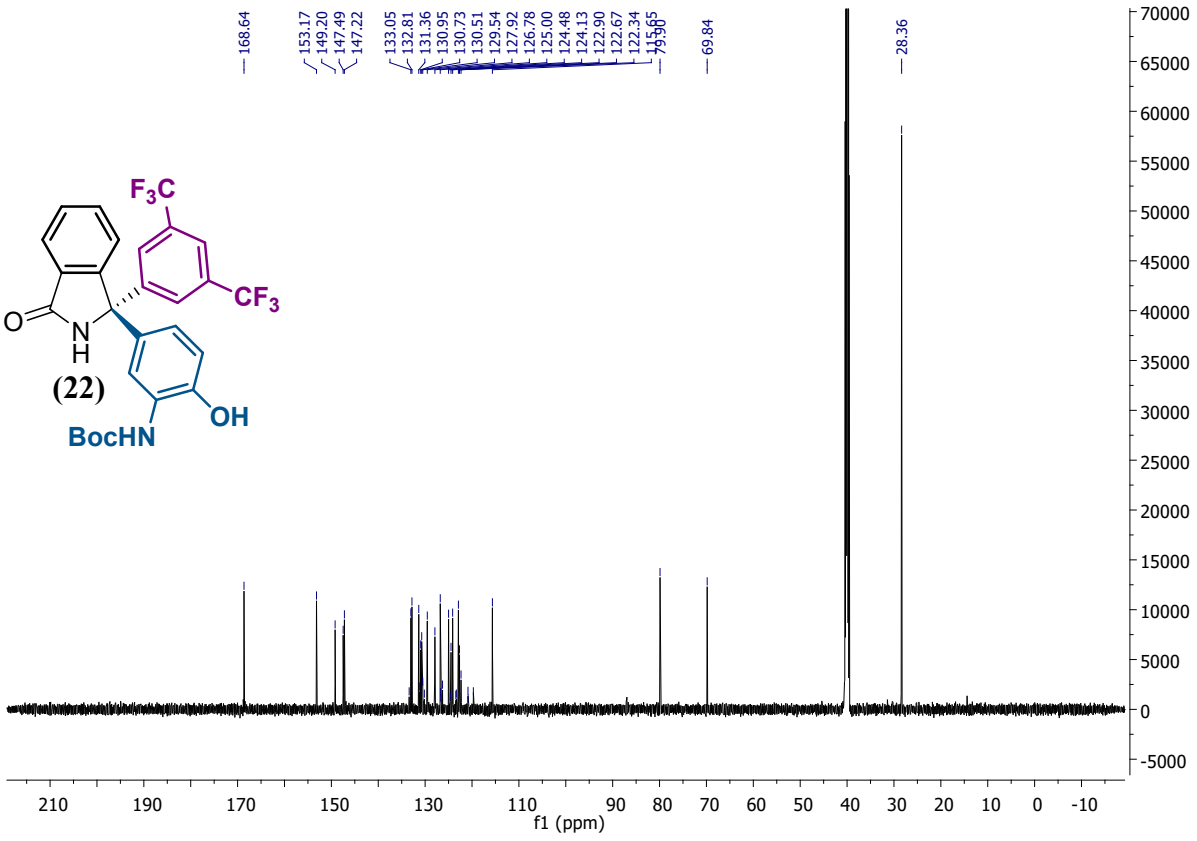
10.00
9.84
8.13
7.89
7.81
7.77
7.74
7.70
7.69
7.60
7.59
7.58
7.57
7.56
6.82
6.79
6.70
6.69
6.67
6.66
1.37
F3C
CF3
O
N
H
(22)
OH
BocHN
1.05
1.00
1.14
1.97
1.13
1.21
1.98
2.17
1.14
1.00
9.24
f1 (ppm)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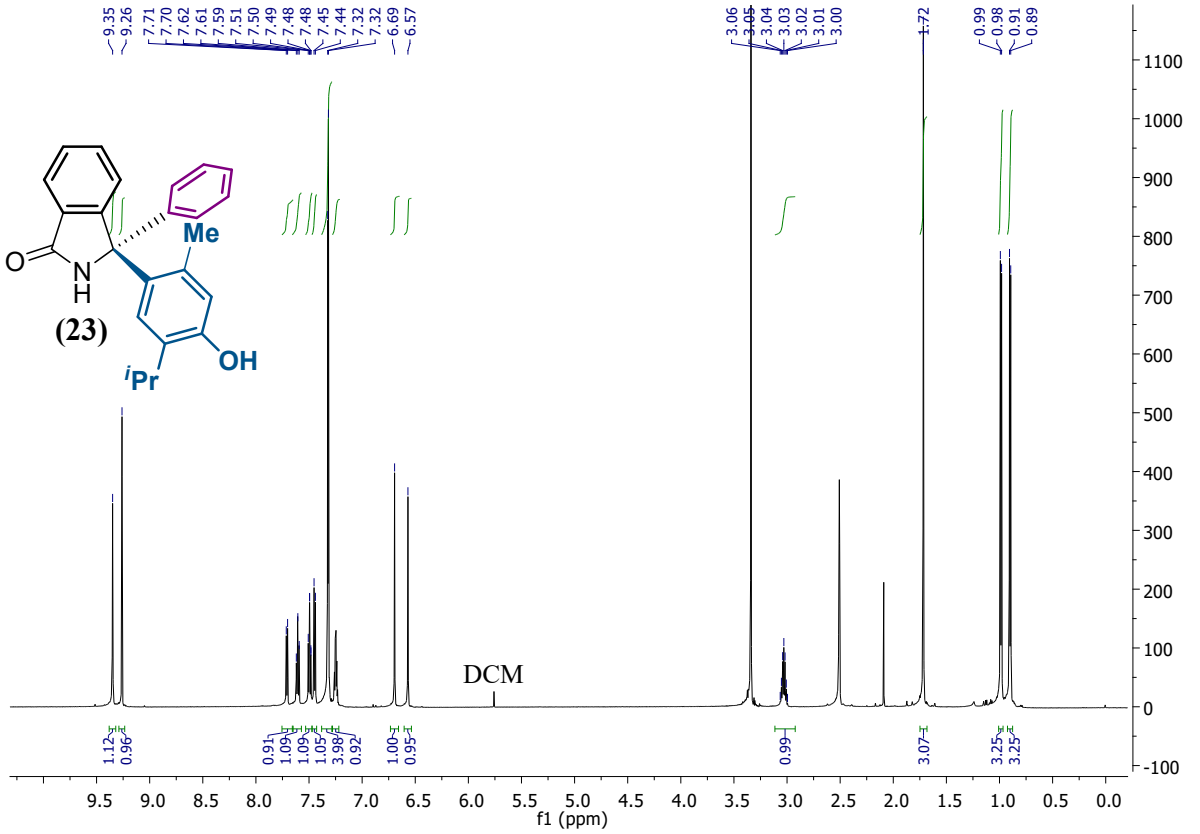
153.17
149.20
147.49
147.22
133.05
132.81
131.36
130.95
130.73
130.51
129.54
127.92
126.78
125.00
124.48
124.13
122.90
122.67
122.34
79.90
69.84
28.36
F3C
CF3
O
N
H
(22)
OH
BocHN
f1 (ppm)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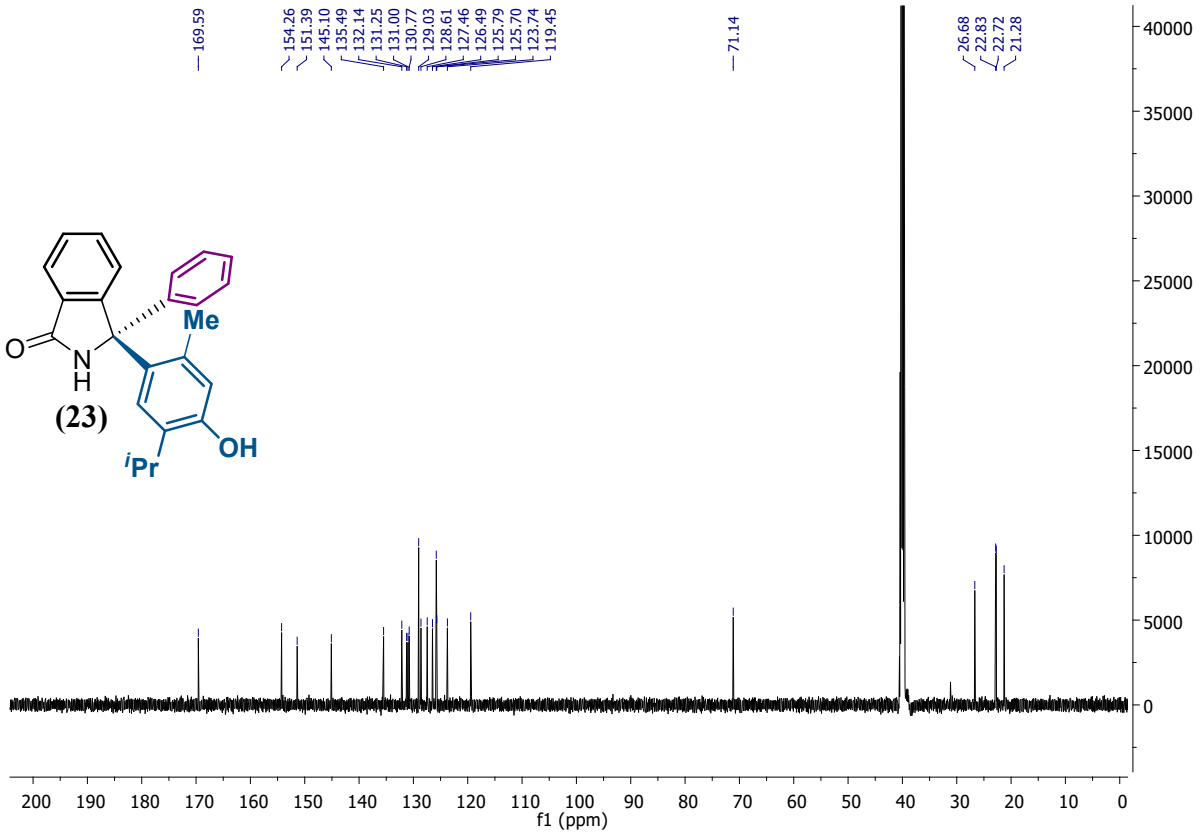
9.26
7.71
7.70
7.62
7.61
7.59
7.51
7.50
7.49
7.48
7.48
7.45
7.44
7.32
7.32
6.69
6.57
3.06
3.05
3.04
3.03
3.02
3.01
3.00
1.72
0.99
0.98
0.91
0.89
Me
O
N
H
(23)
OH
iPr
DCM
1.12
0.96
0.91
1.09
1.09
1.05
3.98
0.92
1.00
0.95
0.99
3.07
3.25
3.25
f1 (ppm)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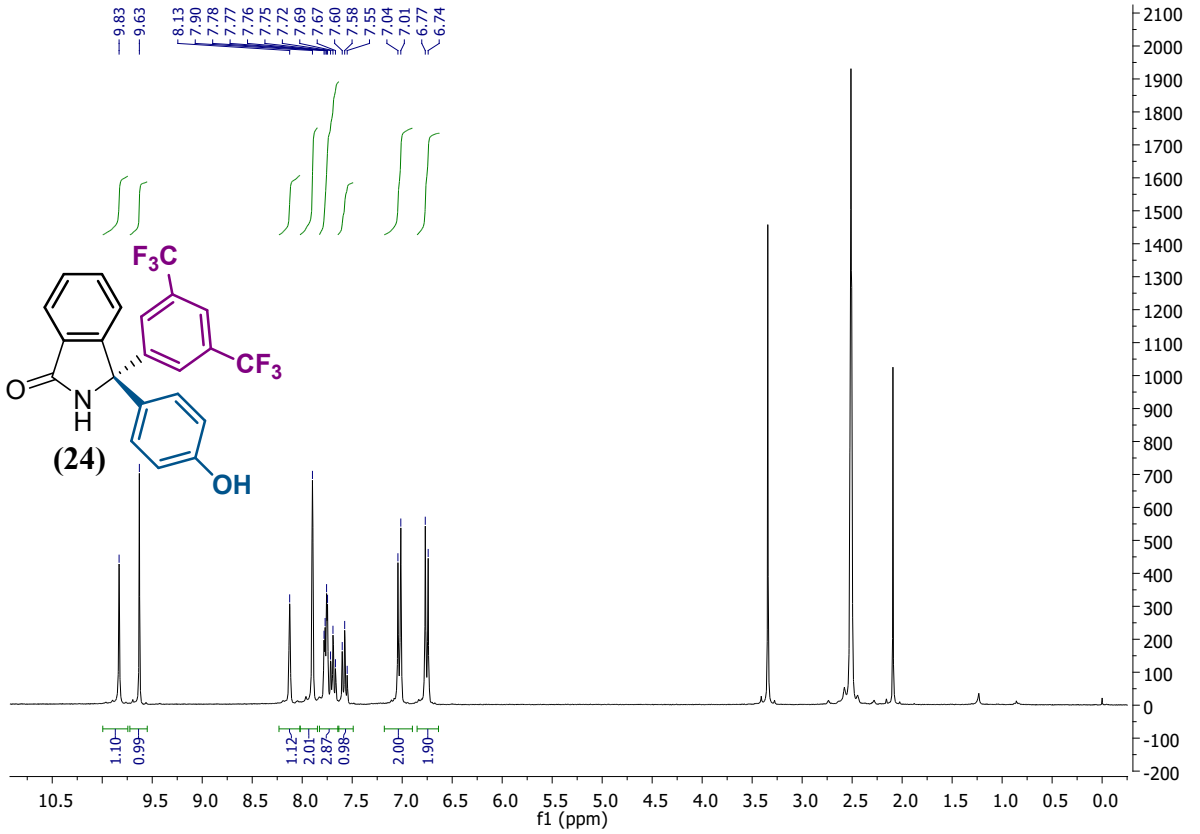
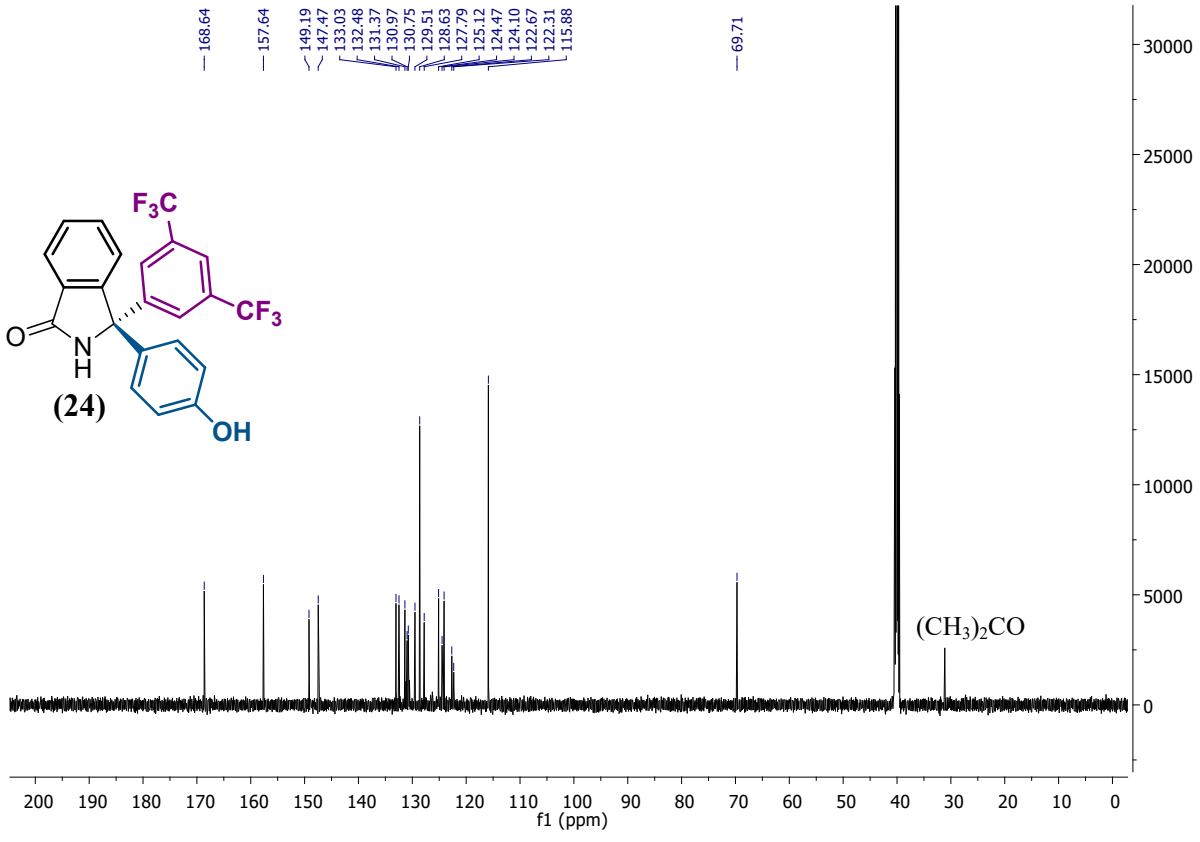
151.39
145.10
135.49
132.14
131.25
131.00
130.77
129.03
128.61
127.46
126.49
125.79
125.70
123.74
119.45
71.14
26.68
22.83
22.72
21.28
Me
O
N
H
(23)
OH
iPr
f1 (ppm)


9.83
9.63
8.13
7.90
7.78
7.77
7.76
7.75
7.72
7.69
7.67
7.60
7.58
7.55
7.04
7.01
6.77
6.74
F3C
CF3
O
N
H
OH
(24)
1.10
0.99
1.12
2.01
2.87
0.98
2.00
1.90
f1 (ppm)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157.64
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147.47
133.03
132.48
131.37
130.97
130.75
129.51
128.63
127.79
125.12
124.47
124.10
122.67
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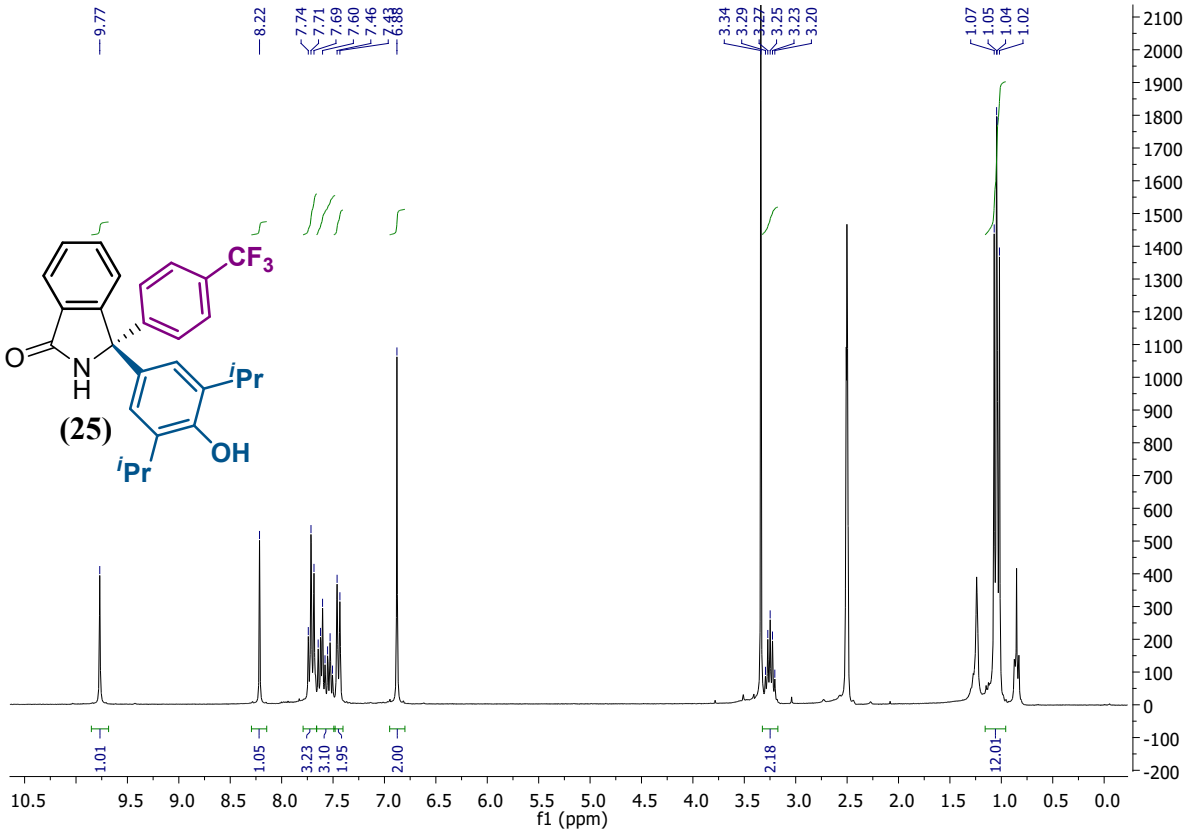
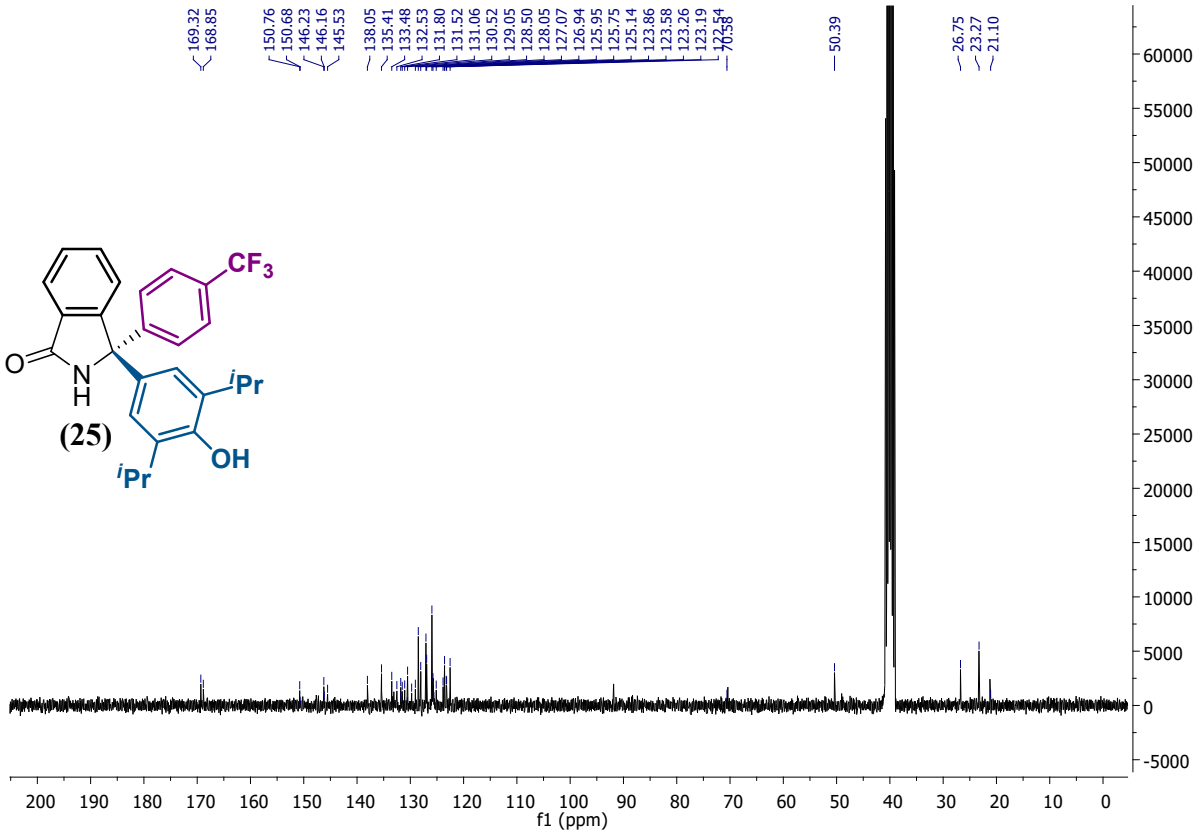
69.71
F3C
CF3
O
N
H
OH
(24)
(CH3)2CO
f1 (ppm)


9.77
8.22
7.74
7.71
7.69
7.60
7.46
3.34
3.29
3.25
3.23
3.20
1.07
1.05
1.04
1.02
CF3
O
N
H
(25)
iPr
OH
iPr
1.01
1.05
3.23
3.10
1.95
2.00
2.18
12.01
f1 (ppm)


169.32
168.85
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150.68
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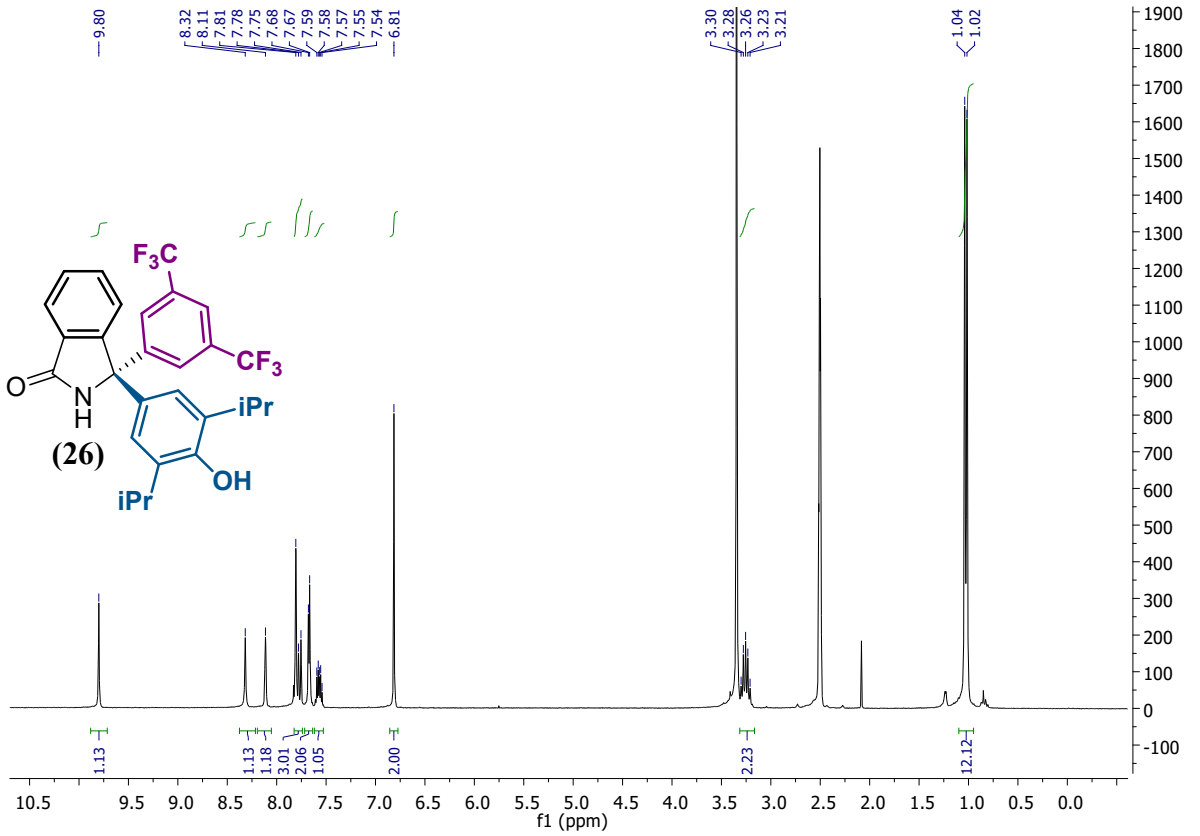
146.16
145.53
138.05
135.41
133.48
132.53
131.80
131.52
131.06
130.52
129.05
128.50
128.05
127.07
126.94
125.95
125.75
125.14
123.86
123.58
123.26
123.19
122.54
70.58
50.39
26.75
23.27
21.10
CF3
O
N
H
(25)
iPr
OH
iPr
f1 (ppm)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8.32
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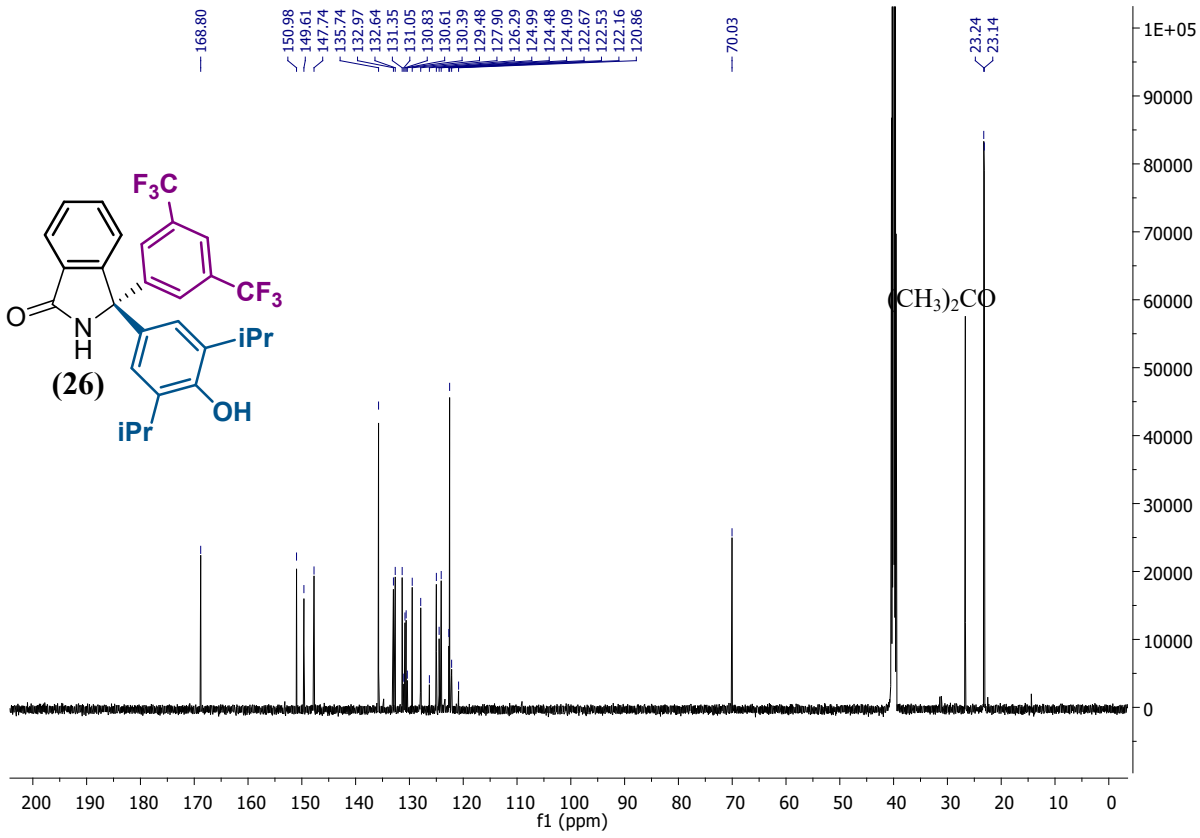
7.81
7.78
7.75
7.68
7.67
7.59
7.58
7.57
7.55
7.54
6.81
3.30
3.28
3.26
3.23
3.21
1.04
1.02
F3C
CF3
O
N
H
iPr
OH
iPr
(26)
1.13
1.13
1.18
3.01
2.06
1.05
2.00
2.23
12.12
f1 (ppm)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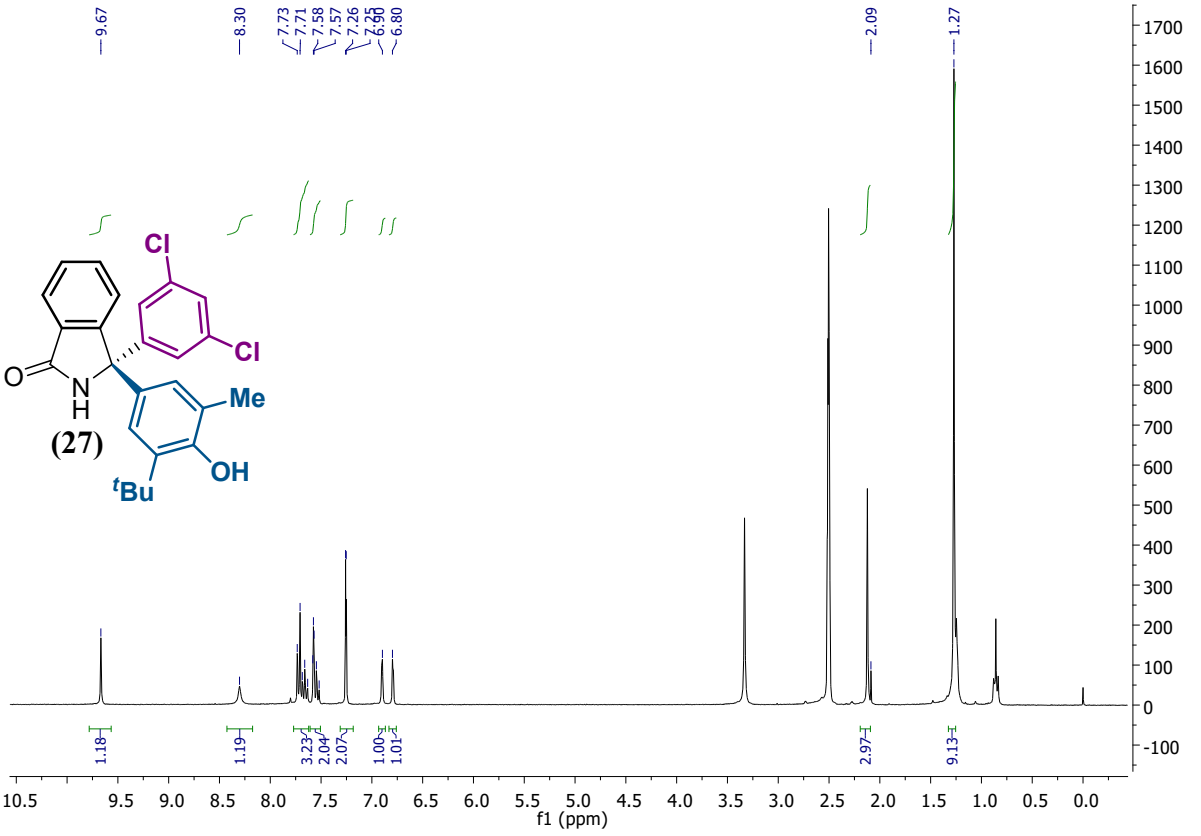
147.74
135.74
132.97
132.64
131.35
131.05
130.83
130.61
130.39
129.48
127.90
126.29
124.99
124.48
124.09
122.67
122.53
122.16
120.86
70.03
23.24
23.14
(CH3)2CO
F3C
CF3
O
N
H
iPr
OH
iPr
(26)
f1 (ppm)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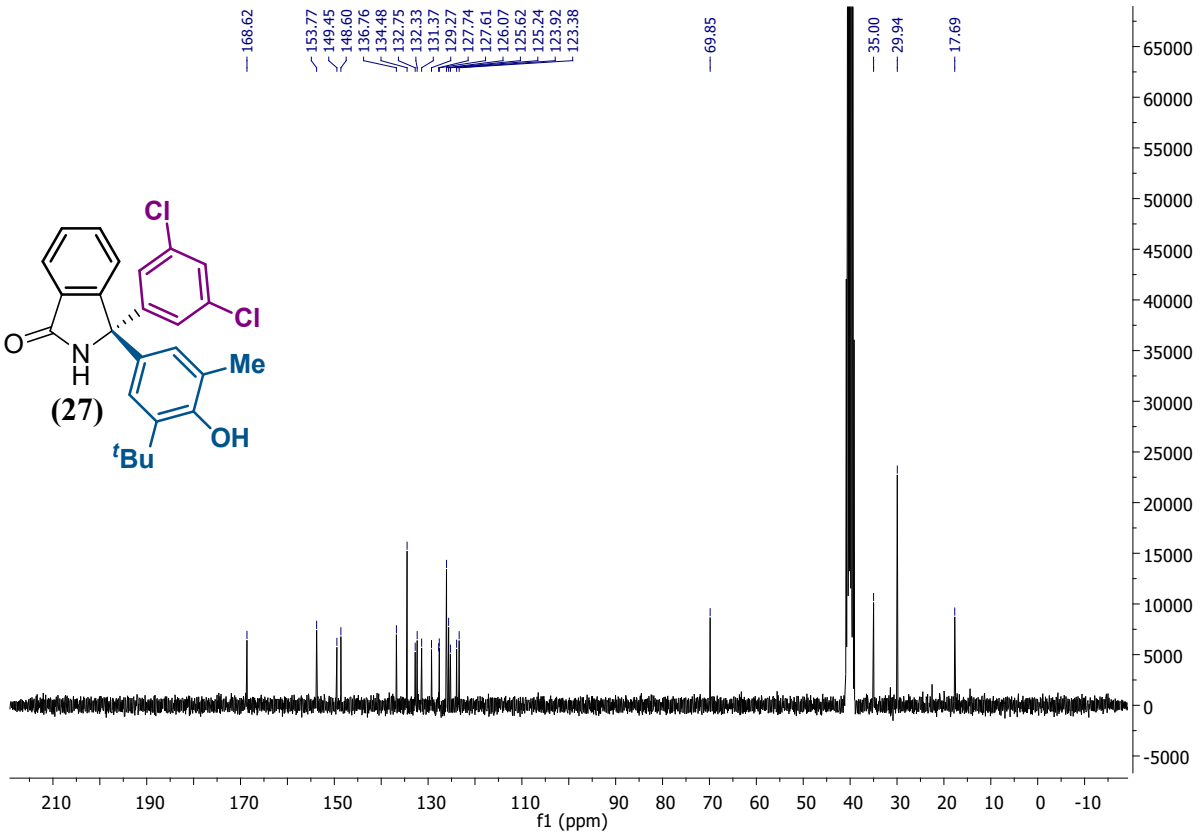
8.30
7.73
7.71
7.58
7.57
7.26
6.80
2.09
1.27
Cl
Cl
O
N
H
Me
OH
tBu
(27)
1.18
1.19
3.23
2.04
2.07
1.00
1.01
2.97
9.13
f1 (ppm)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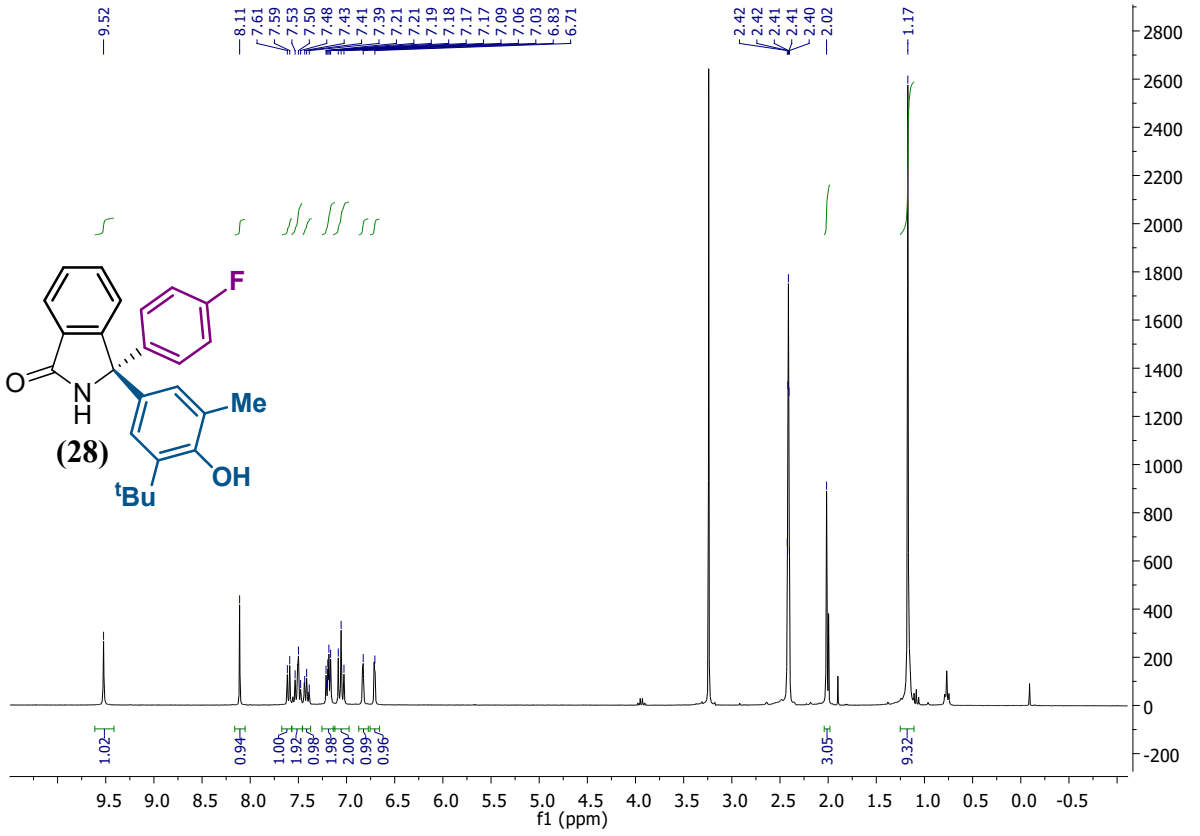
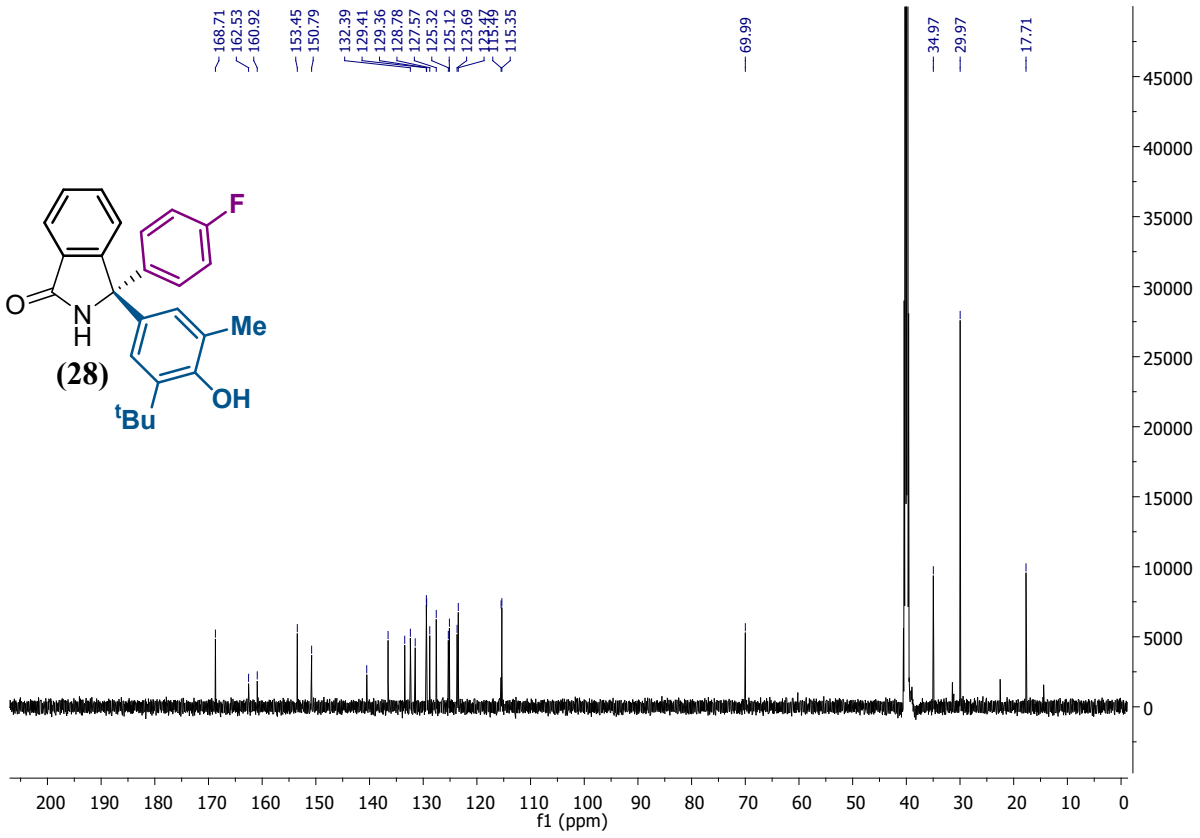
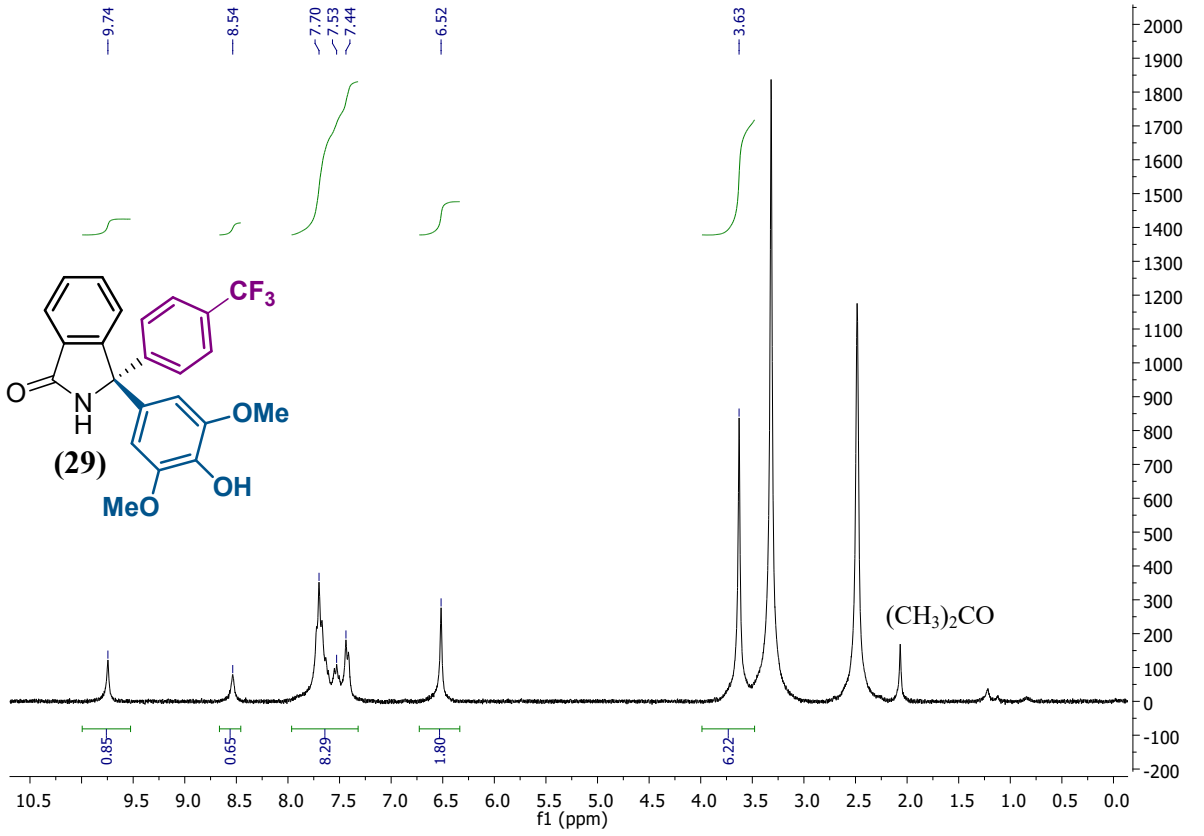
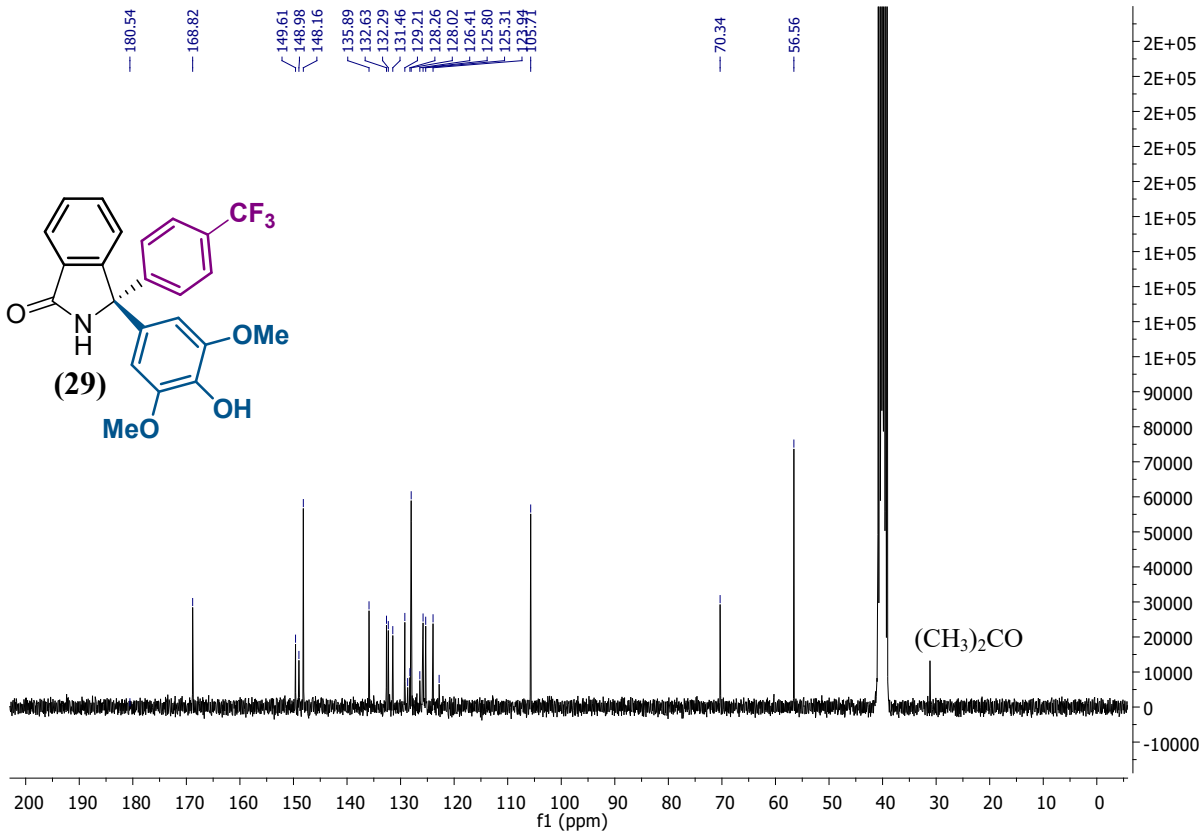
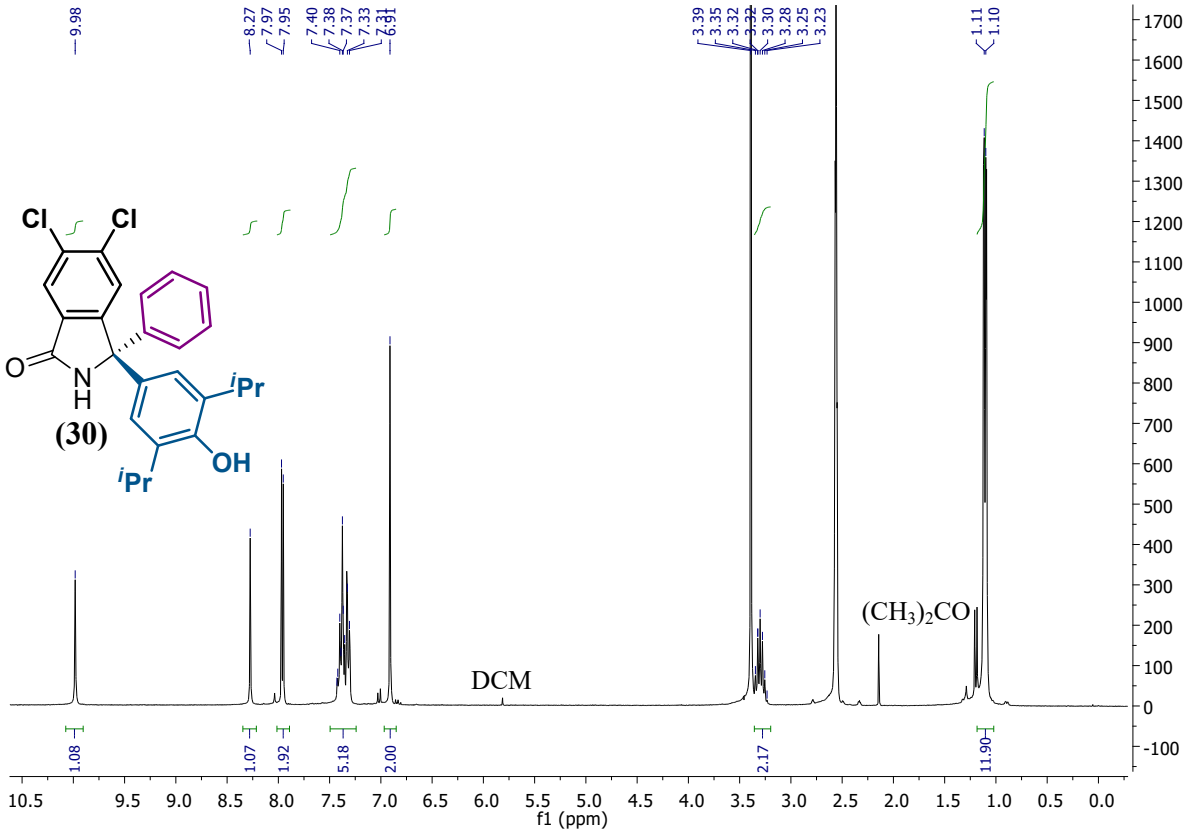
148.60
136.76
134.48
132.75
132.33
131.37
129.27
127.74
127.61
126.07
125.62
125.24
123.92
123.38
69.85
35.00
29.94
17.69
Cl
Cl
O
N
H
Me
OH
tBu
(27)
f1 (ppm)

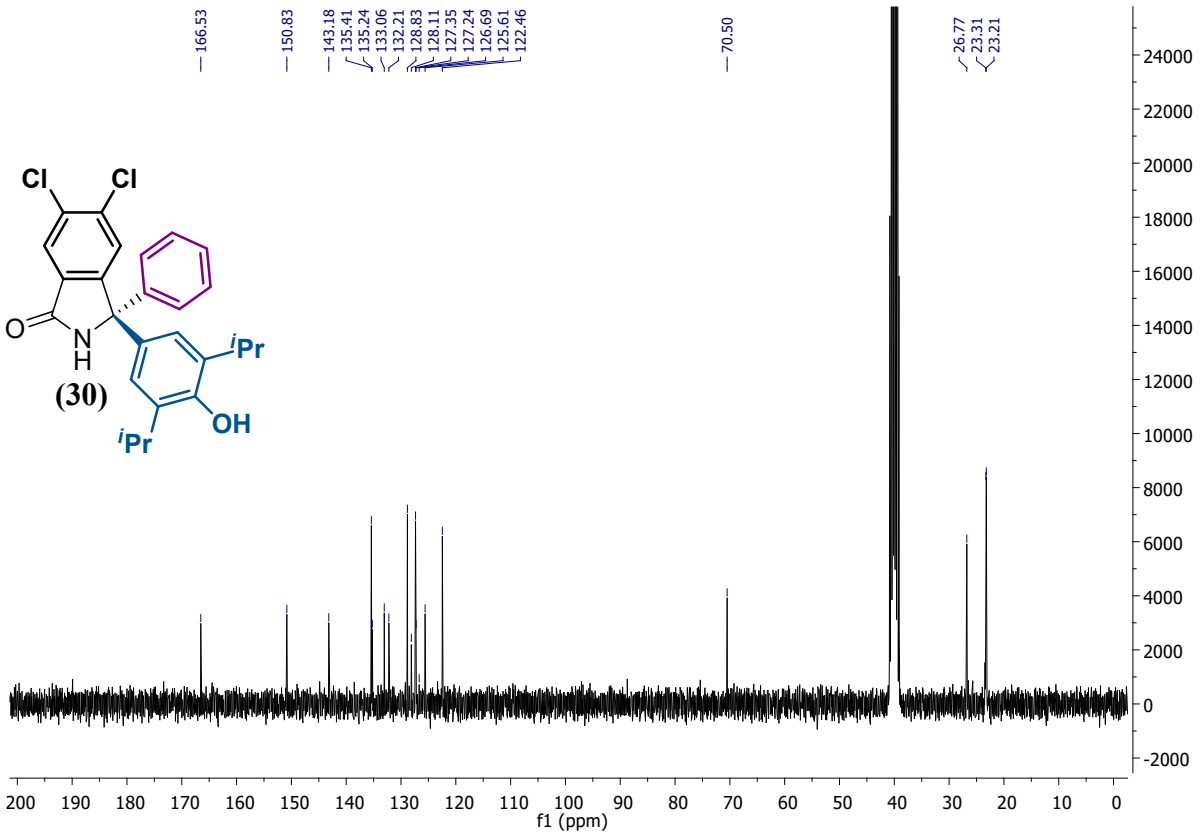

9.52
8.11
7.61
7.59
7.53
7.50
7.48
7.43
7.41
7.39
7.21
7.21
7.19
7.18
7.17
7.17
7.09
7.06
7.03
6.83
6.71
2.42
2.42
2.41
2.41
2.40
2.02
1.17
F
O
N
H
Me
OH
tBu
(28)
1.02
0.94
1.00
1.92
0.98
1.98
2.00
0.99
0.96
3.05
9.32
f1 (ppm)

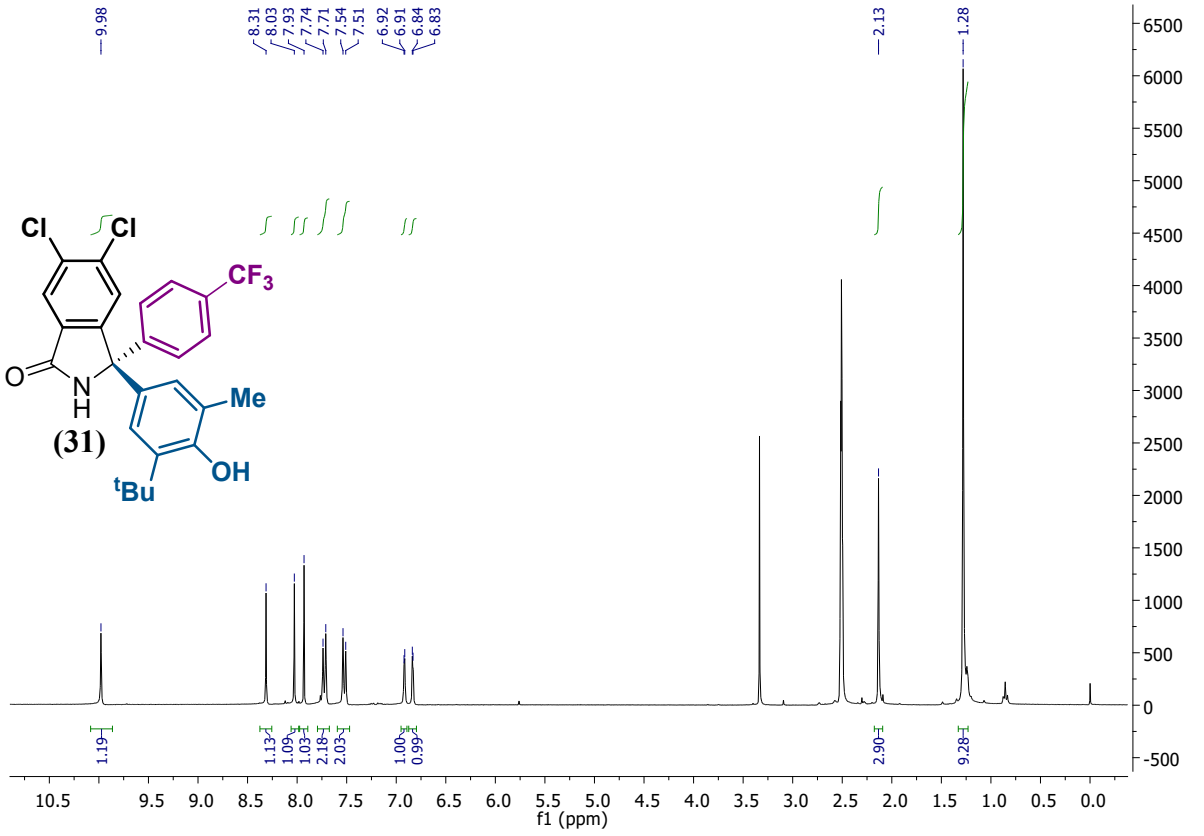

168.71
162.53
160.92
153.45
150.79
132.39
129.41
129.36
128.78
127.57
125.32
125.12
123.69
115.35
69.99
34.97
29.97
17.71
F
O
N
H
Me
OH
tBu
(28)
f1 (ppm)

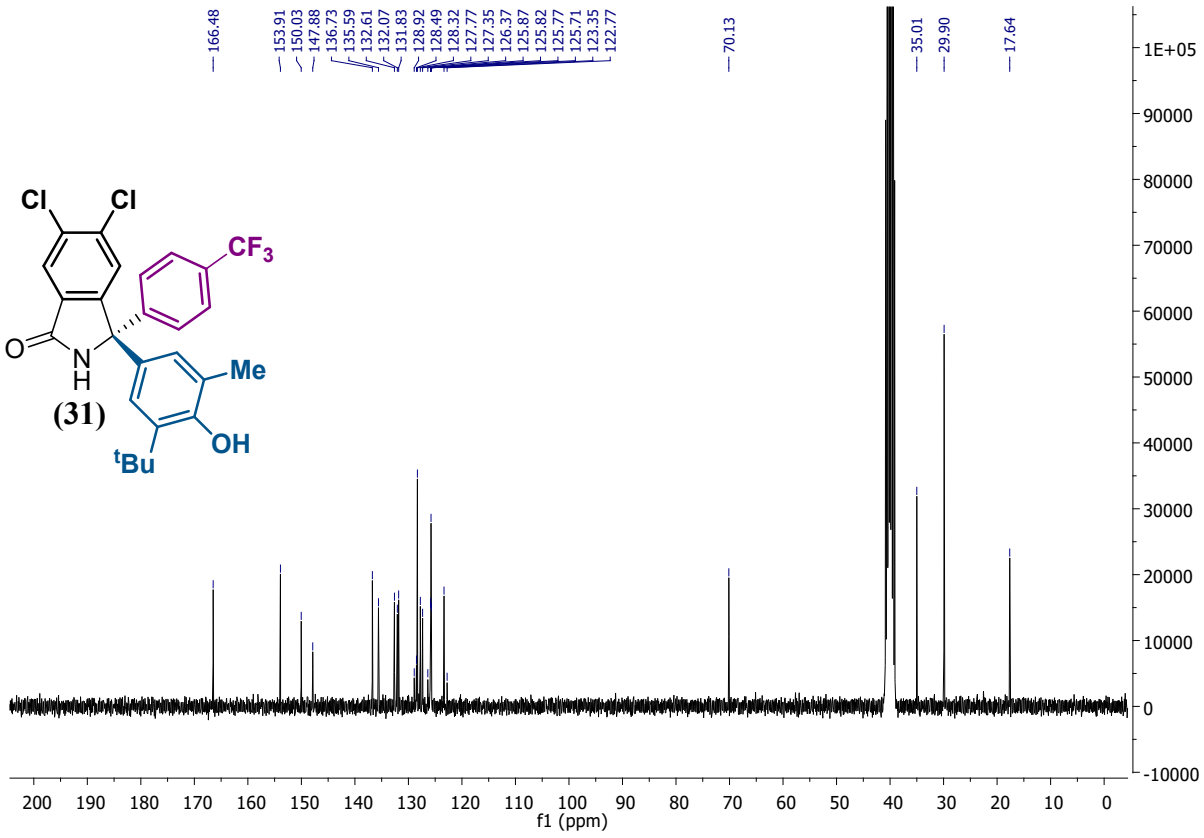

9.74
8.54
7.70
7.53
7.44
6.52
3.63
CF3
O
N
H
OMe
OH
MeO
(29)
(CH3)2CO
0.85
0.65
8.29
1.80
6.22
f1 (ppm)


180.54
168.82
149.61
148.98
148.16
135.89
132.63
132.29
131.46
129.21
128.26
128.02
126.41
125.80
125.31
123.94
105.71
70.34
56.56
CF3
O
N
H
OMe
OH
MeO
(29)
(CH3)2CO
f1 (ppm)


9.98
8.27
7.97
7.95
7.40
7.38
7.37
7.33
7.31
6.91
3.39
3.35
3.32
3.32
3.30
3.28
3.25
3.23
1.11
1.10
Cl
Cl
O
N
H
(30)
iPr
OH
iPr
DCM
(CH3)2CO
1.08
1.07
1.92
5.18
2.00
2.17
11.90
f1 (ppm)


166.53
150.83
143.18
135.41
135.24
133.06
132.21
128.83
128.11
127.35
127.24
126.69
125.61
122.46
70.50
26.77
23.31
23.21
Cl
Cl
O
N
H
(30)
iPr
OH
iPr
f1 (ppm)


9.98
8.31
8.03
7.93
7.74
7.71
7.54
7.51
6.92
6.91
6.84
6.83
2.13
1.28
Cl
Cl
CF3
O
N
H
Me
OH
tBu
(31)
1.19
1.13
1.09
1.03
2.18
2.03
1.00
0.99
2.90
9.28
f1 (ppm)


166.48
153.91
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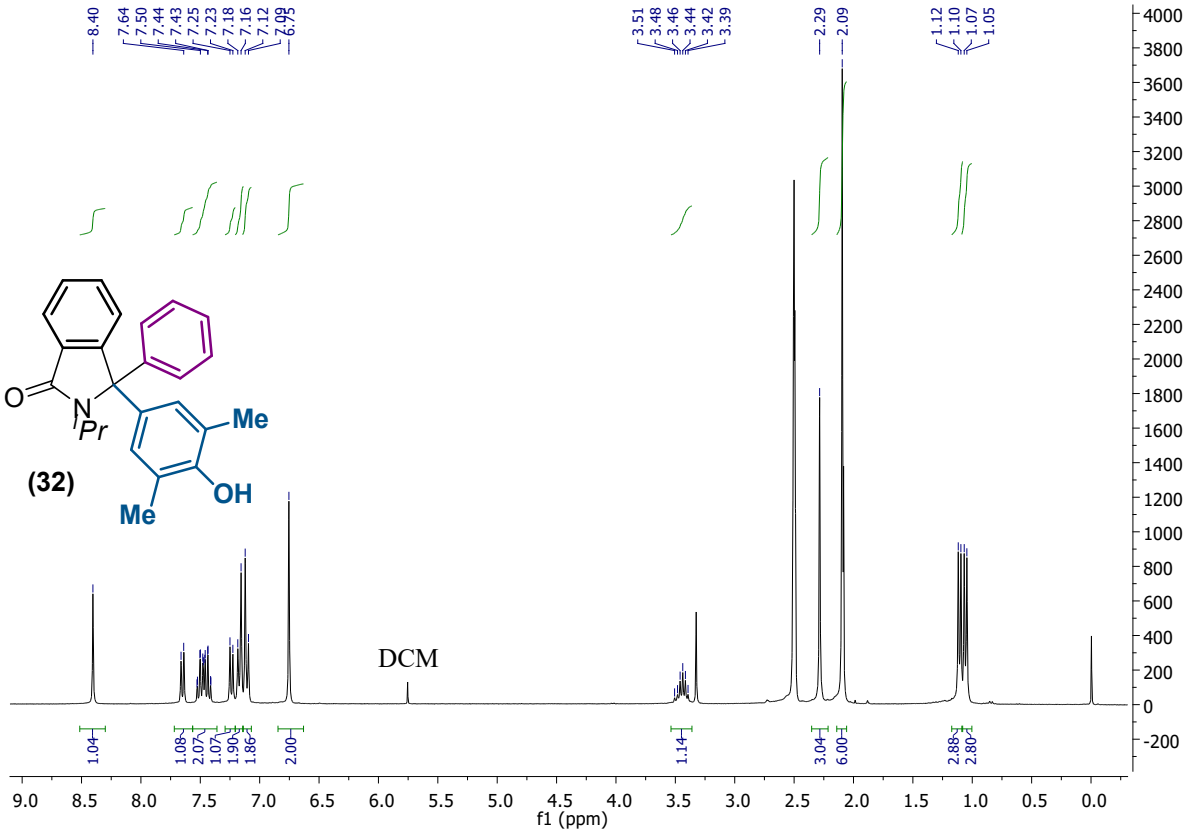
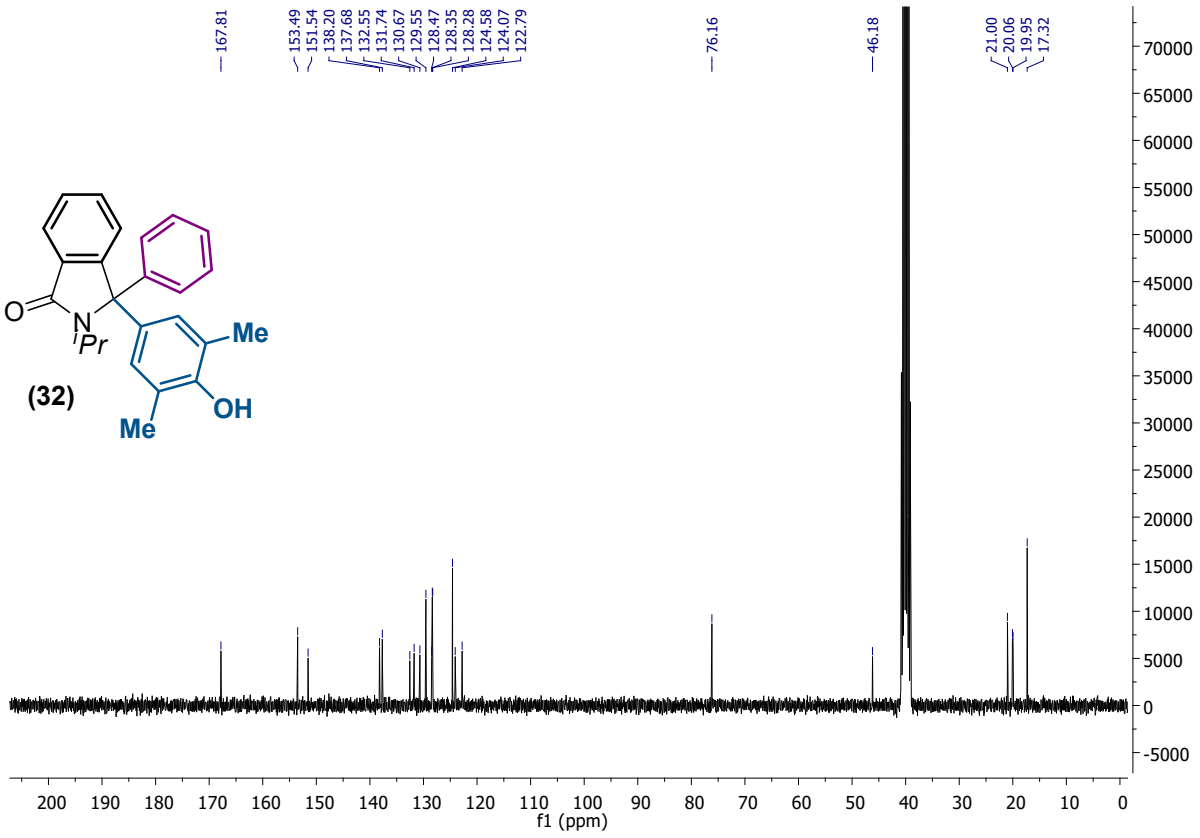
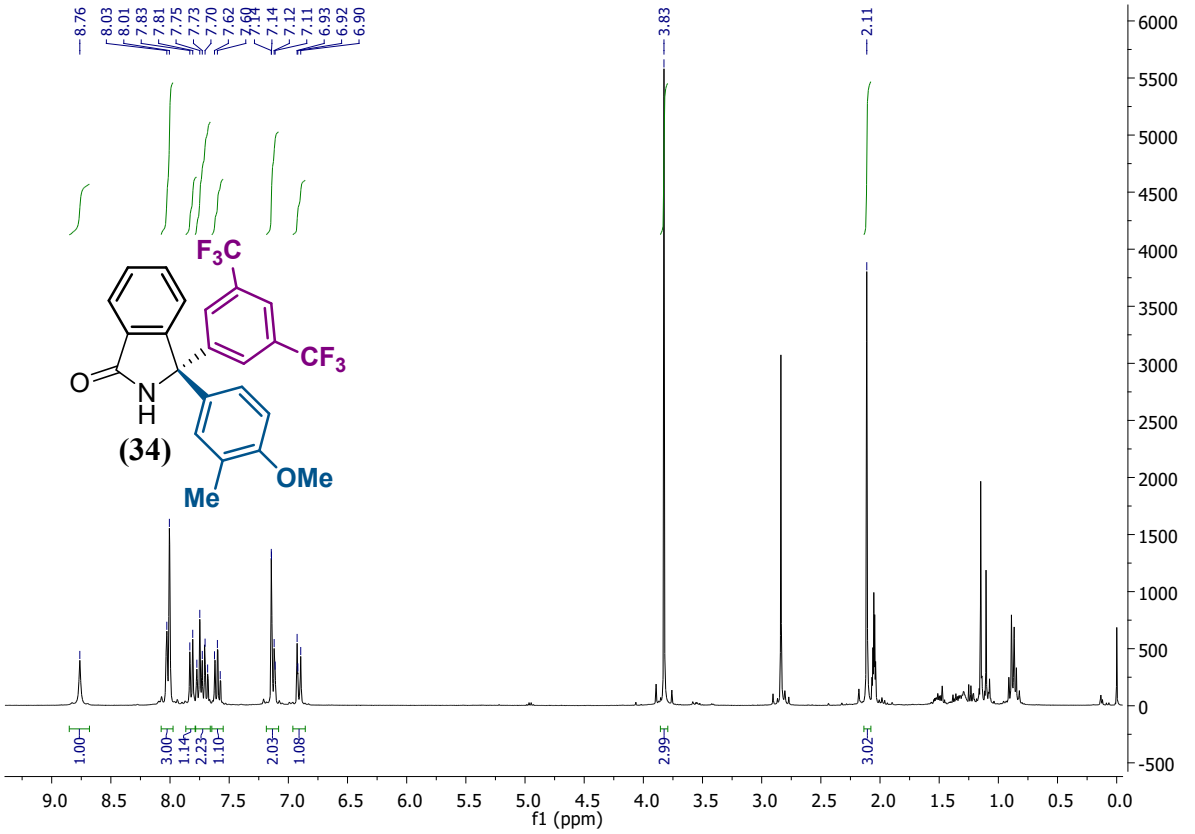
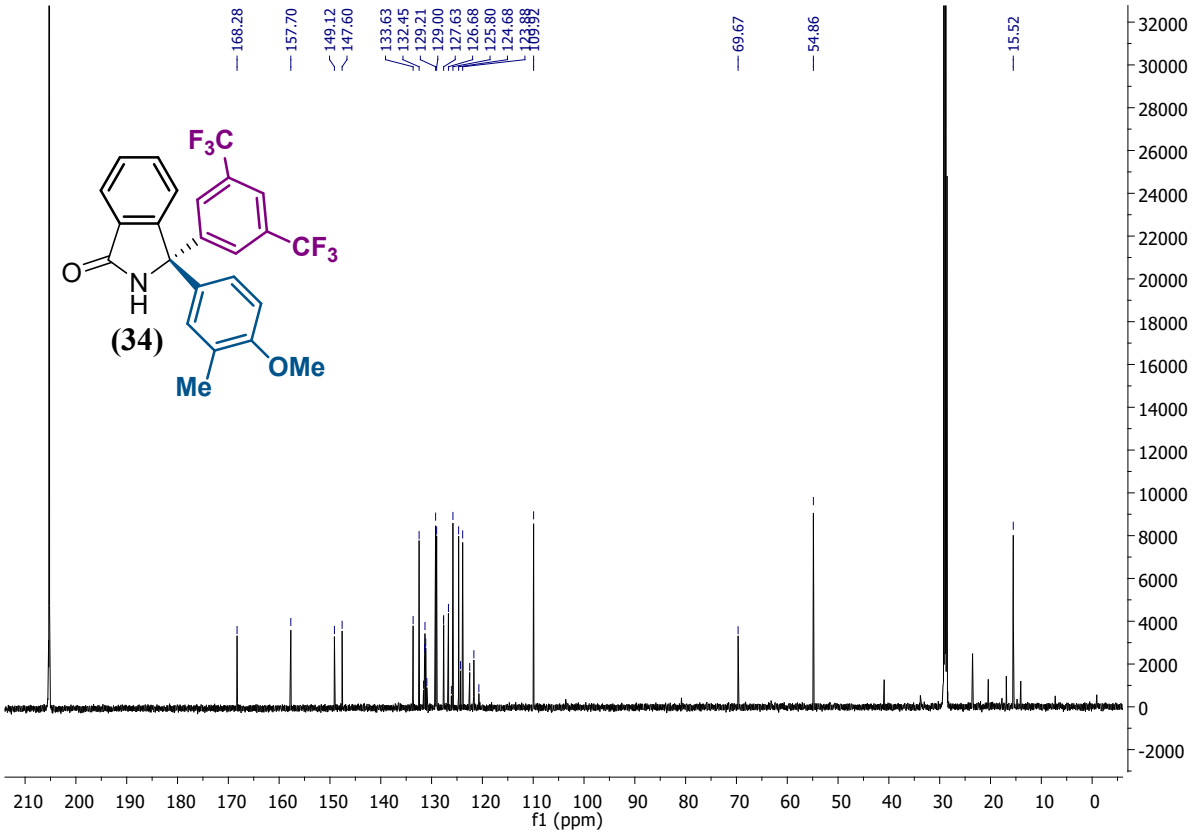
147.88
136.73
135.59
132.61
132.07
131.83
128.92
128.49
128.32
127.77
127.35
126.37
125.87
125.82
125.77
125.71
123.35
122.77
70.13
35.01
29.90
17.64
Cl
Cl
CF3
O
N
H
Me
OH
tBu
(31)
f1 (ppm)

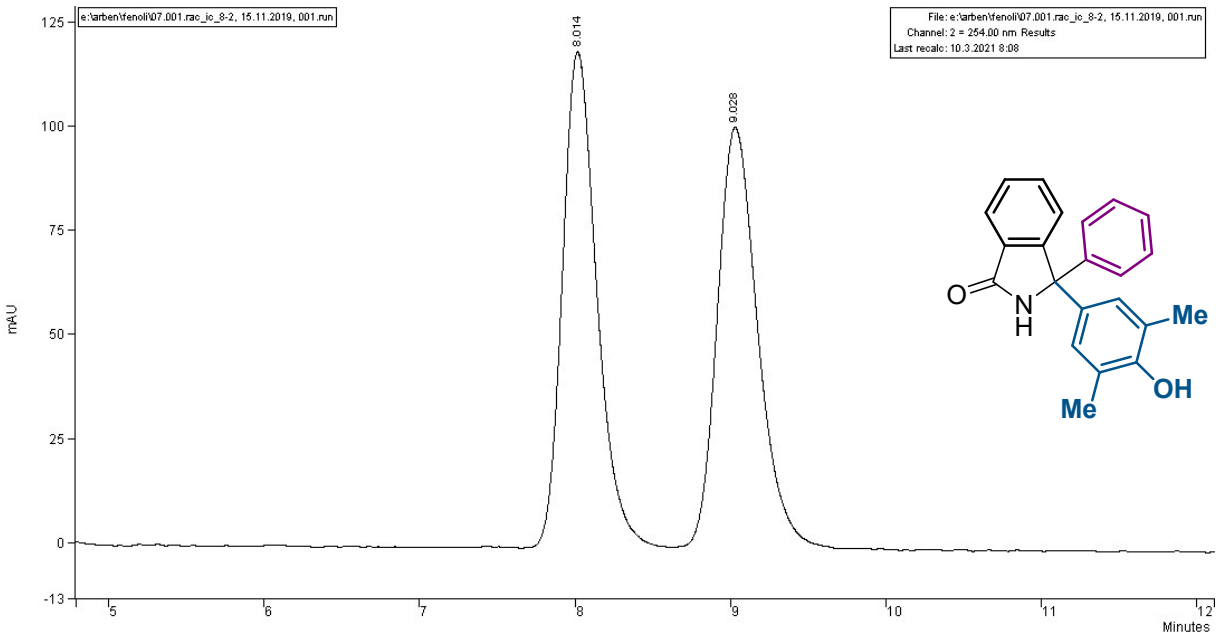

8.40
7.64
7.50
7.44
7.43
7.25
7.23
7.18
7.16
7.12
7.09
6.75
3.51
3.48
3.46
3.44
3.42
3.39
2.29
2.09
1.12
1.10
1.07
1.05
DCM
(32)
Me
OH
Me
iPr
N
O
1.04
1.08
2.07
1.07
1.90
1.86
2.00
1.14
3.04
6.00
2.88
2.80
f1 (ppm)


167.81
153.49
151.54
138.20
137.68
132.55
131.74
130.67
129.55
128.47
128.35
128.28
124.58
124.07
122.79
76.16
46.18
21.00
20.06
19.95
17.32
(32)
Me
OH
Me
iPr
N
O
f1 (ppm)

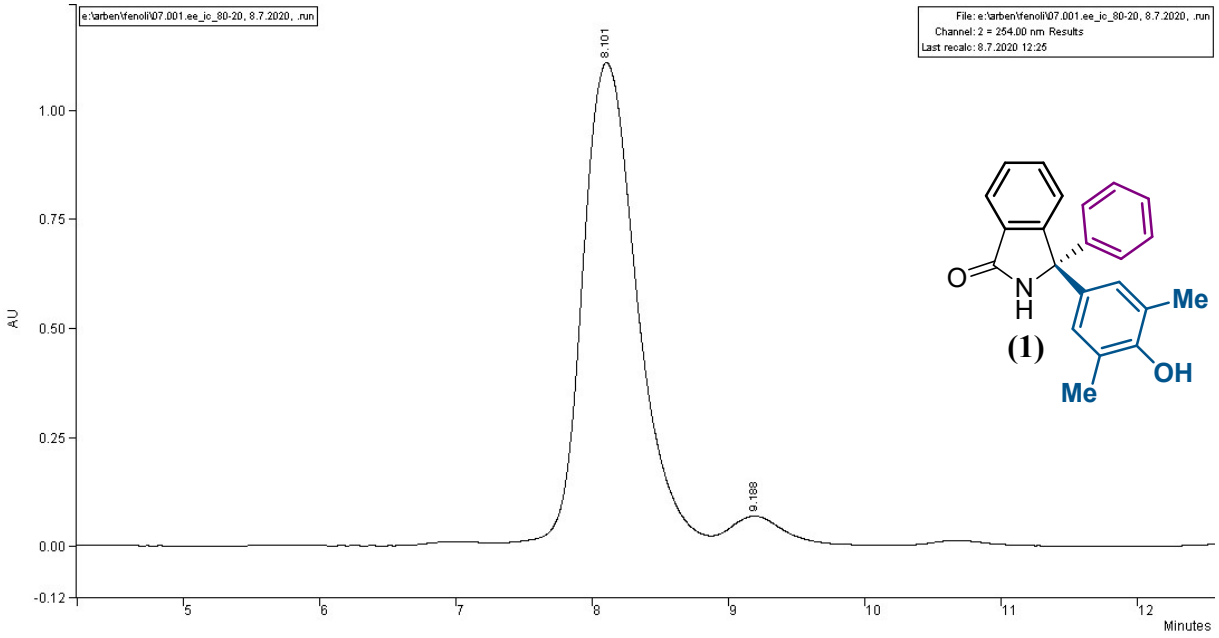

8.76
8.03
8.01
7.83
7.81
7.75
7.73
7.70
7.62
7.60
7.14
7.12
7.11
6.93
6.92
6.90
3.83
2.11
F3C
CF3
O
N
H
(34)
Me
OMe
1.00
3.00
1.14
2.23
1.10
2.03
1.08
2.99
3.02
f1 (ppm)


168.28
157.70
149.12
147.60
133.63
132.45
129.21
129.00
127.63
126.68
125.80
124.68
69.67
54.86
15.52
F3C
CF3
O
N
H
(34)
Me
OMe
f1 (ppm)

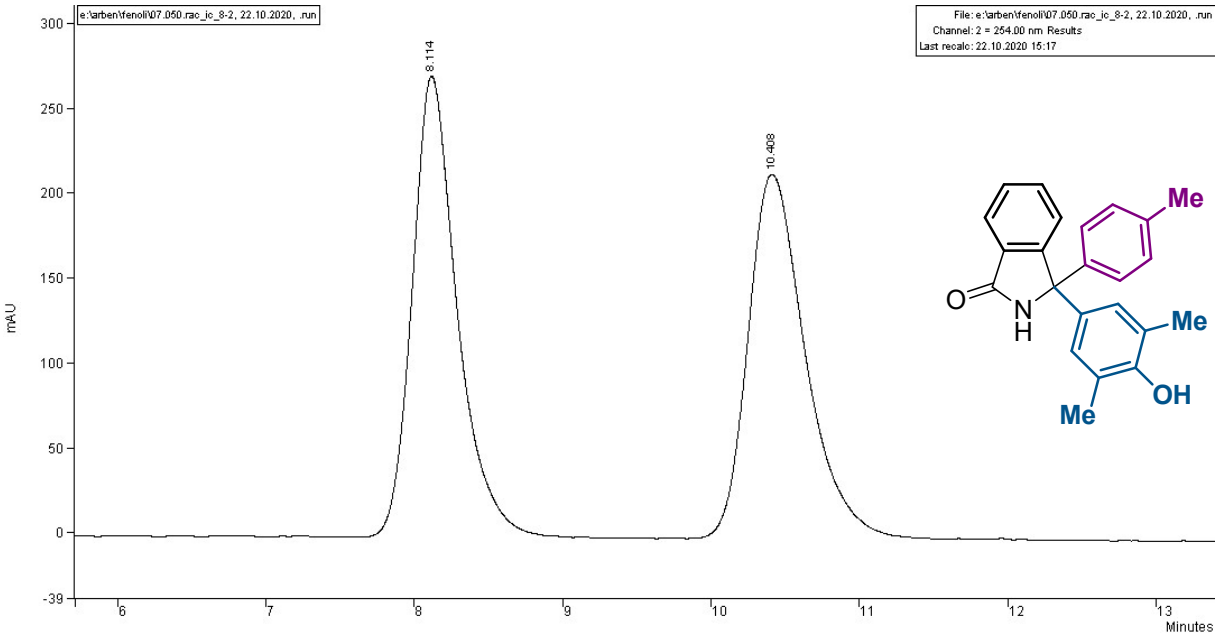
8. HPLC Traces



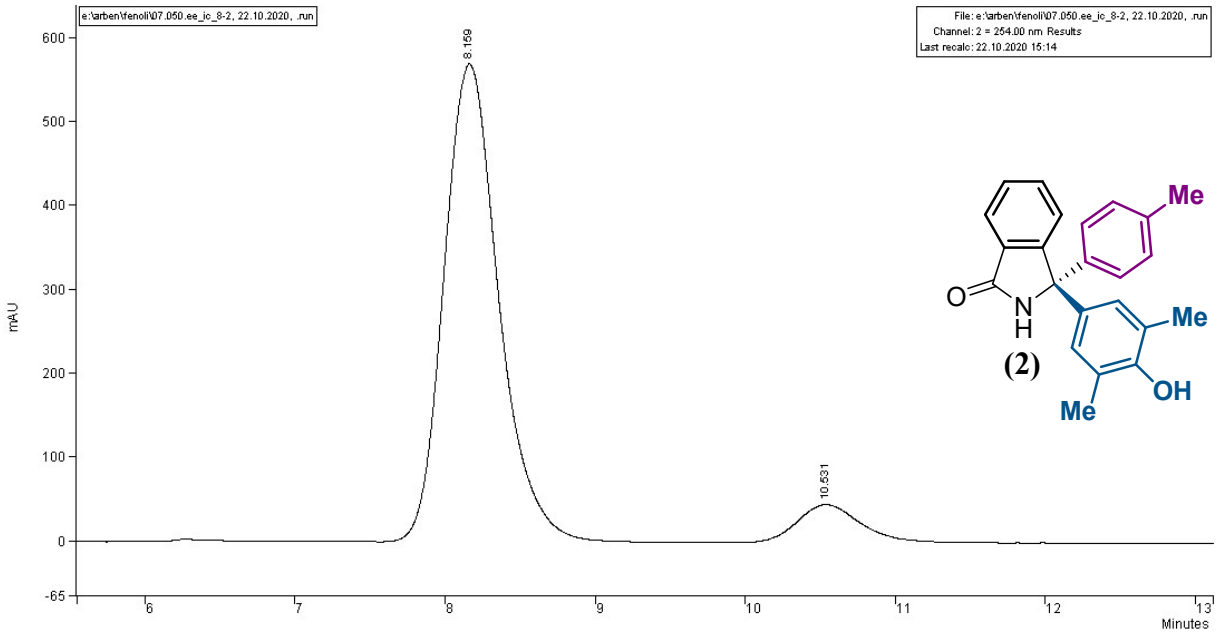
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.4822	8.014	0.000	18140270	BB	13.9	
2		49.5178	9.028	0.000	17793690	BB	16.4	
	Totals:	100.0000		0.000	35933960			



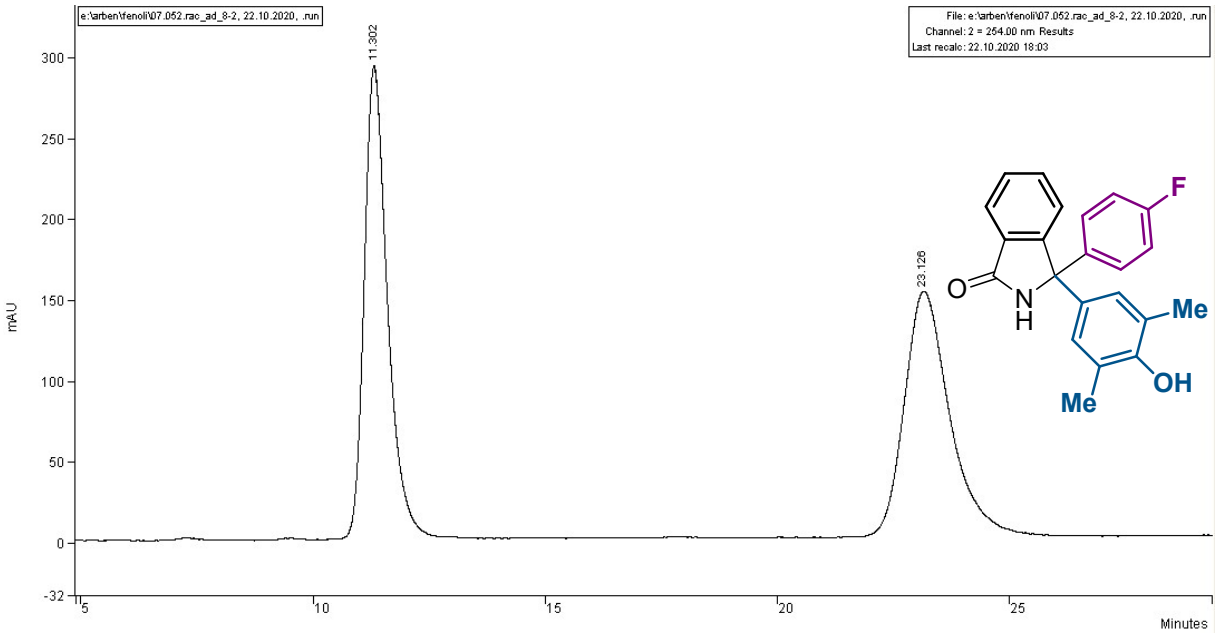
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		96.4054	8.101	0.000	293095712	BB	24.9	
2		3.5946	9.188	0.000	10928432	BB	19.6	
	Totals:	100.0000		0.000	304024144			



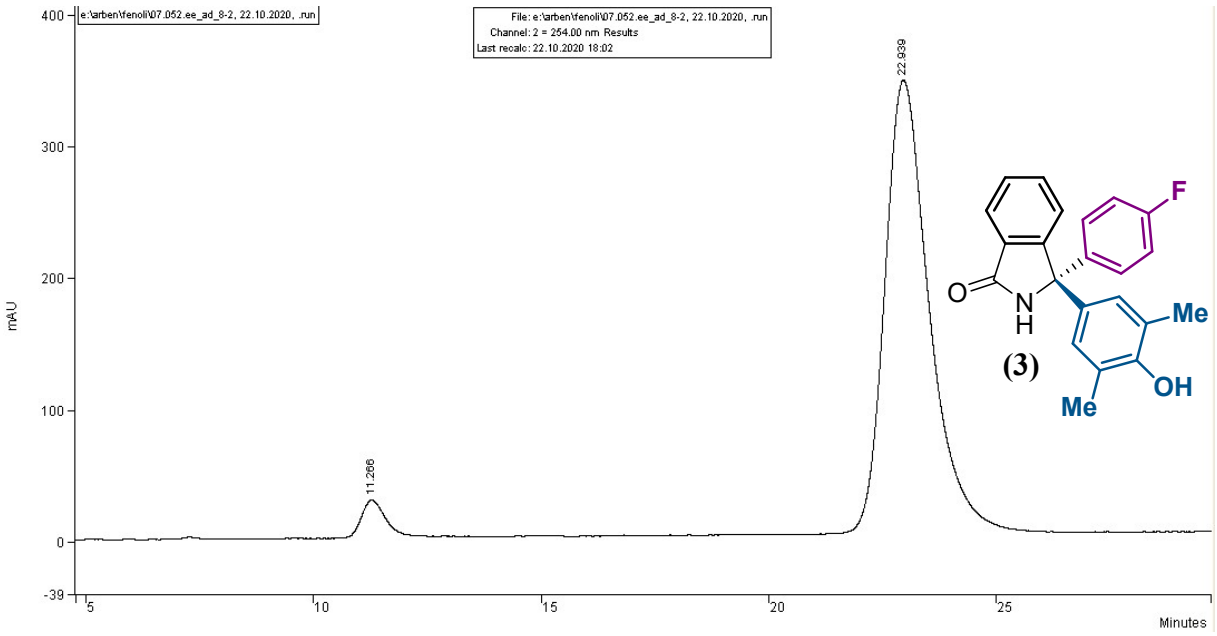
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.7761	8.114	0.000	56942932	BB	18.5	
2		50.2239	10.408	0.000	57455264	BB	24.1	
Totals:		100.0000		0.000	114398196			



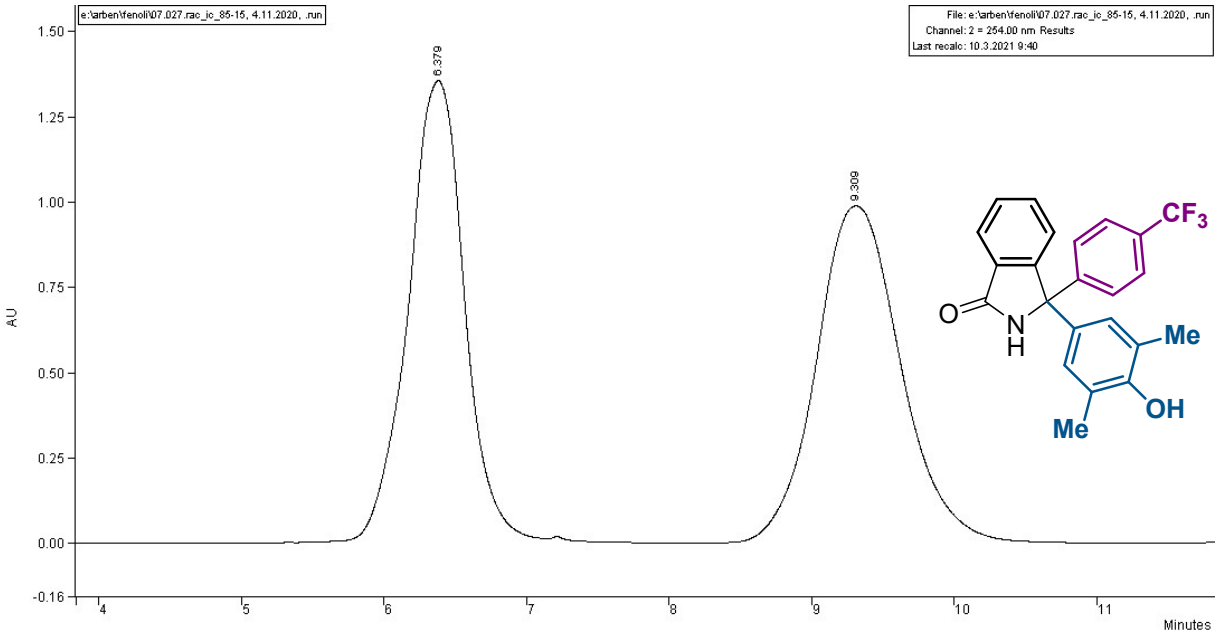
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		91.6357	8.159	0.000	143969440	BB	23.0	
2		8.3643	10.531	0.000	13141173	BB	26.3	
Totals:		100.0000		0.000	157110613			



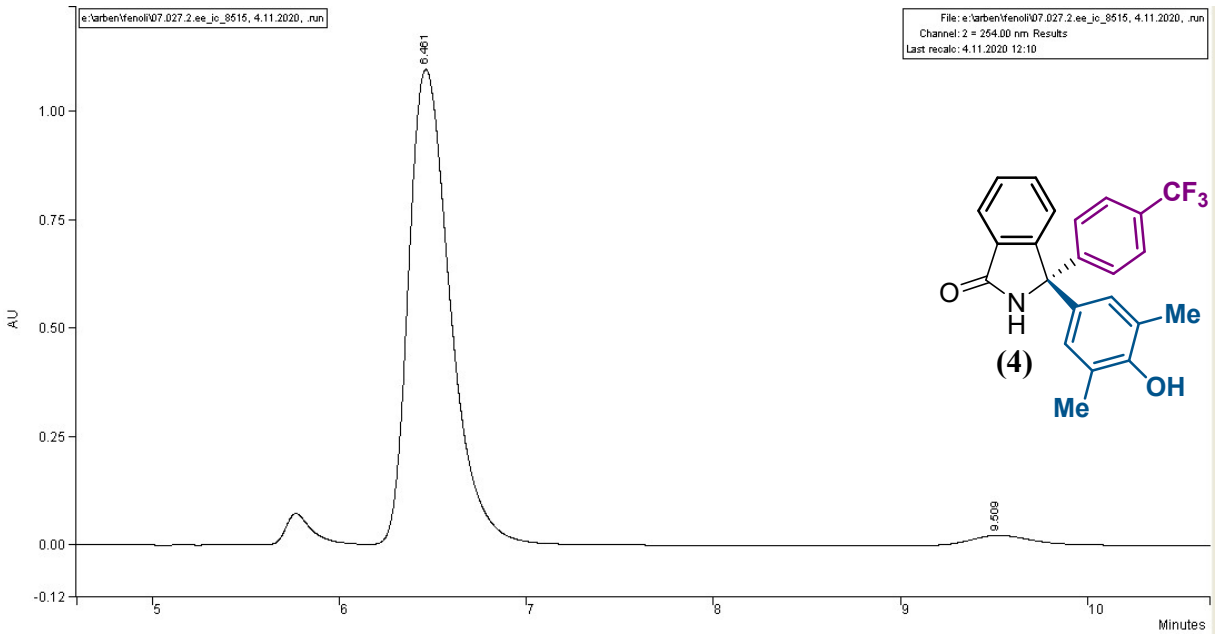
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.8170	12.847	0.000	108906600	BB	29.4	
2		50.1830	14.811	0.000	109706904	BB	33.6	
Totals:		100.0000		0.000	218613504			



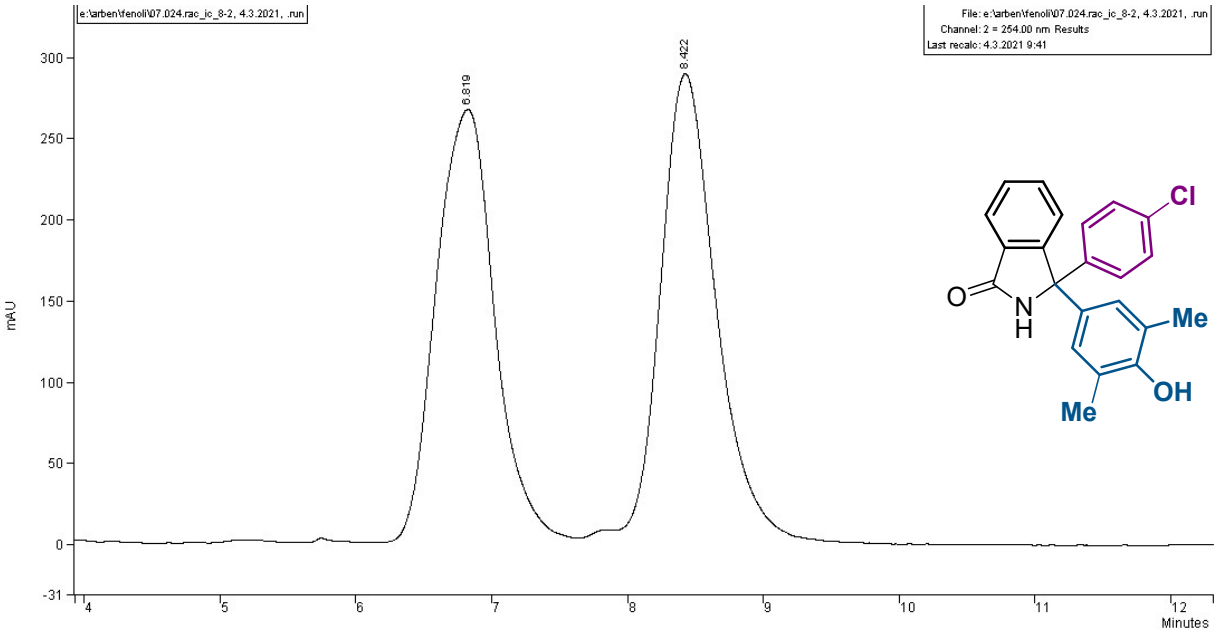
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		4.1514	11.266	0.000	10093745	BB	33.5	
2		95.8486	22.939	0.000	233044896	BB	60.2	
Totals:		100.0000		0.000	243138641			



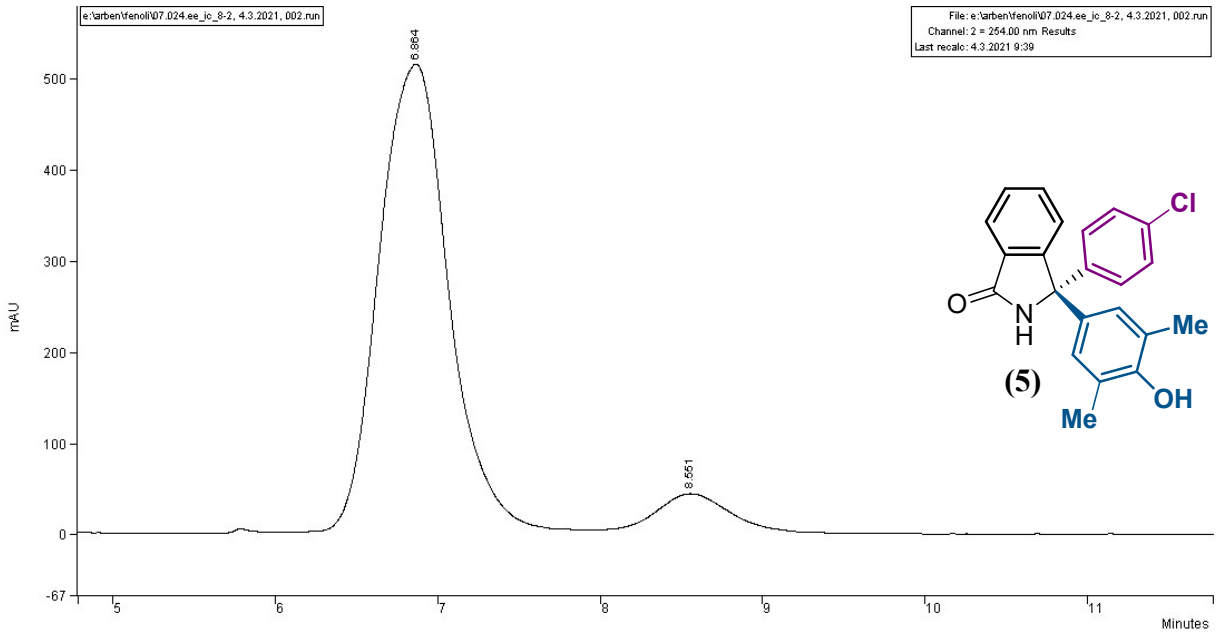
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		48.2282	6.379	0.000	365978464	BB	24.2	
2		51.7718	9.309	0.000	392869056	BB	37.2	
	Totals:	100.0000		0.000	758847520			



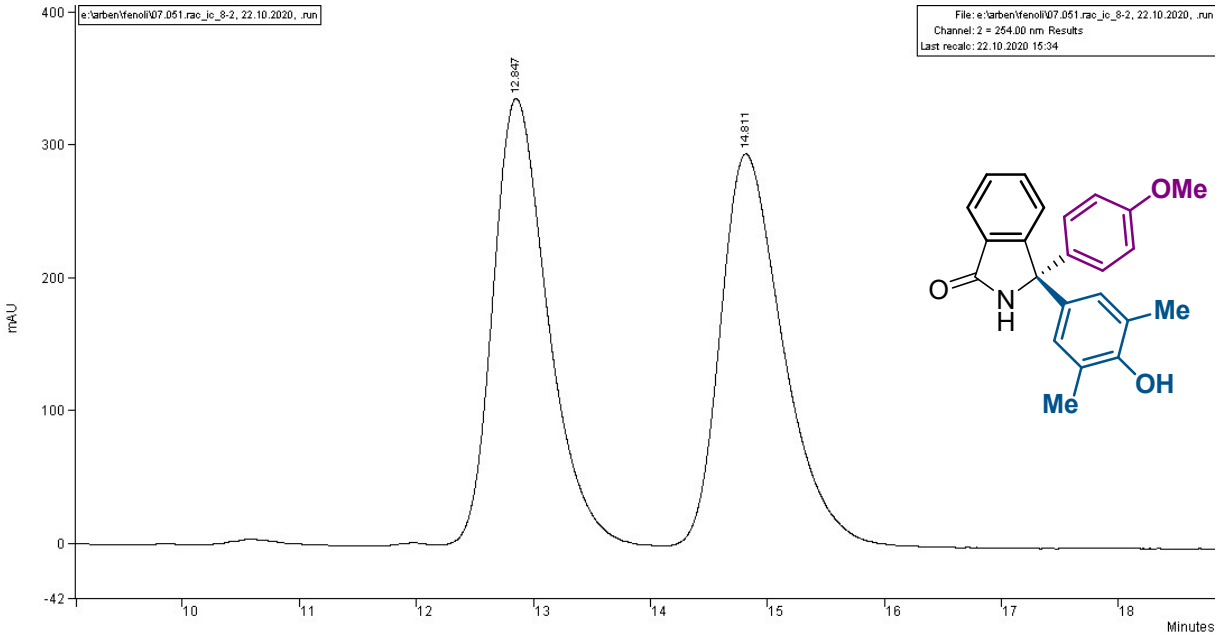
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		97.5581	6.461	0.000	167518144	BB	14.0	
2		2.4419	9.509	0.000	4193067	BB	20.4	
	Totals:	100.0000		0.000	171711211			



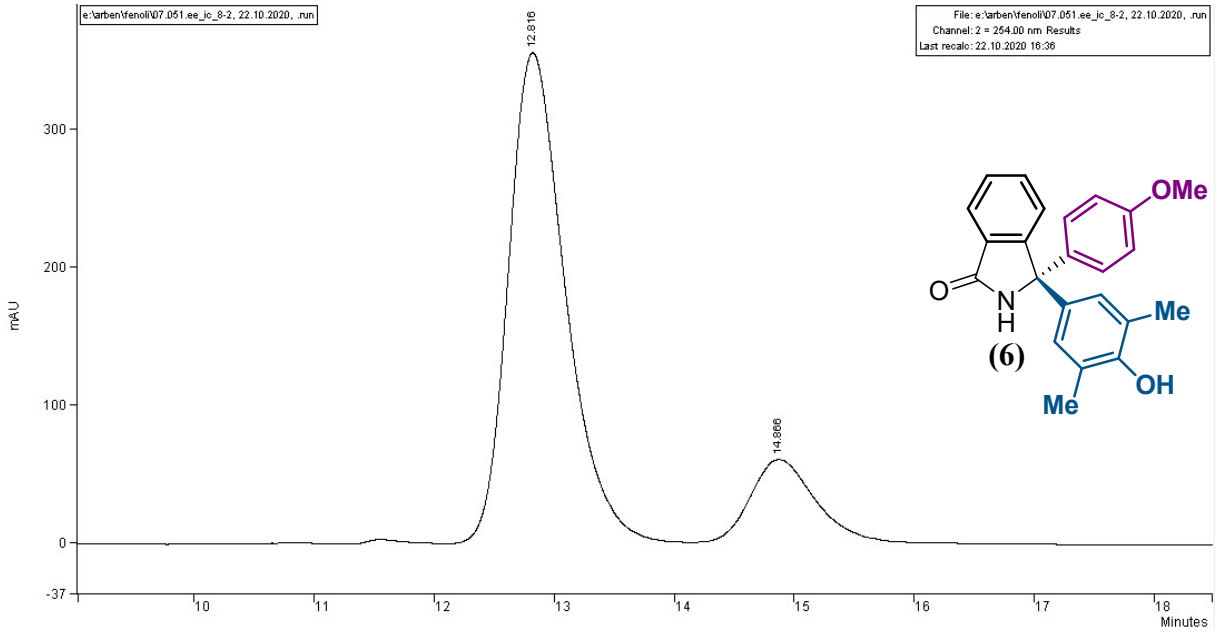
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.3498	6.819	0.000	76696448	BB	27.9	
2		50.6502	8.422	0.000	78717584	BB	25.0	
	Totals:	100.0000		0.000	155414032			



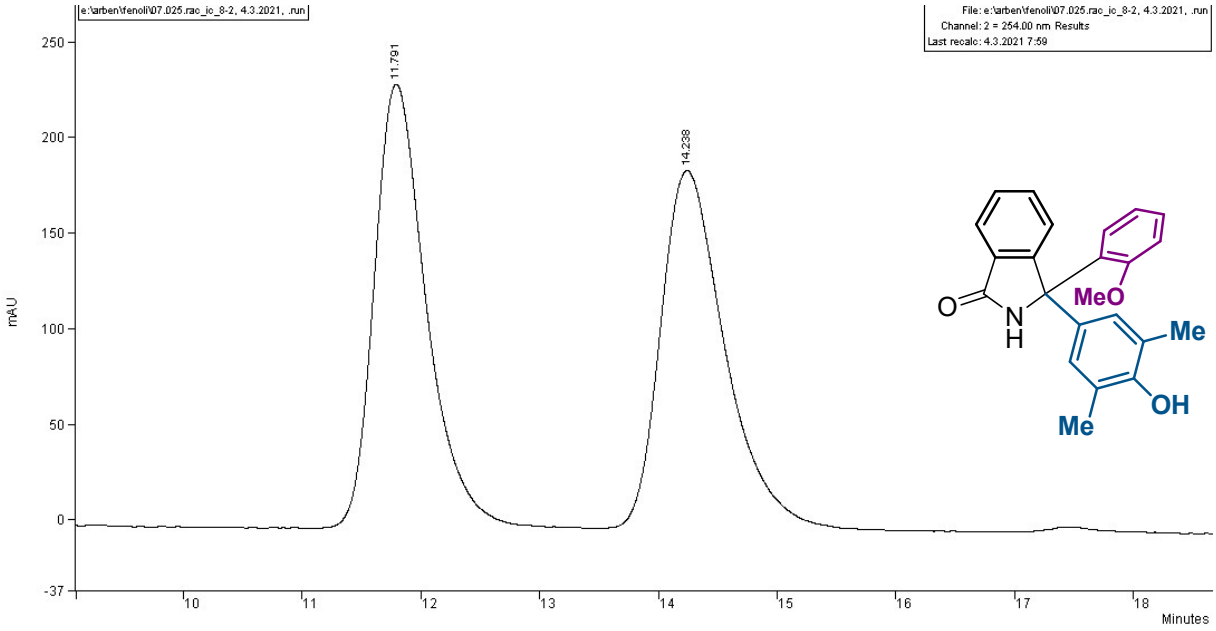
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		92.2833	6.864	0.000	152110944	BB	27.4	
2		7.7167	8.551	0.000	12719440	BB	27.3	
	Totals:	100.0000		0.000	164830384			



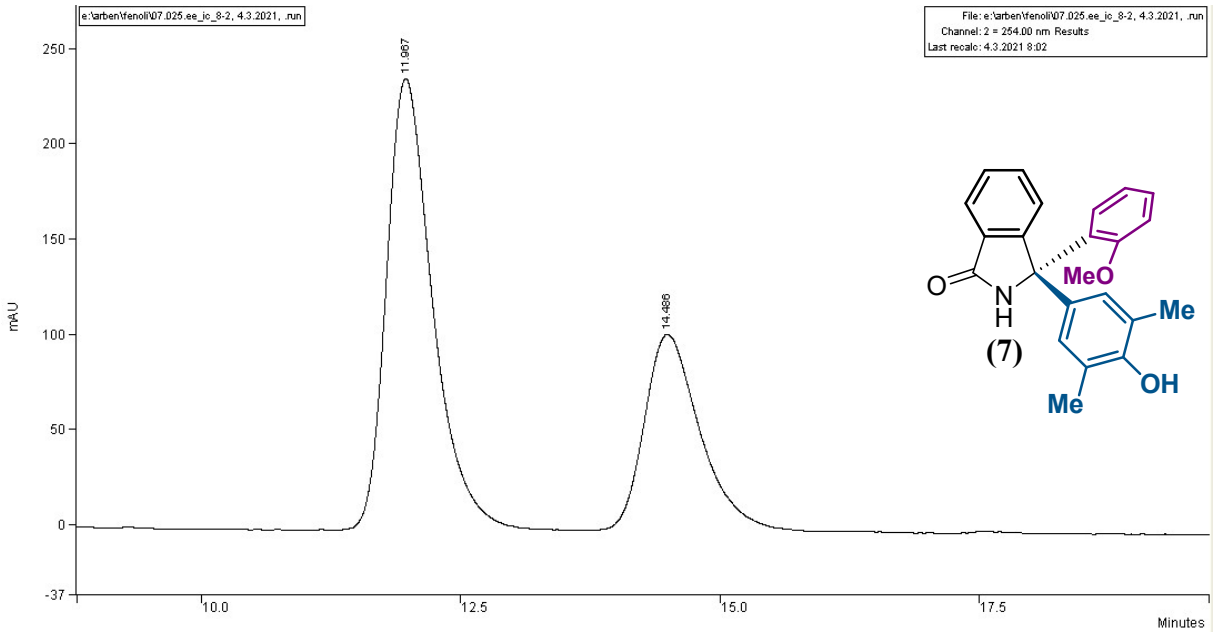
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.8170	12.847	0.000	108906600	BB	29.4	
2		50.1830	14.811	0.000	109706904	BB	33.6	
	Totals:	100.0000		0.000	218613504			



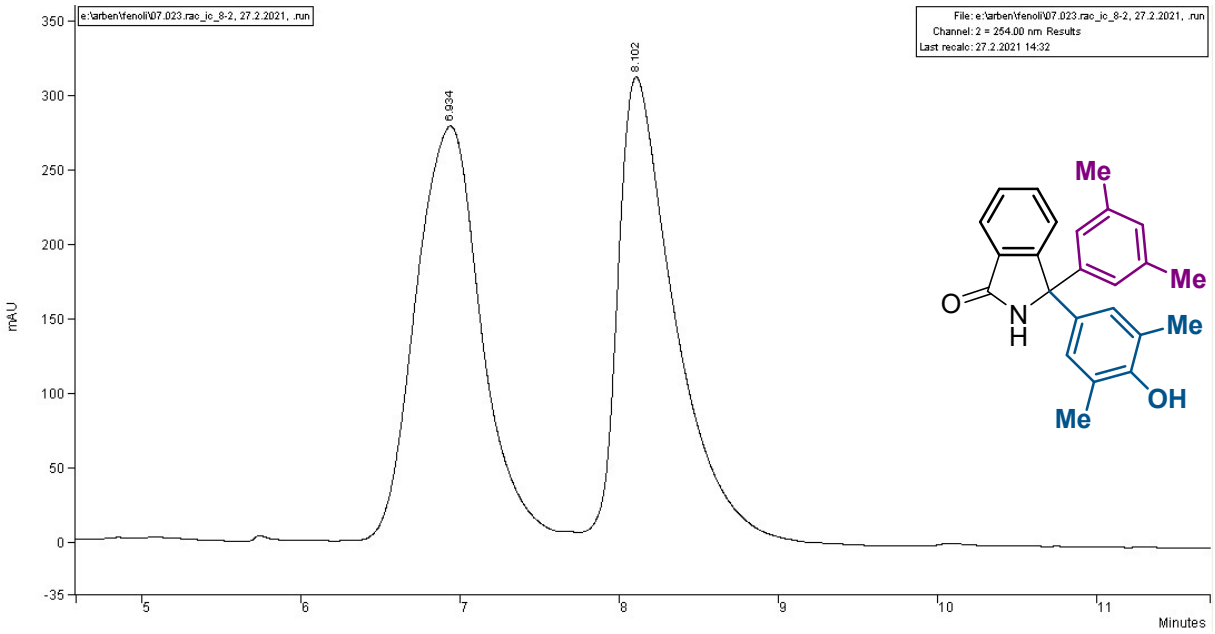
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		83.9382	12.816	0.000	117078120	BB	29.9	
2		16.0618	14.866	0.000	22403244	BB	34.0	
	Totals:	100.0000		0.000	139481364			



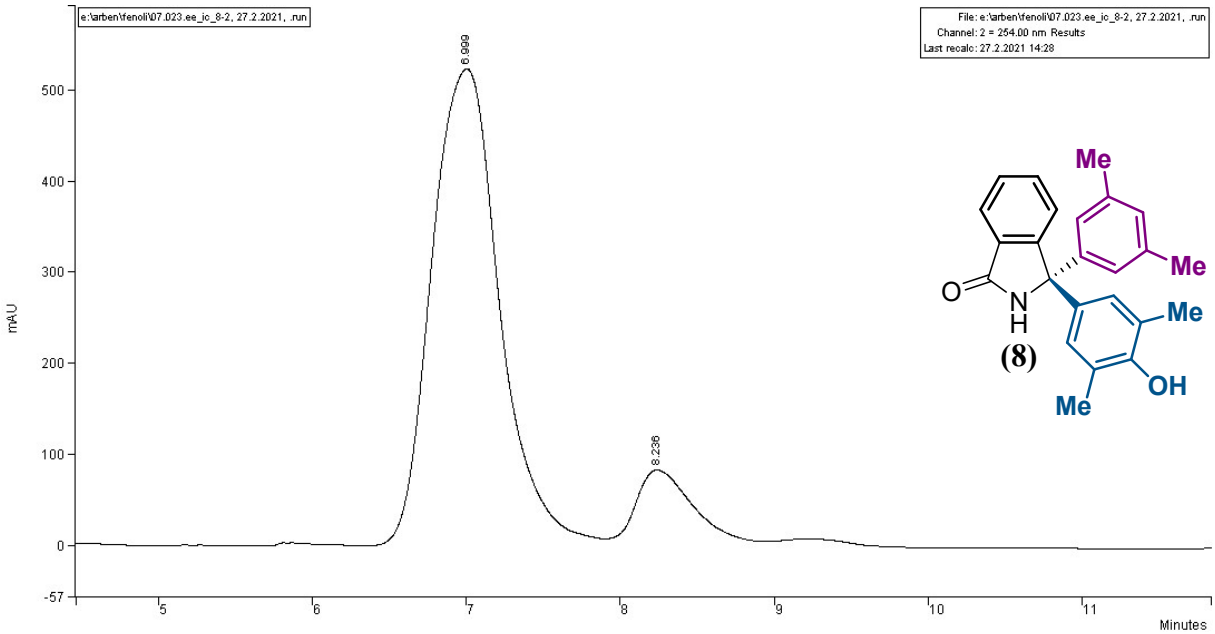
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.0444	11.791	0.000	70452336	BB	27.2	
2		49.9556	14.238	0.000	70327200	BB	33.7	
	Totals:	100.0000		0.000	140779536			



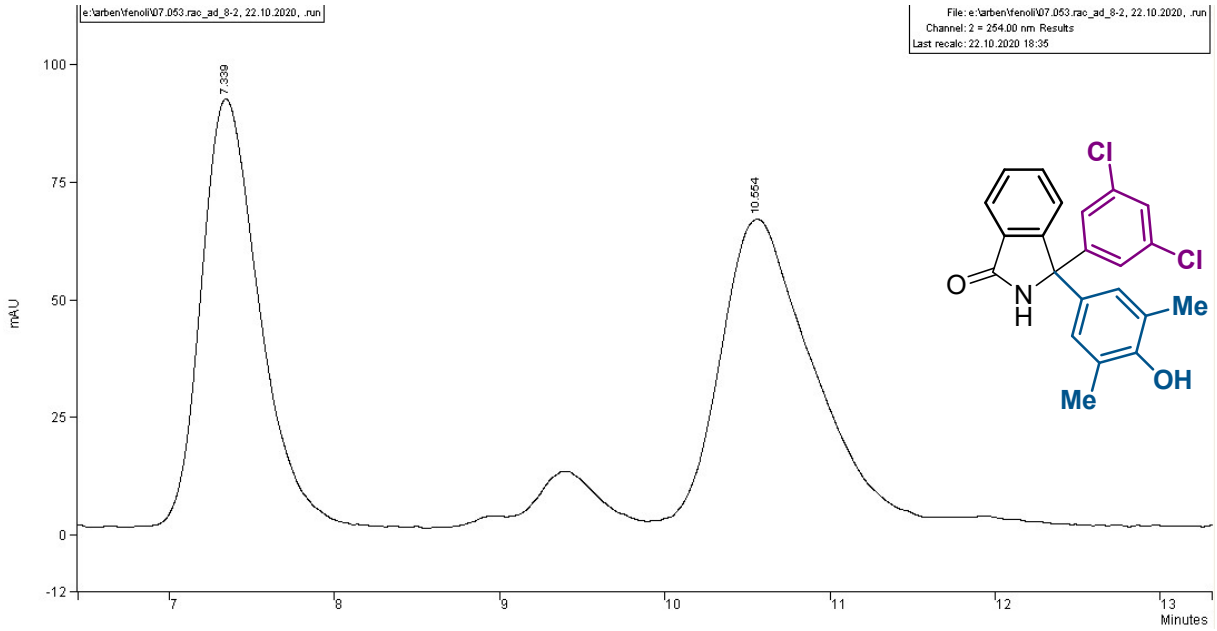
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		65.5944	11.967	0.000	72867112	BB	27.7	
2		34.4056	14.486	0.000	38220360	BB	33.4	
	Totals:	100.0000		0.000	111087472			



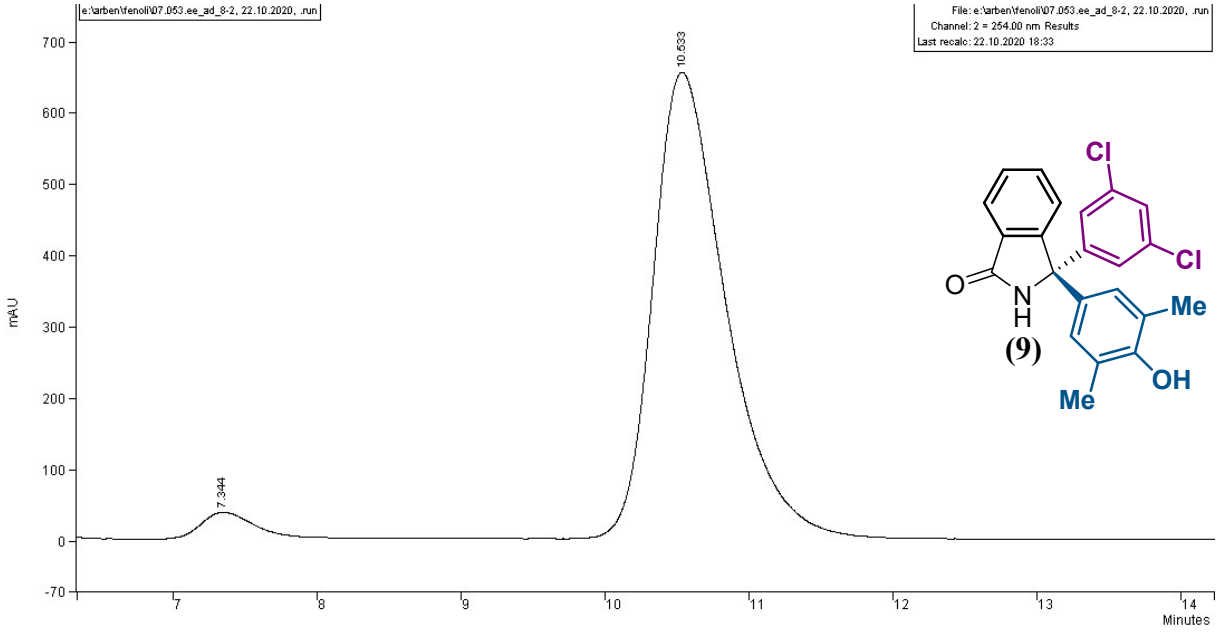
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.7627	6.934	0.000	77143856	BB	26.4	
2		49.2373	8.102	0.000	74825856	BB	21.2	
Totals:		100.0000		0.000	151969712			



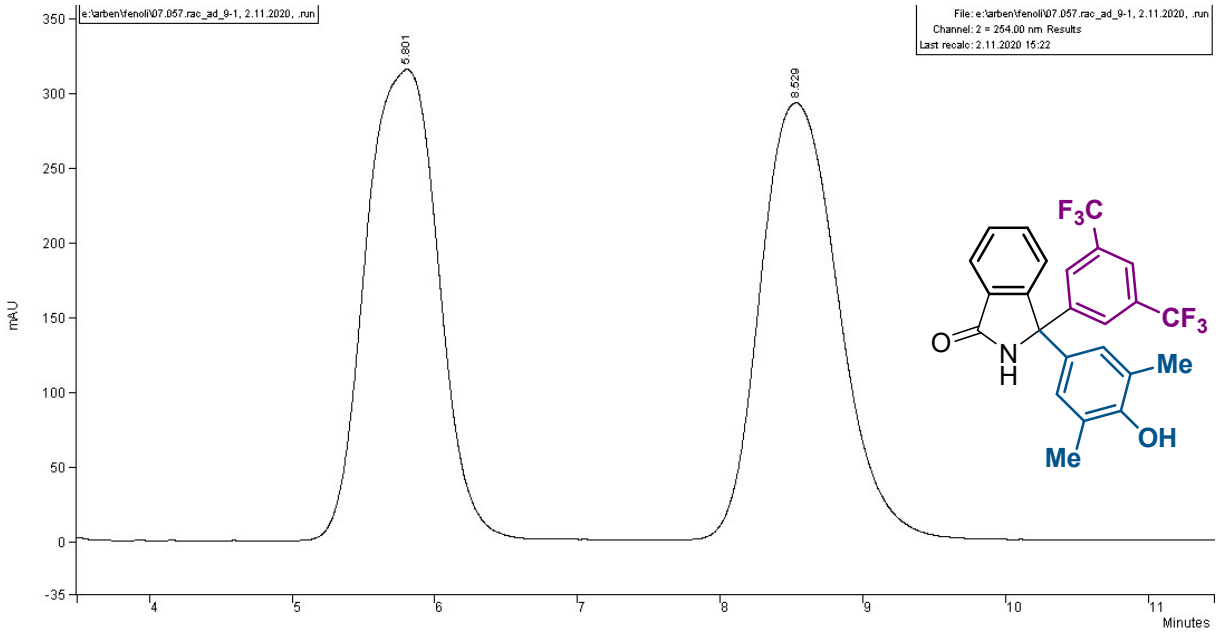
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		89.5572	6.999	0.000	156559296	BB	28.0	
2		10.4428	8.236	0.000	18255534	BB	22.1	
Totals:		100.0000		0.000	174814830			



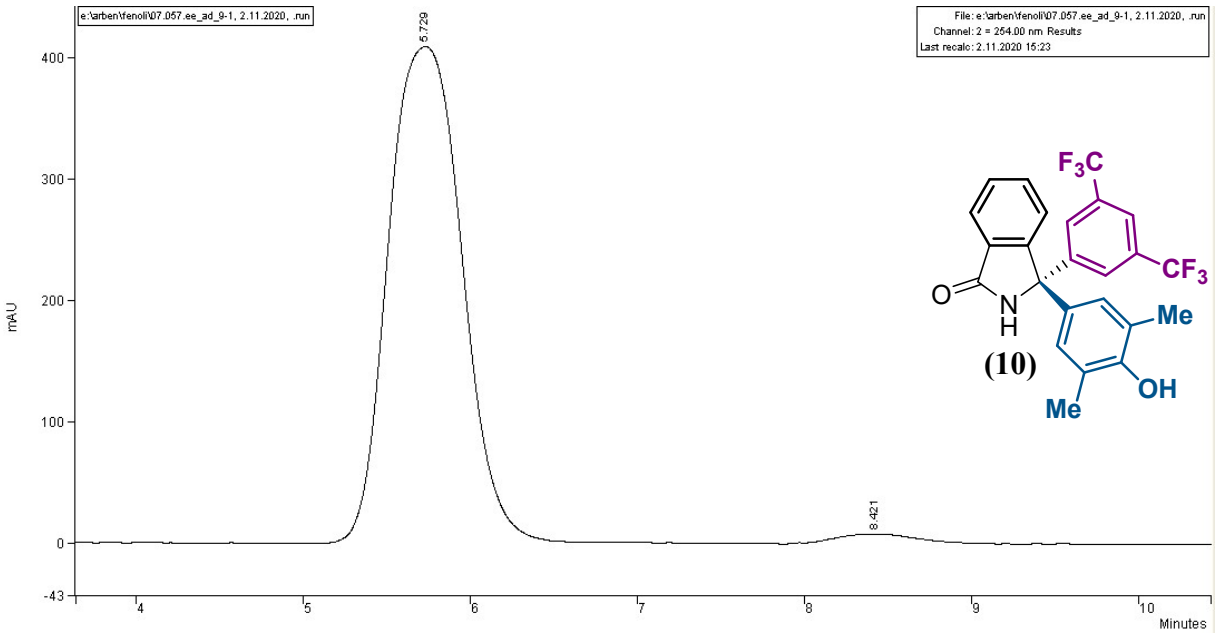
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.5703	7.339	0.000	21839780	BB	22.1	
2		50.4297	10.554	0.000	22218396	BB	33.7	
	Totals:	100.0000		0.000	44058176			



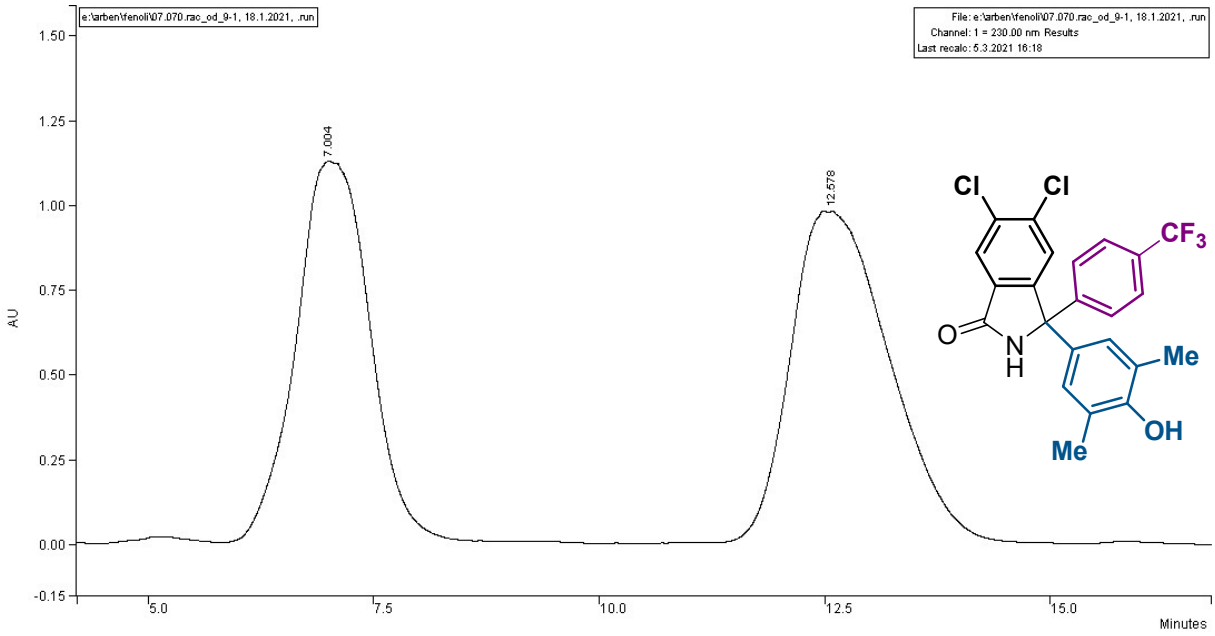
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		3.8881	7.344	0.000	9286061	BB	23.5	
2		96.1119	10.533	0.000	229545712	BB	31.4	
	Totals:	100.0000		0.000	238831773			



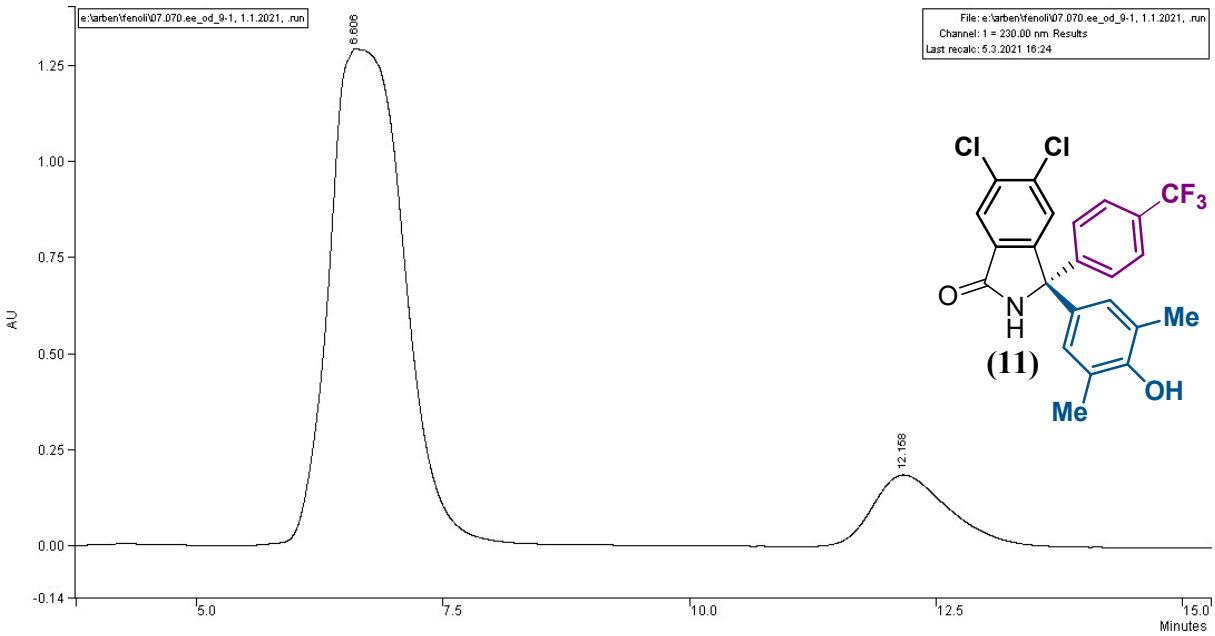
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.0281	5.801	0.000	111002920	BB	34.0	
2		49.9719	8.529	0.000	110878408	BB	35.6	
Totals:		100.0000		0.000	221881328			



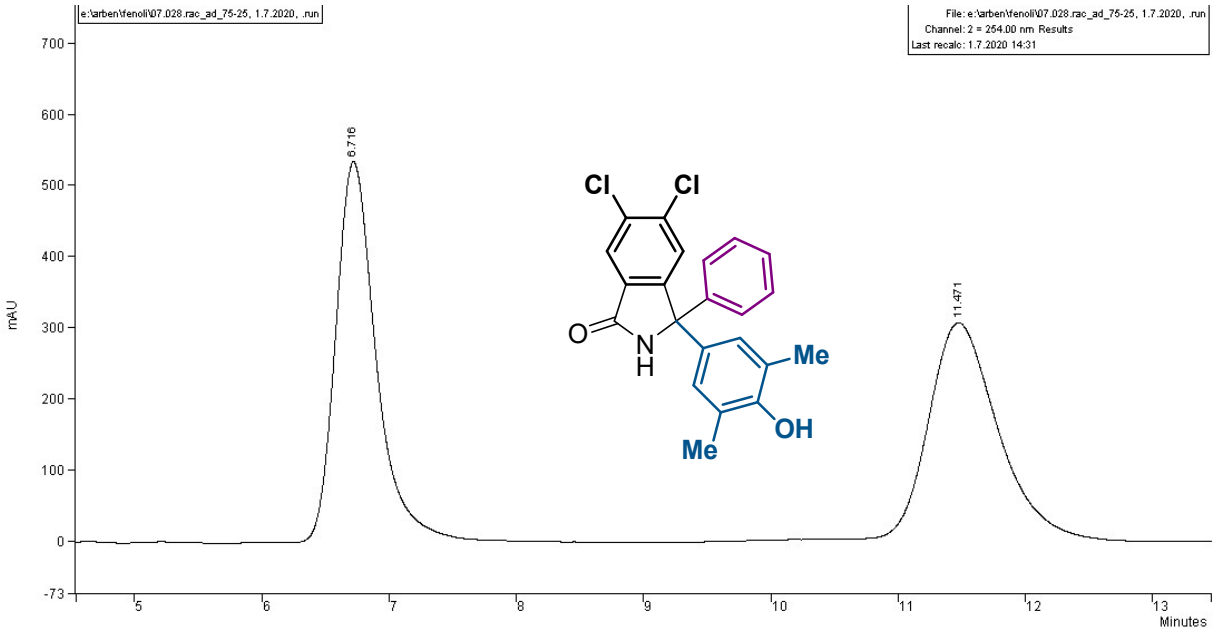
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		97.8734	5.729	0.000	124857464	BB	29.3	
2		2.1266	8.421	0.000	2712920	BB	32.5	
Totals:		100.0000		0.000	127570384			



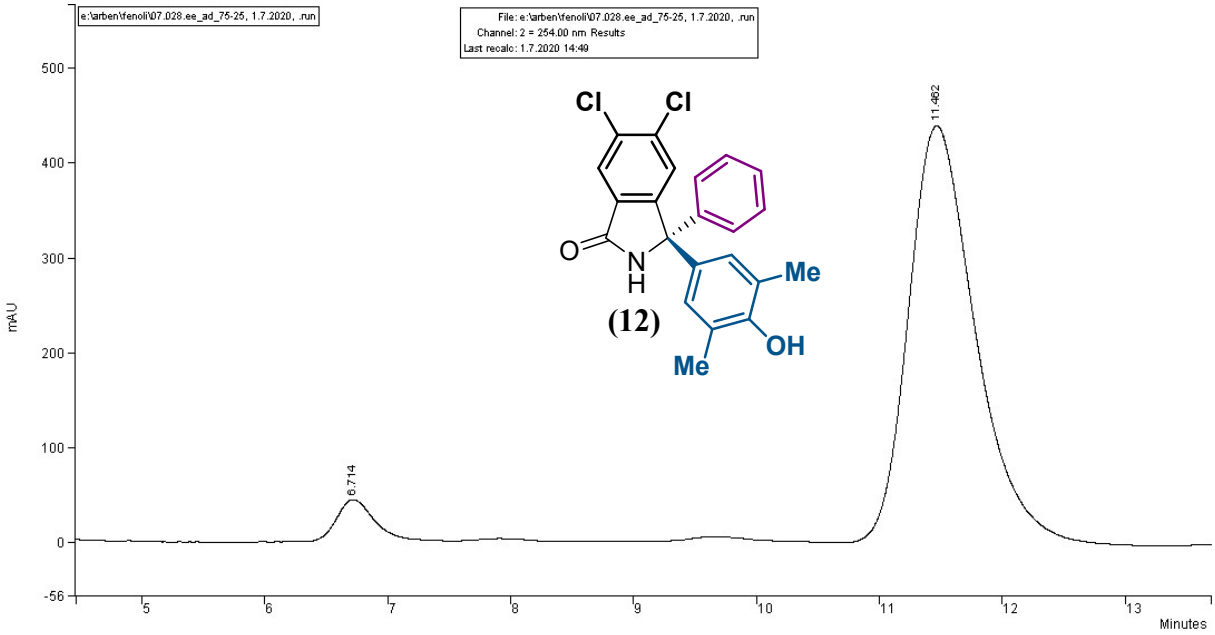
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.3759	7.004	0.000	634180096	BB	52.1	
2		50.6241	12.578	0.000	650210944	BB	69.3	
	Totals:	100.0000		0.000	1284391040			



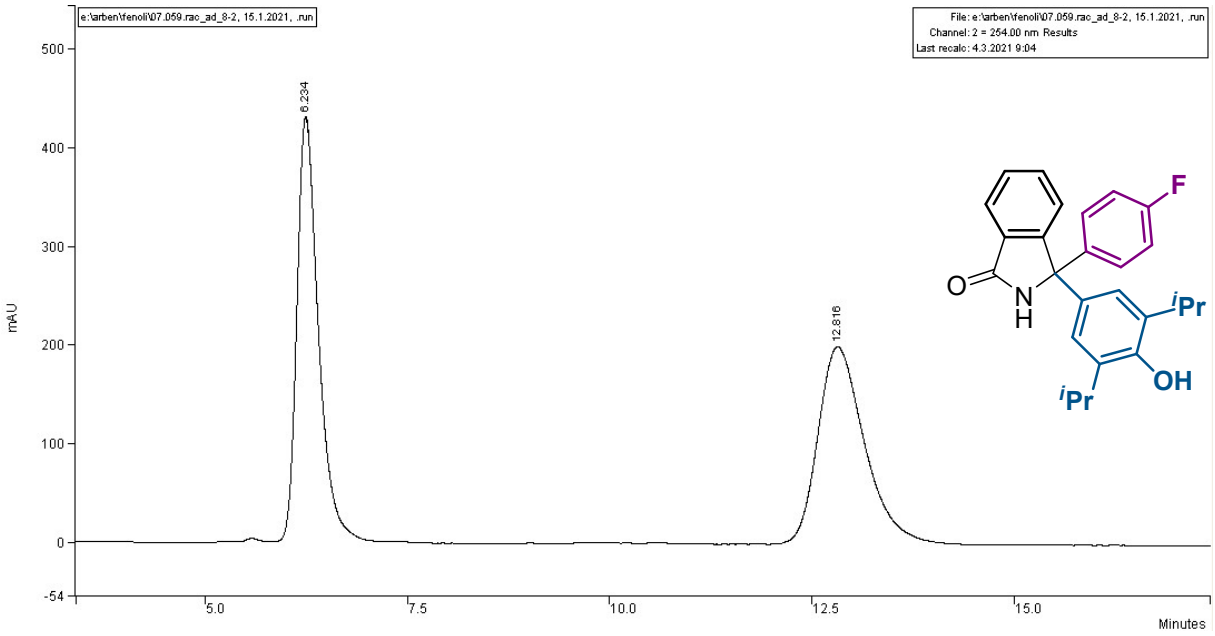
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		92.1750	6.606	0.000	675109440	BB	48.7	
2		7.8250	12.158	0.000	57312092	BB	39.4	
	Totals:	100.0000		0.000	732421532			



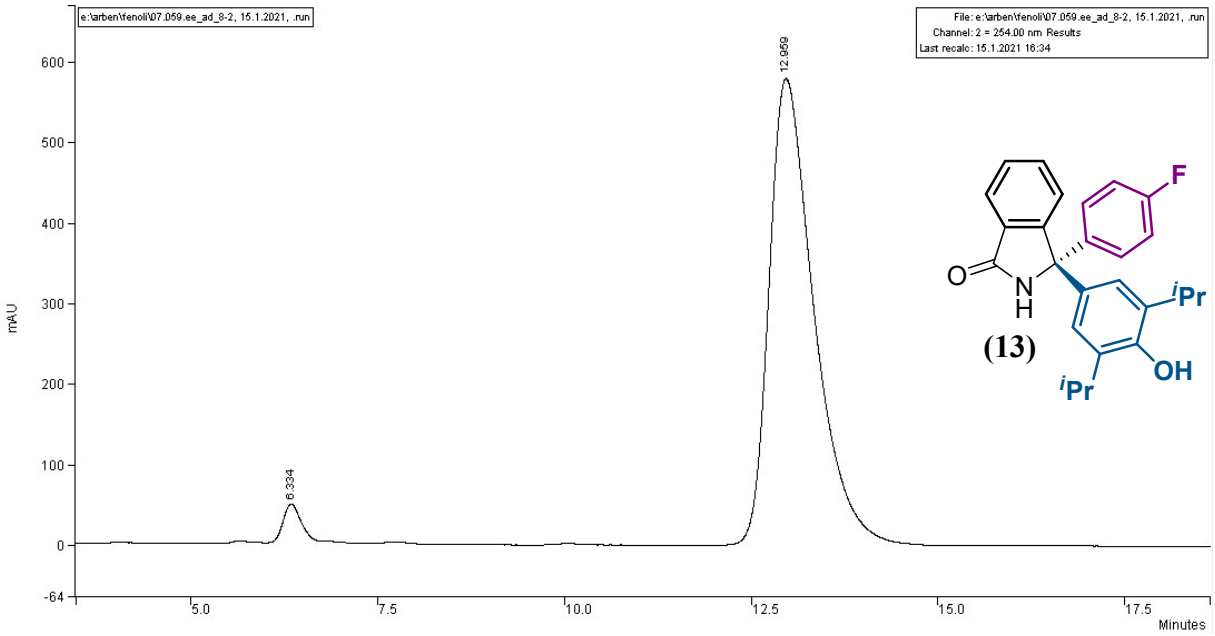
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.7086	6.716	0.000	113594888	BB	19.4	
2		50.2914	11.471	0.000	114926648	BB	34.1	
Totals:		100.0000		0.000	228521536			



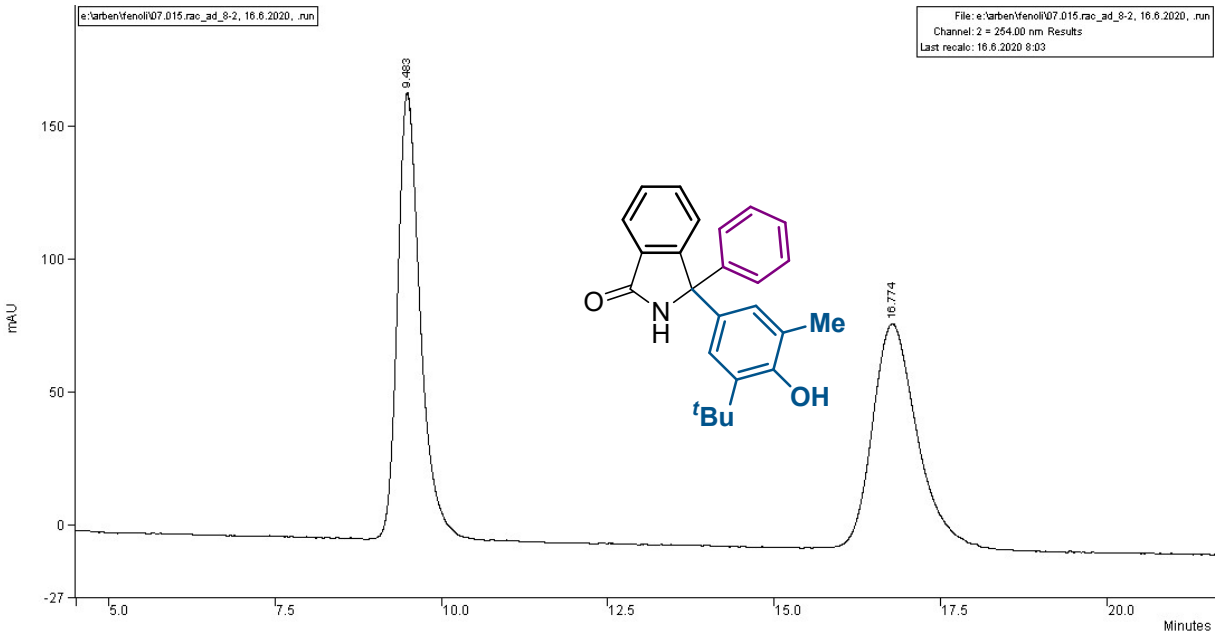
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		5.1870	6.714	0.000	9058787	BB	19.2	
2		94.8130	11.462	0.000	165585248	BB	33.9	
Totals:		100.0000		0.000	174644035			



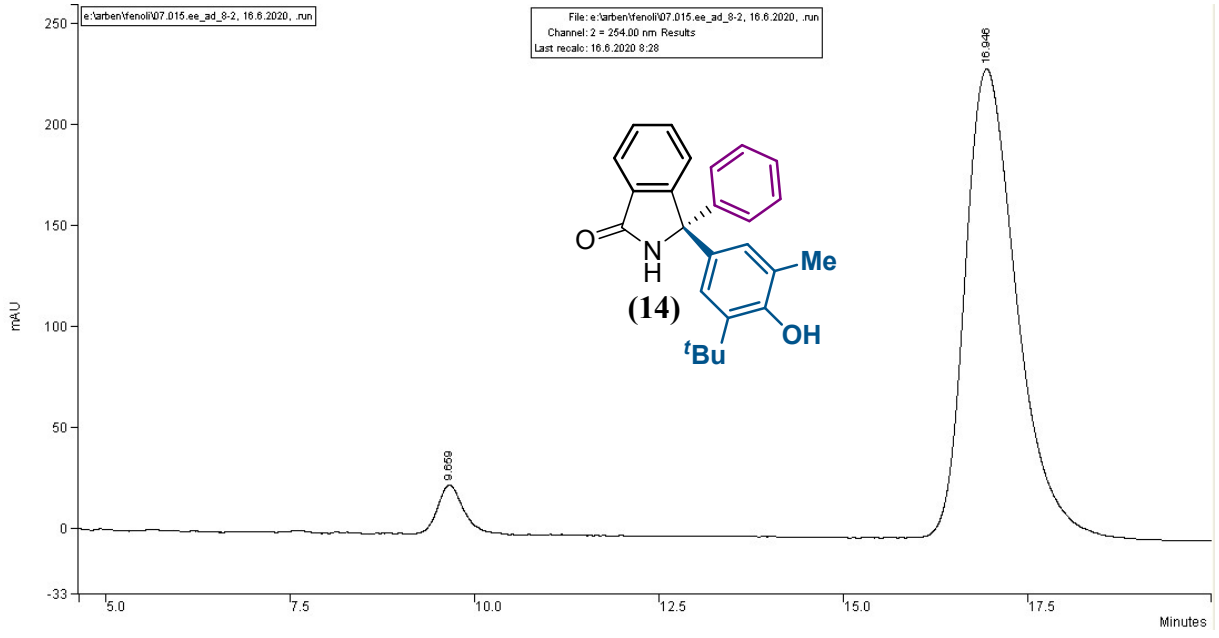
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.7129	6.234	0.000	78808912	BB	16.3	
2		50.2871	12.816	0.000	79719128	BB	36.3	
Totals:		100.0000		0.000	158528040			



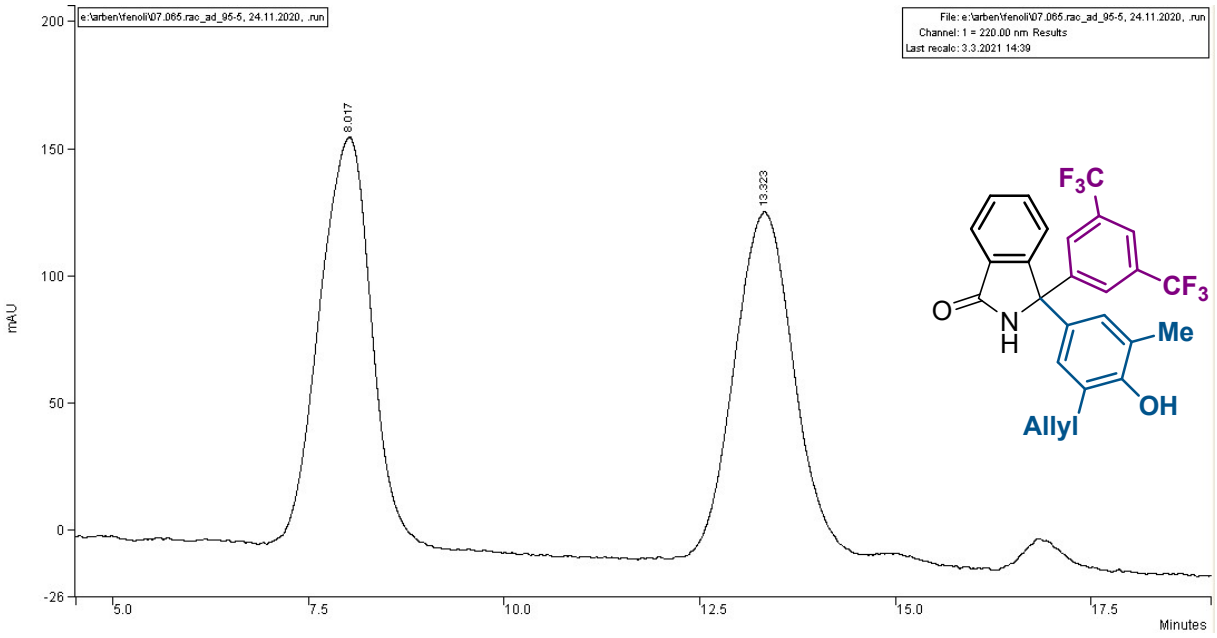
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		3.1066	6.334	0.000	7765268	BB	15.6	
2		96.8934	12.959	0.000	242193280	BB	37.4	
Totals:		100.0000		0.000	249958548			



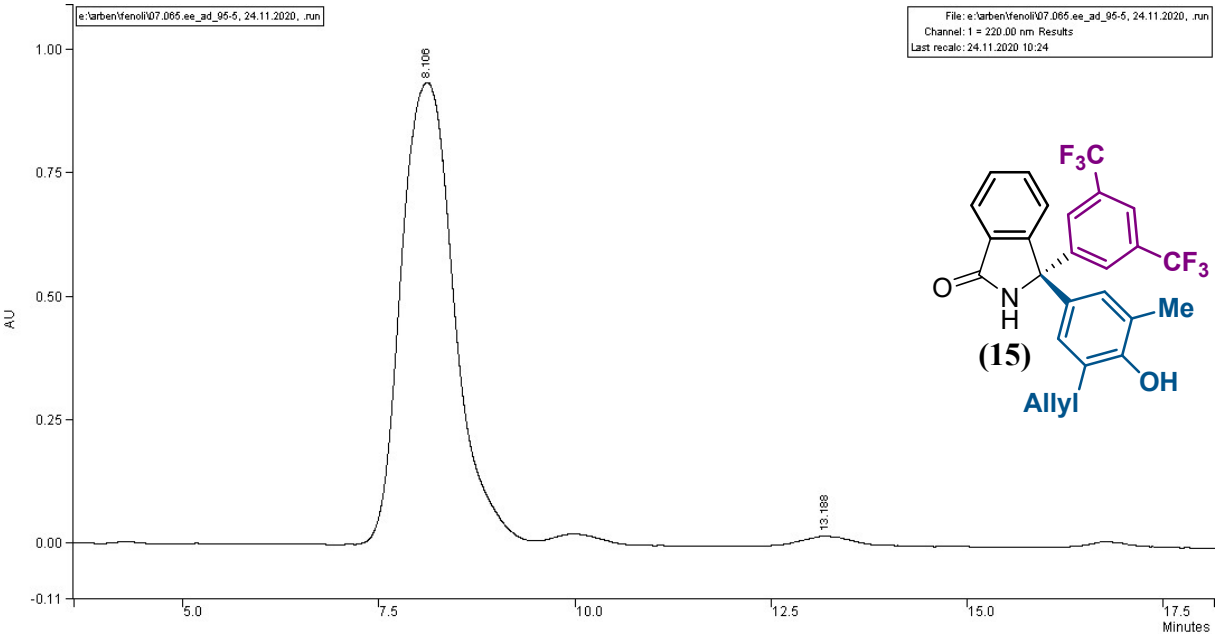
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.2854	9.483	0.000	39878076	BB	20.9	
2		49.7147	16.774	0.000	39425496	BB	41.7	
	Totals:	100.0001		0.000	79303572			



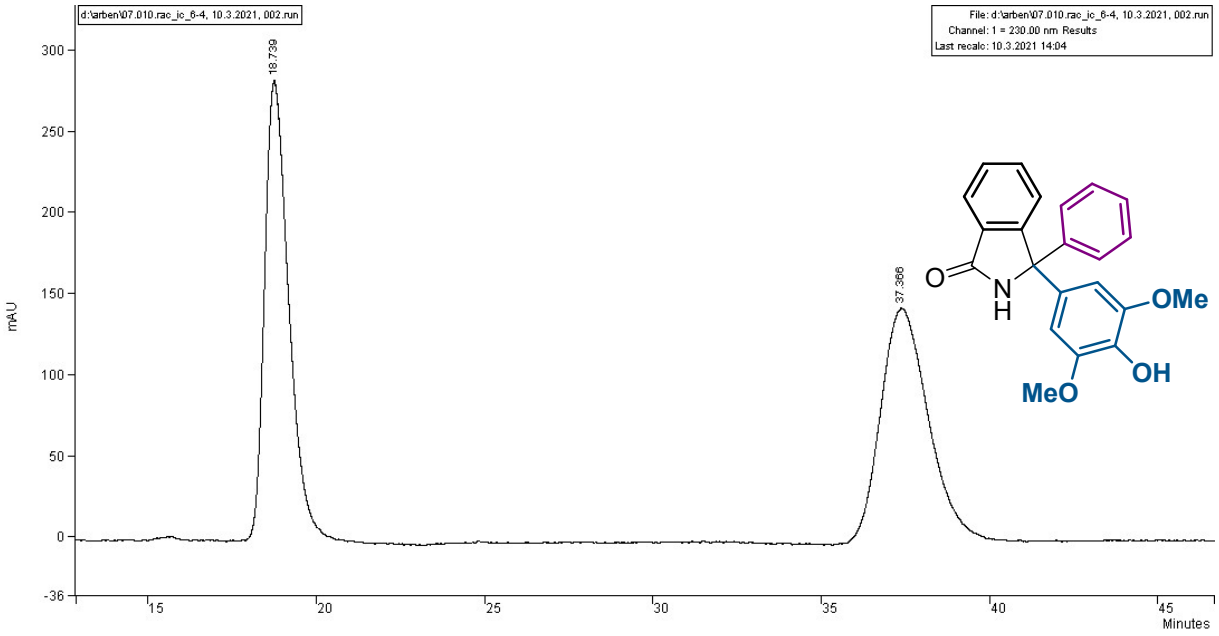
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		4.9691	9.659	0.000	5918597	BB	21.4	
2		95.0309	16.946	0.000	113190176	BB	43.6	
	Totals:	100.0000		0.000	119108773			



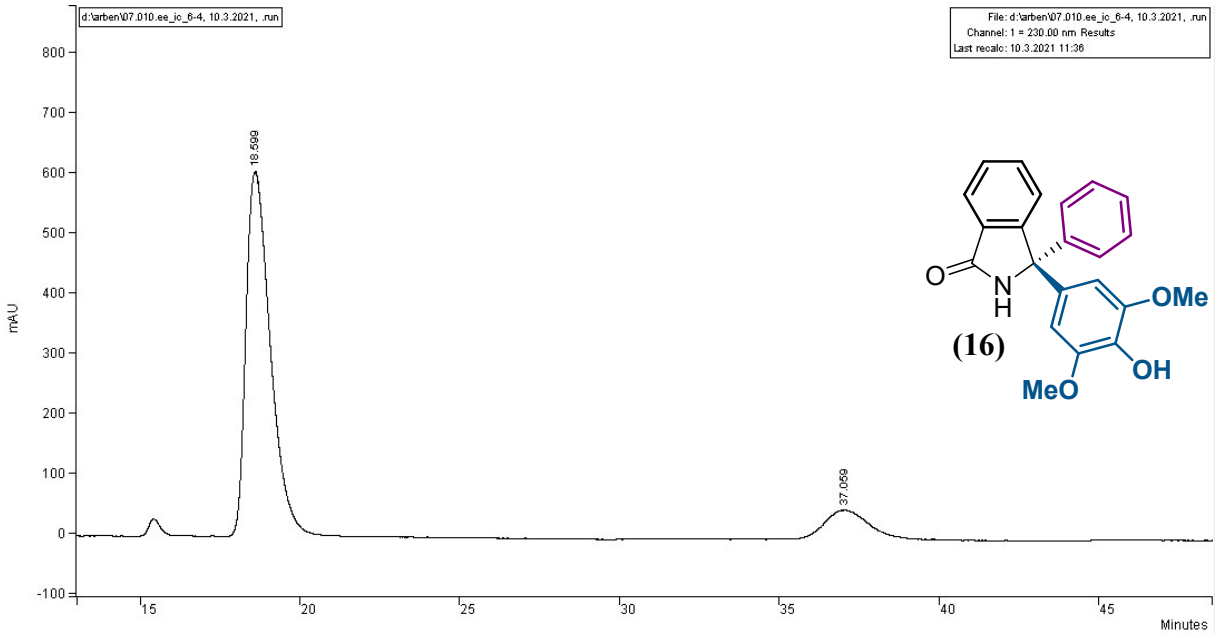
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.9161	8.017	0.000	74116808	BB	43.2	
2		49.0839	13.323	0.000	71449744	BB	49.5	
	Totals:	100.0000		0.000	145566552			



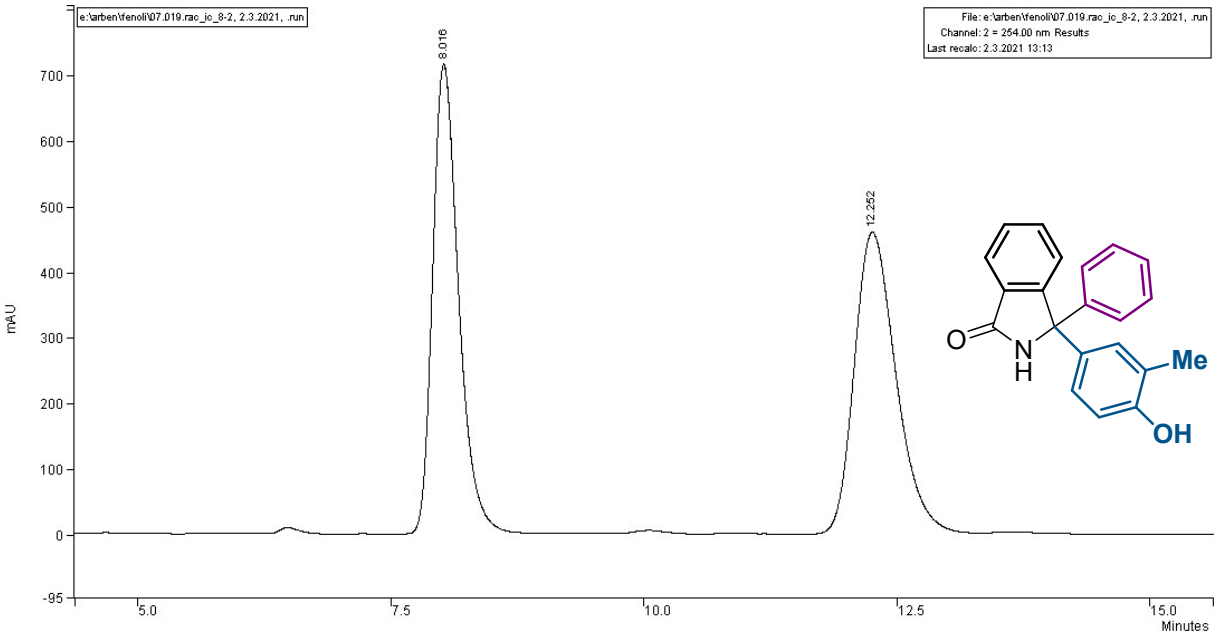
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		98.1600	8.106	0.000	436117888	BB	43.2	
2		1.8400	13.188	0.000	8175144	BB	43.1	
	Totals:	100.0000		0.000	444293032			



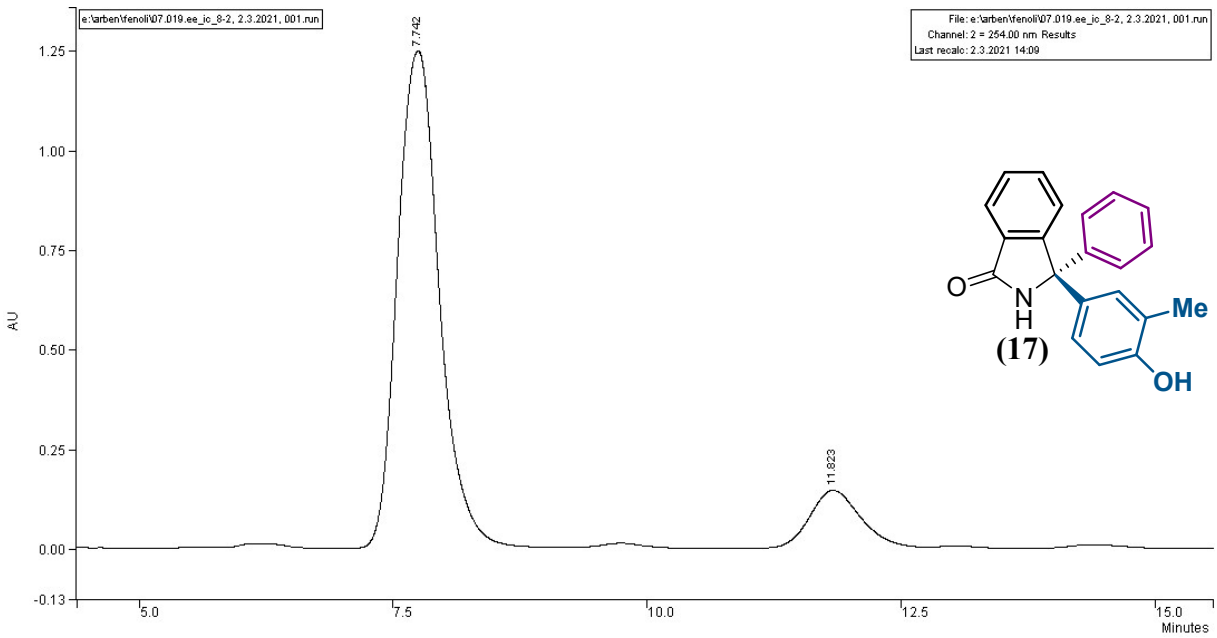
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.0083	18.739	0.000	143063040	BB	45.4	
2		49.9917	37.366	0.000	143015760	BB	91.6	
	Totals:	100.0000		0.000	286078800			



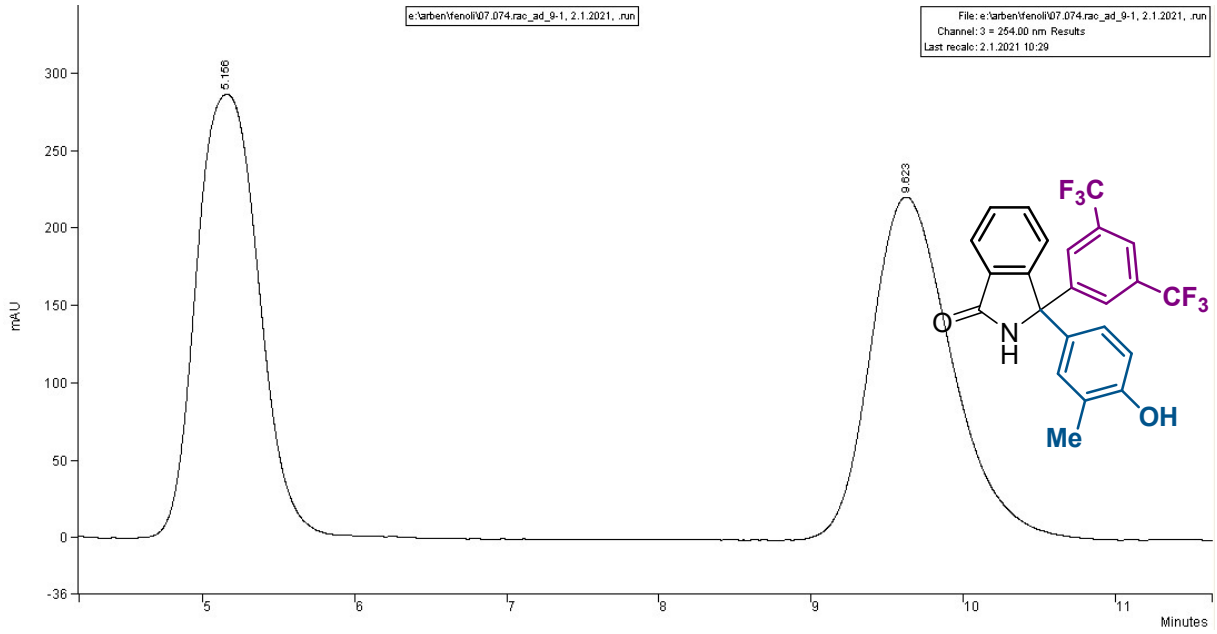
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		89.4671	18.599	0.000	320220512	BB	48.4	
2		10.5329	37.059	0.000	37699512	BB	85.1	
	Totals:	100.0000		0.000	357920024			



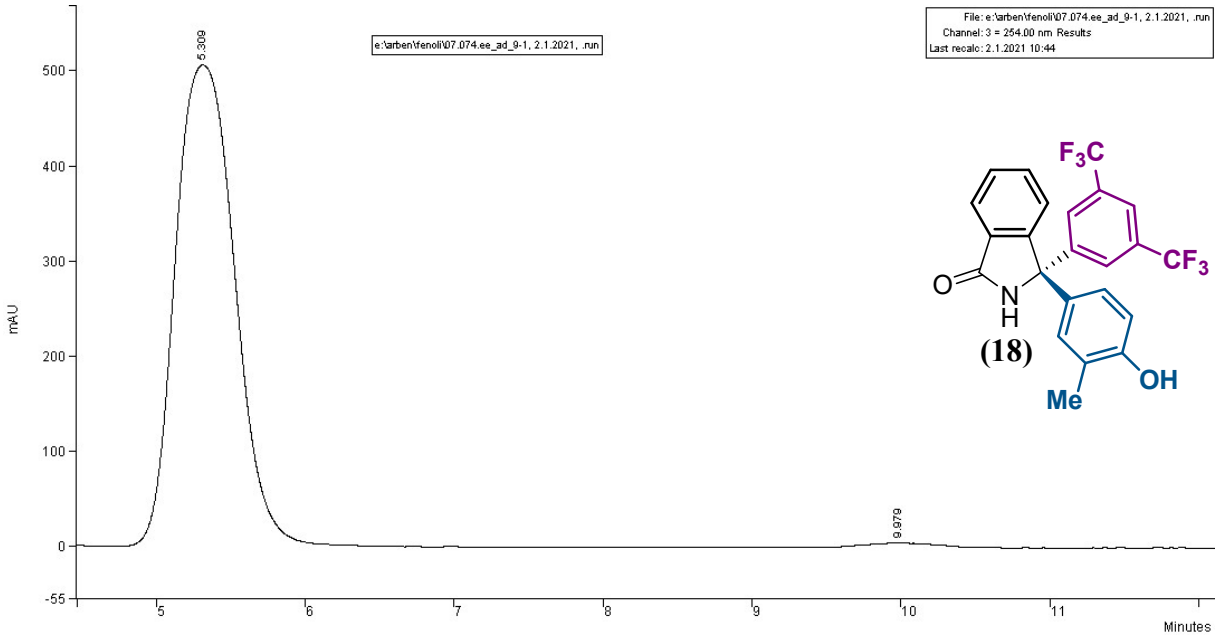
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.4099	8.016	0.000	127531688	BB	16.1	
2		50.5901	12.252	0.000	130578016	BB	26.3	
Totals:		100.0000		0.000	258109704			



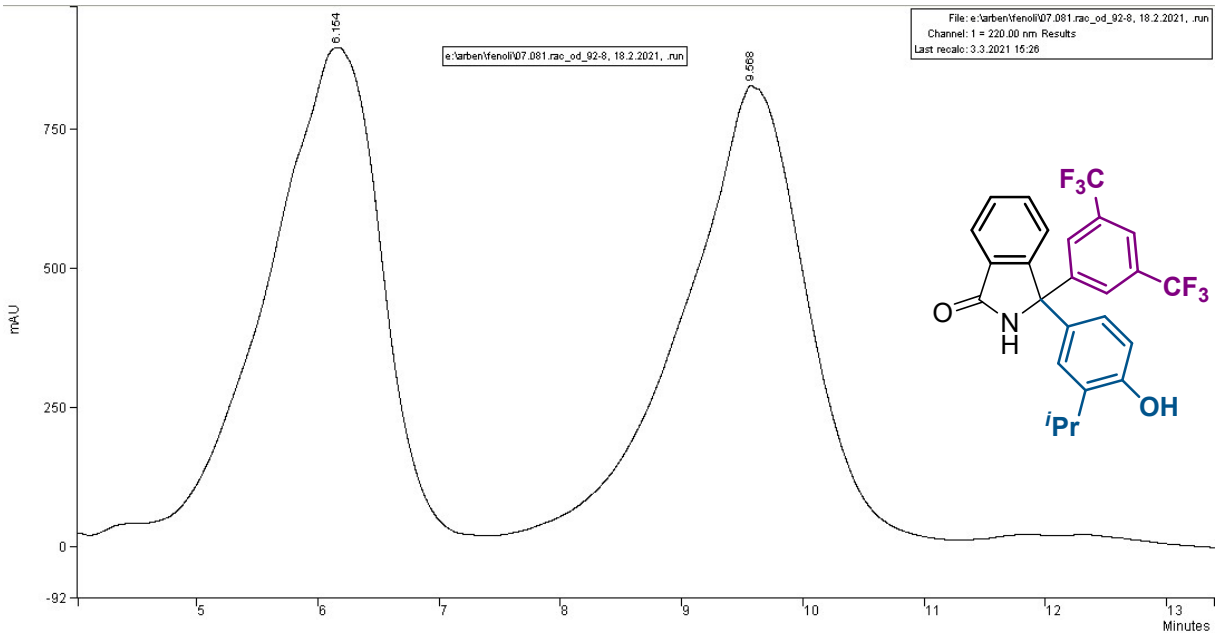
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		87.7631	7.742	0.000	356584736	BB	26.1	
2		12.2369	11.823	0.000	49719052	BB	32.1	
Totals:		100.0000		0.000	406303788			



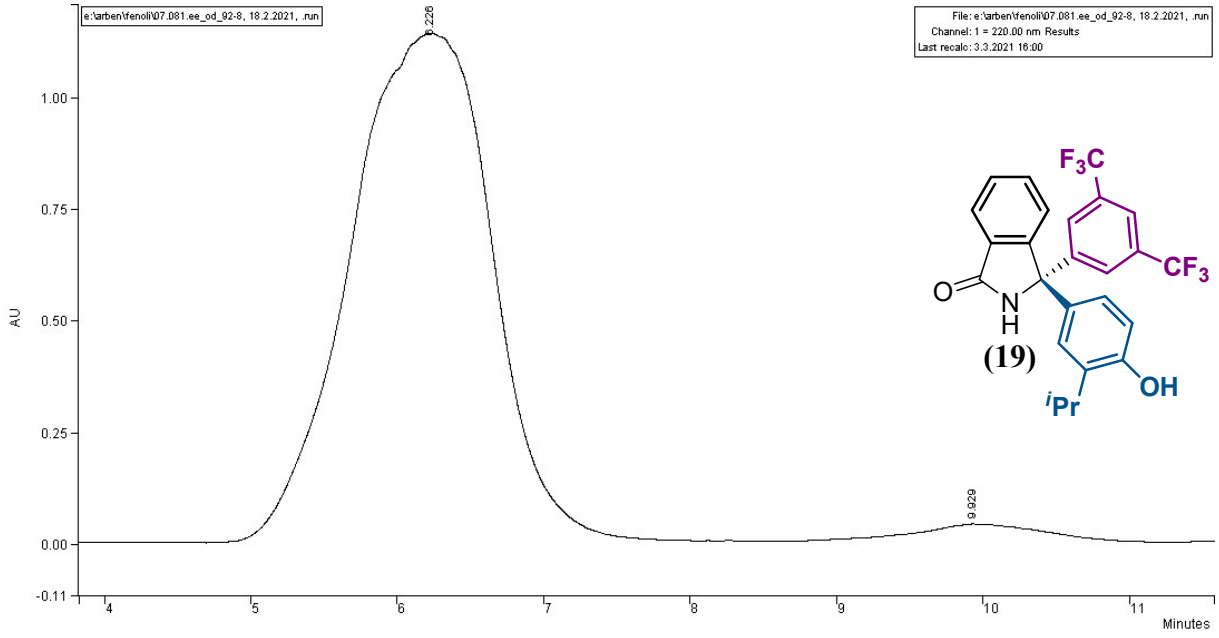
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.8423	5.156	0.000	81144664	BB	27.1	
2		50.1577	9.623	0.000	81658160	BB	33.9	
	Totals:	100.0000		0.000	162802824			



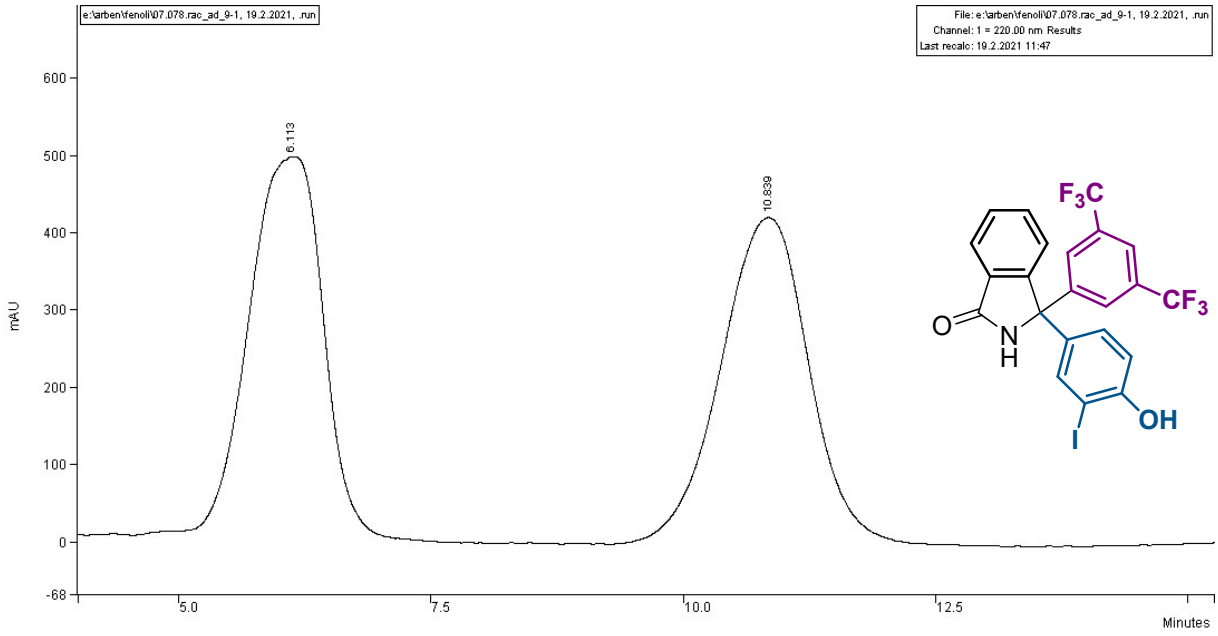
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		98.7516	5.309	0.000	139295616	BB	26.3	
2		1.2484	9.979	0.000	1760952	BB	32.4	
	Totals:	100.0000		0.000	141056568			



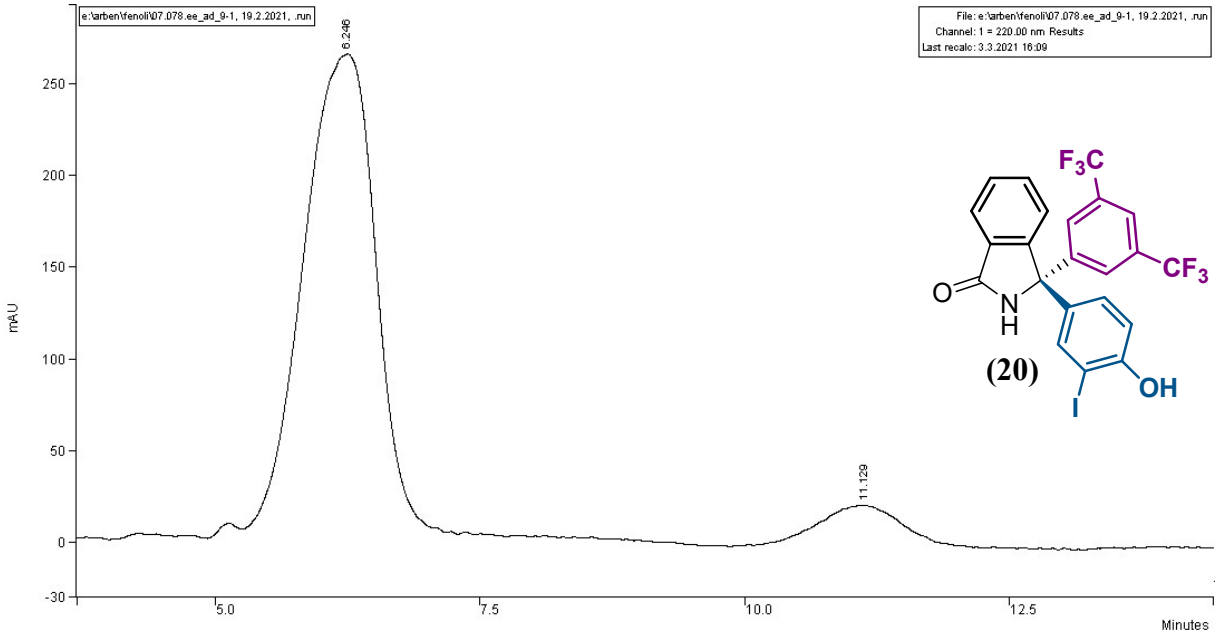
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.6048	6.154	0.000	560471232	BB	59.1	
2		50.3952	9.568	0.000	569402048	BB	62.4	
	Totals:	100.0000		0.000	1129873280			



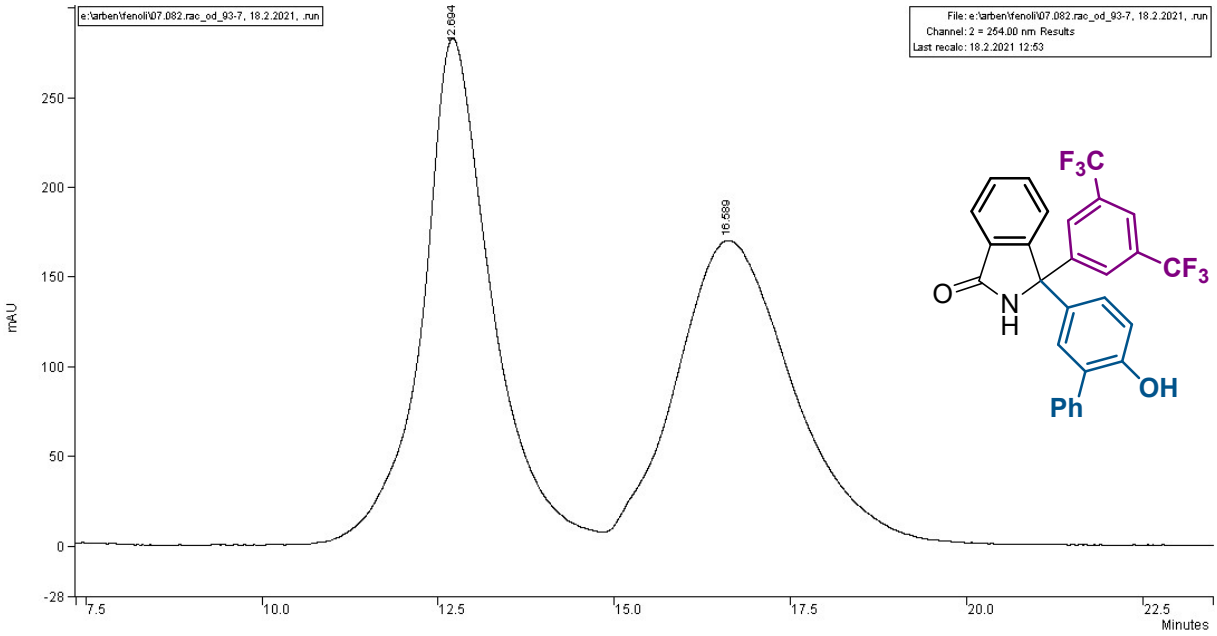
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		98.3415	6.226	0.000	763758144	BB	62.9	
2		1.6585	9.929	0.000	12880652	BB	39.8	
	Totals:	100.0000		0.000	776638796			



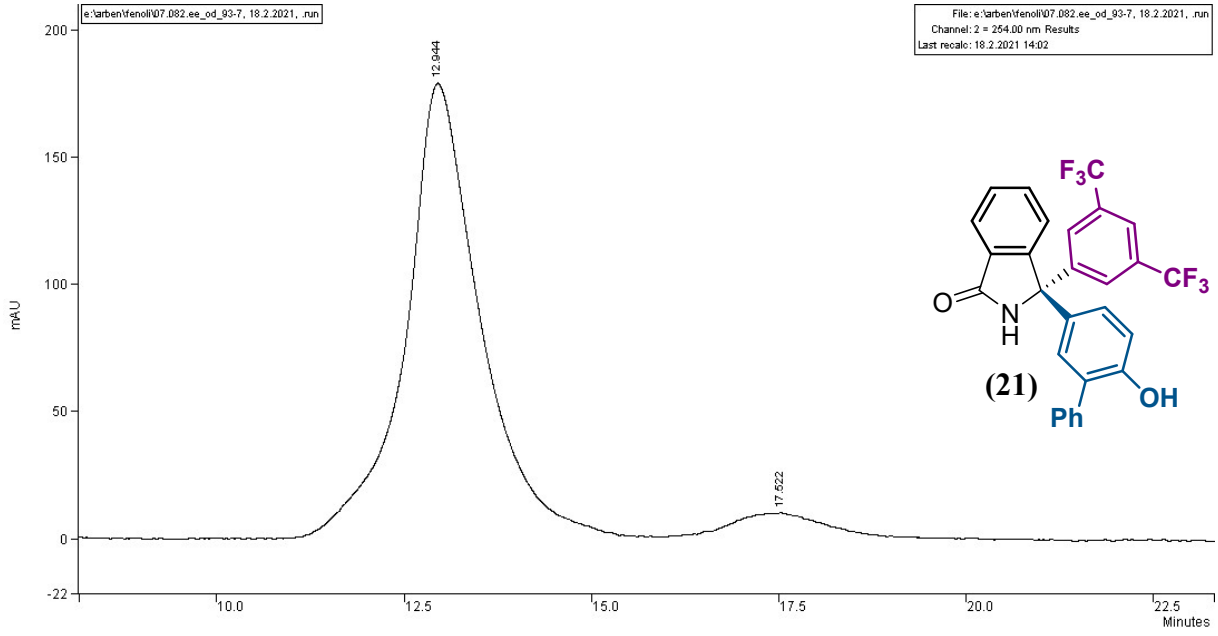
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.3479	6.113	0.000	247231952	BB	47.8	
2		50.6521	10.839	0.000	253766256	BB	55.8	
Totals:		100.0000		0.000	500998208			



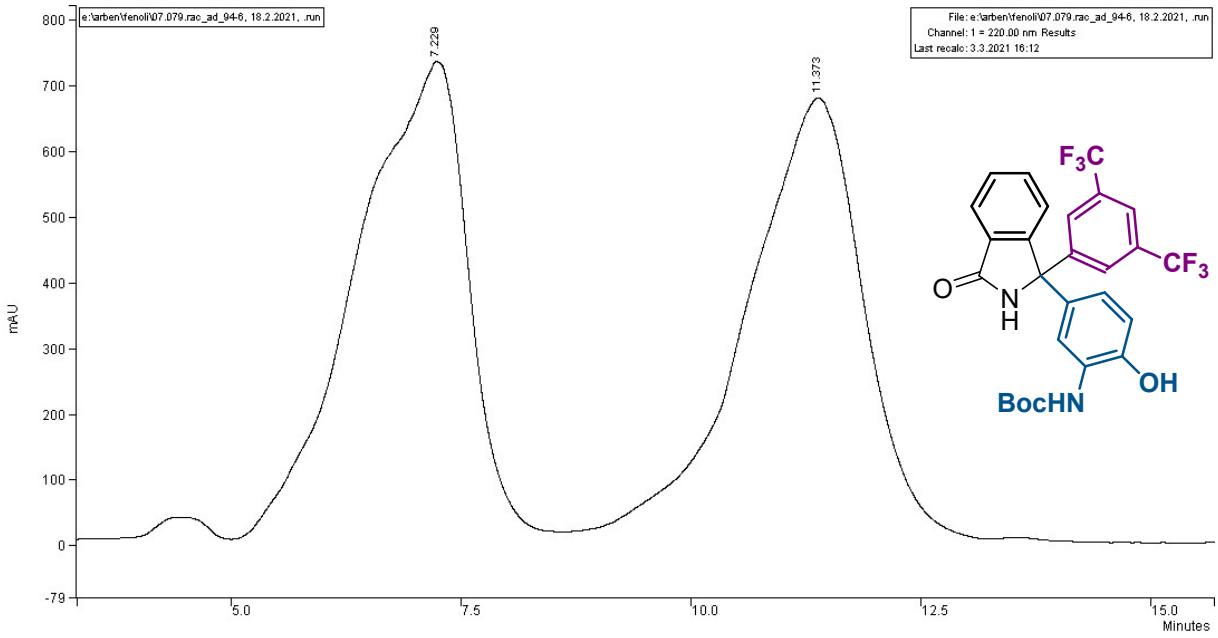
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		91.0666	6.246	0.000	122098536	BB	44.6	
2		8.9334	11.129	0.000	11977523	BB	50.4	
Totals:		100.0000		0.000	134076059			



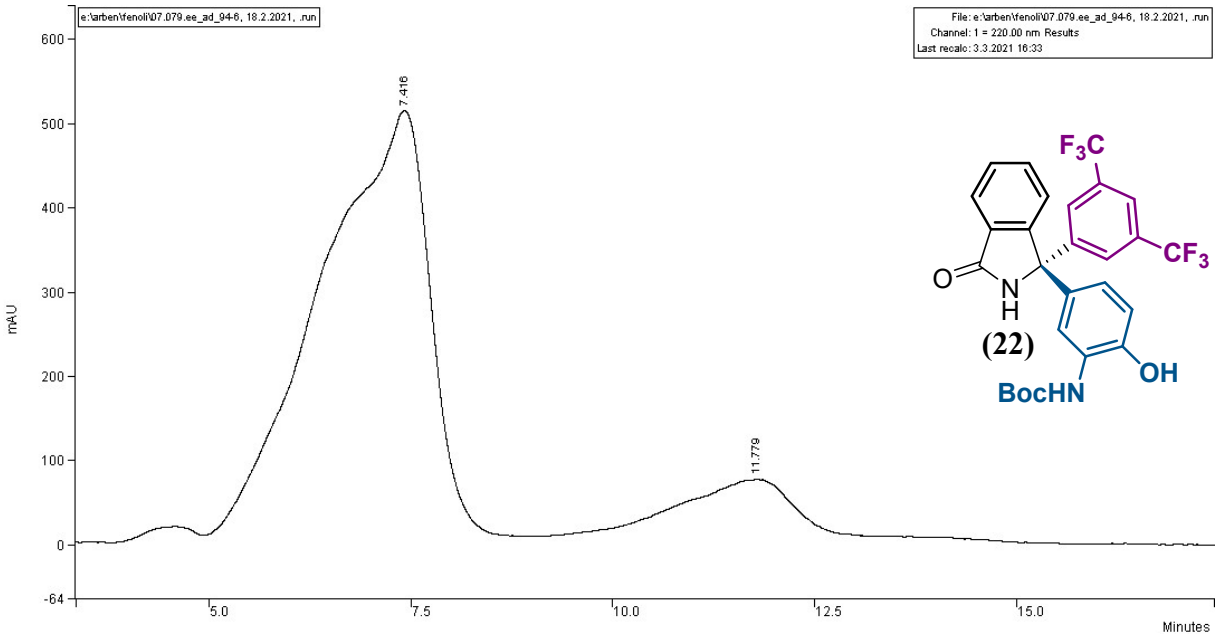
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.4483	12.694	0.000	185781184	BB	55.8	
2		49.5517	16.589	0.000	182479600	BB	100.7	
	Totals:	100.0000		0.000	368260784			



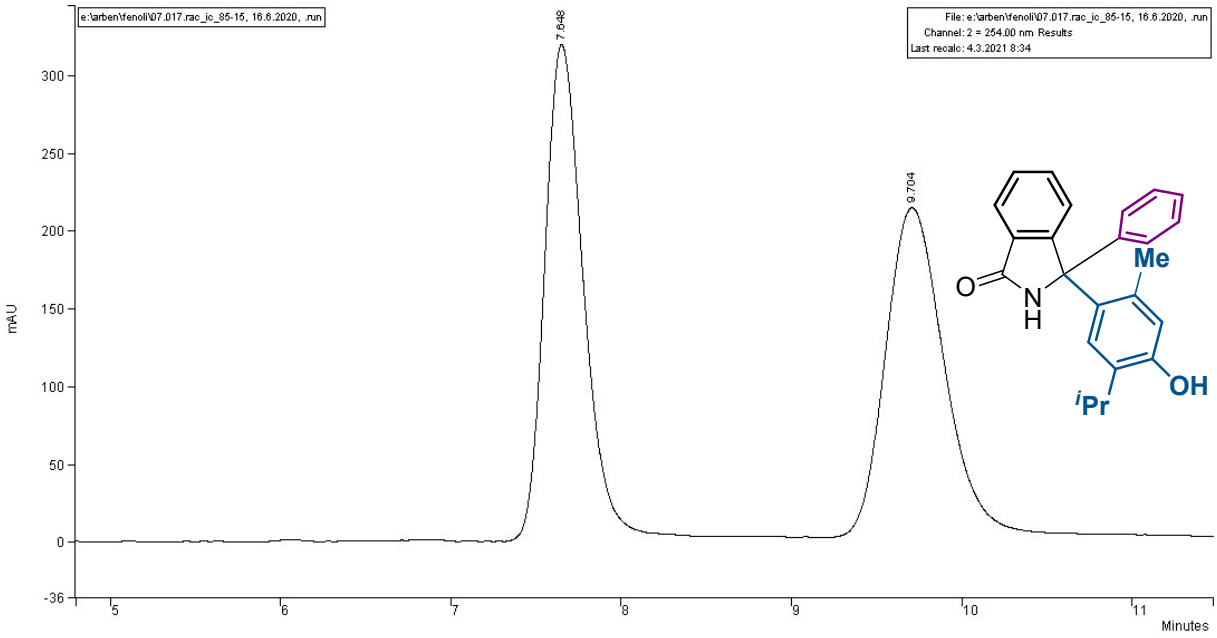
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		94.0490	12.944	0.000	123818328	BB	55.6	
2		5.9510	17.522	0.000	7834630	BB	78.9	
	Totals:	100.0000		0.000	131652958			



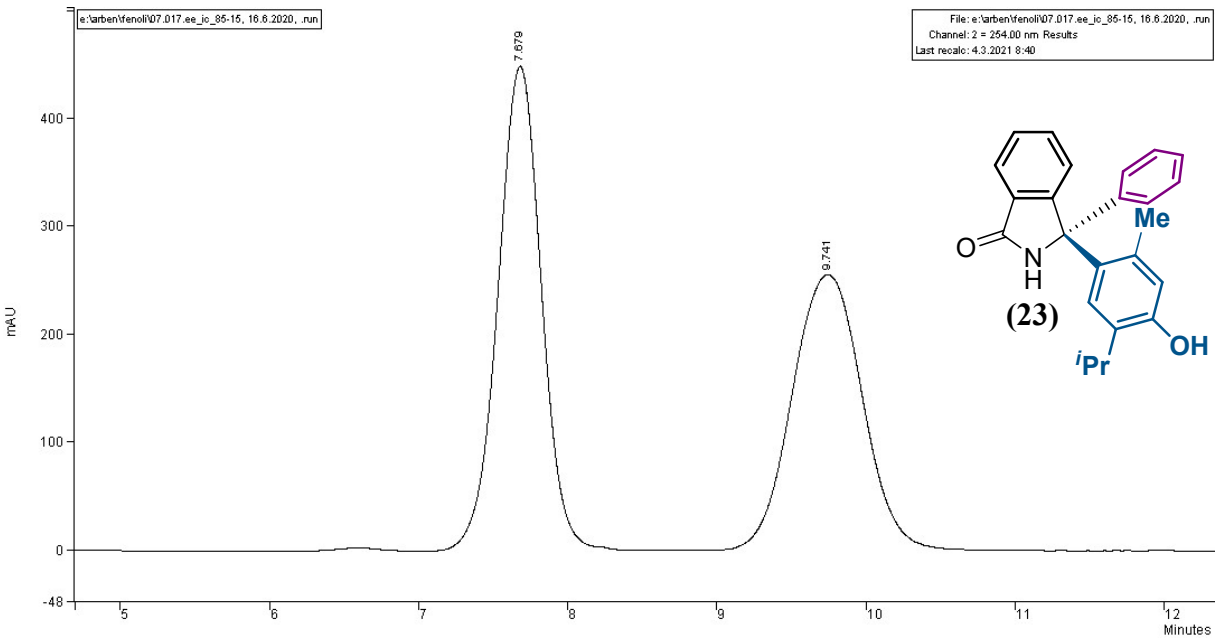
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		51.6393	7.229	0.000	595637376	BB	80.8	
2		48.3607	11.373	0.000	557820096	BB	78.1	
	Totals:	100.0000		0.000	1153457472			



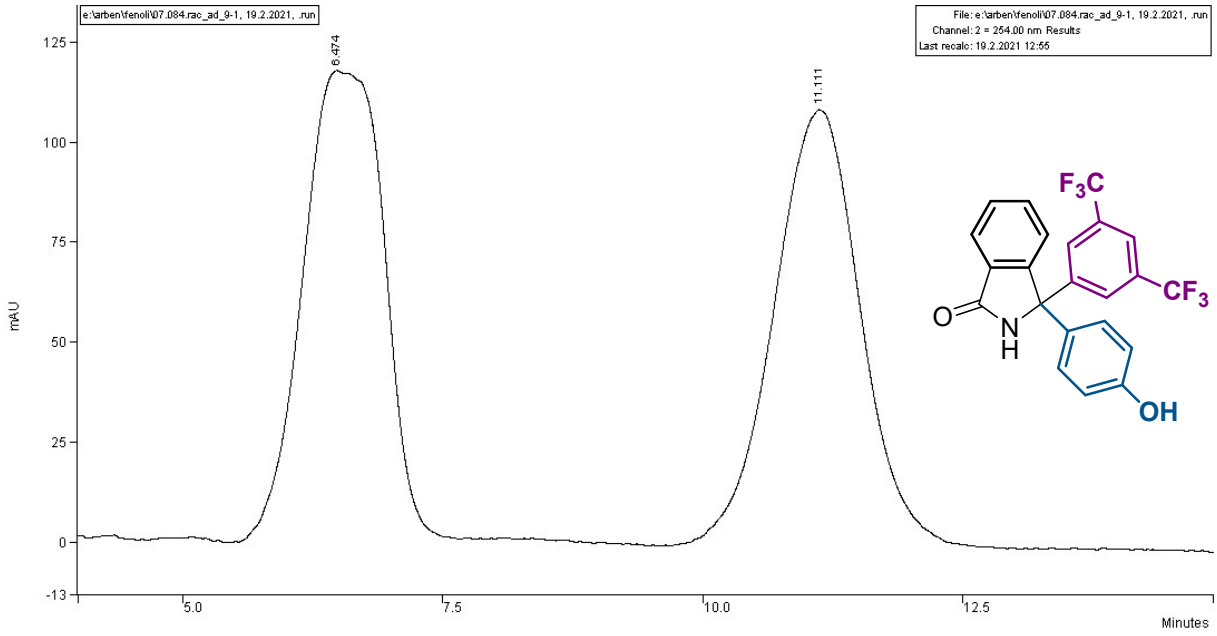
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		89.7638	7.416	0.000	470025536	BB	93.1	
2		10.2362	11.779	0.000	53599384	BB	82.0	
	Totals:	100.0000		0.000	523624920			



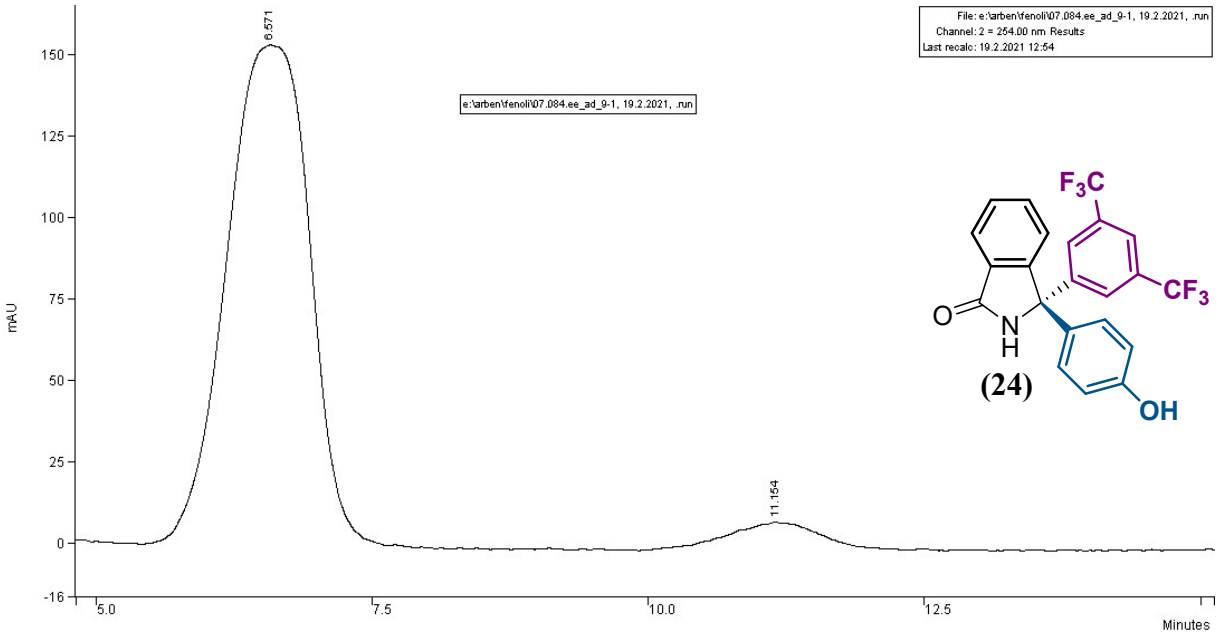
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.5877	7.648	0.000	48632740	BB	14.4	
2		50.4123	9.704	0.000	49441480	BB	22.0	
	Totals:	100.0000		0.000	98074220			



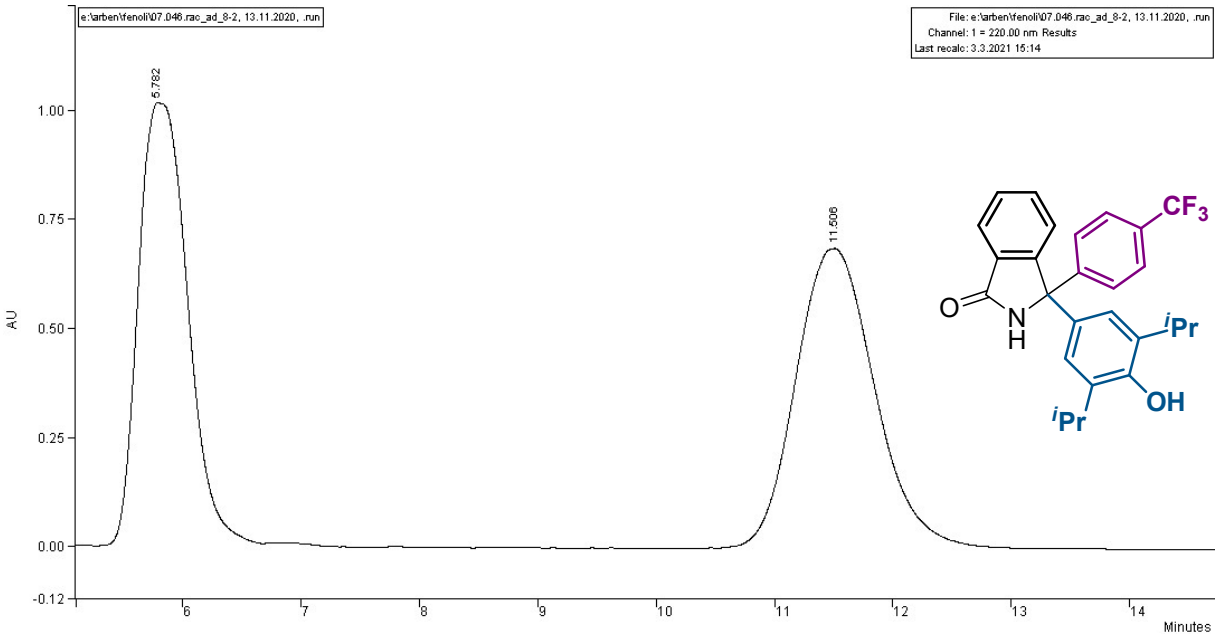
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		51.8170	7.679	0.000	89912440	BB	18.5	
2		48.1830	9.741	0.000	83606624	BB	30.8	
	Totals:	100.0000		0.000	173519064			



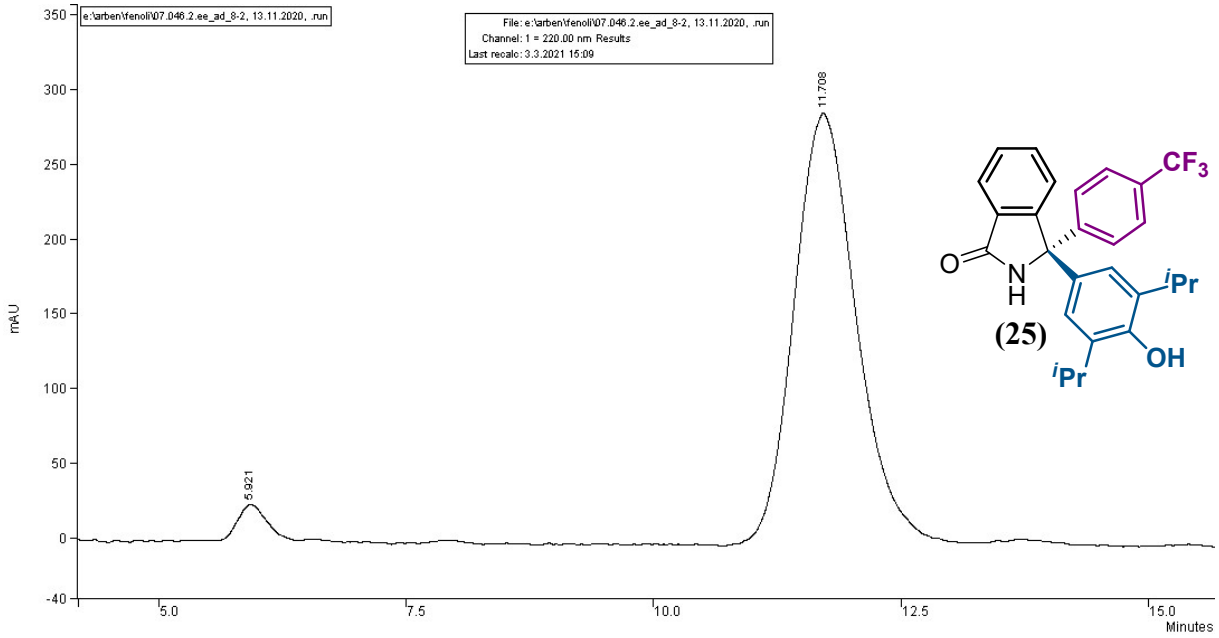
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.1671	6.474	0.000	62661992	BB	51.6	
2		49.8329	11.111	0.000	62244476	BB	53.0	
	Totals:	100.0000		0.000	124906468			



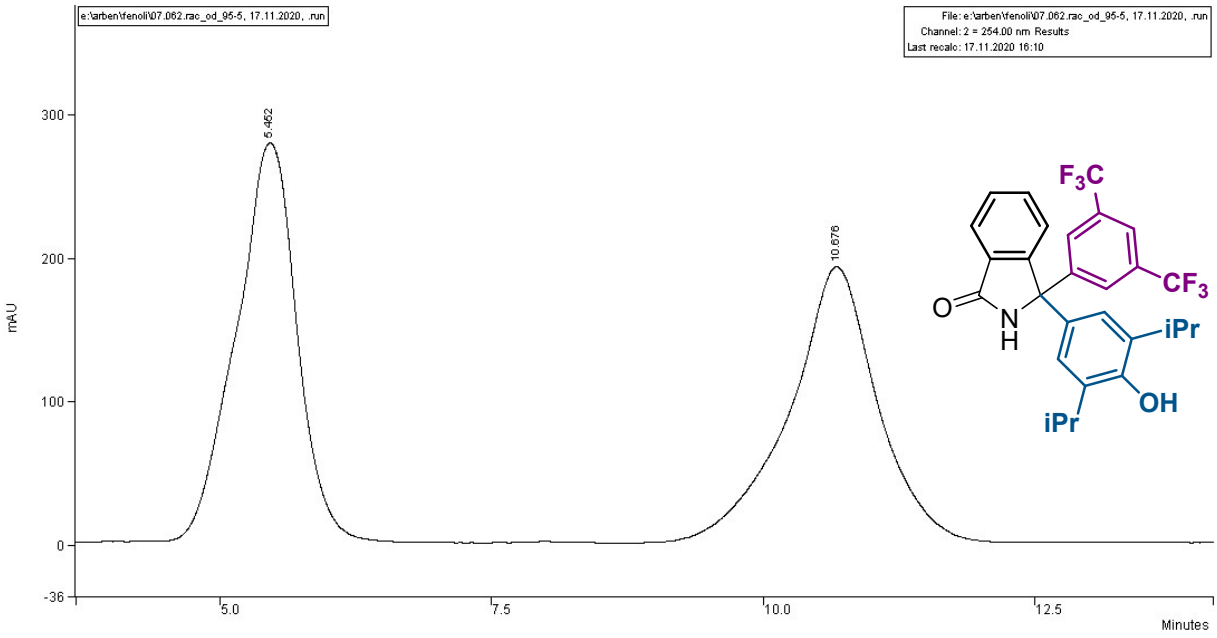
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		94.2973	6.571	0.000	79904136	BB	49.6	
2		5.7027	11.154	0.000	4832267	BB	55.1	
	Totals:	100.0000		0.000	84736403			



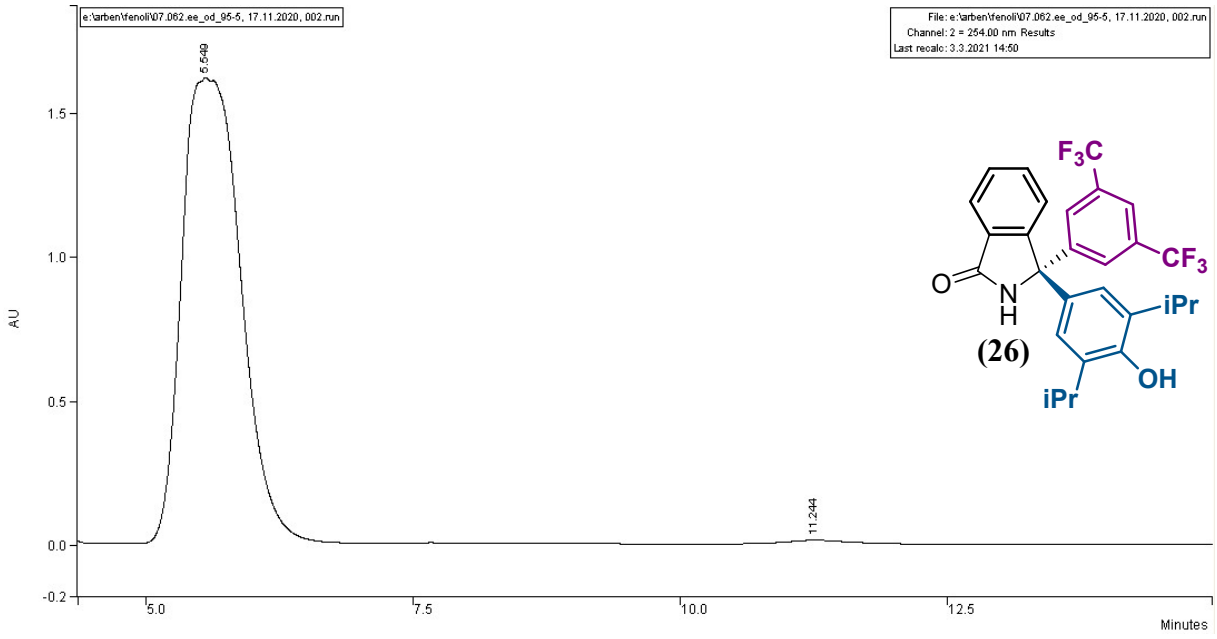
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		48.9599	5.782	0.000	292669664	BB	27.1	
2		51.0401	11.506	0.000	305104512	BB	42.6	
	Totals:	100.0000		0.000	597774176			



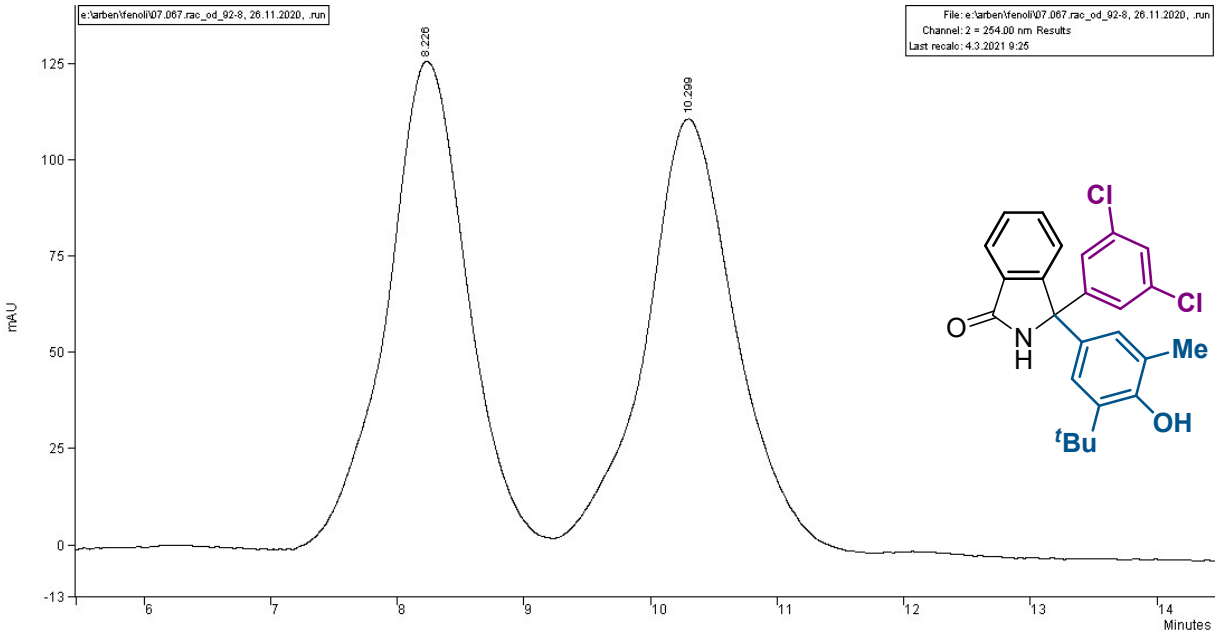
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		3.5125	5.921	0.000	4506751	BB	19.2	
2		96.4875	11.708	0.000	123800480	BB	40.0	
	Totals:	100.0000		0.000	128307231			



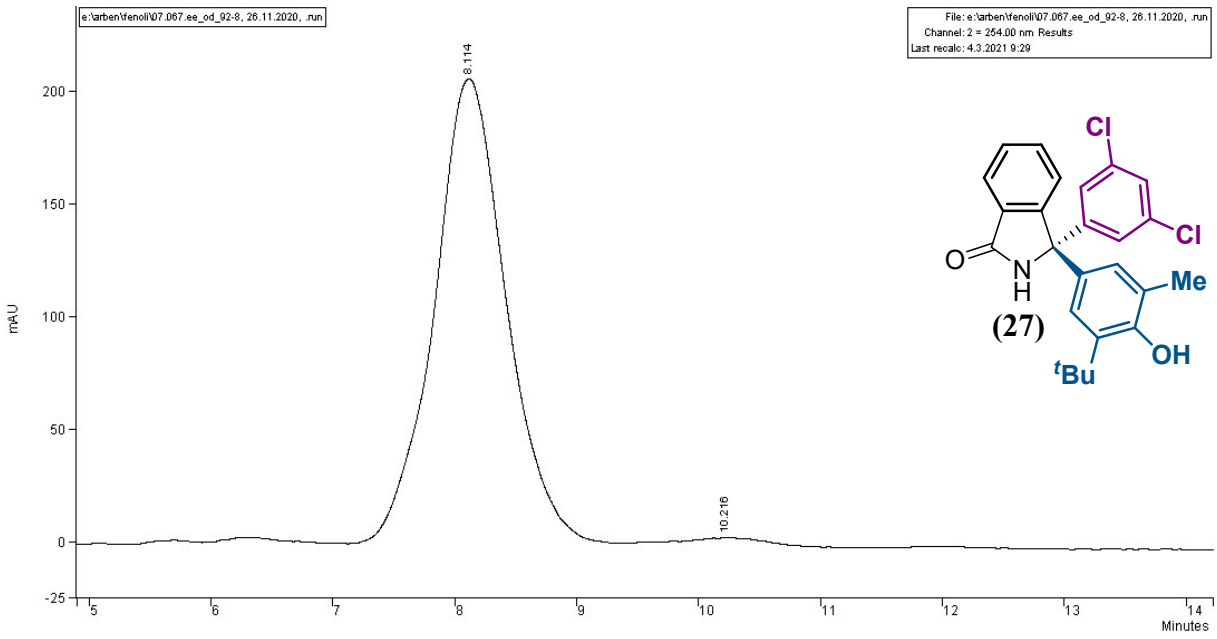
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.6658	5.452	0.000	107723224	BB	35.5	
2		50.3342	10.676	0.000	109173136	BB	47.4	
	Totals:	100.0000		0.000	216896360			



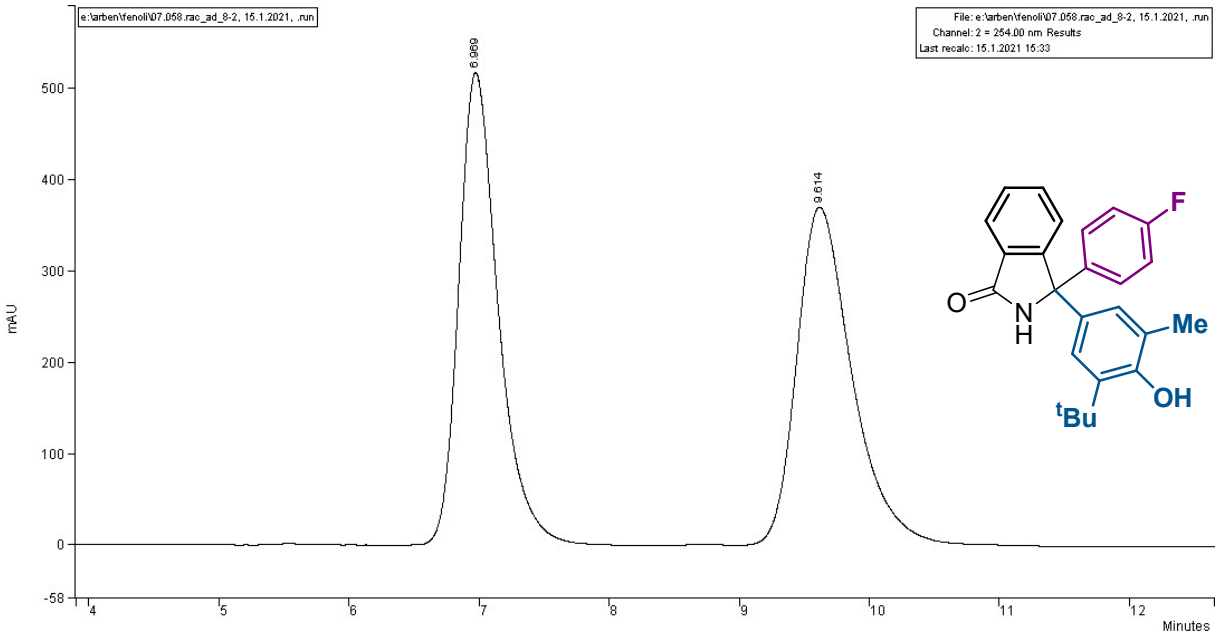
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		99.4177	5.549	0.000	618163648	BB	36.0	
2		0.5823	11.244	0.000	3620707	BB	33.0	
	Totals:	100.0000		0.000	621784355			



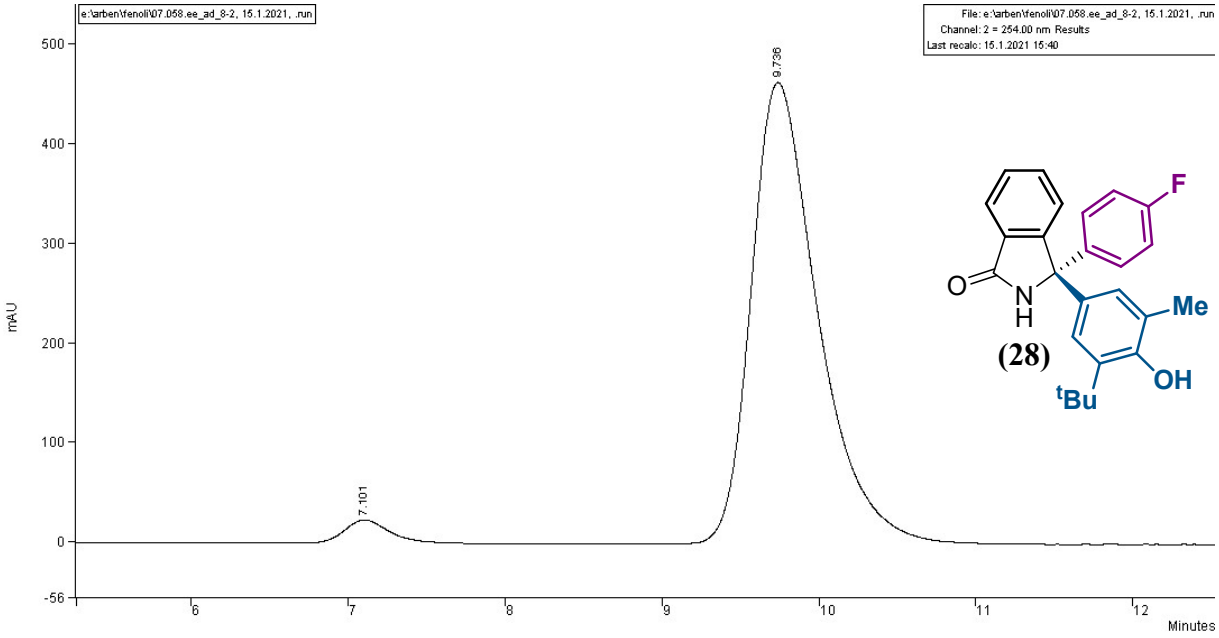
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.1244	8.226	0.000	54274352	BB	38.8	
2		49.8756	10.299	0.000	54005012	BB	41.7	
Totals:		100.0000		0.000	108279364			



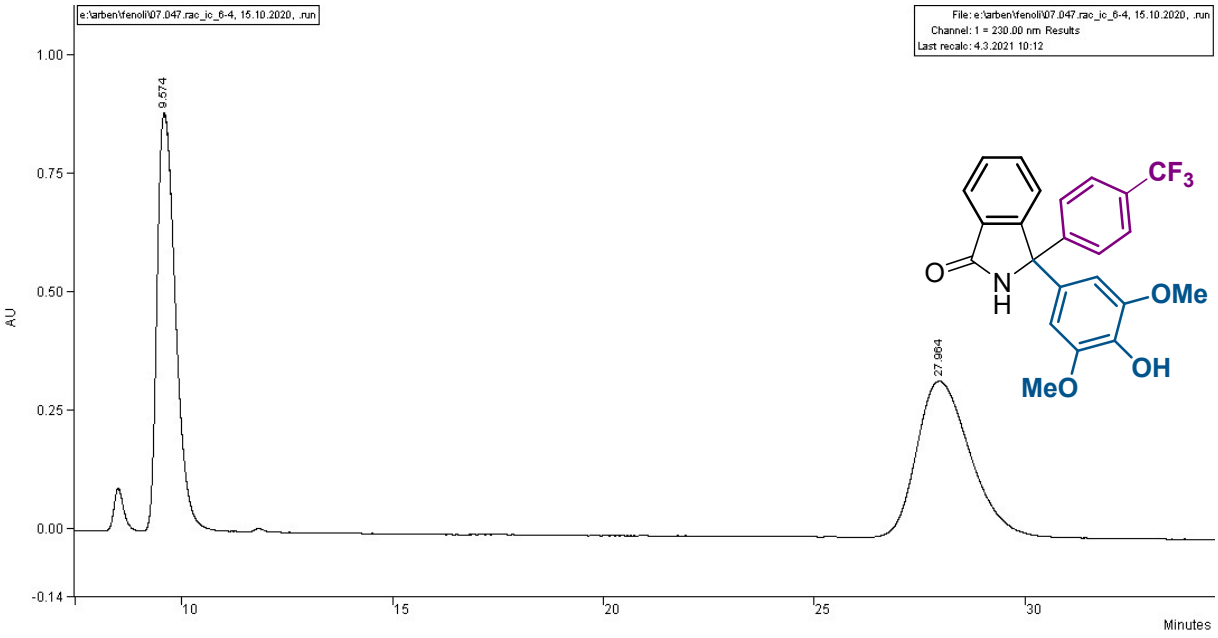
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		98.4421	8.114	0.000	83933880	BB	36.2	
2		1.5579	10.216	0.000	1328288	BB	29.3	
Totals:		100.0000		0.000	85262168			



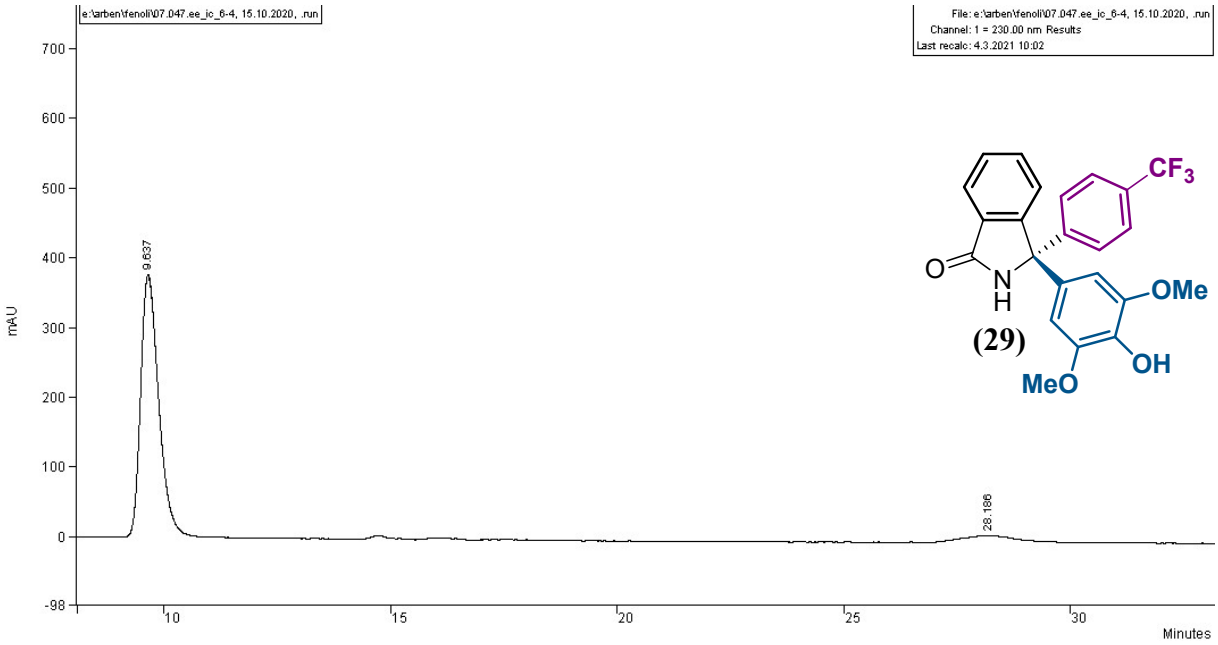
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.8852	6.969	0.000	108202064	BB	18.8	
2		50.1148	9.614	0.000	108699992	BB	26.4	
	Totals:	100.0000		0.000	216902056			



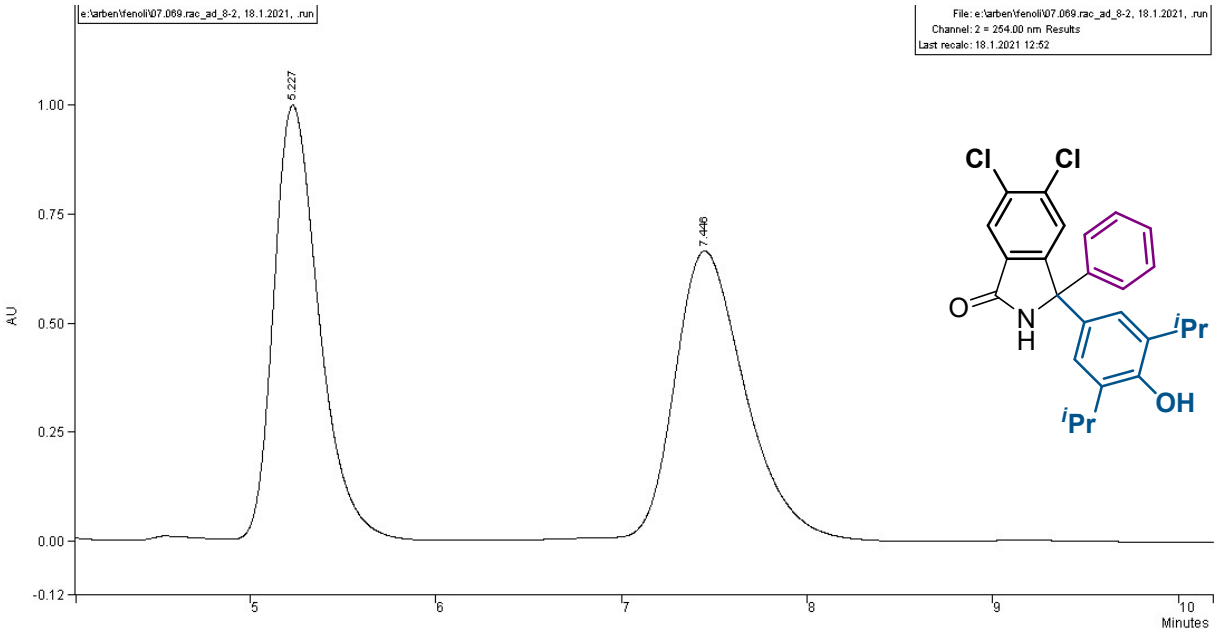
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		3.2629	7.101	0.000	4600420	BB	17.8	
2		96.7371	9.736	0.000	136390704	BB	26.3	
	Totals:	100.0000		0.000	140991124			



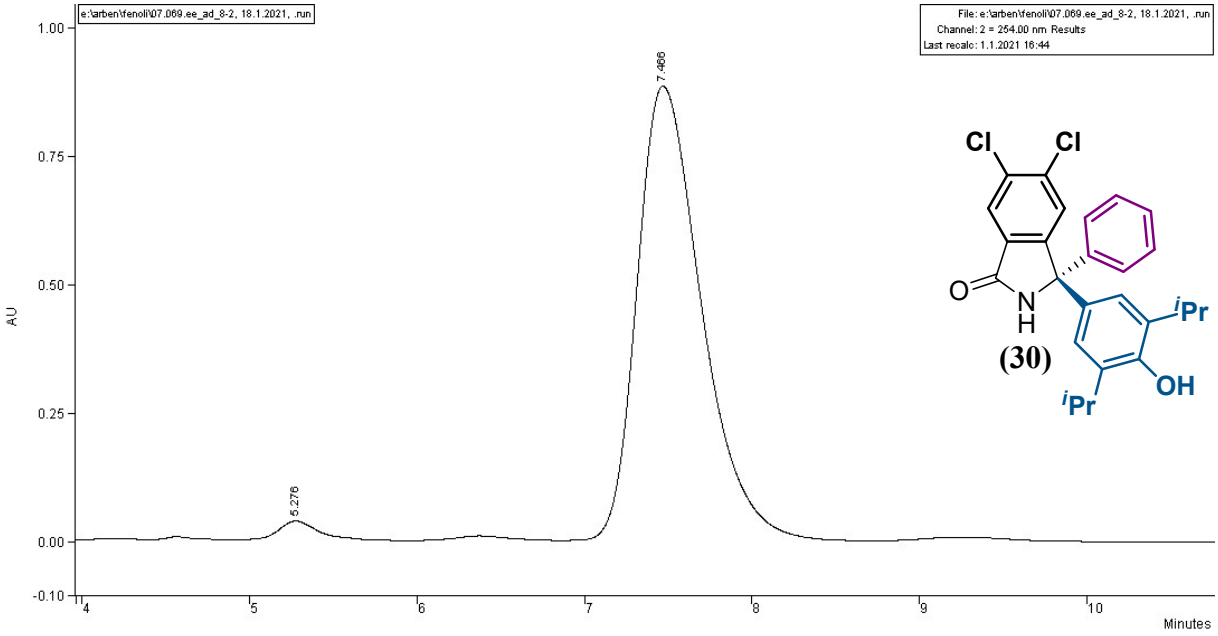
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		47.9635	9.574	0.000	262313984	BB	27.9	
2		52.0365	27.964	0.000	284589024	BB	81.5	
	Totals:	100.0000		0.000	546903008			



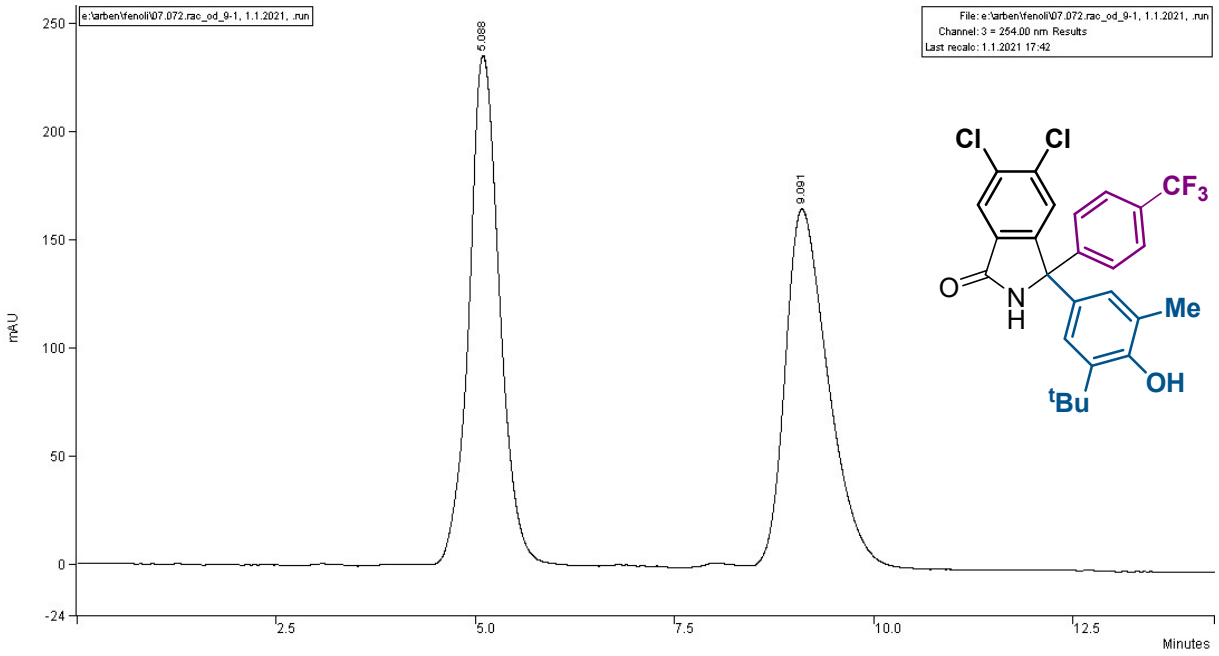
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		94.7394	9.637	0.000	102420392	BB	25.1	
2		5.2606	28.186	0.000	5687079	BB	67.8	
	Totals:	100.0000		0.000	108107471			



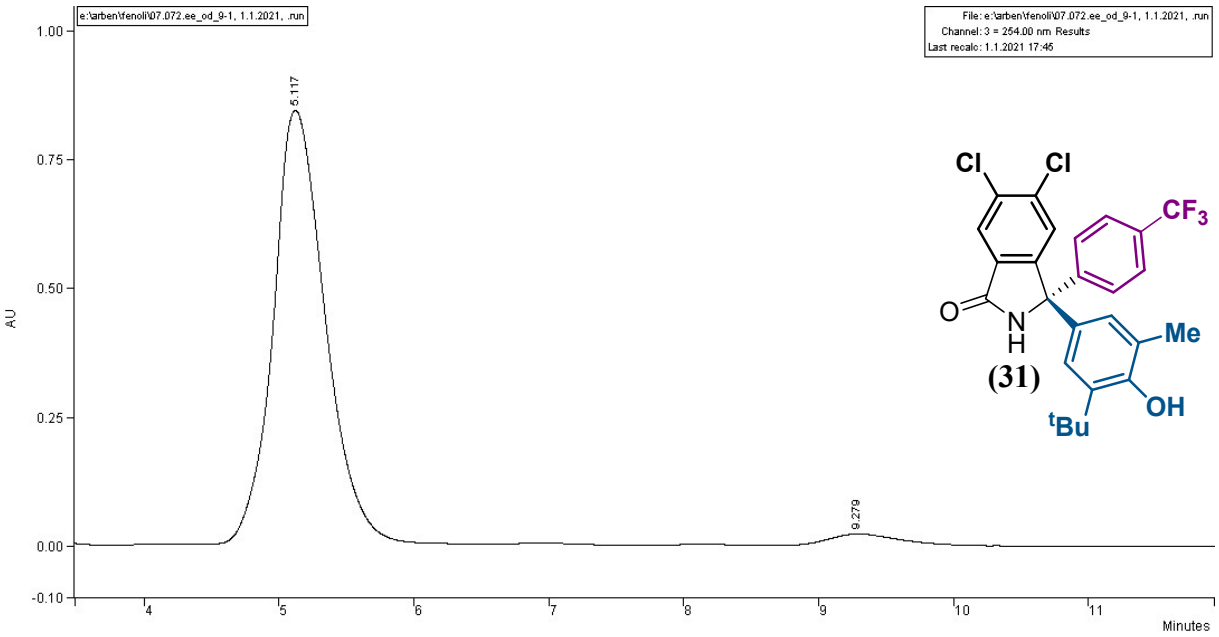
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		49.1359	5.227	0.000	167394880	BB	15.3	
2		50.8641	7.446	0.000	173282320	BB	23.8	
	Totals:	100.0000		0.000	340677200			



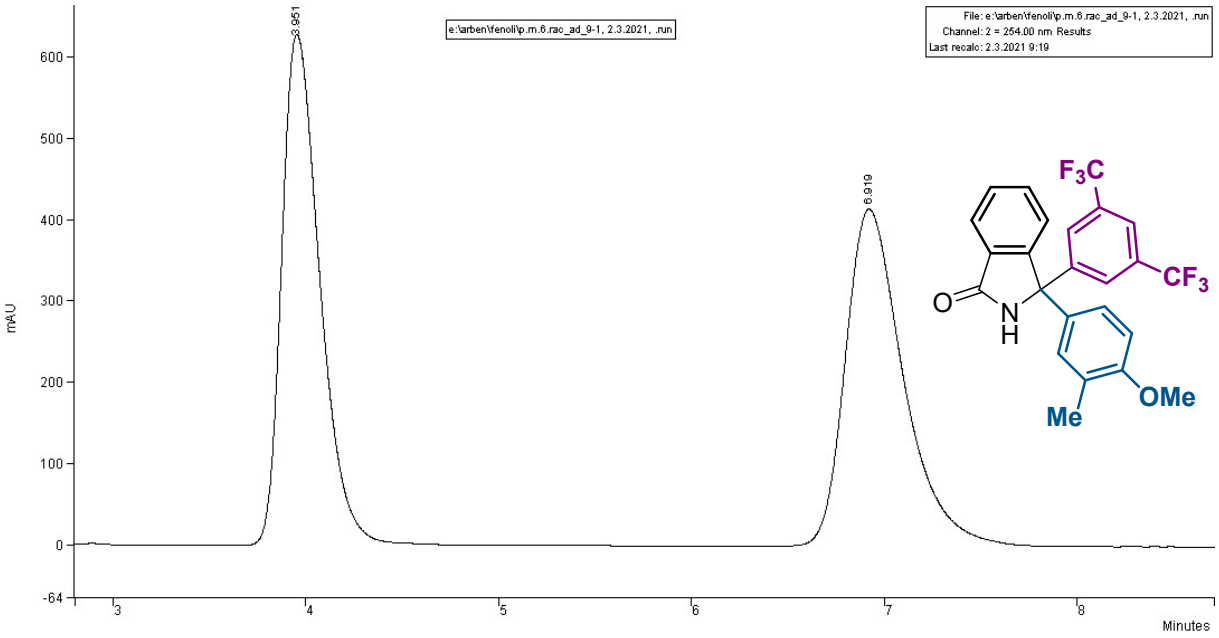
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		2.3043	5.276	0.000	5560391	BB	14.0	
2		97.6957	7.466	0.000	235744432	BB	24.2	
	Totals:	100.0000		0.000	241304823			



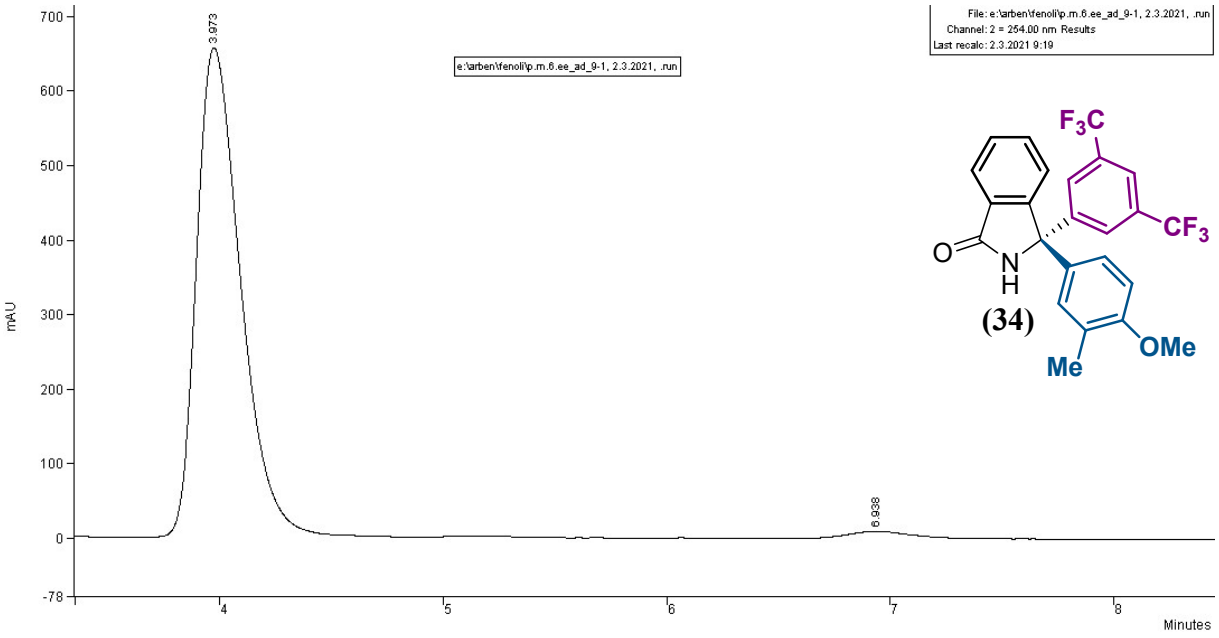
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.3726	5.088	0.000	62419072	BB	23.4	
2		49.6274	9.091	0.000	61495576	BB	34.1	
Totals:		100.0000		0.000	123914648			



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		96.5075	5.117	0.000	224878368	BB	23.7	
2		3.4925	9.279	0.000	8138061	BB	32.9	
Totals:		100.0000		0.000	233016429			



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		50.8167	3.951	0.000	86139792	BB	12.6	
2		49.1833	6.919	0.000	83370832	BB	18.7	
	Totals:	100.0000		0.000	169510624			



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		97.9155	3.973	0.000	90056952	BB	12.5	
2		2.0845	6.938	0.000	1917232	BB	16.9	
	Totals:	100.0000		0.000	91974184			