Supporting Information

Acyl transfer-enabled catalytic asymmetric Michael addition of α-hydroxy-1-indanones to nitroolefins

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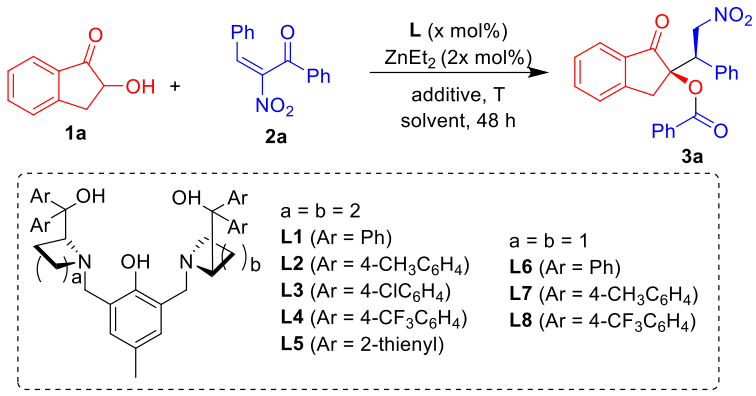
General Information

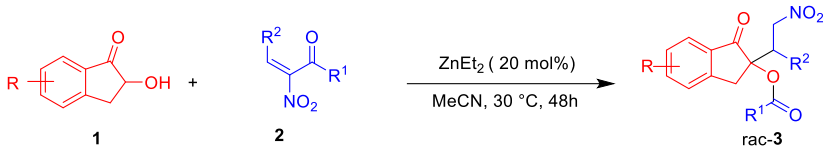
All reactions were carried out under an atmosphere of argon using oven-dried glassware. Super dry solvents, metal catalysts, were purchased from chemical companies and used without further treatment. Flash column chromatography was performed using silica gel (300-400 mesh). ^{1}H NMR ,^{13}C NMR, ^{19}F NMR spectra were recorded in $CDCl_3$ on a 400 MHz spectrometer; chemical shifts are reported in ppm with the solvent signals as reference, and coupling constants (*J*) are given in Hertz. The peak information is described as: s = singlet, d = doublet, t = triplet, q = quartet, m= multiplet. High-resolution mass spectra (HRMS) were obtained using an Agilent LC-MSAD-Trap-XCT instrument using electrospray ionization time-of-flight (ESI-TOF). High performance liquid chromatography (HPLC) was performed on instrument consisted of JASCO model PU-1580 intelligent HPLC pump and JASCO model UV-1575 intelligent UV-vis detector (254 nm) using Daicel Chiralpak IB, IC, ID, IE, IF (4.6 mm × 250 mm) columns. Melting points were determined using YRT-3 melting point apparatus. Optical rotations were measured with Perkin Elmer, model 341 Polarimeter. The instrumentation used for the crystal measurement is Oxford Gemini E X-ray single-crystal diffractometer. Chiral ligand[1-3], α-hydroxy-1-indanones[4] and nitroolefins[5] were synthesized according to the literature. Other reagents were obtained from commercial sources and used without further purification.

General Procedure for optimization of the reaction conditions



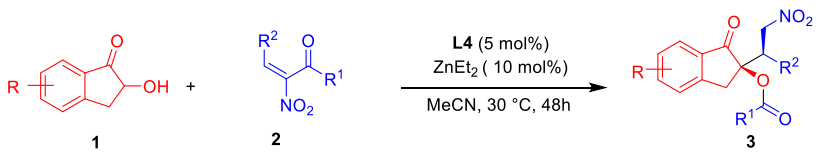
Under a nitrogen atmosphere, a solution of diethylzinc (20 μL, 1.0 M in hexane, 0.02 mmol) was added dropwise to a solution of **L** (0.01 mmol) in solvent (2 mL). After the mixture was stirred for 30 min, α-hydroxy-1-indanone **1a** (0.1 mmol, 14.8 mg) and (Z)-2-nitro-1,3-diphenylprop-2-en-1-one **2a** (0.1 mmol, 25.3 mg) were added. The reaction mixture was stirred for 48 h at the same temperature. The reaction was quenched with NH_4Cl solution (2 mL), and the organic layer was extracted with CH_2Cl_2 (3 × 5 mL). The combined organic layer was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure by using a rotary evaporator. The residue was purified by flash chromatography with petroleum ether/ethyl acetate (4:1) to afford the desired product **3a**.

General Procedure Synthesis of rac-3



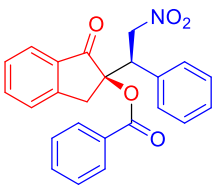
Under a nitrogen atmosphere, a solution of diethylzinc (40 μL, 1.0 M in hexane, 0.04 mmol) was added in MeCN (2 mL). After the mixture was stirred for 30 min at 30 ºC, α-hydroxy-1-indanone **1a** (0.2 mmol, 29.6 mg) and (Z)-2-nitro-1,3-diphenylprop-2-en-1-one **2a** (0.2 mmol, 50.6 mg) were added. The reaction mixture was stirred for 48 h at the same temperature. The reaction was quenched with HCl solution (1 M, 2 mL), and the organic layer was extracted with CH_2Cl_2 (3 × 5 mL). The combined organic layer was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure by using a rotary evaporator. The residue was purified by flash chromatography with petroleum ether/ethyl acetate (4:1) to afford the desired racemic product **3a**.

General Procedure Synthesis of chiral 3



Under a nitrogen atmosphere, a solution of diethylzinc (20 μL, 1.0 M in hexane, 0.02 mmol) was added dropwise to a solution of **L4** (0.01 mmol, 9.6 mg) in MeCN (2 mL). After the mixture was stirred for 30 min at 30 ºC, α-hydroxy-1-indanone **1** (0.2 mmol, 29.6 mg) and (Z)-2-nitro-1,3-diphenylprop-2-en-1-one **2** (0.2 mmol, 50.6 mg) were added. The reaction mixture was stirred for 48 h at the same temperature. The reaction was quenched with HCl solution (1 M, 2 mL), and the organic layer was extracted with CH_2Cl_2 (3 × 5 mL). The combined organic layer was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure by using a rotary evaporator. The residue was purified by flash chromatography with petroleum ether/ethyl acetate (4:1) to afford the desired chiral product **3**.

(*R*)-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3a)

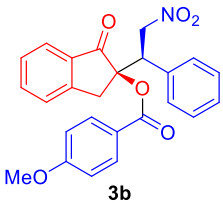


3a

Pale yellow solid (65.8 mg), 3:1 dr, **mp**. 60.2-61.0 ºC; $[\alpha]_D^{20}$ = +49.0 (c = 1.00, in THF); **HPLC**: Chiralpak IC column (hexane/i-PrOH = 90/10, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 26.04 min (minor), t_4 = 48.46 min (major), ee = 43%; ***major product***: t_2 = 31.33 min (minor), t_3 = 34.11 min (major), ee = 88%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.3 Hz, 2.0H), 8.01 (d, *J* = 7.3 Hz, 0.66H), 7.86 (d, *J* = 7.6 Hz, 1.33H), 7.72 (d, *J* = 7.7 Hz, 0.66H), 7.69 - 7.61 (m, 2.33H),7.59 -7.49 (m, 2.33H), 7.49 – 7.39 (m, 3.66H), 7.38 - 7.29 (m, 3.99H), 7.11 – 7.02 (m, 1.66H), 5.58 (dd, *J* =

13.7, 3.8 Hz, 1H), 5.49 (dd, *J* = 13.7, 4.7 Hz, 0.33H), 5.12(dd, *J* = 13.7, 10.5, 1H), 5.05(dd, *J* = 13.7, 9.3 Hz, 0.33H), 4.41 (dd, *J* = 9.3, 4.7 Hz, 0.33H), 3.79 (dd, *J* = 10.4, 3.8 Hz, 1H), 3.58 (d, *J* = 17.3 Hz, 0.33H), 3.42 (d, *J* = 17.3 Hz, 1.33H), 3.25 (d, *J* = 17.5 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.0, 200.3, 165.1, 165.0, 149.0, 148.8, 136.2, 136.0, 135.7, 135.6, 134.0, 133.9, 133.8, 132.4, 129.9, 129.8, 129.3, 129.25, 129.15, 128.89, 128.86, 128.77, 128.73, 128.69, 128.6, 128.4, 128.3, 127.8, 126.2, 125.6, 125.1, 123.7, 85.3, 84.2, 75.8, 75.4, 50.8, 48.0, 38.1, 37.2. **HRMS** (ESI): m/z $[M + H]^+$ calcd for $[C_{24}H_{20}NO_5]^+$: 402.1336, found: 402.1337.

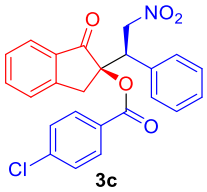
(*R*)-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl4-methoxybenzoate (3b)



3b

White solid (63.9 mg), 74% yield, 8.3:1 dr, **mp**. 134.3-134.9 ºC; $[\alpha]_D^{20}$ = +99.0 (c = 0.98, in THF); **HPLC:** Chiralpak IC column (hexane/i-PrOH = 90/10, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 33.25 min (minor), t_4 = 61.00 min (major), ee = 45%; ***major product***: t_2 = 35.74 min (minor), t_3 = 42.39 min (major), ee = 88%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.03 – 7.97 (m, 2H), 7.97 – 7.92 (m, 0.24H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.71 (d, *J* = 7.7 Hz, 0.12H), 7.62 (td, *J* = 7.5, 1.1 Hz, 1H), 7.51 – 7.26 (m, 7.36H), 7.10 - 7.03 (m, 0.60H), 7.02 – 6.98 (m, 2H), 6.97 – 6.93 (m, 0.24H), 5.58 (dd, *J* = 13.7, 3.9 Hz, 1H), 5.51 (dd, *J* = 13.7, 4.8 Hz, 0.12H), 5.10 (dd, *J* = 13.7, 10.5 Hz, 1H), 5.02 (dd, *J* = 13.7, 9.1 Hz, 0.12H), 4.39 (dd, *J* = 9.1, 4.8 Hz, 0.12H), 3.90 (s, 3H), 3.88 (s, 0.36H), 3.78 (dd, *J* = 10.4, 3.9 Hz, 1H), 3.57 (d, *J* = 17.2 Hz, 0.12H), 3.45 – 3.34 (m, 1.12H), 3.23 (d, *J* = 17.5 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.5, 164.8, 164.2, 148.8, 135.9, 135.8, 133.8, 132.0, 129.3, 129.1, 128.7, 128.2, 126.2, 125.1, 121.1, 114.1, 85.0, 75.9, 55.6, 48.0, 37.3. **HRMS** (ESI): m/z $[M + H]^+$ calcd for $[C_{25}H_{22}NO_6]^+$: 432. 1442, found: 432.1438.

(*R*)-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl 4-chlorobenzoate (3c)

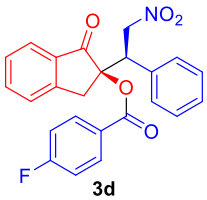


3c

Pale yellow solid (57.6 mg), 66% yield, 1.5:1 dr, **mp**. 180.1-180.8 ºC; $[\alpha]_D^{20}$ = +18.0 (c = 0.99, in THF); **HPLC:** Chiralpak IC column (hexane/i-PrOH = 80/20, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 10.42 min (minor), t_4 = 35.92 min (major), ee = 30%; ***major product***: t_2 = 11.86 min (minor), t_3 = 22.15 min (major), ee = 82%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.00 – 7.94 (m, 2H), 7.94 – 7.89 (m, 1H), 7.84 (d, J = 7.7 Hz, 1H), 7.71 (d, J = 7.7 Hz, 0.5H), 7.63 (td, J = 7.5, 1.1 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.47 – 7.43 (m, 2H), 7.43 – 7.35 (m, 3.0H), 7.35 – 7.27 (m, 4H), 7.11 – 7.00 (m, 3H), 5.57 – 5.46 (m, 1.5H), 5.08 (dd, J = 13.7, 10.2 Hz, 1H), 4.98 (dd, J = 13.7, 8.7 Hz, 0.5H), 4.41 (dd, J = 8.7, 5.1 Hz, 0.5H), 3.82 (dd, J = 10.2, 4.1 Hz, 1H), 3.56 (d, J = 17.2 Hz, 0.5H), 3.41 (d, J = 19.2 Hz, 1.5H), 3.27 (d, J = 17.5 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.9, 200.1, 164.3, 164.2, 149.0, 148.7, 140.6, 140.5, 136.1, 136.1, 135.6, 135.4, 133.7, 131.3, 131.1, 129.3, 129.2, 129.2, 129.2, 129.1, 128.8, 128.6, 128.4, 128.3, 127.9, 127.3, 127.1, 126.2, 126.1, 125.6, 125.1, 123.8, 85.6, 84.5, 75.7, 75.2,

50.7, 47.9, 38.1, 37.0. **HRMS** (ESI): m/z[M + H]$^+$ calcd for [$C_{24}H_{19}ClNO_5$]$^+$: 436.0946, found: 436.0945.

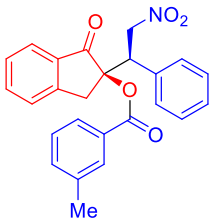
(*R*)-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl 4-fluorobenzoate (3d)



3d

Pale yellow solid (60.7 mg), 72% yield, 3:1 dr, **mp**. 154.1-155.0 °C; $[\alpha]_D^{20}$ = +49.0 (c = 0.95, in THF); **HPLC**: Chiralpak IE column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 9.43 min (minor), t_4 = 34.41 min (major), ee = 29%; ***major product***: t_2 = 10.37 min (minor), t_3 = 21.78 min (major), ee = 82%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.10 – 8.03 (m, 2H), 8.03 – 7.98 (m, 0.72H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 7.7 Hz, 0.36H), 7.63 (td, *J* = 7.5, 1.1 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.41 – 7.27 (m, 6.44H), 7.23 – 7.11 (m, 3.08H), 7.10 – 7.01 (m, 2.08H), 5.59 -5.46 (m, 1.36H), 5.09 (dd, *J* = 13.7, 10.2 Hz, 1H), 4.99 (dd, *J* = 13.7, 8.8 Hz, 0.36H), 4.41 (dd, *J* = 8.7, 5.1 Hz, 0.36H), 3.82 (dd, *J* = 10.2, 4.1 Hz, 1H), 3.57 (d, *J* = 17.2 Hz, 0.36H), 3.41 (d, *J* = 17.4 Hz, 1.36H), 3.27 (d, *J* = 17.5 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.0, 200.2, 166.3 (*J* = 254 Hz), 164.1, 164.0, 149.0, 148.7, 136.1, 135.6, 135.5, 133.8, 132.6, 132.54, 132.48, 132.4, 129.3, 129.22, 129.15, 128.8, 128.6, 128.4, 128.3, 127.9, 126.2, 125.6, 125.2, 125.16, 125.13, 125.11, 123.8, 116.1 (*J* = 22 Hz), 116.0, 85.5, 84.4, 75.7, 75.3, 50.7, 47.9, 38.1, 37.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -103.41, -103.62. **HRMS** (ESI): m/z [M + H]$^+$ calcd for [$C_{24}H_{19}FNO_5$]$^+$: 420.1242, found: 420.1237.

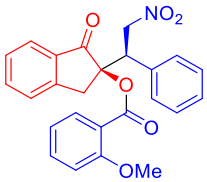
(*R*)-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl 3-methylbenzoate (3e)



3e

Pale yellow solid (46.5 mg), 56% yield, 5:1 dr, **mp**. 130.3 - 131.0 °C; $[\alpha]_D^{20}$ = +37.0 (c = 0.89, in THF); **HPLC**: Chiralpak IC column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 9.20 min (minor), t_4 = 12.52 min (major), ee = 45%; ***major product***: t_2 = 10.26 min (minor), t_3 = 11.16 min (major), ee = 84%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 – 7.77 (m, 3.4H), 7.76 – 7.68 (m, 0.4H), 7.68 – 7.59 (m, 1H), 7.57 – 7.50 (m, 0.4H), 7.49 – 7.39 (m, 4.8H), 7.40 – 7.26 (m, 4.6H), 7.12 – 6.99 (m, 1H), 5.57 (dd, *J* = 13.7, 3.9 Hz, 1H), 5.48 (dd, *J* = 13.7, 4.7 Hz, 0.2H), 5.16 - 5.09 (m, 1.2H), 4.41 (dd, *J* = 9.3, 4.7 Hz, 0.2H), 3.79 (dd, *J* = 10.4, 3.9 Hz, 1H), 3.56 (d, *J* = 17.2 Hz, 0.2H), 3.40 (d, *J* = 17.5 Hz, 1.2H), 3.25 (d, *J* = 17.5 Hz, 1H), 2.44 (s, 3H), 2.41 (s, 0.6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.1, 200.3, 165.3, 165.2, 149.0, 148.8, 138.7, 138.6, 136.2, 136.0, 135.7, 135.5, 134.72, 134.68, 133.8, 132.5, 130.5, 130.4, 129.4, 129.3, 129.1, 128.8, 128.74, 128.73, 128.62, 128.56, 128.4, 128.3, 127.8, 127.0, 126.9, 126.2, 125.6, 125.1, 123.7, 85.2, 84.2, 75.8, 75.4, 50.8, 48.0, 38.1, 37.2, 21.4, 21.3. **HRMS** (ESI): m/z [M + Na]$^+$ calcd for [$C_{25}H_{21}NaNO_5$]$^+$: 438.1312, found: 438.1308.

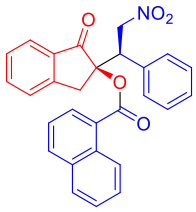
(*R*)-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl 2-methoxybenzoate (3f)



3f

White solid (52.6 mg), 61% yield, 8.3:1 dr, **mp**. 133.3-133.9 ºC; $[\alpha]_D^{20}$ = +55.0 (c = 0.99, in THF); **HPLC**: Chiralpak ID column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2 = 21.46 min (minor), t_4 = 31.79 min (major), ee = 77%; ***major product***: t_1= 19.76 min (minor), t_3 = 25.48 min (major), ee = 94%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 – 7.81 (m, 2H), 7.75 – 7.66 (m, 0.24H), 7.64 – 7.53 (m, 1H), 7.51 – 7.40 (m, 5.36H), 7.37 – 7.28 (m, 3.84H), 7.13 – 6.94 (m, 3.12H), 5.65 -5.53 (m, 1H), 5.29 – 5.13 (m, 1.12H), 4.30 (dd, *J* = 10.6, 3.6 Hz, 0.12H), 4.03 (s, 3H), 3.97 – 3.84 (m, 0.48H), 3.72 – 3.59 (m, 1.12H), 3.41 (d, *J* = 17.6 Hz, 1H), 3.35 (d, *J* = 5.6 Hz, 0.12H), 3.17 (d, *J* = 17.5 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.5, 165.0, 159.7, 148.9, 136.3, 135.9, 135.0, 133.8, 133.0, 129.5, 129.0, 128.6, 128.1, 126.2, 125.2, 120.5, 117.9, 112.2, 85.2, 76.2, 55.9, 48.0, 37.3. **HRMS** (ESI): m/z [M + H]$^+$ calcd for $[C_{25}H_{22}NO_6]^+$: 432.1442, found: 432.1437.

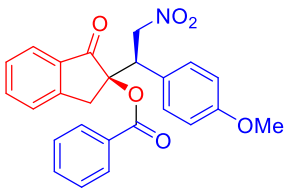
(*R*)-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl 1-naphthoate (3g)



3g

Pale yellow solid (51.6 mg), 54% yield, 3.3:1 dr, **mp**. 133.6-134.5 ºC; $[\alpha]_D^{20}$ = +31.0 (c = 0.96, in THF); **HPLC**: Chiralpak IC column (hexane/i-PrOH = 60/40, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 9.77 min (minor), t_4 = 12.02 min (major), ee = 17%; ***major product***: t_2 = 10.53 min (minor), t_3 = 11.23 min (major), ee = 82%; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.63 – 8.56 (m, 1.3H), 8.06 – 7.94 (m, 3.3H), 7.94 – 7.83 (m, 3H), 7.73 (d, *J* = 7.6 Hz, 0.3H), 7.69 – 7.52 (m, 3.6H), 7.50 – 7.41 (m, 3H), 7.40 – 7.26 (m, 4.5H), 7.16 – 6.99 (m, 1.5H), 5.65 – 5.53 (m, 1.3H), 5.18 (dd, *J* = 13.7, 10.3 Hz, 1H), 5.07 (dd, *J* = 13.7, 9.1 Hz, 0.3H), 4.48 (dd, *J* = 9.0, 4.9 Hz, 0.3H), 3.86 (dd, *J* = 10.2, 3.9 Hz, 1H), 3.63 (d, *J* = 17.2 Hz, 0.3H), 3.53 – 3.37 (m, 1.3H), 3.30 (d, *J* = 17.5 Hz, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 201.1, 200.4, 165.3, 165.2, 149.1, 148.8, 136.2, 136.0, 135.9, 135.7, 135.6, 133.9, 132.5, 132.4, 131.9, 131.8, 129.62, 129.58, 129.4, 129.3, 129.2, 129.0, 128.9, 128.8, 128.7, 128.6, 128.4, 128.3, 127.9, 127.8, 127.1, 127.0, 126.2, 126.0, 125.8, 125.6, 125.1, 125.0, 124.8, 123.8, 85.5, 84.4, 75.9, 75.4, 50.8, 48.0, 38.2, 37.2. **HRMS** (ESI): m/z [M + H]$^+$ calcd for $[C_{28}H_{22}NO_5]^+$: 452.1492, found: 452.1487.

(*R*)-2-((*R*)-1-(4-methoxyphenyl)-2-nitroethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3h)

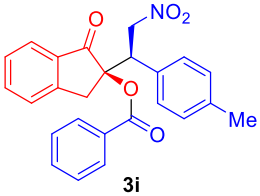


3h

Pale yellow solid (48.3 mg), 56% yield, 9:1 dr, **mp**. 134.5 - 135.6 ºC; $[\alpha]_D^{20}$ = +7.0 (c = 1.01, in THF);

HPLC: Chiralpak IC column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), t_1= 11.71 min (minor), t_4 = 20.05 min (major), ee = 20%;major product: t_2 = 13.84 min (major), t_3 = 16.31 min (minor), ee = 91%; **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.07 – 8.03 (m, 2H), 8.02 – 7.98 (m, 0.22H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.72 (d, J = 7.6 Hz, 0.11H), 7.69 – 7.61 (m, 2H), 7.52 (t, J = 7.7 Hz, 2.11H), 7.49 – 7.42 (m, 1.11H), 7.36 – 7.32 (m, 3.33H), 7.07 (d, J = 7.6 Hz, 0.11H), 7.00 (d, *J* = 8.7 Hz, 0.22H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.57 (d, J = 8.7 Hz, 0.22H) 5.53 (dd, *J* = 13.5, 3.9 Hz, 1H), 5.44 (dd, *J* = 13.5, 4.6 Hz, 0.11H), 5.08 (dd, J = 13.5, 10.7 Hz, 1H), 5.03 – 4.98 (m, 0.11H), 4.34 (dd, *J* = 9.6, 4.7 Hz, 0.11H), 3.79 (s, 3H), 3.73 (dd, *J* = 10.7, 3.9 Hz, 1H), 3.64 (s, 0.33H), 3.57 (d, *J* = 17.1 Hz, 0.11H), 3.45 – 3.35 (m, 1.11H), 3.26 (d, *J* = 17.5 Hz, 1H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ 200.4, 165.1, 159.8, 148.8, 136.0, 133.9, 133.8, 130.4, 129.8, 128.9, 128.8, 128.3, 127.5, 126.2, 125.1, 114.5, 85.5, 76.0, 55.3, 47.33, 37.2. **HRMS** (ESI): m/z [M + H]$^+$ calcd for [$C_{25}H_{22}NO_6$]$^+$: 432.1442, found: 432.1439.

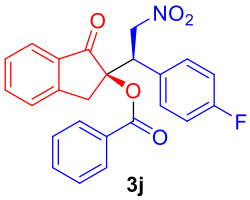
(*R*)-2-((*R*)-2-nitro-1-(p-tolyl)ethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3i)



3i

Pale yellow solid (49.8 mg), 60% yield, 6.7:1 dr, **mp**. 99.2-100.1 ºC; $[\alpha]_D^{20}$ = +8.0 (c = 1.10, in THF); **HPLC**: Chiralpak IC column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 9.58 min (minor), t_4 = 14.78 min (major), ee = 37%; ***major product***: t_2 = 10.47 min (minor), t_3 = 11.55 min (major), ee = 89%; **^{1}H NMR** (400 MHz, CDCl$_3$) δ 8.07 – 8.03 (m, 2H), 8.02 – 7.98 (m, 0.30H), 7.85 (d, J = 7.7 Hz, 1H), 7.71 (d, J = 7.4 Hz, 0.15H), 7.67 – 7.59 (m, 2.15H), 7.51 (t, J = 7.7 Hz, 2.15H), 7.47 – 7.39 (m, 1.30H), 7.36 – 7.26 (m, 3.15H), 7.16 (d, J = 7.9 Hz, 2H), 7.05 (d, J = 7.6 Hz, 0.15H), 6.96 (d, J = 8.1 Hz, 0.30H), 6.85 (d, J = 7.9 Hz, 0.30H), 5.55 (dd, J = 13.6, 3.8 Hz, 1H), 5.45 (dd, J = 13.6, 4.7 Hz, 0.15H), 5.10 (dd, J = 13.6, 10.6 Hz, 1H), 5.02 (dd, J = 13.6, 9.5 Hz, 0.15H), 4.36 (dd, J = 9.4, 4.6 Hz, 0.15H), 3.73 (dd, J = 10.5, 3.8 Hz, 1H), 3.56 (d, J = 17.2 Hz, 0.15H), 3.44 – 3.35 (m, 1.15H), 3.26 (d, J = 17.5 Hz, 1H), 2.32 (s, 3H), 2.13 (s, 0.45H). **^{13}C NMR** (101 MHz, CDCl$_3$) δ 165.1, 148.8, 138.6, 136.0, 133.9, 133.8, 132.6, 129.8, 129.8, 129.2, 129.1, 128.9, 128.8, 128.3, 126.2, 125.2, 85.4, 75.9, 47.6, 37.3, 21.1. **HRMS** (ESI): m/z [M + H]$^+$ calcd for [$C_{25}H_{22}NO_5$]$^+$: 416.1492, found: 416.1489.

(*R*)-2-((*R*)-1-(4-fluorophenyl)-2-nitroethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3j)

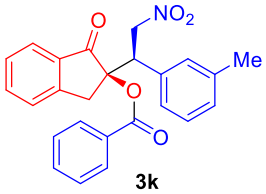


3j

Pale yellow solid (66.3 mg), 79% yield, 2.8:1 dr, **mp**. 144.4 - 144.9 ºC; $[\alpha]_D^{20}$ = +99.0 (c = 1.11, in THF); **HPLC**: Chiralpak IF column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 5.62 min (minor), t_4 = 15.37 min (major), ee = 55%; ***major product***: t_2 = 6.05 min (minor), t_3 = 9.43 min (major), ee = 79%; **^{1}H NMR** (400 MHz, CDCl$_3$) δ 8.07 – 7.96 (m, 2.70H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.72 (d, J = 7.6 Hz, 0.35H), 7.68 – 7.60 (m, 2.35H), 7.56 – 7.49 (m, 2.35H), 7.48 – 7.45 (m, 1.35H), 7.44 – 7.37 (m, 2.35H), 7.34 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 7.5 Hz, 0.35H), 7.10 – 7.01 (m, 3.05H), 6.75 (t, *J* = 8.5 Hz, 0.70H), 5.56 (dd, *J* = 13.7, 3.8 Hz, 1H), 5.46 (dd, *J* = 13.7, 4.5 Hz, 0.35H), 5.13 - 4.97 (m, 1.35H), 4.39 (dd, *J* = 9.6, 4.6 Hz, 0.35H), 3.80 (dd, *J* = 10.6, 3.8 Hz, 1H), 3.60

(d, J = 17.2 Hz, 0.35H), 3.46 – 3.34 (m, 1.35H). 3 22 (d, J = 17.5 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.9, 200.1, 165.0, 164.9, 162.8 (d, J = 248.6 Hz), 162.5 (d, J = 248.8 Hz), 148.9, 148.6, 136.1, 135.8, 134.0, 134.0, 133.7, 131.4, 131.4, 131.0 (d, J = 8.2 Hz), 130.9, 129.9, 129.8, 128.9, 128.8, 128.8, 128.4, 128.0, 126.2, 125.6, 125.2, 123.8, 116.2 (d, J = 21.6 Hz), 115.6, 115.4, 85.2, 75.8, 75.4, 50.1, 47.3, 38.1, 37.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.57, -112.60. **HRMS** (ESI): m/z $[M + H]^+$ calcd for $[C_{24}H_{19}FNO_5]^+$: 420.1242, found: 420.1237.

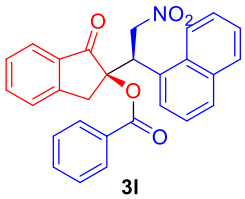
(*R*)-2-((*R*)-2-nitro-1-(m-tolyl)ethyl)-1-oxo-2,3-dihydro-1H-inden-2-ylbenzoate (3k)



3k

Pale yellow solid (54.8 mg), 66% yield, 4:1 dr, **mp**. 130.3 - 131.0 °C; $[\alpha]_D^{20}$ = +52.0 (c = 0.99, in THF); **HPLC**: Chiralpak IE column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 11.20 min (minor), t_4 = 49.69 min (major), ee = 50%; ***major product***: t_2 = 12.69 min (minor), t_3 = 29.66 min (major), ee = 82%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 – 8.04 (m, 2H), 8.02 – 7.99 (m, 0.5H), 7.86 (d, J = 7.7 Hz, 1H), 7.75 – 7.71 (m, 0.25H), 7.68 – 7.58 (m, 2.25H), 7.56 - 7.49 (m, 2.5H), 7.48 - 7.41 (m, 2H), 7.34 (d, J = 7.7 Hz, 1H), 7.25 (d, J = 3.9 Hz, 1.25H), 7.20 (s, 1H), 7.15 - 7.11 (m 1H), 7.04 (d, J = 7.6 Hz, 0.25H), 6.97 – 6.82 (m, 1H), 5.56 (dd, J = 13.7, 3.9 Hz, 1H), 5.47 (dd, J = 13.7, 4.7 Hz, 0.25H), 5.11 (dd, J = 13.7, 10.4 Hz, 1H), 5.01 (dd, J = 13.7, 9.3 Hz, 0.25H), 4.36 (dd, J = 9.3, 4.7 Hz, 0.25H), 3.74 (dd, J = 10.4, 3.8 Hz, 1H), 3.56 (d, J = 17.1 Hz, 0.25H), 3.43 - 3.36(m, 1.25H), 3.26 (d, J = 17.5 Hz, 1H), 2.33 (s, 3H), 2.10 (s, 0.75H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.0, 200.3, 165.3, 165.2, 149.0, 148.7, 138.7, 136.0, 135.7, 135.5, 134.7, 133.8, 130.5, 130.4, 129.4, 129.3, 129.1, 128.8, 128.7, 128.7, 128.6, 128.6, 128.4, 128.3, 127.8, 127.1, 126.9, 126.2, 125.6, 125.1, 123.7, 85.2, 84.2, 75.8, 75.4, 50.7, 48.0, 38.1, 37.2, 21.4, 21.3. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{25}H_{21}NaNO_5]^+$: 438.1312, found: 438.1308.

(*R*)-2-((*R*)-1-(naphthalen-1-yl)-2-nitroethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3l)

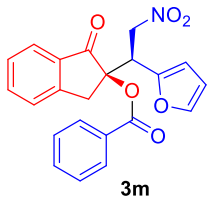


3l

Pale yellow solid (58.4 mg), 61% yield, 4.5:1 dr, **mp**. 123.1-123.8 °C; $[\alpha]_D^{20}$ = +46.0 (c = 0.97, in THF); **HPLC**: Chiralpak IB column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2 = 20.43 min (major), t_4= 28.36 min (minor), ee = 17%; ***major product***: t_1 = 11.16 min (major), t_3 = 25.79 min (minor), ee = 83%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17 – 8.04 (m, 2.22H), 8.05 – 7.99 (m, 0.44H), 7.92 – 7.84 (m, 2.22H), 7.84 – 7.75 (m, 3.22H), 7.73 (d, J = 7.6 Hz, 0.44H), 7.69 – 7.57 (m, 3.44H), 7.56 – 7.35 (m, 5.88H), 7.28 (d, J = 7.7 Hz, 1H), 7.22 – 7.08 (m, 0.44H), 6.92 (d, J = 7.5 Hz, 0.22H), 5.67 (dd, J = 13.8, 3.7 Hz, 1H), 5.55 (dd, J = 13.7, 4.6 Hz, 0.22H), 5.34 – 5.19 (m, 1H), 5.20 – 5.09 (m, 0.22H), 4.57 (dd, J = 9.4, 4.6 Hz, 0.22H), 3.94 (dd, J = 10.5, 3.7 Hz, 1H), 3.59 (d, J = 17.2 Hz, 0.22H), 3.47 (d, J = 17.2 Hz, 0.22H), 3.39 (d, J = 17.5 Hz, 1H), 3.27 (d, J = 17.6 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.3, 200.4, 165.2, 165.0, 149.1, 148.8, 136.1, 135.6, 134.1, 134.0, 133.7, 133.25, 133.19, 133.18, 132.9, 132.7, 130.7, 130.3, 130.2, 130.00, 129.97, 129.8, 129.4, 129.31, 129.26, 128.9, 128.8, 128.7, 128.5, 128.4, 128.3, 128.0, 127.9, 127.8, 127.6, 126.8, 126.6, 126.5, 126.3, 126.0,

125.7, 125.2, 123.7, 85.4, 84.4, 75.9, 75.6, 51.0, 48.2, 38.2, 37.4. **HRMS** (ESI): m/z $[M + H]^+$ calcd for $[C_{28}H_{22}NO_5]^+$: 452.1492, found: 452.1494.

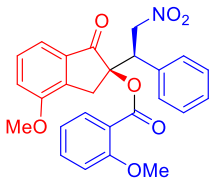
(*R*)-2-((*R*)-1-(furan-2-yl)-2-nitroethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3m)



3m

Blacksolid (47.0 mg), 60% yield, 5:1 dr, **mp**. 71.2-71.9 ºC; $[\alpha]_D^{20}$ = -20.0 (c = 0.96, in THF); **HPLC**: Chiralpak IC column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_1= 8.84 min (minor), t_4 = 12.94 min (major), ee = 31%; ***major product***: t_2 = 9.65 min (minor), t_3 = 11.49 min (major), ee = 79%; **^{1}H NMR** (400 MHz, $CDCl_3$)) δ 8.06 – 8.00 (m, 2H), 8.00 – 7.96 (m, 0.34H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 7.7 Hz, 0.17H), 7.67 – 7.56 (m, 2.17H), 7.54 – 7.44 (m, 2.51H), 7.42 – 7.34 (m, 2H), 7.33 – 7.19 (m, 1.34H), 6.97 (s, 0.17H), 6.31 – 6.28 (m, 1H), 6.25 – 6.20 (m, 1H), 6.16 (d, *J* = 3.0 Hz, 0.17H), 6.01 (s, 0.17H), 5.46 – 5.24 (m, 1.17H), 5.18 – 5.04 (m, 1H), 5.05 – 4.91 (m, 0.17H), 4.66 – 4.49 (m, 0.17H), 4.27 – 4.07 (m, 1H), 3.67 – 3.52 (m, 0.37H), 3.51 – 3.42 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.1, 164.9, 148.8, 148.7, 148.0, 146.5, 143.2, 142.9, 135.9, 135.4, 134.02, 133.9, 129.9, 128.7, 128.2, 127.8, 126.5, 126.2, 125.7, 124.8, 124.0, 110.7, 110.6, 110.3, 84.3, 83.4, 73.7, 73.4, 44.4, 42.6, 38.5, 36.6. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{22}H_{17}NaNO_6]^+$: 414.0948, found: 414.0944.

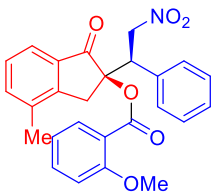
(*R*)-4-methoxy-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3n)



3n

White solid (72.8 mg), 79% yield, 5:1 dr, **mp**. 84.2-85.1 ºC; $[\alpha]_D^{20}$ = +69.0 (c = 0.98, in THF); **HPLC**: Chiralpak ID column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2= 29.74 min (minor), t_4 = 41.70 min (major), ee = 85%; ***major product***: t_1 = 24.18 min (minor), t_3 = 33.12 min (major), ee = 95%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92 – 7.84 (m, 1.2H), 7.59 – 7.52 (m, 1.2H), 7.52 - 7.46 (m, 2H), 7.46 – 7.36 (m, 2.2H), 7.35 – 7.26 (m, 3.2H), 7.13 – 7.09 (m, 0.4H), 7.09 – 6.97 (m, 4H), 6.83 (d, *J* = 7.9 Hz, 0.2H), 5.65 – 5.53 (m, 1.2H), 5.25 – 5.14 (m, 1.2H), 4.27 (dd, *J* = 10.7, 3.7 Hz, 0.2H), 4.02 (s, 3H), 3.92 (s, 0.6H), 3.81 (s, 3H), 3.74 – 3.63 (m, 1.6H), 3.44 (d, *J* = 17.5 Hz, 0.2H), 3.35 (d, *J* = 17.5 Hz, 0.2H), 3.27 – 3.11 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.2, 200.7, 165.0, 164.6, 159.9, 159.6, 156.4, 155.9, 137.9, 137.7, 136.3, 135.1, 134.92, 134.87, 133.0, 132.8, 132.5, 129.6, 129.5, 129.21, 129.18, 129.0, 128.5, 128.4, 128.2, 120.5, 120.4, 118.0, 117.8, 116.5, 116.1, 115.8, 115.4, 112.1, 85.2, 84.4, 76.3, 75.8, 55.9, 55.9, 55.5, 51.0, 48.0, 34.8, 34.2. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{26}H_{23}NaNO_7]^+$: 484.1367, found: 484.1363.

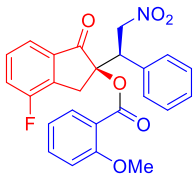
(*R*)-4-methyl-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3o)



3o

Pale yellow solid (66.7 mg), 75% yield, 4.3:1 dr, **mp**. 76.2 - 76.9 ºC; $[\alpha]_D^{20}$ = +78.0 (c = 0.99, in THF); **HPLC**: Chiralpak ID column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2= 23.23 min (minor), t_4 = 36.86 min (major), ee = 78%; ***major product***: t_1 = 19.07 min (minor), t_3 = 29.53 min (major), ee = 95%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 7.8, 1.8 Hz, 1.23H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.59 – 7.52 (m, 1.46H), 7.52 – 7.46 (m, 2.23H), 7.43 (d, *J* = 7.4 Hz, 1.23H), 7.37 – 7.30 (m, 4.46H), 7.17 – 7.14 (m, 0.46H), 7.09 – 6.97 (m, 3.68H), 5.65 – 5.56 (m, 1.23H), 5.27 – 5.13 (m, 1.23H), 4.30 (dd, *J* = 10.6, 3.7 Hz, 0.23H), 4.03 (s, 3H), 3.92 (s, 0.69H), 3.67 (dd, *J* = 10.9, 3.7 Hz, 1H), 3.47 (d, *J* = 17.0 Hz, 0.23H), 3.29 – 3.22 (m, 1.23H), 3.08 (d, *J* = 17.4 Hz, 1H), 2.18 (s, 3H), 2.01 (s, 0.69H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.3, 200.8, 165.0, 164.6, 160.0, 159.7, 148.0, 147.8, 136.4, 136.3, 135.9, 135.4, 135.0, 134.9, 134.8, 133.6, 133.0, 132.8, 132.4, 129.5, 129.1, 129.0, 128.6, 128.5, 128.3, 128.1, 127.8, 122.5, 121.2, 120.5, 120.4, 118.0, 117.8, 112.2, 85.3, 84.5, 76.0, 75.7, 55.9, 55.9, 51.2, 48.0, 36.8, 36.1, 17.8, 17.5. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{26}H_{23}NaNO_6]^+$: 468.1418, found: 468.1415.

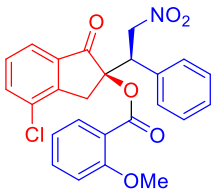
(*R*)-4-fluoro-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate(3p)



3p

Pale yellow solid (60.4 mg), 72% yield, 5:1 dr, **mp**. 87.2-88.1 ºC; $[\alpha]_D^{20}$ = +89.0 (c = 1.11, in THF); **HPLC**: Chiralpak ID column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2= 12.36 min (minor), t_4 = 20.93 min (major), ee = 88%; ***major product***: t_1 = 11.62 min (minor), t_3 = 15.86 min (major), ee = 94%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 - 7.83 (m, 1.21H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.62 - 7.55 (m, 1.21H), 7.50 – 7.40 (m, 3.21H), 7.37 – 7.27 (m, 4.05H), 7.14 – 6.96 (m, 3.84H), 5.70 – 5.46 (m, 1.21H), 5.28 – 5.12 (m, 1.21H), 4.31 (dd, *J* = 10.4, 3.8 Hz, 0.21H), 4.04 (s, 3H), 3.93 (s, 0.63H), 3.71 (dd, *J* = 10.7, 3.7 Hz, 1H), 3.55 (d, *J* = 17.4 Hz, 0.21H), 3.44 (d, *J* = 17.4 Hz, 0.21H)., 3.29 (q, *J* = 17.8 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.38, 199.35, 165.1, 164.7, 160.0, 159.7, 159.4, 136.4, 135.7, 135.2, 134.9, 134.7, 133.1, 132.8, 132.0, 130.0, 129.6, 129.4, 129.2, 129.1, 128.72, 128.69, 128.4, 122.0, 121.5, 121.3, 120.90, 120.86, 120.4, 119.5, 117.6, 117.3, 112.2, 84.8, 83.9, 76.0, 75.5, 55.9, 50.9, 47.8, 33.9, 33.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.57, -112.60. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{25}H_{20}FNaNO_6]^+$: 472.1167, found: 472.1164.

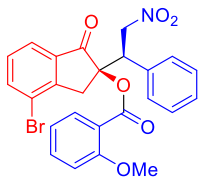
(*R*)-4-chloro-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3q)



3q

Pale yellow solid (75.4 mg), 81% yield, 10:1 dr, **mp**. 144.5-145.6 ºC; $[\alpha]_D^{20}$ = +81.0 (c = 1.08, in THF); **HPLC**: Chiralpak ID column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2= 13.18 min (minor), t_4 = 20.41 min (major), ee = 82%; ***major product***: t_1 = 11.73 min (minor), t_3 = 14.87 min (major), ee = 96%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 – 7.87 (m, 1.1H), 7.74 (d, *J* = 7.5 Hz, 1H), 7.61 – 7.54 (m, 2.2H), 7.47 (dd, *J* = 7.5, 1.7 Hz, 2H), 7.39 (t, *J* = 7.8 Hz, 1.1H), 7.36 – 7.26 (m, 3.3H), 7.12 – 6.97 (m, 2.5H), 5.64 – 5.55 (m, 1.1H), 5.25 - 5.14 (m, 1.1H), 4.32 (dd, *J* = 10.4, 3.9 Hz, 0.1H), 4.02 (s, 3H), 3.92 (s, 0.3H), 3.73 (dd, *J* = 10.7, 3.8 Hz, 1H), 3.54 (d, *J* = 17.6 Hz, 0.1H), 3.42 (d, *J* = 17.6 Hz, 0.1H), 3.29 (q, *J* = 18.0 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.8, 165.0, 159.8, 146.7, 135.8, 135.5, 135.4, 135.2, 133.0, 132.3, 129.6, 129.4, 129.1, 128.7, 123.3, 121.9, 120.6, 117.6, 117.3, 112.2, 84.8, 75.9, 55.9, 47.9, 36.2. **HRMS** (ESI): m/z [M + Na]$^+$ calcd for $[C_{25}H_{20}ClNaNO_6]^+$: 488.0871, found: 488.0870, 490.0854.

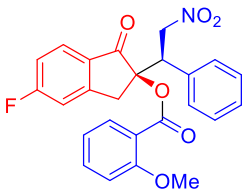
(*R*)-4-bromo-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3r)



3r

Pale yellow solid (76.5 mg), 75% yield, 5:1 dr, **mp**. 64.2-64.9 ºC; $[\alpha]_D^{20}$ = +99.0 (c = 0.95, in THF); **HPLC**: Chiralpak ID column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2= 16.04 min (minor), t_4 = 25.32 min (major), ee = 79%; **major product**: t_1 = 13.63 min (minor), t_3 = 17.84 min (major), ee = 94%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 7.8, 1.8 Hz, 1.2H), 7.78 (dd, *J* = 7.6, 4.4 Hz, 2H), 7.65 – 7.55 (m, 1.4H), 7.52 (d, *J* = 7.5 Hz, 0.2H), 7.49 – 7.42 (m, 2.2H), 7.38 – 7.27 (m, 3.8H), 7.11 – 6.97 (m, 3.8H), 5.63 - 5.51 (m, 1.2H), 5.29 - 5.07 (m 1.2H), 4.32 (dd, *J* = 10.3, 3.9 Hz, 0.20H), 4.03 (s, 3H), 3.93 (s, 0.6H), 3.73 (dd, *J* = 10.7, 3.8 Hz, 1H), 3.50 (d, *J* = 17.6 Hz, 0.2H), 3.37 (d, *J* = 17.5 Hz, 0.2H), 3.29 (d, *J* = 17.9 Hz, 1H), 3.19 (d, *J* = 18.0 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.9, 165.0, 164.6, 160.1, 159.7, 148.8, 148.7, 138.4, 138.1, 137.9, 135.9, 135.4, 135.1, 133.0, 132.8, 131.9, 129.8, 129.4, 129.3, 129.0, 128.7, 128.4, 123.8, 122.5, 121.5, 120.5, 120.4, 117.6, 117.3, 112.1, 110.5, 107.7, 84.9, 84.1, 75.9, 75.3, 67.4, 55.9, 50.8, 47.9, 39.1, 38.2. **HRMS** (ESI): m/z [M + Na]$^+$ calcd for $[C_{25}H_{20}BrNaNO_6]^+$: 532.0366, found: 532.0361.

(*R*)-5-fluoro-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3s)

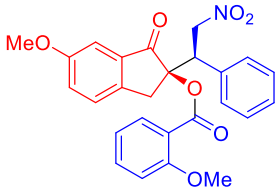


3s

Pale yellow solid (55.8 mg), 62% yield, 10:1 dr, **mp**. 63.8-64.5 ºC; $[\alpha]_D^{20}$ = +88.0 (c = 0.98, in THF); **HPLC**: Chiralpak IC column (hexane/i-PrOH = 80/20, flow rate 0.5 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2= 29.06 min (minor), t_4 = 35.32 min (major), ee = 88%; ***major product***: t_1 = 27.60 min (minor), t_3 = 33.52 min (major), ee = 94%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 – 7.82 (m, 2H), 7.71 – 7.65 (m, 1H), 7.61 – 7.55 (m, 1H), 7.51 – 7.44 (m, 2H), 7.39 – 7.28 (m, 3H), 7.13 (td, *J* = 6.9, 3.4 Hz, 1H), 7.10 – 6.94 (m, 4H), 6.68 (d, 0H), 5.66 – 5.50 (m, 1.06H), 5.26 – 5.11 (m, 1.07H), 4.30 (dd, *J* = 10.5, 3.7 Hz, 0.11H), 4.04 (s, 3H), 3.93 (s, 0.28H), 3.68 (dd, *J* = 10.8, 3.7 Hz, 1H),3.61 (d, *J* = 17.3 Hz,

0.12H),3.39 (d, J = 18.1 Hz, 1.12H), 3.16 (d, J = 17.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 198.6, 167.7 (d, J = 257.9 Hz), 165.1, 159.7, 151.8 (d, J = 10.4 Hz), 136.0, 135.1, 133.1, 129.5, 129.1, 128.7, 127.8, 127.7, 120.6, 117.7, 116.5 (d, J = 23.7 Hz), 113.1 (d, J = 22.7 Hz), 112.2, 85.1, 76.1, 55.9, 48.0, 37.2. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -100.13, -100.69. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{25}H_{20}FNaNO_6]^+$: 472.1167, found: 472.1164.

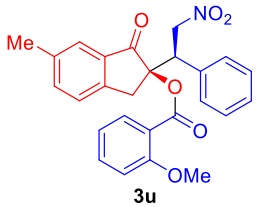
(*R*)-6-methoxy-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3t)



3t

White solid (64.5 mg), 70% yield, 10:1 dr, **mp**. 68.2-68.8 ºC; $[\alpha]_D^{20}$ = +106.0 (c = 1.05, in THF); **HPLC**: Chiralpak IE column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2= 30.16 min (minor), t_4 = 38.04 min (major), ee = 69%; ***major product***: t_1 = 26.51 min (minor), t_3 = 33.84 min (major), ee = 94%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 – 7.82 (m, 1.1H), 7.76 – 7.69 (m, 0.1H), 7.59 – 7.54 (m, 1.2H), 7.52 – 7.45 (m, 2.1H), 7.40 – 7.27 (m, 4H), 7.23 – 7.20 (m, 2H), 7.13 – 6.95 (m, 2.6H), 6.94 – 6.88 (m, 0.1H), 5.59 (dd, J = 13.8, 3.6 Hz, 1.1H), 5.27 - 5.11 (m, 1.1H), 4.28 (dd, J = 10.6, 3.6 Hz, 0.1H), 4.04 (s, 3H), 3.92 (s, 0.3H), 3.86 (s, 3H), 3.80 (s, 0.3H), 3.69 (dd, J = 10.8, 3.6 Hz, 1H), 3.53 (d, J = 16.8 Hz, 0.1H), 3.36 – 3.25 (m, 1.1H), 3.10 (d, J = 17.1 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.5, 165.0, 159.9, 159.7, 141.6, 136.4, 135.0, 134.8, 133.1, 129.5, 129.0, 128.5, 127.1, 125.3, 120.5, 118.0, 112.2, 106.3, 85.8, 76.2, 55.9, 55.7, 48.0, 36.7. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{26}H_{23}NaNO_7]^+$: 484.1367, found: 484.1365.

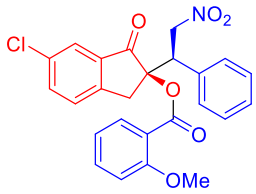
(*R*)-6-methyl-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3u)



3u

White solid (67.6 mg), 76% yield, 7:1 dr, **mp**. 78.4-79.1 ºC; $[\alpha]_D^{20}$ = +104.0 (c = 1.02, in THF); **HPLC**: Chiralpak IE column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), ***minor product***: t_2= 21.51 min (minor), t_4 = 31.85 min (major), ee = 67%; ***major product***: t_1 = 18.23 min (minor), t_3 = 28.62 min (major), ee = 92%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.93 – 7.85 (m, 1.15H), 7.67 (s, 1H), 7.59 – 7.52 (m, 1.15H), 7.51 – 7.42 (m, 3.15H), 7.37 – 7.28 (m, 3.15H), 7.20 (d, J = 7.8 Hz, 1.15H), 7.10 – 6.96 (m, 2.9H), 6.94 – 6.90 (m, 0.15H), 5.60 (dd, J = 13.8, 3.6 Hz, 1.15H), 5.26 – 5.12 (m, 1.15H), 4.28 (dd, J = 10.7, 3.6 Hz, 0.15H), 4.03 (s, 3H), 3.92 (s, 0.45H), 3.66 (dd, J = 10.9, 3.6 Hz, 1H), 3.56 (d, J = 16.9 Hz, 0.15H), 3.38 – 3.29 (m, 1.15H), 3.11 (d, J = 17.4 Hz, 1H), 2.43 (s, 3H), 2.32 (s, 0.45H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.5, 165.0, 159.6, 146.2, 138.2, 137.1, 136.5, 134.9, 133.8, 133.1, 129.5, 129.0, 128.5, 126.0, 125.1, 120.5, 118.0, 112.1, 85.5, 76.3, 55.9, 48.0, 37.1, 21.2. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{26}H_{23}NaNO_6]^+$: 468.1418, found: 468.1414.

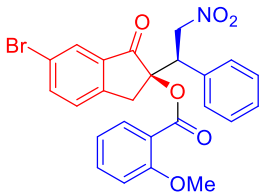
(*R*)-6-chloro-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3v)



3v

White solid (67.1 mg), 72% yield, 13:1 dr, **mp**. 70.1-70.8 °C; $[\alpha]_D^{20}$ = +90.0 (c = 0.98, in THF); **HPLC**: Chiralpak IE column (hexane/i-PrOH = 60/40, flow rate 1.0 mL/min^{-1}, λ = 254 nm), t_1 = 13.96 min (minor), t_2 = 24.29 min (major) ee = 90%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.82 (d, *J* = 1.9 Hz, 1H), 7.61 – 7.52 (m, 2H), 7.50 – 7.43 (m, 2H), 7.37 – 7.29 (m, 3H), 7.28 – 7.24 (m, 1H) 7.09 – 7.01 (m, 2. H), 5.64 – 5.51 (m, 1.08H), 5.24 – 5.11 (m, 1.08H), 4.29 (dd, *J* = 10.4, 3.8 Hz, 0.08H), 4.03 (s, 3H), 3.92 (s, 0.24H), 3.68 (dd, *J* = 10.8, 3.7 Hz, 1H), 3.56 (d, *J* = 17.3 Hz, 0.08H), 3.45 (d, *J* = 12.6 Hz, 0.08H), 3.35 (d, *J* = 17.5 Hz, 1H), 3.15 (d, *J* = 17.6 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.3, 165.1, 159.7, 146.9, 136.0, 135.8, 135.2, 135.0, 134.5, 133.1, 129.5, 129.1, 128.7, 127.5, 124.9, 120.6, 117.6, 112.2, 85.3, 76.0, 55.9, 47.8, 37.0. **HRMS** (ESI): m/z [M + Na]$^+$ calcd for $[C_{25}H_{20}ClNaNO_6]^+$: 488.0871, found: 488.0868.

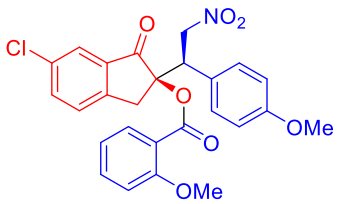
(*R*)-6-bromo-2-((*R*)-2-nitro-1-phenylethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl benzoate (3w)



3w

White solid (74.5 mg), 73% yield, 13:1 dr, **mp**. 79.8-80.9 °C; $[\alpha]_D^{20}$ = +61.0 (c = 1.05, in THF); **HPLC**: Chiralpak IE column (hexane/i-PrOH = 70/30, flow rate 1.0 mL/min^{-1}, λ = 254 nm), t_1 = 19.18 min (minor), t_2 = 33.13 min (major), ee = 90%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 1.6 Hz, 1H), 7.88 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.71 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.61 – 7.53 (m, 1H), 7.50 – 7.44 (m, 2H), 7.38 – 7.28 (m, 3H), 7.20 (d, *J* = 8.1 Hz, 1H), 7.12 – 6.95 (m, 2H), 5.65 – 5.50 (m, 1.08H), 5.26 – 5.10 (m, 1.08H), 4.29 (dd, *J* = 10.4, 3.7 Hz, 0.08H), 4.02 (s, 3H), 3.91 (s, 0.24H), 3.68 (dd, *J* = 10.7, 3.7 Hz, 1H), 3.53 (d, *J* = 17.4 Hz, 0.08H), 3.38 – 3.26 (m, 1.08H), 3.13 (d, *J* = 17.7 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.2, 165.1, 159.7, 147.4, 138.6, 136.0, 135.5, 135.2, 133.1, 129.5, 129.1, 128.7, 128.0, 127.9, 122.2, 120.6, 117.6, 112.2, 85.2, 76.0, 55.9, 47.8, 37.0. **HRMS** (ESI): m/z [M + Na]$^+$ calcd for $[C_{25}H_{20}BrNaNO_6]^+$: 532.0362, found: 532.0362, 534.0340.

(R)-6-chloro-2-((R)-1-(4-methoxyphenyl)-2-nitroethyl)-1-oxo-2,3-dihydro-1H-inden-2-yl 2-methoxybenzoate (3x)

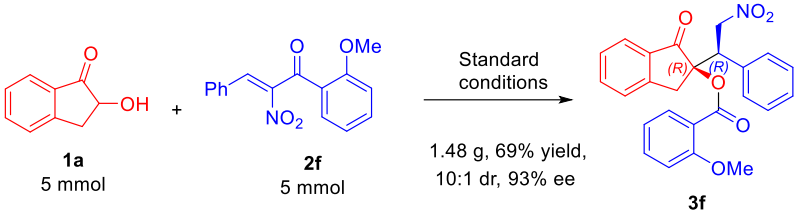


3x

White solid (67.4 mg), 68% yield, 10:1 dr, **mp**. 93.0-93.9 °C; $[\alpha]_D^{20}$ = +23.0 (c = 0.97, in THF); **HPLC**: Chiralpak IF column (hexane/i-PrOH = 90/10, flow rate 1.0 mL/min^{-1}, λ = 254 nm), t_1 = 46.41 min (minor), t_2 = 50.02 min (major), ee = 86%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 – 7.84 (m, 1H), 7.82 (d,

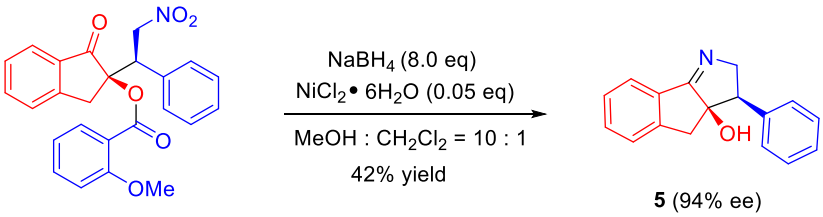
J = 1.9 Hz, 1H), 7.60 – 7.50 (m, 2H), 7.39 (d, J = 8.6 Hz, 2H), 7.33 – 7.22 (m, 1H), 7.12 – 6.93 (m, 2H), 6.85 (d, J = 8.8 Hz, 2H), 5.56 – 5.44 (m, 1H), 5.23 – 5.10 (m, 1H), 4.03 (s, 3H), 3.78 (s, 3H), 3.69 – 3.56 (m, 1H), 3.34 (d, J = 17.6 Hz, 1H), 3.16 (d, J = 17.7 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.4, 165.1, 159.7, 159.7, 147.0, 135.8, 135.3, 135.1, 134.4, 133.1, 130.6, 127.8, 127.5, 124.9, 120.6, 117.6, 114.4, 112.2, 85.5, 76.2, 55.9, 55.3, 47.2, 37.0. **HRMS** (ESI): m/z $[M + Na]^+$ calcd for $[C_{26}H_{22}ClNaNO_7]^+$: 518.0977, found: 518.0977.

Gram-scale reaction



Under a nitrogen atmosphere, a solution of diethylzinc (500 μL, 1.0 M in hexane, 0.5 mmol) was added dropwise to a solution of **L4** (0.25 mmol, 247 mg) in MeCN (15 mL). After the mixture was stirred for 30 min at 30 °C, α-hydroxy-1-indanone **1a** (5 mmol, 0.74g) and (Z)-2-nitro-1,3-diphenylprop-2-en-1-one **2f** (5 mmol, 1.41g) were added. The reaction mixture was stirred for 48 h at the same temperature. The reaction was quenched with NH_4Cl solution (25 mL), and the organic layer was extracted with CH_2Cl_2 (3 × 15 mL). The combined organic layer was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure by using a rotary evaporator. The residue was purified by flash chromatography with petroleum ether/ethyl acetate (4:1) to afford the desired product **3f** (1.48 g) as a white solid.

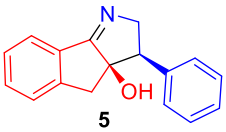
Derivatization



3f (93% ee) **5** (94% ee)

Synthesis of **5**: Compound **3f** (0.2 mmol, 86.2 mg) and $NiCl_2{\cdot}6H_2O$ (0.01 mmol, 2.5 mg) were added to a mixture of 1 mL MeOH/ CH_2Cl_2 (10:1), and $NaBH_4$ (1.6 mmol, 60.2 mg) was added in portions, then the mixture was stirred at rt for 12 h. The reaction was quenched with water, and extracted with CH_2Cl_2 (3 × 5 mL). The organic layers were dried over Na_2SO_4 and concentrated. Then the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give the product **5** as a white solid.

(3*R*,3a*R*)-3-phenyl-2,4-dihydroindeno[1,2-b]pyrrol-3a(3H)-ol (4)



5

White solid (21.3 mg), 42% yield, **mp**. 216.0-216.9 °C; $[\alpha]_D^{20}$ = +169.0 (c = 1.05, in THF); **HPLC**: Chiralpak IF column (hexane/i-PrOH = 7/3, flow rate 1.0 mL/min^{-1}, λ = 254 nm), t_1 = 11.13 min (major), t_2 = 14.86 min (minor), ee = 94%; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.7 Hz, 1H),

7.52 – 7.40 (m, 4H), 7.38 – 7.31 (m, 1H), 7.25 – 7.16 (m, 2H), 6.89 (t, *J* = 7.1 Hz, 1H), 5.80 (s, 1H), 5.38 (dd, *J* = 13.1, 10.4 Hz, 1H), 4.43 (dd, *J* = 13.1, 7.7 Hz, 1H), 3.93 (dd, *J* = 10.0, 7.9 Hz, 1H), 3.20 (d, *J* = 16.2 Hz, 1H), 3.09 (d, *J* = 16.2 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.1, 149.0, 134.2, 131.6, 128.8, 128.7, 127.9, 127.3, 127.3, 126.0, 86.8, 70.9, 51.5, 42.6. **HRMS** (ESI): m/z $[M + H]^+$ calcd for $[C_{17}H_{16}NO]^+$: 250.1226, found: 250.1229.

References

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2. Trost BM, Ito H. A Direct Catalytic Enantioselective Aldol Reaction via a Novel Catalyst Design. *J Am Chem Soc* 2000;122:12003–4.
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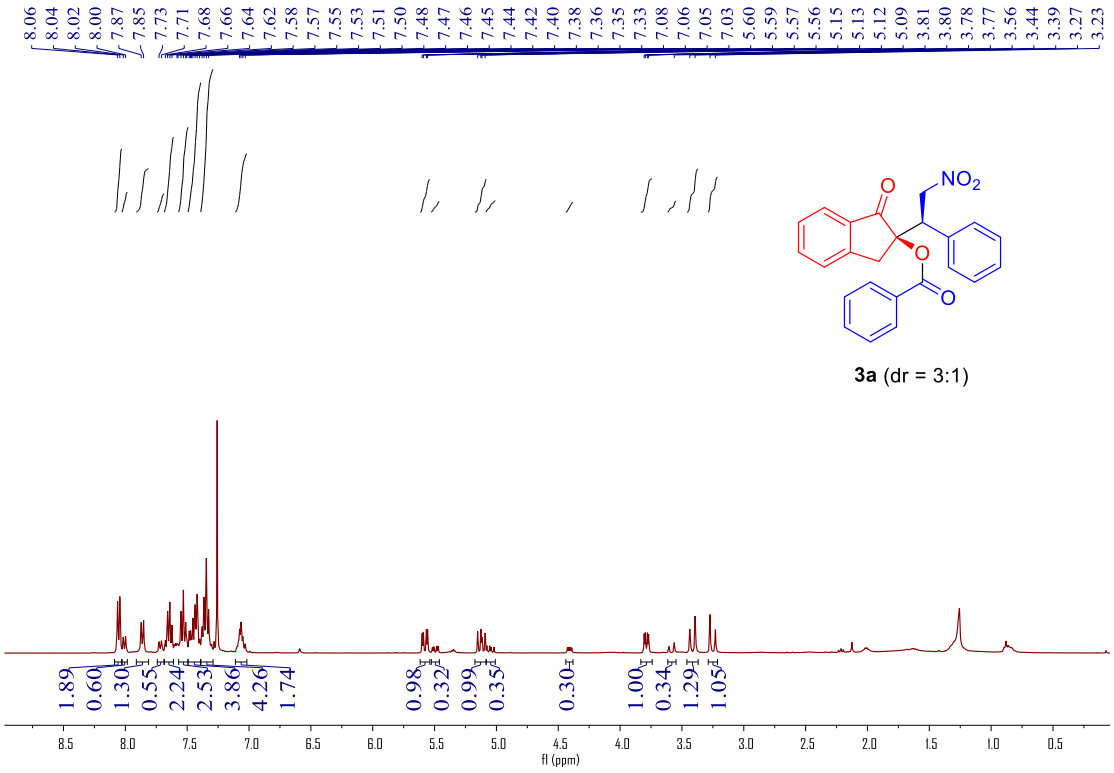
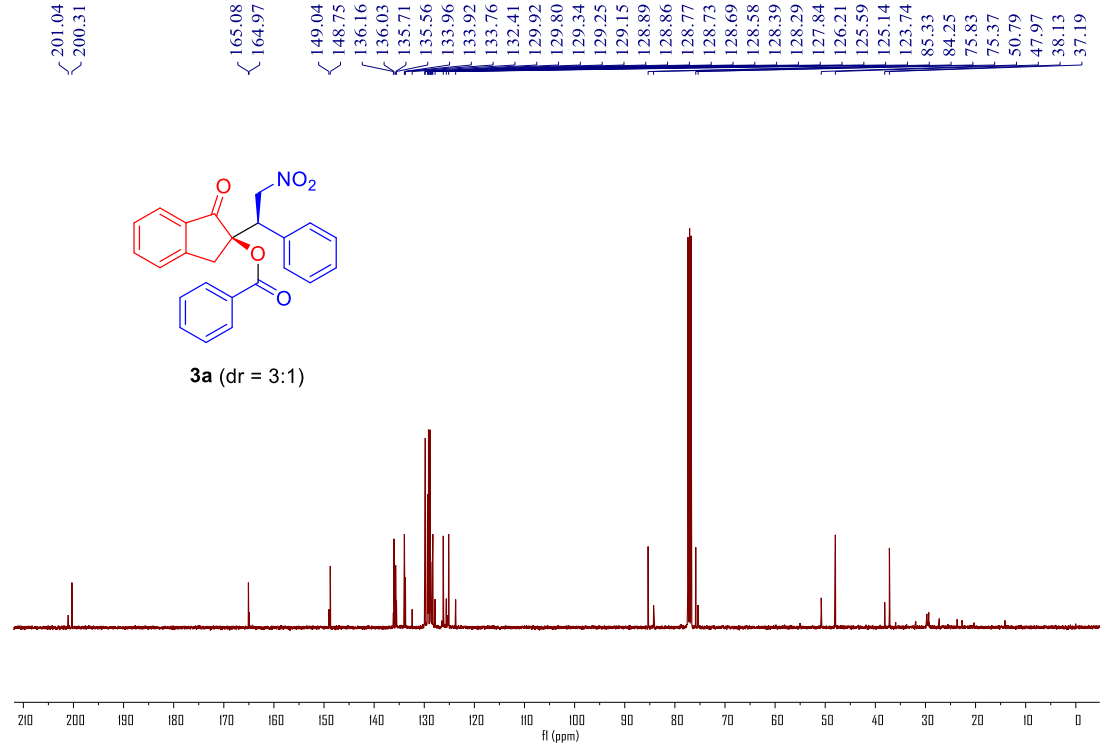
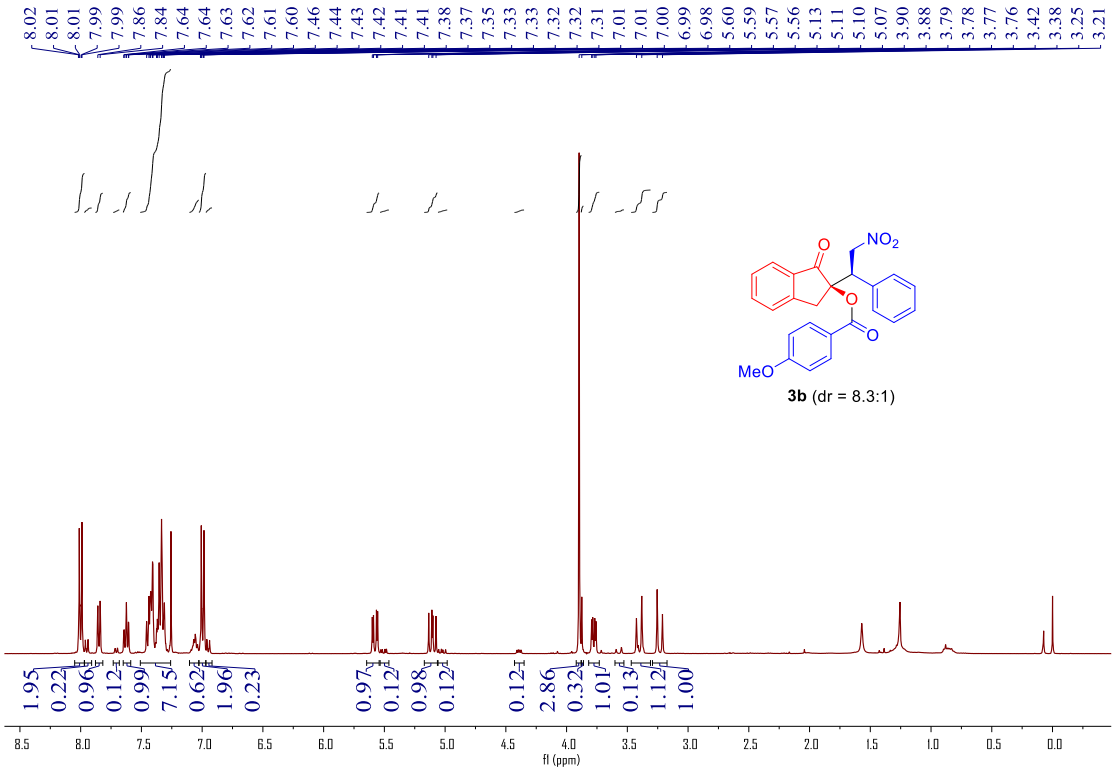
4. Matsuo K, Shindo M. Cu(II)-Catalyzed Acylation by Thiol Esters Under Neutral Conditions: Tandem Acylation-Wittig Reaction Leading to a One-Pot Synthesis of Butenolides. *Org Lett* 2010;12:5346–9.
5. Parida C, Maity R, Chandra Sahoo S, Chandra Pan S. α-Nitro-α,β-Unsaturated Ketones: An Electrophilic Acyl Transfer Reagent in Catalytic Asymmetric Friedel–Crafts and Michael Reactions. *Org Lett* 2019;21:6700-4.

NMR Spectra of compounds



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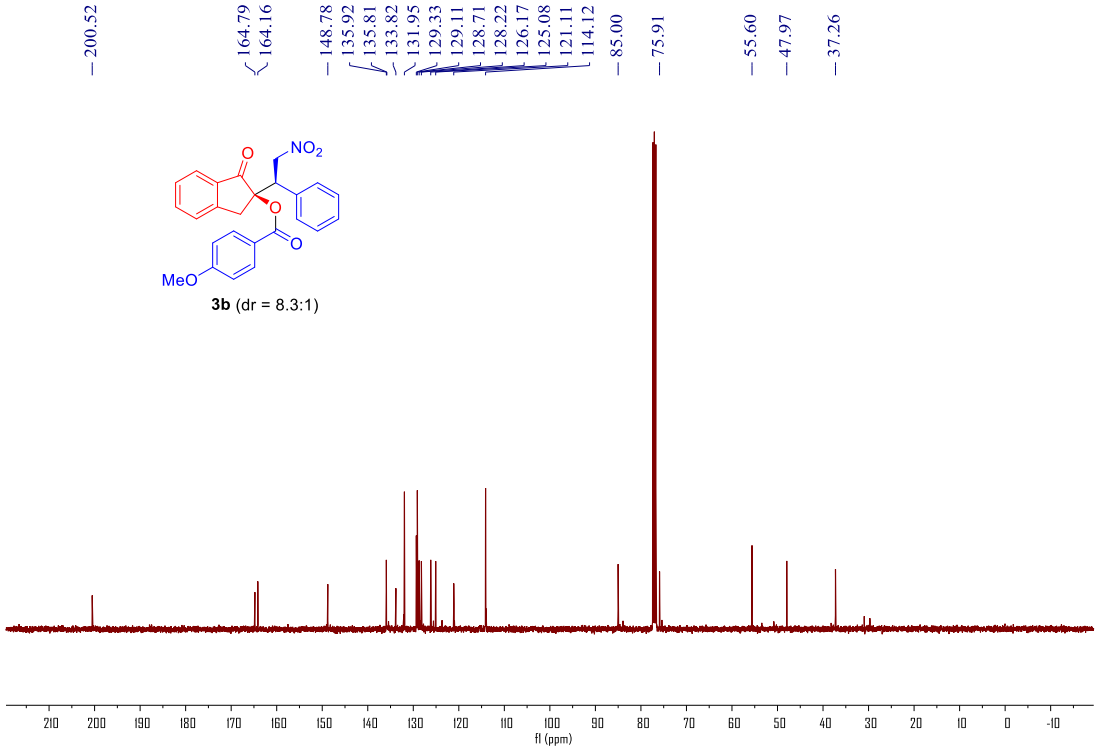
NO2
O
O
O
MeO
3b (dr = 8.3:1)
1.95 0.22 0.96 0.12 0.99 7.15 0.62 1.96 0.23 0.97 0.12 0.98 0.12 0.12 2.86 0.32 1.01 0.13 1.12 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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NO2
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O
O
MeO
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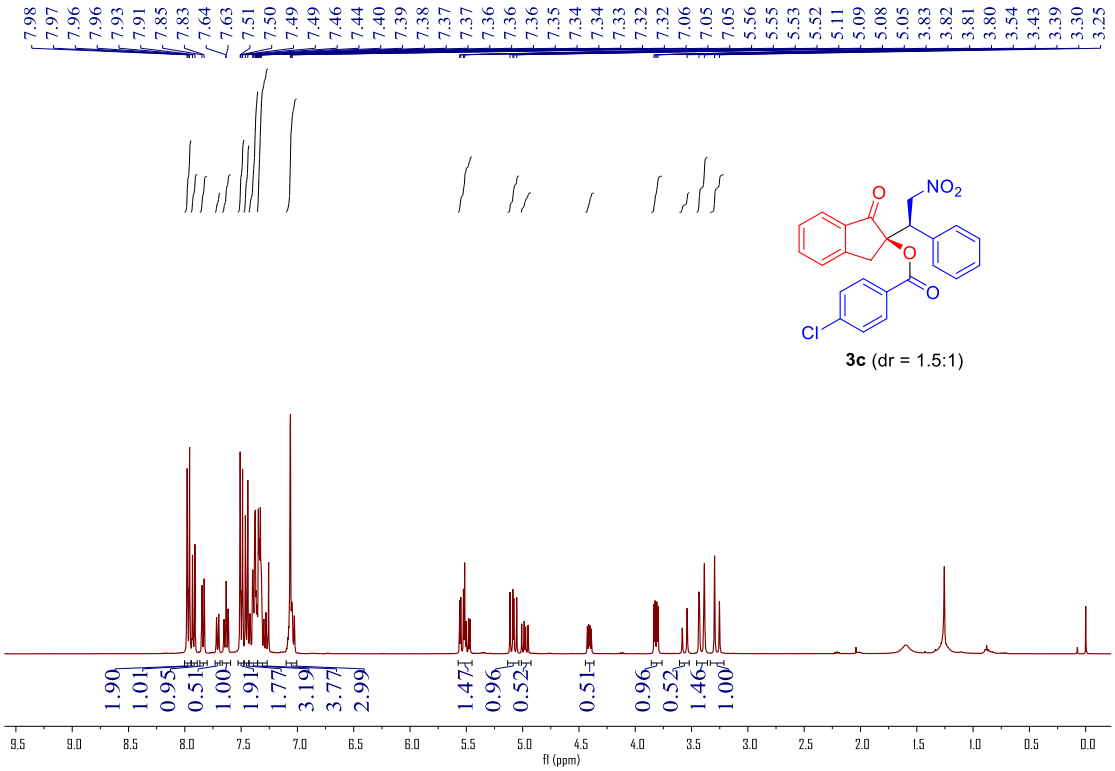
f1 (ppm)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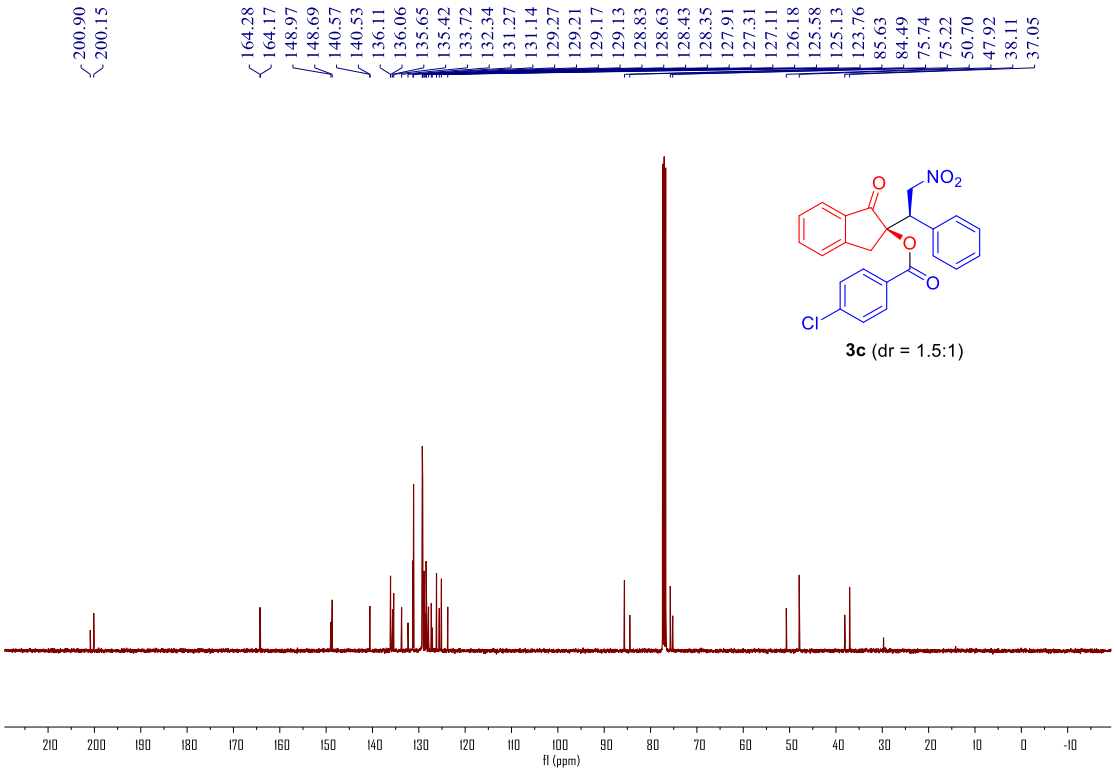
NO2
O
O
O
Cl
3c (dr = 1.5:1)
1.90 1.01 0.95 0.51 1.00 1.91 1.77 3.19 3.77 2.99 1.47 0.96 0.52 0.51 0.96 0.52 1.46 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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NO2
O
O
O
Cl
3c (dr = 1.5:1)
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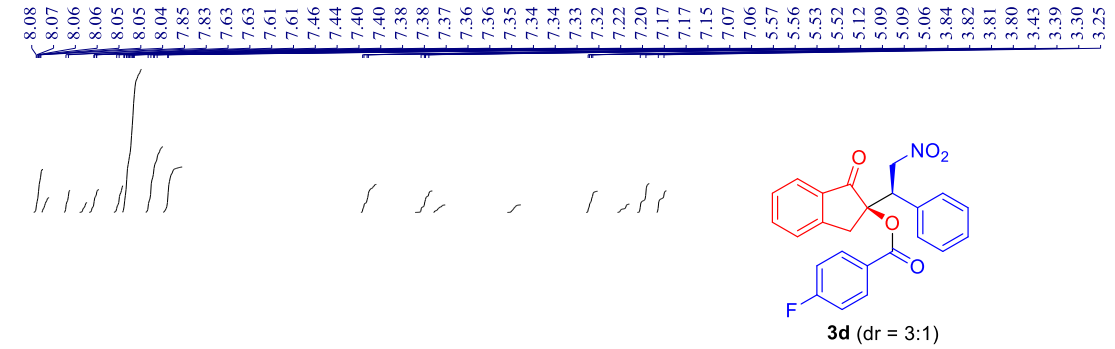
f1 (ppm)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O
NO2
O
O
F
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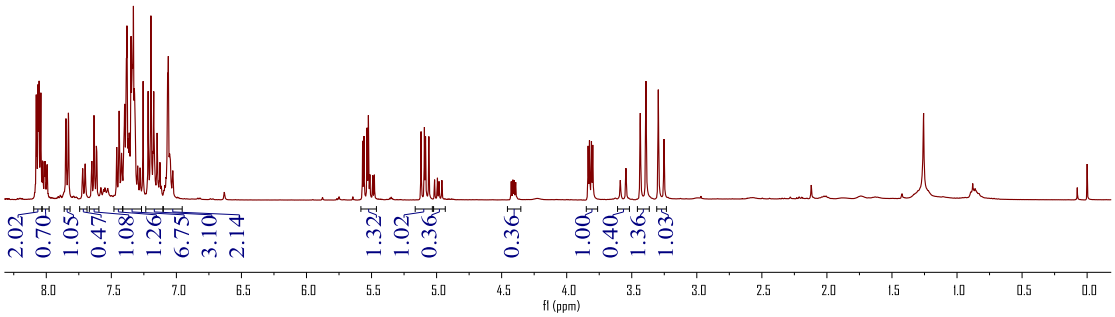
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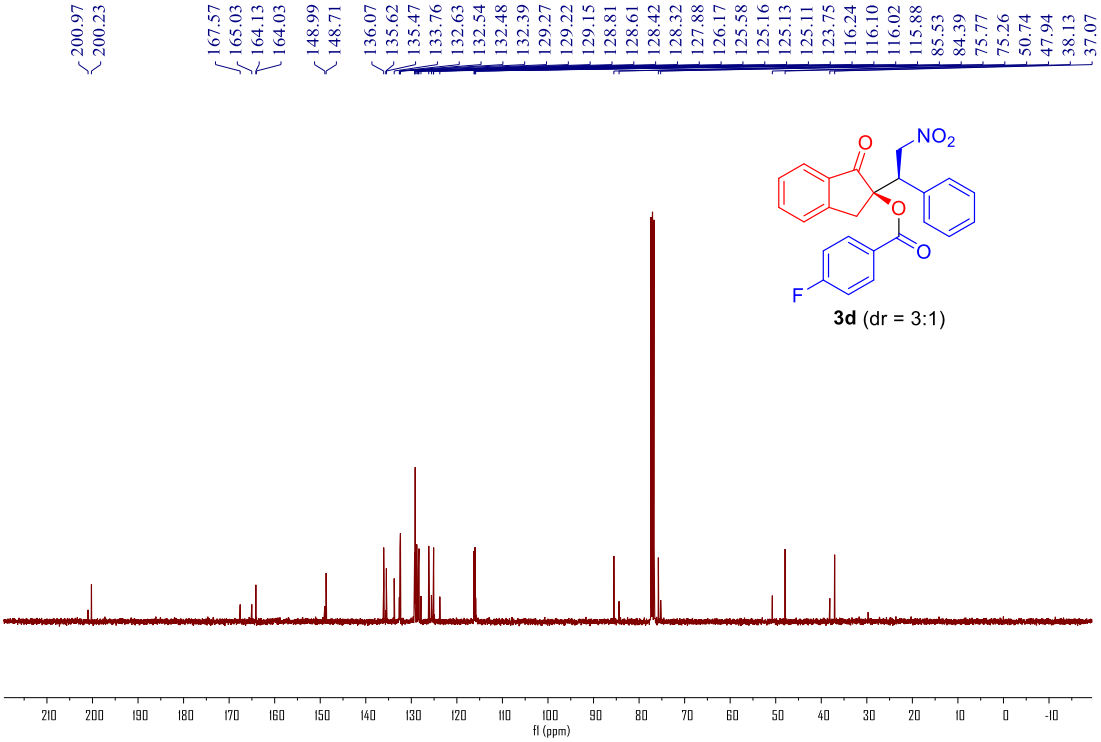
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


200.97 200.23 167.57 165.03 164.13 164.03 148.99 148.71 136.07 135.62 135.47 133.76 132.63 132.54 132.48 132.39 129.27 129.22 129.15 128.81 128.61 128.42 128.32 127.88 126.17 125.58 125.16 125.13 125.11 123.75 116.24 116.10 116.02 115.88 85.53 84.39 75.77 75.26 50.74 47.94 38.13 37.07
O
NO2
O
O
F
3d (dr = 3:1)
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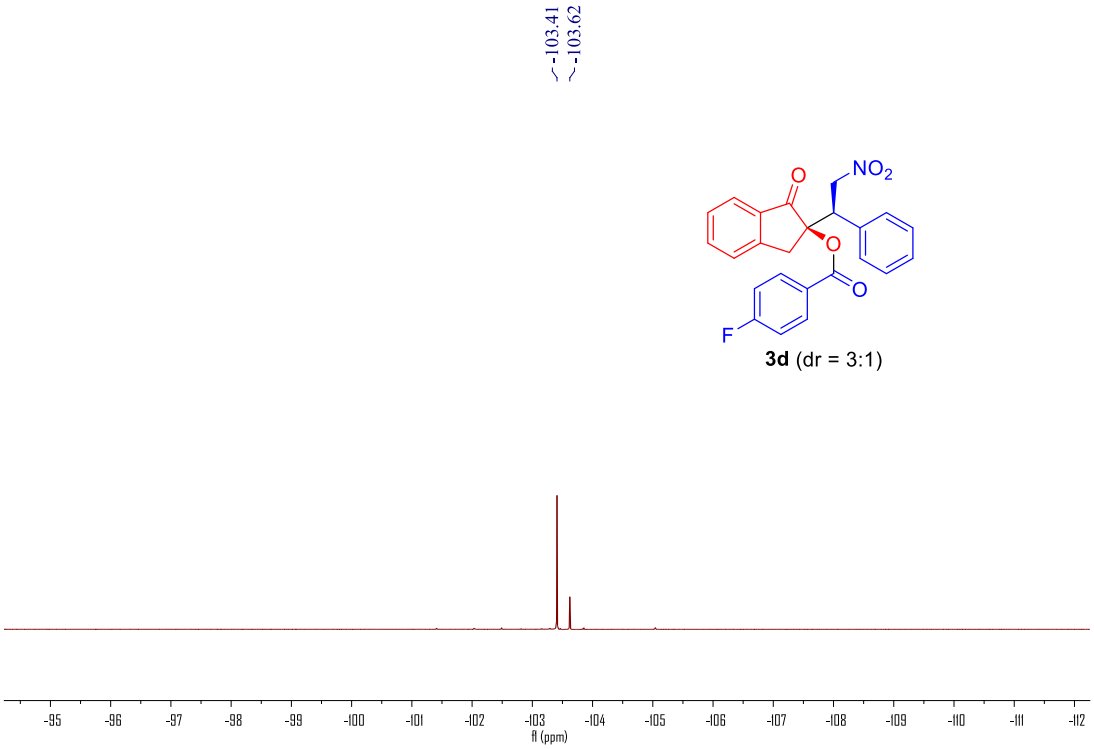
f1 (ppm)


-103.41
-103.62
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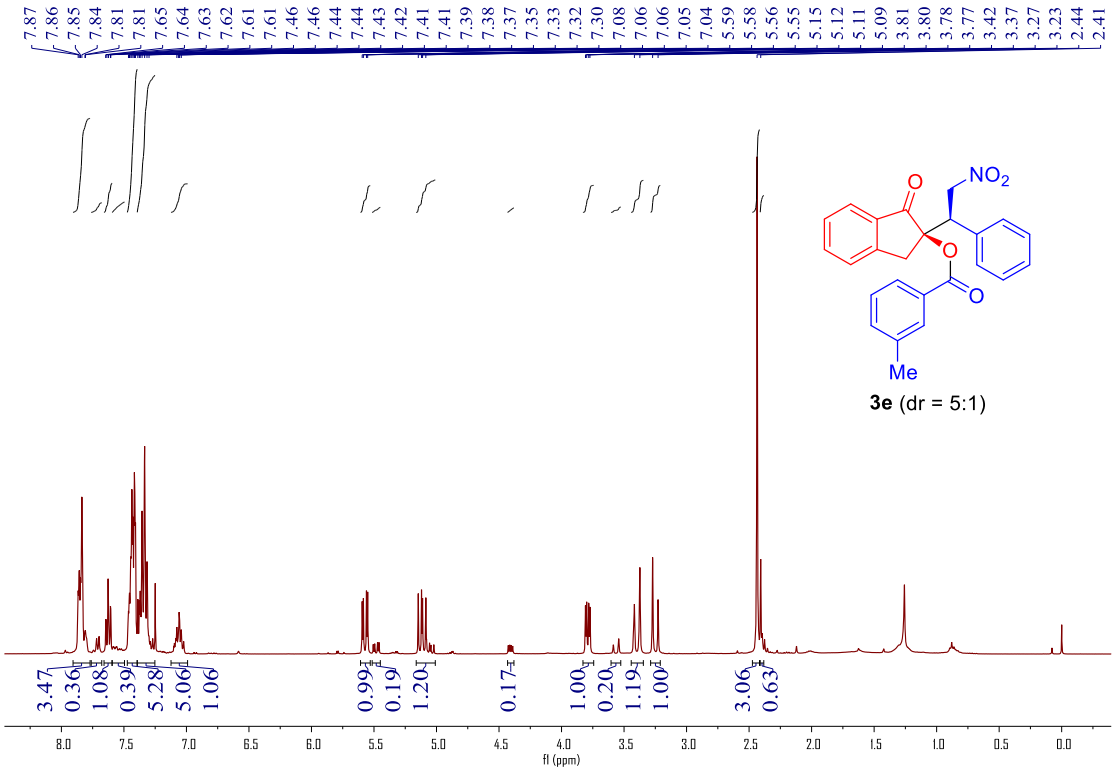
O
O
F
-95
-96
-97
-98
-99
-100
-101
-102
-103
-104
-105
-106
-107
-108
-109
-110
-111
-112
f1 (ppm)

3d (dr = 3:1)



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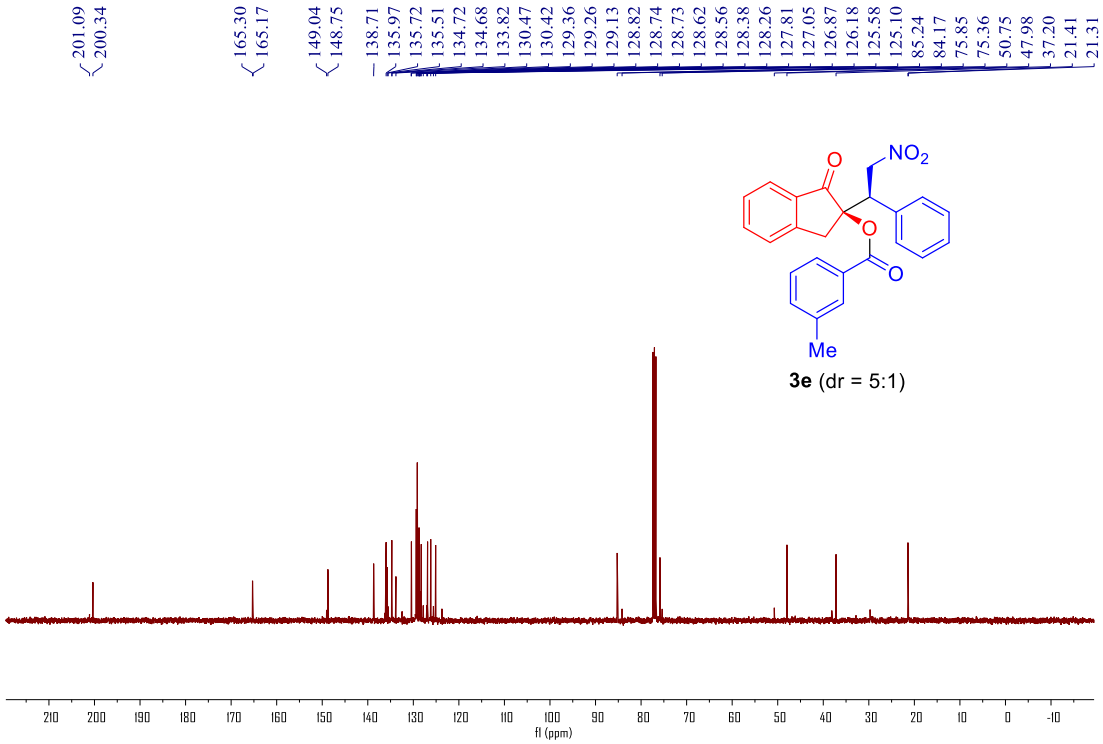

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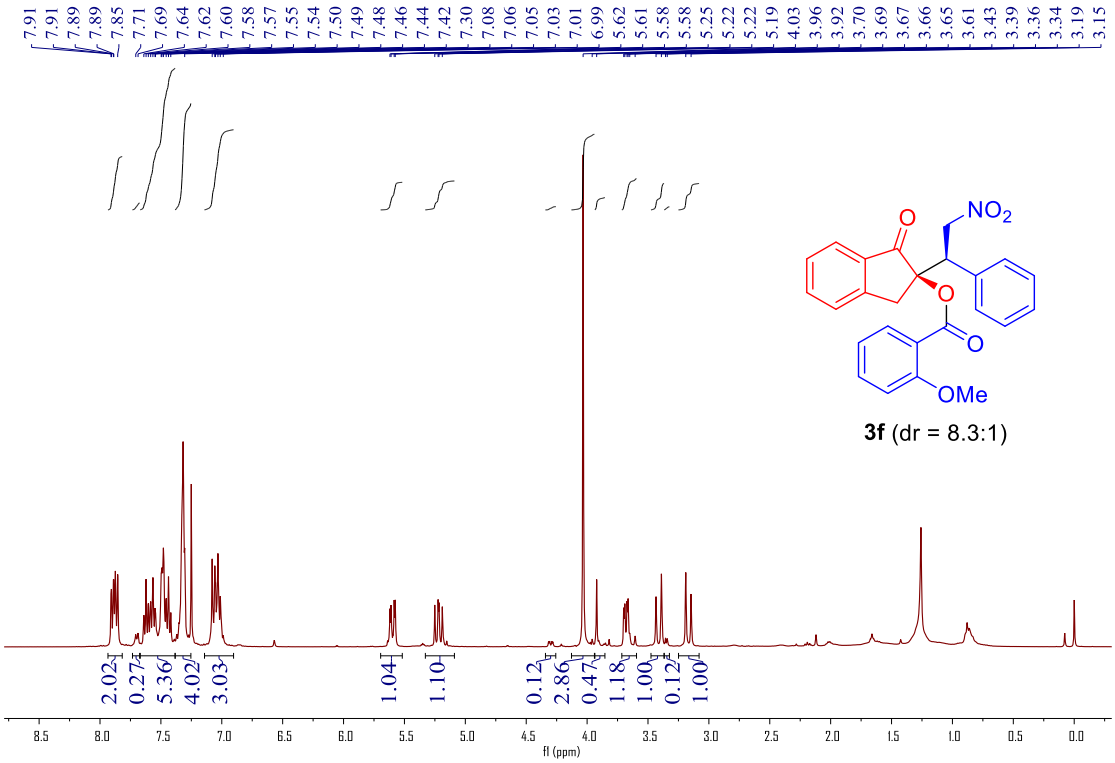

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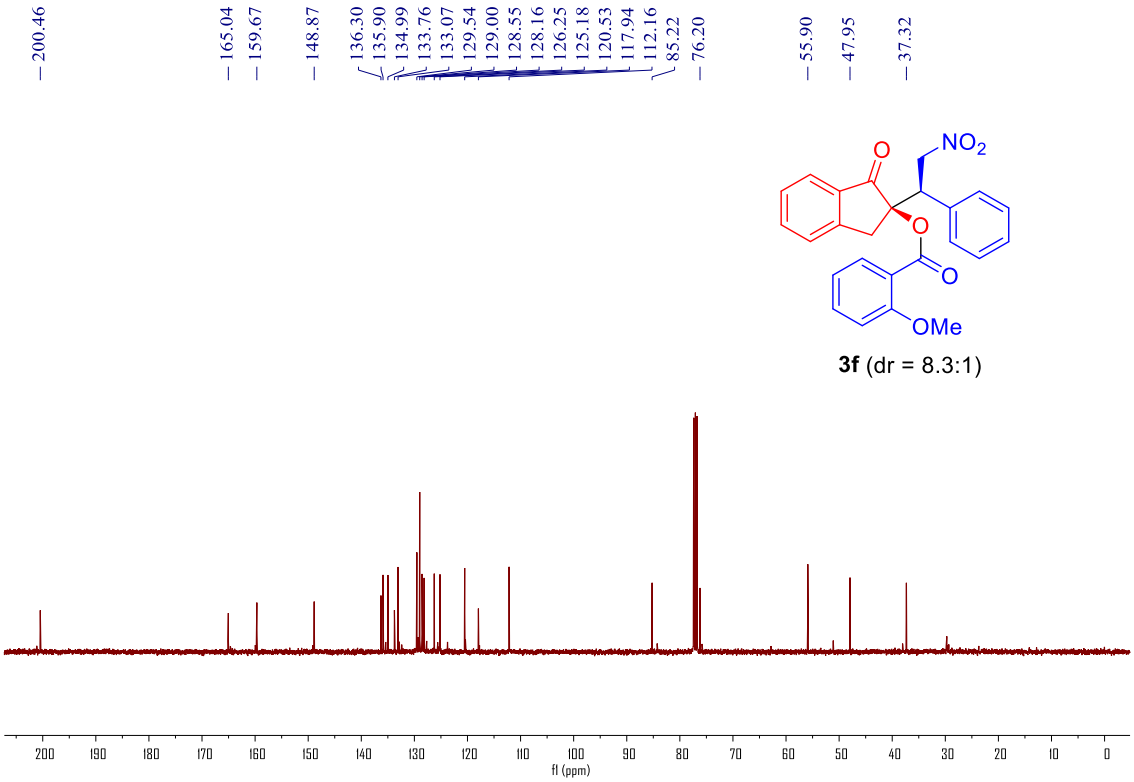

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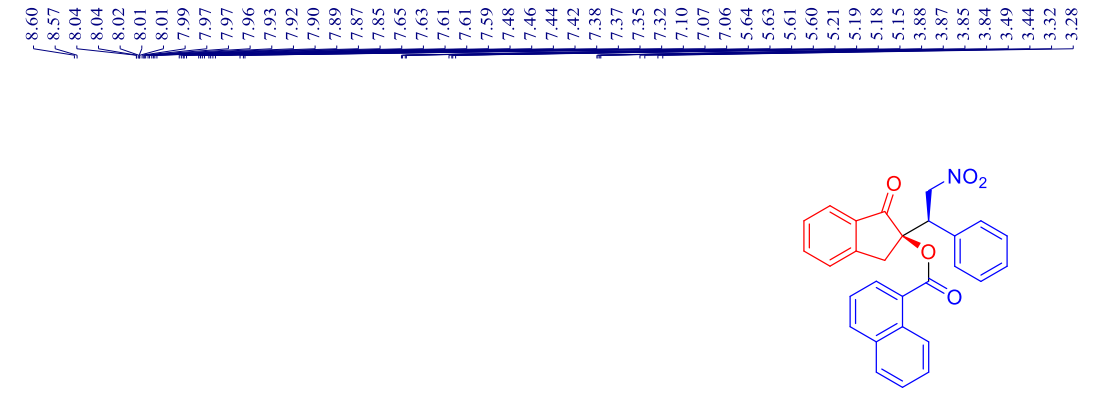
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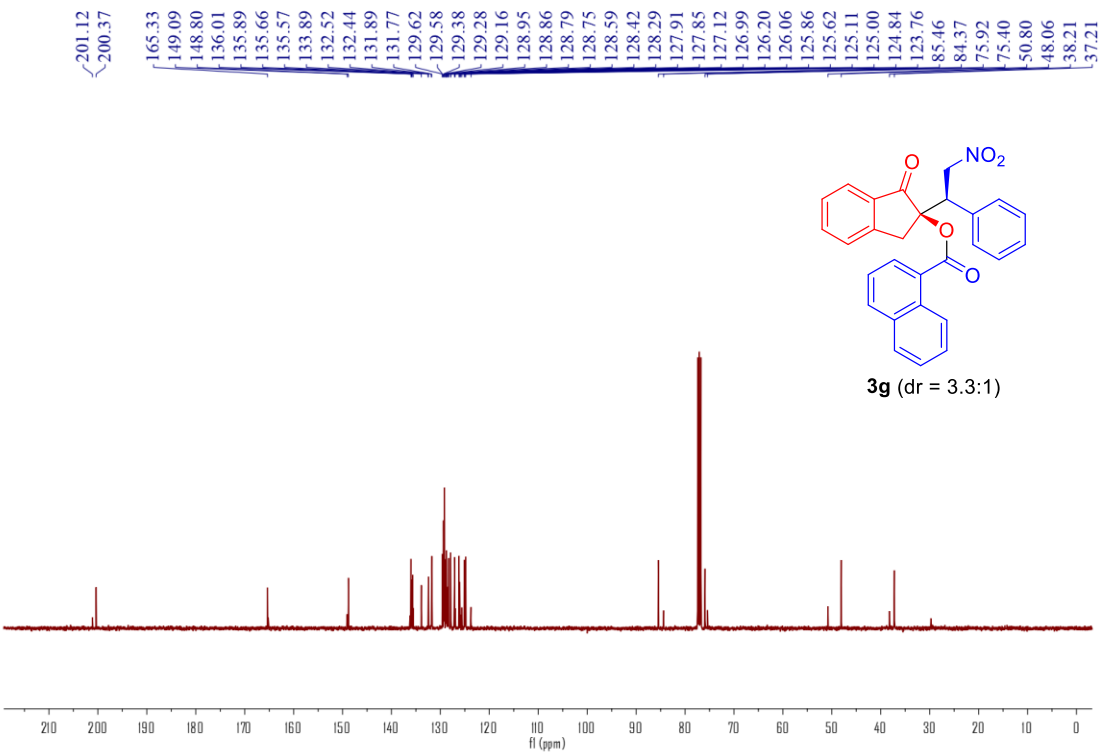
NO2
O
O
O
3g (dr = 3.3:1)
1.25 3.23 3.04 0.29 3.72 3.10 4.69 1.77 1.28 1.00 0.30 0.30 1.00 0.29 1.28 1.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


201.12 200.37 165.33 149.09 148.80 136.01 135.89 135.66 135.57 133.89 132.52 132.44 131.89 131.77 129.62 129.58 129.38 129.28 129.16 128.95 128.86 128.79 128.75 128.59 128.42 128.29 127.91 127.85 127.12 126.99 126.20 126.06 125.86 125.62 125.11 125.00 124.84 123.76 85.46 84.37 75.92 75.40 50.80 48.06 38.21 37.21
NO2
O
O
O
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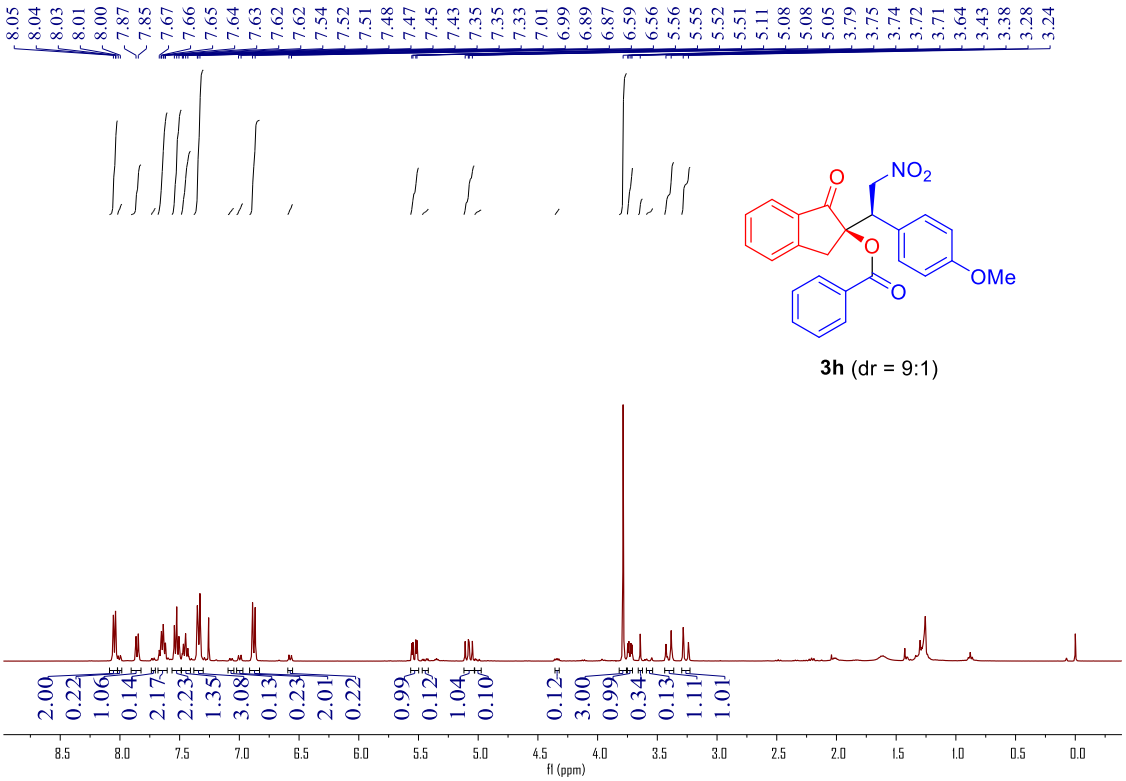
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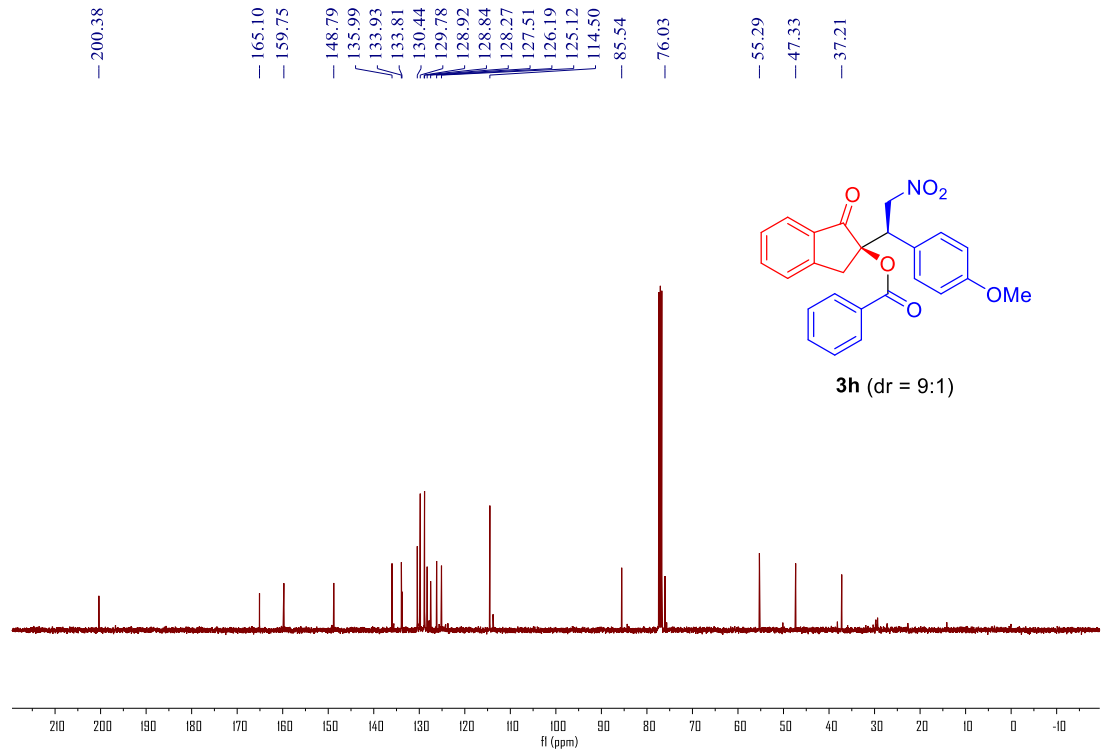
NO2
O
O
O
OMe
3h (dr = 9:1)
2.00 0.22 1.06 0.14 2.17 2.23 1.35 3.08 0.13 0.23 2.01 0.22 0.99 0.12 1.04 0.10 0.12 3.00 0.99 0.34 0.13 1.11 1.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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NO2
O
O
O
OMe
3h (dr = 9:1)
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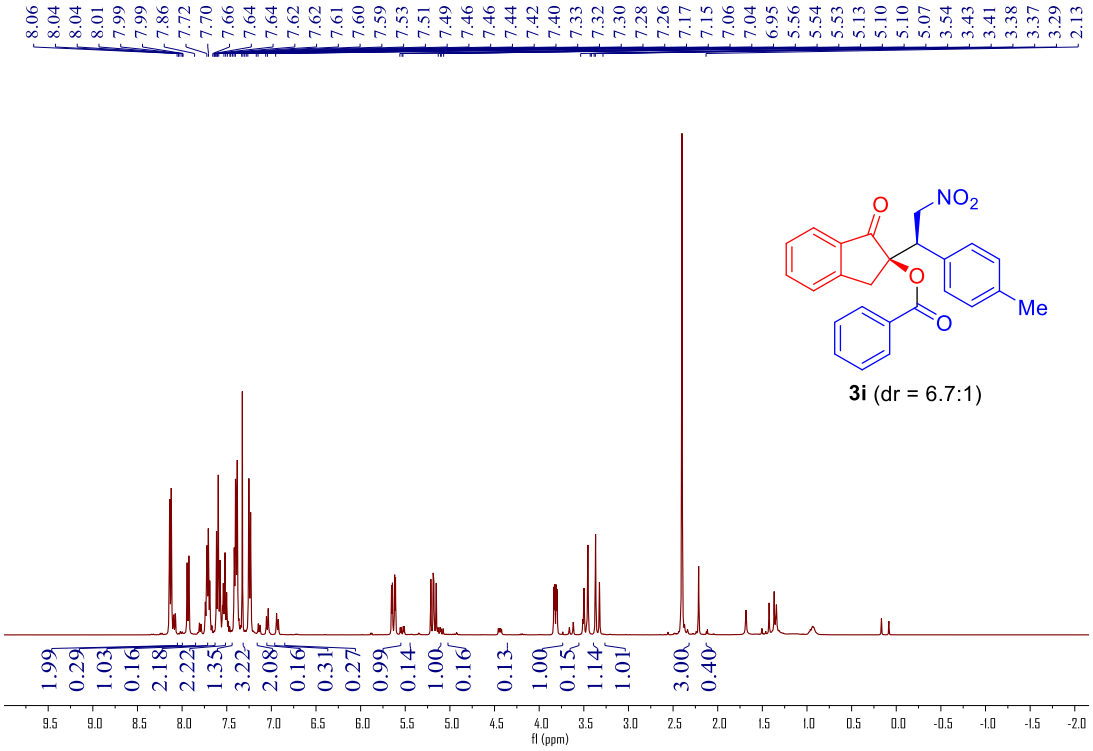
f1 (ppm)



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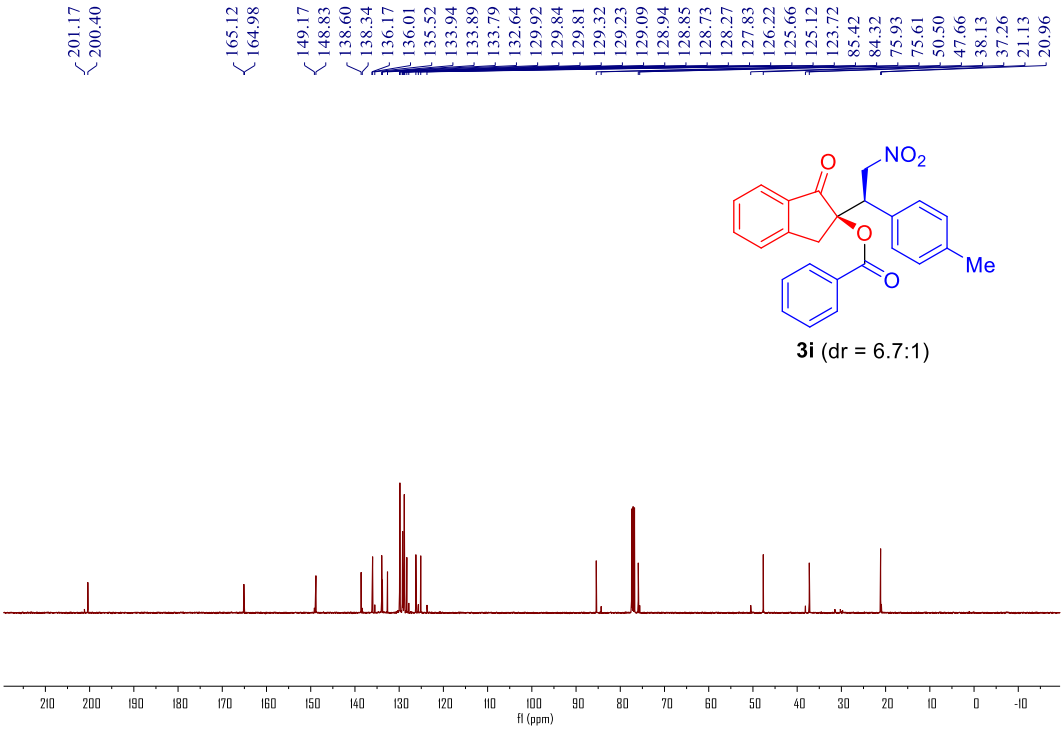

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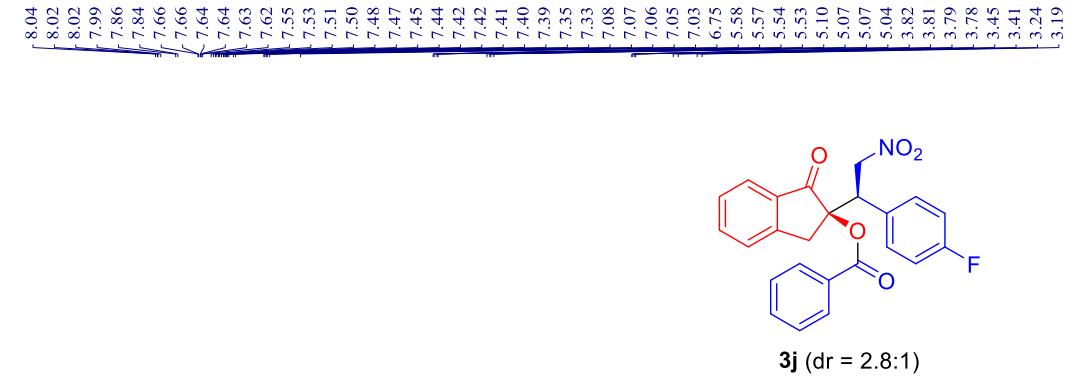

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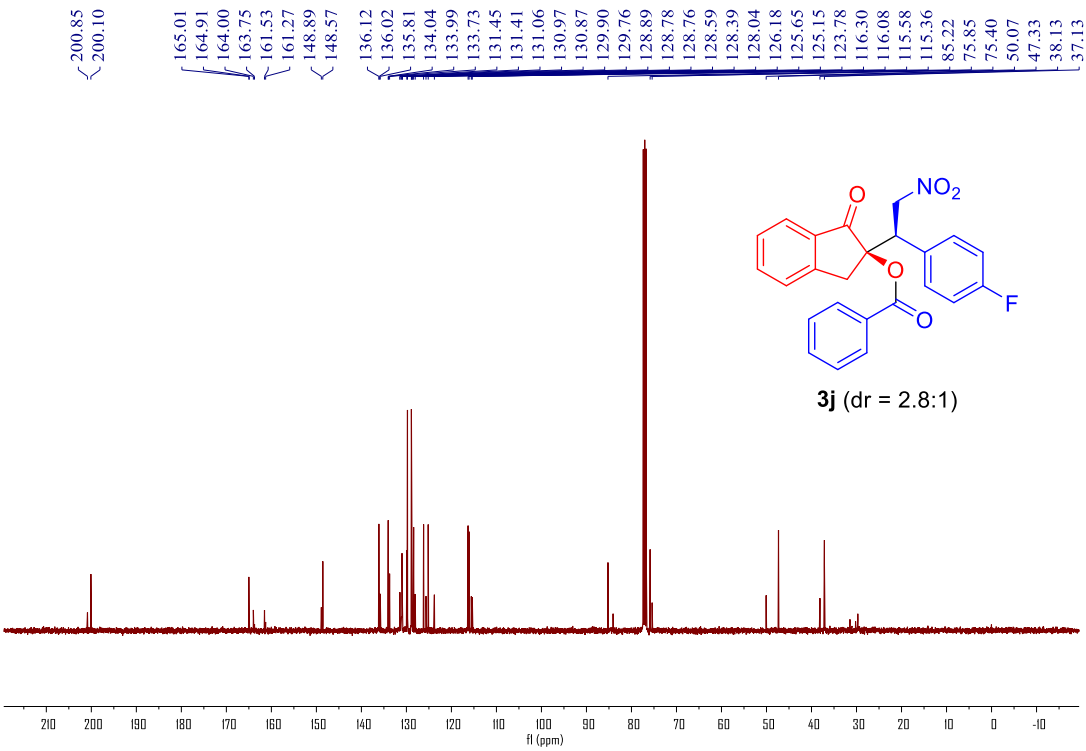
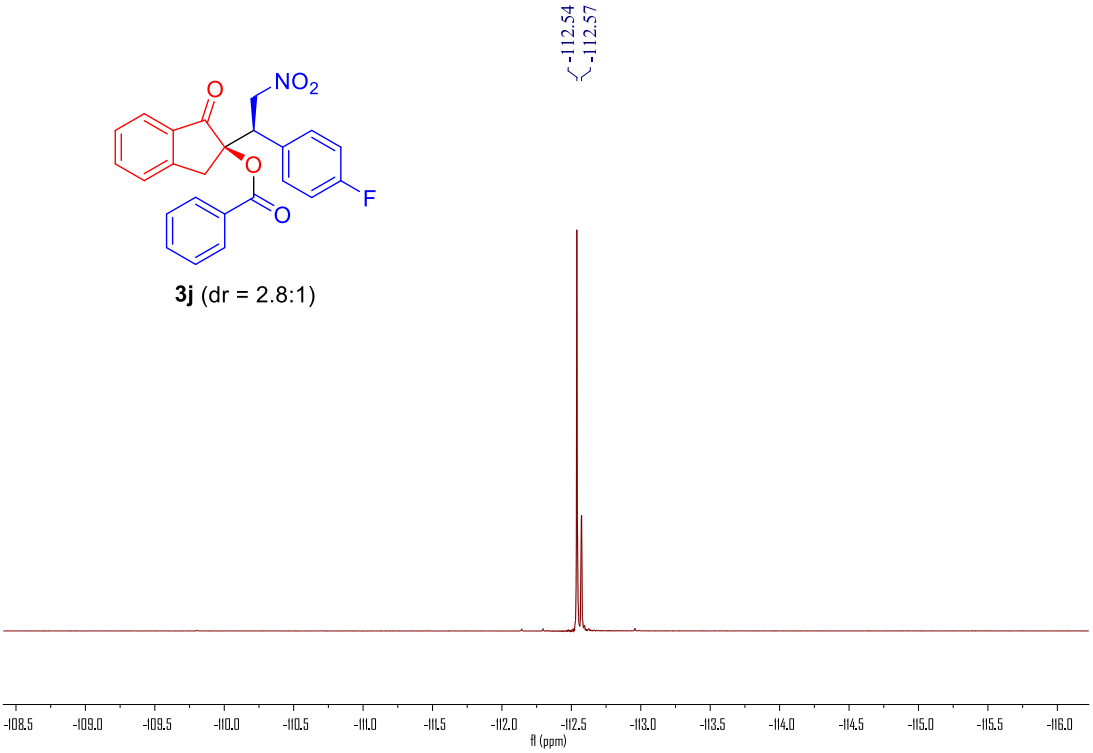


3j (dr = 2.8:1)

O
NO2
O
O
F

3j (dr = 2.8:1)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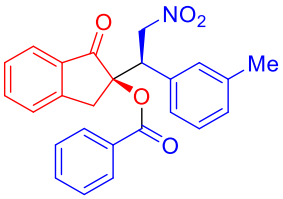
-116.0
f1 (ppm)



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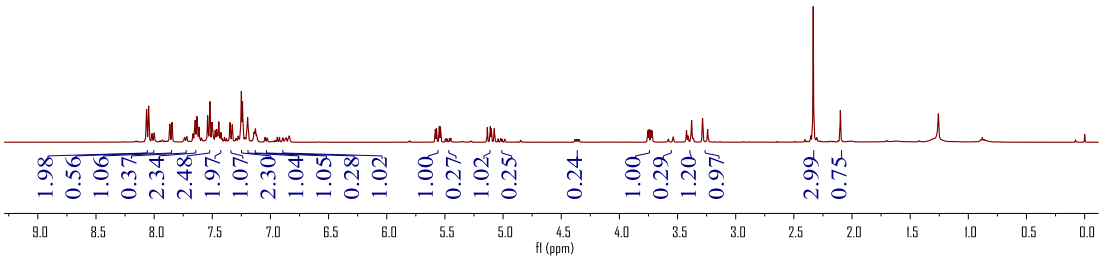

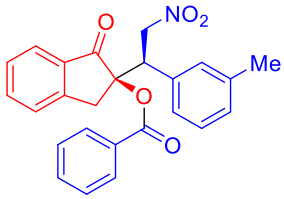

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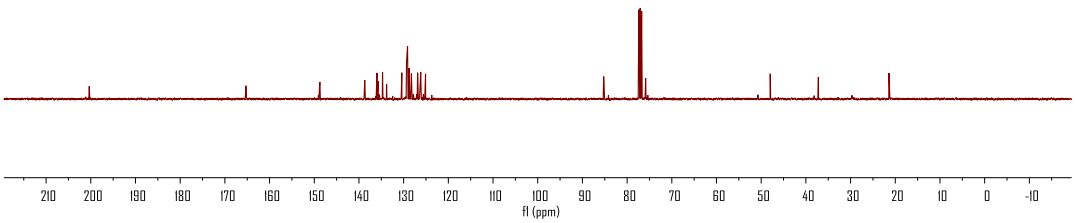

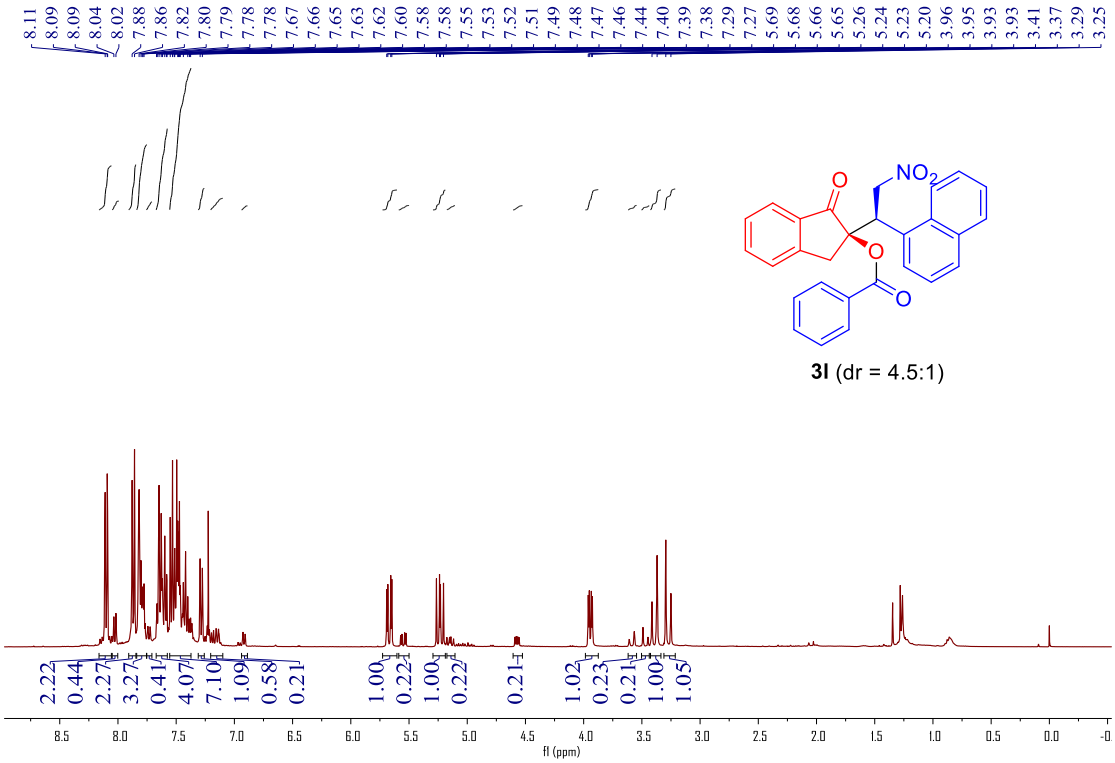
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NO2
O
O
O
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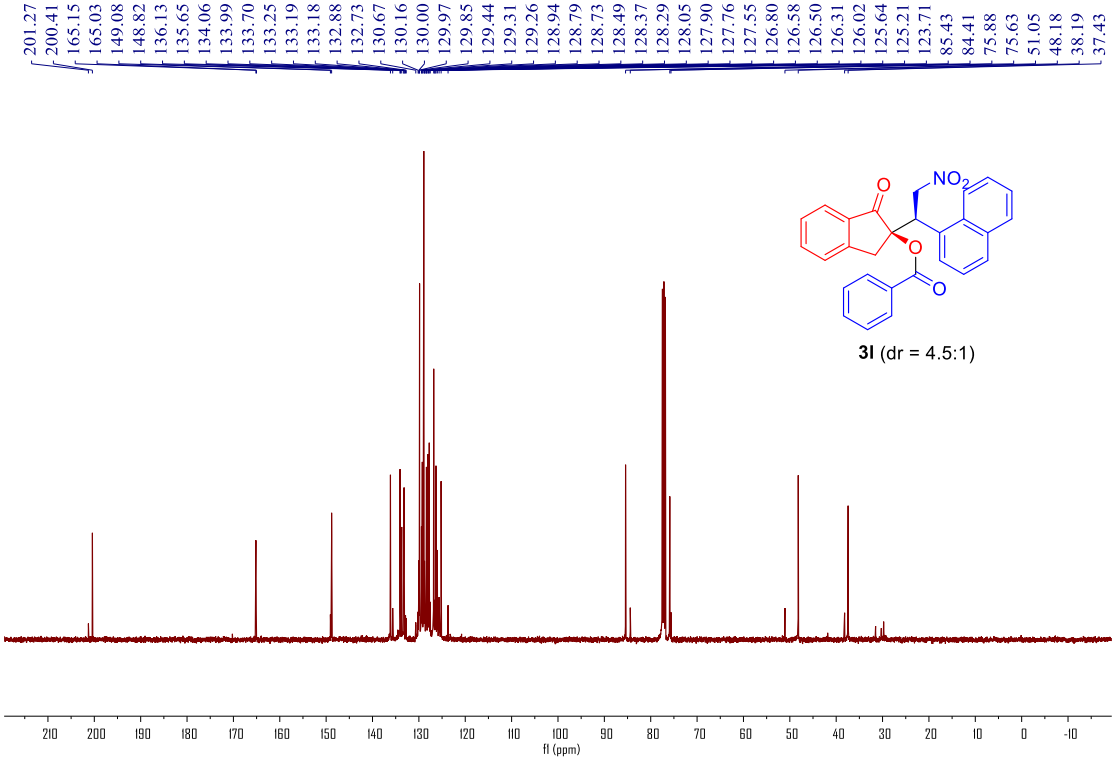
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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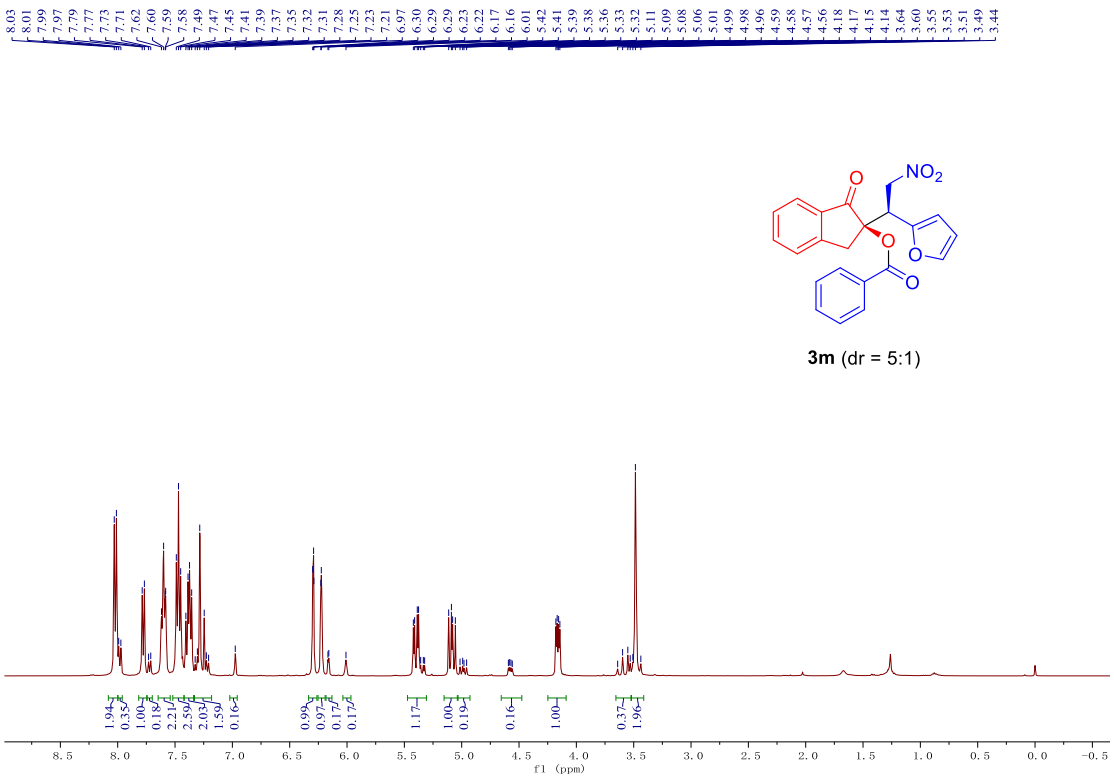
NO2
O
O
O
3l (dr = 4.5:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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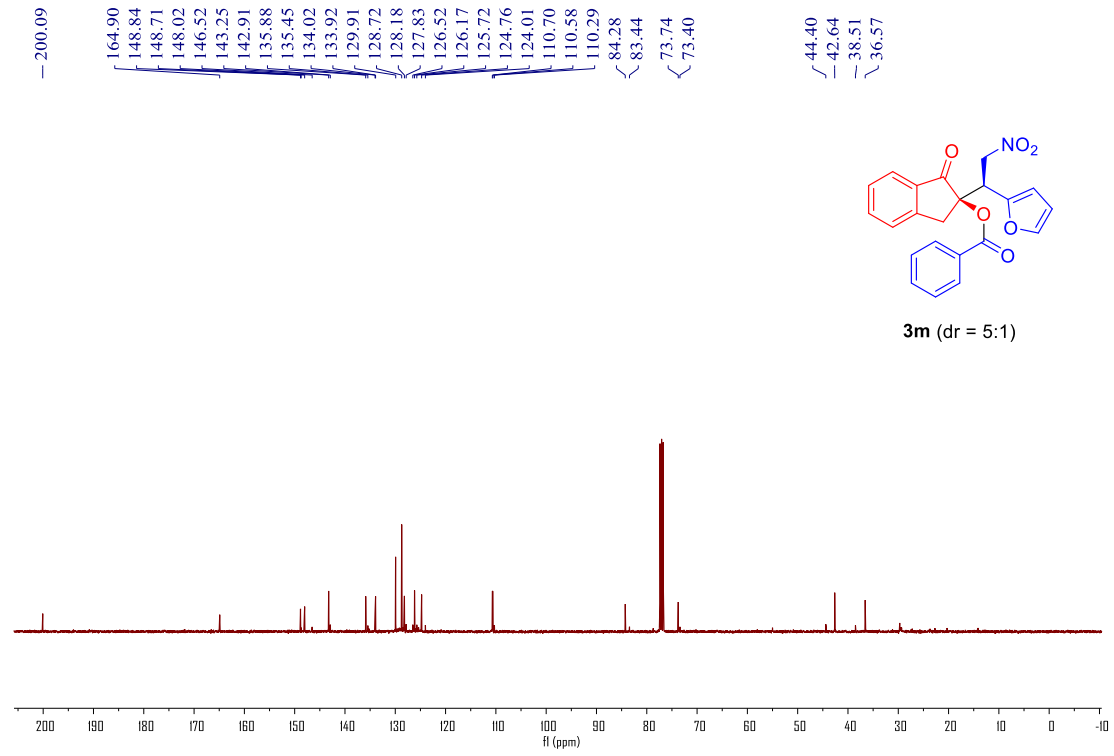
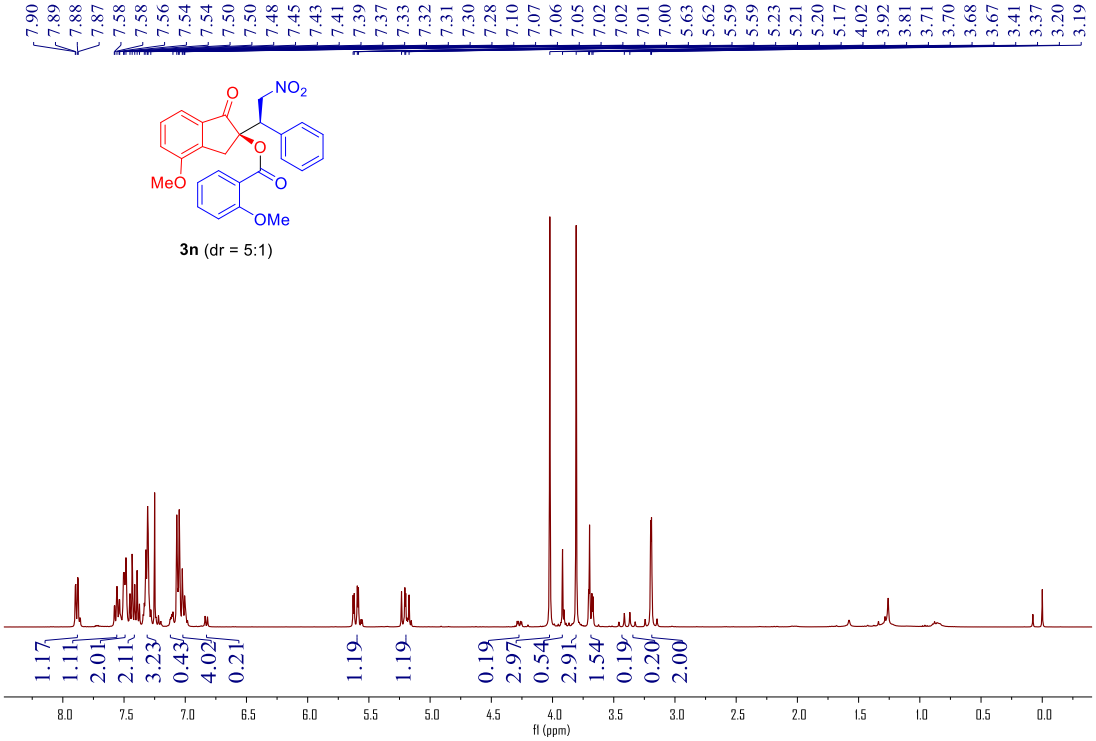
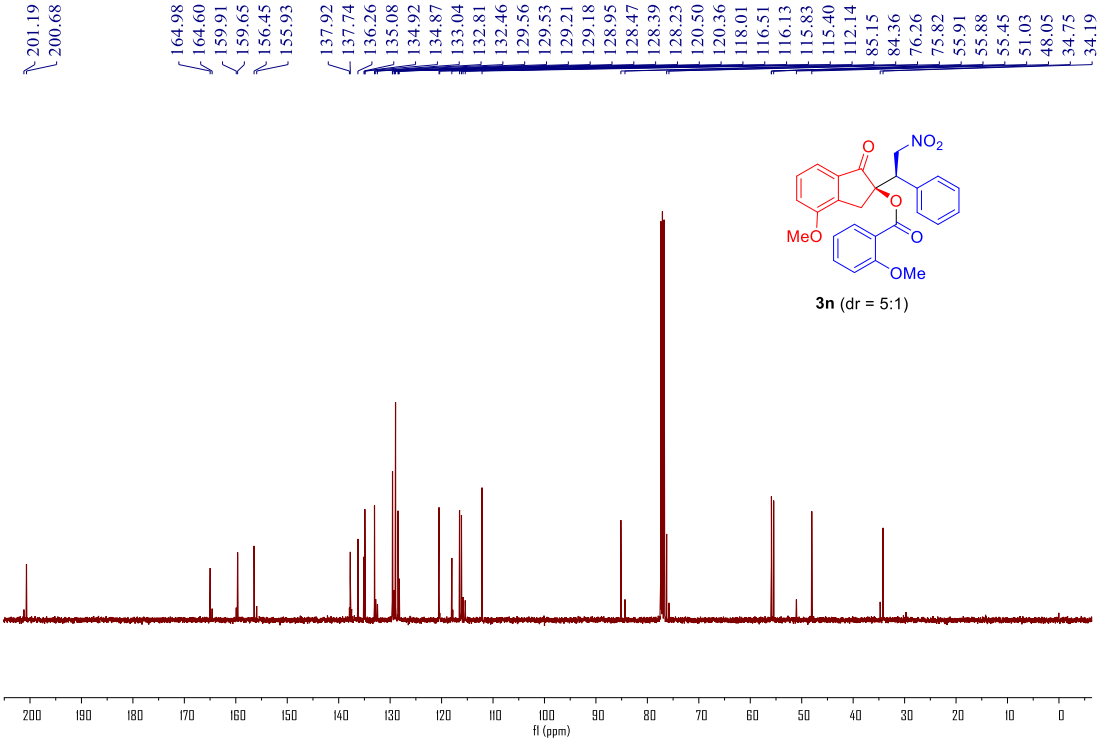
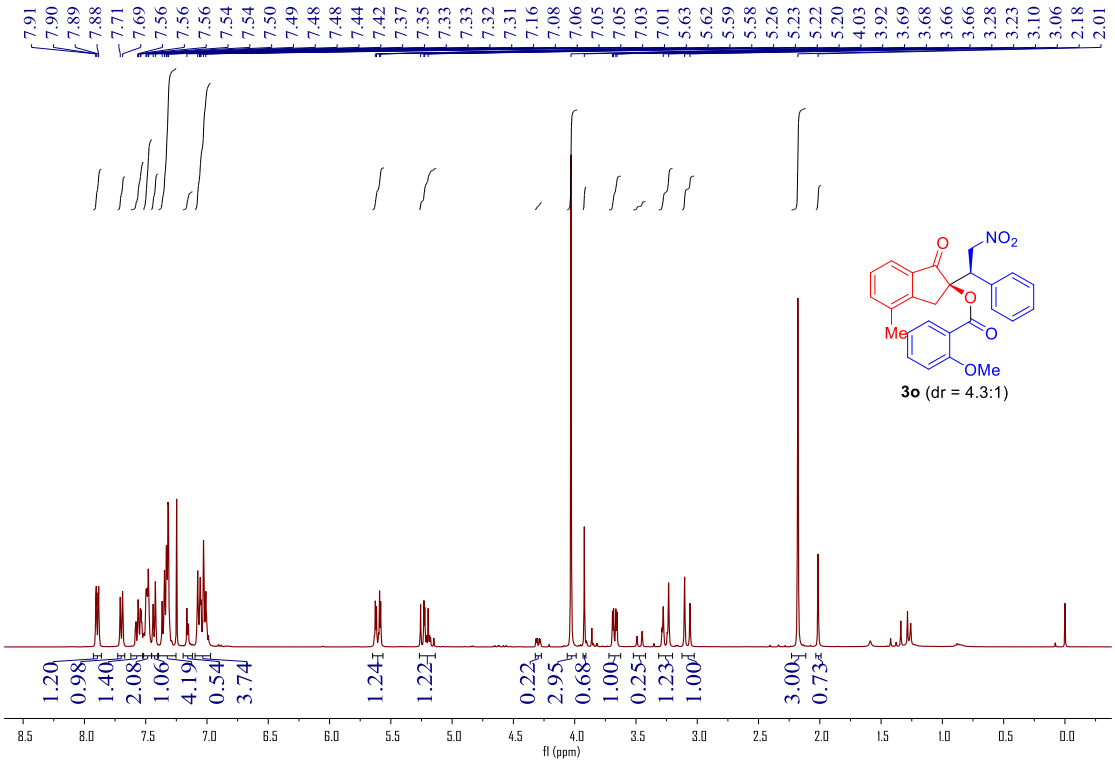
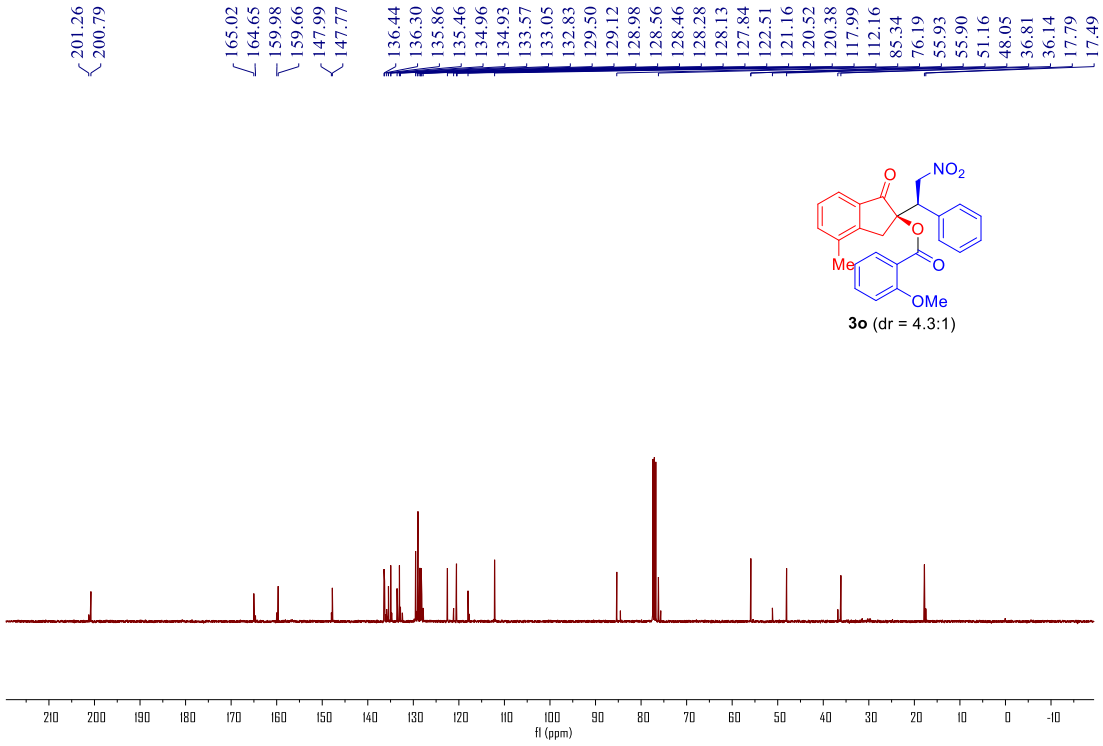
NO2
O
O
O
O
3m (dr = 5:1)
1.94 0.35 1.00 0.18 2.21 2.59 2.03 1.59 0.16 0.99 0.97 0.17 0.17 1.17 1.00 0.19 0.16 1.00 0.37 1.96
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

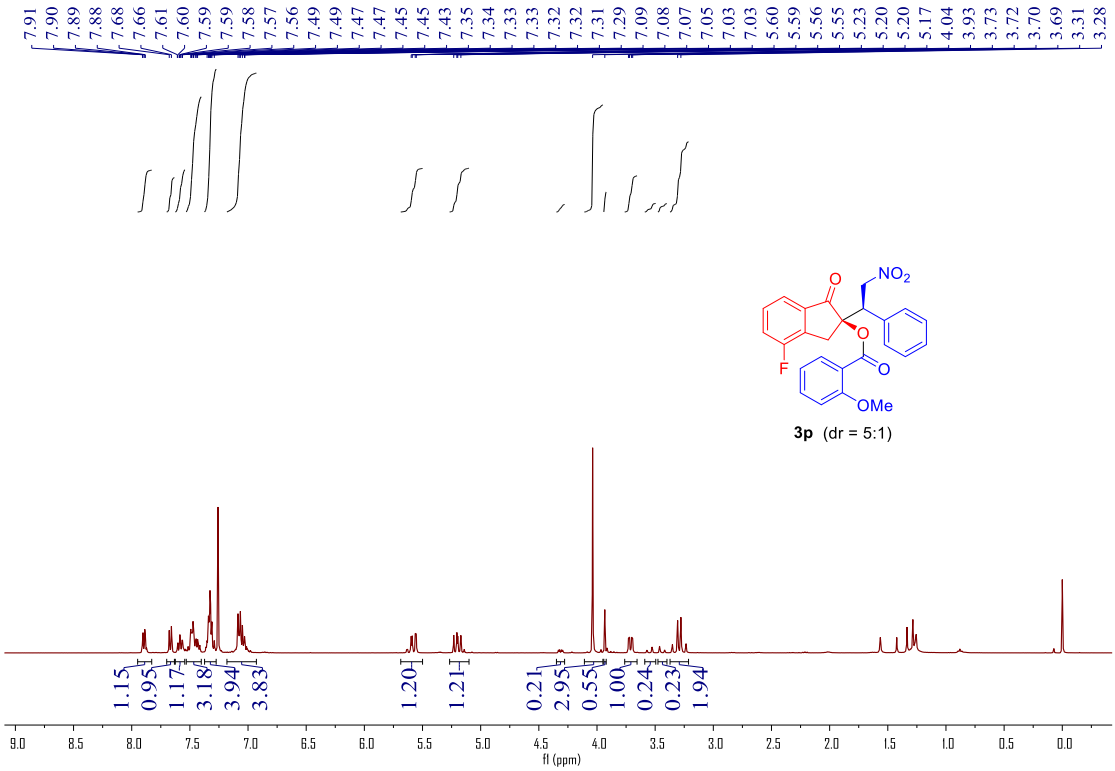

200.09
164.90 148.84 148.71 148.02 146.52 143.25 142.91 135.88 135.45 134.02 133.92 129.91 128.72 128.18 127.83 126.52 126.17 125.72 124.76 124.01 110.70 110.58 110.29
84.28 83.44
73.74 73.40
44.40 42.64 38.51 36.57
NO2
O
O
O
O
3m (dr = 5:1)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

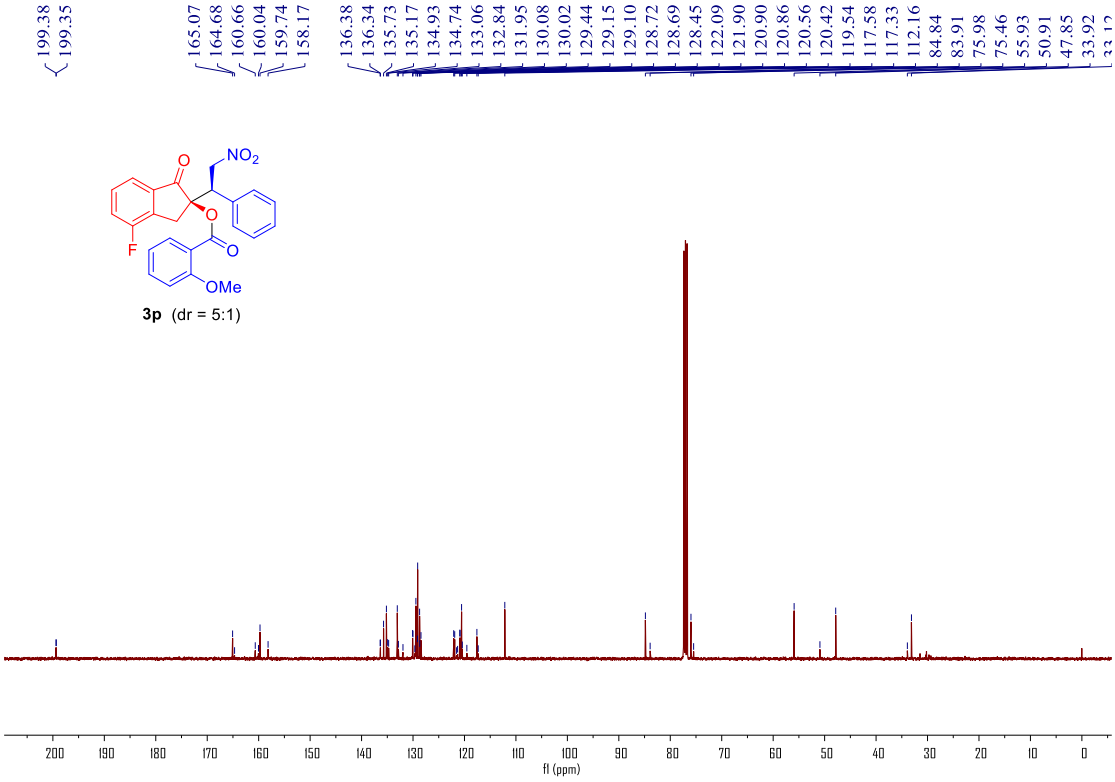

7.90 7.89 7.88 7.87 7.58 7.58 7.56 7.54 7.54 7.50 7.50 7.48 7.45 7.43 7.41 7.39 7.37 7.33 7.32 7.31 7.30 7.28 7.10 7.07 7.06 7.05 7.02 7.02 7.01 7.00 5.63 5.62 5.59 5.59 5.23 5.21 5.20 5.17 4.02 3.92 3.81 3.71 3.70 3.68 3.67 3.41 3.37 3.20 3.19
NO2
O
O
MeO
O
OMe
3n (dr = 5:1)
1.17 1.11 2.01 2.11 3.23 0.43 4.02 0.21 1.19 1.19 0.19 2.97 0.54 2.91 1.54 0.19 0.20 2.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

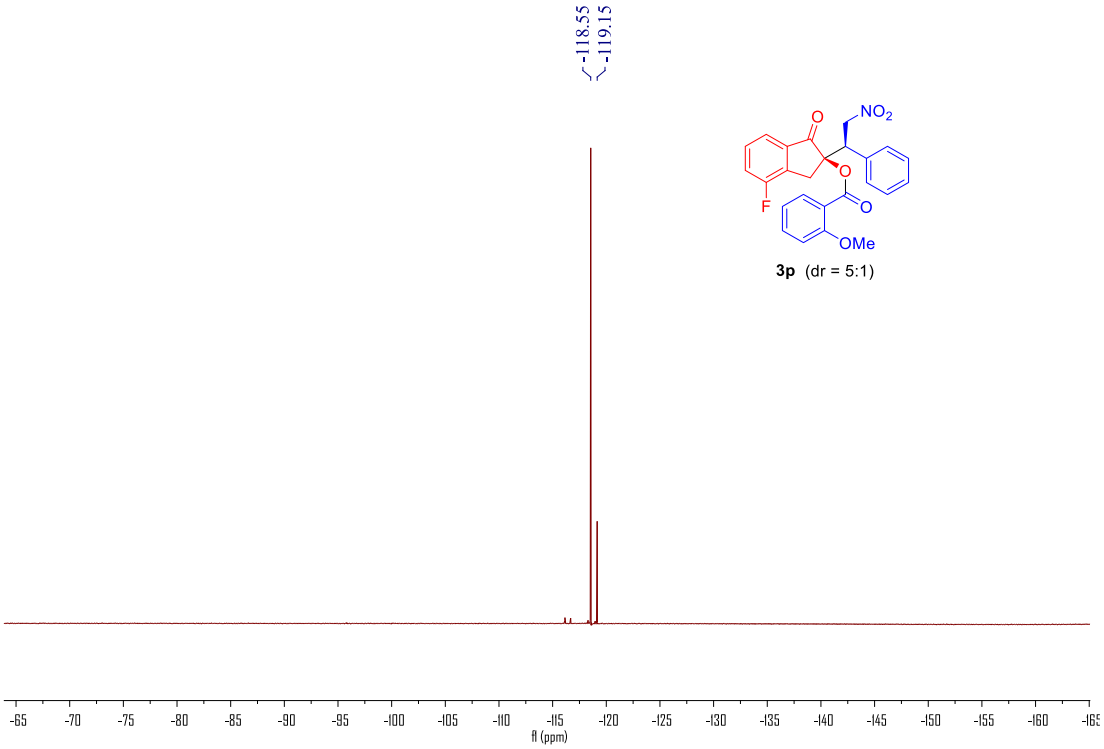

201.19 200.68 164.98 164.60 159.91 159.65 156.45 155.93 137.92 137.74 136.26 135.08 134.92 134.87 133.04 132.81 132.46 129.56 129.53 129.21 129.18 128.95 128.47 128.39 128.23 120.50 120.36 118.01 116.51 116.13 115.83 115.40 112.14 85.15 84.36 76.26 75.82 55.91 55.88 55.45 51.03 48.05 34.75 34.19
NO2
O
O
MeO
O
OMe
3n (dr = 5:1)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

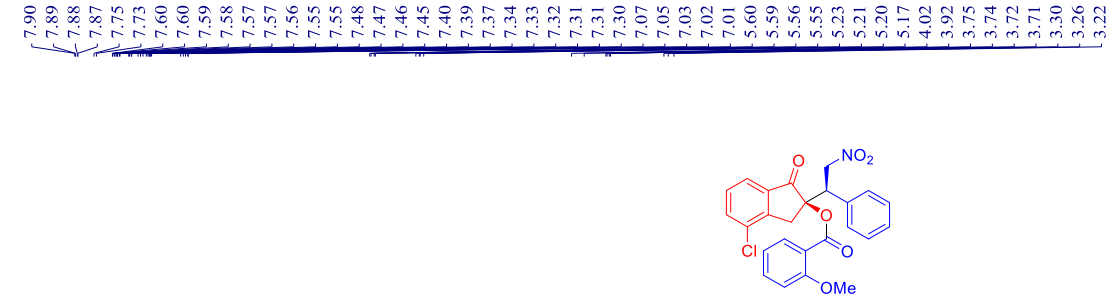

7.91 7.90 7.89 7.88 7.71 7.69 7.56 7.56 7.56 7.54 7.54 7.50 7.49 7.48 7.48 7.44 7.42 7.37 7.35 7.33 7.33 7.32 7.31 7.16 7.08 7.06 7.05 7.05 7.03 7.01 5.63 5.62 5.59 5.58 5.26 5.23 5.22 5.20 4.03 3.92 3.69 3.68 3.66 3.66 3.28 3.23 3.10 3.06 2.18 2.01
1.20 0.98 1.40 2.08 1.06 4.19 0.54 3.74 1.24 1.22 0.22 2.95 0.68 1.00 0.25 1.23 1.00 3.00 0.73
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
O
NO2
O
Me
O
OMe
3o (dr = 4.3:1)


201.26 200.79 165.02 164.65 159.98 159.66 147.99 147.77 136.44 136.30 135.86 135.46 134.96 134.93 133.57 133.05 132.83 129.50 129.12 128.98 128.56 128.46 128.28 128.13 127.84 122.51 121.16 120.52 120.38 117.99 112.16 85.34 76.19 55.93 55.90 51.16 48.05 36.81 36.14 17.79 17.49
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
O
NO2
O
Me
O
OMe
3o (dr = 4.3:1)

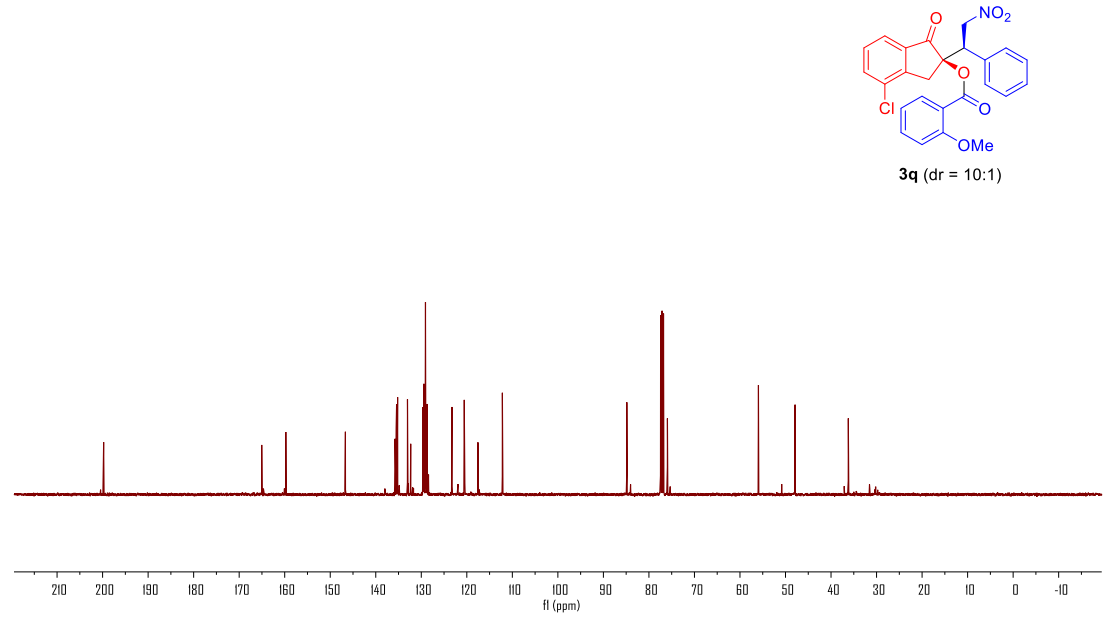

7.91 7.90 7.89 7.88 7.68 7.66 7.61 7.60 7.59 7.59 7.58 7.57 7.56 7.49 7.49 7.47 7.47 7.45 7.45 7.43 7.35 7.34 7.33 7.33 7.32 7.32 7.31 7.29 7.09 7.08 7.07 7.05 7.03 7.03 5.60 5.59 5.56 5.55 5.23 5.20 5.20 5.17 4.04 3.93 3.73 3.72 3.70 3.69 3.31 3.28
NO2
O
F
OMe
3p (dr = 5:1)
1.15 0.95 1.17 3.18 3.94 3.83 1.20 1.21 0.21 2.95 0.55 1.00 0.24 0.23 1.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


199.38 199.35 165.07 164.68 160.66 160.04 159.74 158.17 136.38 136.34 135.73 135.17 134.93 134.74 133.06 132.84 131.95 130.08 130.02 129.44 129.15 129.10 128.72 128.69 128.45 122.09 121.90 120.90 120.86 120.56 120.42 119.54 117.58 117.33 112.16 84.84 83.91 75.98 75.46 55.93 50.91 47.85 33.92
NO2
O
F
OMe
3p (dr = 5:1)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

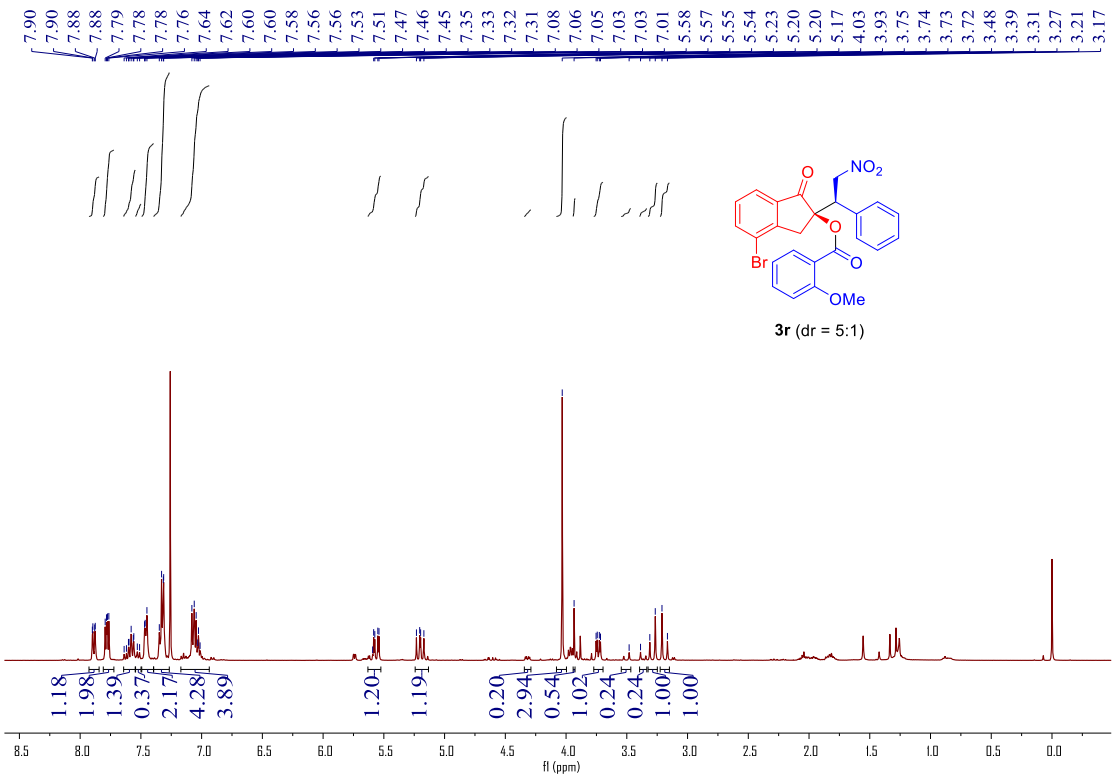

-118.55
-119.15
NO2
O
O
F
O
OMe
3p (dr = 5:1)
-65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160
f1 (ppm)

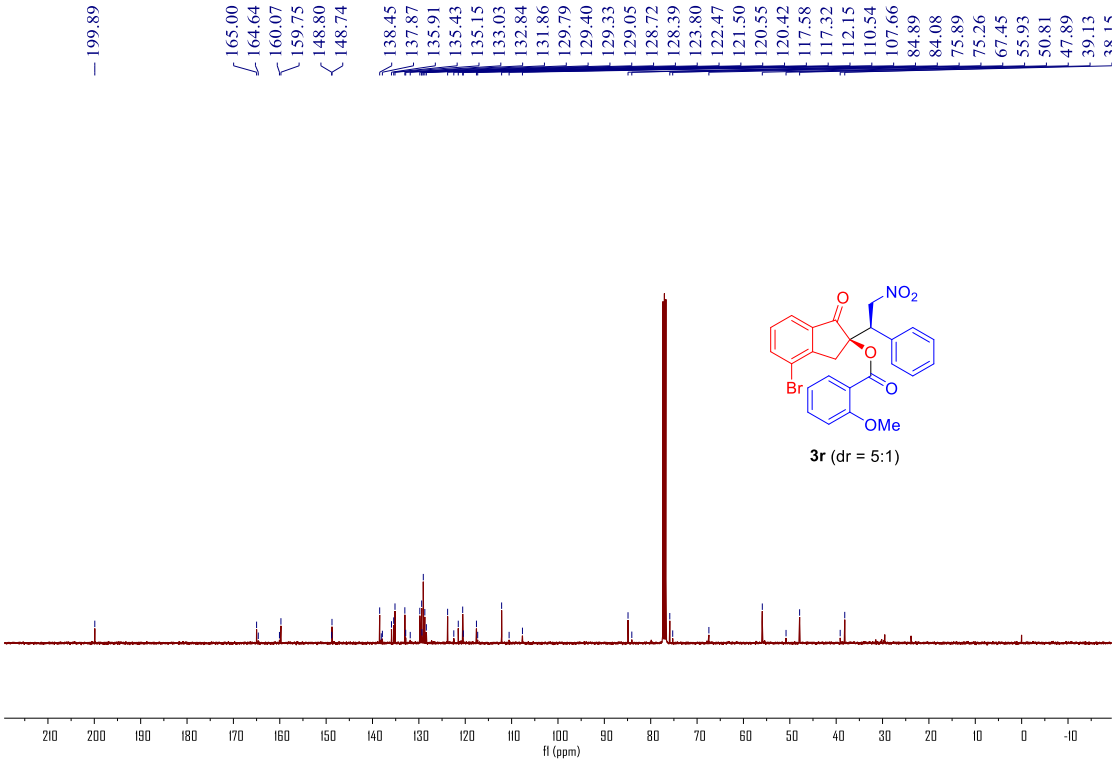


3q (dr = 10:1)

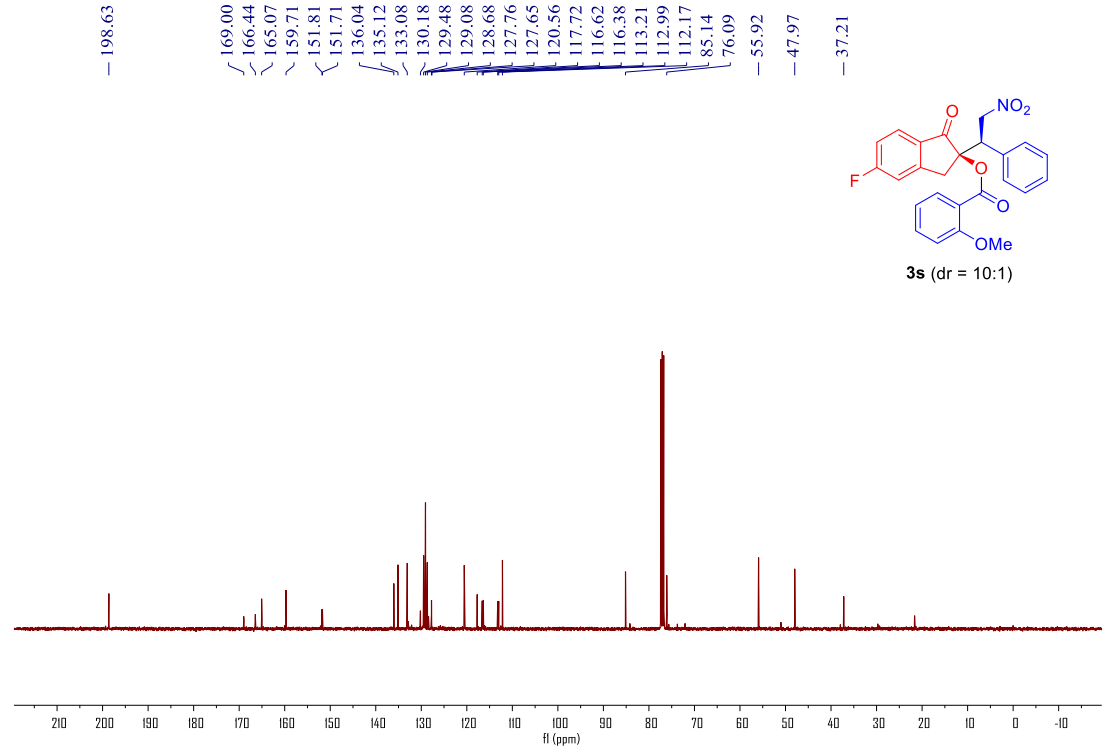


3q (dr = 10:1)

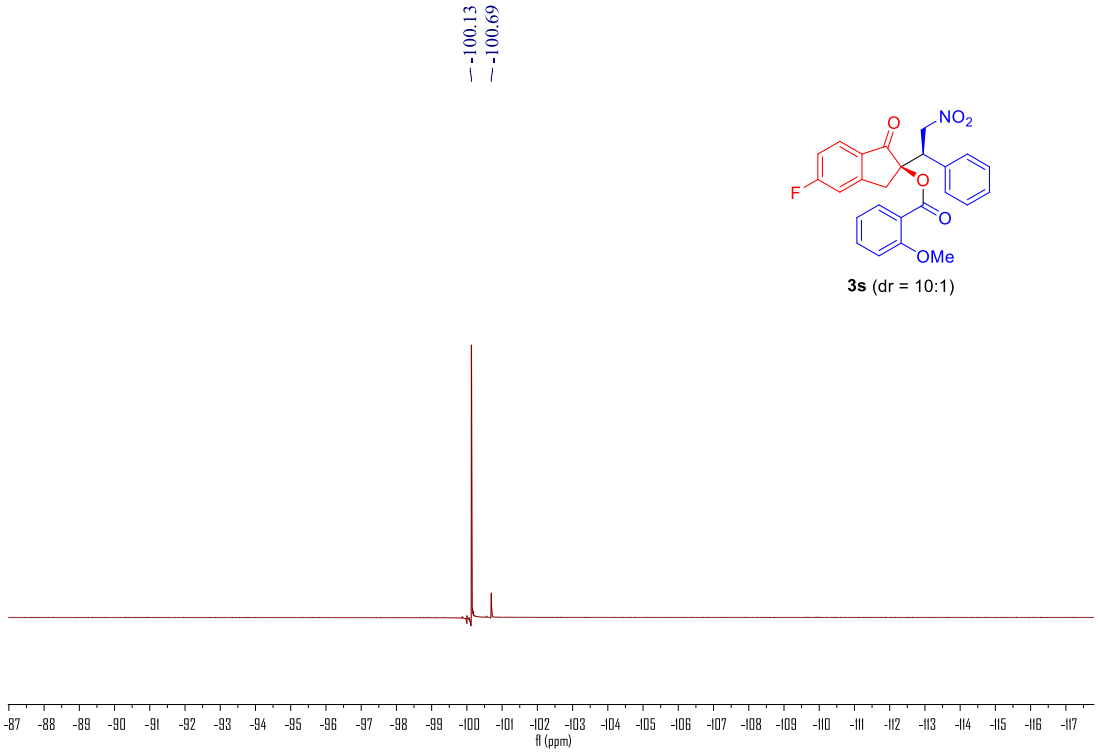

7.90 7.90 7.88 7.88 7.79 7.78 7.78 7.76 7.64 7.62 7.60 7.60 7.58 7.56 7.56 7.53 7.51 7.47 7.46 7.45 7.35 7.33 7.32 7.31 7.08 7.06 7.05 7.03 7.03 7.01 5.58 5.57 5.55 5.54 5.23 5.20 5.20 5.17 4.03 3.93 3.75 3.74 3.73 3.72 3.48 3.39 3.31 3.27 3.21 3.17
NO2
O
O
Br
O
OMe
3r (dr = 5:1)
1.18 1.98 1.39 0.37 2.17 4.28 3.89 1.20 1.19 0.20 2.94 0.54 1.02 0.24 0.24 1.00 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


199.89
165.00 164.64 160.07 159.75 148.80 148.74
138.45 137.87 135.91 135.43 135.15 133.03 132.84 131.86 129.79 129.40 129.33 129.05 128.72 128.39 123.80 122.47 121.50 120.55 120.42 117.58 117.32 112.15 110.54 107.66 84.89 84.08 75.89 75.26 67.45 55.93 50.81 47.89 39.13
NO2
O
O
Br
O
OMe
3r (dr = 5:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

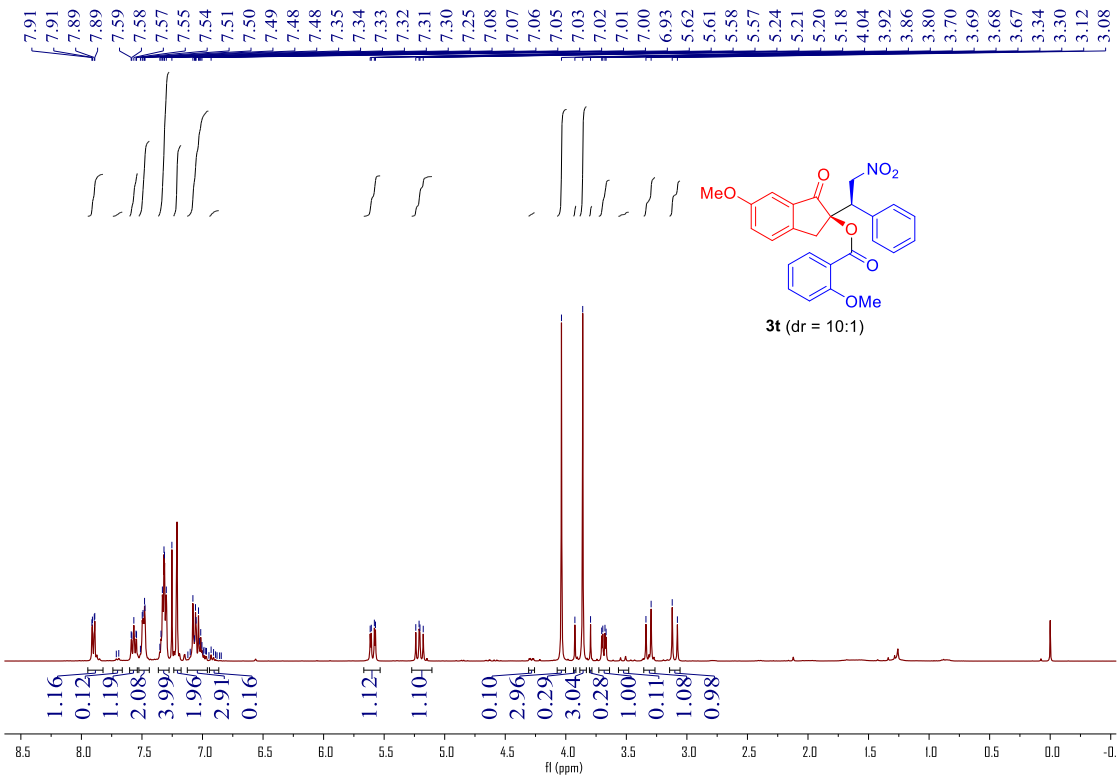
3s (dr = 10:1)

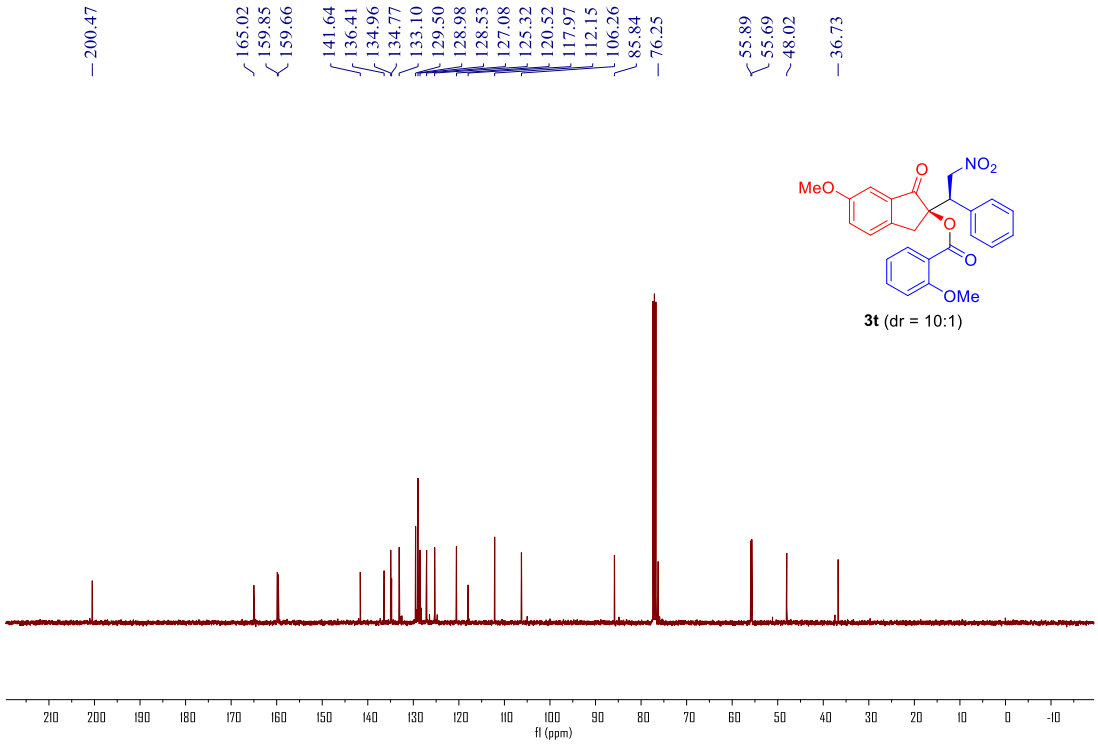


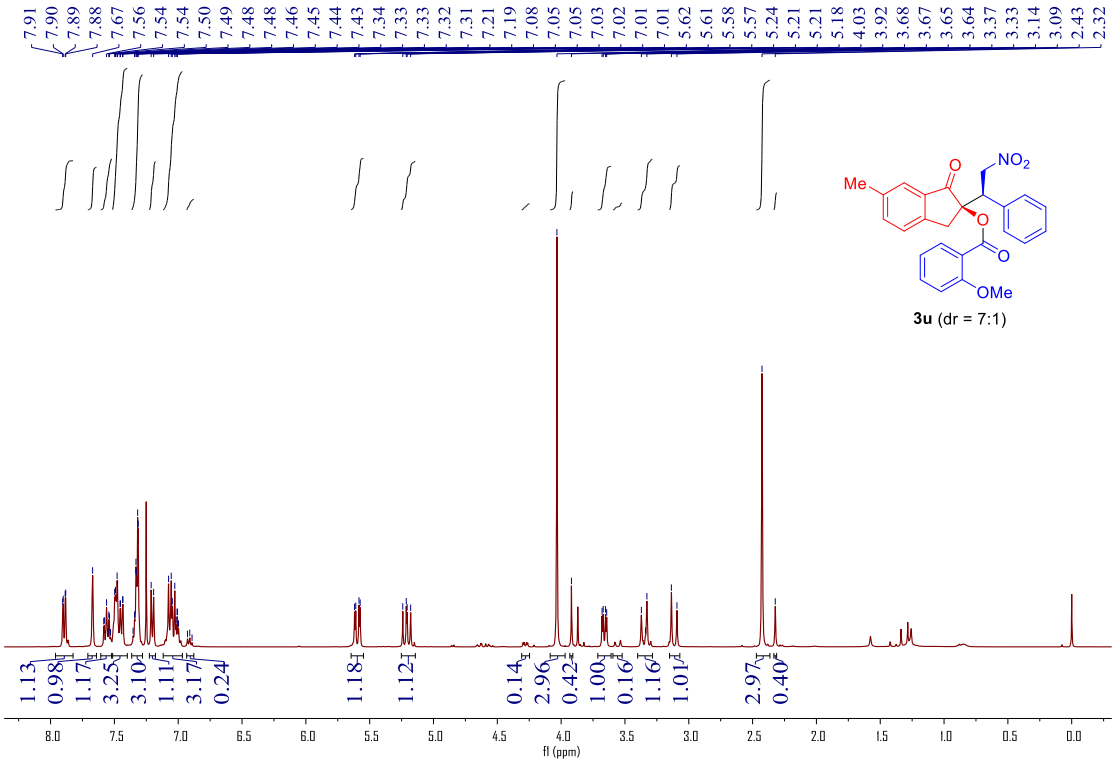
3s (dr = 10:1)

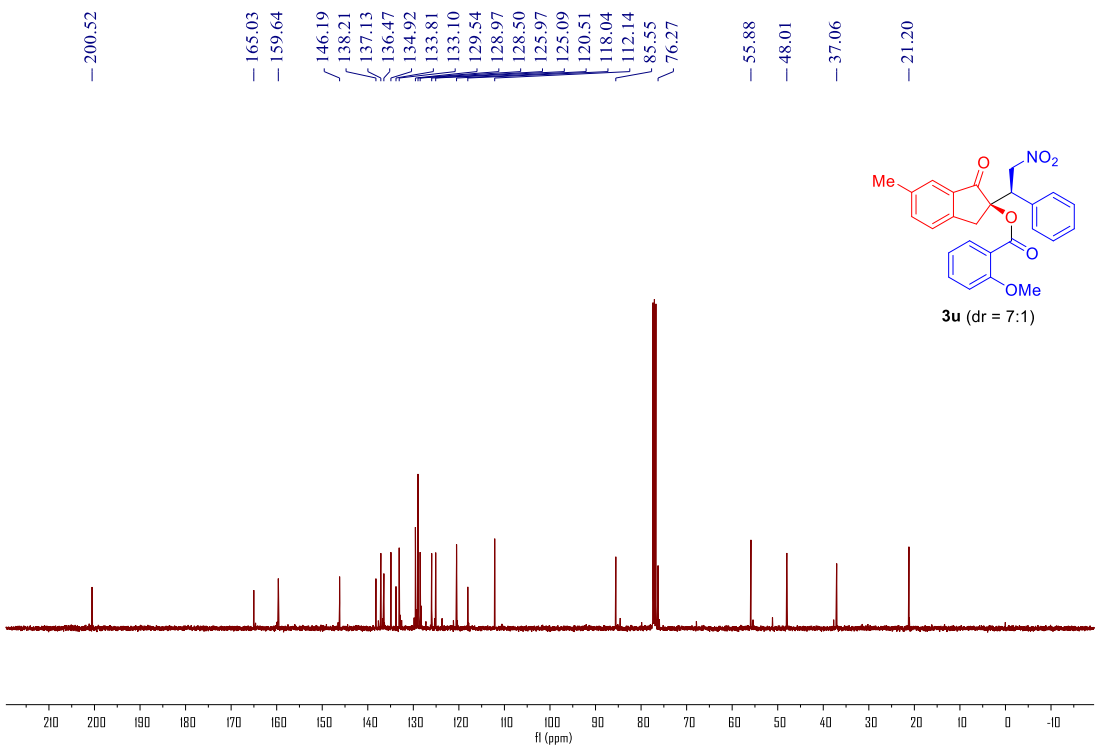

-100.13
-100.69
NO2
O
F
O
O
OMe
-87 -88 -89 -90 -91 -92 -93 -94 -95 -96 -97 -98 -99 -100 -101 -102 -103 -104 -105 -106 -107 -108 -109 -110 -111 -112 -113 -114 -115 -116 -117
f1 (ppm)

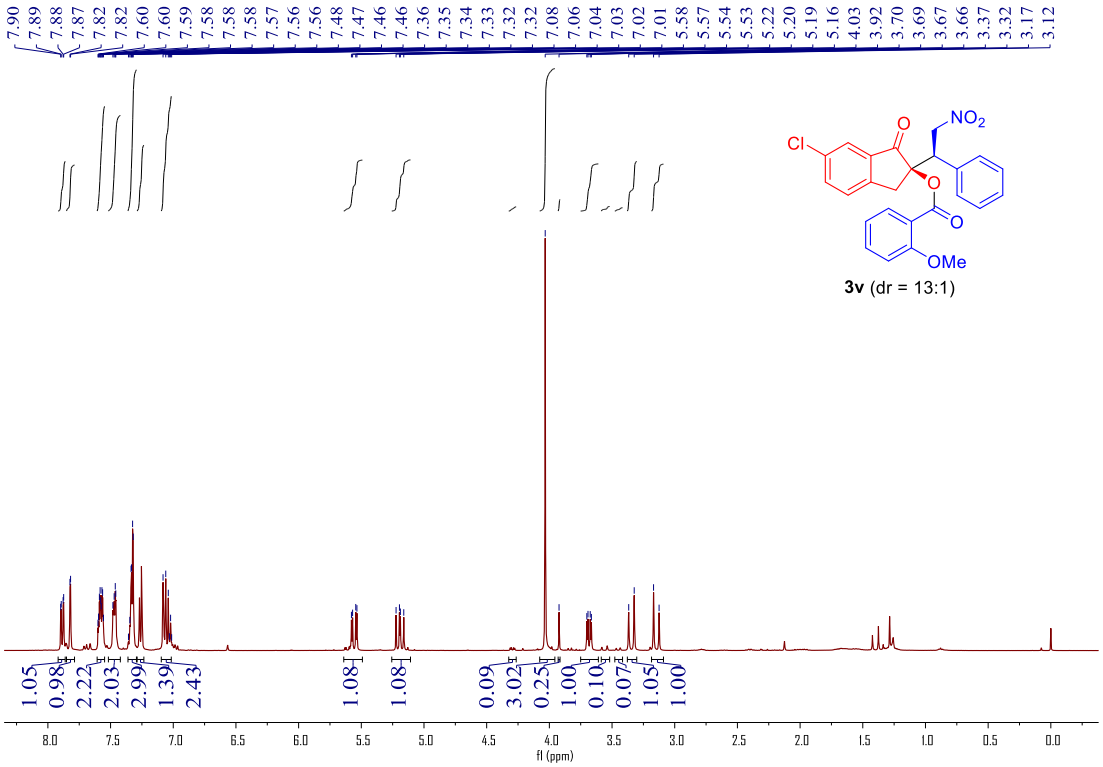
3s (dr = 10:1)

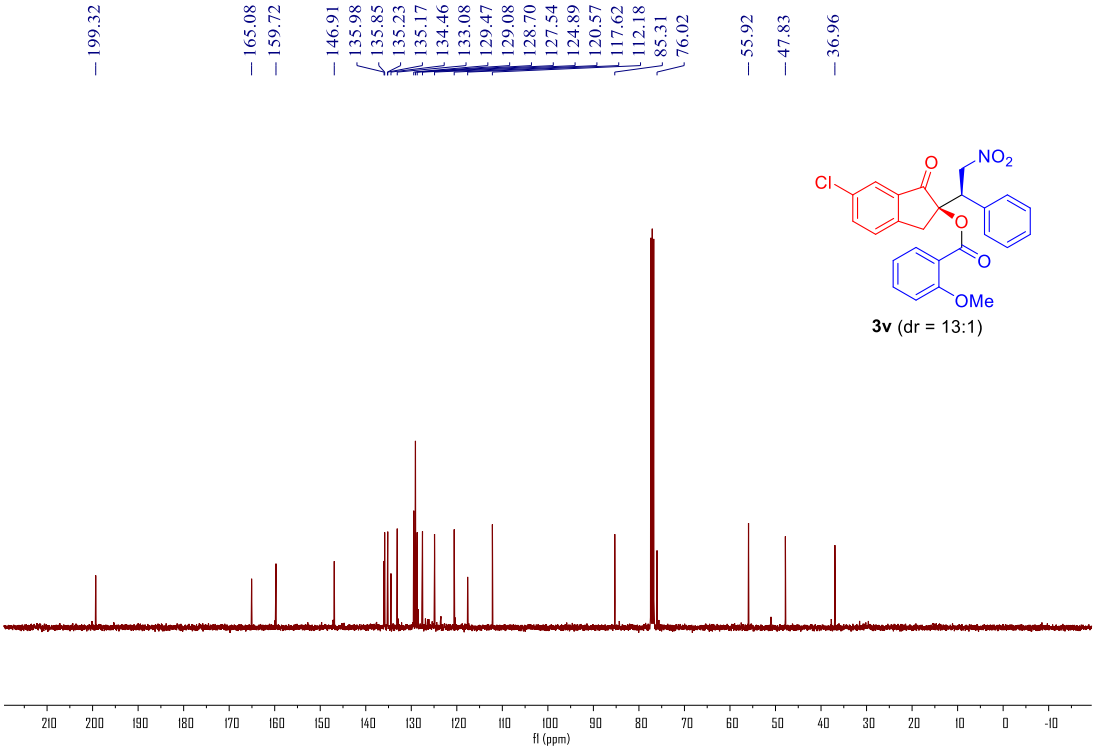

7.91 7.91 7.89 7.89 7.59 7.58 7.57 7.55 7.54 7.51 7.50 7.49 7.48 7.48 7.35 7.34 7.33 7.32 7.31 7.30 7.25 7.08 7.07 7.06 7.05 7.03 7.02 7.01 7.00 6.93 5.62 5.61 5.58 5.57 5.24 5.21 5.20 5.18 4.04 3.92 3.86 3.80 3.70 3.69 3.68 3.67 3.34 3.30 3.12 3.08
MeO
NO2
O
OMe
3t (dr = 10:1)
1.16 0.12 1.19 2.08 3.99 1.96 2.91 0.16 1.12 1.10 0.10 2.96 0.29 3.04 0.28 1.00 0.11 1.08 0.98
f1 (ppm)

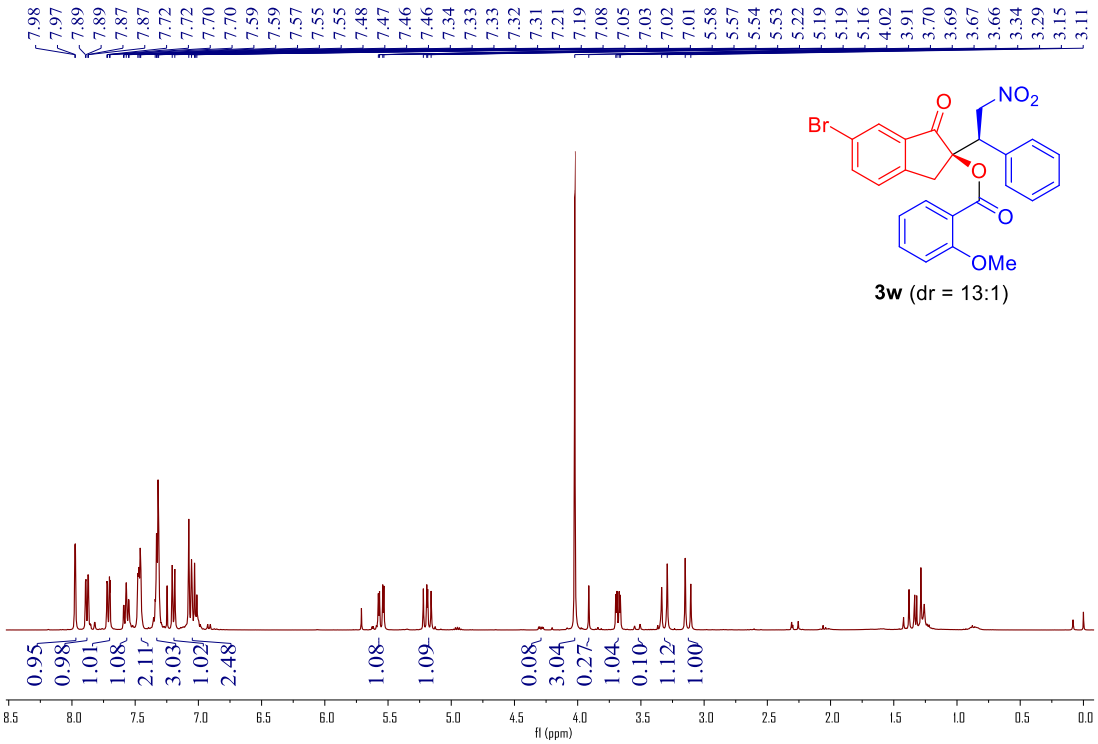

200.47
165.02 159.85 159.66
141.64 136.41 134.96 134.77 133.10 129.50 128.98 128.53 127.08 125.32 120.52 117.97 112.15 106.26 85.84 76.25
55.89 55.69 48.02
36.73
MeO
NO2
O
OMe
3t (dr = 10:1)
f1 (ppm)

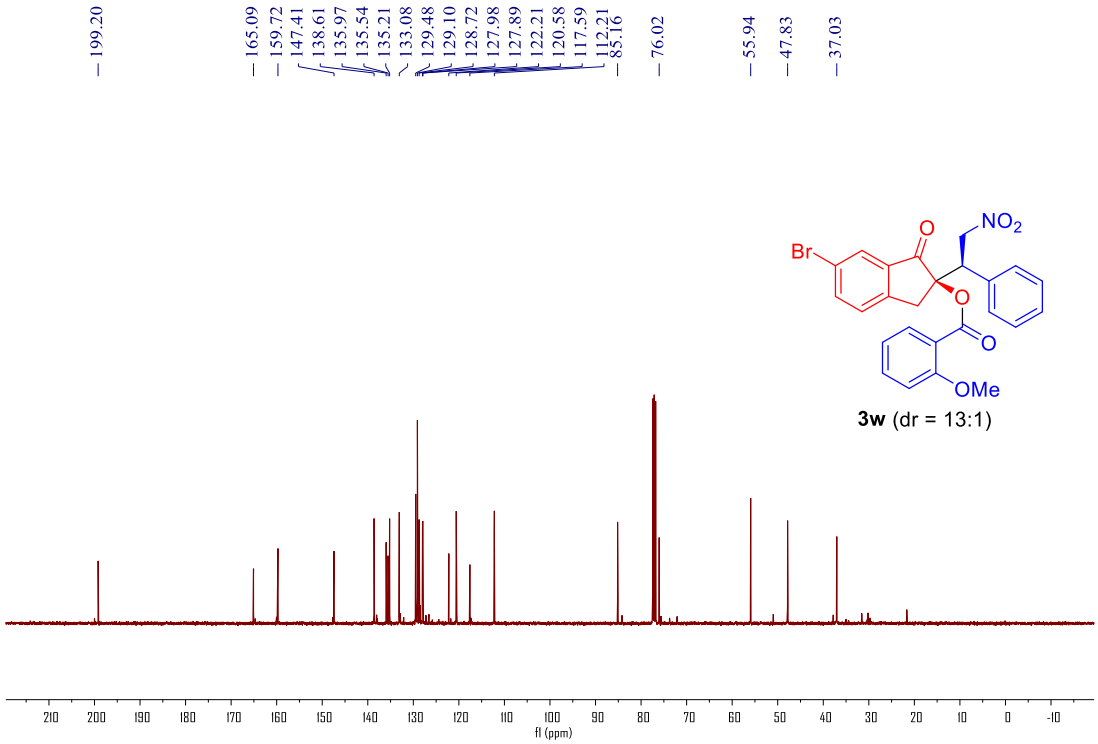

7.91 7.90 7.89 7.88 7.67 7.56 7.54 7.54 7.50 7.49 7.48 7.48 7.46 7.45 7.44 7.43 7.34 7.33 7.33 7.32 7.31 7.21 7.19 7.08 7.05 7.05 7.03 7.02 7.01 7.01 5.62 5.61 5.58 5.57 5.24 5.21 5.21 5.18 4.03 3.92 3.68 3.67 3.65 3.64 3.37 3.33 3.14 3.09 2.43 2.32
1.13 0.98 1.17 3.25 3.10 1.11 3.17 0.24 1.18 1.12 0.14 2.96 0.42 1.00 0.16 1.16 1.01 2.97 0.40
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
Me
O
NO2
O
O
OMe
3u (dr = 7:1)

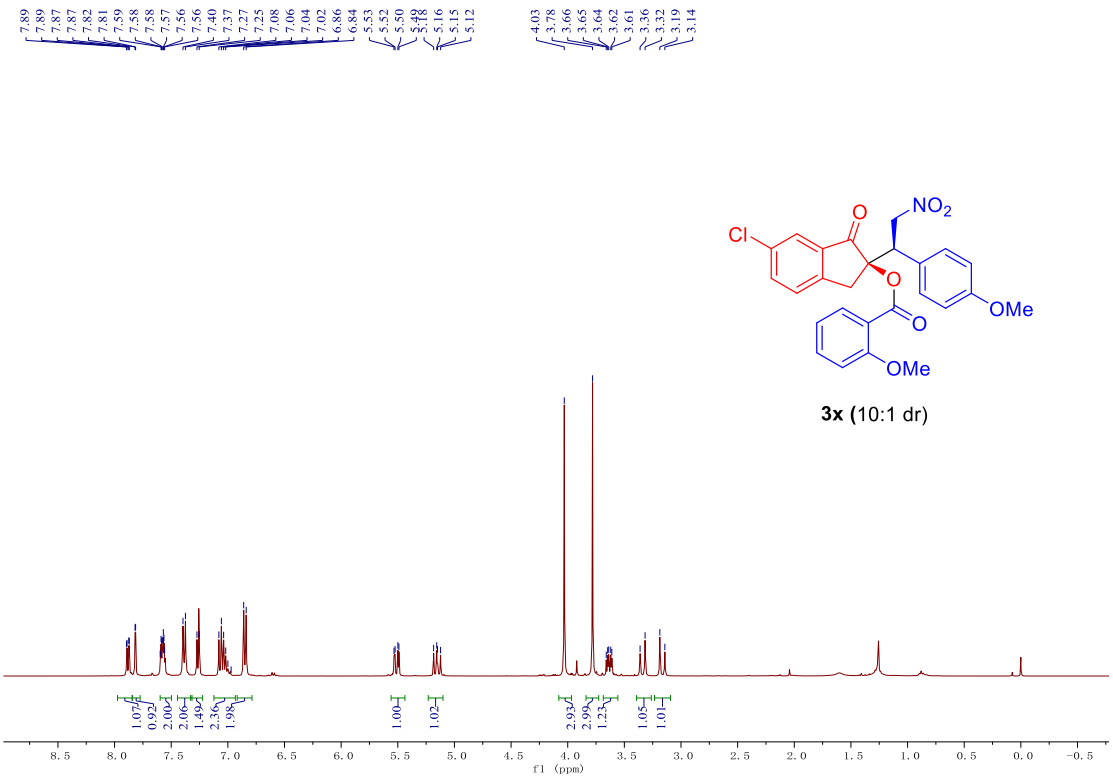

200.52
165.03
159.64
146.19
138.21
137.13
136.47
134.92
133.81
133.10
129.54
128.97
128.50
125.97
125.09
120.51
118.04
112.14
85.55
76.27
55.88
48.01
37.06
21.20
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
Me
O
NO2
O
O
OMe
3u (dr = 7:1)

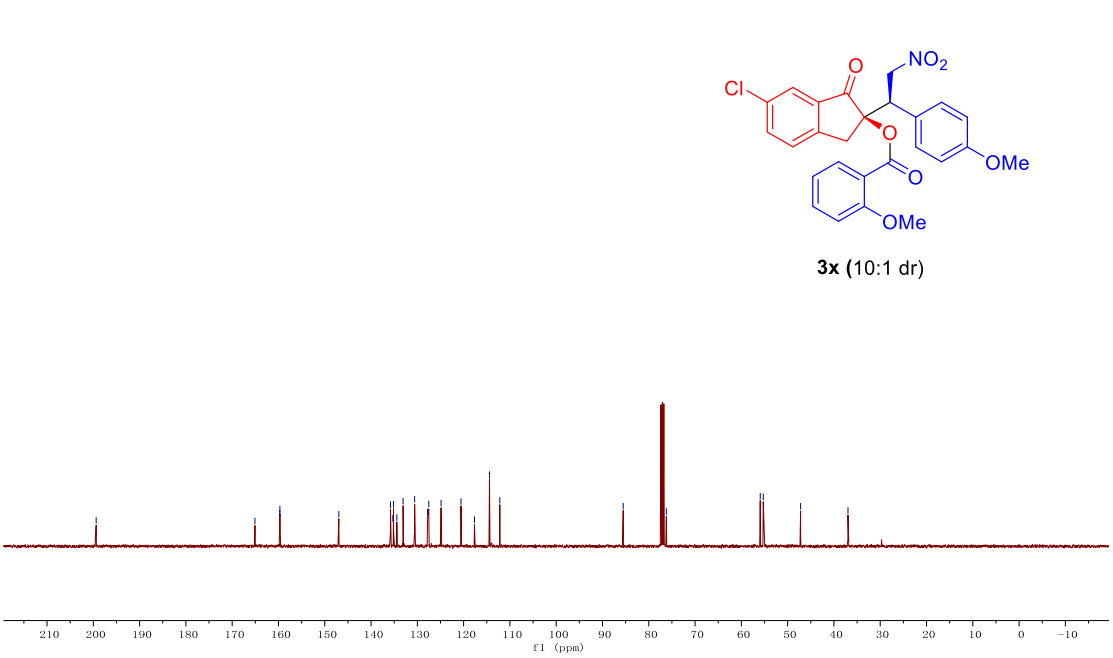

7.90 7.89 7.88 7.87 7.82 7.82 7.60 7.60 7.59 7.58 7.58 7.58 7.57 7.56 7.56 7.48 7.47 7.46 7.46 7.36 7.35 7.34 7.33 7.32 7.32 7.08 7.06 7.04 7.03 7.02 7.01 5.58 5.57 5.54 5.53 5.22 5.20 5.19 5.16 4.03 3.92 3.70 3.69 3.67 3.66 3.37 3.32 3.17 3.12
1.05 0.98 2.22 2.03 2.99 1.39 2.43 1.08 1.08 0.09 3.02 0.25 1.00 0.10 0.07 1.05 1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
Cl
O
NO2
O
O
OMe
3v (dr = 13:1)

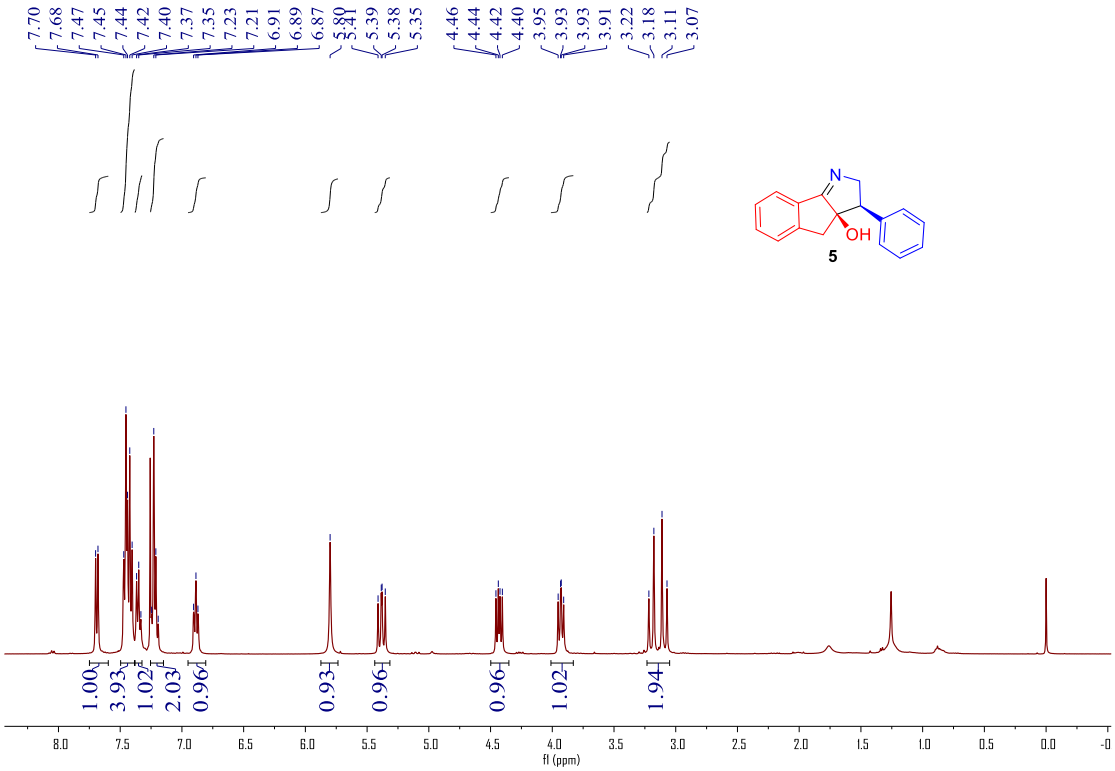

199.32
165.08
159.72
146.91
135.98
135.85
135.23
135.17
134.46
133.08
129.47
129.08
128.70
127.54
124.89
120.57
117.62
112.18
85.31
76.02
55.92
47.83
36.96
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
Cl
O
NO2
O
O
OMe
3v (dr = 13:1)


7.98 7.97 7.89 7.89 7.87 7.87 7.72 7.72 7.70 7.70 7.59 7.59 7.57 7.55 7.55 7.48 7.47 7.46 7.46 7.34 7.33 7.33 7.32 7.31 7.21 7.19 7.08 7.05 7.03 7.02 7.01 5.58 5.57 5.54 5.53 5.22 5.19 5.19 5.16 4.02 3.91 3.70 3.69 3.67 3.66 3.34 3.29 3.15 3.11
Br
O
NO2
O
O
OMe
3w (dr = 13:1)
0.95 0.98 1.01 1.08 2.11 3.03 1.02 2.48 1.08 1.09 0.08 3.04 0.27 1.04 0.10 1.12 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


199.20
165.09 159.72 147.41 138.61 135.97 135.54 135.21 133.08 129.48 129.10 128.72 127.98 127.89 122.21 120.58 117.59 112.21 85.16
76.02
55.94 47.83 37.03
Br
O
NO2
O
O
OMe
3w (dr = 13:1)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.89 7.89 7.87 7.87 7.82 7.81 7.59 7.58 7.58 7.57 7.56 7.56 7.40 7.37 7.27 7.25 7.08 7.06 7.04 7.02 6.86 6.84 5.53 5.52 5.50 5.48 5.18 5.16 5.15 5.12
4.03 3.78 3.66 3.65 3.64 3.62 3.61 3.36 3.32 3.19 3.14
Cl
O
NO2
O
O
OMe
OMe
3x (10:1 dr)
1.07 0.92 2.00 2.06 1.49 2.36 1.98 1.00 1.02 2.93 2.99 1.23 1.05 1.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


199.38
165.08 159.71 159.69
146.96 135.81 135.29 135.14 134.43 133.08 130.58 127.78 127.53 124.87 120.57 117.65 114.41 112.18
85.52
76.20
55.92 55.27
47.20
36.97
Cl
O
NO2
O
O
OMe
OMe
3x (10:1 dr)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.70
7.68
7.47
7.45
7.44
7.42
7.40
7.37
7.35
7.23
7.21
6.91
6.89
6.87
5.80
5.41
5.39
5.38
5.35
4.46
4.44
4.42
4.40
3.95
3.93
3.93
3.91
3.22
3.18
3.11
3.07
N
OH
5
1.00
3.93
1.02
2.03
0.96
0.93
0.96
0.96
1.02
1.94
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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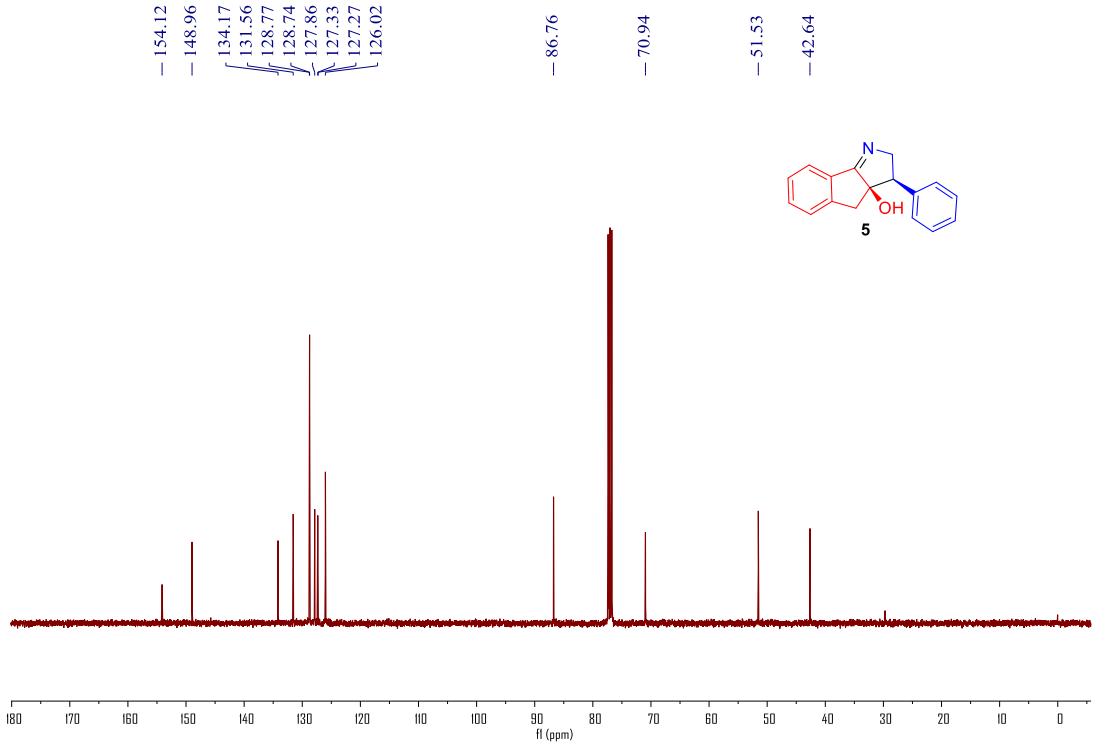
f1 (ppm)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134.17
131.56
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127.86
127.33
127.27
126.02
86.76
70.94
51.53
42.64
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OH
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170
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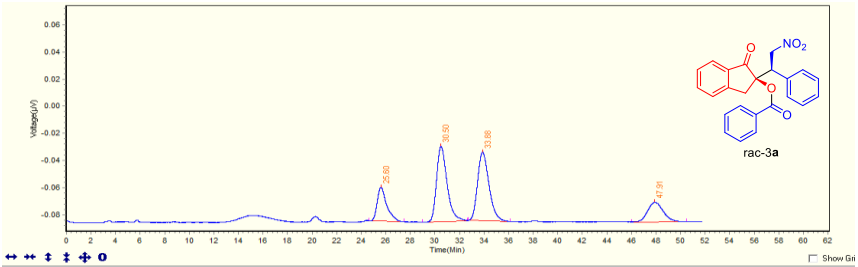
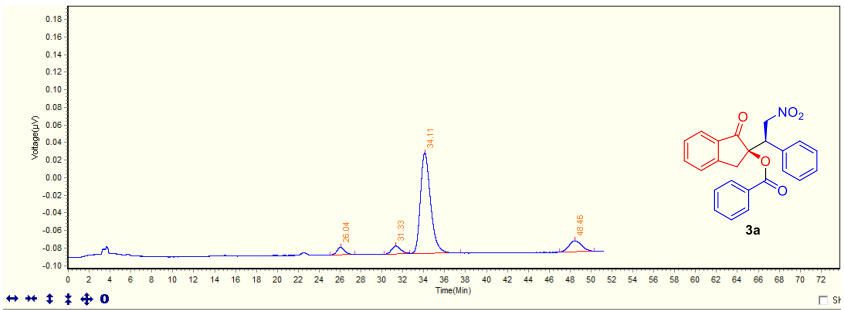
HPLC spectra of compounds



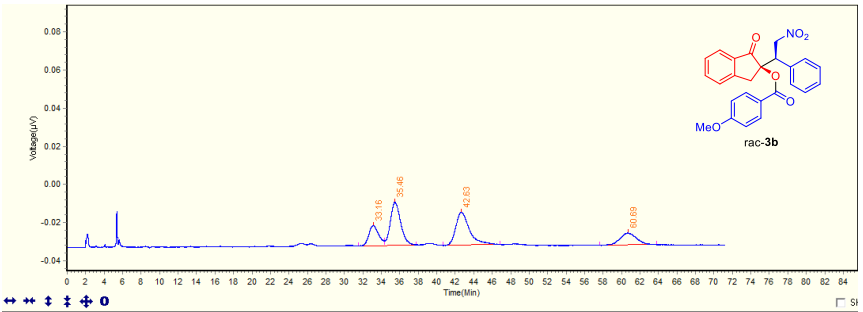
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	25.60	668182	12399	14.65%	2.861	BB
2	30.50	1637401	27521	35.90%	3.668	BB
3	33.88	1629502	25162	35.73%	3.42	BB
4	47.91	625514	7171	13.72%	4.477	BB
Total		4,560,599	72,253	100.00%		



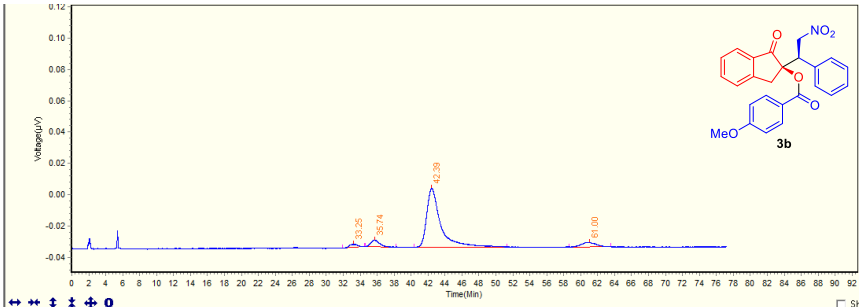
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	26.04	211521	4266	4.37%	2.339	BB
2	31.33	258982	4415	5.35%	2.462	BB
3	34.11	3841418	57151	79.40%	4.802	BB
4	48.46	526342	6233	10.88%	3.323	BB
Total		4,838,263	72,065	100.00%		



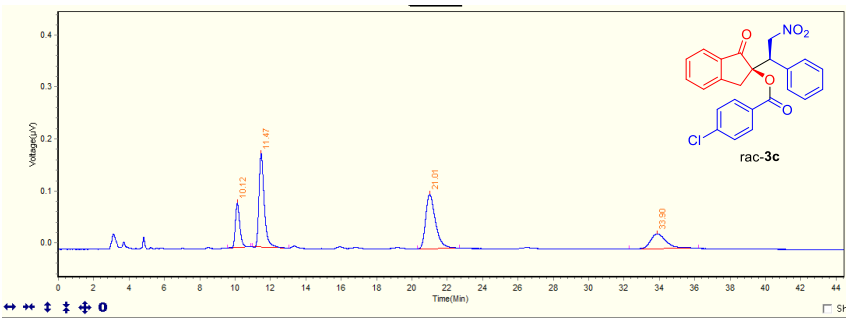
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	33.16	386900	5293	15.32%	2.825	BV
2	35.46	869764	11283	34.43%	3.426	VB
3	42.63	885199	8582	35.05%	6.166	BB
4	60.69	383958	3108	15.20%	6.166	BB
Total		2,525,821	28,266	100.00%		



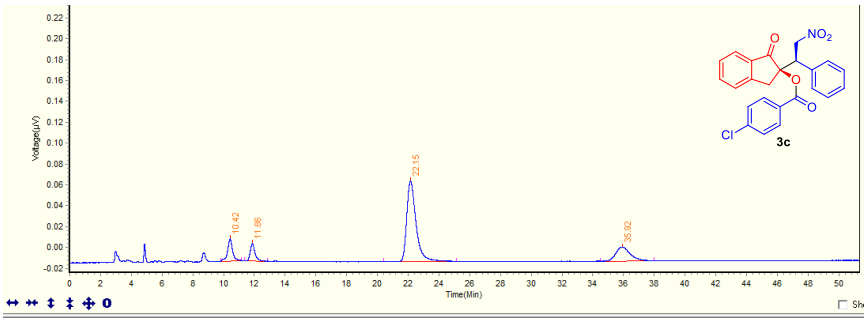
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	33.25	67054	980	2.68%	2.598	BB
2	35.74	150780	2139	6.02%	3.618	BB
3	42.39	2117832	18599	84.56%	10.947	BB
4	61.00	168968	1408	6.75%	4.917	BB
Total		2,504,634	23,126	100.00%		



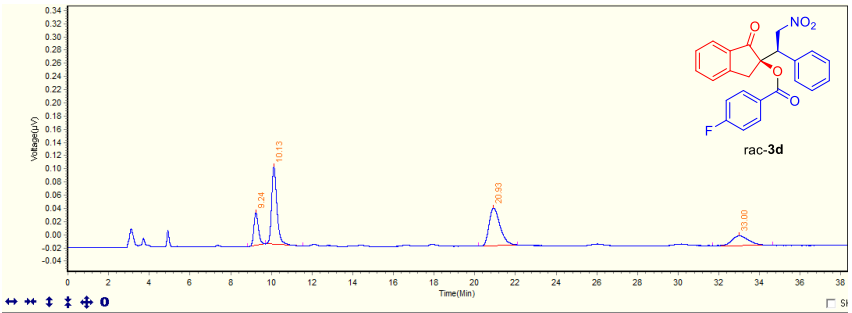
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.12	728640	42377	13.29%	1.322	BB
2	11.47	1863908	89491	34.00%	2.04	BB
3	21.01	1999189	51768	36.47%	2.379	BB
4	33.90	889988	14228	16.24%	3.921	BB
Total		5,481,725	197,864	100.00%		



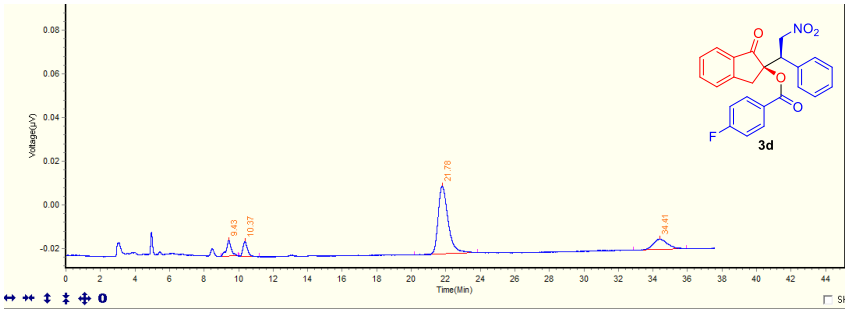
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.42	230411	10460	9.37%	1.337	BB
2	11.86	173134	8236	7.04%	1.49	BB
3	22.15	1618731	38598	65.82%	4.728	BB
4	35.92	437007	6713	17.77%	3.496	BB
Total		2,459,283	64,007	100.00%		



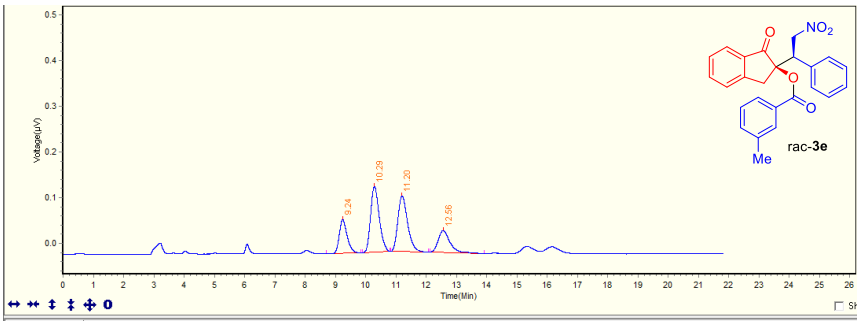
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.24	378032	24476	12.90%	0.883	BB
2	10.13	1071729	58801	36.56%	1.842	BB
3	20.93	1064906	28526	36.33%	1.918	BB
4	33.00	416900	7371	14.22%	2.955	BB
Total		2,931,567	119,174	100.00%		



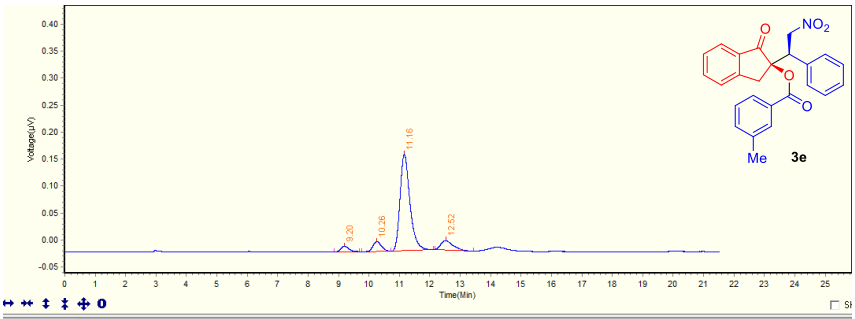
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.43	71201	3544	8.07%	0.978	BB
2	10.37	60836	3432	6.89%	1.166	BB
3	21.78	613071	15455	69.46%	3.656	BB
4	34.41	137498	2325	15.58%	3.07	BB
Total		882,606	24,756	100.00%		



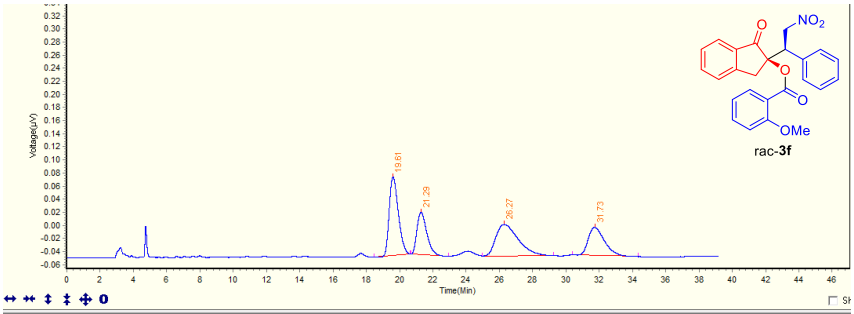
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.24	661716	36701	16.16%	1.128	BB
2	10.29	1431790	71789	34.97%	0.911	BB
3	11.20	1369999	61072	33.46%	1.258	BB
4	12.56	631192	23708	15.41%	1.785	BB
Total		4,094,697	193,270	100.00%		



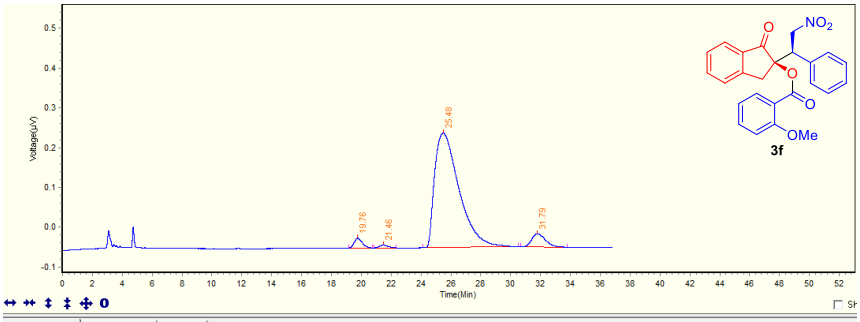
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.20	89073	5135	3.53%	0.828	BB
2	10.26	174011	9067	6.90%	0.958	BB
3	11.16	2021400	89384	80.14%	1.398	BB
4	12.52	237985	8765	9.43%	1.268	BB
Total		2,522,469	112,351	100.00%		



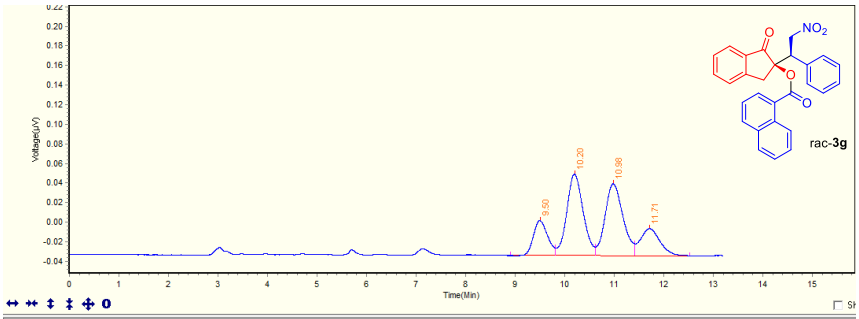
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	19.61	2284423	60166	31.27%	2.168	BB
2	21.29	1325466	32340	18.14%	2.262	BB
3	26.27	2243782	24034	30.71%	4.287	BB
4	31.73	1452699	21458	19.88%	3.957	BB
Total		7,306,370	137,998	100.00%		



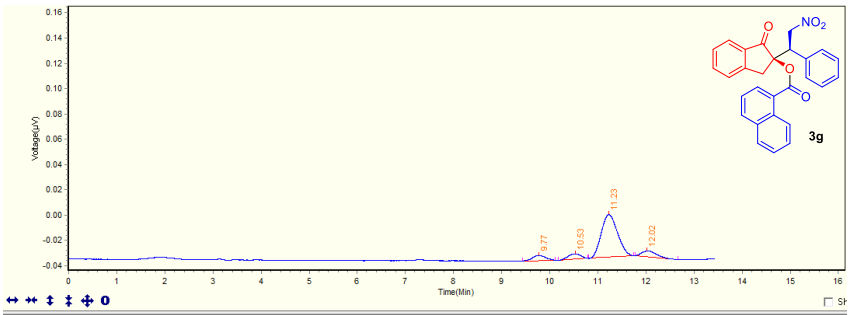
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	19.76	464564	12243	2.58%	1.593	BB
2	21.46	133566	3352	0.74%	1.505	BB
3	25.48	16331370	143871	90.84%	6.416	BB
4	31.79	1047897	16539	5.83%	3.098	BB
Total		17,977,397	176,005	100.00%		



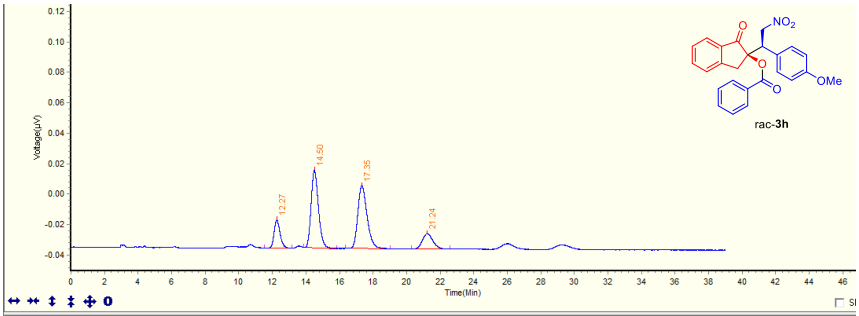
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.50	354328	17824	13.51%	0.904	BV
2	10.20	963065	41507	36.73%	0.809	VV
3	10.98	923286	36714	35.21%	0.793	VV
4	11.71	381529	13825	14.55%	1.111	VB
Total		2,622,208	109,870	100.00%		



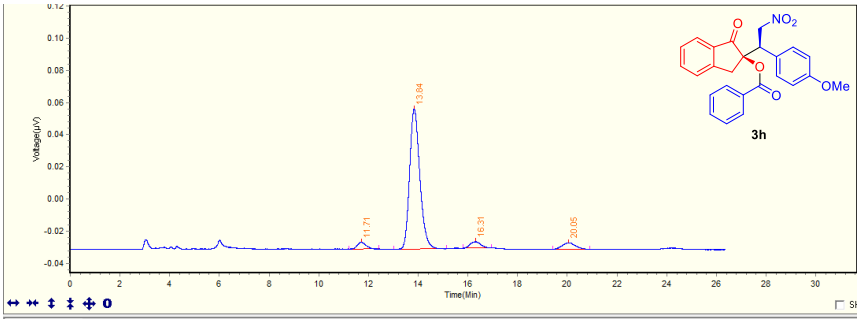
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.77	37140	1992	7.13%	0.678	BB
2	10.53	39649	2158	7.61%	0.613	BB
3	11.23	396141	16826	76.07%	0.937	BB
4	12.02	47827	2257	9.18%	0.888	BB
Total		520,757	23,233	100.00%		



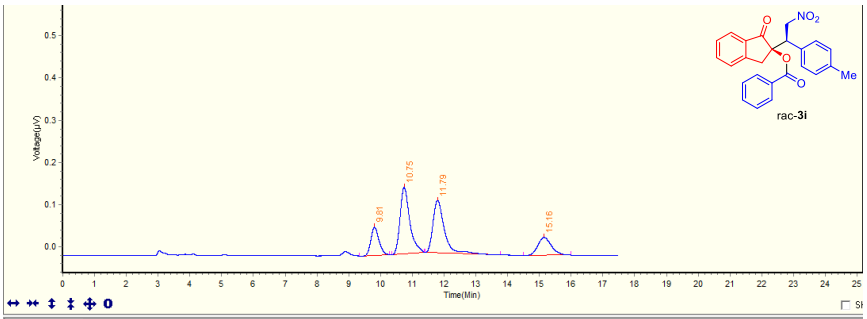
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.27	226268	9208	11.28%	1.639	BB
2	14.50	772414	25393	38.50%	1.968	BB
3	17.35	794551	20684	39.60%	2.67	BB
4	21.24	213162	4977	10.62%	2.296	BB
Total		2,006,395	60,262	100.00%		



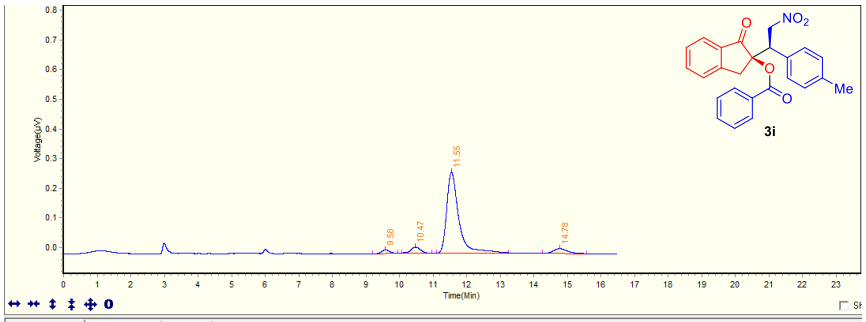
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.71	49264	2154	3.45%	1.203	BB
2	13.84	1247070	43657	87.37%	2.123	BB
3	16.31	57139	1964	4.00%	1.14	BB
4	20.05	73938	2029	5.18%	1.488	BB
Total		1,427,411	49,804	100.00%		



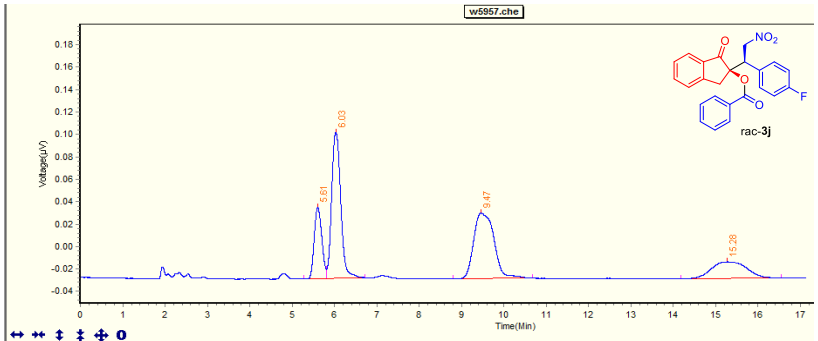
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.81	589835	33278	13.35%	0.956	BB
2	10.75	1668033	78475	37.75%	1.039	BB
3	11.79	1538940	61974	34.83%	2.37	BB
4	15.16	622241	20984	14.08%	1.497	BB
Total		4,419,049	194,711	100.00%		



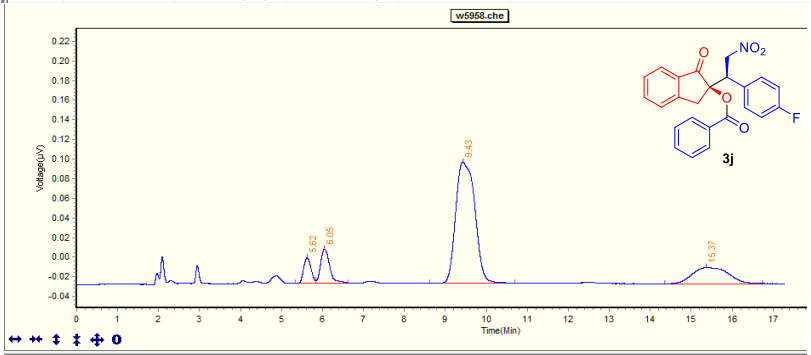
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.58	106703	6399	2.70%	0.753	BB
2	10.47	200328	10107	5.07%	0.891	BB
3	11.55	3411610	137073	86.36%	2.14	BB
4	14.78	231859	8179	5.87%	1.317	BB
Total		3,950,500	161,758	100.00%		



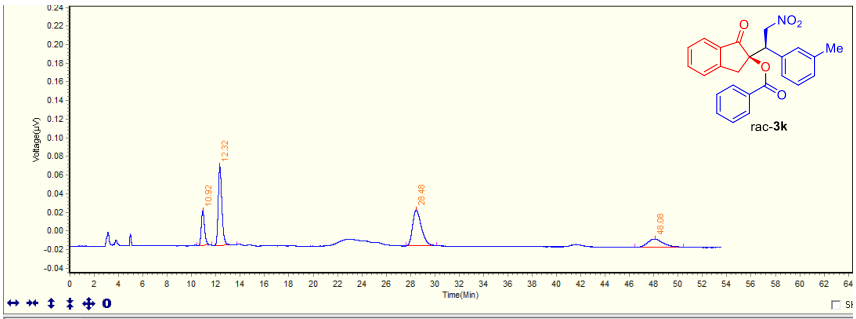
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Ty
1	5.61	397385	31823	14.44%	0.543	BV
2	6.03	970769	65083	35.27%	0.915	VB
3	9.47	973440	29243	35.37%	1.88	BB
4	15.28	410743	7283	14.92%	2.374	BB
Total		2,752,337	133,432	100.00%		



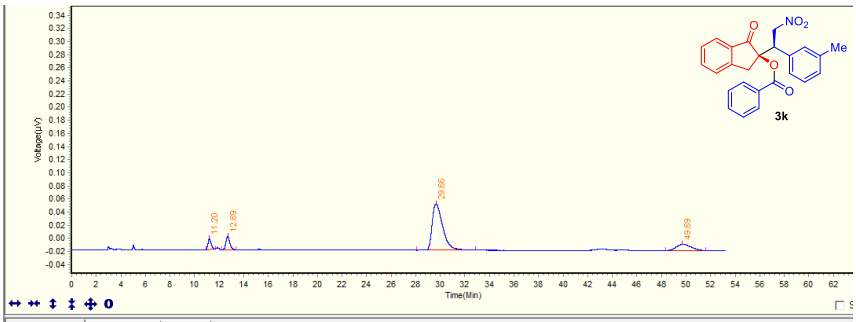
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.62	162237	12964	5.54%	0.497	BV
2	6.05	263542	17275	9.00%	0.789	VB
3	9.43	2004808	61589	68.45%	2.077	BB
4	15.37	498093	8170	17.01%	2.388	BB
Total		2,928,680	99,998	100.00%		



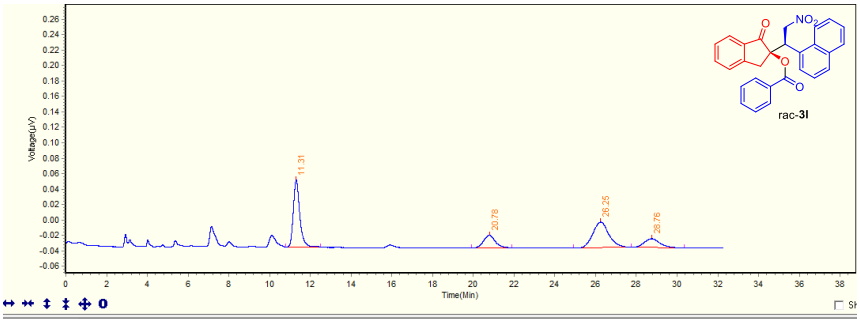
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.92	344413	18389	13.46%	1.193	BB
2	12.32	871573	42186	34.06%	2.05	BB
3	28.48	961780	19013	37.58%	2.497	BB
4	48.08	381499	4361	14.91%	4.026	BB
Total		2,559,265	83,949	100.00%		



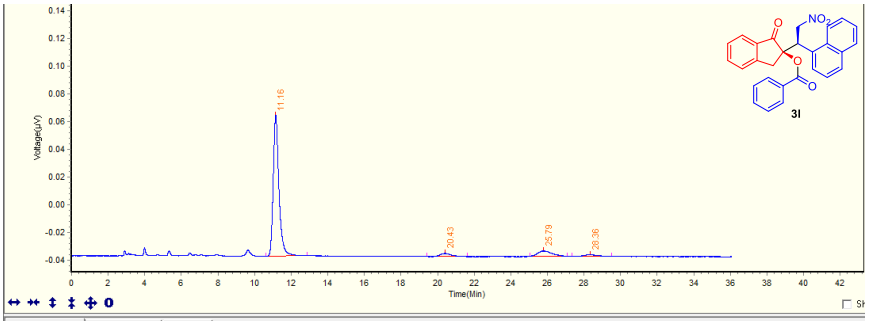
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.20	142222	7871	4.98%	0.777	BB
2	12.69	221825	10314	7.77%	1.184	BB
3	29.66	2086761	35198	73.07%	4.796	BB
4	49.69	404890	4845	14.18%	3.261	BB
Total		2,855,698	58,228	100.00%		



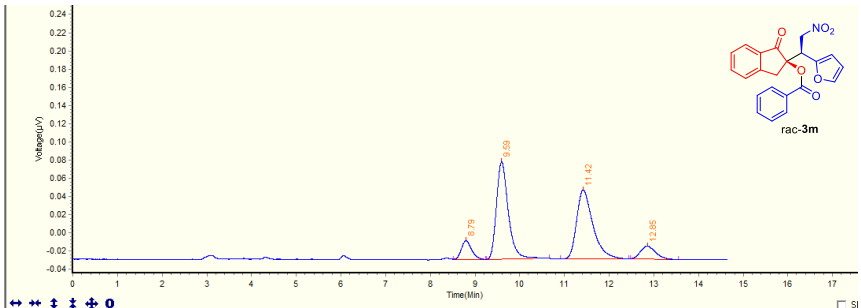
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.31	946455	43374	38.06%	1.708	BB
2	20.78	332825	8279	13.38%	1.979	BB
3	28.76	297199	5685	11.95%	2.6	BB
4	26.25	910183	16591	36.60%	2.833	BB
Total		2,486,662	73,929	100.00%		



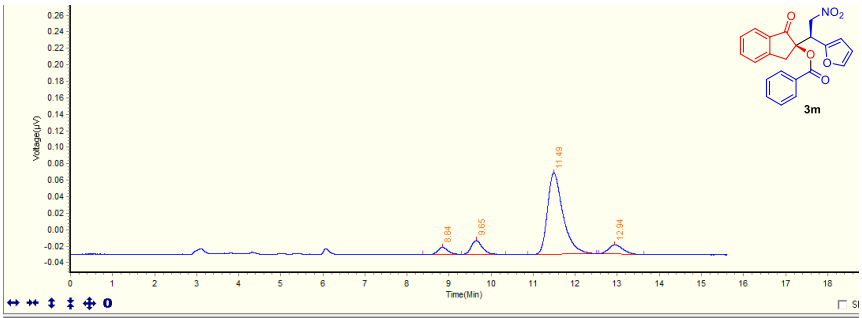
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.16	1099694	50787	86.35%	2.253	BB
2	20.43	41735	1147	3.28%	2.21	BB
3	25.79	100218	1907	7.87%	2.037	BB
4	28.36	31871	634	2.50%	2.167	BB
Total		1,273,518	54,475	100.00%		



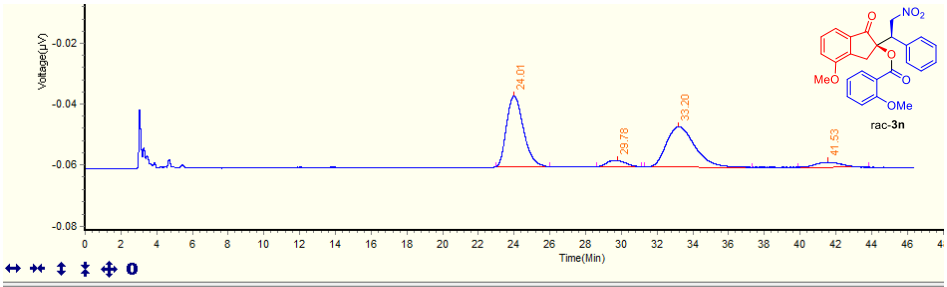
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.79	160419	10078	7.07%	0.722	BB
2	9.59	983553	53340	43.37%	1.408	BB
3	11.42	958588	37920	42.27%	1.53	BB
4	12.85	165204	7022	7.28%	1.073	BB
Total		2,267,764	108,360	100.00%		



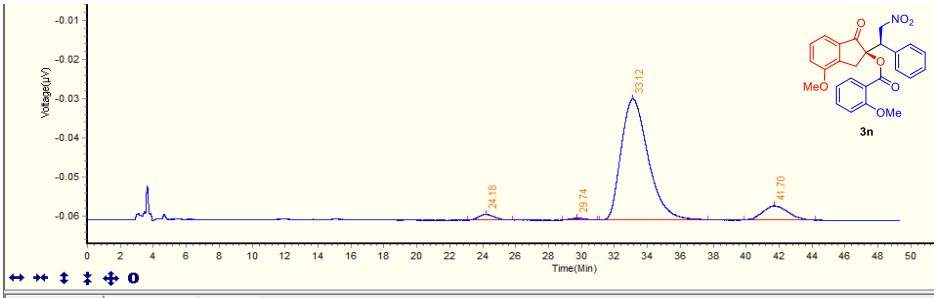
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.84	63405	4134	3.96%	0.92	BB
2	9.65	145660	8254	9.09%	1.052	BB
3	11.49	1259038	49239	78.61%	1.633	BB
4	12.94	133541	5631	8.34%	1.07	BB
Total		1,601,644	67,258	100.00%		



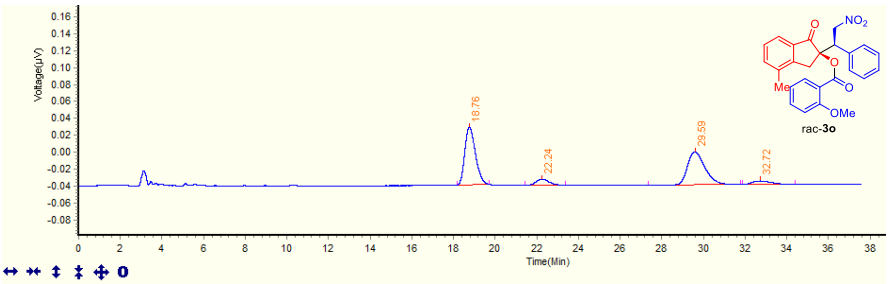
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	24.01	762352	11632	45.96%	3.012	BB
2	29.78	77978	1074	4.70%	2.509	BB
3	33.20	736054	6648	44.37%	6.023	BB
4	41.53	82403	831	4.97%	3.96	BB
Total		1,658,787	20,185	100.00%		



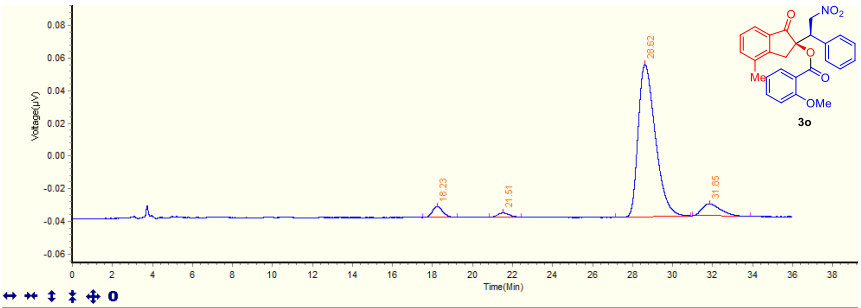
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	24.18	48087	750	2.39%	2.728	BB
2	29.74	14653	228	0.73%	2.136	BB
3	33.12	1755296	15462	87.27%	6.585	BB
4	41.70	193356	1819	9.61%	4.331	BB
Total		2,011,392	18,259	100.00%		



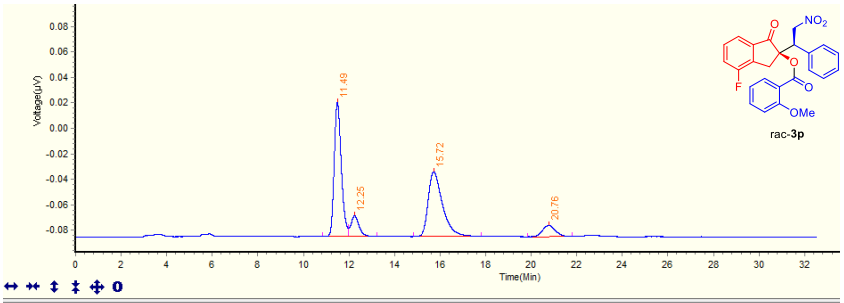
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	18.76	1210632	34188	46.12%	1.537	BB
2	22.24	153470	3615	5.85%	1.944	BB
3	29.59	1125876	19334	42.89%	4.43	BB
4	32.72	134752	2099	5.13%	2.532	BB
Total		2,624,730	59,236	100.00%		



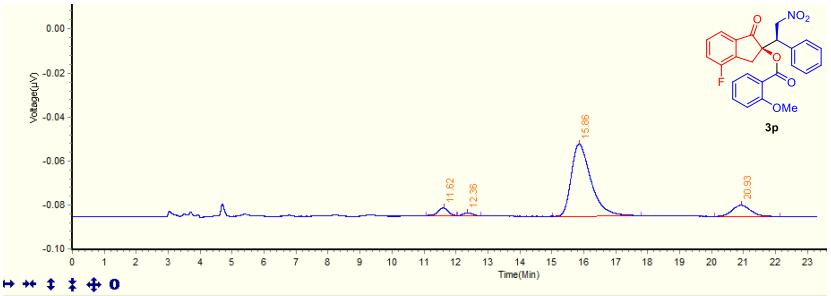
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	18.23	119611	3354	3.76%	1.728	BB
2	21.51	50242	1286	1.58%	1.599	BB
3	28.62	2775514	46494	87.16%	3.76	BB
4	31.85	239131	3679	7.51%	2.896	BB
Total		3,184,498	54,813	100.00%		



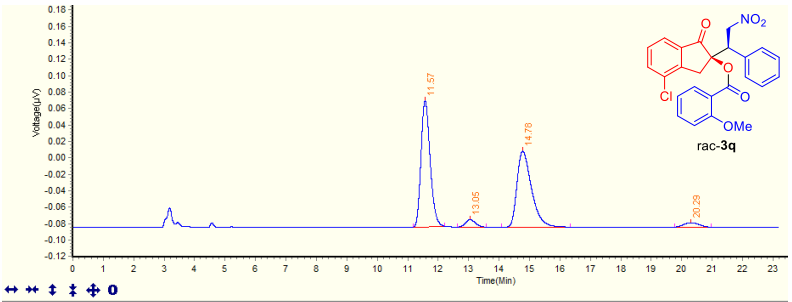
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.49	1141366	52799	43.47%	1.135	BV
2	12.25	202261	8097	7.70%	1.251	VB
3	15.72	1108311	25361	42.21%	2.974	BB
4	20.76	173772	4357	6.62%	1.956	BB
Total		2,625,710	90,614	100.00%		



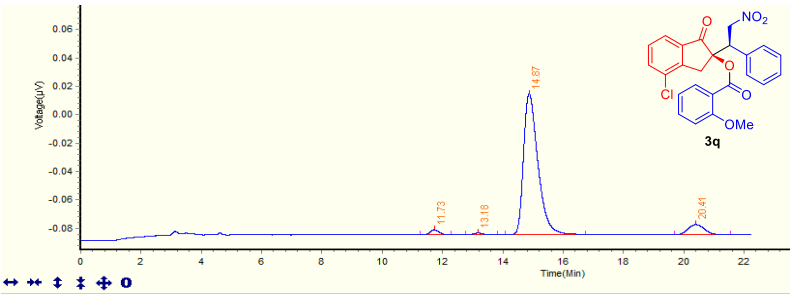
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Ty
1	11.62	37603	1747	4.44%	0.952	BB
2	12.36	13449	673	1.59%	0.728	BB
3	15.86	696160	16385	82.29%	2.774	BB
4	20.93	98803	2506	11.68%	2.046	BB
Total		846,015	21,311	100.00%		



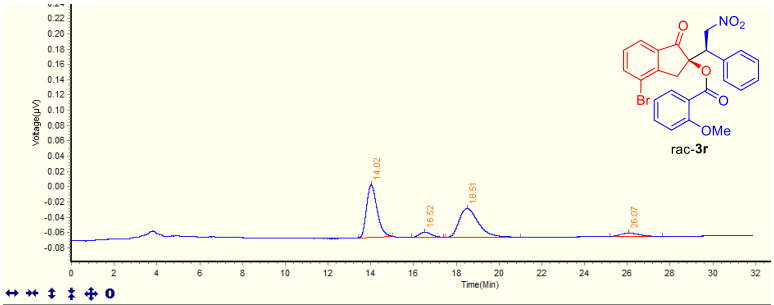
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width		Peak Ty
1	11.57	1597432	76583	47.92%	1.032	BB	
2	13.05	102453	4525	3.07%	0.947	BB	
3	14.78	1539290	46362	46.18%	2.259	BB	
4	20.29	94100	2664	2.82%	1.199	BB	
Total		3,333,275	130,134	100.00%			



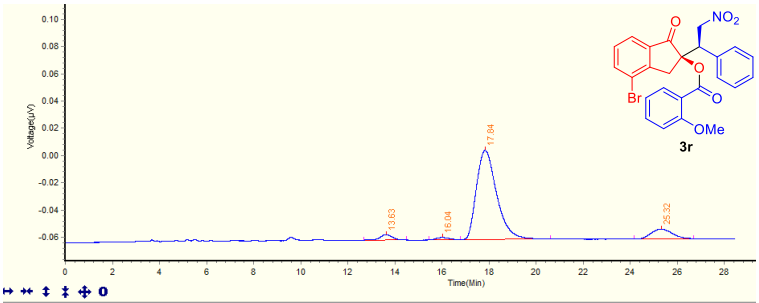
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	
1	11.73	36754	1787	2.01%	1.016	BB
2	13.18	13840	619	0.76%	1.043	BB
3	14.87	1643107	49692	89.87%	2.646	BB
4	20.41	134617	3598	7.36%	1.843	BB
Total		1,828,318	55,696	100.00%		



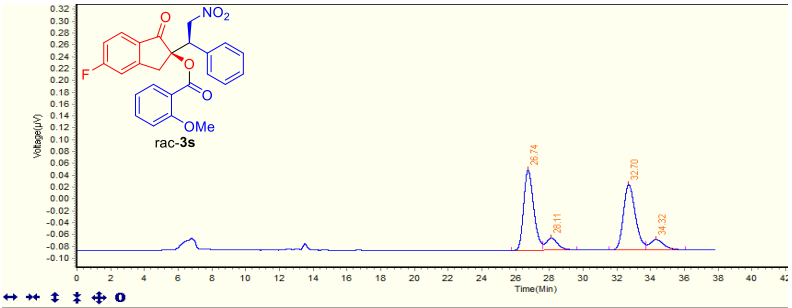
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width		Peak Type
1	14.02	1179250	34305	45.23%	1.61	BB	
2	16.52	133622	3410	5.13%	1.495	BB	
3	18.51	1163672	18844	44.64%	3.527	BB	
4	26.07	130447	2147	5.00%	2.453	BB	
Total		2,606,991	58,706	100.00%			



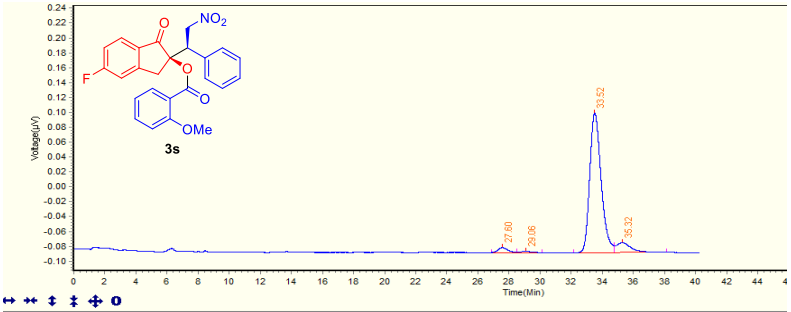
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width		Peak Type
1	13.63	73235	2000	3.21%	1.812	BB	
2	16.04	31829	868	1.40%	1.333	BB	
3	17.84	1948871	32684	85.52%	3.829	BB	
4	25.32	224824	3577	9.87%	2.529	BB	
Total		2,278,759	39,129	100.00%			



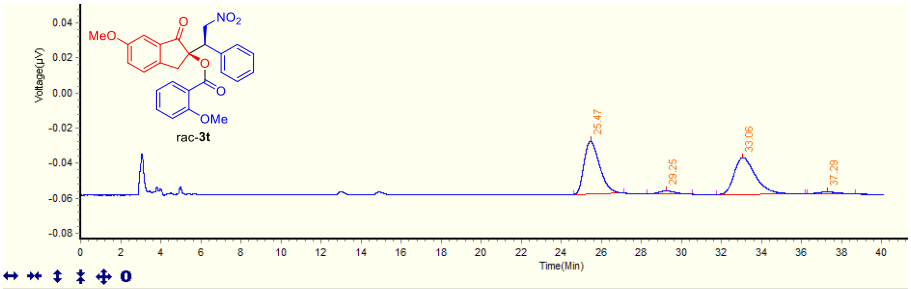
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	
1	26.74	2789534	67438	42.86%	1.855	BV
2	28.11	496274	10187	7.62%	2.018	VB
3	32.70	2718727	54952	41.77%	2.182	BV
4	34.32	504215	8578	7.75%	2.345	VB
Total		6,508,750	141,155	100.00%		



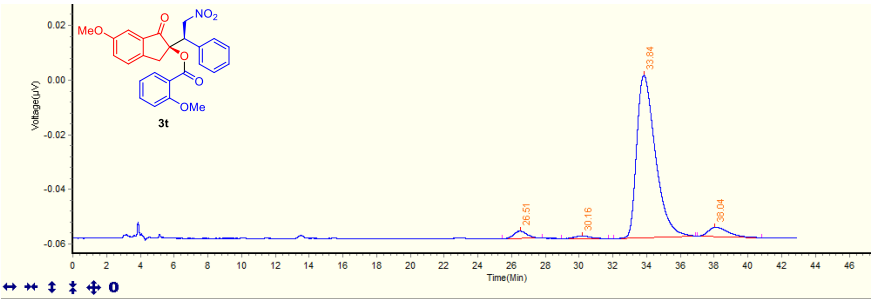
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	
1	27.60	137892	3261	2.56%	1.596	BV
2	29.06	37902	844	0.70%	1.644	VB
3	33.52	4780546	93666	88.61%	2.612	BV
4	35.32	438567	6597	8.13%	3.337	VB
Total		5,394,907	104,368	100.00%		



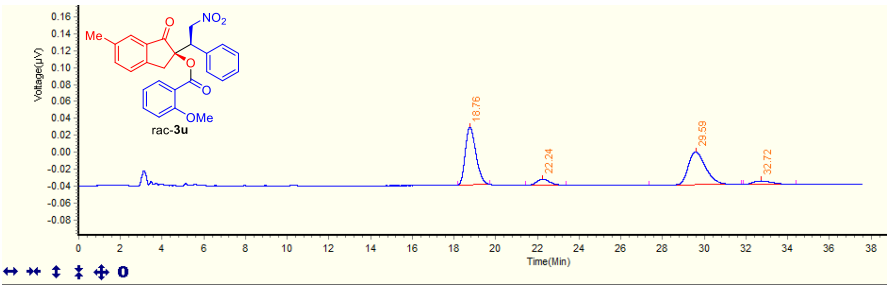
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	25.47	811501	15096	48.65%	2.504	BB
2	29.25	47993	848	2.88%	2.263	BB
3	33.06	770794	10443	46.21%	4.432	BB
4	37.29	37643	554	2.26%	2.408	BB
Total		1,667,931	26,941	100.00%		



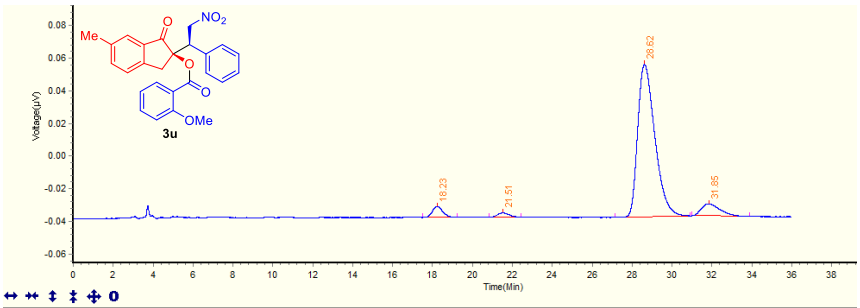
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	26.51	71934	1357	2.86%	2.373	BB
2	30.16	28210	484	1.12%	2.787	BB
3	33.84	2275659	29704	90.55%	4.85	BB
4	38.04	137425	1695	5.47%	3.818	BB
Total		2,513,228	33,240	100.00%		



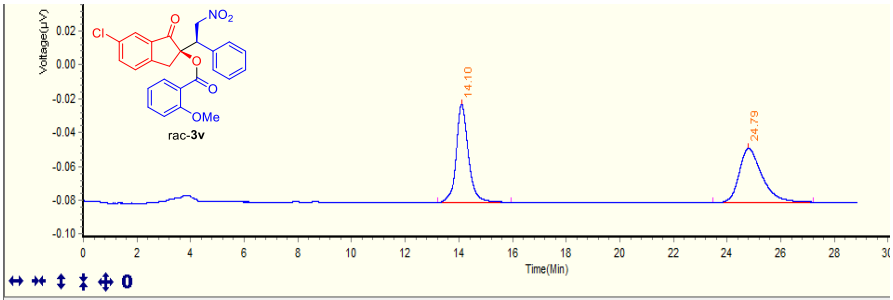
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	18.76	1210632	34188	46.12%	1.537	BB
2	22.24	153470	3615	5.85%	1.944	BB
3	29.59	1125876	19334	42.89%	4.43	BB
4	32.72	134752	2099	5.13%	2.532	BB
Total		2,624,730	59,236	100.00%		



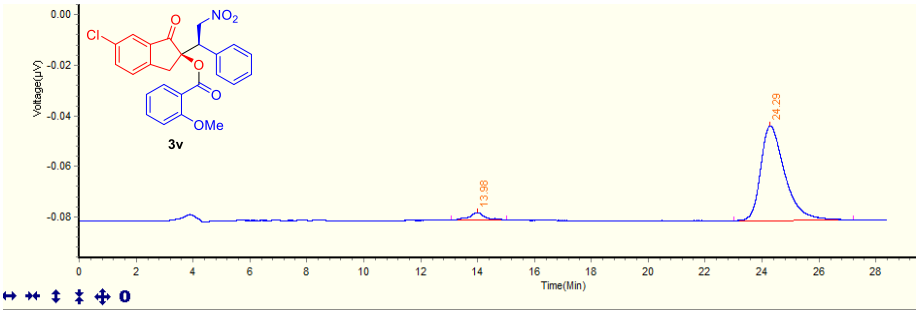
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	18.23	119611	3354	3.76%	1.728	BB
2	21.51	50242	1286	1.58%	1.599	BB
3	28.62	2775514	46494	87.16%	3.76	BB
4	31.85	239131	3679	7.51%	2.896	BB
Total		3,184,498	54,813	100.00%		



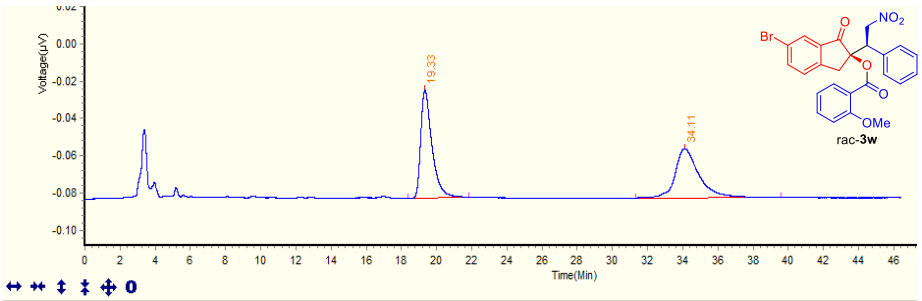
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	14.10	915632	29076	49.23%	2.738	BB
2	24.79	944321	15967	50.77%	3.743	BB
Total		1,859,953	45,043	100.00%		



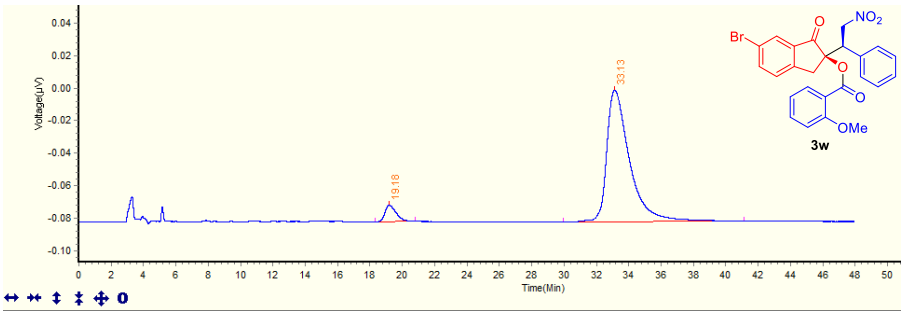
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.98	57539	1473	4.98%	1.946	BB
2	24.29	1098093	18730	95.02%	4.199	BB
Total		1,155,632	20,203	100.00%		



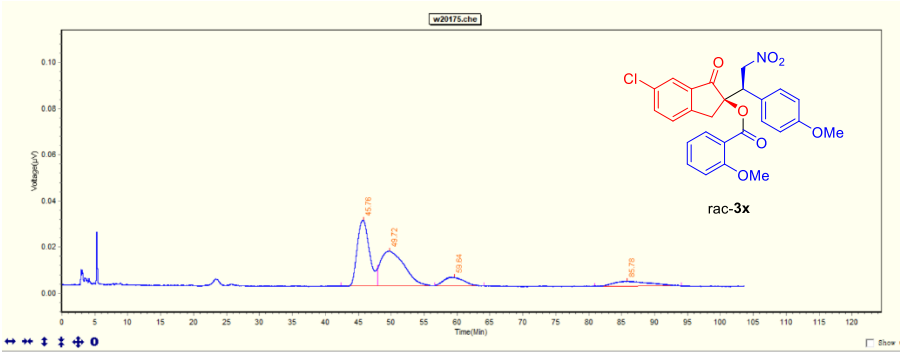
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Typ
1	19.33	1277470	28813	50.64%	3.463	BB
2	34.11	1245279	13145	49.36%	8.264	BB
Total		2,522,749	41,958	100.00%		



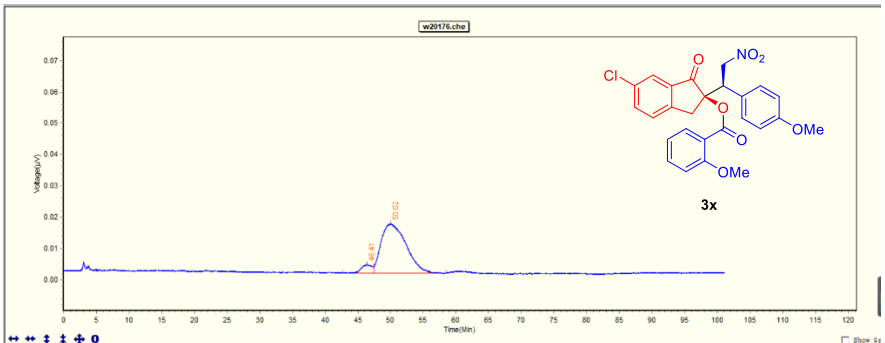
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	19.18	240333	4999	5.76%	2.477	BB
2	33.13	3931602	40358	94.24%	11.175	BB
Total		4,171,935	45,357	100.00%		



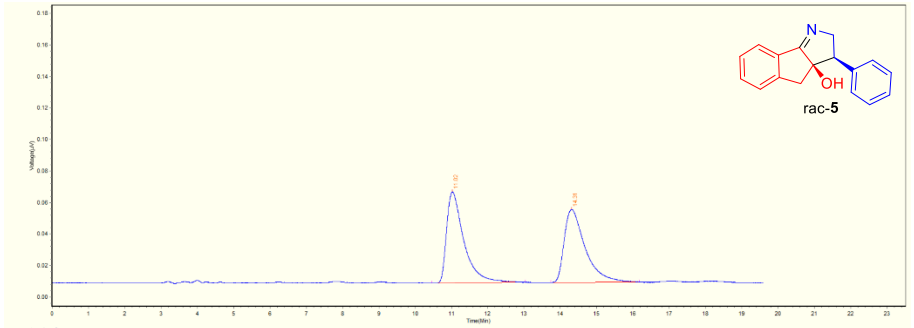
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	45.76	1849335	14257	41.17%	5.593	BV
2	49.72	1864062	7556	41.50%	8.605	VV
3	59.64	386956	1827	8.62%	7.529	VB
4	85.78	391238	1046	8.71%	13.123	BB
Total		4,491,591	24,686	100.00%		



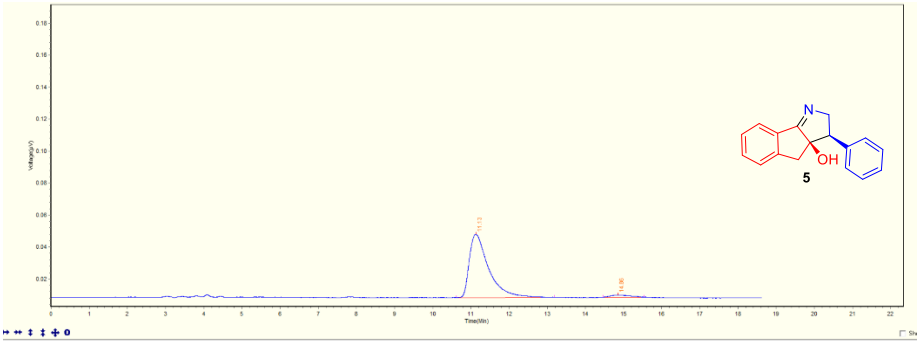
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	46.41	159681	1378	7.10%	4.797	BV
2	50.02	2089641	7856	92.90%	11.054	VB
Total		2,249,322	9,234	100.00%		



Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.02	953262	28869	50.64%	2.573	BB
2	14.31	929188	23205	49.36%	2.444	BB
Total		1,882,450	52,074	100.00%		



Integration Result | Calculation Result | TimeTable

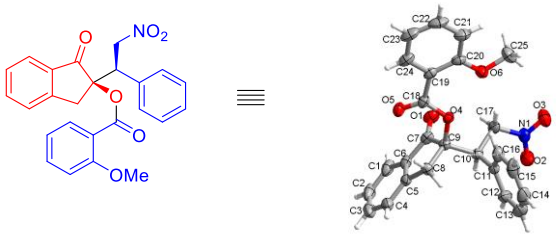
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.13	692870	19766	96.83%	2.566	BB
2	14.86	22706	656	3.17%	1.973	BB
Total		715,576	20,422	100.00%		

Single-crystal X-ray diffraction of 3f (CCDC 2097558)

3f with ellipsoid contour at 30% probability level

X-ray analysis was carried out using the single crystal which was grown in Hexane/DCM.

The instrumentation used for the crystal measurement is Oxford Gemini E X-ray single-crystal diffractometer.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 202107196

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 202107196

```
Bond precision:  C-C = 0.0069 A          Wavelength=1.54184

Cell:            a=10.1810(17)    b=11.2267(15)     c=10.4811(18)
                 alpha=90         beta=115.00(2)    gamma=90
Temperature:     293 K

                 Calculated                Reported
Volume           1085.7(3)                 1085.8(3)
Space group      P 21                      P 1 21 1
Hall group       P 2yb                     P 2yb
Moiety formula   C25 H21 N O6              C25 H21 N O6
Sum formula      C25 H21 N O6              C25 H21 N O6
Mr               431.43                    431.43
Dx,g cm-3        1.320                     1.320
Z                2                         2
Mu (mm-1)        0.784                     0.784
F000             452.0                     452.0
F000'            453.50
h,k,lmax         12,13,12                  12,13,12
Nref             4292[ 2261]               4074
Tmin,Tmax        0.910,0.932               0.886,1.000
Tmin'            0.896

Correction method= # Reported T Limits: Tmin=0.886 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.80/0.95      Theta(max)= 72.447

R(reflections)= 0.0450( 3373)     wR2(reflections)= 0.1157( 4074)

S = 1.039                 Npar= 290
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00688 Ang.
```

Alert level G

```
PLAT012_ALERT_1_G No        _shelx_res_checksum Found in CIF ......     Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT791_ALERT_4_G Model has Chirality at C9          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C10         (Sohnke SpGr)          R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         45 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 Check
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  8 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  3 ALERT type 2 Indicator that the structure model may be wrong or deficient
  1 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Density functional theory (DFT) calculations

Possible coordination modes of 1a with the catalyst.

During the complexation reaction, **1a** has to be deprotonated by the catalyst and forms intermediate 2. Either deprotonation of the hydroxyl group or deprotonation of the C-H bond connecting the hydroxyl group was possible. However, although the former could lead to a slightly more stable intermediate (**IN2_a**, **Figure S1** below), it could not undergo the subsequent Michael addition reaction to form the carbon-carbon bond. In other words, this is a non-productive intermediate. On the other hand, deprotonation of the C-H bond of **1a** would directly lead to the carbanion-coordinating complex. Our calculations indicate that this complex is high unstable (**IN2_b**, 9.5 kcal/mol). Alternatively, the carbanion could isomerize to the enolate form. Here possible coordination modes of the enolate to the catalyst have also been considered. We have calculated the structure with two oxygen atoms of **1a** binding with the two Zn centers, respectively (i.e., **IN2_c**). However, this structure cannot be located computationally, and it was optimized to the stable structure with one anionic oxygen binding with both Zn centers while the other oxygen of the OH group forming H-bonding with the catalyst (i.e., **IN2**).

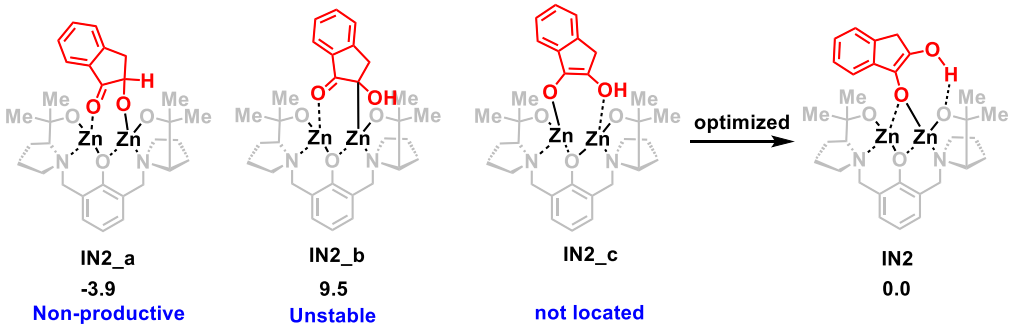


Figure S1. Possible coordination modes of **1a** with the catalyst.

Energetics and Cartesian Coordinates for All Calculated Species.

Species	Electronic Energy (EE)	High-Level Single Point Energies	△△E	△△H	△△G	Imaginary Frequency (cm-1*i)
1a	-498.259105	-498.033063	0.159095	0.160039	0.116882	
2a	-858.592412	-858.185074	0.243488	0.244433	0.181348	
IN1	-1404.063583	-1726.532555	0.626526	0.627470	0.529898	
IN2	-1822.578329	-2144.829011	0.707650	0.708594	0.601565	
IN2_a	-1822.589716	-2144.833095	0.707922	0.708867	0.599486	
IN2_b	-1822.558070	-2144.814598	0.708167	0.709111	0.602298	
TS3_RR	-2681.240572	-3003.023115	0.951920	0.952864	0.813867	-125.34
IN4_RR	-2681.258768	-3003.049348	0.955128	0.956072	0.815787	
TS3_SS	-2681.243807	-3003.020638	0.950655	0.951599	0.815145	-177.20
IN4_SS	-2681.262654	-3003.049930	0.955597	0.956542	0.818101	

1a

C	-0.33044200	0.53661600	-0.04551900
C	-0.49502000	-0.85684900	-0.00315400
C	-1.77942700	-1.39500100	0.04067000
C	-2.87277800	-0.52514500	0.05371700
C	-2.69872700	0.86735100	0.02765300
C	-1.41850000	1.41155500	-0.01810800
C	1.10916400	0.84290800	-0.09441400
C	1.84343600	-0.47528900	-0.38675200
C	0.84213500	-1.57111400	0.02871100
H	-1.93232300	-2.46993900	0.07046500
H	-3.87858800	-0.93369200	0.08796800
H	-3.56826500	1.51695000	0.04050600
H	-1.25321200	2.48409400	-0.04096700
H	1.97416900	-0.51468800	-1.48430100
H	1.08607000	-1.89365800	1.04757500
O	1.68567000	1.90177700	0.08871800
O	3.08097800	-0.54239900	0.27429600
H	3.36953900	0.38029100	0.37284200
H	0.87037700	-2.45458200	-0.61502700

2a

C	4.00479200	-1.87047100	0.04957700
C	4.22104700	-0.80114000	-0.82112100
C	3.30834500	0.24744000	-0.86886900
C	2.15537800	0.24215900	-0.05992100
C	1.95809900	-0.83605200	0.82571100
C	2.87629400	-1.87915500	0.87400000
H	4.71687000	-2.68875000	0.09401100
H	5.10033700	-0.78271100	-1.45714800
H	3.47490200	1.08156700	-1.54444800
H	1.11033100	-0.84439700	1.49746600
H	2.71524500	-2.70066300	1.56488100
C	1.23648600	1.36413000	-0.20463000
H	1.60910700	2.22220300	-0.75963300
C	-0.03692700	1.47700700	0.20773500
C	-0.87367500	0.49503000	1.00160500
N	-0.76795600	2.69760400	-0.12337300
O	-1.96290100	2.69819000	0.19056300
O	-0.18948800	3.62298900	-0.69023000
O	-0.80847700	0.51077800	2.22103600
C	-1.69513800	-0.48474900	0.25090500
C	-2.48647500	-1.38625600	0.97887100
C	-1.68688000	-0.53891500	-1.14929700
C	-3.26031400	-2.32871200	0.31238800
H	-2.47612300	-1.32270600	2.06141500
C	-2.46180600	-1.48590200	-1.81489500
H	-1.07152000	0.15335400	-1.71385600
C	-3.24833000	-2.37939800	-1.08554800
H	-3.87452500	-3.02412900	0.87588800
H	-2.45401100	-1.52664700	-2.89943100
H	-3.85336800	-3.11609000	-1.60553700

IN1

C	-0.07214800	1.38110400	-0.12626600
C	-1.18421300	2.08205200	0.39327600
C	-1.13999300	3.47998500	0.44215700
C	-0.03106400	4.18931400	-0.01258100

C	1.04784400	3.48769500	-0.55010100
C	1.04197700	2.09368200	-0.61946700
H	-1.99439100	4.01396800	0.85056100
H	1.90652600	4.02707200	-0.94183400
O	-0.02096400	0.02730900	-0.17305600
C	-2.40219600	1.35054300	0.89798800
H	-3.11029300	2.06531800	1.33548600
H	-2.12253700	0.65469400	1.69577700
C	-4.20893500	-0.28701100	0.34384300
C	-3.64552300	1.41448500	-1.22954400
C	-5.49478200	0.53861100	0.07152700
H	-4.04125100	-0.41772400	1.41674300
C	-5.03376900	1.79610800	-0.69897400
H	-3.73042300	0.84387900	-2.15651000
H	-2.98298900	2.26186300	-1.41147000
H	-6.20630700	-0.04187600	-0.51903300
H	-5.99976300	0.80065000	1.00403300
H	-5.71702600	2.07595400	-1.50476500
H	-4.95757400	2.65658900	-0.02697700
N	-3.06420600	0.54113100	-0.17751300
C	-4.17359100	-1.74118800	-0.25347600
O	-2.89473400	-2.30731000	-0.05502500
Zn	-1.59615000	-1.01367600	-0.38222200
H	-0.01418200	5.27283900	0.03778800
C	-4.50573700	-1.78880600	-1.75698800
H	-4.47512000	-2.83154800	-2.08184200
H	-5.48980300	-1.38050200	-2.00777200
H	-3.75185700	-1.24817300	-2.34132900
C	-5.18334100	-2.59032800	0.53164800
H	-6.20784700	-2.21604100	0.43155100
H	-5.15189900	-3.61879200	0.16371200
H	-4.91343700	-2.60298500	1.59143500
C	2.15586000	1.32818200	-1.28398800
H	2.73907800	2.00957400	-1.92042000
H	1.71228400	0.56647200	-1.92879900
C	3.94468800	-0.34917400	-1.10303500
C	3.93936900	1.51944400	0.39761700
C	5.35884500	0.29023000	-1.08657400
H	3.56531000	-0.38492500	-2.12769300
C	5.16240900	1.70272000	-0.50660200
H	4.22850500	1.04306700	1.34013900
H	3.40750800	2.44101700	0.64427400
H	6.03303100	-0.28335300	-0.44667200
H	5.80320200	0.30755900	-2.08501500
H	6.03711000	2.07272400	0.03608600
H	4.94189200	2.42378000	-1.30192700
N	3.04481700	0.59703500	-0.34163900
C	3.80079200	-1.81706200	-0.56451700
O	2.44774400	-2.10083700	-0.39225500
Zn	1.74637000	-0.79640300	0.86931200
C	4.56039900	-2.02558400	0.77068600
H	4.29845500	-3.01754600	1.14726300
H	5.65041600	-1.97208700	0.67875500
H	4.25151600	-1.29610600	1.53014500
C	4.39380500	-2.76087600	-1.62416700
H	5.44716700	-2.54308800	-1.84020100
H	4.31805200	-3.79401500	-1.27337000
H	3.81903700	-2.67796000	-2.55191500

C	1.43839000	-0.53051200	2.88334700
H	2.24093600	0.12263300	3.25709000
H	1.59178700	-1.49539400	3.38475100
C	0.08205400	0.05522800	3.29905700
H	-0.08773800	1.03763300	2.84207800
H	-0.74852000	-0.59466000	2.98819300
H	-0.02290900	0.18833600	4.38650600

IN2

C	0.93947100	-2.53397700	-0.15227600
C	2.32079500	-2.81694600	-0.02431700
C	2.75800700	-4.13777500	-0.16410600
C	1.86378900	-5.18096700	-0.38976700
C	0.50371900	-4.89403600	-0.48236900
C	0.02349700	-3.58580100	-0.37952200
H	3.82096700	-4.34741900	-0.07458100
H	-0.20774500	-5.69839500	-0.65108600
O	0.49491500	-1.27509400	-0.05233300
C	3.32925100	-1.76245600	0.37144700
H	4.33135600	-2.21091100	0.33981600
H	3.16546500	-1.46004900	1.41397600
C	4.40391700	0.43628800	0.08008500
C	3.58381500	-0.72710900	-1.86439200
C	5.44558100	0.53035400	-1.05939800
H	4.85122600	-0.04237300	0.95631800
C	5.10511100	-0.63515300	-2.00271600
H	3.09990500	0.06627500	-2.44403400
H	3.15141000	-1.68168500	-2.16969500
H	5.34683400	1.47822000	-1.59472100
H	6.46653900	0.48155900	-0.67396900
H	5.42675000	-0.46387500	-3.03343100
H	5.57286300	-1.56491000	-1.66024000
N	3.31736900	-0.49256400	-0.42135100
C	3.78885700	1.77051000	0.60259800
O	2.71182000	1.42384200	1.45776500
Zn	1.49735900	0.40207300	0.35366300
H	2.21988200	-6.20107600	-0.48524000
C	3.26461900	2.66837100	-0.53815100
H	2.69565100	3.48961400	-0.09751000
H	4.06040900	3.09349200	-1.15574300
H	2.58793500	2.12245100	-1.21207400
C	4.84278800	2.52748000	1.41525400
H	5.71818300	2.78856100	0.81029600
H	4.40439700	3.44838000	1.80902500
H	5.16729000	1.91763200	2.26329400
C	-1.44949900	-3.32887900	-0.59346800
H	-1.96333700	-4.29951500	-0.63890600
H	-1.61695100	-2.84920300	-1.56565300
C	-3.60202400	-2.36987100	0.07031600
C	-2.01607200	-2.95902900	1.79333600
C	-4.34000200	-2.96592100	1.28809000
H	-3.76613600	-3.01244100	-0.80111000
C	-3.27360700	-3.80435100	2.00826400
H	-2.01090000	-2.10698000	2.48260800
H	-1.07548000	-3.49874000	1.91905500
H	-4.69332900	-2.17425000	1.95437700
H	-5.21239800	-3.54876500	0.98297800
H	-3.49534900	-3.97558100	3.06541600

H	-3.15814000	-4.78344800	1.52916700
N	-2.12596500	-2.44550400	0.40331900
C	-3.97478600	-0.92721800	-0.39367700
O	-2.98217200	-0.50010400	-1.29602900
Zn	-1.36334100	-0.45666200	-0.27166400
C	-4.06284800	0.05365400	0.79812200
H	-4.11773800	1.07241500	0.40926200
H	-4.92904400	-0.12022000	1.44369300
H	-3.16991100	-0.00630500	1.44140000
C	-5.32347800	-0.96765300	-1.12065200
H	-6.12741100	-1.34724700	-0.47926100
H	-5.58826700	0.04042100	-1.45102000
H	-5.24648700	-1.60494600	-2.00651700
C	-1.75264500	3.17078600	-0.35109300
C	-1.82199100	4.51666100	0.07490600
C	-2.80039700	5.36761400	-0.40877500
C	-3.73112200	4.87736700	-1.33874900
C	-3.66278700	3.54904900	-1.76060800
C	-2.67526100	2.67919500	-1.27803700
C	-0.63261800	2.52075100	0.34055800
C	-0.01291300	3.43193600	1.14957800
C	-0.70903600	4.76882300	1.05983300
H	-2.84855900	6.40143600	-0.07509500
H	-4.50425700	5.53332500	-1.72803200
H	-4.38921100	3.17464200	-2.47711200
H	-2.67452300	1.64043000	-1.59262300
H	-0.01395500	5.54790100	0.71924500
O	-0.30121700	1.20168100	0.15092300
O	1.04912500	3.35085200	1.97192500
H	-1.07850200	5.08791600	2.04347100
H	1.66764800	2.57822200	1.79060000

IN2_a

C	-1.58798700	2.08470300	0.16939500
C	-0.98120400	3.33370800	-0.10459500
C	-1.69423800	4.50857400	0.14575000
C	-2.99829800	4.47940200	0.63694600
C	-3.59352400	3.24557000	0.89223000
C	-2.90814800	2.04702900	0.67771400
H	-1.21631900	5.46251700	-0.06371700
H	-4.60848900	3.20391000	1.28013100
O	-0.92399400	0.95120800	-0.05730100
C	0.38805000	3.40909600	-0.73188200
H	0.66253400	4.46549600	-0.85821500
H	0.35860400	2.97594400	-1.74014500
C	2.79546800	2.90503400	-0.65808200
C	1.61294900	3.15675600	1.39583400
C	3.48567000	4.03927400	0.14986400
H	2.58582100	3.22927300	-1.68123100
C	2.51140900	4.39547500	1.29405500
H	2.09814500	2.37215700	1.98141400
H	0.63084500	3.34670200	1.83208200
H	4.44170900	3.69531200	0.54993800
H	3.70148600	4.90439000	-0.48225500
H	3.02050300	4.61678900	2.23609600
H	1.91154900	5.27462700	1.03585600
N	1.46241600	2.67477300	0.00124400
C	3.58860000	1.56106300	-0.82467500

O	2.73701300	0.60783100	-1.38768600
Zn	1.04486900	0.56673800	-0.47548400
H	-3.54039100	5.40146900	0.81776700
C	4.15866900	1.02466000	0.50816200
H	4.66431200	0.07796300	0.29871100
H	4.88136300	1.69601300	0.98404900
H	3.36368000	0.80563300	1.22644000
C	4.75078900	1.83194500	-1.79477500
H	5.44588000	2.59236400	-1.41930700
H	5.30732400	0.90429900	-1.95526300
H	4.35803900	2.16004500	-2.76217500
C	-3.55164500	0.73850300	1.05881400
H	-4.55665800	0.93826800	1.45444500
H	-2.98754600	0.26566200	1.87240000
C	-4.35600800	-1.51014200	0.45906700
C	-4.38256300	0.21071900	-1.20929900
C	-5.75672600	-1.47472700	-0.20608500
H	-4.44767600	-1.40831500	1.54411500
C	-5.84831300	-0.10008600	-0.89311800
H	-4.05809600	-0.34657000	-2.09390200
H	-4.16488300	1.26731300	-1.37451300
H	-5.84768300	-2.27092300	-0.94923600
H	-6.55227900	-1.63000300	0.52665600
H	-6.47964900	-0.10563000	-1.78600200
H	-6.25404700	0.65352300	-0.20933900
N	-3.62349000	-0.28364600	-0.03348300
C	-3.48717700	-2.79297900	0.24789000
O	-2.21142100	-2.55366100	0.77277300
Zn	-1.53309100	-0.97990400	-0.08847200
C	-3.36759100	-3.17798400	-1.24508700
H	-2.66154700	-4.00842700	-1.32369500
H	-4.31168300	-3.48505300	-1.70660200
H	-2.96142100	-2.34985400	-1.84230200
C	-4.14227400	-3.94657800	1.02096700
H	-5.15789600	-4.16323100	0.66970500
H	-3.53535800	-4.84905800	0.90726000
H	-4.18189100	-3.70058300	2.08634100
C	3.00480300	-2.65580900	0.80802900
C	3.17835000	-3.29339900	-0.43562500
C	4.27066900	-4.13841700	-0.61998800
C	5.17310600	-4.31206800	0.43195200
C	5.00508300	-3.65098000	1.65949800
C	3.91724200	-2.80658200	1.85527000
C	1.80903500	-1.82191000	0.71689800
C	1.00502100	-2.28449500	-0.50351700
C	2.11345300	-2.86469900	-1.42043000
H	4.42781800	-4.64356400	-1.56836600
H	6.02949000	-4.96640600	0.29627200
H	5.72848500	-3.80312800	2.45425500
H	3.76340800	-2.28183600	2.79266600
H	0.37724200	-3.12083600	-0.14441600
H	2.48993500	-2.04035400	-2.03831600
O	1.50744400	-0.82407400	1.38170900
O	0.21690800	-1.26291800	-1.02416900
H	1.76589600	-3.66982300	-2.07292900

IN2_b

C	0.71431600	2.35538200	-1.09506000

C	2.12659900	2.21245300	-1.01926600
C	2.89263300	3.24448900	-0.47256600
C	2.30127100	4.36496700	0.11227000
C	0.91222500	4.41170200	0.20376100
C	0.11116700	3.41343200	-0.35817400
H	3.97650400	3.15497600	-0.48654200
H	0.43398500	5.22979100	0.73787900
O	-0.00912400	1.49531400	-1.79686300
C	2.76717700	0.91393800	-1.43542700
H	3.76484600	1.10250000	-1.84883700
H	2.16088300	0.42006800	-2.19573200
C	-1.38454600	3.51612100	-0.19545300
H	-1.61599000	4.34814100	0.48378200
H	-1.83415000	3.75808400	-1.16590700
C	-2.08227700	1.81668800	1.69922400
C	-3.60444500	2.61432400	0.05669700
C	-3.37410800	0.96372100	1.80641400
H	-2.13433600	2.68558800	2.37079000
C	-4.35989500	1.47814800	0.73660000
H	-3.80753700	2.70759100	-1.01369100
H	-3.83891900	3.58059500	0.52794300
H	-3.13467300	-0.08220300	1.60439900
H	-3.78254700	1.01152500	2.81711400
H	-4.59740600	0.68211400	0.02392900
H	-5.30536100	1.82692600	1.15774300
C	3.59332000	-1.30889300	-0.66405900
C	3.70447000	0.45091300	0.83809200
C	5.07296200	-0.86321000	-0.69689500
H	3.23805000	-1.59054500	-1.65867300
C	5.16437100	0.25442900	0.37558900
H	3.48218200	-0.18703700	1.69551400
H	3.44262200	1.47669500	1.08933200
H	5.76066200	-1.68666200	-0.50999000
H	5.32119800	-0.46550000	-1.68556900
H	5.80587000	-0.02561300	1.21475300
H	5.57429400	1.17568400	-0.04977600
N	-2.16278500	2.31215800	0.26795400
N	2.85934800	-0.05226300	-0.27976100
C	-0.81157500	0.95329000	2.05825100
C	3.24187600	-2.52821700	0.34242300
O	-0.55031100	0.11035000	0.95353700
O	2.15799700	-2.24211500	1.18037000
Zn	-1.42912800	0.63810800	-0.77057400
Zn	1.02000300	-0.94268100	0.37757000
H	2.91069200	5.15995800	0.52832500
C	4.42353700	-2.91703800	1.25271900
H	4.06297500	-3.69410000	1.93109400
H	5.28223500	-3.31828300	0.70456600
H	4.75969000	-2.07649200	1.86588700
C	2.89868700	-3.73341900	-0.55781700
H	3.71528000	-3.97893900	-1.24933700
H	2.69788800	-4.60948400	0.06589800
H	2.00003900	-3.51236200	-1.14191500
C	0.41614700	1.80153700	2.41329300
H	1.22818500	1.13422500	2.72000300
H	0.76381700	2.39819900	1.57824200
H	0.20053100	2.46917900	3.25480200
C	-1.11405800	0.07199400	3.28780900

H	-1.44426200	0.66821600	4.14589200
H	-1.86492900	-0.68733900	3.06951200
H	-0.19539600	-0.44873200	3.57226900
C	-2.05344600	-2.38740500	-0.46973100
C	-3.38794600	-2.22018900	-0.88335000
C	-4.42115700	-2.74294300	-0.11683700
C	-4.10059500	-3.45757400	1.04675900
C	-2.76864500	-3.64231400	1.43501700
C	-1.72404600	-3.10430600	0.67732600
C	-1.16131300	-1.66068100	-1.40448900
C	-1.99679500	-0.91888700	-2.27549100
C	-3.43190700	-1.39295500	-2.15286800
H	-5.45874300	-2.61056600	-0.41180500
H	-4.89797300	-3.87850400	1.65197400
H	-2.54569800	-4.20587300	2.33587900
H	-0.68544500	-3.23138700	0.97153000
H	-3.69731200	-2.01426100	-3.02028100
O	0.12513000	-1.61953200	-1.34812500
O	-1.58141900	-0.31833900	-3.44803700
H	-4.17129200	-0.58372000	-2.11333500
H	-0.69484800	0.05309300	-3.29053700

TS3_RR

C	-3.23689300	1.02307800	-0.18141900
C	-4.07450700	-0.10886500	0.01168900
C	-5.36994200	0.07408200	0.51039000
C	-5.85441500	1.32756200	0.86614100
C	-5.01145300	2.42739400	0.72978900
C	-3.72224500	2.29476900	0.21597600
H	-6.00294700	-0.80121500	0.63387300
H	-5.35403900	3.41583700	1.02471000
O	-2.01692300	0.92742000	-0.74537300
C	-3.62340900	-1.53806500	-0.19925400
H	-4.50142500	-2.19527300	-0.13729700
H	-2.95786500	-1.84778100	0.61819200
C	-2.52801900	-3.22840300	-1.64058400
C	-3.68377800	-1.40640200	-2.66133700
C	-3.54614100	-3.81101800	-2.65656400
H	-2.63458100	-3.70110100	-0.66027000
C	-4.51699800	-2.65467000	-2.97095500
H	-3.00555500	-1.17895400	-3.48784600
H	-4.26959400	-0.51182700	-2.44730400
H	-3.03576200	-4.13842900	-3.56565400
H	-4.06115700	-4.68469900	-2.25047300
H	-4.88076900	-2.66999500	-4.00169500
H	-5.39298700	-2.69283800	-2.31496200
N	-2.88009800	-1.77870400	-1.47082700
C	-1.02132400	-3.37869400	-2.00517100
O	-0.29864200	-2.65360000	-1.02647100
Zn	-1.03828500	-0.85017300	-0.83164700
H	-6.86163700	1.44284200	1.25214600
C	-0.66698100	-2.82376000	-3.39785300
H	0.41151800	-2.91991300	-3.54621800
H	-1.17178600	-3.34701700	-4.21495800
H	-0.91075800	-1.75807800	-3.47519300
C	-0.62858000	-4.85742000	-1.91393000
H	-1.15250200	-5.46746700	-2.65741800
H	0.44757800	-4.95990000	-2.07582000

H	-0.85550000	-5.24819600	-0.91799200
C	-2.83541900	3.50816800	0.11151000
H	-3.40814400	4.40846700	0.38048200
H	-2.47800400	3.62611900	-0.91293000
C	-0.75949600	4.60186200	1.01917400
C	-1.96672400	3.09319200	2.38835000
C	0.17196400	4.25546200	2.19676600
H	-1.36966600	5.48196700	1.28196300
C	-0.66179700	3.36816400	3.15112400
H	-2.31335000	2.06240000	2.47471000
H	-2.77769700	3.75488700	2.73167900
H	1.03264100	3.68833100	1.83348800
H	0.55691400	5.15820800	2.67550900
H	-0.13366300	2.43462900	3.35397600
H	-0.86531100	3.85758400	4.10683800
N	-1.64135000	3.39953600	0.98006700
C	-0.04292500	4.85902100	-0.36397000
O	0.15552900	3.65957400	-1.05255000
Zn	-0.37244600	2.04041900	-0.14489800
C	1.32179300	5.54251200	-0.12576100
H	1.74418000	5.82562700	-1.09465200
H	1.23709300	6.44841500	0.48615700
H	2.02367900	4.85763600	0.35454600
C	-0.88204900	5.82803900	-1.22602400
H	-0.97315300	6.81168800	-0.75002800
H	-0.38476200	5.95536400	-2.19152200
H	-1.88774300	5.45218100	-1.41963300
C	2.94652800	1.12784400	-1.73457600
C	4.19964800	0.49754200	-1.88928700
C	5.34548400	1.25717500	-2.07883500
C	5.22183700	2.64963600	-2.14717800
C	3.97136300	3.26849600	-2.02331900
C	2.81391800	2.51900000	-1.81320600
C	1.92787900	0.10704700	-1.46917200
C	2.62779300	-1.18260200	-1.30236300
C	4.04653600	-0.99596100	-1.81327400
H	6.31602100	0.78016800	-2.17680400
H	6.10864000	3.25797300	-2.30104100
H	3.89940500	4.35044700	-2.08000700
H	1.84742700	3.00913800	-1.68871300
H	4.09260900	-1.45001000	-2.81163400
O	0.67280700	0.30931800	-1.37074200
O	2.10713300	-2.38074700	-1.45862900
H	4.79603000	-1.49320000	-1.19582400
H	1.07079600	-2.49238600	-1.25519800
C	6.77461200	-2.10392900	1.67005500
C	5.76352700	-3.04644200	1.46682000
C	4.45639800	-2.64779100	1.19884300
C	4.12704700	-1.27897200	1.14586600
C	5.16341300	-0.33940700	1.33464100
C	6.46898400	-0.74443000	1.59735600
H	7.79113600	-2.42649100	1.87504000
H	5.99646900	-4.10658900	1.50617400
H	3.68481600	-3.37864200	1.00639500
H	4.93170700	0.71967900	1.27200300
H	7.24490900	0.00099200	1.74455300
C	2.80794600	-0.72351400	0.79818400
H	2.85493700	0.35728900	0.79819600

C	1.49327300	-1.12513800	1.29553100
C	1.04700900	-2.51106900	1.60454800
N	0.56229000	-0.15236500	1.31324200
O	-0.71117900	-0.42078400	1.25798700
O	0.88502500	1.11295200	1.27628900
O	1.66356500	-3.48103400	1.18183800
C	-0.13699800	-2.74165300	2.49236400
C	-0.36580300	-1.99790200	3.65443800
C	-0.99712900	-3.79283200	2.15878100
C	-1.45688600	-2.29402500	4.46769000
H	0.30718200	-1.18736200	3.91744800
C	-2.10345200	-4.07088100	2.95904300
H	-0.78724700	-4.36210700	1.26125600
C	-2.33527100	-3.32157400	4.11519100
H	-1.62773700	-1.71903900	5.37273400
H	-2.77933300	-4.87711400	2.68845700
H	-3.19342400	-3.54143100	4.74337400

IN4_RR

C	-3.38294500	-0.12168000	-0.19274300
C	-3.77017800	-1.48177200	-0.05154700
C	-5.04154200	-1.78388100	0.45052800
C	-5.92714600	-0.79463000	0.86313200
C	-5.51917900	0.53446200	0.78670900
C	-4.27137200	0.88281200	0.27090400
H	-5.32819200	-2.82948800	0.53212400
H	-6.17849600	1.32691700	1.13144400
O	-2.21608700	0.23682800	-0.76278800
C	-2.84317600	-2.65123000	-0.30465000
H	-3.43373300	-3.57767700	-0.27988100
H	-2.11993700	-2.73853800	0.51815100
C	-1.19159200	-3.79176200	-1.75324300
C	-2.91598100	-2.47845600	-2.76229500
C	-1.89673400	-4.65605700	-2.83148100
H	-1.16032900	-4.31447700	-0.79320900
C	-3.22549200	-3.93351100	-3.12919900
H	-2.35715700	-1.98858200	-3.56429000
H	-3.79299500	-1.86949800	-2.53896400
H	-1.28527500	-4.71383000	-3.73523900
H	-2.05028500	-5.68109000	-2.48592900
H	-3.55043200	-4.04425500	-4.16718700
H	-4.02921800	-4.31833700	-2.49234800
N	-2.04852000	-2.57114000	-1.56242000
C	0.28235100	-3.37283900	-2.04243900
O	0.66447900	-2.47421300	-1.02240300
Zn	-0.65584400	-1.06097300	-0.87589600
H	-6.90688400	-1.05456400	1.24957500
C	0.45844700	-2.68464500	-3.41104100
H	1.49313800	-2.34481600	-3.49502500
H	0.23790000	-3.33827200	-4.26020700
H	-0.17945400	-1.79657900	-3.49407600
C	1.17878600	-4.61409100	-1.96309000
H	0.93164400	-5.35169300	-2.73447200
H	2.22281500	-4.31526200	-2.08741100
H	1.08290000	-5.08674800	-0.98131900
C	-3.85867600	2.33167300	0.24009600
H	-4.70507400	2.96535900	0.54379900
H	-3.55911800	2.61950000	-0.76884800

C	-2.26456000	4.02283400	1.21448100
C	-2.89797900	2.15715600	2.51909100
C	-1.26893400	3.96805800	2.39488400
H	-3.13406100	4.63591200	1.50199000
C	-1.69751200	2.75607300	3.26040700
H	-2.94465400	1.06850600	2.56773500
H	-3.84962500	2.55922300	2.90226700
H	-0.25329100	3.80991300	2.02662700
H	-1.27012900	4.90962900	2.94807900
H	-0.88669800	2.02484100	3.30907500
H	-1.95970300	3.03445100	4.28387100
N	-2.69872900	2.59675700	1.12498400
C	-1.68775300	4.55375000	-0.16040000
O	-1.14718000	3.50808700	-0.91214200
Zn	-1.05627700	1.79962900	-0.01130800
C	-0.59648700	5.61494200	0.10021300
H	-0.31782100	6.07147600	-0.85429600
H	-0.93430100	6.41275400	0.77250300
H	0.30114600	5.15555100	0.51915000
C	-2.81025700	5.25039700	-0.96127000
H	-3.18278400	6.14019300	-0.43975400
H	-2.40752400	5.55996000	-1.92963900
H	-3.65837000	4.59035900	-1.15102100
C	2.29820000	2.23782400	-1.87088800
C	3.70134300	2.16296500	-1.95155500
C	4.43562000	3.30145500	-2.26719900
C	3.74663000	4.49361400	-2.50604400
C	2.34635500	4.55900300	-2.42679000
C	1.59749200	3.43051600	-2.11047900
C	1.77928000	0.93905200	-1.48629200
C	2.97493200	0.03495400	-1.04543400
C	4.18767400	0.76708300	-1.68354600
H	5.51902100	3.26560300	-2.32929300
H	4.30747300	5.39100600	-2.75252400
H	1.84353800	5.50546400	-2.59903300
H	0.51707400	3.48687300	-1.97693000
H	4.41896700	0.24429900	-2.61736500
O	0.57680400	0.59678100	-1.53148000
O	2.89044500	-1.25605900	-1.54961900
H	5.08003700	0.73600400	-1.05672600
H	2.05397900	-1.74452800	-1.25917400
C	6.87438500	-1.10890100	2.25483100
C	6.37117700	-1.78833700	1.14322400
C	5.15052100	-1.42165100	0.57990400
C	4.42116500	-0.35210000	1.11511700
C	4.93746000	0.33086900	2.22237100
C	6.15147300	-0.04721600	2.79720700
H	7.82289400	-1.40483100	2.69348200
H	6.92722400	-2.61857900	0.71756400
H	4.74583600	-1.95839900	-0.26758200
H	4.38034600	1.16669900	2.63915000
H	6.53314300	0.49270400	3.65887500
C	3.09716400	0.13023300	0.54664500
H	3.03539200	1.19608600	0.77415600
C	1.87010400	-0.50083200	1.16714200
C	1.79670400	-1.94231800	1.52025400
N	0.77806100	0.25063800	1.18079400
O	-0.43661100	-0.25540100	1.16184400

O	0.81189700	1.54577600	1.03234600
O	2.67187500	-2.70420900	1.13398200
C	0.69136300	-2.46021900	2.38752000
C	0.21637500	-1.76933400	3.50705600
C	0.16362700	-3.71647300	2.07164100
C	-0.79184800	-2.32223200	4.29254800
H	0.63438700	-0.79986100	3.76045500
C	-0.86221600	-4.25847300	2.84409900
H	0.56076300	-4.23493300	1.20742000
C	-1.34312700	-3.56090000	3.95472600
H	-1.15371600	-1.78544700	5.16424300
H	-1.28144100	-5.22678400	2.58610400
H	-2.13963400	-3.98352700	4.55996200

TS3_SS

C	1.01115700	-2.62752500	-0.59661800
C	0.20265900	-3.67581900	-1.10197000
C	0.46530300	-5.00002300	-0.74110500
C	1.52812000	-5.32209500	0.09758500
C	2.34445200	-4.29335800	0.56216200
C	2.10977600	-2.95481600	0.23881400
H	-0.17418300	-5.78501400	-1.13731600
H	3.19090700	-4.52529600	1.20331900
O	0.71015700	-1.35592500	-0.92060100
C	-0.93960600	-3.37151200	-2.03217900
H	-1.30590800	-4.30499100	-2.47963400
H	-0.59905000	-2.73021800	-2.85219200
C	-3.19001200	-2.39604400	-2.31514200
C	-2.64540800	-3.42498200	-0.24473900
C	-4.20233200	-3.55317000	-2.09982800
H	-2.76649900	-2.42503500	-3.32279800
C	-3.65717800	-4.36920100	-0.90622700
H	-3.13244600	-2.73487500	0.44443600
H	-1.85467500	-3.93920300	0.30168800
H	-5.19720000	-3.15887600	-1.88285700
H	-4.29663400	-4.16708900	-2.99866100
H	-4.44153900	-4.68014500	-0.21141700
H	-3.15614000	-5.27785300	-1.25533000
N	-2.05791600	-2.63807500	-1.35999400
C	-3.76074400	-0.95741700	-2.15772100
O	-2.63695900	-0.08268300	-2.24433700
Zn	-1.20519900	-0.65475300	-0.99593600
H	1.72927800	-6.35335100	0.36776900
C	-4.50401600	-0.71352100	-0.83030700
H	-4.89783600	0.30501900	-0.81874000
H	-5.34357700	-1.40095400	-0.69372900
H	-3.84002000	-0.79851100	0.03229100
C	-4.69074100	-0.66522300	-3.34062600
H	-5.56645800	-1.32272600	-3.34498400
H	-5.04010600	0.36904600	-3.28058000
H	-4.15238400	-0.78847500	-4.28488300
C	3.03918900	-1.90370800	0.79794400
H	3.85871200	-2.40791100	1.32943100
H	2.52119000	-1.27697300	1.53075500
C	4.53464100	-0.00418500	0.19889200
C	4.25913800	-1.73461700	-1.34002200
C	5.85708200	-0.79611800	0.26517100
H	4.21485100	0.33345300	1.18738400

C	5.72126700	-1.86983700	-0.84694000
H	4.19927300	-1.12258100	-2.24131300
H	3.77394700	-2.68994400	-1.54075500
H	6.73409600	-0.16031600	0.13987400
H	5.95242100	-1.27446700	1.24527000
H	6.42674400	-1.70768300	-1.66545200
H	5.91108000	-2.87160100	-0.45054700
N	3.53898000	-1.00734000	-0.26749400
C	4.51795900	1.27435000	-0.76383500
O	3.31324400	1.36236100	-1.47456900
Zn	1.87425200	0.33090400	-0.71901500
C	5.66008000	1.28806400	-1.80057800
H	5.52231000	2.17612700	-2.42267500
H	6.65469600	1.34541000	-1.34677600
H	5.62610100	0.41974000	-2.46213900
C	4.68293800	2.50379200	0.15381600
H	5.58767900	2.43089400	0.77092100
H	4.75831400	3.41291200	-0.45078100
H	3.81549700	2.59671900	0.81223900
C	0.22007500	3.62000200	-1.09929900
C	-0.64248200	4.72172900	-0.92534400
C	-0.13506200	6.01122500	-0.85633600
C	1.24239700	6.19759900	-1.01082200
C	2.09133200	5.10542500	-1.22930200
C	1.59763200	3.80398700	-1.27422500
C	-0.56645700	2.38640200	-1.07650400
C	-1.96062700	2.73482300	-0.85760500
C	-2.06741100	4.25993900	-0.83305400
H	-0.79501300	6.85993000	-0.70061400
H	1.65556000	7.20139600	-0.97093100
H	3.15676500	5.27126500	-1.35642700
H	2.27710400	2.96548700	-1.42734400
H	-2.57562100	4.65128300	0.05274500
O	-0.09456400	1.19044300	-1.17267100
O	-3.01491500	2.05789400	-1.22881300
H	-2.65764500	4.57033900	-1.70351900
H	-2.84507400	1.05677400	-1.73938000
C	-5.49328900	1.43885000	2.93771300
C	-5.35087300	2.33458700	1.88007000
C	-4.09139000	2.62485300	1.35837100
C	-2.92840200	2.02160200	1.87186800
C	-3.09643000	1.13588100	2.95689900
C	-4.35158900	0.84899800	3.48178400
H	-6.47602000	1.21177700	3.33994200
H	-6.22535500	2.81295200	1.44888900
H	-4.03210100	3.30557500	0.52527200
H	-2.22779400	0.68757900	3.42328200
H	-4.43420900	0.16798100	4.32374600
C	-1.56424300	2.33078400	1.36149100
H	-1.23330500	3.35839000	1.46734500
C	-0.50662000	1.38492800	1.61364400
C	-0.69303400	-0.04258900	1.70808200
N	0.80446400	1.85444500	1.66357400
O	1.75258300	1.03181200	1.34616100
O	1.06467700	3.02954700	1.94041900
O	-1.58944700	-0.61868200	1.01903800
C	0.03681800	-0.86179300	2.70545200
C	0.01102500	-2.25658100	2.56665900

C	0.69913300	-0.29457400	3.80836200
C	0.67080200	-3.07028100	3.48276800
H	-0.50956100	-2.68553300	1.72203400
C	1.35388800	-1.10866000	4.72496400
H	0.69330500	0.78016800	3.95072600
C	1.34916400	-2.49799600	4.55958600
H	0.66732700	-4.14629700	3.34374500
H	1.86526900	-0.66295700	5.57221700
H	1.86692700	-3.13025600	5.27476700

IN4_SS

C	1.48167000	-2.45275200	-0.32364100
C	0.90841100	-3.66887200	-0.77081500
C	1.36814900	-4.88879000	-0.26994100
C	2.41805900	-4.94047900	0.64264700
C	3.03048300	-3.74799300	1.02050900
C	2.59175400	-2.50325000	0.55975400
H	0.90469900	-5.80685100	-0.62291000
H	3.87613900	-3.77197200	1.70294800
O	0.95224800	-1.29517400	-0.76669600
C	-0.14538100	-3.64603500	-1.84323200
H	-0.27698600	-4.65840700	-2.24786400
H	0.18946100	-3.00683100	-2.66628100
C	-2.42856500	-3.06730200	-2.54757300
C	-2.09210400	-3.94630800	-0.35892700
C	-3.24428200	-4.38508900	-2.45396500
H	-1.82796600	-3.04197100	-3.46041500
C	-2.81165000	-5.06079600	-1.13158100
H	-2.79647300	-3.33670600	0.20859300
H	-1.33005900	-4.30659300	0.33391600
H	-4.31588100	-4.17713000	-2.45720800
H	-3.04776800	-5.03009800	-3.31390900
H	-3.65495300	-5.46737700	-0.56746100
H	-2.12578600	-5.89097700	-1.32826900
N	-1.46049600	-3.09311700	-1.39733900
C	-3.24819300	-1.73817100	-2.57309700
O	-2.32437700	-0.67041400	-2.48372800
Zn	-1.08144100	-0.99754900	-0.98814400
H	2.77525100	-5.89081800	1.02517400
C	-4.28445200	-1.64444000	-1.43314400
H	-4.85990300	-0.72326300	-1.55021900
H	-4.98842000	-2.48187500	-1.43300900
H	-3.80701600	-1.58871300	-0.45178300
C	-3.96549200	-1.65080400	-3.92732700
H	-4.68311400	-2.46590800	-4.07298800
H	-4.50711100	-0.70277400	-3.98744400

H	-3.23434200	-1.67469000	-4.74085400
C	3.32617100	-1.26799400	1.03529300
H	4.21099200	-1.58586300	1.60461200
H	2.69845500	-0.68301300	1.71332700
C	4.41941900	0.85944700	0.29407700
C	4.60749700	-1.04113200	-1.06308600
C	5.87849600	0.39409700	0.46995500
H	3.98512300	1.19769700	1.23686600
C	6.04190100	-0.77102700	-0.54130600
H	4.44838800	-0.57615100	-2.03773800
H	4.36245400	-2.10052500	-1.14720600
H	6.59927400	1.19799600	0.31559300
H	6.02542800	0.03090000	1.49223400
H	6.71157500	-0.50936700	-1.36406000
H	6.45875100	-1.65757900	-0.05502500
N	3.69491400	-0.38452000	-0.09803300
C	4.16657300	2.02952300	-0.77532500
O	2.97244100	1.83859000	-1.48818800
Zn	1.83853100	0.53106700	-0.67051700
C	5.29828800	2.17215400	-1.81273100
H	5.01514000	2.97650400	-2.49680900
H	6.26410000	2.43292700	-1.36836600
H	5.41960700	1.26620400	-2.41069200
C	4.07313400	3.33480600	0.03982500
H	4.96362200	3.49703700	0.66078300
H	3.97168700	4.18779400	-0.63875500
H	3.19145900	3.30273400	0.68544400
C	-0.50950800	3.45128200	-1.50737300
C	-1.62183800	4.30230200	-1.33193000
C	-1.47608800	5.66646400	-1.55688900
C	-0.22754800	6.14561300	-1.96446400
C	0.87233000	5.28854100	-2.13711200
C	0.75162300	3.92348600	-1.90953800
C	-0.89936000	2.11311900	-1.14888600
C	-2.28100600	2.13408800	-0.48137100
C	-2.84225000	3.52714200	-0.90471600
H	-2.31129900	6.34679900	-1.42173600
H	-0.10263000	7.20970900	-2.14495700
H	1.83107600	5.70195000	-2.43334700
H	1.60960800	3.25054500	-1.97156800
H	-3.40372900	4.02013300	-0.10643700
O	-0.23364600	1.05874600	-1.27459200
O	-3.08927000	1.06243700	-0.82644200
H	-3.52646200	3.37218300	-1.74552200

H	-2.81643900	0.52892900	-1.65258100
C	-5.37223900	1.55547000	3.76039200
C	-5.59672900	1.62089600	2.38718300
C	-4.53321100	1.78195900	1.49536300
C	-3.21901600	1.87991300	1.96660400
C	-3.00677400	1.82036100	3.35287600
C	-4.06592100	1.65776500	4.24159800
H	-6.20235200	1.42506000	4.44829600
H	-6.60717600	1.53815100	1.99698800
H	-4.72712000	1.79429300	0.43274000
H	-1.99512100	1.90447200	3.73779800
H	-3.86985300	1.61295700	5.30898600
C	-1.99610800	2.13592900	1.08763300
H	-1.66089300	3.15428600	1.30671700
C	-0.80973800	1.28618200	1.48870700
C	-0.85014600	-0.13893800	1.70498100
N	0.40789800	1.90503400	1.47348300
O	1.47499600	1.16070300	1.35220400
O	0.53243600	3.14491500	1.45839600
O	-1.61497300	-0.87272800	1.01116300
C	-0.06705300	-0.78651400	2.78509100
C	0.13688200	-2.17151300	2.72029700
C	0.44887700	-0.06612800	3.87435800
C	0.87108000	-2.82336000	3.70672500
H	-0.26417400	-2.71901000	1.87792500
C	1.17538500	-0.71860300	4.86339300
H	0.28015400	1.00255800	3.94161800
C	1.39435800	-2.09777300	4.77782100
H	1.04745000	-3.89087700	3.62707000
H	1.57145800	-0.15566500	5.70271700
H	1.96861000	-2.60355700	5.5485000