

Supporting Information

Metal-free catalytic asymmetric fluorination of keto esters using a combination of hydrogen fluoride (HF) and oxidant: Experiment and computation

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General: Unless otherwise noted, all commercially available compounds were used as purchased without further purification. Solvents used in the reactions were p.a. grade and dried and degassed only if indicated. Acetonitrile was distilled over P₄O₁₀ prior to use. Solvents for chromatography were technical grade and distilled prior to use. Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminum plates with F-254 indicator, visualized by irradiation with UV light or by basic potassium permanganate stain. Column chromatography was performed using silica gel Merck 60 (particle size 0.063-0.2 mm). Solvent mixtures are understood as volume/volume. ¹H-NMR, ¹⁹F-NMR and ¹³C-NMR were recorded on a Varian VNMR 400, VNMR 600 and Mercury 300 spectrometer in CDCl₃, C₆D₆ and D₆-DMSO. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); coupling constants (*J*) are in Hertz (Hz). Mass spectra EI/CI (methane) were conducted on a Finnigan SSQ 7000 mass spectrometer. ESI spectra were recorded in positive mode on a ThermoFinnigan LCQ Deca XP plus. The high resolution mass spectra (HRMS) were recorded on a ThermoFisher Scientific LTQ-Orbitrap XL. IR spectra were recorded on a Perkin Elmer Spectrum 100 FT-IR spectrometer and are reported in terms of frequency of absorption (cm⁻¹). Optical rotations were measured on a Perkin Elmer 343 Plus polarimeter and are reported as [deg·cm³·dm⁻¹·g⁻¹]. HPLC analysis was performed using chiral stationary phase columns (columns: Daicel Co. Chiralcel[®] OD-H, Chiralpak[®] AD-H, Chiralpak[®] AS-H, Chiralpak[®] IA; 250 mm × 4.6 mm; eluent: *n*-hexane/2-propanol mixtures, isocratic). Gas Chromatography was performed using a chiral stationary phase column (column: Lipodex[®] E; 25 m × 0.25 mm; carrier gas: hydrogen 100 kPa). The programs are displayed in the following manner: initial temperature (hold time) – temperature gradient – hold temperature (hold time). The chiral HPLC and GC methods were calibrated with the corresponding racemic mixtures. Compounds **3a**¹, **3b**², **3c**³, **3d**³, **3k**⁴, **5a**⁵, **5b**⁶, **5d**⁷, **5f**⁵, **5i**⁸ were prepared according to the reported procedures.

¹ Brown, D. S.; Marples, B. A.; Smith, P.; Walton, L. *Tetrahedron* **1995**, *51*, 3587-3606.

² Smith, A. M. R.; Billen, D.; Hii, K. K. *Chem. Commun.* **2009**, *26*, 3925-3927.

³ Smith, A. M. R.; Rzepa, H. S.; White, A. J. P.; Billen, D.; Hii, K. K. *J. Org. Chem.* **2010**, *75*, 3085-3096.

⁴ Vita, M. V.; Caramenti, P.; Waser, J. *Org. Lett.* **2015**, *17*, 5832-5835.

⁵ Uyanik, M.; Yasui, T.; Ishihara, K. *Angew. Chem. Int. Ed.* **2010**, *49*, 2175-2177.

⁶ Kong, W.; Feige, P.; De Haro, T.; Nevado, C. *Angew. Chem. Int. Ed.* **2013**, *52*, 2469-2473.

⁷ Wöste, T. H.; Muniz, K. *Synthesis* **2016**, *48*, 816-827.

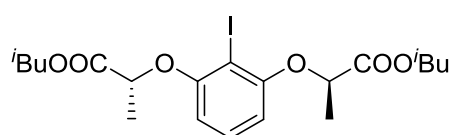
⁸ Shimogaki, M.; Fujita, M.; Sugimura, T. *Eur. J. Org. Chem.* **2013**, 7128-7138.

Preparation of the catalysts

General procedure I

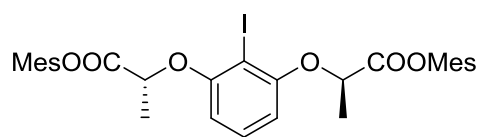
To a solution of (2*R*,2'*R*)-2,2'-((2-iodo-1,3-phenylene)bis(oxy))dipropionic acid⁵ (114.0 mg, 0.30 mmol, 1 equiv), appropriate alcohol (1.20 mmol, 2.5 equiv), triethylamine (84 μ L, 0.60 mmol, 2 equiv) and 4-(dimethylamino)pyridine (9.0 mg, 0.25 equiv) in dichloromethane (6 mL) was added *N*-(3-Dimethylaminopropyl)-*N'*-ethylcarbodiimide hydrochloride (144.0 mg, 0.75 mmol, 2.5 equiv) and the reaction mixture was stirred at RT for 6 h. 1 M HCl_{aq} (10 mL) was added and the product was extracted into dichloromethane (3 $\times$ 5 mL). The combined organic phases were dried over Na₂SO₄, filtered, concentrated under reduced pressure and the residue purified by flash chromatography.

Diisobutyl 2,2'-((2-iodo-1,3-phenylene)bis(oxy))(2*R*,2'*R*)-dipropionate (3c):



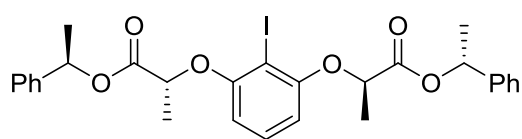
Isolated as a colorless oil. $[\alpha]_D^{RT} -36.4$ ($c = 1.0$, CHCl₃). ¹H NMR (400 MHz, CDCl₃) δ 7.10 (t, $J = 8.3$ Hz, 1H), 6.35 (d, $J = 8.3$ Hz, 2H), 4.76 (q, $J = 6.8$ Hz, 2H), 3.96 – 3.83 (m, 4H), 1.88 (hept, $J = 6.7$ Hz, 2H), 1.68 (d, $J = 6.8$ Hz, 6H), 0.87 – 0.80 (m, 12H). ¹³C NMR (101 MHz, CDCl₃) δ 171.7, 158.2, 129.4, 106.7, 80.5, 74.1, 71.2, 27.6, 18.9, 18.9, 18.6. IR (ATR) ν_{max} 2956, 2328, 2095, 1742, 1584, 1457, 1247, 1105, 764 cm⁻¹. MS (EI): m/z (%) 224.9 (100), 491.8 (81) [M]⁺, (MW = 492.35). HRMS (ESI): calc. for [C₂₀H₂₉O₆I+Na]⁺ 515.0901; found 515.08917.

Dimesityl 2,2'-((2-iodo-1,3-phenylene)bis(oxy))(2*R*,2'*R*)-dipropionate (3e):



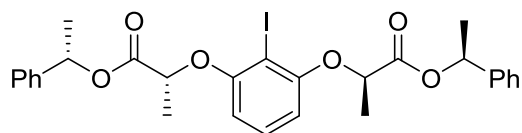
Isolated as a colorless solid, m.p. 154-155 °C. $[\alpha]_D^{RT} -2.0$ ($c = 1.0$, CHCl₃). ¹H NMR (600 MHz, CDCl₃) δ 7.22 (t, $J = 8.3$ Hz, 1H), 6.85 (s, 4H), 6.63 (d, $J = 8.3$ Hz, 2H), 5.09 (q, $J = 6.8$ Hz, 2H), 2.26 (s, 6H), 2.02 (s, 12H), 1.92 (d, $J = 6.8$ Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 169.6, 158.3, 145.3, 135.6, 129.5, 129.5, 129.4, 107.3, 80.9, 74.2, 20.7, 18.9, 16.3. IR (ATR) ν_{max} 2929, 2304, 2096, 1907, 1761, 1585, 1456, 1373, 1248, 1111, 854, 757 cm⁻¹. MS (CI): m/z (%) 253.6 (100), 617.0 (13) [M]⁺, (MW = 616.49). HRMS (ESI): calc. for [C₃₀H₃₃O₆I+Na]⁺ 639.12140; found 639.12146.

bis((*R*)-1-phenylethyl) 2,2'-((2-iodo-1,3-phenylene)bis(oxy))(2*R*,2'*R*)-dipropionate (3g):



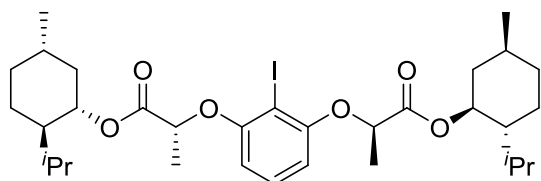
Isolated as a colorless oil. $[\alpha]_D^{RT} +36.7$ ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.30 – 7.22 (m, 6H), 7.22 – 7.17 (m, 4H), 6.99 (t, $J = 8.3$ Hz, 1H), 6.30 (d, $J = 8.3$ Hz, 2H), 5.91 (q, $J = 6.6$ Hz, 2H), 4.79 (q, $J = 6.8$ Hz, 2H), 1.69 (d, $J = 6.8$ Hz, 6H), 1.56 (d, $J = 6.6$ Hz, 6H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 170.9, 158.2, 140.9, 129.5, 128.4, 127.9, 126.0, 106.8, 80.5, 74.1, 73.4, 22.2, 18.5. **IR** (ATR) ν_{max} 3470, 2981, 2331, 2092, 1739, 1584, 1456, 1243, 1097, 880, 745 cm^{-1} . **MS** (ESI): m/z (%) 610.69 (99) $[\text{M}+\text{Na}]^+$, 1198.06 (100) $[2\text{M}+\text{Na}-1]^+$, (MW = 588.44). **HRMS** (ESI): calc. for $[\text{C}_{28}\text{H}_{29}\text{O}_6\text{I}+\text{Na}]$ 611.09010; found 611.09131.

bis((*S*)-1-phenylethyl) 2,2'-((2-iodo-1,3-phenylene)bis(oxy))(2*R*,2'*R*)-dipropionate (3h):



Isolated as a colorless oil. $[\alpha]_D^{RT} -95.3$ ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.38 – 7.33 (m, 8H), 7.33 – 7.27 (m, 2H), 6.94 (t, $J = 8.3$ Hz, 1H), 6.24 (d, $J = 8.3$ Hz, 2H), 5.92 (q, $J = 6.6$ Hz, 2H), 4.77 (q, $J = 6.8$ Hz, 2H), 1.70 (d, $J = 6.8$ Hz, 6H), 1.44 (d, $J = 6.6$ Hz, 6H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 170.9, 158.1, 140.9, 129.3, 128.5, 128.0, 126.1, 106.7, 80.4, 74.2, 73.3, 22.0, 18.4. **IR** (ATR) ν_{max} 2981, 2333, 2092, 1739, 1584, 1456, 1240, 1096, 867, 747 cm^{-1} . **MS** (ESI): m/z (%) 253.86 (100) $[\text{C}_{12}\text{H}_{14}\text{O}_6]^+$, 357.80 (95) $[\text{C}_{20}\text{H}_{22}\text{O}_6]^+$, 610.68 (57) $[\text{M}+\text{Na}]^+$, 1197.76 (76) $[2\text{M}+\text{Na}-1]^+$, (MW = 588.44). **HRMS** (ESI): calc. for $[\text{C}_{28}\text{H}_{29}\text{O}_6\text{I}+\text{Na}]^+$ 611.09010; found 611.09119.

bis((1*S*,2*R*,5*S*)-2-isopropyl-5-methylcyclohexyl) 2,2'-((2-iodo-1,3-phenylene)bis(oxy))(2*R*,2'*R*)-dipropionate (3j):



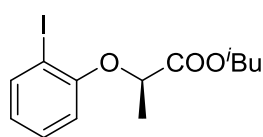
Isolated as a colorless solid, m.p. 95-96 °C. $[\alpha]_D^{RT} +12.2$ ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.08 (t, $J = 8.3$ Hz, 1H), 6.35 (d, $J = 8.3$ Hz, 2H), 4.76 – 4.68 (m, 4H), 1.92 (dtd, $J = 14.0$, 7.0, 2.7 Hz, 2H), 1.88 – 1.83 (m, 2H), 1.70 – 1.63 (m, 10H), 1.07 – 0.98 (m, 2H), 0.90 (d, $J = 7.0$ Hz, 6H), 0.88 – 0.79 (m, 10H), 0.75 (d, $J = 7.0$ Hz, 6H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.2, 158.2, 129.1, 106.8, 80.8, 75.3, 74.2, 46.8, 40.3, 34.1, 31.3, 26.3, 23.3, 21.9, 20.7, 18.5, 16.2. **IR** (ATR) ν_{max} 3460, 2952, 2197, 2088, 2009, 1917, 1742, 1581, 1444, 1369, 1205, 1101, 980, 752 cm^{-1} . **MS** (CI): m/z (%) 253.1 (100) $[\text{C}_{12}\text{H}_{13}\text{O}_6]^+$, 656.3 (46) $[\text{M}]^+$, (MW = 656.64). **HRMS** (ESI): calc. for $[\text{C}_{32}\text{H}_{49}\text{O}_6\text{I}+\text{Na}]^+$ 679.24660; found 679.24323.

General procedure II

To a solution of the appropriate resorcinol (0.50 mmol, 1 equiv) in methanol (5 mL) cooled to $-20\text{ }^{\circ}\text{C}$ and protected from direct light with aluminum foil was added dropwise a solution of *N*-iodosuccinimide (117.0 mg, 0.52 mmol, 1.04 equiv) in methanol (2 mL). The reaction mixture was warmed to $0\text{ }^{\circ}\text{C}$ and stirred at this temperature until TLC and NMR analyses indicated complete conversion of starting material and product formation (15 min – 48 h). Methanol was evaporated under reduced pressure at RT and the residue was dissolved in ethyl acetate (10 mL). The organic phase was washed with $\text{Na}_2\text{S}_2\text{O}_3$ solution and brine, dried over Na_2SO_4 , filtered and evaporated under reduced pressure. The crude product was immediately used in the next step without further purification.

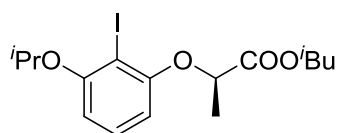
To a solution of 2-iodoresorcinol derivative (prepared according to reported procedures *or* crude from the previous step, assumed 0.50 mmol), triphenylphosphine (315.0 mg, 1.20 mmol, 2.4 equiv) and isobutyl (*S*)-lactate (175 μL , 1.50 mmol, 3 equiv) in dry THF (6 mL) cooled to $0\text{ }^{\circ}\text{C}$, under argon, was added dropwise diisopropyl azodicarboxylate (237 μL , 1.20 mmol, 2.4 equiv). The reaction mixture was stirred at RT for 15 h and the solvent was evaporated under reduced pressure. The residue was dried under high vacuum for 1 h and a hexane/diethyl ether 4:1 (10 mL) mixture was added with strong stirring. The resulting suspension was filtrated, the solids were washed with hexane (2 mL) and the clear solution was evaporated under reduced pressure. The residue was purified by flash chromatography.

isobutyl (*R*)-2-(2-iodophenoxy)propanoate (**4a**):



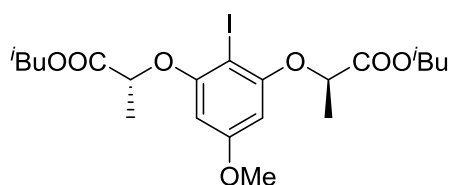
Isolated as a colorless oil. $[\alpha]_D^{RT} -13.2$ ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.78 (dd, $J = 8.1, 1.6\text{ Hz}$, 1H), 7.27 – 7.19 (m, 1H), 6.75 – 6.68 (m, 2H), 4.79 (q, $J = 6.8\text{ Hz}$, 1H), 3.98 – 3.86 (m, 2H), 1.90 (hept, $J = 6.7\text{ Hz}$, 1H), 1.70 (d, $J = 6.8\text{ Hz}$, 3H), 0.88 – 0.83 (m, 6H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.6, 156.5, 139.8, 129.3, 123.3, 113.1, 87.1, 73.9, 71.3, 27.7, 18.9, 18.9, 18.6. **IR** (ATR) ν_{max} 2957, 2320, 2092, 1741, 1579, 1462, 1371, 1256, 1109, 746 cm^{-1} . **MS** (CI): m/z (%) 292.9 (27), 49.0 (100) $[\text{M}]^+$, (MW = 348.18). **HRMS** (ESI): calc. for $[\text{C}_{13}\text{H}_{17}\text{O}_3\text{I} + \text{Na}]^+$ 371.01146; found 371.01190.

isobutyl (R)-2-(2-iodo-3-isopropoxyphenoxy)propanoate (4b):



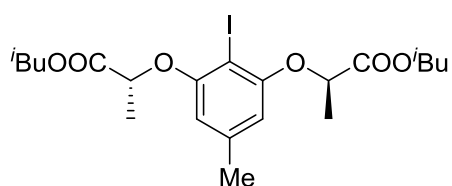
Isolated as a colorless oil. $[\alpha]_D^{RT} -25.4$ ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.13 (t, $J = 8.2$ Hz, 1H), 6.49 (d, $J = 7.9$ Hz, 1H), 6.33 (dd, $J = 8.3$, 0.8 Hz, 1H), 4.78 (q, $J = 6.8$ Hz, 1H), 4.55 (hept, $J = 6.1$ Hz, 1H), 3.93 (dd, $J = 10.6$, 6.6 Hz, 1H), 3.88 (dd, $J = 10.6$, 6.5 Hz, 1H), 1.89 (hept, $J = 6.7$ Hz, 1H), 1.69 (d, $J = 6.8$ Hz, 3H), 1.39 – 1.34 (m, 6H), 0.86 – 0.82 (m, 6H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 171.8, 158.5, 158.2, 129.3, 108.0, 105.8, 81.8, 74.1, 72.2, 71.2, 27.7, 22.2, 22.1, 18.9, 18.9, 18.6. **IR** (ATR) ν_{max} 2961, 2330, 2102, 1742, 1582, 1455, 1370, 1247, 1104, 763 cm^{-1} . **MS** (EI): m/z (%) 181.1 (100), 280.2 (28) $[\text{M}-\text{I}+1]^+$, 406.1 (87) $[\text{M}]^+$, (MW = 406.26). **HRMS** (ESI): calc. for $[\text{C}_{16}\text{H}_{23}\text{O}_4\text{I}+\text{Na}]^+$ 429.05332; found 429.05334.

diisobutyl 2,2'-((2-iodo-5-methoxy-1,3-phenylene)bis(oxy))(2R,2'R)-dipropionate (5a):



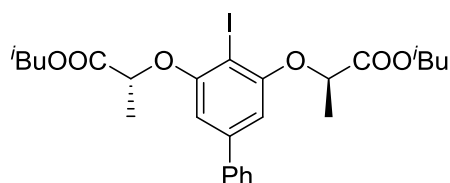
Isolated as a colorless oil. $[\alpha]_D^{RT} -3.2$ ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 6.01 (s, 2H), 4.71 (q, $J = 6.8$ Hz, 2H), 3.96 – 3.82 (m, 4H), 3.67 (s, 3H), 1.87 (hept, $J = 6.7$ Hz, 2H), 1.65 (d, $J = 6.8$ Hz, 6H), 0.86 – 0.80 (m, 12H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.6, 161.6, 158.4, 94.2, 74.2, 71.2, 69.8, 55.4, 27.6, 18.9, 18.9, 18.6. **IR** (ATR) ν_{max} 3459, 2951, 2312, 2093, 1919, 1735, 1585, 1439, 1361, 1200, 1116, 807, 759, 693 cm^{-1} . **MS** (EI): m/z (%) 253.7 (100), 522 (25) $[\text{M}]^+$, (MW = 522.38). **HRMS** (ESI): calc. for $[\text{C}_{21}\text{H}_{31}\text{O}_7\text{I}+\text{Na}]^+$ 545.10067; found 545.10065.

diisobutyl 2,2'-((2-iodo-5-methyl-1,3-phenylene)bis(oxy))(2R,2'R)-dipropionate (5b):



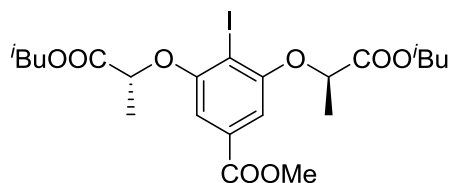
Isolated as a colorless oil. $[\alpha]_D^{RT} -14.7$ ($c = 0.986$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 6.21 (s, 2H), 4.75 (q, $J = 6.8$ Hz, 2H), 3.97 – 3.88 (m, 4H), 2.22 (s, 3H), 1.91 (hept, $J = 6.7$ Hz, 2H), 1.68 (d, $J = 6.8$ Hz, 6H), 0.90 – 0.84 (m, 12H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 171.8, 157.9, 139.9, 108.0, 76.6, 74.1, 71.2, 27.7, 21.7, 18.9, 18.9, 18.6. **IR** (ATR) ν_{max} 2956, 2329, 2102, 1742, 1578, 1446, 1208, 1113, 815 cm^{-1} . **MS** (CI): m/z (%) 239.1 (100), 506.2 (5) $[\text{M}]^+$, (MW = 506.38). **HRMS** (ESI): calc. for $[\text{C}_{21}\text{H}_{31}\text{O}_6\text{I}+\text{Na}]^+$ 529.10575; found 529.10583.

diisobutyl 2,2'-((4-iodo-[1,1'-biphenyl]-3,5-diyl)bis(oxy))(2*R*,2'*R*)-dipropionate (5c):



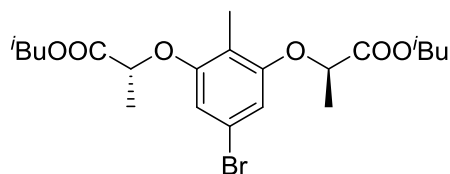
Isolated as a colorless solid, m.p. 70-71 °C. $[\alpha]_D^{RT} +32.3$ (c = 1.0, CHCl₃). ¹H NMR (600 MHz, CDCl₃) δ 7.46 – 7.42 (m, 2H), 7.42 – 7.38 (m, 2H), 7.37 – 7.33 (m, 1H), 6.60 (s, 2H), 4.87 (q, *J* = 6.8 Hz, 2H), 3.99 – 3.88 (m, 4H), 1.90 (hept, *J* = 6.7 Hz, 2H), 1.73 (d, *J* = 6.8 Hz, 6H), 0.87 – 0.83 (m, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 171.7, 158.4, 143.2, 140.3, 128.8, 127.9, 126.9, 106.1, 79.4, 74.3, 71.3, 27.7, 18.9, 18.9, 18.6. IR (ATR) ν_{max} 3475, 2954, 2328, 2091, 1742, 1573, 1451, 1381, 1201, 1121, 992, 832, 757, 686 cm⁻¹. MS (CI): *m/z* (%) 442.2 (14) [M-I+1]⁺, 569.0 (100) [M+1]⁺, (MW = 568.45). HRMS (ESI): calc. for [C₂₆H₃₃O₆I+Na]⁺ 591.12140; found 591.12122.

diisobutyl 2,2'-((2-iodo-5-(methoxycarbonyl)-1,3-phenylene)bis(oxy))(2*R*,2'*R*)-dipropionate (5d):



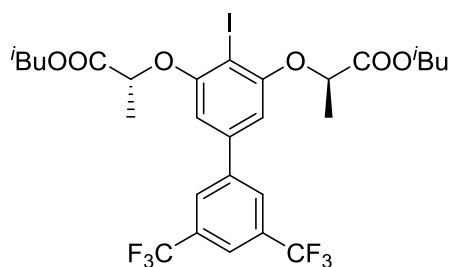
Isolated as a colorless solid, m.p. 56-57 °C. $[\alpha]_D^{RT} -3.6$ (c = 1.0, CHCl₃). ¹H NMR (600 MHz, CDCl₃) δ 7.02 (s, 2H), 4.88 (q, *J* = 6.8 Hz, 2H), 3.93 (d, *J* = 6.6 Hz, 4H), 3.85 (s, 3H), 1.91 (hept, *J* = 6.7 Hz, 2H), 1.71 (d, *J* = 6.8 Hz, 6H), 0.87 (d, *J* = 6.7 Hz, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 171.2, 166.0, 158.2, 131.6, 107.0, 87.1, 74.0, 71.4, 52.4, 27.7, 18.9, 18.9, 18.5. IR (ATR) ν_{max} 3476, 2954, 2325, 2097, 1916, 1742, 1570, 1449, 1403, 1202, 1121, 993, 833, 758, 686 cm⁻¹. MS (ESI): *m/z* (%) 572.86 (4) [M+Na]⁺, 1122.09 (100) [2M+Na-1]⁺. (MW = 550.39). HRMS (ESI): calc. for C₂₂H₃₁O₈INa 573.09558; found 573.09467.

diisobutyl 2,2'-((5-bromo-2-iodo-1,3-phenylene)bis(oxy))(2*R*,2'*R*)-dipropionate (5e):



Isolated as a colorless solid, m.p. 44-45 °C. $[\alpha]_D^{RT} +7.7$ (c = 1.0, CHCl₃). ¹H NMR (600 MHz, CDCl₃) δ 6.52 (s, 2H), 4.75 (q, *J* = 6.8 Hz, 2H), 3.98 – 3.91 (m, 4H), 1.92 (hept, *J* = 6.7 Hz, 2H), 1.70 (d, *J* = 6.8 Hz, 6H), 0.90 – 0.87 (m, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 171.1, 158.6, 122.8, 110.3, 79.1, 74.3, 71.5, 27.7, 18.9, 18.9, 18.5. IR (ATR) ν_{max} 3475, 2958, 2323, 2097, 1741, 1566, 1403, 1196, 1117, 993, 824, 692 cm⁻¹. MS (CI): *m/z* (%) 303.0 (87), 304.9 (84), 570.0 (99) [M]⁺, 572.0 (100) [M+2]⁺, (MW = 571.25). HRMS (ESI): calc. for [C₂₀H₂₈O₆⁷⁹BrI+Na]⁺ 593.00062; found 593.00049.

diisobutyl 2,2'-((4-iodo-3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-3,5-diyl)bis(oxy)) (2*R*,2'*R*)-dipropionate (5f):

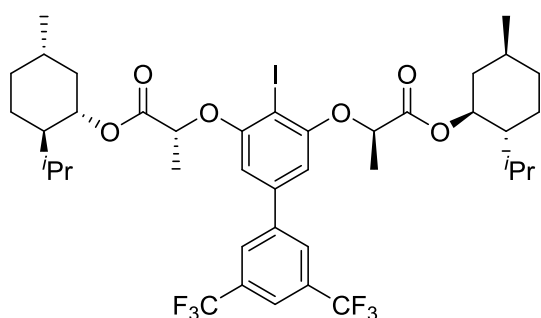


Isolated as a colorless solid, m.p. 91-92 °C. $[\alpha]_D^{RT} +29.3$ ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.86 (s, 1H), 7.83 (s, 2H), 6.54 (s, 2H), 4.89 (q, $J = 6.8$ Hz, 2H), 3.99 – 3.90 (m, 4H), 1.91 (hept, $J = 6.7$ Hz, 2H), 1.75 (d, $J = 6.8$ Hz, 6H), 0.89 – 0.82 (m, 12H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 171.4, 158.9, 142.6, 140.1, 132.3 (q, $J = 33.4$ Hz), 127.1 (q, $J = 3.1$ Hz), 123.1 (q, $J = 272.8$ Hz), 121.5 (hept, $J = 3.9$ Hz), 106.0, 81.7, 74.4, 71.5, 27.7, 18.8, 18.8, 18.6. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -62.9 (s, 6F). **IR** (ATR) ν_{max} 2957, 2320, 2092, 1738, 1573, 1382, 1123, 914, 830, 690 cm^{-1} . **MS** (ESI): m/z (%) 704.42 (19) $[\text{M}]^+$, 1429.78 (100) $[2\text{M}+\text{Na}-1]^+$, (MW = 704.44). **HRMS** (ESI): calc. for $[\text{C}_{28}\text{H}_{31}\text{O}_6\text{F}_6\text{I}+\text{Na}]^+$ 727.09617; found 727.09619.

Synthesis of bis((1*S*,2*R*,5*S*)-2-isopropyl-5-methylcyclohexyl 2,2'-((4-iodo-3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-3,5-diyl)bis(oxy))(2*R*,2'*R*)-dipropionate (6):

5f (211.0 mg, 0.30 mmol, 1 equiv) was dissolved in THF (2 mL) and methanol (2 mL) followed by addition of 3 M NaOH_{aq} (2 mL). After 2 h of stirring at RT the organic solvents were evaporated under reduced pressure and 1 M HCl_{aq} was added (10 mL). The product was extracted into ethyl acetate (3×10 mL) and the combined organic phases were dried over Na_2SO_4 , filtered, concentrated and dried under high vacuum for 1 h.

The crude acid was dissolved in dichloromethane (10 mL), *D*-menthol (188.0 mg, 1.20 mmol, 4 equiv), triethylamine (84 μL , 0.60 mmol, 2 equiv) and 4-(dimethylamino)pyridine (9.0 mg, 0.075 mmol, 0.25 equiv) were added, followed by solid *N*-(3-Dimethylaminopropyl)-*N'*-ethylcarbodiimide hydrochloride (144.0 mg, 0.75 mmol, 2.5 equiv) and the reaction mixture was stirred at RT for 6 h. 1 M HCl_{aq} (10 mL) was added and the product was extracted into dichloromethane (3×5 mL). The combined organic phases were dried over Na_2SO_4 , filtered, concentrated in vacuo and the residue was purified by flash chromatography and crystallized from hot methanol to provide the product as a colorless solid.



m.p. 111-112 °C. $[\alpha]_D^{RT} +69.5$ (c = 1.0, CHCl₃).

¹H NMR (400 MHz, CDCl₃) δ 7.85 (s, 1H), 7.80 (s, 2H), 6.45 (s, 2H), 4.87 (q, *J* = 6.7 Hz, 2H), 4.70 – 4.60 (m, 2H), 1.85 – 1.77 (m, 2H), 1.72 (d, *J* = 6.8 Hz, 6H), 1.70 – 1.54 (m, 6H), 1.47 – 1.27 (m, 4H), 1.02 – 0.88 (m, 2H), 0.85 – 0.72 (m, 10H),

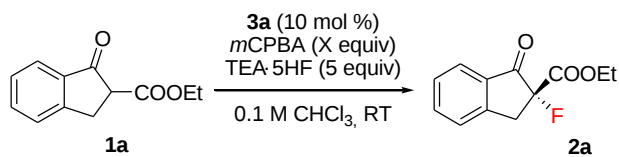
0.66 (d, *J* = 7.0 Hz, 6H), 0.47 (d, *J* = 7.0 Hz, 6H). **¹³C NMR** (101 MHz, CDCl₃) δ 170.8, 158.8, 143.0, 140.1, 132.3 (q, *J* = 33.4 Hz), 127.2, 123.1 (q, *J* = 272.9 Hz), 121.4 (hept, *J* = 3.5 Hz), 105.9, 81.7, 75.5, 74.2, 46.6, 40.4, 34.0, 31.2, 26.3, 23.3, 21.8, 20.3, 18.5, 15.9. **¹⁹F NMR** (376 MHz, CDCl₃) δ –62.8. **IR** (ATR) $\nu_{\max}$ 3465, 2940, 2322, 2096, 1745, 1574, 1381, 1127, 956, 831, 690 cm^{–1}. **MS** (CI): *m/z* (%) 139.2 (100) [C₁₀H₁₉]⁺, 868.5 (23) [M]⁺, (MW = 868.74). **HRMS** (ESI): calc. for [C₄₀H₅₁F₆IO₆+Na]⁺ 891.25323; found 891.24701.

Table 1. Screening of the oxidants.^[a]

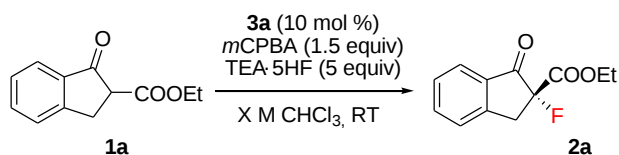
Entry	oxidant	Yield (%)	ee (%)
1	<i>m</i> CPBA	38	12
2	MeCOOOH	< 5	-
3	NaBO ₃ · 4H ₂ O	0	-
4	K ₂ S ₂ O ₈	0	-
5	KHSO ₅	0	-
6	<i>t</i> BuOOH	0	-
7	(<i>t</i> BuO) ₂	0	-

Table 2. Evaluation of the catalyst loading.

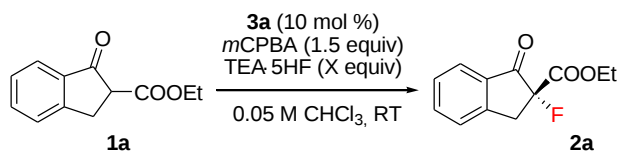
Entry	Catalyst loading (mol %)	Yield (%)	ee (%)
1	100	85	68
2	50	79	66
3	20	73	64
4	10	67	61
5	5	57	60
6	2	42	60
7	1	29	60

Table 3. Evaluation of the amount of *m*CPBA.

Entry	Amount of <i>m</i> CPBA (equiv)	Yield (%)	<i>ee</i> (%)
1	10	61	61
2	5	66	61
3	2.5	67	61
4	2	67	61
5	1.5	67	61
6	1	62	61

Table 4. Evaluation of the concentration.

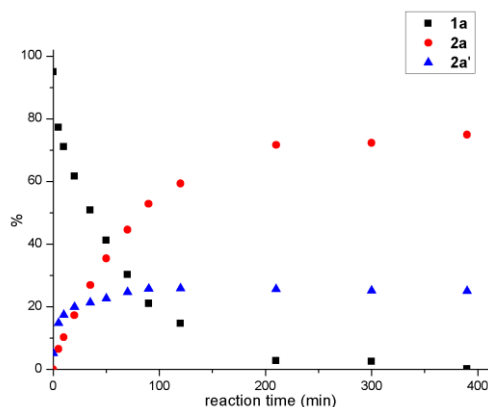
Entry	concentration	Yield (%)	<i>ee</i> (%)
1	0.2	75	60
2	0.1	67	61
3	0.05	65	64
4	0.02	56	70
5	0.01	47	70

Table 5. Asymmetric fluorination. Evaluation of the amount of TEA 5HF.

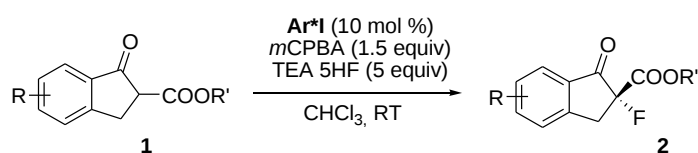
Entry	Amount of TEA 5HF	Yield (%)	<i>ee</i> (%)
1	25	70	62
2	10	67	62
3	5	65	64
4	2.5	65	67
5	1	62	70
7	0.5	51	70

To get a deeper understanding of the reaction's progress, we studied the kinetics of the chiral fluorination reaction of indanone based β -ketoester **1a**. The distribution of the reaction products was recorded as a function of time (Figure 1). The background hydroxylation (formation of **2a'**) is faster than the fluorination reaction during the first 30 minutes. From this point the rate constant of the fluorination process is higher and the yield of hydroxylated product stays constant at about 25% and the reaction is finished after 6 hours. It is also noteworthy, that the ee of the fluorinated product is not changing, while for the formation of the hydroxylated product a minimal chiral induction ($ee = 11\%$, after 5 minutes) is observed at the beginning which is disappearing after 30 minutes.

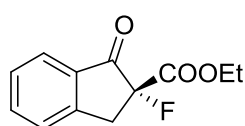
Figure 1. Distribution of the reaction products.



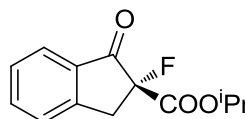
General procedure for the asymmetric fluorination



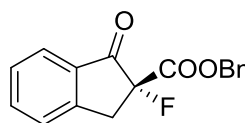
A 10 mL FEP tube was charged with the β -ketoester (0.10 mmol) and the catalyst (0.01 mmol, 10 mol%). CHCl_3 (1 mL) was added followed by $5\text{HF} \cdot \text{NEt}_3$ (100 mg, 0.50 mmol). Solid $m\text{CPBA}$ (26.0 mg, 0.15 mmol) was added in one portion and the reaction mixture was stirred at RT for 4 – 18 h. $1\text{M K}_2\text{CO}_3$ (5 mL) was added to neutralize the mixture. The product was extracted with chloroform ($3 \times 5\text{ mL}$), the combined organic layers were dried over MgSO_4 , filtered and concentrated under reduced pressure. The residue was purified by flash chromatography.

ethyl (R)-2-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2a):

Isolated as a colorless solid, m.p. 27-28 °C. $[\alpha]_D^{RT} -17.7$ (c = 1.0, CHCl₃) [lit.⁹ -43.6 (c = 0.9, CHCl₃, R 86% ee)]. ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, J = 7.9 Hz, 1H), 7.68 (td, J = 7.6, 1.1 Hz, 1H), 7.50 – 7.40 (m, 2H), 4.25 (q, J = 7.1 Hz, 2H), 3.76 (dd, J = 17.7, 11.6 Hz, 1H), 3.40 (dd, J = 23.3, 17.7 Hz, 1H), 1.23 (t, J = 7.1 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 195.2 (d, J = 18.2 Hz), 167.3 (d, J = 28.0 Hz), 150.9 (d, J = 3.5 Hz), 136.7, 133.2, 128.6, 126.6, 125.6, 94.5 (d, J = 201.6 Hz), 62.6, 38.2 (d, J = 23.9 Hz), 14.0. ¹⁹F NMR (564 MHz, CDCl₃) δ -164.45 (dd, J = 23.3, 11.6 Hz). IR (ATR) ν_{max} 3442, 2985, 2325, 2091, 2001, 1936, 1759, 1724, 1603, 1467, 1372, 1288, 1192, 1069, 1107, 918, 858, 807, 751, 689 cm⁻¹. MS (EI): m/z (%) 149.4 (100) [C₉H₆FO]⁺, 223.5.0 (18) [M+1]⁺, (MW = 222.22). HRMS (ESI): calc. for [C₁₂H₁₁O₃F+Na]⁺ 245.05844; found 245.05869. GC (Lipodex E, 80 °C (5 min) – 10 K/min – 180 °C (20 min)), t_R 15.8 min (minor) t_R 16.2 min (major).

isopropyl (R)-2-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2b):

Isolated as a colorless solid, m.p. 55-57 °C. $[\alpha]_D^{RT} -10.2$ (c = 1.1, CHCl₃) [lit.⁹ -23.2 (c = 1.0, CHCl₃, R 60% ee)]. ¹H NMR (400 MHz, CDCl₃) δ 7.84 (d, J = 7.7 Hz, 1H), 7.73 – 7.67 (m, 1H), 7.52 – 7.43 (m, 2H), 5.14 (hept, J = 6.3 Hz, 1H), 3.76 (dd, J = 17.6, 11.8 Hz, 1H), 3.42 (dd, J = 23.2, 17.6 Hz, 1H), 1.23 (d, J = 6.3 Hz, 3H), 1.21 (d, J = 6.3 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 195.5 (d, J = 18.2 Hz), 167.0 (d, J = 27.6 Hz), 151.1 (d, J = 3.4 Hz), 136.8, 133.5, 128.7, 126.7, 125.8, 94.6 (d, J = 201.6 Hz), 70.9, 38.4 (d, J = 24.0 Hz), 21.7, 21.6. ¹⁹F NMR (376 MHz, CDCl₃) δ -164.4 (dd, J = 23.2, 11.8 Hz). IR (ATR) ν_{max} 2984, 2929, 2326, 2118, 1751, 1722, 1605, 1462, 1426, 1377, 1343, 1274, 1191, 1136, 1102, 1067, 919, 828, 753, 719, 673 cm⁻¹. MS (EI): m/z (%) 149.4 (100) [M-COOⁱPr]⁺, 216.5 (29) [M-HF]⁺, 237.5 (49) [M+1]⁺, (MW = 236.24). HRMS (ESI): calc. for [C₁₃H₁₃O₃F+Na]⁺ 259.07409; found 259.07413. HPLC (Chiralpak AS-H, n-hexane/2-propanol 98/2, flow rate 1.0 mL/min) t_R 17.2 min (minor); t_R 18.0 min (major).

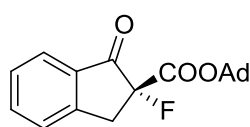
benzyl (R)-2-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2c):

Isolated as a colorless oil. $[\alpha]_D^{RT} -11.3$ (c = 1.0, CHCl₃) [lit.⁹ -10.9 (c = 1.1, CHCl₃, R 82% ee)]. ¹H NMR (400 MHz, CDCl₃) δ 7.82 (d, J = 7.7 Hz, 1H), 7.68 (td, J = 7.7, 1.1 Hz, 1H), 7.53 – 7.38 (m, 2H), 7.35 – 7.19 (m, 5H), 5.23 (q, J = 12.3 Hz, 2H), 3.75 (dd, J = 17.6, 11.5 Hz, 1H), 3.42 (dd, J = 23.2, 17.6

⁹ Mori, K.; Miyake, A.; Akiyama, T. *Chem. Lett.* **2014**, 43, 137–139.

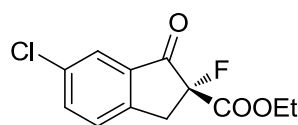
Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 195.0 (d, $J = 18.1$ Hz), 167.1 (d, $J = 28.2$ Hz), 150.8 (d, $J = 3.8$ Hz), 136.7, 134.6, 133.3, 128.6, 128.6, 128.5, 128.0, 126.6, 125.6, 94.6 (d, $J = 202.2$ Hz), 67.8, 38.2 (d, $J = 23.8$ Hz). ^{19}F NMR (376 MHz, CDCl_3) δ -164.5 (dd, $J = 23.2, 11.5$ Hz). IR (ATR) ν_{max} 3888, 3439, 3058, 2916, 2660, 2327, 2185, 2104, 1997, 1842, 1728, 1597, 1462, 1381, 1276, 1191, 1079, 921, 808, 739, 694 cm^{-1} . MS (CI): m/z (%) 91.4 (100) $[\text{C}_7\text{H}_7]^+$, 285.6 (4) $[\text{M}]^+$, (MW = 284.29). HRMS (ESI): calc. for $[\text{C}_{17}\text{H}_{13}\text{O}_3\text{F}+\text{Na}]^+$ 307.07409; found 307.07440. HPLC (Chiralcel OD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_R 17.3 min (major); t_R 20.1 min (minor).

adamantan-1-yl (*R*)-2-fluoro-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (2d):



Isolated as a colorless oil. $[\alpha]_D^{RT} +0.8$ ($c = 1.0$, CHCl_3) [lit.¹⁰ -4.12 ($c = 1.4$, S 99% *ee*)]. ^1H NMR (400 MHz, CDCl_3) δ 7.80 (d, $J = 7.7$ Hz, 1H), 7.65 (td, $J = 7.6, 1.1$ Hz, 1H), 7.50 – 7.38 (m, 2H), 3.70 (dd, $J = 17.5, 10.5$ Hz, 1H), 3.37 (dd, $J = 22.8, 17.5$ Hz, 1H), 2.11 (s, 3H), 2.01 (d, $J = 3.0$ Hz, 6H), 1.59 (t, $J = 3.0$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 195.8 (d, $J = 18.4$ Hz), 165.8 (d, $J = 27.9$ Hz), 151.0 (d, $J = 4.1$ Hz), 136.4, 133.6, 128.4, 126.4 (d, $J = 1.1$ Hz), 125.4 (d, $J = 0.8$ Hz), 94.3 (d, $J = 201.6$ Hz), 84.1, 41.0, 38.4 (d, $J = 24.1$ Hz), 35.9, 30.8. ^{19}F NMR (376 MHz, CDCl_3) δ -164.2 (dd, $J = 22.8, 10.5$ Hz). IR (ATR) ν_{max} 3441, 2913, 2858, 2668, 2325, 2087, 1995, 1939, 1724, 1604, 1460, 1276, 1191, 1052, 964, 917, 873, 833, 806, 731 cm^{-1} . MS (EI): m/z (%) 135.5 (100) $[\text{C}_{10}\text{H}_{15}]^+$, 328.6 (1) $[\text{M}]^+$, (MW = 328.38). HRMS (ESI): calc. for $[\text{C}_{20}\text{H}_{21}\text{O}_3\text{F}+\text{Na}]^+$ 351.13669; found 351.13644. HPLC (Chiralpak AD-H, *n*-hexane/2-propanol 98/2, flow rate 1.0 mL/min) t_R 14.0 min (minor); t_R 18.3 min (major).

ethyl (*R*)-6-chloro-2-fluoro-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (2e):

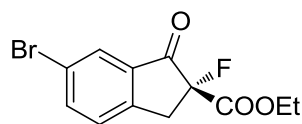


Isolated as a colorless oil. $[\alpha]_D^{RT} +2.9$ ($c = 1.0$, CHCl_3). ^1H NMR (600 MHz, CDCl_3) δ 7.80 (d, $J = 2.0$ Hz, 1H), 7.66 (dd, $J = 8.2, 2.0$ Hz, 1H), 7.46 (t, $J = 6.4$ Hz, 1H), 4.28 (q, $J = 7.1$ Hz, 2H), 3.75 (dd, $J = 17.6, 11.0$ Hz, 1H), 3.40 (dd, $J = 22.9, 17.6$ Hz, 1H), 1.26 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 194.2 (d, $J = 18.2$ Hz), 167.0 (d, $J = 27.6$ Hz), 149.0 (d, $J = 4.0$ Hz), 136.8, 135.2, 134.9 (d, $J = 1.1$ Hz), 127.9, 125.4, 94.8 (d, $J = 202.9$ Hz), 62.9, 38.0 (d, $J = 24.2$ Hz), 14.2. ^{19}F NMR (564 MHz, CDCl_3) δ -164.1 (dd, $J = 22.9, 11.0$ Hz). IR (ATR) ν_{max} 2976, 2813, 2022, 1909, 1747, 1602, 1538, 1472, 1346, 1275, 1190, 1133, 952, 829, 737, 665 cm^{-1} .

¹⁰ Shibata, N.; Kohno, J.; Takai, K.; Ishimaru, T.; Nakamura, S.; Toru, T.; Kanemasa, S. *Angew. Chem. Int. Ed.* **2005**, *44*, 4204-4207.

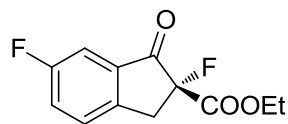
MS (EI): m/z (%) 183.0 (100) $[M-COOEt]^+$, 236.0 (44) $[M-HF]^+$, 257.0 (14) $[M]^+$, (MW = 256.66). **HRMS** (ESI): calc. for $[C_{12}H_{10}O_3^{35}ClF+Na]^+$ 279.01947; found 279.01947. **GC** (Lipodex E, 100 °C (5 min) – 7 K/min – 180 °C (20 min)), t_R 18.9 min (minor) t_R 19.3 min (major).

ethyl (R)-6-bromo-2-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2f):



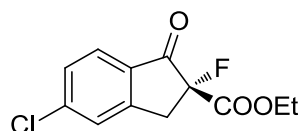
Isolated as a colorless oil. $[\alpha]_D^{RT} +6.1$ ($c = 1.0$, $CHCl_3$). **1H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, $J = 1.7$ Hz, 1H), 7.80 (dd, $J = 8.2$, 1.9 Hz, 1H), 7.40 (d, $J = 8.2$ Hz, 1H), 4.28 (q, $J = 7.1$ Hz, 2H), 3.73 (dd, $J = 17.7$, 11.0 Hz, 1H), 3.37 (dd, $J = 22.9$, 17.7 Hz, 1H), 1.27 (t, $J = 7.1$ Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.1 (d, $J = 18.6$ Hz), 167.0 (d, $J = 27.3$ Hz), 149.5 (d, $J = 3.7$ Hz), 139.6, 135.1, 128.4 (d, $J = 48.8$ Hz), 122.9, 94.6 (d, $J = 203.2$ Hz), 62.9, 38.1 (d, $J = 24.0$ Hz), 14.2. **^{19}F NMR** (564 MHz, $CDCl_3$) δ -164.09 (dd, $J = 22.9$, 11.0 Hz). **IR** (ATR) ν_{max} 3457, 2976, 2325, 2094, 1738, 1599, 1440, 1278, 1189, 1080, 934, 817, 692 cm^{-1} . **MS** (EI): m/z (%) 227.0 (74) $[M-COOEt]^+$, 229.0 (37) $[M-COOEt+2]^+$, 282.0 (99) $[M-HF+2]^+$, 282.0 (100) $[M-HF]^+$, 301.0 (24) $[M]^+$, 303.0 (23) $[M+2]^+$, (MW = 301.66). **HRMS** (ESI): calc. for $[C_{12}H_{10}O_3^{79}BrF+Na]^+$ 322.96896; found 322.96841. **HPLC** (Chiralpak AS-H, *n*-hexane/2-propanol 98/2, flow rate 1.0 mL/min) t_R 22.2 min (major); t_R 32.7 min (minor).

ethyl (R)-6-bromo-2-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2g):



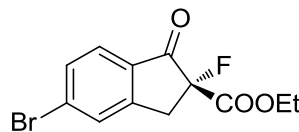
Isolated as a colorless oil. $[\alpha]_D^{RT} -12.9$ ($c = 1.0$, $CHCl_3$). **1H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.38 (m, 3H), 4.28 (q, $J = 7.1$ Hz, 2H), 3.75 (dd, $J = 17.5$, 11.1 Hz, 1H), 3.38 (ddd, $J = 22.3$, 17.5, 1.1 Hz, 1H), 1.27 (t, $J = 7.1$ Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 194.6 (dd, $J = 18.4$, 2.9 Hz), 167.1 (d, $J = 27.5$ Hz), 162.9 (d, $J = 250.3$ Hz), 146.5 (dd, $J = 3.5$, 2.3 Hz), 135.1 (d, $J = 7.8$ Hz), 128.2 (d, $J = 7.7$ Hz), 124.6 (d, $J = 23.7$ Hz), 111.5 (d, $J = 22.7$ Hz), 95.1 (d, $J = 202.7$ Hz), 62.9, 37.9 (d, $J = 24.1$ Hz), 14.2. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.07 (q, $J = 4.7$ Hz, 1F), -163.91 (dd, $J = 22.9$, 11.0 Hz, 1F). **IR** (ATR) ν_{max} 3429, 3311, 3093, 3067, 2986, 2927, 2857, 2187, 2072, 1755, 1721, 1610, 1542, 1483, 1438, 1368, 1335, 1263, 1194, 1135, 1098, 1072, 1010, 971, 905, 865, 841, 796, 764, 712, 679 cm^{-1} . **MS** (EI): m/z (%) 167.0 (22) $[M-COOEt]^+$, 220.0 (61) $[M-HF]^+$, 241.1 (100) $[M+1]^+$, (MW = 240.20). **HRMS** (ESI): calc. for $[C_{12}H_{10}O_3F_2+Na]^+$ 263.04902; found 263.04892. **GC** (Lipodex E, 100 °C (5 min) – 7 K/min – 180 °C (20 min)), t_R 15.3 min (minor) t_R 15.8 min (major).

ethyl (R)-5-chloro-2-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2h):



Isolated as a yellow solid, m.p. 55-56 °C. $[\alpha]_D^{RT}$ -43.5 (c = 1.2, CHCl₃) [lit.¹¹ -62.7 (c = 2.11, CH₂Cl₂, 99% ee)]. **¹H NMR** (600 MHz, CDCl₃) δ 7.77 (d, *J* = 8.3 Hz, 1H), 7.51 (d, *J* = 0.6 Hz, 1H), 7.45 (dd, *J* = 8.3, 0.6 Hz, 1H), 4.29 (q, *J* = 7.1 Hz, 2H), 3.77 (dd, *J* = 17.7, 11.3 Hz, 1H), 3.41 (dd, *J* = 22.9, 17.7 Hz, 1H), 1.27 (t, *J* = 7.1 Hz, 3H). **¹³C NMR** (151 MHz, CDCl₃) δ 194.0 (d, *J* = 18.4 Hz), 167.1 (d, *J* = 27.6 Hz), 152.4 (d, *J* = 3.6 Hz), 143.6, 131.8, 129.7, 127.0, 126.8, 94.5 (d, *J* = 203.0 Hz), 62.9, 38.1 (d, *J* = 24.2 Hz), 14.2. **¹⁹F NMR** (376 MHz, CDCl₃) δ -163.98 (dd, *J* = 22.9, 11.3 Hz). **IR** (ATR) ν_{max} 3153, 3434, 3093, 2948, 2331, 2195, 2119, 1762, 1722, 1598, 1465, 1419, 1373, 1326, 1273, 1194, 1066, 1013, 918, 866, 835, 780, 712, 671 cm⁻¹. **MS** (EI): *m/z* (%) 183.0 (83) [M-COOEt]⁺, 185.0 (28) [M-COOEt+2]⁺, 236.0 (100) [M-HF]⁺, 238.0 (34) [M-HF+2]⁺, 257.0 (56) [M+1]⁺, 259.0 (18) [M+3]⁺, (MW = 256.03). **HRMS** (ESI): calc. for [C₁₂H₁₀O₃³⁵ClF+Na]⁺ 279.01947; found 279.01917. **GC** (Lipodex E, 100 °C (5 min) – 10 K/min – 180 °C (20 min)), *t_R* 19.2 min (minor) *t_R* 20.1 min (major).

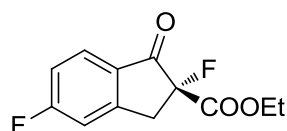
ethyl (R)-5-bromo-2-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2i):



Isolated as a yellow solid, m.p. 76-78 °C. $[\alpha]_D^{RT}$ -51.9 (c = 1.4, CHCl₃) [lit.¹¹ -75.6 (c = 3.00, CH₂Cl₂, 99% ee)]. **¹H NMR** (600 MHz, CDCl₃) δ 7.71 – 7.68 (m, 2H), 7.63 – 7.60 (m, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 3.77 (dd, *J* = 17.7, 11.2 Hz, 1H), 3.40 (dd, *J* = 22.9, 17.7 Hz, 1H), 1.27 (t, *J* = 7.1 Hz, 3H). **¹³C NMR** (151 MHz, CDCl₃) δ 194.2 (d, *J* = 18.3 Hz), 167.0 (d, *J* = 27.9 Hz), 152.4 (d, *J* = 3.6 Hz), 132.5, 132.5, 132.2, 130.1, 126.8, 94.4 (d, *J* = 203.2 Hz), 62.9, 38.0 (d, *J* = 24.3 Hz), 14.2. **¹⁹F NMR** (564 MHz, CDCl₃) δ -164.07 (dd, *J* = 22.9, 11.2 Hz). **IR** (ATR) ν_{max} 3270, 3089, 2984, 2940, 2328, 2115, 1932, 1762, 1724, 1592, 1466, 1416, 1370, 1274, 1192, 1104, 1059, 1012, 917, 859, 781, 735, 706, 668, 594, 549 cm⁻¹. **MS** (EI): *m/z* (%) 225.0 (42) [M-COOEt-2]⁺, 227.0 (100) [M-COOEt]⁺, 229.0 (56) [M-COOEt+2]⁺, 280.0 (20) [M-HF]⁺, 282.0 (20) [M-HF+2]⁺, 301.6 (19) [M-2]⁺, 300.0 (23) [M]⁺, 301.6 [M+2]⁺, (MW = 301.11). **HRMS** (ESI): calc. for [C₁₂H₁₀O₃⁷⁹BrF+Na]⁺ 322.96896; found 322.96924. **HPLC** (Chiralcel OD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) *t_R* 12.3 min (major); *t_R* 14.8 min (minor).

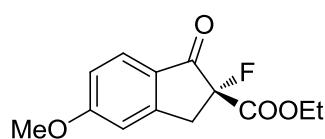
¹¹ Peng, J.; Du, D.-M. *RSC Adv.* **2014**, *4*, 2061–2067.

ethyl (*R*)-2,5-difluoro-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (2j):



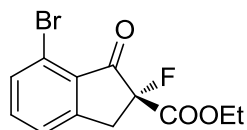
Isolated as a colorless oil. $[\alpha]_D^{RT} +8.8$ ($c = 0.8$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.85 (dd, $J = 8.1, 5.3$ Hz, 1H), 7.20 – 7.13 (m, 2H), 4.28 (q, $J = 7.1$ Hz, 2H), 3.78 (dd, $J = 17.8, 11.2$ Hz, 1H), 3.41 (dd, $J = 22.9, 17.8$ Hz, 1H), 1.26 (t, $J = 7.1$ Hz, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 193.3 (d, $J = 18.3$ Hz), 168.1 (d, $J = 260.2$ Hz), 167.0 (d, $J = 27.6$ Hz), 153.9 (dd, $J = 10.7, 3.8$ Hz), 129.6, 128.2 (d, $J = 10.8$ Hz), 117.1 (d, $J = 23.9$ Hz), 113.5 (d, $J = 22.8$ Hz), 94.5 (d, $J = 202.6$ Hz), 62.7, 38.1 (dd, $J = 24.4, 1.6$ Hz), 14.0. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -98.27 – -98.34 (m, 1F), -163.77 (dd, $J = 22.9, 11.2$ Hz, 1F). **IR** (ATR) ν_{max} 3435, 2980, 2670, 2336, 2075, 1932, 1726, 1596, 1477, 1432, 1342, 1259, 1190, 1074, 1011, 931, 854, 789, 699 cm^{-1} . **MS** (EI): m/z (%) 167.1 (57) $[\text{M}-\text{COOEt}]^+$, 220.1 (100) $[\text{M}-\text{HF}]^+$, 241.1 (39) $[\text{M}+1]^+$, (MW = 240.20). **HRMS** (ESI): calc. for $[\text{C}_{12}\text{H}_{10}\text{O}_3\text{F}_2+\text{Na}]^+$ 263.04902; found 263.04892. **HPLC** (Chiralcel OD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_R 11.9 min (major); t_R 13.8 min (minor).

ethyl (*R*)-2-fluoro-5-methoxy-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (2k):



Isolated as a colorless oil. $[\alpha]_D^{RT} -79.1$ ($c = 1.4$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.77 (d, $J = 8.6$ Hz, 1H), 6.97 (dd, $J = 8.6, 2.2$ Hz, 1H), 6.92 – 6.90 (m, 1H), 4.32 – 4.24 (m, 2H), 3.92 (s, 3H), 3.73 (dd, $J = 17.6, 11.3$ Hz, 1H), 3.37 (dd, $J = 23.0, 17.6$ Hz, 1H), 1.26 (t, $J = 7.1$ Hz, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 193.2 (d, $J = 18.3$ Hz), 167.7 (d, $J = 27.9$ Hz), 167.0, 154.2 (d, $J = 3.8$ Hz), 127.6, 126.5, 116.9, 109.9, 95.1 (d, $J = 201.1$ Hz), 62.7, 56.0, 38.4 (d, $J = 24.1$ Hz), 14.2. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -163.51 (dd, $J = 23.0, 11.3$ Hz). **IR** (ATR) ν_{max} 3426, 2979, 2849, 2620, 2108, 1920, 1756, 1716, 1595, 1454, 1261, 1190, 1080, 1016, 921, 850, 787, 735, 690 cm^{-1} . **MS** (EI): m/z (%) 179.1 (73) $[\text{M}-\text{COOEt}]^+$, 232.1 (100) $[\text{M}-\text{HF}]^+$, 252.1 (39) $[\text{M}]^+$, (MW = 252.24). **HRMS** (ESI): calc. for $[\text{C}_{13}\text{H}_{13}\text{NO}_4\text{F}+\text{Na}]^+$ 275.06901; found 275.06897. **HPLC** (Chiralpak AD-H, *n*-hexane/2-propanol 97/3, flow rate 1.0 mL/min) t_R 24.4 min (major); t_R 28.1 min (minor).

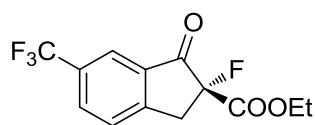
ethyl (*R*)-7-bromo-2-fluoro-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (2l):



Isolated as a colorless oil. $[\alpha]_D^{RT} +22.3$ ($c = 0.9$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.63 (dd, $J = 7.7, 0.7$ Hz, 1H), 7.52 (t, $J = 7.7$ Hz, 1H), 7.45 (dd, $J = 7.7, 0.7$ Hz, 1H), 4.34 – 4.25 (m, 2H), 3.75 (dd, $J = 17.6, 11.6$ Hz, 1H), 3.39 (dd, $J = 23.3, 17.6$ Hz, 1H), 1.28 (t, $J = 7.1$ Hz, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 192.7 (d, $J = 18.9$ Hz), 167.0 (d, $J = 27.6$ Hz), 153.5 (d, $J = 3.4$ Hz), 136.9, 133.7,

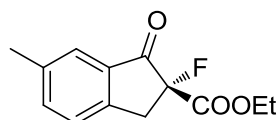
131.3, 125.5, 121.7, 94.8 (d, $J = 202.4$ Hz), 62.9, 37.5 (d, $J = 23.8$ Hz), 14.2. **^{19}F NMR** (564 MHz, CDCl_3) δ -162.99 (dd, $J = 23.3, 11.6$ Hz). **IR** (ATR) ν_{max} 3455, 2972, 2326, 2094, 1737, 1586, 1446, 1280, 1194, 1079, 906, 779, 684 cm^{-1} . **MS** (EI): m/z (%) 120.3 (100), 227.3 (44) $[\text{M}-\text{COOEt}]^+$, 229.3 (42) $[\text{M}-\text{COOEt}+2]^+$, 280.4 (11) $[\text{M}-\text{HF}]^+$, 282.3 (12) $[\text{M}-\text{HF}+2]^+$, 301.4 (42) $[\text{M}+1]^+$, 303.4 (37) $[\text{M}+3]^+$, (MW = 301.66). **HRMS** (ESI): calc. for $[\text{C}_{12}\text{H}_{10}\text{O}_3^{79}\text{BrF}+\text{Na}]^+$ 322.96896; found 322.96912. **HPLC** (Chiralcel OD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_R 15.6 min (major); t_R 18.7 min (minor).

ethyl (*R*)-2-fluoro-1-oxo-6-(trifluoromethyl)-2,3-dihydro-1H-indene-2-carboxylate (2m)



Isolated as a colorless oil. $[\alpha]_D^{RT} -5.4$ ($c = 1.0$, CHCl_3). **^1H NMR** (600 MHz, CDCl_3) δ 8.11 (s, 1H), 7.95 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.66 (d, $J = 8.1$ Hz, 1H), 4.30 (q, $J = 7.1$ Hz, 2H), 3.86 (dd, $J = 17.9, 11.2$ Hz, 1H), 3.50 (dd, $J = 22.8, 18.0$ Hz, 1H), 1.27 (t, $J = 7.1$ Hz, 3H). **^{13}C NMR** (151 MHz, CDCl_3) δ 194.2 (d, $J = 18.6$ Hz), 166.7 (d, $J = 27.3$ Hz), 153.9, 133.7, 133.0 (d, $J = 3.1$ Hz), 131.5 (q, $J = 33.5$ Hz), 127.4, 123.3 (q, $J = 272.7$ Hz), 122.8 (d, $J = 3.6$ Hz), 94.3 (d, $J = 203.3$ Hz), 62.9, 38.3 (d, $J = 24.2$ Hz), 14.0. **^{19}F NMR** (564 MHz, CDCl_3) δ -62.77 (s, 3F), -164.16 (dd, $J = 22.8, 11.2$ Hz, 1F). **IR** (ATR) ν_{max} 3070, 2978, 2325, 2089, 1766, 1733, 1626, 1590, 1446, 1372, 1329, 1260, 1189, 1125, 1073, 1010, 949, 911, 841, 796, 697 cm^{-1} . **MS** (EI): m/z (%) 198.1 (33) $[\text{C}_{10}\text{H}_5\text{F}_3\text{O}]^+$, 217.1 (100) $[\text{M}-\text{COOEt}]^+$, 270.1 (35) $[\text{M}-\text{HF}]^+$, 291.1 (16) $[\text{M}+1]^+$, (MW = 290.21). **HRMS** (ESI): calc. for $[\text{C}_{13}\text{H}_{10}\text{O}_3\text{F}_4+\text{Na}]^+$ 313.04583; found 313.04526. **HPLC** (Chiralpak IA, *n*-hexane/2-propanol 98/2, flow rate 1.0 mL/min) t_R 10.0 min (major); t_R 11.8 min (minor).

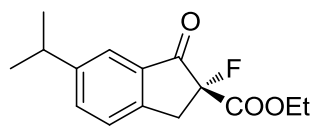
ethyl (*R*)-2-fluoro-6-methyl-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2n):



Isolated as a colorless oil. $[\alpha]_D^{RT} -9.3$ ($c = 1.0$, CHCl_3) [lit.¹¹ -19.7 ($c = 2.35$, CH_2Cl_2 , 99% ee)]. **^1H NMR** (600 MHz, CDCl_3) δ 7.63 (s, 1H), 7.51 (dd, $J = 7.9, 1.0$ Hz, 1H), 7.38 (d, $J = 7.8$ Hz, 1H), 4.27 (q, $J = 7.1$ Hz, 2H), 3.73 (dd, $J = 17.4, 11.3$ Hz, 1H), 3.38 (dd, $J = 23.3, 17.4$ Hz, 1H), 2.43 (s, 3H), 1.26 (t, $J = 7.1$ Hz, 3H). **^{13}C NMR** (151 MHz, CDCl_3) δ 195.5 (d, $J = 18.3$ Hz), 167.6 (d, $J = 28.0$ Hz), 148.5 (d, $J = 3.6$ Hz), 138.9, 138.1, 133.6, 126.4, 125.6, 95.0 (d, $J = 201.1$ Hz), 62.7, 38.1 (d, $J = 23.8$ Hz), 21.3, 14.2. **^{19}F NMR** (564 MHz, CDCl_3) δ -164.34 (dd, $J = 23.3, 11.3$ Hz). **IR** (ATR) ν_{max} 3425, 2962, 2925, 2854, 2329, 2165, 2115, 1982, 1756, 1721, 1614, 1581, 1493, 1431, 1387, 1331, 1267, 1222, 1185, 1078, 1050, 1004, 959, 891, 855, 827, 794, 760, 716, 688, 665 cm^{-1} . **MS** (EI): m/z (%) 163.1 (16) $[\text{M}-\text{COOEt}]^+$, 216.1 (100) $[\text{M}-\text{HF}]^+$, 237.2 (14) $[\text{M}+1]^+$, (MW = 236.24). **HRMS** (ESI): calc. for $[\text{C}_{13}\text{H}_{13}\text{O}_3\text{F}+\text{Na}]^+$ 259.07409; found

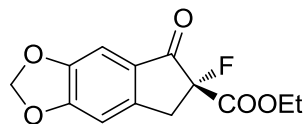
259.07367. **HPLC** (Chiralcel OD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_R 10.1 min (major); t_R 12.8 min (minor).

ethyl (R)-2-fluoro-6-isopropyl-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (2o):



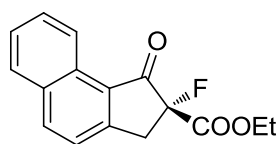
Isolated as a colorless oil. $[\alpha]_D^{RT}$ -2.4 ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.70 (s, 1H), 7.58 (dd, $J = 7.9, 1.7$ Hz, 1H), 7.41 (d, $J = 7.9$ Hz, 1H), 4.34 – 4.23 (m, 2H), 3.75 (dd, $J = 17.4, 11.6$ Hz, 1H), 3.38 (dd, $J = 23.3, 17.4$ Hz, 1H), 2.99 (hept, $J = 6.9$ Hz, 1H), 1.30 – 1.24 (m, 9H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 195.4 (d, $J = 18.2$ Hz), 167.5 (d, $J = 27.9$ Hz), 149.8, 148.7 (d, $J = 3.5$ Hz), 135.9, 133.4, 126.3, 122.8, 94.9 (d, $J = 201.1$ Hz), 62.6, 37.9 (d, $J = 23.9$ Hz), 33.8, 23.8, 14.0. $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -164.1 (dd, $J = 23.3, 11.7$ Hz). **IR** (ATR) ν_{max} 3441, 2965, 2094, 1764, 1723, 1616, 1580, 1491, 1464, 1438, 1369, 1290, 1189, 1101, 1071, 1011, 960, 889, 837, 792, 742, 712, 676 cm^{-1} . **MS** (EI): m/z (%) 191.1 (40) $[\text{M}-\text{COOEt}]^+$, 244.1 (100) $[\text{M}-\text{HF}]^+$, 265.1 (61) $[\text{M}+1]^+$, (MW = 264.29). **HRMS** (ESI): calc. for $[\text{C}_{15}\text{H}_{17}\text{O}_3\text{F}+\text{Na}]^+$ 287.10539; found 287.10443. **HPLC** (Chiralcel OD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_R 7.5 min (major); t_R 9.3 min (minor).

ethyl (R)-6-fluoro-5-oxo-6,7-dihydro-5H-indeno[5,6-d][1,3]dioxole-6-carboxylate (2p):



Isolated as a yellow oil. $[\alpha]_D^{RT}$ -41.8 ($c = 1.2$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.14 (s, 1H), 6.85 (s, 1H), 6.12 (dd, $J = 2.8, 1.0$ Hz, 1H), 4.33 – 4.23 (m, 2H), 3.65 (dd, $J = 17.4, 10.6$ Hz, 1H), 3.29 (dd, $J = 22.4, 17.4$ Hz, 1H), 1.27 (t, $J = 7.1$ Hz, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 192.9 (d, $J = 18.5$ Hz), 167.4 (d, $J = 27.8$ Hz), 155.9, 149.2, 149.2, 127.8, 105.7, 103.6, 102.8, 94.9 (d, $J = 201.1$ Hz), 62.6, 38.1 (d, $J = 24.1$ Hz), 14.0. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -163.29 (dd, $J = 22.4, 10.6$ Hz). **IR** (ATR) ν_{max} 2984, 2917, 2782, 2655, 2340, 2107, 1759, 1710, 1609, 1501, 1469, 1392, 1322, 1260, 1192, 1130, 1070, 1030, 933, 862, 793, 735, 679 cm^{-1} . **MS** (EI): m/z (%) 193.1 (34) $[\text{M}-\text{COOEt}]^+$, 246.1 (100) $[\text{M}-\text{HF}]^+$, 266.1 (15) $[\text{M}]^+$, (MW = 266.22). **HRMS** (ESI): calc. for $[\text{C}_{13}\text{H}_{11}\text{O}_5\text{F}+\text{Na}]^+$ 289.04827; found 289.04776. **HPLC** (Chiralpak AS-H, *n*-hexane/2-propanol 80/20, flow rate 1.0 mL/min) t_R 24.0 min (major); t_R 26.2 min (minor).

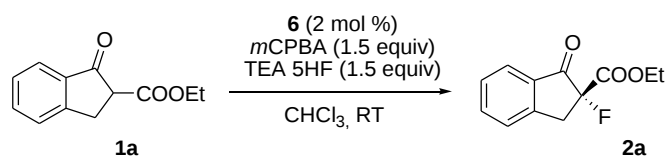
ethyl (R)- 2-fluoro-1-oxo-2,3-dihydro-1H-cyclopenta[a]naphthalene-2-carboxylate (2q):



Isolated as a colorless solid, m.p. 90-91 °C. $[\alpha]_D^{RT}$ $+27.2$ ($c = 1.0$, CHCl_3). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 9.02 (d, $J = 8.4$ Hz, 1H), 8.17 (d, $J = 8.4$ Hz, 1H), 7.94 (d, $J = 8.2$ Hz, 1H), 7.73 (ddd, $J = 8.3, 7.0, 1.1$ Hz, 1H), 7.65 – 7.60 (m, 1H), 7.54 (d, $J = 8.4$ Hz, 1H), 4.36 – 4.23 (m, 2H), 3.89 (dd, $J = 17.7$,

10.8 Hz, 1H), 3.54 (dd, $J = 22.5, 17.7$ Hz, 1H), 1.27 (t, $J = 7.1$ Hz, 3H). **^{13}C NMR** (151 MHz, CDCl_3) δ 195.4 (d, $J = 18.4$ Hz), 167.6 (d, $J = 28.2$ Hz), 154.8 (d, $J = 3.5$ Hz), 138.2, 133.2, 130.0, 129.7, 128.7, 127.9, 127.6, 124.3, 123.5, 94.7 (d, $J = 200.8$ Hz), 62.8, 38.7 (d, $J = 23.8$ Hz), 14.2. **^{19}F NMR** (564 MHz, CDCl_3) δ -163.76 (dd, $J = 22.5, 10.8$ Hz). **IR** (ATR) ν_{max} 3497, 2988, 2328, 2057, 1954, 1754, 1707, 1628, 1576, 1516, 1442, 1375, 1278, 1188, 1071, 1009, 961, 897, 814, 758, 684 cm^{-1} . **MS** (EI): m/z (%) 251.9 (16) $[\text{M}-\text{HF}]^+$, 272.9 (100) $[\text{M}+1]^+$, (MW = 272.27). **HRMS** (ESI): calc. for $[\text{C}_{16}\text{H}_{13}\text{O}_3\text{F}+\text{Na}]^+$ 295.07409; found 295.07434. **HPLC** (Chiralcel OD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_R 14.7 min (major); t_R 19.1 min (minor).

Scale-up experiment

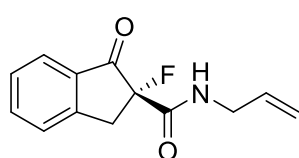


A 100 mL PTFE flask was charged with **6** (86.9 mg, 0.10 mmol, 2 mol %). CHCl₃ (50 mL) was added followed by 5HF·NEt₃ (750 mg, 7.5 mmol) and *m*CPBA (1.290 g, 7.50 mmol, 1.5 equiv). **1a** (1.022 g, 5.0 mmol) in CHCl₃ (10 mL) was added dropwise over 12 h via syringe pump at RT and the reaction mixture was stirred for additional 2 h. 2M K₂CO₃ (25 mL) was added to neutralize the reaction mixture. The product was extracted into chloroform (3 × 25 mL), the combined organic layers were dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography to provide **2a** (700 mg, 63%, 95:5 *er*) and catalyst **6** (75 mg, 86% recovery).

Functionalization of products

Synthesis of (*R*)-*N*-allyl-2-fluoro-1-oxo-2,3-dihydro-1*H*-indene-2-carboxamide (**8a**):

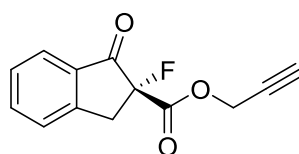
A 10 mL microwave vial was charged with a solution of **2a** (22.0 mg, 0.10 mmol, 1 equiv) and allylamine (38 μ L, 29.0 mg, 0.50 mmol, 5 equiv) in toluene (1 mL). The mixture was heated at 135 °C under microwave irradiation (200 W) for 30 min and subsequently cooled to RT. Volatiles were removed under reduced pressure and the residue was purified by flash chromatography to provide the product as a pale yellow solid.



m.p. 89-90 °C. $[\alpha]_D^{RT}$ -30.0 (c = 1.0, CHCl_3). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.80 (d, J = 7.7 Hz, 1H), 7.68 (td, J = 7.5, 1.0 Hz, 1H), 7.50 (d, J = 7.8 Hz, 1H), 7.43 (t, J = 7.5 Hz, 1H), 6.70 (s, 1H), 5.91 – 5.82 (m, 1H), 5.29 (ddd, J = 17.1, 2.6, 1.3 Hz, 1H), 5.20 (ddd, J = 10.2, 2.6, 1.3 Hz, 1H), 4.01 – 3.93 (m, 3H), 3.33 (dd, J = 24.1, 17.3 Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 196.6 (d, J = 18.0 Hz), 166.7 (d, J = 22.7 Hz), 151.9 (d, J = 4.1 Hz), 136.7, 133.2, 133.0, 128.4, 126.5, 125.5, 117.1, 96.9 (d, J = 203.0 Hz), 41.8, 37.4 (d, J = 22.8 Hz). $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -163.23 (dd, J = 24.0, 11.6 Hz). **IR** (ATR) ν_{max} 3448, 3265, 3079, 2925, 2855, 2692, 2442, 2325, 2198, 2163, 2076, 1993, 1956, 1815, 1730, 1652, 1605, 1544, 1466, 1418, 1294, 1207, 1152, 1070, 993, 911, 881, 801, 720 cm^{-1} . **MS** (EI): m/z (%) 56.3 (29) $[\text{C}_3\text{H}_6\text{N}]^+$, 130.1 (52) $[\text{C}_9\text{H}_6\text{O}]^+$, 150.1 (42) $[\text{C}_9\text{H}_7\text{FO}]^+$, 234.1 (100) $[\text{M}+1]^+$, (MW = 233.24). **HRMS** (ESI): calc. for $\text{C}_{13}\text{H}_{12}\text{NO}_2\text{FNa}$ 256.07443; found 256.07422. **HPLC** (Chiralpak AD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_R 18.0 min (major); t_R 30.0 min (minor).

Synthesis of prop-2-yn-1-yl (*R*)-2-fluoro-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (**8b**):

A 10 mL microwave vial was charged with a solution of **2a** (22.0 mg, 0.10 mmol, 1 equiv), dibutyltin oxide (1.2 mg, 5 μ mol, 5 mol %) and propargyl alcohol (58 μ L, 56.0 mg, 1.0 mmol, 10 equiv) in toluene (1 mL). The mixture was heated at 135 °C under microwave irradiation (200W) for 45 min and cooled to RT. Volatiles were removed under reduced pressure and the residue was purified by flash chromatography to provide the product as a colorless oil.

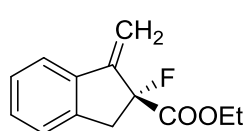


$[\alpha]_D^{RT}$ +3.9 (c = 1.0, CHCl_3). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 (d, J = 7.7 Hz, 1H), 7.71 (td, J = 7.6, 1.1 Hz, 1H), 7.51 (d, J = 7.7 Hz, 1H), 7.48 (t, J = 7.5 Hz, 1H), 4.84 (dd, J = 15.5, 2.5 Hz, 1H), 4.74 (dd, J = 15.5, 2.5 Hz, 1H), 3.82 (dd, J = 17.7, 11.8 Hz, 1H), 3.46 (dd, J = 23.4, 17.7 Hz, 1H), 2.50 (t, J = 2.5 Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 194.6 (d, J = 18.2 Hz), 166.6 (d, J =

28.2 Hz), 150.7 (d, $J = 3.1$ Hz), 136.9, 133.1, 128.7, 126.6, 125.8, 94.4 (d, $J = 201.8$ Hz), 76.2, 76.1, 53.6, 38.1 (d, $J = 23.7$ Hz). **^{19}F NMR** (376 MHz, CDCl_3) δ -164.47 (dd, $J = 23.4, 11.8$ Hz). **IR** (ATR) ν_{max} 3440, 3292, 3075, 2951, 2661, 2327, 2257, 2191, 2125, 1996, 1948, 1769, 1724, 1606, 1468, 1429, 1372, 1279, 1183, 1069, 1012, 976, 917, 806, 731, 692 cm^{-1} . **MS** (EI): m/z (%) 45.3 (100) $[\text{C}_2\text{H}_5\text{O}]^+$, 149.2 (46) $[\text{C}_9\text{H}_6\text{FO}]^+$, 233.2 (46) $[\text{M}+1]^+$, (MW = 232.21). **HRMS** (ESI): calc. for $\text{C}_{13}\text{H}_9\text{O}_3\text{FNa}$ 255.04279; found 255.04274. **HPLC** (Chiralpak AD-H, n -hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_{R} 16.5 min (minor); t_{R} 19.8 min (major).

Synthesis of ethyl (*R*)-2-fluoro-1-methylene-2,3-dihydro-1*H*-indene-2-carboxylate (**9**):

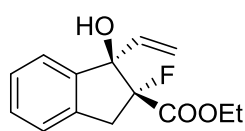
A 5 mL flask was charged with methyltriphenylphosphonium bromide (99.0 mg, 0.275 mmol, 2.75 equiv), sealed with a rubber stopper, evacuated and back-filled with argon (three times). Dry toluene (1 mL) was added and the suspension was cooled to 0 °C. n -BuLi (156 μL , 1.6 M in hexanes, 2.5 equiv) was added dropwise and the resulting yellow suspension was stirred for 2 h. A solution of **2a** (22.0 mg, 0.10 mmol, 1 equiv) in dry toluene (1 mL) was added and stirring was continued for 15 h. Volatiles were removed in vacuo and the residue purified by flash chromatography to provide the product as a pale yellow oil.



$[\alpha]_{\text{D}}^{25} -9.6$ ($c = 0.9$, CHCl_3). **^1H NMR** (600 MHz, CDCl_3) δ 7.50 (dd, $J = 6.4, 2.8$ Hz, 1H), 7.34 – 7.22 (m, 2H), 5.79 (d, $J = 4.8$ Hz, 1H), 5.48 (d, $J = 4.8$ Hz, 1H), 4.35 – 4.19 (m, 2H), 3.74 (dd, $J = 18.6, 17.6$ Hz, 1H), 3.35 (dd, $J = 27.0, 17.6$ Hz, 1H), 1.27 (t, $J = 7.1$ Hz, 3H). **^{13}C NMR** (101 MHz, CDCl_3) δ 170.1 (d, $J = 30.4$ Hz), 148.5 (d, $J = 17.3$ Hz), 141.1, 137.2, 129.7, 127.5, 125.1, 121.1, 109.2 (d, $J = 4.9$ Hz), 98.2 (d, $J = 194.7$ Hz), 62.0, 41.9 (d, $J = 24.5$ Hz), 14.05. **^{19}F NMR** (376 MHz, CDCl_3) δ -143.50 (ddt, $J = 27.1, 18.6, 4.8$ Hz). **IR** (ATR) ν_{max} 2481, 2983, 2937, 2328, 2256, 2056, 1996, 1944, 1738, 1604, 1465, 1370, 1297, 1250, 1193, 1063, 1017, 949, 909, 860, 729 cm^{-1} . **MS** (EI): m/z (%) 147.0 (100) $[\text{C}_{10}\text{H}_8\text{F}]^+$, 200.0 (65) $[\text{M}-\text{HF}]^+$, 220.0 (16) $[\text{M}]^+$, (MW = 220.24). **HRMS** (ESI): calc. for $\text{C}_{13}\text{H}_{13}\text{O}_2\text{FNa}$ 243.07918; found 243.07956. **HPLC** (Chiralpak AS-H, n -hexane/2-propanol 97/3, flow rate 1.0 mL/min) t_{R} 6.4 min (minor); t_{R} 7.2 min (major).

Synthesis of ethyl (1*R*,2*R*)-2-fluoro-1-hydroxy-1-vinyl-2,3-dihydro-1*H*-indene-2-carboxylate (**10**):

A 5 mL flask was charged with **2a** (22.0 mg, 0.10 mmol, 1 equiv), sealed with a rubber stopper, evacuated and back-filled with argon (three times). Dry THF (2 mL) was added and the solution was cooled to $-20\text{ }^{\circ}\text{C}$. Vinyl magnesium bromide (110 μL , 1.0 M in THF, 1.1 equiv) was added dropwise and the resulting solution was gradually warmed to RT and stirred for 2 h. $\text{NH}_4\text{Cl}_{\text{aq}}$ (2 mL) was added and the product was extracted into ethyl acetate ($3 \times 5\text{ mL}$). The combined organic layers were dried over Na_2SO_4 , filtered and concentrated under reduced pressure. The residue was purified by flash chromatography to provide the product as a colorless solid.

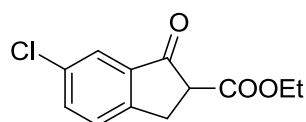


m.p. $54\text{--}55\text{ }^{\circ}\text{C}$. $[\alpha]_D^{RT} -100.5$ ($c = 1.0$, CHCl_3). **^1H NMR** (400 MHz, CDCl_3) δ 7.34 – 7.26 (m, 3H), 7.26 – 7.21 (m, 1H), 5.79 (dd, $J = 17.0$, 10.6 Hz, 1H), 5.22 (dd, $J = 17.0$, 1.2 Hz, 1H), 5.16 (dt, $J = 10.6$, 1.2 Hz, 1H), 4.37 – 4.21 (m, 2H), 3.74 (dd, $J = 34.4$, 17.3 Hz, 1H), 3.27 (dd, $J = 20.1$, 17.4 Hz, 1H), 3.01 (s, 1H), 1.31 (t, $J = 7.1$ Hz, 3H). **^{13}C NMR** (101 MHz, CDCl_3) δ 167.8 (d, $J = 26.9$ Hz), 142.6, 137.2, 136.0, 129.2, 127.9, 125.0, 124.5, 115.9, 104.1 (d, $J = 199.3$ Hz), 86.4 (d, $J = 20.3$ Hz), 62.0, 38.8 (d, $J = 23.3$ Hz), 14.2. **^{19}F NMR** (376 MHz, CDCl_3) δ -167.01 (dd, $J = 34.3$, 20.1 Hz). **IR** (ATR) ν_{max} 3508, 2990, 2927, 2855, 2324, 2191, 2162, 2057, 1998, 1944, 1873, 1722, 1638, 1605, 1507, 1466, 1405, 1371, 1315, 1285, 1238, 1194, 1156, 1115, 1067, 987, 938, 911, 892, 859, 766, 726, 656 cm^{-1} . **MS** (EI): m/z (%) 157.2 (100) $[\text{C}_{11}\text{H}_9\text{O}]^+$, 177.1 (48) $[\text{C}_{11}\text{H}_{10}\text{FO}]^+$, 230.2 (57) $[\text{M}-\text{HF}]^+$, 250.1 (59) $[\text{M}]^+$, (MW = 250.27). **HRMS** (ESI): calc. for $\text{C}_{14}\text{H}_{15}\text{O}_3\text{FNa}$ 273.08974; found 273.08972. **HPLC** (Chiralcel OD-H, *n*-hexane/2-propanol 95/5, flow rate 1.0 mL/min) t_R 7.5 min (minor); t_R 8.7 min (major).

Preparation of starting materials

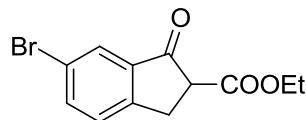
Starting materials were prepared in analogy to the reported procedures: An oven-dried round bottom flask was charged with sodium hydride (60% in oil, 2.2 equiv). The flask was evacuated and back-filled with nitrogen. After addition of diethyl carbonate (10 equiv) and a catalytic amount of sodium tert-butoxide (0.1 equiv.) the mixture was cooled in an ice bath and the indanone was added portionwise. After TLC analysis confirmed complete conversion of the starting materials 1 M HCl_{aq} was added until pH = 1 and the product was extracted into ethyl acetate. The combined organic layers were dried over Na₂SO₄ and concentrated under reduced pressure. The residue was purified by flash chromatography.

ethyl 6-chloro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**1e**):



Isolated as a beige solid, m.p. 104-105 °C. Mixture of tautomers (keto/enol 2:1). ¹H NMR (600 MHz, CDCl₃) δ 10.34 (s, 0.3H), 7.73 (d, *J* = 1.9 Hz, 0.6H), 7.61 (t, *J* = 1.2 Hz, 0.3H), 7.58 (dd, *J* = 8.2, 2.1 Hz, 0.7H), 7.45 (dd, *J* = 8.2, 0.6 Hz, 0.7H), 7.38 (d, *J* = 1.3 Hz, 0.7H), 4.33 (q, *J* = 7.1 Hz, 0.6H), 4.27 – 4.22 (m, 1.4H), 3.75 (dd, *J* = 8.2, 4.0 Hz, 0.7H), 3.52 (dd, *J* = 17.3, 3.9 Hz, 0.7H), 3.50 (s, 0.6H), 3.34 (dd, *J* = 17.3, 8.3 Hz, 0.7H), 1.37 (t, *J* = 7.1 Hz, 1H), 1.31 (t, *J* = 7.1 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 198.2, 168.6, 151.6, 141.2, 138.6, 136.8, 135.4, 134.2, 133.0, 129.3, 127.7, 125.7, 124.4, 120.8, 104.0, 61.9, 60.3, 53.7, 32.3, 29.9, 14.4, 14.2. IR (ATR) ν_{max} 3824, 3067, 2986, 2285, 2105, 1899, 1740, 1637, 1562, 1471, 1411, 1330, 1244, 1134, 1099, 1023, 943, 894, 855, 778, 723 cm⁻¹. MS (EI): *m/z* (%) 164.0 (52) [M-HCOOEt]⁺, 166.0 [M-HCOOEt+2]⁺, 238.0 (100) [M]⁺, 240.0 (35) [M+2]⁺, (MW = 238.67). HRMS (ESI) calc for [C₁₂H₁₁O₃³⁵Cl+Na]⁺ 261.02889; found 261.02881.

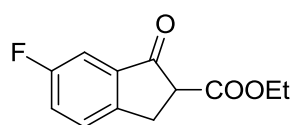
ethyl 6-bromo-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**1f**):



Isolated as a beige solid, m.p. 89-88 °C. Mixture of tautomers (keto/enol 2:1). ¹H NMR (600 MHz, CDCl₃) δ 10.32 (s, 0.3H), 7.90 (d, *J* = 1.8 Hz, 0.7H), 7.77 (d, *J* = 1.8 Hz, 0.3H), 7.72 (dd, *J* = 8.1, 1.9 Hz, 0.7H), 7.53 (dd, *J* = 8.0, 1.9 Hz, 0.3H), 7.40 (d, *J* = 8.1 Hz, 0.7H), 7.33 (d, *J* = 8.0 Hz, 0.3H), 4.33 (q, *J* = 7.1 Hz, 0.6H), 4.27 – 4.22 (m, 1.4H), 3.74 (dd, *J* = 8.3, 4.0 Hz, 0.7H), 3.50 (dd, *J* = 17.4, 4.0 Hz, 0.7H), 3.48 (s, 0.6H), 3.32 (dd, *J* = 17.4, 8.3 Hz, 0.7H), 1.36 (t, *J* = 7.1 Hz, 1H), 1.31 (t, *J* = 7.1 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 198.2, 168.8, 152.3, 141.8, 139.1, 138.3, 137.2, 132.2, 128.2, 127.7, 126.3, 124.0, 122.1, 121.0, 103.9, 62.1, 60.5, 53.6,

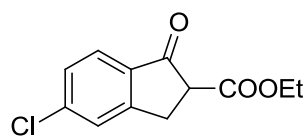
32.5, 30.1, 14.6, 14.3. **IR** (ATR) $\nu_{\max}$ 3434, 3062, 2982, 2911, 2321, 2083, 1991, 1899, 1749, 1714, 1643, 1585, 1557, 1471, 1414, 1378, 1334, 1244, 1208, 1179, 1134, 1096, 1030, 939, 891, 861, 834, 804, 777, 724 cm^{-1} . **MS** (EI): m/z (%) 208.0 (59) $[\text{M}-\text{HCOOEt}]^+$, 210.0 (61) $[\text{M}-\text{HCOOEt}]^+$, 282.0 (100), $[\text{M}]^+$, 284.0 (96) $[\text{M}+1]^+$, (MW = 283.12). **HRMS** (ESI) calc for $[\text{C}_{12}\text{H}_{11}\text{O}_3^{79}\text{Br}+\text{Na}]^+$ 304.97838; found 304.97833.

ethyl 6-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (1g):



Isolated as a brown solid, m.p. 80-81 °C. Mixture of tautomers (keto/enol 2.5:1). **^1H NMR** (600 MHz, CDCl_3) δ 10.34 (s, 0.3H), 7.47 (dd, J = 8.4, 4.5 Hz, 0.7H), 7.36 – 7.41 (m, 1H), 7.33 (tt, J = 7.4, 3.7 Hz, 0.7H), 7.30 (dd, J = 8.2, 2.5 Hz, 0.3H), 7.10 (ddd, J = 9.2, 8.3, 2.5 Hz, 0.3H), 4.32 (q, J = 7.1 Hz, 0.6H), 4.28 – 4.20 (m, 1.4H), 3.76 (dd, J = 8.2, 4.0 Hz, 0.7H), 3.51 (dd, J = 17.0, 3.9 Hz, 0.7H), 3.48 (s, 0.6H), 3.34 (dd, J = 17.0, 8.2 Hz, 0.7H), 1.36 (t, J = 7.1 Hz, 0.9H), 1.30 (t, J = 7.2 Hz, 2.1H). **^{13}C NMR** (151 MHz, CDCl_3) δ 198.7 (d, J = 3.0 Hz), 168.9, 162.6 (d, J = 248.8 Hz), 162.4 (d, J = 244.4 Hz), 149.2 (d, J = 2.0 Hz), 138.8 (d, J = 9.2 Hz), 138.5 (d, J = 2.3 Hz), 137.1 (d, J = 7.6 Hz), 128.1 (d, J = 8.1 Hz), 125.9 (d, J = 8.5 Hz), 123.3 (d, J = 23.8 Hz), 116.5 (d, J = 23.4 Hz), 110.5 (d, J = 22.1 Hz), 107.7 (d, J = 23.6 Hz), 104.5, 62.0, 60.4, 54.2, 32.2, 29.9, 14.6, 14.3. **^{19}F NMR** (564 MHz, CDCl_3) δ -113.89 (dd, J = 12.0, 7.8 Hz, 0.7F), -115.42 – -115.49 (m, 0.3F). **IR** (ATR) $\nu_{\max}$ 3458, 3277 3065, 2992, 2914, 2665, 2286, 2230, 2109, 1997, 1901, 1730, 1636, 1572, 1471, 1415, 1344, 1307, 1257, 1191, 1083, 1020, 871, 780, 734 cm^{-1} . **MS** (EI): m/z (%) 148.1 (100) $[\text{M}-\text{COOEt}]^+$, 222.1 (76) $[\text{M}]^+$, (MW = 222.21). **HRMS** (ESI) calc for $[\text{C}_{12}\text{H}_{11}\text{O}_3\text{F}+\text{Na}]^+$ 245.05844; found 245.05812.

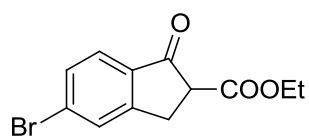
ethyl 5-chloro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (1h):



Isolated as a yellow solid, m.p. 38-39 °C. Mixture of tautomers (keto/enol 3.5:1). **^1H NMR** (600 MHz, CDCl_3) δ 10.41 (s, 0.2H), 7.70 (d, J = 8.2 Hz, 0.8H), 7.55 (d, J = 8.2 Hz, 0.2H), 7.50 (d, J = 0.9 Hz, 0.8H), 7.45 (d, J = 1.1 Hz, 0.2H), 7.39 – 7.36 (m, 1H), 7.36 (d, J = 1.8 Hz, 1H), 4.32 (q, J = 7.1 Hz, 0.4H), 4.28 – 4.22 (m, 1.6H), 3.73 (dd, J = 8.3, 4.0 Hz, 0.8H), 3.54 (dd, J = 17.4, 4.0 Hz, 0.8H), 3.51 (s, 0.4H), 3.35 (dd, J = 17.4, 8.3 Hz, 0.8H), 1.36 (t, J = 7.1 Hz, 0.6H), 1.31 (t, J = 7.1 Hz, 2.4H). **^{13}C NMR** (151 MHz, CDCl_3) δ 198.2, 168.9, 155.2, 144.8, 142.2, 135.6, 133.9, 128.8, 127.5, 126.9, 125.9, 125.3, 121.8, 103.0, 62.1, 60.4, 53.5, 32.6, 30.1, 14.6, 14.3. **IR** (ATR) $\nu_{\max}$ 3835, 3296, 2975, 2910, 2659, 2322, 2096, 1995, 1892, 1721, 1660, 1612, 1507, 1416, 1332, 1271, 1198, 1111, 1017, 922, 827, 752 cm^{-1} . **MS** (EI): m/z (%) 164.0 (53)

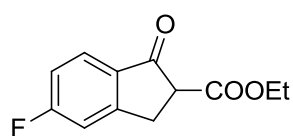
$[M-HCO_2Et]^+$, 166.0 (23) $[M-HCO_2Et+2]^+$, 238.0 (100) $[M]^+$, 240.0 (38) $[M+2]^+$, (MW = 238.67). **HRMS** (ESI) calc for $[C_{12}H_{11}O_3^{35}Cl+Na]^+$ 261.02889; found 261.02878.

ethyl 5-bromo-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (1i):



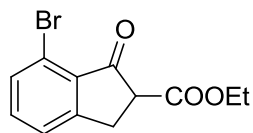
Isolated as a brown solid, m.p. 49-51 °C. Mixture of tautomers (keto/enol 3:1). **¹H NMR** (600 MHz, CDCl₃) δ 10.40 (s, 0.25H), 7.69 (s, 0.75H), 7.64 – 7.60 (m, 1H), 7.55 – 7.48 (m, 1.25H), 4.32 (q, J = 7.1 Hz, 0.5H), 4.28 – 4.21 (m, 1.5H), 3.71 (dd, J = 8.3, 4.0 Hz, 0.75H), 3.54 (dd, J = 17.4, 3.9 Hz, 0.75H), 3.50 (s, 0.5H), 3.35 (dd, J = 17.4, 8.3 Hz, 0.75H), 1.36 (t, J = 7.1 Hz, 0.75H), 1.31 (t, J = 7.1 Hz, 2.25H). **¹³C NMR** (151 MHz, CDCl₃) δ 198.2, 168.6, 155.1, 144.9, 135.9, 134.1, 131.5, 130.9, 130.1, 129.9, 128.1, 125.8, 123.8, 121.9, 102.8, 61.9, 60.3, 53.3, 32.4, 29.9, 14.4, 14.2. **IR** (ATR) ν_{max} 3787, 3476, 2980, 2650, 2321, 2215, 2159, 2079, 1969, 1937, 1901, 1714, 1622, 1590, 1559, 1462, 1406, 1374, 1347, 1280, 1246, 1212, 1174, 1128, 1095, 1054, 1012, 915, 853, 824, 776, 727 cm⁻¹. **MS** (EI): m/z (%) 102.3 (100), 208.3 (41) $[M-HCOOEt]^+$, 210.3 (45) $[M-HCOOEt+2]^+$, 282.4 (24) $[M]^+$, 284.4 (24) $[M+2]^+$, (MW = 283.12). **HRMS** (ESI) calc for $[C_{12}H_{11}O_3^{79}Br+Na]^+$ 304.97838; found 304.97855.

ethyl 5-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (1j):

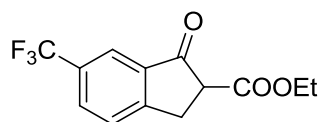


Isolated as a brown oil.¹² Mixture of tautomers (keto/enol 9:1). **¹H NMR** (600 MHz, CDCl₃) δ 10.44 (s, 0.1H), 7.76 (dd, J = 8.5, 5.3 Hz, 0.9H), 7.57 (ddd, J = 8.4, 5.1, 1.4 Hz, 0.1H), 7.18 – 7.14 (m, 1H), 7.11 – 7.05 (m, 1.0H), 4.31 (q, J = 7.1 Hz, 0.2H), 4.28 – 4.20 (m, 1.8H), 3.72 (dt, J = 8.9, 4.4 Hz, 0.9H), 3.54 (dd, J = 17.4, 3.9 Hz, 0.9H), 3.50 (s, 0.2H), 3.34 (dd, J = 17.4, 8.3 Hz, 0.9H), 1.35 (t, J = 7.1 Hz, 0.3H), 1.30 (t, J = 7.1 Hz, 2.7H). **¹³C NMR** (151 MHz, CDCl₃) δ 197.7, 168.9, 168.5, 166.8, 165.1 (d, J = 248.7 Hz), 156.7 (d, J = 10.4 Hz), 145.7 (d, J = 9.0 Hz), 131.8, 131.8, 127.1 (d, J = 10.7 Hz), 122.1 (d, J = 9.4 Hz), 116.4 (d, J = 23.8 Hz), 114.5 (d, J = 23.6 Hz), 113.4 (d, J = 22.4 Hz), 112.4 (d, J = 23.4 Hz), 102.3, 62.0, 60.3, 53.6, 32.7, 30.3, 30.3, 14.6, 14.3. **¹⁹F NMR** (564 MHz, CDCl₃) δ -101.49 (dd, J = 13.7, 8.2 Hz, 0.9F), -111.05 – -111.11 (m, 0.1F).

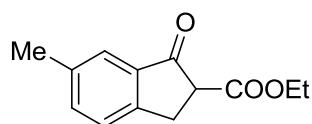
¹² Ishihara, M.; Nakayama, G. *Chem. Pharm. Bull.* **1993**, 41, 529-538.

ethyl 7-bromo-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (1l):

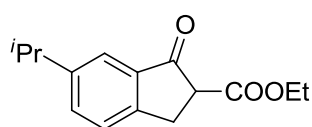
Isolated as an orange solid, m.p. 66-68 °C. Mixture of tautomers (keto/enol 3:1). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 10.82 (s, 0.25H), 7.58 – 7.53 (m, 0.75H), 7.51 (d, $J = 7.9$ Hz, 0.25H), 7.47 – 7.42 (m, 1.5H), 7.41 – 7.38 (m, 0.25H), 7.23 (d, $J = 7.6$ Hz, 0.25H), 4.33 (q, $J = 7.1$ Hz, 0.5H), 4.29 – 4.19 (m, 1.5H), 3.75 (dd, $J = 8.4, 4.3$ Hz, 0.75H), 3.56 – 3.45 (m, 1.25H), 3.31 (dd, $J = 17.4, 8.5$ Hz, 0.75H), 1.36 (t, $J = 7.1$ Hz, 0.75H), 1.32 (t, $J = 7.1$ Hz, 2.25H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 196.8, 168.9, 156.4, 146.1, 135.8, 133.0, 132.8, 132.0, 130.4, 125.7, 123.9, 120.6, 115.9, 103.8, 62.0, 60.5, 54.1, 32.4, 29.4, 14.6, 14.3. **IR** (ATR) ν_{max} 3273, 3061, 2980, 2900, 2800, 2327, 2079, 2003, 1932, 1847, 1715, 1643, 1616, 1556, 1469, 1442, 1412, 1374, 1350, 1311, 1251, 1206, 1140, 1104, 1019, 932, 875, 788, 765, 743 cm^{-1} . **MS** (EI): m/z (%) 209.0 (100) $[\text{M}-\text{COOEt}]^+$, 211.0 (94) $[\text{M}-\text{COOEt}+2]^+$, 282.0 (99) $[\text{M}]^+$, 284.0 (92) $[\text{M}+2]^+$, (MW = 283.12). **HRMS** (ESI) calc for $[\text{C}_{12}\text{H}_{11}\text{O}_3^{79}\text{Br}+\text{Na}]^+$ 304.97838; found 304.97849.

ethyl 1-oxo-6-(trifluoromethyl)-2,3-dihydro-1H-indene-2-carboxylate (1m):

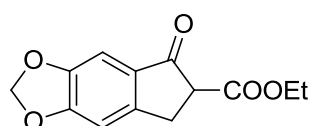
Isolated as an orange solid, m.p. 68-69 °C. Mixture of tautomers (keto/enol 1.3:1). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.36 (s, 0.4H), 8.04 (s, 0.6H), 7.91 – 7.84 (m, 1H), 7.69 – 7.62 (m, 1H), 7.56 (t, $J = 9.6$ Hz, 0.4H), 4.34 (q, $J = 7.1$ Hz, 0.8H), 4.29 – 4.23 (m, 1.2H), 3.78 (dd, $J = 8.3, 3.8$ Hz, 0.6H), 3.64 (dd, $J = 17.6, 3.8$ Hz, 0.6H), 3.58 (s, 0.8H), 3.44 (dd, $J = 17.7, 8.3$ Hz, 0.6H), 1.37 (t, $J = 7.1$ Hz, 1.2H), 1.32 (t, $J = 7.1$ Hz, 1.8H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 198.4, 168.6, 156.9, 146.6, 137.7, 135.8, 132.0 (q, $J = 3.2$ Hz), 130.9 (q, $J = 33.3$ Hz), 129.8 (q, $J = 32.4$ Hz), 127.5, 125.2, 124.3 (q, $J = 272.1$ Hz), 123.7 (q, $J = 272.6$ Hz), 122.1 (q, $J = 4.0$ Hz), 117.9 (q, $J = 3.9$ Hz), 104.2, 62.2, 60.6, 53.6, 32.9, 30.5, 14.6, 14.3. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -62.1 (s, 1.2F), -62.6 (s, 1.8F). **IR** (ATR) ν_{max} 3285, 2995, 2323, 2108, 1925, 1740, 1662, 1600, 1480, 1419, 1372, 1323, 1265, 1219, 1102, 1021, 940, 902, 832, 771, 717 cm^{-1} . **MS** (EI): m/z (%) 198.4 (54) $[\text{M}-\text{HCOOEt}]^+$, 272.5 (92) $[\text{M}]^+$, (MW = 272.22). **HRMS** (ESI) calc for $[\text{C}_{13}\text{H}_{11}\text{O}_3\text{F}_3+\text{Na}]^+$ 295.05525; found 295.05582.

ethyl 6-methyl-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (1n):

Isolated as a light brown solid, m.p. 48-49 °C. Mixture of tautomers (keto/enol 9:1). ^1H NMR (400 MHz, CDCl_3) δ 10.43 (s, 0.1H), 7.56 (s, 0.9H), 7.44 (dd, J = 7.9, 1.3 Hz, 1H), 7.38 (d, J = 7.9 Hz, 0.9H), 7.34 (d, J = 7.6 Hz, 0.1H), 7.25 – 7.21 (m, 0.1H), 4.29 (q, J = 7.1, 0.2H), 4.28 – 4.19 (m, 1.8H), 3.70 (dd, J = 8.2, 4.0 Hz, 0.9H), 3.52 – 3.43 (m, 1.1H), 3.32 (dd, J = 17.1, 8.2 Hz, 0.9H), 2.42 (s, 0.3H), 2.40 (s, 2.7H), 1.36 (t, J = 7.1 Hz, 0.3H), 1.30 (t, J = 7.1 Hz, 2.7H). ^{13}C NMR (101 MHz, CDCl_3) δ 199.8, 169.4, 151.2, 140.5, 137.9, 136.8, 135.6, 130.5, 126.3, 124.7, 124.5, 121.2, 61.8, 60.2, 53.8, 32.3, 30.1, 21.5, 21.2, 14.6, 14.3. IR (ATR) ν_{max} 3809, 3460, 2983, 2926, 2326, 2105, 1992, 1904, 1738, 1630, 1574, 1467, 1412, 1370, 1253, 1201, 1083, 1026, 953, 881, 779, 713 cm^{-1} . MS (EI): m/z (%) 144.4 (100) $[\text{M}-\text{HCOOEt}]^+$, 218.5 (35) $[\text{M}]^+$, (MW = 218.25). HRMS (ESI) calc for $[\text{C}_{13}\text{H}_{14}\text{O}_3+\text{Na}]^+$: 241.08352; found: 241.08427.

ethyl 6-isopropyl-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (1o):

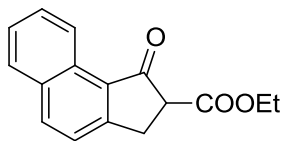
Isolated as a brown oil. Mixture of tautomers (keto/enol 8:1). ^1H NMR (600 MHz, CDCl_3) δ 10.50 (s, 0.1H), 7.64 (d, J = 1.4 Hz, 0.9H), 7.53 – 7.49 (m, 1H), 7.42 (d, J = 7.9 Hz, 0.9H), 7.38 (d, J = 7.8 Hz, 0.9H), 7.30 (dd, J = 7.8, 1.6 Hz, 0.1H), 4.32 (q, J = 7.1 Hz, 0.2H), 4.29 – 4.21 (m, 1.8H), 3.71 (dd, J = 8.2, 4.0 Hz, 0.9H), 3.50 (dd, J = 17.1, 4.0 Hz, 0.9H), 3.48 (s, 0.2H), 3.33 (dd, J = 17.1, 8.2 Hz, 0.9H), 3.02 – 2.93 (m, 1H), 1.36 (t, J = 7.1 Hz, 0.3H), 1.31 (t, J = 7.1 Hz, 2.7H), 1.29 (d, J = 6.9 Hz, 0.6H), 1.26 (d, J = 6.9 Hz, 5.4H). ^{13}C NMR (151 MHz, CDCl_3) δ 199.9, 169.4, 151.6, 149.1, 148.1, 141.0, 135.6, 134.8, 128.2, 126.5, 124.7, 122.0, 118.5, 61.8, 60.2, 53.9, 34.3, 34.0, 32.3, 30.1, 24.3, 24.1, 24.1, 14.6, 14.4. IR (ATR) ν_{max} 3433, 2962, 2324, 2098, 1995, 1921, 1711, 1648, 1580, 1461, 1371, 1318, 1256, 1164, 1100, 1015, 830, 786, 708, 673 cm^{-1} . MS (EI): m/z (%) 172.1 (82) $[\text{M}-\text{HCOOEt}]^+$, 246.0 (100) $[\text{M}]^+$, (MW = 246.30). HRMS (ESI) calc for $[\text{C}_{15}\text{H}_{18}\text{O}_3+\text{Na}]^+$: 269.11482; found: 269.11475.

ethyl 5-oxo-6,7-dihydro-5H-indeno[5,6-d][1,3]dioxole-6-carboxylate (1p):

Isolated as a yellow solid, m.p. 80-81 °C. Mixture of tautomers (keto/enol >20:1). ^1H NMR (600 MHz, CDCl_3) δ 7.09 (s, 1H), 6.85 (s, 1H), 6.08 (d, J = 2.6 Hz, 1H), 4.28 – 4.18 (m, 2H), 3.70 (dd, J = 7.9, 3.6 Hz, 1H), 3.41 (dd, J = 17.0, 3.5 Hz, 1H), 3.23 (dd, J = 17.1, 7.9 Hz, 1H), 1.30 (t, J = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 197.5, 169.4, 155.0, 151.7, 148.8, 129.9, 105.7, 103.1, 102.6, 61.9, 53.9, 30.3, 14.4. IR (ATR) ν_{max} 3450, 2982, 2928, 2780, 2329, 2100, 1866, 1695, 1606, 1467, 1374, 1309, 1254, 1211, 1076, 1027, 932, 865, 806, 765, 733, 672 cm^{-1} . MS

(EI): m/z (%) 174.1 (99) $[M-HCOOEt]^+$, 248.1 (100) $[M]^+$, (MW = 248.23). **HRMS** (ESI) calc for $[C_{13}H_{12}O_5+H]^+$: 249.07575; found: 249.07578.

ethyl 1-oxo-2,3-dihydro-1H-cyclopenta[a]naphthalene-2-carboxylate (1q):



Isolated as a yellow solid, m.p. 93-94 °C. Mixture of tautomers (keto/enol >20:1). **1H NMR** (600 MHz, $CDCl_3$) δ 9.08 (d, J = 8.4 Hz, 1H), 8.08 (d, J = 8.4 Hz, 1H), 7.90 (d, J = 8.2 Hz, 1H), 7.68 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.59 – 7.52 (m, 2H), 4.32 – 4.23 (m, 2H), 3.83 (dd, J = 7.8, 3.6 Hz, 1H), 3.64 (dd, J = 17.5, 3.6 Hz, 1H), 3.45 (dd, J = 17.5, 7.8 Hz, 1H), 1.33 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.0, 169.5, 157.4, 136.8, 133.0, 129.7, 129.5, 129.4, 128.4, 127.0, 124.0, 123.8, 61.9, 54.0, 30.8, 14.40. **IR** (ATR) ν_{max} 3456, 2987, 2324, 2087, 1945, 1689, 1574, 1516, 1440, 1368, 1321, 1206, 1159, 1078, 1015, 931, 863, 824, 754, 676 cm^{-1} . **MS** (EI): m/z (%) 180.0 (100) $[M-HCOOEt]^+$, 254.0 (83) $[M]^+$, (MW = 254.28). **HRMS** (ESI) calc for $[C_{16}H_{14}O_3+Na]^+$: 277.08352; found: 277.08359.

Computational details.

Geometries were optimized with Gaussian09¹ package using the PBE0² functional with D3 empirical corrections with Becke-Johnson damping.³ The electronic configuration of the systems was described with the split-valence SVP⁴ basis set for H, C, O and F while for I we adopted the quasi-relativistic SDD⁵ effective core potential with the associated valence basis set. All geometries were characterized as minimum or transition state through frequency calculations. The reported free energies were built through single point energy calculations on the PBE/SVP geometries using the M06 functional and the triple- ζ TZVP basis set for H, C and O, augmented with a diffuse basis function for F.⁶ Solvent effects were included with the PCM model using CH₂Cl₂ as the solvent.⁷ To this M06/TZVP electronic energy in solvent, thermal corrections were added from the gas-phase frequency calculations at the PBE-D3/SVP level.

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Cartesian coordinates of species reported in Scheme 7 with solvent energies (in a.u.).

1a							
E=-689.9726055				C	-5.839366	-2.734568	0.918558
C	-4.231717	-0.308484	-0.192012	C	-6.858837	-1.699268	0.464030
C	-3.226657	-1.224890	0.116023	C	-6.234358	-0.593189	-0.387893
C	-1.917297	-0.764526	0.244952	C	-5.082122	0.031403	0.382524
C	-1.646222	0.593392	0.067424	C	-4.056691	-0.989982	0.841868
C	-2.644368	1.515946	-0.248548	C	-4.683406	-2.097817	1.686651
C	-3.948252	1.052553	-0.375651	O	-4.428884	0.972881	-0.505838
C	-0.206046	0.856392	0.253704	C	-3.778024	1.994919	0.020883
C	0.433690	-0.489494	0.687535	O	-3.671747	2.256743	1.187764
C	-0.663620	-1.544096	0.536239	C	-7.258875	0.442512	-0.825387
C	1.675897	-0.759262	-0.125974	C	-3.643005	-3.124485	2.109665
O	1.725769	-1.484630	-1.086066	C	-3.139770	2.829050	-1.090541
O	0.376289	1.899146	0.108825	C	-4.006974	4.011304	-1.455297
O	2.704198	-0.055037	0.332891	O	-1.886986	3.345413	-0.637372
C	3.905524	-0.100960	-0.436350	C	-0.929404	2.521515	-0.258325
C	4.885588	0.861062	0.181548	C	0.275855	3.114107	0.231391
H	-2.386142	2.568795	-0.384025	C	1.395117	2.318689	0.626111
H	-4.757619	1.745065	-0.617531	C	1.239476	0.939380	0.640499
H	-5.262316	-0.657751	-0.294743	C	0.056376	0.346956	0.173109
H	-3.465099	-2.283015	0.249531	C	-1.006400	1.136086	-0.294595
H	0.742874	-0.340850	1.734547	O	2.500225	2.957001	0.960696
H	4.285103	-1.135687	-0.445461	C	3.701614	2.219042	1.202249
H	3.668243	0.162045	-1.479280	C	4.800569	3.222467	1.461824
H	5.823792	0.865565	-0.392161	I	0.426847	5.125264	0.284050
H	4.473930	1.880712	0.186669	C	-0.067144	-1.120331	0.166373
H	5.115795	0.577443	1.219037	C	-0.892647	-1.765977	-0.764741
H	-0.417660	-2.209522	-0.307209	C	-1.026290	-3.147900	-0.751407
H	-0.770069	-2.174433	1.432099	C	-0.329205	-3.918830	0.177469
Ar*-I-F				C	0.504823	-3.285775	1.094639
E=-2558.6048058				C	0.629558	-1.901108	1.097842
				C	-1.910059	-3.823944	-1.769784

F	-2.866945	-2.995076	-2.202087	H	-6.327089	-3.500699	1.541960
C	1.329844	-4.100211	2.059661	H	-5.430210	-3.264214	0.038370
F	0.780090	-5.284035	2.299884	H	5.736560	-2.045947	0.770933
C	4.013418	1.359349	-0.025694	H	-5.794231	-1.063601	-1.287210
O	4.546029	0.209498	0.348534	H	-5.099809	-1.629035	2.598040
C	4.864464	-0.764587	-0.678438	H	-3.598725	-1.442128	-0.055164
C	6.045457	-1.584070	-0.185498	H	7.609573	-0.241274	-0.875710
C	6.314688	-2.707547	-1.188398	H	7.076921	0.065360	0.797144
C	5.085263	-3.566789	-1.449717	H	8.110849	-1.332730	0.433943
C	3.899162	-2.735260	-1.934693	H	7.146314	-3.327660	-0.818793
C	3.627586	-1.604818	-0.942888	H	1.801603	-2.980977	-2.500047
C	7.276013	-0.723738	0.057428	H	2.836107	-4.368036	-2.905890
C	2.655748	-3.584715	-2.154668	H	2.359785	-4.084029	-1.218399
O	3.779783	1.710991	-1.149082	H	2.816741	-0.957149	-1.314926
F	1.088933	5.576983	-1.541246	H	-6.804673	1.216006	-1.461585
F	2.554028	-4.314377	1.557200	H	-8.070236	-0.028563	-1.399334
F	1.485766	-3.463653	3.219881	H	-7.713294	0.940304	0.046654
F	-2.504039	-4.897051	-1.250563	H	-7.666571	-2.180203	-0.109540
F	-1.208704	-4.217603	-2.830446	H	-2.803404	-2.655536	2.646753
H	3.554528	1.564202	2.076470	H	-4.081855	-3.885891	2.771592
H	5.738903	2.694118	1.679565	H	-3.232814	-3.648692	1.231597
H	4.947476	3.857407	0.576910	H	-3.258640	-0.481653	1.407181
H	4.547003	3.852634	2.325402	A E=-3248.6137909			
H	2.066423	0.303143	0.949271				
H	-1.916478	0.650101	-0.639167	C	-1.533140	-3.373802	1.040857
H	-2.964639	2.186764	-1.968884	C	-0.763271	-3.499203	2.345057
H	-4.975370	3.655850	-1.833192	C	0.583405	-4.184868	2.168406
H	-4.180529	4.639213	-0.570119	C	0.367406	-5.541641	1.497847
H	-3.524204	4.610833	-2.239193	C	-0.406954	-5.435950	0.191474
H	-1.433441	-1.191867	-1.517760	C	-1.748493	-4.727502	0.367703
H	1.253918	-1.431479	1.859216	O	-0.501613	-2.183148	2.864006
H	-0.444266	-5.004010	0.194099	C	-1.437303	-1.591211	3.595943
H	5.140969	-0.205763	-1.587461	O	-2.459554	-2.091248	3.975467
H	3.295123	-2.043758	0.014618	C	1.341526	-4.306886	3.481152
H	6.663892	-2.262166	-2.137808	C	-2.496452	-4.579023	-0.948429
H	4.181200	-2.273775	-2.899732	C	-1.042842	-0.152639	3.924977
H	5.319024	-4.350632	-2.187584	C	-0.309424	-0.067978	5.245139
H	4.794313	-4.090397	-0.520704	O	-0.181722	0.380576	2.925572
H	-5.461847	0.601213	1.246776	C	-0.557812	0.329743	1.650185
H	-7.342014	-1.242417	1.346975	C	-1.875692	0.182110	1.216241

C	-2.162053	0.108470	-0.148562	C	5.485536	-0.541271	-2.379165
C	-1.138900	0.195046	-1.100726	C	6.882193	-0.339854	-1.856729
C	0.179700	0.389148	-0.695259	C	6.892628	-0.066934	-0.483839
C	0.448187	0.447075	0.678476	C	5.530922	-0.027832	0.032227
O	1.210680	0.515489	-1.553391	C	8.079785	0.141570	0.226996
C	0.951830	1.159003	-2.801031	C	9.275500	0.072570	-0.473160
C	2.270000	1.327227	-3.521143	C	9.272388	-0.195922	-1.850885
C	-3.561647	-0.061883	-0.586599	C	8.085434	-0.402917	-2.553544
C	-3.887326	-0.974473	-1.595178	O	5.152992	0.179607	1.164526
C	-5.210722	-1.141109	-1.990698	H	0.274050	0.545221	-3.415279
C	-6.224696	-0.378021	-1.413974	H	2.095145	1.791318	-4.501178
C	-5.899796	0.541314	-0.420814	H	2.945881	1.976205	-2.944793
C	-4.581568	0.689967	0.003229	H	2.743898	0.347710	-3.679788
I	2.377993	0.811742	1.348802	H	-1.390626	0.164884	-2.160540
F	1.789121	2.484045	2.253296	H	-2.685195	0.079637	1.938676
C	-5.535609	-2.199475	-3.013355	H	-1.974869	0.433842	3.975184
F	-6.708435	-1.981192	-3.598050	H	-0.949877	-0.455152	6.048825
C	-6.956325	1.412222	0.211477	H	0.616355	-0.659588	5.207614
F	-6.995818	1.227793	1.532594	H	-0.055323	0.977946	5.465314
C	0.257497	2.504065	-2.583452	H	2.688063	-3.798591	-0.424016
O	-0.490998	2.983641	-3.388620	H	1.497899	-2.806794	-1.292921
O	0.616313	3.028769	-1.423235	H	8.107006	-0.611008	-3.625654
C	-0.086087	4.196040	-0.937985	H	10.224251	-0.243998	-2.385315
C	-1.382921	3.738344	-0.292432	H	10.224452	0.229466	0.043424
C	-2.130169	4.884019	0.384912	H	8.048542	0.353009	1.297891
C	-1.200859	5.590010	1.370908	H	-4.340490	1.423837	0.775207
C	0.089720	6.048080	0.705302	H	-3.106610	-1.580715	-2.058094
C	0.844103	4.897504	0.039182	H	-7.258875	-0.495533	-1.739438
C	2.128580	5.362098	-0.630454	H	1.739050	-5.069712	-2.378380
C	-3.407457	4.389941	1.047971	H	2.281784	-3.789842	-3.490257
F	-8.165959	1.160998	-0.277622	H	3.479448	-4.784328	-2.613231
F	-6.688020	2.705593	0.002940	H	-1.372167	-4.040118	3.088486
F	-5.584610	-3.409211	-2.442873	H	1.168813	-3.542788	1.482255
F	-4.599037	-2.253113	-3.964304	H	1.343716	-6.025663	1.331483
O	2.795770	-1.198160	0.146144	H	-0.179891	-6.199952	2.196179
C	3.542445	-1.294736	-0.830585	H	0.190047	-4.868796	-0.546609
O	3.477660	-2.314832	-1.630140	H	-0.563236	-6.436660	-0.242287
C	2.465097	-3.322166	-1.390232	H	-2.365523	-5.345298	1.046484
C	2.499643	-4.292177	-2.536964	H	-0.962276	-2.712083	0.362836
C	4.581476	-0.271389	-1.173060	H	-2.500450	-2.882786	1.231697

H	-0.298230	4.842383	-1.805912	C	-0.261853	0.466216	-0.234520
H	1.099413	4.155758	0.817357	C	-1.135091	-0.553011	0.164655
H	0.751109	6.532933	1.440498	C	-0.788585	-1.906543	0.050581
H	-0.139479	6.816667	-0.055492	C	0.472706	-2.234585	-0.451978
H	-0.961395	4.894349	2.196269	C	1.372520	-1.224907	-0.808727
H	-1.719601	6.448284	1.827165	C	0.994157	0.115984	-0.723559
H	-2.408441	5.615042	-0.397266	I	-2.921240	-0.005309	1.072416
H	-1.134835	2.972788	0.463938	F	-1.854087	0.484394	2.734908
H	-2.021823	3.257491	-1.050289	C	2.753754	-1.556397	-1.215025
H	2.320605	-4.784803	3.327109	C	3.040189	-2.602500	-2.094916
H	1.513799	-3.321106	3.936392	C	4.359231	-2.880233	-2.452186
H	0.781352	-4.922152	4.203522	C	5.409798	-2.131928	-1.928868
H	-3.476250	-4.098237	-0.810651	C	5.126840	-1.098089	-1.036645
H	-1.917004	-3.965011	-1.659703	C	3.813853	-0.810417	-0.684449
H	-2.671312	-5.555961	-1.423555	O	-1.678502	-2.813862	0.475187
H	2.795227	5.847635	0.097767	C	-1.201786	-4.045346	0.989754
H	2.675338	4.518442	-1.078136	C	-2.388523	-4.759809	1.600287
H	1.919302	6.091415	-1.429946	C	4.638959	-3.964661	-3.459146
H	-4.092013	3.925360	0.321647	F	3.752000	-4.957960	-3.364279
H	-3.175896	3.643147	1.826937	C	6.260960	-0.328934	-0.413631
H	-3.951249	5.213940	1.533636	F	6.861657	-1.040708	0.543272
H	5.264658	0.140956	-3.213971	O	-3.465718	2.031743	-1.226438
H	5.349867	-1.563541	-2.760652	C	-4.668316	2.048288	-1.329058
H	4.013909	0.670215	-1.287825	O	-5.389499	3.155911	-1.503589
A-B				C	-4.686780	4.398912	-1.406729
E=-3449.1020855				C	-3.937010	4.738134	-2.673796
C	3.083652	5.210876	-0.336611	C	-5.542493	0.852220	-1.240698
C	3.029373	3.688462	-0.254248	C	-6.853188	0.805224	-2.015308
C	3.595032	3.021589	-1.494067	C	-6.945244	-0.619890	-2.474807
C	5.032390	3.456149	-1.772042	C	-5.808570	-1.340189	-2.082842
C	5.102275	4.978849	-1.859074	C	-4.922081	-0.448751	-1.338561
C	4.523804	5.642627	-0.616910	C	-7.957086	-1.272827	-3.175757
O	1.659404	3.274868	-0.114063	C	-7.795084	-2.623735	-3.481730
C	1.247822	2.771754	1.047412	C	-6.650014	-3.332956	-3.088388
O	1.949083	2.597736	2.012464	C	-5.642994	-2.695494	-2.375030
C	5.588483	2.774952	-3.012841	C	-0.097948	-3.832905	2.027403
C	2.520221	5.874925	0.910820	O	0.777460	-4.634953	2.217831
C	-0.242869	2.459813	1.036687	O	-0.270111	-2.690613	2.668741
C	-1.091627	3.709647	1.095289	C	0.735987	-2.246783	3.601802
O	-0.624639	1.755833	-0.146671	C	1.812940	-1.487189	2.845381

C	2.854279	-0.897165	3.795209	H	5.645410	3.142506	-0.907428
C	2.156796	-0.014989	4.829878	H	2.953420	3.274044	-2.357049
C	1.074282	-0.779380	5.579126	H	3.554455	1.927514	-1.376220
C	0.031816	-1.389472	4.643192	H	1.172561	-3.145034	4.070675
C	3.942529	-0.148518	3.040497	H	-0.466130	-0.573204	4.091635
C	-1.029386	-2.173208	5.399506	H	0.564900	-0.119460	6.299776
F	5.856033	-4.485500	-3.296722	H	1.539293	-1.586485	6.176256
F	4.571419	-3.493174	-4.707961	H	1.716499	0.854880	4.310451
F	5.840747	0.811207	0.143834	H	2.898921	0.387343	5.539014
F	7.192625	-0.017653	-1.319062	H	3.326024	-1.740514	4.335864
F	-5.538542	0.866146	1.281986	H	1.331201	-0.673150	2.275018
H	-0.764927	-4.661406	0.185852	H	2.292957	-2.161059	2.117277
H	-2.074538	-5.732660	2.001973	H	2.602158	6.970057	0.839471
H	-2.815178	-4.153191	2.411624	H	1.457295	5.631911	1.053822
H	-3.162069	-4.920160	0.836316	H	3.063788	5.550469	1.812226
H	0.789169	-3.277149	-0.497360	H	5.574072	1.679041	-2.911438
H	1.657905	0.918005	-1.042683	H	4.997546	3.037628	-3.905715
H	-0.437900	1.827468	1.915915	H	6.630472	3.076785	-3.199499
H	-0.817796	4.311883	1.973277	H	-1.540598	-1.529227	6.130708
H	-0.942040	4.304273	0.182931	H	-1.792413	-2.572565	4.715574
H	-2.151500	3.427064	1.174564	H	-0.584850	-3.020001	5.949023
H	-5.702826	0.862516	0.075600	H	4.460457	-0.805959	2.325240
H	-5.472334	5.137467	-1.195498	H	3.516231	0.707898	2.493943
H	-4.019654	4.342570	-0.535349	H	4.701771	0.248588	3.731761
H	-4.743615	-3.219055	-2.043505	H	-7.722104	1.085104	-1.397443
H	-6.558246	-4.391267	-3.342347	H	-6.844563	1.503741	-2.867652
H	-8.578161	-3.144051	-4.038986	O	-3.851758	-0.858883	-0.817076
H	-8.859302	-0.739671	-3.484933	F	-4.512492	3.082136	1.529358
H	3.609038	-0.019839	0.038032	H	-4.990414	2.252087	1.496546
H	2.228857	-3.196254	-2.520350	B			
H	6.439854	-2.357922	-2.209238	E=-3248.1813710			
H	-3.491237	5.740621	-2.584544	C	1.933695	-3.310620	-0.878353
H	-3.128524	4.015555	-2.850195	C	1.137717	-3.664463	-2.123755
H	-4.611745	4.741450	-3.543455	C	-0.109178	-4.476933	-1.806260
H	3.576373	3.352419	0.641650	C	0.295705	-5.719117	-1.011051
H	2.463241	5.502803	-1.204885	C	1.103326	-5.385243	0.235734
H	4.559558	6.739783	-0.713201	C	2.340288	-4.549629	-0.085562
H	5.148054	5.391223	0.260202	O	0.707794	-2.450459	-2.760251
H	4.541811	5.312737	-2.751786	C	1.571825	-1.794012	-3.521823
H	6.146399	5.298161	-2.010624	O	2.650501	-2.194860	-3.869747

C	-0.895492	-4.828422	-3.059503	F	4.882891	-1.558544	4.000231
C	3.118615	-4.177849	1.167257	O	-2.715871	-1.509712	-0.271973
C	1.015452	-0.432487	-3.936458	C	-3.478779	-1.635295	0.754264
C	0.260170	-0.527979	-5.245371	O	-3.031139	-2.409129	1.747250
O	0.115334	0.074446	-2.972871	C	-1.752884	-3.024646	1.647057
C	0.499884	0.144914	-1.693618	C	-1.191012	-3.183693	3.037094
C	1.834131	0.190975	-1.280909	C	-4.736810	-1.082451	0.930771
C	2.147374	0.217287	0.080654	C	-5.596885	-1.287088	2.149115
C	1.134639	0.194034	1.043487	C	-6.900498	-0.649986	1.751351
C	-0.202337	0.186448	0.641227	C	-6.818291	-0.140483	0.450445
C	-0.504909	0.175349	-0.721954	C	-5.464088	-0.388733	-0.097156
O	-1.234166	0.172768	1.501782	C	-7.894508	0.501456	-0.157884
C	-1.113490	0.853642	2.740498	C	-9.077214	0.630559	0.565077
C	-2.484692	0.838510	3.380426	C	-9.167726	0.125148	1.868333
C	3.561634	0.262170	0.504551	C	-8.084136	-0.516374	2.471614
C	4.012392	-0.523093	1.571249	O	-5.092130	-0.042225	-1.230159
C	5.346787	-0.485081	1.962880	H	-0.382277	0.350453	3.395450
C	6.252054	0.355739	1.317818	H	-2.455080	1.352256	4.350870
C	5.804497	1.146683	0.263830	H	-3.208817	1.338160	2.721530
C	4.474967	1.093831	-0.149423	H	-2.810718	-0.200444	3.528288
I	-2.495474	0.415203	-1.334759	H	1.390144	0.236437	2.102386
F	-1.823698	2.132920	-2.243274	H	2.639337	0.159457	-2.014917
C	5.814153	-1.409550	3.054804	H	1.882886	0.239053	-4.053979
F	6.925988	-0.965927	3.640014	H	0.924884	-0.901901	-6.035717
C	6.734245	2.101972	-0.436142	H	-0.595442	-1.209514	-5.137177
F	6.711852	1.914067	-1.758296	H	-0.114550	0.465199	-5.528567
C	-0.601882	2.276035	2.521062	H	-1.878415	-4.003420	1.153093
O	0.118629	2.848830	3.294175	H	-1.096552	-2.417018	1.010234
O	-1.072811	2.755470	1.382469	H	-8.169452	-0.905531	3.489675
C	-0.539070	3.986199	0.855065	H	-10.103642	0.235297	2.422049
C	0.765756	3.666825	0.143651	H	-9.941465	1.128201	0.118655
C	1.331965	4.867702	-0.607908	H	-7.792404	0.886584	-1.175070
C	0.270438	5.415155	-1.559851	H	4.135770	1.729270	-0.970066
C	-1.018675	5.756543	-0.824580	H	3.318475	-1.189060	2.086154
C	-1.596504	4.553720	-0.079569	H	7.293966	0.397121	1.636047
C	-2.881634	4.893501	0.659039	H	-0.230081	-3.717995	2.997037
C	2.622958	4.502685	-1.326501	H	-1.018477	-2.202327	3.503112
F	7.994314	1.964215	-0.025468	H	-1.875816	-3.755053	3.680445
F	6.373165	3.371205	-0.216318	H	1.779687	-4.211402	-2.835260
F	6.078718	-2.630118	2.570599	H	-0.744100	-3.838507	-1.164680

H	-0.609768	-6.287279	-0.742791	C	4.765021	-0.532312	-0.445596
H	0.889467	-6.383007	-1.666011	C	2.651873	-1.432774	-1.472864
H	0.470171	-4.817483	0.940962	O	2.043292	-1.764555	-2.637454
H	1.397412	-6.309442	0.759650	C	0.798127	-2.424772	-2.523253
H	2.998784	-5.160328	-0.732055	C	0.191599	-2.539986	-3.899298
H	1.309025	-2.654502	-0.245757	O	4.442766	-0.516976	0.736934
H	2.824685	-2.730485	-1.164467	O	2.066554	-1.552421	-0.384506
H	-0.357548	4.667562	1.703835	I	1.733690	0.631698	1.045786
H	-1.806805	3.763328	-0.821387	F	0.822237	2.345364	2.310077
H	-1.774215	6.135917	-1.531102	C	-0.264205	0.303301	0.576150
H	-0.829545	6.575951	-0.105540	C	-1.196799	0.005981	1.579559
H	0.056730	4.652393	-2.330162	C	-2.539046	-0.169593	1.235296
H	0.658392	6.302551	-2.086759	C	-2.957391	-0.058589	-0.094751
H	1.560773	5.658551	0.131994	C	-2.018587	0.229713	-1.090630
H	0.563100	2.856599	-0.577386	C	-0.673528	0.406140	-0.762982
H	1.498306	3.287263	0.873812	O	-0.769527	-0.037289	2.853880
H	-1.805969	-5.391827	-2.805687	C	-1.243515	-1.017233	3.738569
H	-1.200698	-3.922772	-3.602536	C	-0.996869	-0.512279	5.148036
H	-0.293428	-5.451158	-3.741650	O	0.276033	0.587117	-1.693194
H	4.020184	-3.592971	0.931285	C	0.090260	1.475716	-2.775563
H	2.493794	-3.573053	1.846655	C	1.296309	1.331666	-3.683130
H	3.438066	-5.072613	1.722916	C	-4.377148	-0.261645	-0.445726
H	-3.645585	5.268080	-0.038928	C	-4.739366	-0.870959	-1.656446
H	-3.295690	4.008570	1.164419	C	-6.076065	-1.064281	-1.988260
H	-2.711612	5.672571	1.421104	C	-7.090942	-0.656410	-1.123865
H	3.398765	4.163442	-0.621965	C	-6.741254	-0.054483	0.081216
H	2.444251	3.691495	-2.052591	C	-5.403542	0.145217	0.416332
H	3.030692	5.361698	-1.881239	C	-6.441324	-1.771254	-3.263891
H	-5.182861	-0.809833	3.055580	F	-5.467355	-1.699169	-4.173774
H	-5.728623	-2.354810	2.397308	C	-7.812991	0.358414	1.051676
(S)B-2a				F	-8.006857	-0.576065	1.991196
E=-3348.1151045				C	-0.544275	-2.362912	3.549255
C	7.204482	0.323980	-0.318493	O	-0.943374	-3.370638	4.079381
C	6.087341	-0.149481	-0.999077	O	0.539203	-2.251263	2.808893
C	6.098744	-0.345109	-2.384280	C	1.391678	-3.393794	2.624390
C	7.250608	-0.065228	-3.111308	C	0.947808	-4.144844	1.382001
C	8.377197	0.411664	-2.435424	C	1.888364	-5.305085	1.060491
C	8.356664	0.606658	-1.049623	C	3.324441	-4.794346	0.952378
C	4.763231	-0.851258	-2.860597	C	3.752885	-4.044578	2.206212
C	3.961684	-0.926625	-1.604418	C	2.819903	-2.876762	2.518946

C	3.247178	-2.107216	3.756871	H	0.213580	5.090179	-1.203338
C	1.449368	-6.046035	-0.193602	H	1.764594	3.654633	0.980677
C	-0.032399	2.923374	-2.310781	H	2.765812	5.884088	1.463310
O	-0.352073	3.812542	-3.060732	H	1.689692	6.628361	0.273037
O	0.279995	3.040543	-1.039050	H	0.820710	5.044789	2.758540
C	0.349025	4.330275	-0.414285	H	0.729772	6.816963	2.586780
C	-0.764891	4.400203	0.614269	H	-0.869189	6.545361	0.709243
C	-0.712584	5.701351	1.411118	H	-0.613311	3.544710	1.296746
C	0.674502	5.863576	2.032355	H	-1.740205	4.290913	0.109891
C	1.777617	5.783353	0.984321	H	4.267831	-1.717795	3.626442
C	1.726293	4.458611	0.225845	H	2.585790	-1.244761	3.925358
C	-1.812595	5.744774	2.461613	H	3.229249	-2.743838	4.658986
C	2.855686	4.280511	-0.777078	H	0.417112	-6.419569	-0.101619
F	-7.547353	-1.255963	-3.812886	H	1.486119	-5.379226	-1.070768
F	-6.685567	-3.070864	-3.050597	H	2.105242	-6.906104	-0.402908
F	-8.988420	0.550550	0.444023	H	3.820767	4.539776	-0.312266
F	-7.497750	1.489079	1.688005	H	2.940865	3.234707	-1.119096
F	3.525351	1.124153	-1.634676	H	2.724364	4.936890	-1.655447
H	-0.840618	1.245309	-3.325785	H	-2.810643	5.650646	2.003901
H	1.265156	2.113440	-4.453935	H	-1.692208	4.913195	3.175019
H	2.207824	1.410059	-3.060231	H	-1.789165	6.687159	3.032995
H	1.295130	0.342478	-4.160075	H	0.953546	-3.422538	-2.073596
H	-2.331818	0.332148	-2.130100	H	0.139045	-1.868949	-1.841521
H	-3.264802	-0.404745	2.014396	H	-0.755377	-3.098635	-3.851567
H	-2.320604	-1.213145	3.603357	H	-0.016722	-1.544296	-4.318269
H	-1.315916	-1.267896	5.878226	H	0.869925	-3.064730	-4.588930
H	0.073686	-0.300302	5.282196	H	7.276218	-0.207346	-4.195425
H	-1.553425	0.420994	5.310122	H	9.287118	0.639337	-2.997593
H	-5.153747	0.655288	1.348427	H	9.248838	0.985145	-0.543768
H	-3.962365	-1.211816	-2.342225	H	7.154973	0.468379	0.763546
H	-8.139011	-0.793647	-1.391706	H	4.844440	-1.832723	-3.361835
H	1.276764	-4.038493	3.513986	H	4.296574	-0.150258	-3.569696
H	2.857554	-2.190882	1.657510	(R)B-2a			
H	4.776244	-3.654342	2.086253	E=-3348.1075770			
H	3.778971	-4.741870	3.066369	C	1.864820	-3.826006	1.120212
H	3.395953	-4.112656	0.086647	C	2.242761	-3.065800	2.377593
H	4.008140	-5.637516	0.753335	C	3.577239	-2.347850	2.246083
H	1.850381	-6.016301	1.909290	C	4.661831	-3.355641	1.867819
H	0.943564	-3.426026	0.546193	C	4.295131	-4.148810	0.622416
H	-0.080965	-4.512578	1.528682	C	2.940328	-4.841732	0.739371

O	1.223697	-2.073416	2.643789	F	-5.283382	-2.484198	-4.048791
C	0.182827	-2.413417	3.372388	F	-7.478950	1.036184	1.391256
O	-0.035103	-3.501534	3.847235	F	-7.422382	-0.887473	2.344013
C	3.935430	-1.555281	3.491463	O	-2.190175	2.922777	-2.963413
C	2.568452	-5.592009	-0.531042	H	-0.821443	0.868040	-3.549424
C	-0.748861	-1.231553	3.643471	H	0.710559	2.582603	-4.500542
C	-0.527171	-0.722678	5.054749	H	1.547624	2.711474	-2.916438
O	-0.528119	-0.150227	2.772089	H	1.653555	1.196207	-3.845983
C	-0.991644	-0.185342	1.510992	H	-2.287313	0.007601	-2.158467
C	-0.166566	0.301349	0.491387	H	-2.948768	-0.944972	1.992181
C	-0.615550	0.336457	-0.834000	H	-1.773769	-1.628826	3.551258
C	-1.911684	-0.081179	-1.138783	H	-0.656337	-1.543589	5.772514
C	-2.759453	-0.523739	-0.116659	H	0.490276	-0.315566	5.144265
C	-2.289932	-0.591884	1.198060	H	-1.242160	0.081381	5.277608
I	1.722456	1.031072	0.954457	H	-4.920387	0.066751	1.384717
F	0.359158	2.571969	2.000113	H	-3.763003	-1.816249	-2.305718
O	0.250495	0.781838	-1.764586	H	-7.925155	-1.572099	-1.226154
C	-0.229418	1.510930	-2.874576	H	2.255449	-3.753743	3.241083
C	-1.159032	2.634009	-2.410728	H	3.494314	-1.649429	1.399286
O	-0.656123	3.209464	-1.336260	H	5.579757	-2.791563	1.645909
C	-1.473584	4.072775	-0.520961	H	4.854553	-4.036590	2.721096
C	-2.317331	3.186353	0.380385	H	4.306724	-3.439430	-0.221972
C	-3.093504	3.976331	1.427780	H	5.078330	-4.896247	0.406674
C	-2.107854	4.822085	2.231331	H	3.005888	-5.580151	1.563499
C	-1.300945	5.738133	1.320216	H	1.743147	-3.086700	0.311294
C	-0.516133	4.946822	0.275223	H	0.895968	-4.329322	1.275549
C	-4.167779	-0.849059	-0.415144	H	-2.106339	4.676808	-1.195764
C	-4.534522	-1.502380	-1.601001	H	0.130488	4.233903	0.820754
C	-5.870200	-1.766494	-1.882457	H	-0.593473	6.340847	1.913507
C	-6.876822	-1.380228	-0.996117	H	-1.974670	6.458133	0.814704
C	-6.519842	-0.733273	0.181270	H	-1.408221	4.139156	2.745003
C	-5.181573	-0.472512	0.471906	H	-2.642990	5.408731	2.997896
C	-6.248757	-2.518185	-3.128241	H	-3.796643	4.660995	0.912717
F	-7.357345	-2.017832	-3.685351	H	-1.608962	2.528678	0.909460
C	-7.565063	-0.278312	1.161490	H	-2.995929	2.571537	-0.232387
F	-8.804662	-0.529405	0.730788	H	4.876108	-1.009126	3.329228
C	-3.900843	3.038323	2.314725	H	3.157695	-0.813001	3.726096
C	0.319245	5.842502	-0.624346	H	4.062060	-2.214114	4.369003
C	0.996521	2.039305	-3.589159	H	1.594706	-6.099591	-0.435855
F	-6.498025	-3.807258	-2.864356	H	2.502799	-4.896802	-1.384235

H	3.326017	-6.351062	-0.783115	C	-8.034962	-0.993012	2.083637
H	1.038961	6.429506	-0.032600	C	-7.450881	-1.290566	3.321326
H	0.891717	5.249759	-1.353227	C	-5.015611	-1.811265	-0.094342
H	-0.313113	6.553034	-1.185254	C	-3.787765	-2.242600	0.540041
H	-4.655403	2.483552	1.733601	C	-4.000840	-2.396527	2.022489
H	-3.233473	2.304784	2.796918	I	-2.956720	-0.130033	-1.429235
H	-4.430439	3.588801	3.108730	F	-2.678455	1.727449	-2.274403
F	5.735031	-1.596877	-0.326054	C	-2.711393	-2.931769	-0.125387
O	2.506770	-0.864989	-0.389722	O	-2.161767	-3.903022	0.612249
C	3.181291	-0.711055	-1.441556	C	-1.017276	-4.558241	0.074420
O	2.639870	-1.009364	-2.660117	C	-0.230340	-5.153398	1.213555
C	1.577814	-1.942329	-2.655087	O	-5.241314	-1.556888	-1.288159
C	1.012918	-2.029697	-4.050736	C	-1.068410	0.088275	-0.579728
C	4.500677	-0.269186	-1.445993	C	0.060124	0.062832	-1.413338
C	5.119657	0.423841	-0.297840	C	1.300202	0.393940	-0.866731
C	6.454187	0.874601	-0.788897	C	1.424670	0.663662	0.498085
C	6.613339	0.524063	-2.132040	C	0.297851	0.659117	1.326632
C	5.403532	-0.220058	-2.635120	C	-0.961802	0.389670	0.786946
C	7.778034	0.874493	-2.805005	O	-0.135333	-0.268258	-2.689126
C	8.770413	1.579895	-2.117289	C	0.894369	-0.126951	-3.642925
C	8.598742	1.934167	-0.775735	C	0.270920	-0.336085	-5.007736
C	7.428206	1.585680	-0.101081	C	2.774946	0.889944	1.055292
O	4.596034	0.781691	0.750819	C	3.114187	0.407673	2.324118
H	1.961271	-2.924535	-2.322738	C	4.408630	0.552977	2.815780
H	0.806207	-1.637976	-1.933417	C	5.389880	1.186261	2.058304
H	0.212998	-2.784267	-4.091605	C	5.056075	1.672816	0.796992
H	0.589019	-1.063322	-4.363218	C	3.763873	1.532730	0.301148
H	1.792188	-2.309596	-4.775551	O	-2.089349	0.411205	1.511510
H	7.920597	0.605153	-3.855614	C	-2.204932	1.340544	2.581584
H	9.691266	1.860642	-2.636046	C	-1.757047	2.728656	2.126337
H	9.386276	2.487940	-0.257539	O	-2.233388	2.980009	0.917832
H	7.262000	1.851547	0.945601	C	-1.756128	4.132318	0.196197
H	5.660881	-1.243105	-2.953656	C	-0.505786	3.714619	-0.558889
H	4.928704	0.282133	-3.497499	C	0.005522	4.797905	-1.502007
(S)B-C				C	-1.122174	5.226325	-2.438793
E=-3248.1496962				C	-2.356670	5.668276	-1.663895
C	-6.135806	-1.753952	3.406239	C	-2.879557	4.579699	-0.726841
C	-5.410046	-1.922499	2.230476	C	4.761512	-0.067449	4.140848
C	-5.998432	-1.617850	0.998956	F	3.756959	0.033524	5.013431
C	-7.308015	-1.151713	0.906298	C	6.112815	2.289674	-0.079479

F	5.613033	3.265711	-0.839083	H	0.648711	-5.688641	0.824439
C	1.237320	4.320297	-2.257210	H	0.120390	-4.367454	1.898990
C	-4.105597	5.030752	0.051352	H	-0.838931	-5.866020	1.789287
C	2.075293	-1.072462	-3.440436	H	3.535995	-3.076357	-3.052086
O	3.098310	-0.932932	-4.058771	H	1.784549	-3.796574	-0.665339
O	1.847476	-2.010357	-2.533863	H	3.128694	-5.881916	-0.549241
C	2.959285	-2.838522	-2.142196	H	4.140623	-5.321642	-1.880151
C	3.839069	-2.076700	-1.164079	H	3.859189	-3.977401	0.869740
C	4.987712	-2.934037	-0.638650	H	5.266350	-4.873140	0.288686
C	4.436331	-4.226699	-0.040109	H	5.621968	-3.207818	-1.503267
C	3.540643	-4.973818	-1.019185	H	3.214063	-1.747081	-0.315580
C	2.389567	-4.110915	-1.536020	H	4.237383	-1.172828	-1.651755
C	1.492131	-4.857754	-2.510180	H	-1.520504	4.918869	0.932860
C	5.844522	-2.160968	0.352964	H	-3.139250	3.694650	-1.333693
C	-3.656284	1.342114	3.009455	H	-3.161162	5.960548	-2.357865
F	5.837728	0.498943	4.684509	H	-2.117508	6.572294	-1.072607
F	5.026800	-1.373135	3.998274	H	-1.386809	4.371966	-3.087548
F	6.633798	1.374071	-0.908548	H	-0.776168	6.036305	-3.102073
F	7.117803	2.795621	0.633817	H	0.292459	5.678417	-0.895443
O	-1.076499	3.463357	2.791844	H	-0.768387	2.821310	-1.148198
O	-2.271155	-2.683535	-1.249890	H	0.277318	3.428350	0.161297
H	-1.552045	1.052192	3.422177	H	1.088555	-5.772584	-2.049756
H	-3.808333	2.064826	3.823059	H	0.644057	-4.235168	-2.829327
H	-4.293800	1.614499	2.156949	H	2.054272	-5.159562	-3.409069
H	-3.957459	0.345795	3.359609	H	6.223780	-1.226333	-0.087368
H	0.394683	0.913187	2.381863	H	5.265495	-1.896887	1.252726
H	2.194130	0.381536	-1.485185	H	6.709743	-2.756919	0.681595
H	1.318610	0.891898	-3.581894	H	-4.920255	5.316379	-0.631267
H	1.041200	-0.235116	-5.783157	H	-4.481025	4.228894	0.703897
H	-0.176918	-1.338272	-5.068260	H	-3.875989	5.904367	0.684143
H	-0.516332	0.411717	-5.172927	H	2.052943	4.051815	-1.566739
H	-1.353743	-5.331479	-0.635573	H	0.999106	3.427863	-2.860400
H	-0.431972	-3.828640	-0.504856	H	1.618456	5.093956	-2.941350
H	-5.692625	-1.983249	4.379252	H	-3.274530	-1.808942	2.611190
H	-8.035194	-1.158498	4.235550	H	-3.877707	-3.446875	2.340315
H	-9.065207	-0.630835	2.047264	(R)B-C			
H	-7.731908	-0.918222	-0.073160	E=-3248.1537819			
H	3.521358	1.941869	-0.681301	C	-0.908550	-2.782098	-1.000409
H	2.368084	-0.114288	2.925791	C	0.471147	-2.877556	-1.167868
H	6.402751	1.298788	2.446328	C	1.048215	-3.058526	-2.429361

C	0.234518	-3.127541	-3.557360	F	-5.409032	3.618357	0.970451
C	-1.151485	-3.044498	-3.395105	C	0.806724	5.056191	1.978397
C	-1.722753	-2.885161	-2.125194	C	5.163698	4.188101	-1.842876
C	2.542971	-3.120692	-2.303504	C	-1.248651	0.336396	3.776031
C	2.787890	-2.813507	-0.849502	O	-2.211752	0.704915	4.397835
C	1.534096	-2.678982	-0.154415	O	-1.087503	-0.846304	3.217149
I	3.182190	-0.310588	0.900644	C	-2.191547	-1.768692	3.220990
F	3.764090	1.592347	1.416400	C	-3.189286	-1.359305	2.148821
C	4.055381	-3.072664	-0.223685	C	-4.324041	-2.368819	2.001485
O	4.892515	-3.769109	-1.013073	C	-3.751056	-3.765018	1.765493
C	6.192967	-4.045068	-0.503012	C	-2.747013	-4.159950	2.841629
C	6.196229	-5.258774	0.398496	C	-1.606868	-3.153537	2.989554
C	1.329493	0.393362	0.282739	C	-0.624561	-3.543833	4.082421
C	0.388479	0.761108	1.257982	C	-5.293865	-1.945933	0.907775
C	-0.905271	1.084801	0.848296	C	3.272461	0.452710	-3.914862
C	-1.261532	0.997118	-0.500967	F	-6.168862	-0.232311	-3.856773
C	-0.292329	0.707072	-1.465942	F	-5.153555	-1.871813	-2.900085
C	1.012918	0.405582	-1.082948	F	-6.334229	1.738945	1.459195
O	0.811741	0.792424	2.519919	F	-7.042500	2.873910	-0.226306
C	-0.039547	1.240739	3.554099	O	1.473794	3.183082	-3.518799
C	0.799033	1.334155	4.811520	O	4.413430	-2.695647	0.894888
C	-2.687488	1.084290	-0.880123	H	1.131861	0.668718	-3.792627
C	-3.163797	0.325651	-1.955673	H	3.374446	1.050712	-4.830823
C	-4.520633	0.295122	-2.261308	H	4.153804	0.610835	-3.277591
C	-5.434475	1.026697	-1.508568	H	3.219410	-0.609133	-4.191667
C	-4.965906	1.789988	-0.441299	H	-0.557252	0.682880	-2.521712
C	-3.609828	1.824765	-0.131025	H	-1.668452	1.320094	1.587254
O	1.976105	0.104077	-1.968752	H	-0.441496	2.237204	3.298481
C	2.020577	0.859866	-3.169932	H	0.178625	1.694574	5.642492
C	2.029541	2.354329	-2.849427	H	1.208373	0.346194	5.066349
O	2.747032	2.572912	-1.757855	H	1.633562	2.030330	4.649894
C	2.758903	3.877876	-1.151937	H	6.815691	-4.207688	-1.394558
C	1.763567	3.857667	-0.004428	H	6.563799	-3.159842	0.036065
C	1.787497	5.141685	0.817765	H	-1.322421	-2.618581	-0.004666
C	3.214474	5.411997	1.291888	H	-2.809763	-2.834120	-2.026271
C	4.200131	5.442350	0.131363	H	-1.804199	-3.104051	-4.269907
C	4.181144	4.149163	-0.682898	H	0.666096	-3.252630	-4.554146
C	-4.996690	-0.618903	-3.357193	H	-3.272710	2.442609	0.702931
F	-4.120114	-0.682558	-4.362399	H	-2.473531	-0.287574	-2.535923
C	-5.944530	2.517751	0.440732	H	-6.498289	1.001619	-1.747630

H	7.224076	-5.493164	0.714610	C	-0.581537	-2.468218	1.603876
H	5.593010	-5.068643	1.297229	C	0.805344	-2.493598	1.742144
H	5.787763	-6.135775	-0.125455	C	1.371938	-2.034368	2.930166
H	-2.671717	-1.714384	4.213487	C	0.571305	-1.552690	3.977016
H	-1.039935	-3.101931	2.043397	C	-2.795731	-1.972761	2.251920
H	-2.323327	-5.153722	2.625203	C	-2.823413	-2.396301	0.780470
H	-3.269130	-4.254478	3.812141	C	-1.431661	-2.918447	0.448902
H	-3.260593	-3.787448	0.775145	C	-3.944731	-3.347902	0.478676
H	-4.569388	-4.502199	1.718070	O	-5.107780	-2.698721	0.395553
H	-4.875961	-2.392224	2.960533	C	-6.286043	-3.484711	0.200212
H	-2.651048	-1.268329	1.189084	C	-7.460662	-2.544991	0.143572
H	-3.598328	-0.364768	2.387816	O	-3.748890	-1.695395	2.938009
H	2.458219	4.609756	-1.920256	O	-3.824337	-4.535537	0.330580
H	4.440208	3.310555	-0.012144	I	-3.330376	-0.530924	-0.466689
H	5.222915	5.620956	0.500723	F	-3.338831	1.220552	-1.771868
H	3.961335	6.292110	-0.535366	C	-1.367770	0.113646	-0.146521
H	3.507697	4.612311	1.995688	C	-1.047569	0.725463	1.068018
H	3.253261	6.360652	1.852422	C	0.260860	1.164820	1.277402
H	1.481977	5.981219	0.164184	C	1.211786	1.016395	0.265284
H	2.036744	3.014781	0.649338	C	0.849362	0.493159	-0.979095
H	0.752262	3.662979	-0.399178	C	-0.446797	0.021948	-1.191780
H	-0.207129	-4.543216	3.888959	O	-2.021440	0.821488	1.982165
H	0.214898	-2.835926	4.121888	C	-2.005839	1.898843	2.905898
H	-1.114113	-3.566391	5.070705	C	-3.297117	1.813197	3.688684
H	-5.704996	-0.943689	1.103233	C	2.639579	1.287236	0.532451
H	-4.793603	-1.914243	-0.074235	C	3.183944	0.938226	1.771539
H	-6.137024	-2.648977	0.825872	C	4.550850	1.060046	2.008096
H	6.190499	4.353052	-1.482556	C	5.399947	1.549640	1.021944
H	5.154247	3.243994	-2.407299	C	4.859513	1.913620	-0.210891
H	4.918364	5.003994	-2.542836	C	3.496174	1.785985	-0.456967
H	-0.219880	4.869360	1.625294	O	-0.861234	-0.570604	-2.316211
H	1.086021	4.230645	2.654572	C	-0.111697	-0.440834	-3.502516
H	0.796658	5.984159	2.570624	C	1.177600	-1.252889	-3.495611
O	1.303370	-2.375103	1.028962	O	2.068672	-1.040337	-4.275541
H	2.926700	-4.117794	-2.582734	C	5.090484	0.568457	3.322605
H	3.041514	-2.400917	-2.974669	F	6.375068	0.873074	3.487964
(S)C				C	5.774143	2.363313	-1.318098
E=-3248.2109329				F	6.188666	1.314673	-2.044422
C	-0.812654	-1.525542	3.842250	C	-1.874569	3.215153	2.136329
C	-1.369843	-1.977848	2.646180	O	-1.148887	4.117482	2.461272

O	-2.664180	3.178880	1.077990	H	-7.360008	-1.837128	-0.692765
C	-2.509568	4.145330	0.019636	H	2.871488	-3.085430	-3.341538
C	-1.401460	3.646291	-0.891844	H	1.482708	-4.023895	-0.796709
C	-1.256745	4.477302	-2.162441	H	3.041749	-5.943870	-0.832589
C	-2.605353	4.536294	-2.877053	H	3.858625	-5.286258	-2.250658
C	-3.699465	5.066196	-1.960543	H	3.725832	-3.961116	0.520416
C	-3.850173	4.221951	-0.695151	H	5.140446	-4.740595	-0.191707
C	-4.952310	4.738468	0.215408	H	5.164738	-3.079860	-2.025795
C	-0.161760	3.908992	-3.053063	H	2.805960	-1.772670	-0.581681
F	6.863445	2.969199	-0.845183	H	3.616819	-1.164073	-2.036036
F	5.164878	3.203262	-2.154414	H	-2.245100	5.114017	0.477946
F	4.981298	-0.769216	3.407341	H	-4.070464	3.184083	-1.003724
F	4.410189	1.073095	4.354143	H	-4.665287	5.090110	-2.491164
C	-1.014201	-0.856166	-4.646137	H	-3.477212	6.113442	-1.679510
O	1.187630	-2.188053	-2.554605	H	-2.872591	3.514407	-3.198832
C	2.412316	-2.918318	-2.352681	H	-2.527730	5.158827	-3.784138
C	2.040891	-4.252978	-1.722742	H	-0.973301	5.509747	-1.879394
C	3.315771	-5.000194	-1.331013	H	-1.676683	2.617988	-1.176788
C	4.231046	-4.170107	-0.441241	H	-0.451096	3.618927	-0.334294
C	4.611200	-2.844358	-1.096965	H	0.852145	-6.021563	-2.144042
C	3.347875	-2.083682	-1.492247	H	0.222107	-4.531153	-2.883912
C	1.141626	-5.077861	-2.630186	H	1.658846	-5.329480	-3.570568
C	5.509847	-1.993285	-0.212717	H	5.795589	-1.058473	-0.717913
H	-1.136963	1.821943	3.580461	H	5.000151	-1.723384	0.726789
H	-3.324695	2.592163	4.462916	H	6.433093	-2.530703	0.052870
H	-4.150992	1.944251	3.009847	H	-5.922026	4.742838	-0.305648
H	-3.382121	0.823375	4.158744	H	-5.055418	4.109798	1.112137
H	0.536781	1.625396	2.225189	H	-4.745788	5.770263	0.546625
H	1.607848	0.386421	-1.751579	H	0.806573	3.873580	-2.528409
H	0.194686	0.611384	-3.636076	H	-0.416323	2.880431	-3.358917
H	-0.484689	-0.742342	-5.601050	H	-0.030308	4.507734	-3.967618
H	-1.322520	-1.904936	-4.526426	H	1.441590	-2.861760	0.936421
H	-1.910750	-0.221263	-4.639956	H	2.458753	-2.046741	3.048720
H	-6.170892	-4.070637	-0.725536	H	1.042274	-1.201000	4.898069
H	-6.366467	-4.202428	1.031374	H	-1.462256	-1.152028	4.637299
H	3.095004	2.084930	-1.427505	H	-1.473919	-4.020262	0.401277
H	2.535428	0.522184	2.544381	H	-1.047231	-2.571791	-0.522939
H	6.470507	1.640941	1.207271	(R)C			
H	-8.391062	-3.113477	0.001991	E=-3248.2049727			
H	-7.543126	-1.968831	1.076438	C	0.509701	0.966505	4.186374

C	1.244757	1.529202	3.144746	O	2.569078	-3.405424	0.941587
C	0.578516	2.154313	2.089235	C	2.539556	-4.229519	-0.241464
C	-0.813084	2.247600	2.046594	C	1.524893	-3.624092	-1.195907
C	-1.544601	1.686616	3.087263	C	1.517157	-4.316790	-2.554611
C	-0.882496	1.047168	4.145986	C	2.929884	-4.292421	-3.134830
C	2.733512	1.573598	2.949603	C	3.938542	-4.914044	-2.178430
C	2.918877	2.100738	1.531383	C	3.947666	-4.219791	-0.816748
C	1.553867	2.647754	1.092813	C	4.957394	-4.838386	0.136580
C	4.015472	3.123759	1.399246	C	0.504353	-3.668396	-3.486418
O	4.340083	3.339094	0.127831	F	-6.785528	-2.705557	-1.537937
C	5.280053	4.381587	-0.138701	F	-4.987634	-2.900520	-2.713939
C	5.422029	4.496602	-1.633262	F	-5.229551	0.533906	3.147631
O	4.529976	3.690900	2.329364	F	-4.642765	-1.340818	4.018339
I	3.413129	0.454519	-0.013113	C	1.541147	1.091583	-4.288303
F	3.539364	-1.129726	-1.511763	O	-0.837542	2.306398	-2.315939
C	1.440983	-0.241921	0.121500	C	-2.047612	3.067268	-2.160084
C	1.009073	-0.980090	1.224875	C	-1.685761	4.324554	-1.383578
C	-0.322394	-1.394092	1.273425	C	-2.961380	5.087386	-1.028339
C	-1.183177	-1.104394	0.211867	C	-3.976002	4.221984	-0.292790
C	-0.702760	-0.469150	-0.934011	C	-4.344866	2.975732	-1.093975
C	0.618125	-0.018372	-0.988682	C	-3.079826	2.201395	-1.454253
O	1.890418	-1.235759	2.208611	C	-0.681006	5.182272	-2.135863
C	1.770926	-2.460900	2.914568	C	-5.342266	2.088458	-0.364259
C	2.968084	-2.561571	3.833455	H	0.838068	-2.487910	3.501054
C	-2.635207	-1.347355	0.335436	H	2.930769	-3.502474	4.399481
C	-3.267865	-1.103670	1.557506	H	3.894446	-2.533570	3.242664
C	-4.652476	-1.192310	1.672442	H	2.971892	-1.723325	4.544854
C	-5.433292	-1.547078	0.577566	H	-0.689919	-1.942604	2.139557
C	-4.805143	-1.807517	-0.639665	H	-1.388083	-0.257820	-1.751901
C	-3.422602	-1.709689	-0.763901	H	0.200759	-0.409328	-3.520796
O	1.146903	0.638782	-2.017533	H	1.111765	1.064545	-5.298297
C	0.515365	0.621021	-3.278227	H	1.857430	2.118371	-4.054370
C	-0.749428	1.469878	-3.335640	H	2.417514	0.431112	-4.235542
O	-1.553326	1.356037	-4.224884	H	4.909857	5.312744	0.317924
C	-5.283376	-0.798810	2.979049	H	6.233321	4.136028	0.356515
F	-6.562756	-1.156725	3.052063	H	-2.952656	-1.924340	-1.725746
C	-5.635758	-2.111102	-1.857435	H	-2.672643	-0.792139	2.417056
F	-5.942355	-0.983431	-2.515066	H	-6.517922	-1.613780	0.668231
C	1.718721	-3.627597	1.926093	H	6.137490	5.292877	-1.884323
O	1.005762	-4.586094	2.062425	H	5.786666	3.554264	-2.068245

H	4.454115	4.737368	-2.096130	C	-2.328948	0.554437	3.924129
H	-2.413634	3.332697	-3.166450	C	-2.904660	0.060631	2.755311
H	-1.198333	3.990764	-0.451136	C	-2.217107	-0.813267	1.910641
H	-2.696475	5.970539	-0.424914	C	-0.923800	-1.215656	2.230094
H	-3.418325	5.477069	-1.956952	C	-0.342495	-0.729360	3.401707
H	-3.558501	3.907745	0.682453	C	-1.034378	0.152722	4.242598
H	-4.883653	4.804479	-0.064705	C	-3.087649	-1.231150	0.758224
H	-4.811697	3.313835	-2.038730	C	-4.324622	-0.370435	0.870175
H	-2.624195	1.796894	-0.533041	C	-4.269375	0.335109	2.234572
H	-3.334299	1.340765	-2.094170	I	-3.192621	1.707579	-0.444220
H	2.240831	-5.247199	0.063763	F	-5.550619	1.085296	0.000119
H	4.184808	-3.152743	-0.977758	C	-5.576334	-0.977947	0.338884
H	4.952132	-4.870138	-2.609221	O	-5.406511	-1.354620	-0.934446
H	3.709491	-5.988075	-2.040612	C	-6.545199	-1.923933	-1.570949
H	3.211791	-3.240587	-3.318117	C	-6.136816	-2.341446	-2.959847
H	2.949990	-4.812811	-4.106953	C	-1.134804	1.251283	-0.392784
H	1.225510	-5.375109	-2.408290	C	-0.621839	0.324778	-1.314637
H	1.819978	-2.571924	-1.339556	C	0.697961	-0.118067	-1.200227
H	0.523077	-3.653162	-0.736678	C	1.471813	0.290972	-0.110761
H	-0.420361	6.077694	-1.551810	C	0.966997	1.217507	0.803475
H	0.246571	4.622422	-2.318325	C	-0.326436	1.720606	0.652100
H	-1.089561	5.516376	-3.104240	O	-1.482986	-0.125699	-2.242803
H	-5.615131	1.212155	-0.971278	C	-1.055329	-0.946435	-3.301284
H	-4.922837	1.718654	0.586040	C	-2.240689	-1.108394	-4.234045
H	-6.266660	2.637310	-0.126988	O	-0.868898	2.623928	1.479469
H	5.974529	-4.785096	-0.281104	C	-0.042635	3.300253	2.400490
H	4.964957	-4.315867	1.104701	C	-0.917197	4.291773	3.137943
H	4.729480	-5.900833	0.327031	C	2.786656	-0.337408	0.125926
H	-0.510425	-3.690582	-3.057798	C	3.189152	-0.633056	1.432158
H	0.770819	-2.613430	-3.665234	C	4.384179	-1.302773	1.678194
H	0.470104	-4.173788	-4.463900	C	5.210452	-1.686212	0.627097
H	-1.301813	2.742575	1.206327	C	4.818555	-1.387887	-0.676833
H	-2.636113	1.736886	3.083357	C	3.623659	-0.720479	-0.928833
H	-1.471655	0.608434	4.955745	C	4.726467	-1.639944	3.103786
H	1.011357	0.469296	5.020358	F	3.760768	-2.392096	3.655217
H	3.196458	0.590467	3.108777	C	5.649249	-1.855749	-1.840647
H	3.203436	2.283232	3.651166	F	6.917879	-2.071005	-1.494344
O	1.332771	3.344803	0.133276	C	-0.544454	-2.316780	-2.871860
(S)C-2a				O	0.166905	-2.975281	-3.584740
E=-3248.1624010				O	-0.982365	-2.688265	-1.675599

C	-0.466333	-3.927943	-1.148994	H	-5.776521	-1.476739	-3.536577
C	0.925377	-3.694725	-0.583970	H	-5.334057	-3.094019	-2.924634
C	1.491222	-4.943184	0.087776	H	-0.404123	-4.643296	-1.986196
C	0.507031	-5.456793	1.136280	H	-1.529850	-3.659290	0.670458
C	-0.878034	-5.691584	0.547767	H	-1.574479	-6.041751	1.326374
C	-1.453992	-4.437003	-0.110731	H	-0.827535	-6.499666	-0.204997
C	-2.836319	-4.674566	-0.700292	H	0.439167	-4.716655	1.955401
C	2.872956	-4.674835	0.664729	H	0.890791	-6.384730	1.590391
C	1.129402	3.998766	1.711322	H	1.587982	-5.724501	-0.689923
O	2.194378	4.166880	2.245415	H	0.878002	-2.873000	0.152282
O	0.808490	4.384198	0.484909	H	1.596712	-3.363795	-1.391439
C	1.850333	4.865347	-0.381938	H	2.586307	5.404290	0.238163
C	2.508157	3.670438	-1.052299	H	0.413929	5.243946	-1.893707
C	3.529425	4.076456	-2.111349	H	1.771936	6.895866	-3.159827
C	2.887310	5.035756	-3.111583	H	3.029265	6.834683	-1.924366
C	2.246354	6.231212	-2.419931	H	2.118017	4.487934	-3.686732
C	1.206687	5.817938	-1.378056	H	3.638672	5.374749	-3.843446
C	4.129494	2.852847	-2.788985	H	4.344742	4.623944	-1.600987
C	0.571255	7.016191	-0.690218	H	1.714487	3.059358	-1.518309
F	4.833318	-0.541210	3.853748	H	2.984948	3.040749	-0.285262
F	5.868865	-2.315361	3.202464	H	-3.535771	-5.027761	0.072731
F	5.640042	-0.967085	-2.836844	H	-3.254099	-3.757050	-1.139657
F	5.169024	-3.005095	-2.333289	H	-2.798371	-5.442613	-1.489993
O	-6.500540	-1.300952	1.036276	H	3.564394	-4.310484	-0.110694
H	0.400001	2.586617	3.116610	H	2.827907	-3.910889	1.457849
H	-0.324145	4.835816	3.885488	H	3.306472	-5.585579	1.105372
H	-1.356679	5.008530	2.429942	H	0.084159	7.677259	-1.422705
H	-1.732528	3.756294	3.643764	H	-0.189316	6.699869	0.037903
H	1.597314	1.550207	1.626856	H	1.330038	7.610024	-0.154669
H	1.103331	-0.849226	-1.897866	H	4.615941	2.183041	-2.062802
H	-0.213666	-0.470687	-3.835312	H	3.347070	2.272031	-3.305711
H	-1.967864	-1.752096	-5.080620	H	4.882452	3.137688	-3.539751
H	-3.084594	-1.555376	-3.689012	H	-0.366147	-1.886807	1.575044
H	-2.552944	-0.124984	-4.610497	H	0.668051	-1.048824	3.670975
H	-6.909878	-2.774018	-0.972512	H	-0.556215	0.515190	5.155675
H	-7.348702	-1.170248	-1.590175	H	-2.899175	1.233353	4.562578
H	3.347211	-0.484416	-1.958111	O	-5.145871	0.942840	2.779536
H	2.539890	-0.364227	2.267088	H	-2.602001	-1.251202	-0.227125
H	6.143394	-2.216299	0.819350	H	-3.450322	-2.266800	0.916326
H	-6.993172	-2.779364	-3.493038	(R)C-2a			

E=-3248.1667857				F	4.705801	0.303712	4.061182
C	1.849315	-3.415010	-0.587082	C	6.024915	-0.583215	-1.736436
C	0.541883	-3.936644	-1.160715	F	5.758754	0.270035	-2.729261
C	-0.333415	-4.602549	-0.110318	C	3.256248	3.186005	-2.880732
C	0.473615	-5.707483	0.572021	C	-1.253116	6.479829	-1.086208
C	1.790456	-5.204284	1.150246	C	-4.522455	-0.810557	0.971771
C	2.653519	-4.519291	0.092118	C	-4.908836	-0.128022	2.246392
O	-0.204099	-2.839106	-1.719785	C	-3.642290	-0.061302	3.052527
C	0.171888	-2.382979	-2.899601	C	-2.618880	-0.787269	2.437797
O	1.008762	-2.876096	-3.612448	C	-3.103670	-1.384950	1.178813
C	-1.640014	-5.111375	-0.698916	C	-1.344016	-0.894226	2.989673
C	3.958193	-3.982089	0.661555	C	-1.094754	-0.233693	4.188612
C	-0.578814	-1.121214	-3.317033	C	-2.113286	0.499407	4.811630
C	-1.642991	-1.466892	-4.339809	C	-3.392083	0.589457	4.256033
O	-1.227528	-0.449242	-2.263152	C	-5.502005	-1.689631	0.261379
C	-0.536058	0.081959	-1.249379	O	-6.440553	-2.180466	0.837131
C	-1.263173	0.840606	-0.317616	O	-2.559004	-2.216423	0.498976
C	-0.617742	1.401857	0.793730	O	-5.112415	-1.984332	-0.965228
C	0.744177	1.168256	0.996962	C	-5.944145	-2.872892	-1.703332
C	1.472884	0.428748	0.061235	C	-5.218936	-3.225909	-2.975706
C	0.842326	-0.075320	-1.078579	C	-1.816490	3.938079	3.086977
I	-3.352728	1.041054	-0.528605	F	6.523392	-0.590105	3.318986
F	-5.736191	0.481154	-0.127327	F	4.777801	-1.805232	3.657398
O	-1.364508	2.150916	1.622346	F	5.861530	-1.819045	-2.225211
C	-0.727072	3.117643	2.429447	F	7.311620	-0.448989	-1.415176
C	0.208779	4.005941	1.609114	O	1.229255	4.469075	2.045969
O	-0.268754	4.195881	0.386849	H	-0.104630	2.633962	3.201527
C	0.577396	4.814842	-0.597649	H	-1.373000	4.696177	3.746943
C	1.517170	3.760737	-1.159305	H	-2.427353	4.435165	2.320182
C	2.358571	4.280493	-2.322133	H	-2.463459	3.276868	3.679162
C	1.447971	4.882008	-3.390899	H	1.252826	1.598733	1.858771
C	0.522387	5.944088	-2.812715	H	1.421941	-0.658695	-1.790840
C	-0.332500	5.413932	-1.660199	H	0.182266	-0.462137	-3.773184
C	2.901728	0.132702	0.292176	H	-1.187136	-1.997678	-5.185865
C	3.395413	-0.038633	1.590475	H	-2.408325	-2.105298	-3.876124
C	4.731640	-0.362410	1.809036	H	-2.125986	-0.549325	-4.702436
C	5.608146	-0.521346	0.740030	H	-6.158493	-3.760142	-1.087758
C	5.123535	-0.351695	-0.554512	H	-6.905460	-2.372557	-1.901762
C	3.789602	-0.026882	-0.778532	H	3.442905	0.122976	-1.802056
C	5.195180	-0.610071	3.218862	H	2.722510	0.058458	2.444258

H	6.654684	-0.772796	0.913202	(S)-to-(R)C-D			
H	-5.827135	-3.911930	-3.582275	E=-3248.1861590			
H	-5.015119	-2.324259	-3.570666	C	-1.751920	0.437591	4.046893
H	-4.260767	-3.717013	-2.751349	C	-2.367838	-0.004961	2.875372
H	0.756797	-4.645088	-1.979125	C	-1.815655	-1.019482	2.091471
H	-0.577502	-3.827368	0.637218	C	-0.601205	-1.593507	2.463143
H	-0.142288	-6.167966	1.361294	C	0.027667	-1.147859	3.625626
H	0.677797	-6.508147	-0.162837	C	-0.542992	-0.141657	4.418573
H	1.584818	-4.480256	1.960577	C	-3.595646	0.533635	2.246107
H	2.348461	-6.035391	1.612278	C	-3.778707	-0.274537	0.934750
H	2.898806	-5.274244	-0.678957	C	-2.711943	-1.348841	0.929493
H	1.617312	-2.624210	0.147734	I	-3.425619	1.260829	-0.701662
H	2.446868	-2.954736	-1.389832	C	-1.327569	1.058982	-0.660095
H	1.155907	5.610579	-0.097664	C	-0.624873	1.615529	0.417345
H	-0.951960	4.581816	-2.046210	C	0.697150	1.228872	0.639381
H	-0.138317	6.348014	-3.597021	C	1.327145	0.357799	-0.252337
H	1.123739	6.798332	-2.448655	C	0.658864	-0.101834	-1.391102
H	0.842557	4.071819	-3.839865	C	-0.691110	0.211231	-1.575484
H	2.054392	5.306541	-4.208655	O	-1.303614	2.461771	1.197350
H	3.004214	5.093672	-1.937097	C	-0.638290	3.170764	2.222211
H	0.906227	2.905609	-1.500691	C	-1.673882	4.056776	2.882356
H	2.167709	3.387331	-0.353538	O	-1.461170	-0.293285	-2.549179
H	-2.249908	-5.599607	0.076289	C	-0.920988	-1.113761	-3.558537
H	-2.228420	-4.279585	-1.109600	C	-2.038818	-1.390804	-4.545316
H	-1.455045	-5.849424	-1.497392	C	2.673809	-0.161431	0.063224
H	4.560749	-3.489017	-0.117177	C	3.013804	-0.432929	1.392606
H	3.769238	-3.242118	1.456114	C	4.242419	-1.004093	1.711502
H	4.565754	-4.788655	1.100181	C	5.161979	-1.311292	0.713941
H	-1.926142	6.876278	-1.861962	C	4.831048	-1.036080	-0.611446
H	-1.873646	6.073730	-0.273505	C	3.603995	-0.465415	-0.937147
H	-0.671232	7.325499	-0.682022	C	4.518086	-1.334616	3.153041
H	3.930939	2.781466	-2.109935	F	4.355607	-0.269237	3.939148
H	2.651015	2.348279	-3.269140	C	5.769491	-1.425637	-1.721151
H	3.878769	3.558763	-3.709565	F	5.756734	-0.528344	-2.709495
H	-0.572798	-1.471557	2.474705	C	-5.197374	-0.737118	0.604779
H	-0.107233	-0.289043	4.652792	O	-5.134998	-1.450466	-0.582714
H	-1.902956	1.008429	5.755869	C	-6.342754	-2.095795	-0.930586
H	-4.176198	1.160033	4.759572	C	-6.105427	-2.897474	-2.186731
H	-5.381808	0.839082	2.032863	C	0.536718	3.982098	1.681489
H	-5.687078	-0.753162	2.721447	O	1.517662	4.223650	2.334547

O	0.322575	4.371663	0.432340	H	6.121759	-1.763520	0.964226
C	1.404779	4.976999	-0.296975	H	-7.031155	-3.399566	-2.505254
C	0.790874	5.930677	-1.310911	H	-5.767080	-2.246588	-3.008005
C	1.893271	6.477855	-2.217659	H	-5.336919	-3.668750	-2.022877
C	2.695470	5.372986	-2.891449	H	-0.093954	-4.713301	-2.097634
C	3.310211	4.414295	-1.873696	H	-1.260027	-3.713740	0.535026
C	2.225154	3.874195	-0.945916	H	-1.215441	-6.093142	1.218674
C	-0.004924	7.038683	-0.638538	H	-0.456246	-6.536732	-0.310816
C	4.072821	3.277461	-2.539029	H	0.742598	-4.696353	1.840521
C	-0.335112	-2.430386	-3.061172	H	1.266426	-6.339211	1.469379
O	0.429188	-3.066754	-3.738651	H	1.944110	-5.648773	-0.801582
O	-0.769375	-2.781334	-1.859448	H	1.079081	-2.828321	0.007172
C	-0.197371	-3.974718	-1.284952	H	1.834710	-3.303672	-1.525012
C	1.175767	-3.657010	-0.716748	H	2.026946	5.536562	0.421291
C	1.801168	-4.868801	-0.029718	H	0.102764	5.327901	-1.933061
C	0.840322	-5.428822	1.017421	H	1.443883	7.143613	-2.971936
C	-0.535974	-5.723769	0.434104	H	2.570186	7.110979	-1.614901
C	-1.162777	-4.499216	-0.234461	H	2.034220	4.799000	-3.566700
C	3.163086	-4.525511	0.554722	H	3.486069	5.806073	-3.525715
C	-2.543813	-4.782571	-0.804070	H	4.022887	4.994407	-1.257058
F	5.750724	-1.799353	3.337839	H	1.538220	3.226179	-1.519017
F	3.662815	-2.273350	3.595554	H	2.675649	3.245706	-0.161972
F	5.411570	-2.602020	-2.252297	H	-3.212745	-5.176782	-0.024202
F	7.025313	-1.547610	-1.293324	H	-3.006701	-3.871613	-1.209767
F	-5.774654	0.692538	0.038345	H	-2.492026	-5.532166	-1.610685
O	-5.815704	-1.159981	1.576568	H	3.836317	-4.117427	-0.215053
H	-0.219347	2.464067	2.958747	H	3.070673	-3.770970	1.352514
H	-1.228117	4.586211	3.735108	H	3.645919	-5.412628	0.992282
H	-2.059142	4.791469	2.161020	H	-0.472698	7.696508	-1.386374
H	-2.516248	3.440498	3.228420	H	-0.802679	6.627552	-0.003461
H	1.247020	1.606692	1.500251	H	0.647471	7.661976	-0.005166
H	1.167401	-0.785378	-2.069045	H	4.533230	2.607281	-1.796367
H	-0.089905	-0.591574	-4.065244	H	3.396801	2.668416	-3.162568
H	-1.667058	-2.026951	-5.359091	H	4.874194	3.657366	-3.191057
H	-2.870678	-1.898525	-4.035629	H	-0.142129	-2.378530	1.860006
H	-2.409066	-0.445337	-4.964274	H	0.978824	-1.595451	3.926114
H	-6.672534	-2.732904	-0.093128	H	-0.034454	0.182051	5.329524
H	-7.125996	-1.334050	-1.087517	H	-2.221667	1.223872	4.642686
H	3.375848	-0.244366	-1.981573	O	-4.263611	1.452096	2.632093
H	2.290821	-0.230537	2.184896	H	-2.185216	-1.457952	-0.028673

H -3.236406 -2.305035 1.099541

(R)-to-(S)C-D

E=-3248.1793770

C 0.357729 5.712261 -1.498748

C 1.079857 4.937927 -0.406319

C 1.988844 3.853523 -0.960437

C 3.010670 4.402122 -1.952994

C 2.296722 5.188800 -3.050931

C 1.390371 6.270086 -2.478352

O 0.075538 4.324469 0.422199

C 0.380278 4.049433 1.681814

O 1.374594 4.401702 2.259264

C 3.879901 3.286781 -2.515390

C -0.540196 6.799444 -0.928895

C -0.712499 3.221616 2.357276

C -1.731203 4.115570 3.031977

O -1.412620 2.410694 1.437431

C -0.722364 1.576595 0.645112

C -1.407584 1.004846 -0.435110

C -0.748591 0.192269 -1.369578

C 0.618781 -0.051196 -1.200772

C 1.277150 0.421243 -0.064089

C 0.615027 1.242757 0.851135

I -3.501387 1.215668 -0.522168

F -5.969515 0.808454 0.470032

O -1.490953 -0.317512 -2.354775

C -0.900055 -0.981716 -3.452408

C -0.121601 -2.244380 -3.095487

O -0.536930 -2.805170 -1.976710

C 0.180287 -3.963459 -1.505427

C 1.457153 -3.516301 -0.811971

C 2.210263 -4.689782 -0.191267

C 1.282019 -5.464826 0.741120

C 0.008672 -5.906615 0.031345

C -0.755440 -4.738598 -0.591257

C 2.663254 -0.007364 0.210970

C 3.055079 -0.277478 1.525524

C 4.334418 -0.749393 1.804677

C 5.255680 -0.947757 0.781695

C 4.872430 -0.671671 -0.529573

C 3.591106 -0.210696 -0.816363

C 4.665839 -1.091786 3.231360

F 5.931957 -1.472347 3.379134

C 5.820007 -0.940542 -1.667019

F 5.568385 -2.131720 -2.224032

C 3.481700 -4.224604 0.502127

C -2.014310 -5.185542 -1.316666

C -4.016317 -0.311603 1.110006

C -2.920760 -1.399443 1.007994

C -1.987443 -1.136108 2.121527

C -2.486000 -0.115125 2.936481

C -3.832403 0.352010 2.460066

C -0.763566 -1.756758 2.375671

C -0.018836 -1.327094 3.467938

C -0.508069 -0.298622 4.287111

C -1.740007 0.307509 4.035069

O -2.851639 -2.273273 0.184842

C -5.457500 -0.676290 0.730261

O -6.039353 -1.248010 1.659433

O -5.463720 -1.182694 -0.551689

C -6.440665 -2.156640 -0.845552

C -5.889903 -3.065068 -1.919531

C -2.026361 -1.325851 -4.406766

F 3.887779 -2.095142 3.670350

F 4.449268 -0.055724 4.045140

F 7.090525 -0.948668 -1.265355

F 5.699493 -0.022743 -2.629793

O 0.759645 -2.656001 -3.806915

H -0.206769 2.594483 3.110860

H -1.233892 4.761257 3.768154

H -2.240846 4.742076 2.286271

H -2.483389 3.501756 3.546707

H 1.159150 1.640266 1.706509

H 1.158154 -0.683999 -1.902576

H -0.170481 -0.313025 -3.942479

H -1.624881 -1.848974 -5.284746

H -2.758164 -1.970309 -3.898502

H -2.534253 -0.408418 -4.734128

H -6.678355 -2.709843 0.076781

H -7.370340 -1.661047 -1.180289

H	3.318802	0.008893	-1.850304
H	2.336350	-0.152747	2.337286
H	6.257201	-1.318009	1.001357
H	-6.622730	-3.841850	-2.185781
H	-5.646228	-2.495668	-2.830285
H	-4.968535	-3.551217	-1.566323
H	0.439910	-4.574238	-2.386933
H	-1.063316	-4.045604	0.210322
H	-0.657199	-6.440367	0.728159
H	0.265960	-6.632171	-0.762579
H	1.022799	-4.820449	1.602316
H	1.810822	-6.337239	1.158780
H	2.498604	-5.371123	-1.014326
H	1.195257	-2.786571	-0.025141
H	2.105467	-2.996353	-1.534958
H	1.661897	5.629265	0.226062
H	-0.270261	4.980583	-2.041237
H	0.868855	6.805245	-3.288123
H	2.003244	7.027612	-1.956065
H	1.694170	4.486490	-3.656217
H	3.035921	5.633667	-3.736892
H	3.664084	5.108810	-1.406979
H	1.359516	3.095972	-1.460513
H	2.500338	3.345586	-0.128131
H	-2.681482	-5.733706	-0.634771
H	-2.570402	-4.318710	-1.698426
H	-1.772305	-5.852015	-2.161378
H	4.140984	-3.685689	-0.195643
H	3.251672	-3.544370	1.338427
H	4.046982	-5.075137	0.913197
H	-1.074887	7.328506	-1.732006
H	-1.289479	6.379514	-0.242593
H	0.051283	7.545130	-0.372830
H	4.408577	2.741506	-1.718560
H	3.265608	2.555868	-3.067615
H	4.635969	3.677938	-3.213118
H	-0.409293	-2.552755	1.718199
H	0.945308	-1.789026	3.694388
H	0.084843	0.027617	5.145686
H	-2.112143	1.095410	4.694763

H	-3.954500	1.442139	2.442193
H	-4.646993	-0.062913	3.080921

(R)D

E=-789.17218314

F	-1.988034	1.627771	-0.778194
C	-0.349593	0.313676	0.460640
C	0.234960	-1.063279	0.686403
C	1.670628	-0.897855	0.260976
C	1.979718	0.440853	-0.008822
C	0.786306	1.290038	0.187252
C	2.658267	-1.871225	0.130092
C	3.938538	-1.479203	-0.261130
C	4.242157	-0.135780	-0.521084
C	3.259620	0.839376	-0.394347
C	-1.696640	0.533233	-0.060292
O	-1.452341	0.772743	1.265202
O	-2.456940	-0.517100	-0.406077
C	-3.837421	-0.397105	-0.060441
C	-4.533258	-1.671461	-0.458940
H	-3.917233	-0.217123	1.025600
H	-4.267007	0.473825	-0.582941
H	-5.603251	-1.612233	-0.212523
H	-4.434808	-1.845583	-1.540342
H	-4.102011	-2.533603	0.070620
H	2.439537	-2.922619	0.332408
H	4.721699	-2.234275	-0.366050
H	5.254296	0.139934	-0.825589
H	3.461880	1.894923	-0.590343
H	-0.300566	-1.835814	0.114631
H	0.156751	-1.327867	1.753910
O	0.704697	2.489717	0.148690

(S)D

E=-789.1709789

F	1.862077	-2.196694	-0.727148
C	0.354534	-0.704864	0.395906
C	-0.159796	0.717668	0.450227
C	-1.599992	0.619695	0.146082
C	-1.979746	-0.726223	0.057413
C	-0.820284	-1.652647	0.319665
C	-2.514064	1.658079	-0.034464

C	-3.834121	1.329918	-0.320045
C	-4.220157	-0.013994	-0.418986
C	-3.303133	-1.048553	-0.233168
O	0.497831	1.702013	0.686320
C	1.690856	-0.991829	-0.150990
O	1.505878	-1.030633	1.198889
O	2.493524	-0.079990	-0.705981
C	3.445200	0.592657	0.123089
C	3.842484	1.864573	-0.576611
H	2.982564	0.807128	1.096535
H	4.312148	-0.072323	0.281657
H	4.601372	2.398019	0.014427
H	4.260518	1.655625	-1.572324
H	2.964733	2.516488	-0.690119
H	-2.179684	2.694879	0.046863
H	-4.575986	2.117241	-0.471232
H	-5.261714	-0.255527	-0.645358
H	-3.622123	-2.090784	-0.311178
H	-0.692133	-2.413123	-0.465374
H	-0.936933	-2.185390	1.277908

(R)-to-(S)D-E

E=-889.1310514

C	-3.311313	0.808971	-0.199476
C	-1.997578	0.386087	-0.064108
C	-1.671194	-0.970335	0.013577
C	-2.680172	-1.925813	-0.029564
C	-4.010443	-1.508499	-0.153949
C	-4.326414	-0.150225	-0.237982
C	-0.759989	1.238080	-0.046745
C	0.362712	0.236975	0.024464
C	-0.182021	-1.161299	0.145918
C	1.761777	0.523427	-0.157064
O	2.668792	-0.377573	0.379092
C	3.840287	-0.508149	-0.383983
C	4.622593	-1.688126	0.143205
O	1.348989	0.315429	-1.402579
O	-0.722507	2.425283	-0.276103
F	2.238737	1.783109	0.087975
H	3.574189	-0.651976	-1.447405
H	4.444619	0.417246	-0.320708

H	5.563236	-1.818026	-0.414705
H	4.864010	-1.545759	1.207857
H	4.030815	-2.611945	0.053601
H	-2.441642	-2.992217	0.032413
H	-4.810499	-2.253993	-0.189368
H	-5.371400	0.157953	-0.338000
H	-3.518643	1.879977	-0.271980
H	0.084685	-1.566699	1.131660
H	0.231725	-1.809479	-0.641196
F	-0.339044	0.683919	1.830779

(S)-to-(R)D-E

E=-889.1286962

C	-0.145025	-0.810154	-0.351918
C	-1.608809	-0.548514	-0.188335
C	-1.842064	0.785848	0.144326
C	-0.548421	1.538555	0.269962
C	0.514771	0.511495	-0.044442
C	-2.648562	-1.448441	-0.376262
C	-3.959417	-0.999131	-0.209274
C	-4.204220	0.334643	0.131204
C	-3.148749	1.234825	0.308306
C	1.872580	0.985437	-0.327656
F	2.099148	2.247039	0.212249
O	1.343257	1.021348	-1.536163
O	3.070673	0.358884	-0.097456
C	3.165568	-1.030032	-0.335170
C	2.965268	-1.810705	0.948403
F	0.236947	-0.391952	1.665517
H	2.428684	-1.340833	-1.089477
H	4.175219	-1.199149	-0.750560
H	2.990439	-2.894702	0.749855
H	3.756033	-1.567261	1.677340
H	1.989009	-1.544838	1.385843
H	-2.416102	-2.481473	-0.647578
H	-4.799015	-1.686771	-0.345359
H	-5.234904	0.679007	0.257726
H	-3.351730	2.277195	0.571653
O	0.315169	-1.841800	-0.788944
H	-0.483152	2.380636	-0.434527
H	-0.389645	1.911997	1.290828

(S)E			
E=-889.1849802			
C	-0.171282	-0.522038	1.346734
C	-1.472111	-0.750580	0.632539
C	-1.876065	0.401676	-0.047954
C	-0.851738	1.460306	0.132246
C	0.380699	0.757631	0.709995
C	-2.287746	-1.879722	0.608553
C	-3.494834	-1.828137	-0.091090
C	-3.898070	-0.662968	-0.754978
C	-3.085951	0.468738	-0.730088
O	-0.990540	2.640635	-0.076652
C	1.305908	0.347527	-0.483236
F	1.797858	1.612325	-0.976590
O	0.742015	-0.357736	-1.351113
O	2.470516	-0.217051	0.173316
C	3.326407	-0.880386	-0.701792
C	4.056424	-1.977069	0.045891
F	1.009032	1.561718	1.626824
H	2.731131	-1.297742	-1.534616
H	4.059836	-0.172804	-1.144541
H	4.785292	-2.488874	-0.604875
H	4.597305	-1.564755	0.913373
H	3.342368	-2.726217	0.423913
H	-1.986186	-2.795404	1.124865
H	-4.137858	-2.712807	-0.121912
H	-4.847689	-0.649690	-1.297138
H	-3.365065	1.394660	-1.239600
H	-0.346411	-0.336904	2.421123
H	0.539491	-1.352506	1.241975

(R)E			
E=-889.1840831			
C	3.106075	-0.956156	-0.503125
C	1.860374	-0.714686	0.072621
C	1.489077	0.598396	0.374993
C	2.336252	1.676934	0.142499
C	3.580743	1.432123	-0.433274
C	3.956432	0.121826	-0.755391
C	0.793467	-1.684183	0.488849
C	-0.433114	-0.806458	0.757473

C	0.130325	0.601378	0.969575
C	-1.303926	-0.760014	-0.545112
O	-2.522692	-0.117364	-0.159434
C	-3.020156	0.838385	-1.043330
C	-3.358448	2.109263	-0.287161
F	-1.131683	-1.225947	1.862111
F	-1.723107	-2.159744	-0.680118
O	-0.680830	-0.326374	-1.541229
H	-2.259843	1.024934	-1.822104
H	-3.928217	0.449390	-1.552521
H	-3.773651	2.877686	-0.962011
H	-4.098546	1.907729	0.504465
H	-2.455998	2.505765	0.201623
H	2.004495	2.685663	0.402168
H	4.264880	2.258984	-0.643260
H	4.933684	-0.058829	-1.212980
H	3.412751	-1.974225	-0.758897
O	-0.405779	1.529790	1.528407
H	0.568284	-2.440629	-0.273942
H	1.077077	-2.194494	1.425868

(S)2a			
E=-789.2173929			
C	-2.655275	1.405893	-0.562949
C	-1.661737	0.635755	0.042935
C	-1.839560	-0.723042	0.318099
C	-3.032966	-1.345778	-0.038132
C	-4.026620	-0.584806	-0.653497
C	-3.845886	0.781046	-0.913337
C	-0.324702	1.063532	0.479813
C	0.437481	-0.235691	0.896322
C	-0.646734	-1.308464	1.023652
C	1.402198	-0.556768	-0.240652
O	2.614247	-0.091228	-0.004026
C	3.576446	-0.267586	-1.047623
C	4.860765	0.382330	-0.607431
O	1.057630	-1.128618	-1.242587
O	0.145944	2.167541	0.526463
H	3.697266	-1.346074	-1.238110
H	3.177820	0.178739	-1.972455
H	5.625779	0.268959	-1.389269

H	4.710528	1.455369	-0.420404
H	5.238021	-0.078575	0.316947
H	-3.192727	-2.408195	0.160656
H	-4.967291	-1.062481	-0.938871
H	-4.643493	1.348927	-1.397403
H	-2.478912	2.466495	-0.756060
H	-0.854189	-1.452548	2.096102
H	-0.340887	-2.272542	0.594760
F	1.113895	-0.017573	2.058013

(R)2a

E=-789.2173928

C	3.032970	-1.345774	-0.038145
C	1.839548	-0.723055	0.318047
C	1.661720	0.635745	0.042898
C	2.655273	1.405897	-0.562936
C	3.845905	0.781065	-0.913293
C	4.026642	-0.584786	-0.653469
C	0.646726	-1.308488	1.023608
C	-0.437484	-0.235717	0.896311
C	0.324697	1.063528	0.479820
C	-1.402203	-0.556754	-0.240673
O	-2.614301	-0.091398	-0.003957
C	-3.576506	-0.267716	-1.047553
C	-4.860717	0.382497	-0.607472
O	-1.057583	-1.128440	-1.242685
H	-3.177770	0.178392	-1.972439
H	-3.697541	-1.346209	-1.237879
H	-5.625820	0.268926	-1.389193
H	-5.237917	-0.078063	0.317102
H	-4.710361	1.455583	-0.420815
H	2.478920	2.466501	-0.756045
H	4.643519	1.348971	-1.397318
H	4.967327	-1.062456	-0.938807
H	3.192731	-2.408194	0.160631
F	-1.113894	-0.017614	2.058006
H	0.340869	-2.272562	0.594711
H	0.854221	-1.452589	2.096048
O	-0.145936	2.167534	0.526529

Ar*-I

E=-2459.0412041

C	3.474851	-1.219239	-1.253985
C	4.767931	-0.610072	-0.740246
C	5.680963	-1.640997	-0.093516
C	5.930341	-2.776344	-1.087729
C	4.638849	-3.401517	-1.597808
C	3.716400	-2.363823	-2.234898
O	4.456483	0.380404	0.259188
C	4.084259	1.591095	-0.159103
O	4.056695	1.951469	-1.302713
C	6.976414	-1.022527	0.408222
C	2.400696	-2.970672	-2.699263
C	3.704065	2.478894	1.028751
C	4.795389	3.494823	1.288648
O	2.526267	3.201781	0.750272
C	1.389986	2.536539	0.488164
C	0.264947	3.291361	0.128953
C	-0.938256	2.655406	-0.209395
C	-1.000474	1.257392	-0.210021
C	0.103164	0.501810	0.188783
C	1.288623	1.143127	0.551140
O	-1.980986	3.439862	-0.523241
C	-3.171698	2.859317	-0.996684
C	-4.093995	3.994837	-1.389503
I	0.390219	5.395070	0.074715
C	0.025984	-0.973123	0.222076
C	-0.786463	-1.675892	-0.677288
C	-0.861758	-3.063520	-0.636581
C	-0.103256	-3.793383	0.277675
C	0.721208	-3.103735	1.160383
C	0.771685	-1.711853	1.147271
C	-1.728248	-3.794368	-1.624950
F	-1.030247	-4.188779	-2.693684
C	1.620259	-3.850109	2.106833
F	1.667360	-3.267996	3.306047
C	-3.835559	1.997740	0.077411
O	-3.883429	2.275562	1.242723
O	-4.366452	0.907981	-0.481258
C	-5.014544	-0.049742	0.374807
C	-6.097549	-0.736164	-0.444797
C	-6.718212	-1.858563	0.387107

C	-5.679889	-2.844600	0.904570
C	-4.593020	-2.150110	1.722991
C	-3.973559	-1.023287	0.899778
C	-7.140445	0.249190	-0.949426
C	-3.532028	-3.126629	2.209334
F	-2.730683	-3.026325	-2.067801
F	-2.272161	-4.888039	-1.081596
F	1.234252	-5.113395	2.277666
F	2.880597	-3.879480	1.640256
H	3.557609	1.835132	1.913393
H	5.736105	2.987890	1.546018
H	4.948622	4.105890	0.388267
H	4.502489	4.150362	2.120094
H	2.151029	0.543217	0.832917
H	-1.922252	0.746027	-0.479603
H	-2.959777	2.216114	-1.868563
H	-5.037500	3.599128	-1.790956
H	-4.307957	4.616231	-0.508608
H	-3.610853	4.617078	-2.155063
H	-1.365139	-1.131913	-1.425035
H	1.393002	-1.194872	1.880631
H	-0.161150	-4.881951	0.307858
H	5.294047	-0.099319	-1.564816
H	2.911377	-1.607460	-0.388791
H	6.512296	-2.381040	-1.940866
H	4.237499	-1.946985	-3.117926
H	4.862722	-4.200953	-2.323073
H	4.106351	-3.881259	-0.756961
H	-5.466707	0.502545	1.215970
H	-7.260776	-1.411760	1.240762
H	-6.165151	-3.627275	1.510366
H	-5.203328	-3.361528	0.051202
H	5.126625	-2.059175	0.767434
H	-5.591511	-1.195756	-1.314608
H	-5.077029	-1.693631	2.607434
H	-3.447183	-1.461122	0.034954
H	7.554901	-0.592628	-0.426130
H	6.780076	-0.220179	1.133623
H	7.608429	-1.778075	0.898822
H	6.566253	-3.539825	-0.611196

H	1.754305	-2.216583	-3.174109
H	2.565203	-3.780571	-3.426338
H	1.841651	-3.394174	-1.849463
H	2.859931	-0.433917	-1.719997
H	-6.681291	1.034618	-1.566813
H	-7.900488	-0.260691	-1.560438
H	-7.659199	0.737602	-0.108214
H	-7.477220	-2.379981	-0.218211
H	-2.746786	-2.615052	2.787248
H	-3.971054	-3.906565	2.850293
H	-3.045469	-3.630655	1.359239
H	-3.227385	-0.473575	1.495358

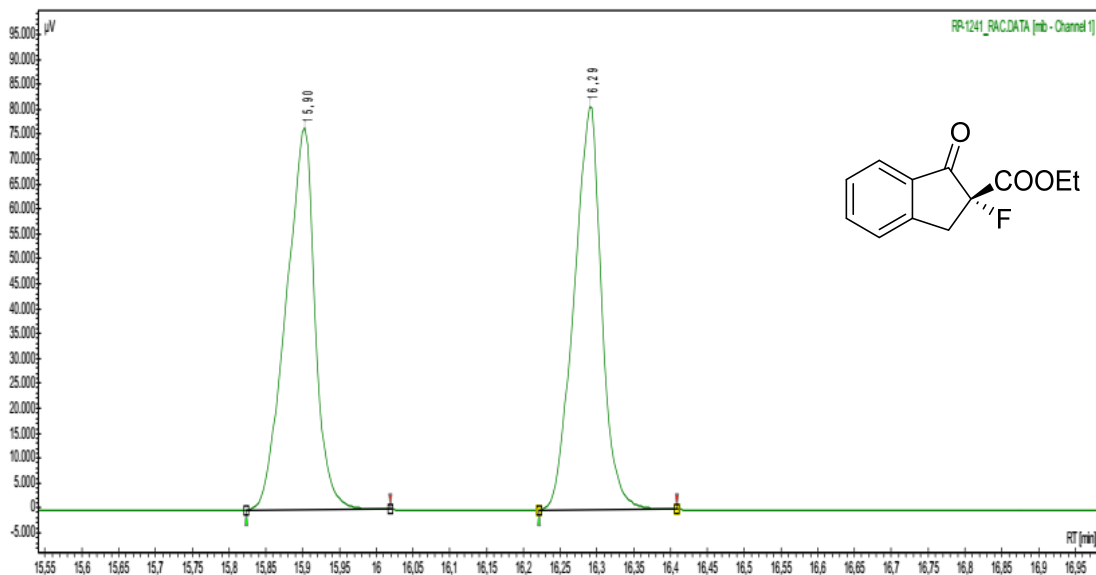
Pro-(R) B-C full catalyst

C	-1.410170	2.175617	1.879391
C	-0.052899	2.458640	2.015432
C	0.591350	2.399096	3.255936
C	-0.126952	2.027028	4.389249
C	-1.491882	1.752473	4.261926
C	-2.134766	1.837834	3.019340
C	2.041237	2.754695	3.095854
C	2.208194	2.891230	1.605190
C	0.938352	2.729005	0.948699
C	3.360482	3.526090	1.025691
O	4.142400	4.120174	1.944706
C	5.333723	4.748305	1.482654
C	5.068583	6.146485	0.972406
O	3.673556	3.531397	-0.166803
H	6.001255	4.761798	2.356389
H	5.787027	4.126636	0.695472
H	-1.874295	2.213689	0.892977
H	-3.205433	1.630798	2.951481
H	-2.071683	1.467425	5.143672
H	0.359981	1.958706	5.365835
H	6.015446	6.634329	0.695292
H	4.423831	6.113675	0.082981
H	4.578375	6.757958	1.744598
O	0.658171	2.723902	-0.263918
H	2.281695	3.695024	3.622566
H	2.704267	1.985021	3.525539

I	2.838000	1.048240	-0.788634	C	-3.688336	4.158249	-1.437418
F	3.681540	-0.492481	-1.855255	C	-2.425350	3.429391	-1.898845
C	1.177179	-0.113156	-0.339459	C	-1.507194	4.256919	-2.818620
C	0.244379	-0.378152	-1.354888	C	-5.739288	1.114595	-0.154477
C	-0.948130	-1.017017	-1.014221	C	3.380297	-0.909567	3.665036
C	-1.219868	-1.341720	0.318533	F	-6.070068	-1.805795	3.952899
C	-0.244326	-1.148479	1.301480	F	-5.298067	0.145272	3.471500
C	0.966171	-0.539046	0.979586	F	-6.194142	-2.433141	-1.678717
O	0.581467	-0.013421	-2.590195	F	-6.647646	-4.028808	-0.307485
C	-0.253219	-0.324491	-3.687243	O	2.407671	-3.739344	2.638772
C	0.508467	0.040975	-4.943946	H	1.334900	-1.541930	3.469991
C	-2.585183	-1.765409	0.694548	H	3.660545	-1.714955	4.357127
C	-3.106795	-1.391633	1.938378	H	4.237673	-0.670310	3.019835
C	-4.428776	-1.672207	2.270285	H	3.114729	-0.017128	4.247653
C	-5.259228	-2.339399	1.375001	H	-0.436524	-1.441121	2.332706
C	-4.743976	-2.720389	0.137842	H	-1.712953	-1.182703	-1.770008
C	-3.422921	-2.442956	-0.199729	H	-0.476530	-1.406306	-3.688076
O	1.931691	-0.320403	1.887206	H	-0.100951	-0.196561	-5.825677
C	2.204750	-1.351639	2.820134	H	0.743434	1.114982	-4.944622
C	2.522784	-2.666041	2.108931	H	1.449058	-0.525311	-4.985637
O	2.961517	-2.431769	0.884320	H	-3.044932	-2.765861	-1.171244
C	3.216884	-3.516122	-0.024771	H	-2.488176	-0.831270	2.640509
C	2.204456	-3.394613	-1.150620	H	-6.295818	-2.556987	1.634380
C	2.437165	-4.419743	-2.254713	H	-3.348225	2.226700	-3.466778
C	3.878658	-4.314991	-2.748643	H	-1.813076	3.183504	-1.013202
C	4.882914	-4.441892	-1.609101	H	-3.408905	5.108267	-0.956829
C	4.650920	-3.388782	-0.524516	H	-4.301980	4.426093	-2.315566
C	-4.973023	-1.153873	3.573510	H	-3.971239	3.133607	0.446564
F	-4.074457	-1.249692	4.556546	H	-5.439945	3.873636	-0.193165
C	-5.646991	-3.360929	-0.881813	H	-5.541319	2.188800	-1.997178
F	-4.981880	-4.209888	-1.666555	H	-3.053481	0.977254	-0.697084
C	1.430798	-4.239201	-3.381854	H	-3.946330	0.305485	-2.077148
C	5.686366	-3.397813	0.615962	H	3.073372	-4.458525	0.526173
C	-1.599442	0.393459	-3.642135	H	4.705485	-2.393070	-1.000759
O	-2.525521	0.054920	-4.333243	H	5.906500	-4.350230	-2.002877
O	-1.591862	1.389246	-2.780083	H	4.808640	-5.452790	-1.170260
C	-2.818792	2.091348	-2.509221	H	4.010851	-3.334977	-3.241744
C	-3.669214	1.245589	-1.573570	H	4.070940	-5.084504	-3.514607
C	-4.922586	1.978173	-1.104012	H	2.300570	-5.430465	-1.824237
C	-4.533341	3.319267	-0.486803	H	2.301133	-2.382901	-1.575094

H	1.185805	-3.486428	-0.737461	O	-4.077154	-2.923885	-1.046014
H	-0.719662	3.559876	-3.150045	O	-0.934893	-2.825381	-0.383107
H	-6.017780	0.157678	-0.622078	H	0.921096	-4.479831	2.320436
H	-5.168641	0.884992	0.760256	H	0.856347	-4.181344	0.563419
H	-6.665039	1.624256	0.153885	H	-5.430720	-2.875786	4.489025
H	5.381138	-2.585434	1.299372	H	-7.836200	-3.052963	3.880442
H	0.395744	-4.334149	-3.016821	H	-8.539701	-3.221606	1.512988
H	1.537706	-3.239267	-3.835292	H	-6.808797	-3.200008	-0.318906
H	1.576843	-4.984330	-4.178948	H	2.436181	-2.591803	1.790186
C	-0.803811	5.364113	-2.041230	H	1.129890	-1.740784	0.924229
H	-0.100696	5.908417	-2.690788	H	1.032941	-1.967111	2.694370
H	-1.516468	6.104261	-1.641463	H	-2.931258	-1.999382	3.066724
H	-0.229782	4.939181	-1.204664	H	-2.856559	-3.760016	3.005160
C	-2.207444	4.801870	-4.059565	I	-2.537609	-0.754455	-1.151467
H	-2.953399	5.570875	-3.802167	F	-2.979308	0.910116	-2.277595
H	-1.478302	5.272980	-4.736697	C	-0.854602	0.203650	-0.380423
H	-2.722774	4.014718	-4.632693	C	0.211065	0.487947	-1.246859
C	7.077806	-3.039115	0.104242	C	1.394252	0.997951	-0.711445
H	7.777083	-2.891372	0.941714	C	1.518309	1.193278	0.667276
H	7.497197	-3.835772	-0.530749	C	0.415640	0.998958	1.506356
H	7.059678	-2.111762	-0.489763	C	-0.779106	0.501984	0.985635
C	5.712965	-4.691118	1.425683	O	0.002796	0.259064	-2.542286
H	6.009182	-5.552422	0.805732	C	0.970830	0.623306	-3.502777
H	6.446390	-4.615150	2.243476	C	0.332167	0.455650	-4.865616
H	4.737783	-4.915910	1.883312	C	2.859414	1.464091	1.227306
Pro-(S) B-C full catalyst				C	3.230242	0.890882	2.448257
C	-5.728087	-2.950440	3.439501	C	4.527071	1.029572	2.936125
C	-4.776826	-2.955641	2.423617	C	5.482023	1.742250	2.218969
C	-5.183395	-3.044807	1.088787	C	5.118465	2.316946	1.002437
C	-6.527839	-3.139131	0.735083	C	3.822718	2.188282	0.513618
C	-7.476705	-3.146322	1.754301	O	-1.857653	0.260750	1.753095
C	-7.077687	-3.050090	3.093491	C	-2.249523	1.255945	2.688051
C	-4.005067	-2.956546	0.194810	C	-2.324729	2.635921	2.038928
C	-2.851295	-2.814995	1.054512	O	-2.707976	2.533860	0.777466
C	-3.280513	-2.876356	2.496830	C	-2.703684	3.695427	-0.073302
C	-1.477349	-3.072910	0.694901	C	-1.490319	3.584190	-0.978558
O	-0.777554	-3.612620	1.703430	C	-1.434877	4.693439	-2.023509
C	0.632508	-3.751562	1.550281	C	-2.753133	4.732464	-2.794755
C	1.348106	-2.433574	1.748641	C	-3.956855	4.852671	-1.867331
				C	-4.009894	3.707684	-0.855248

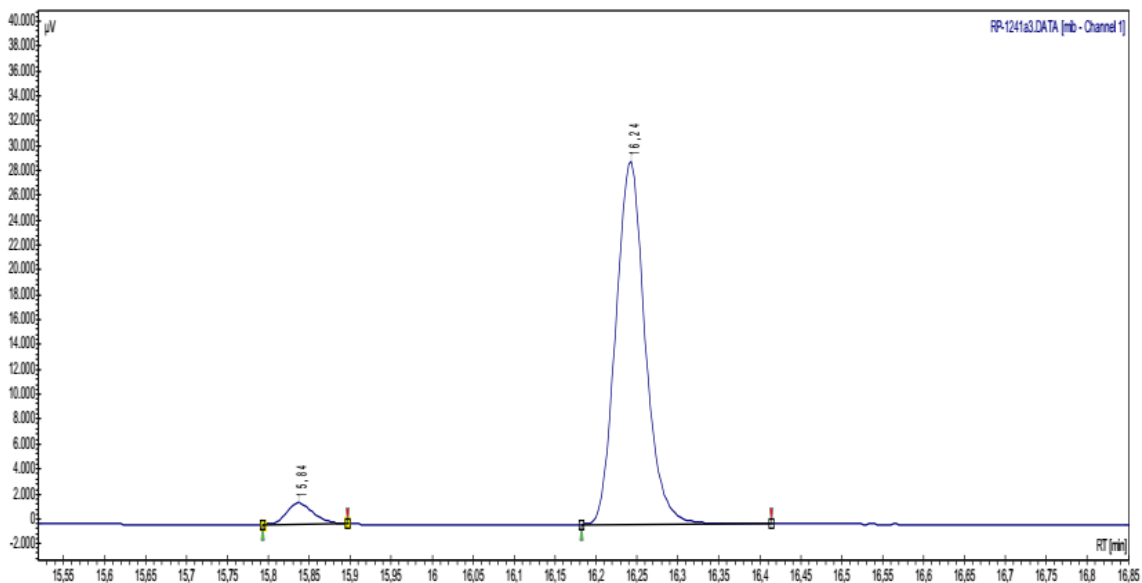
C	4.899410	0.309423	4.203778	H	4.085545	-3.563131	0.535724
F	3.918221	0.376294	5.107031	H	5.552883	-4.314310	-0.096216
C	6.157992	3.011312	0.163776	H	5.896941	-2.417681	-1.638040
F	5.627706	3.990380	-0.569995	H	3.382780	-1.220762	-0.377385
C	-0.240199	4.505177	-2.947099	H	4.425593	-0.438085	-1.585983
C	-5.247536	3.701764	0.061940	H	-2.621982	4.582806	0.572747
C	2.252908	-0.196265	-3.398725	H	-4.023867	2.757933	-1.419725
O	3.263039	0.118563	-3.971999	H	-4.883376	4.865007	-2.460824
O	2.095988	-1.255030	-2.624930	H	-3.915095	5.821194	-1.337272
C	3.239941	-2.075011	-2.334030	H	-2.842306	3.800542	-3.381824
C	4.053516	-1.413342	-1.233036	H	-2.741675	5.564559	-3.518185
C	5.219311	-2.283366	-0.773596	H	-1.319982	5.660966	-1.498012
C	4.705895	-3.665417	-0.373338	H	-1.553231	2.613524	-1.493387
C	3.885488	-4.313279	-1.482675	H	-0.573292	3.579908	-0.364956
C	2.708893	-3.441811	-1.923535	H	1.115207	-3.275511	-3.313654
C	1.802109	-4.077055	-2.995383	H	6.371937	-0.618042	0.027435
C	6.000672	-1.605556	0.342576	H	5.368873	-1.454630	1.233293
C	-3.603652	0.852093	3.232350	H	6.866867	-2.211073	0.650724
F	6.003248	0.807086	4.757045	H	-5.144881	2.796153	0.685165
F	5.120444	-0.990812	3.965677	H	0.705683	4.476885	-2.382875
F	6.731651	2.147341	-0.684684	H	-0.331876	3.556040	-3.501835
F	7.128800	3.535900	0.910994	H	-0.168041	5.317128	-3.686827
O	-2.099125	3.652425	2.640565	C	0.932916	-5.179962	-2.401360
H	-1.520308	1.339502	3.511003	H	0.271099	-5.611490	-3.167934
H	-3.989946	1.637837	3.895879	H	1.536590	-6.006314	-1.990965
H	-4.308274	0.694388	2.403513	H	0.292003	-4.777167	-1.602818
H	-3.519577	-0.082535	3.801898	C	2.559048	-4.563242	-4.227042
H	0.493224	1.200554	2.574683	H	3.193483	-5.434559	-3.998885
H	2.258595	1.163998	-1.351131	H	1.854160	-4.873336	-5.013461
H	1.260864	1.679042	-3.355226	H	3.205445	-3.782390	-4.658268
H	1.046818	0.746718	-5.646372	C	-6.535856	3.543577	-0.738432
H	0.034475	-0.591584	-5.018531	H	-7.390404	3.355669	-0.070232
H	-0.564237	1.087330	-4.931675	H	-6.771474	4.450568	-1.317691
H	3.561650	2.662709	-0.433885	H	-6.468805	2.701396	-1.444945
H	2.508704	0.296761	3.011448	C	-5.330700	4.897342	1.007801
H	6.498510	1.845475	2.599937	H	-6.230273	4.825372	1.638753
H	3.846445	-2.143945	-3.251994	H	-4.463328	4.958649	1.682801
H	2.065649	-3.259568	-1.044068	H	-5.398957	5.848870	0.456265
H	3.514884	-5.297560	-1.156645				
H	4.544840	-4.504782	-2.347031				



Peak results :

RP-1241_RAC.DAT [mib - Channel 1]

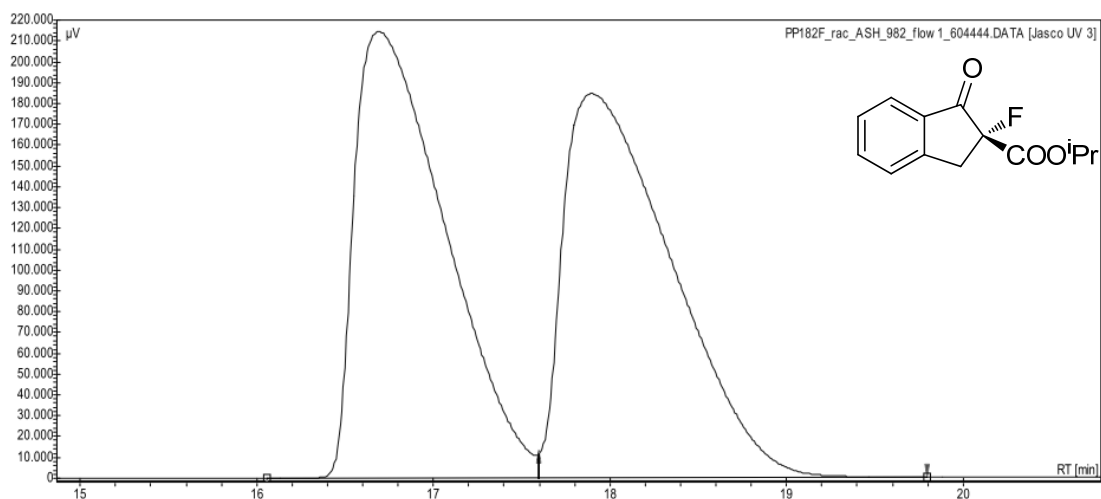
Index	Name	Time [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
2	UNKNOWN	15.90	49.93	76814.7	3508.8	49.929
1	UNKNOWN	16.29	50.07	81071.2	3518.9	50.071
Total			100.00	157885.9	7027.7	100.000



Peak results :

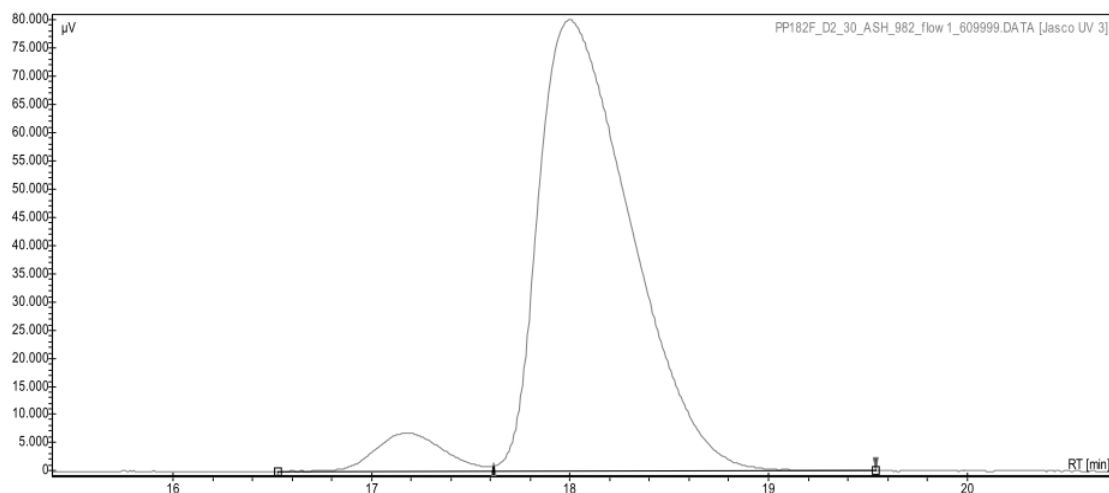
RP-1241a3.DAT [mib - Channel 1]

Index	Name	Time [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	15.84	5.04	1708.7	64.2	5.042
2	UNKNOWN	16.24	94.96	29142.1	1210.1	94.958
Total			100.00	30850.8	1274.3	100.000



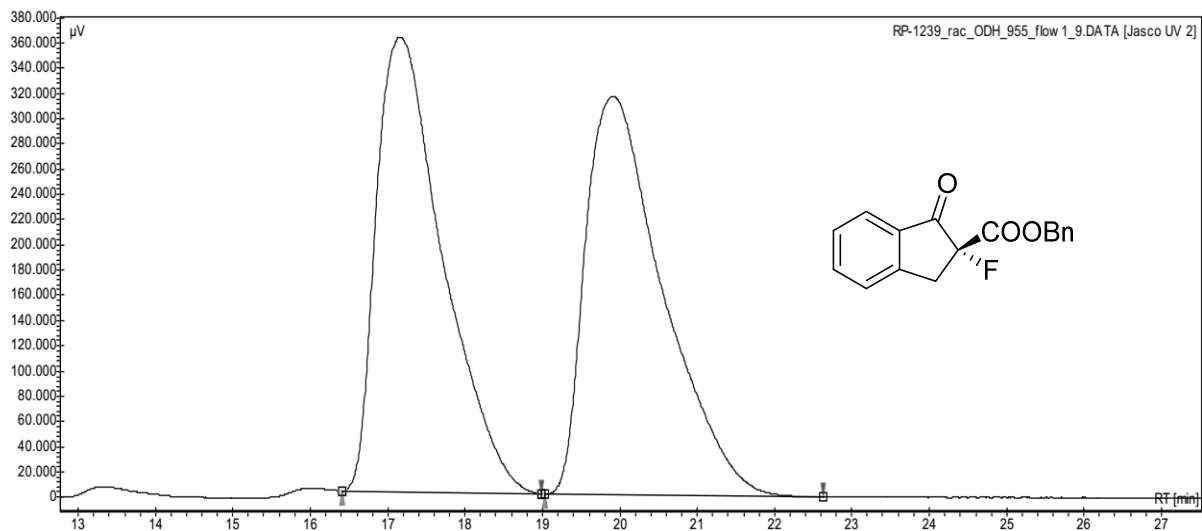
PP182F_rac_ASH_982_flow1_604444.D [Jasco UV 3]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	16,059	16,692	17,598	0,000	49,31	214306,9	127680,9	49,306
2	UNKNOWN	17,598	17,892	19,797	0,000	50,69	184508,9	131273,5	50,694
Total						100,00	398815,8	258954,3	100,000



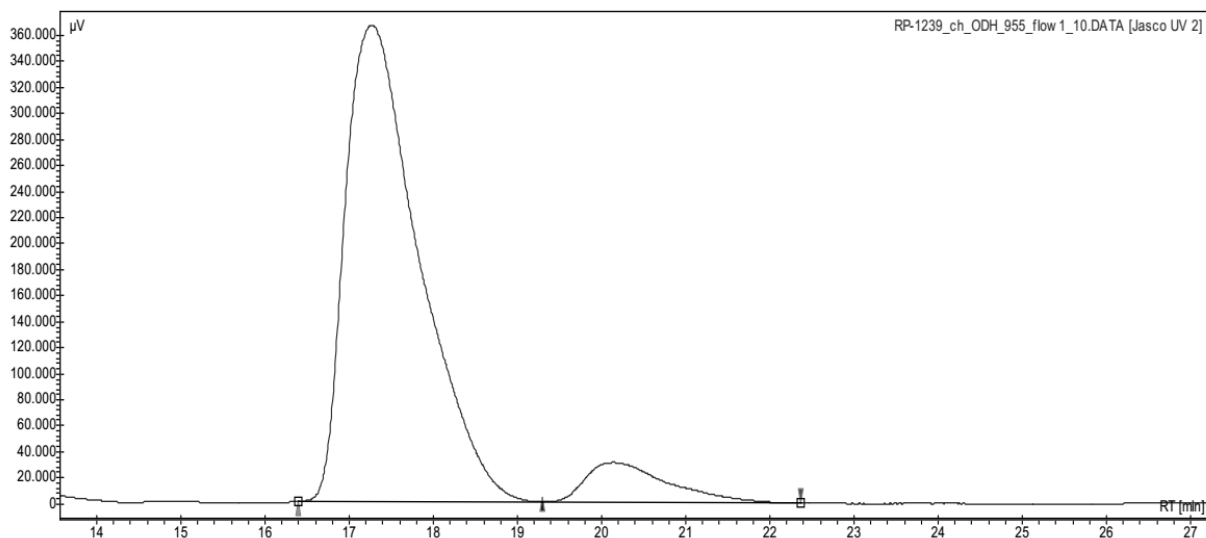
PP182F_D2_30_ASH_982_flow1_609999.D [Jasco UV 3]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	16,527	17,183	17,614	0,000	5,99	6838,1	2733,6	5,987
2	UNKNOWN	17,614	17,992	19,540	0,000	94,01	80140,6	42926,7	94,013
Total						100,00	86978,8	45660,3	100,000



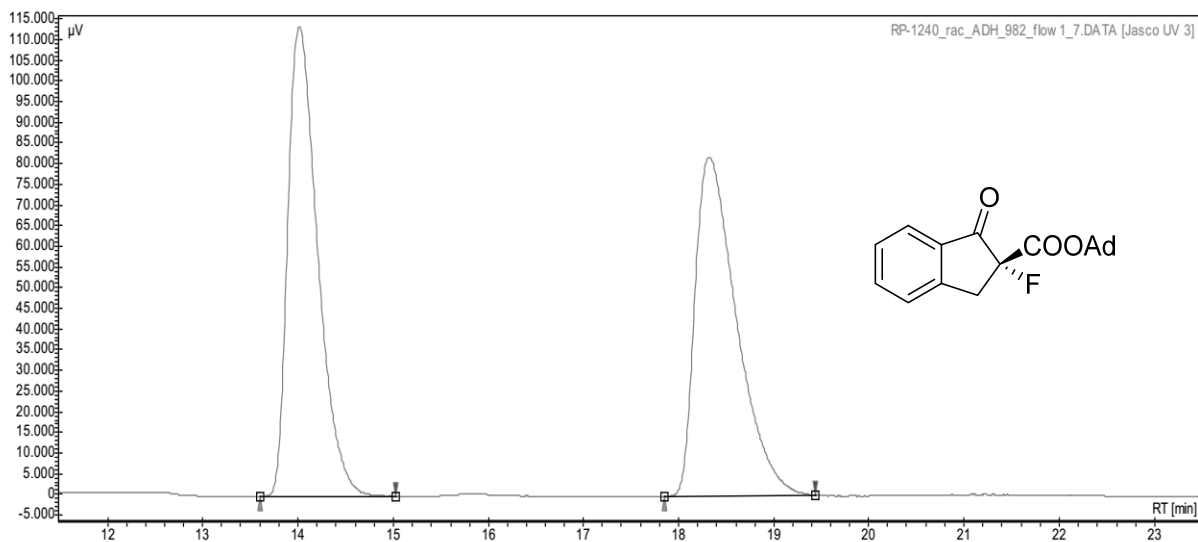
RP-1239_rac_ODH_955_flow1_9.DATA [Jasco UV 2]

Index	Start	Time	End	Area %
	[Min]	[Min]	[Min]	[%]
1	16,415	17,158	18,992	49,438
2	19,037	19,908	22,636	50,562
Total				100,000



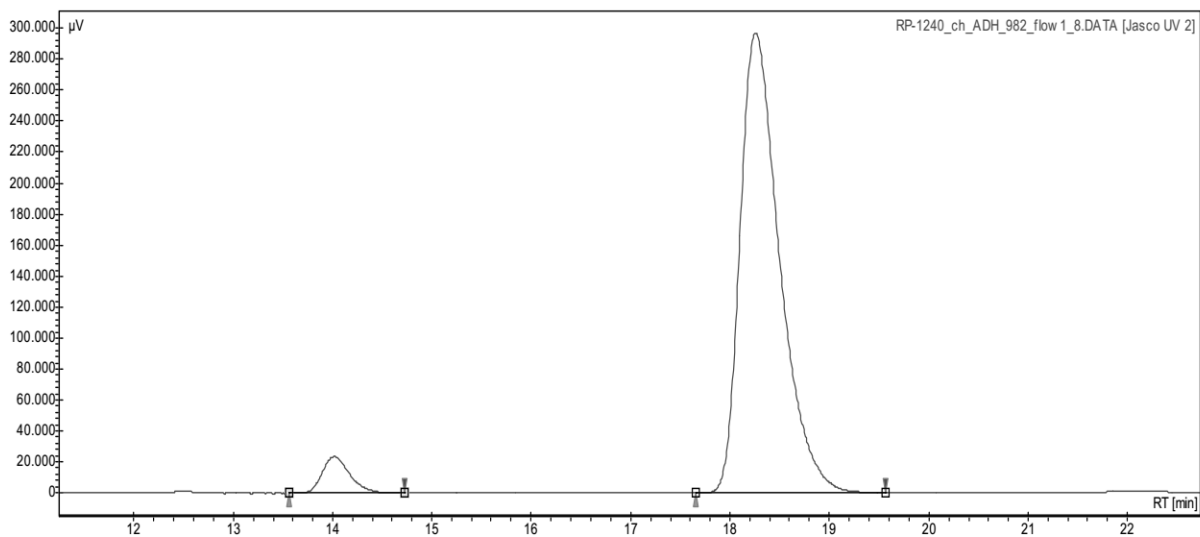
RP-1239_ch_ODH_955_flow1_10.DATA [Jasco UV 2]

Index	Start	Time	End	Area %
	[Min]	[Min]	[Min]	[%]
1	16,386	17,267	19,293	91,440
2	19,293	20,142	22,362	8,560
Total				100,000



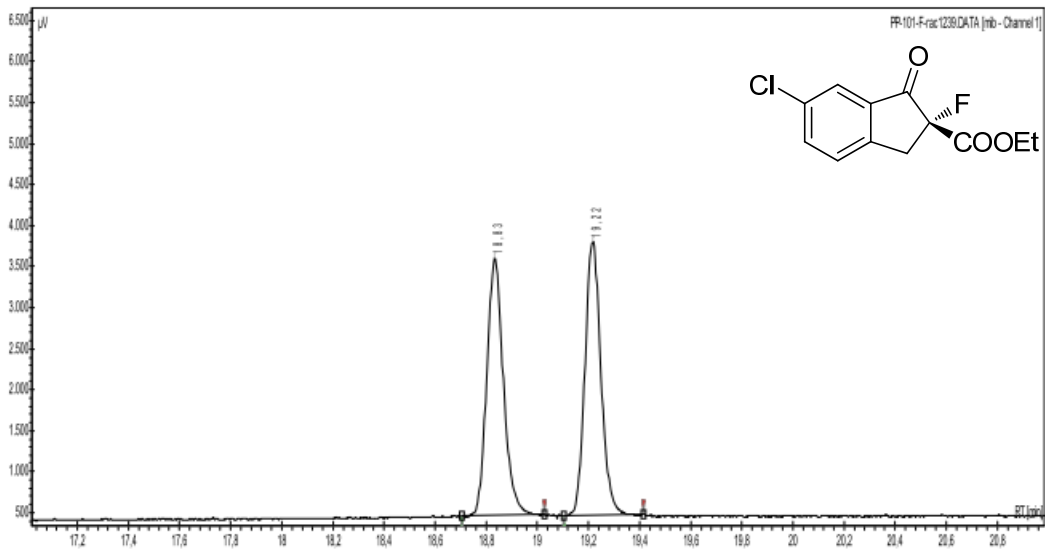
RP-1240_rac_ADH_982_flow1_7.D [Jasco UV 3]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	13,601	14,008	15,026	0,000	49,84	113545,8	41156,5	49,835
2	UNKNOWN	17,851	18,325	19,437	0,000	50,16	81959,4	41428,6	50,165
Total						100,00	195505,1	82585,1	100,000



RP-1240_ch_ADH_982_flow1_8.D [Jasco UV 2]

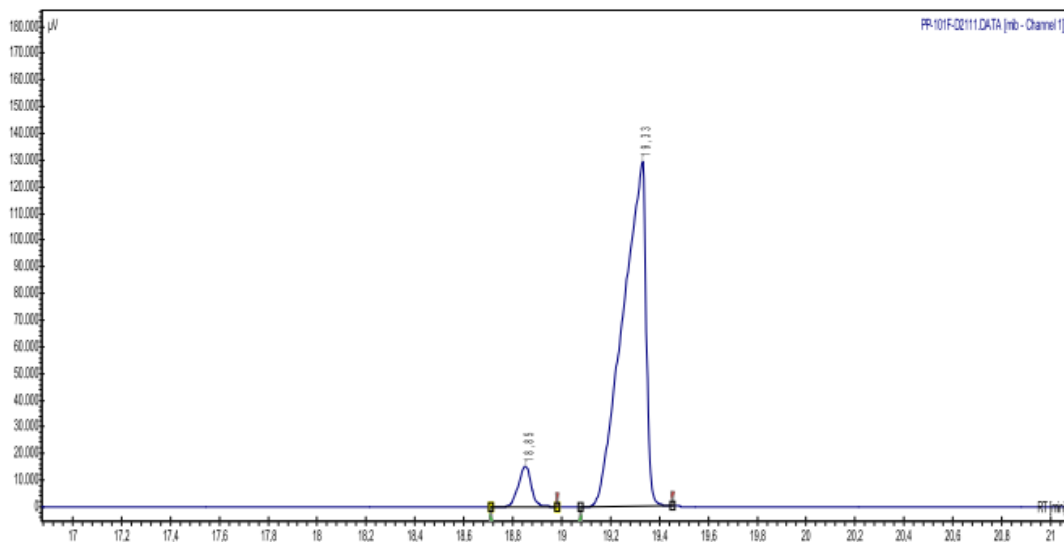
Index	Start [Min]	Time [Min]	End [Min]	Area % [%]
1	13,562	14,017	14,720	5,248
2	17,651	18,258	19,560	94,752
Total				100,000



Peak results :

PP-101-Frac1239.D [mib - Channel 1]

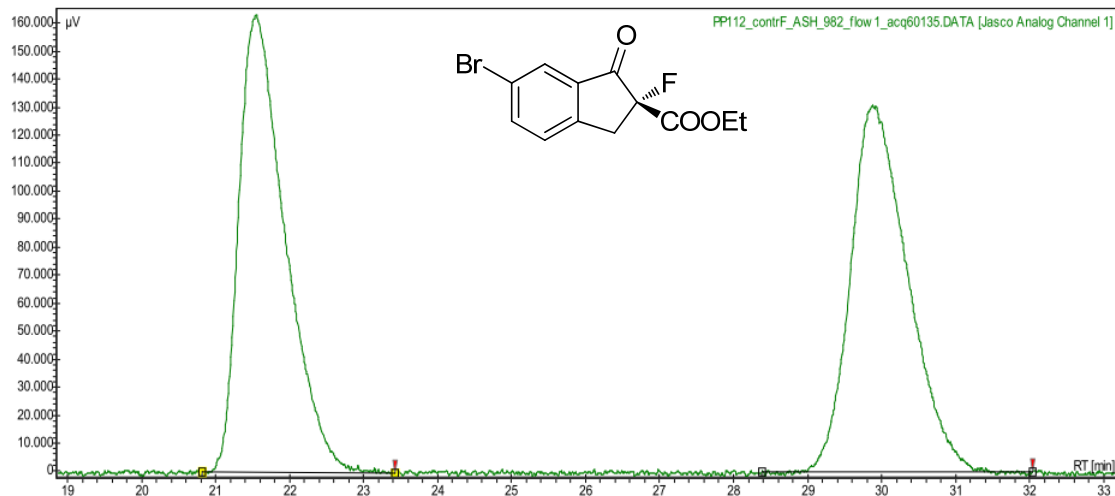
Index	Name	Time [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	18.83	49.70	3140.9	237.6	49.705
2	UNKNOWN	19.22	50.30	3336.9	240.4	50.295
Total			100.00	6477.9	478.0	100.000



Peak results :

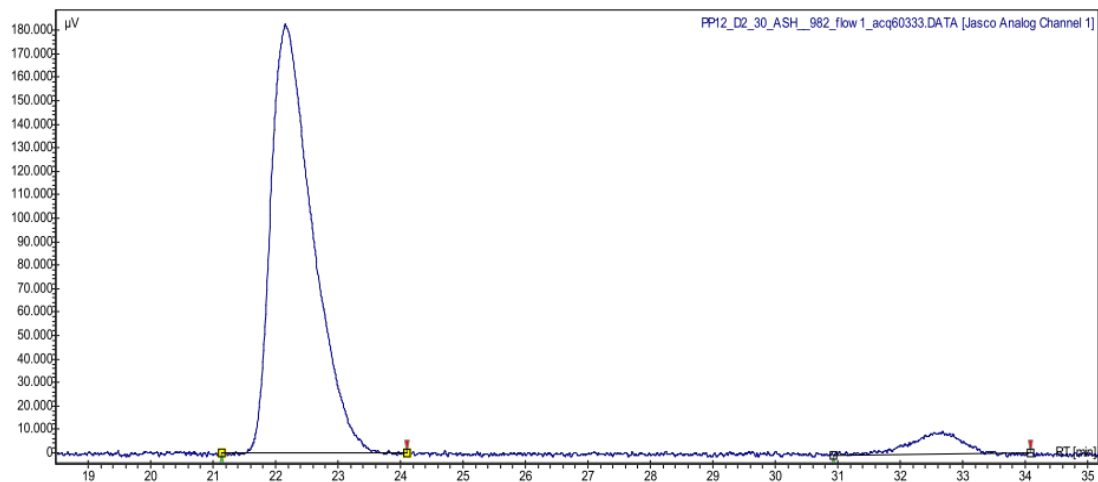
PP-101F-D2111.D [mib - Channel 1]

Index	Name	Time [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	18.85	6.13	15300.4	923.7	6.132
2	UNKNOWN	19.33	93.87	129258.1	14138.6	93.868
Total			100.00	144558.4	15062.2	100.000



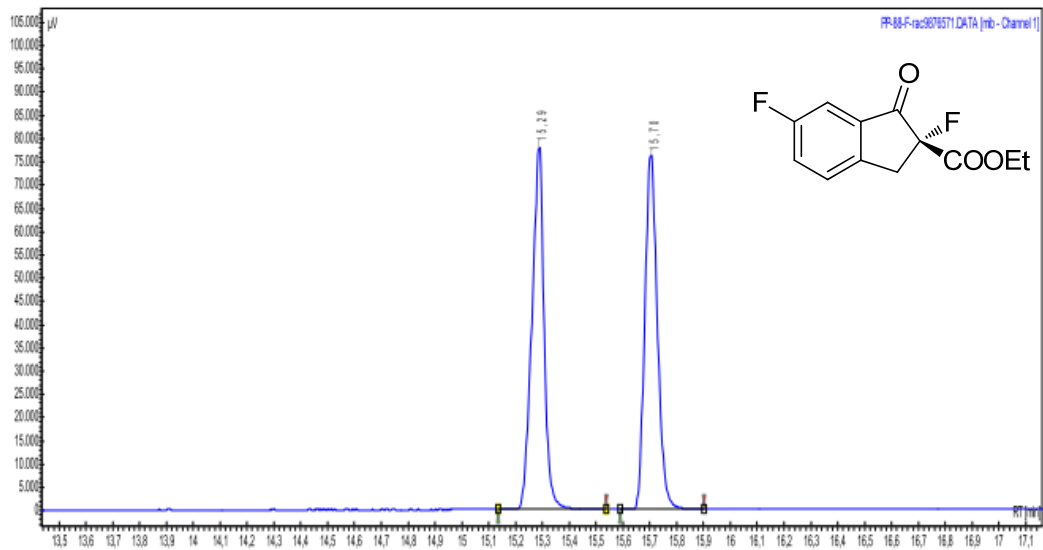
PP112_contrF_ASH_982_flow1_acq60135.DATA [Jasco Analog Channel 1]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	20,826	21,542	23,430	0,000	50,46	163262,6	118235,1	50,455
2	UNKNOWN	28,388	29,867	32,045	0,000	49,54	130428,2	116102,1	49,545
Total						100,00	293690,8	234337,2	100,000



PP12_D2_30_ASH_982_flow1_acq60333.DATA [Jasco Analog Channel 1]

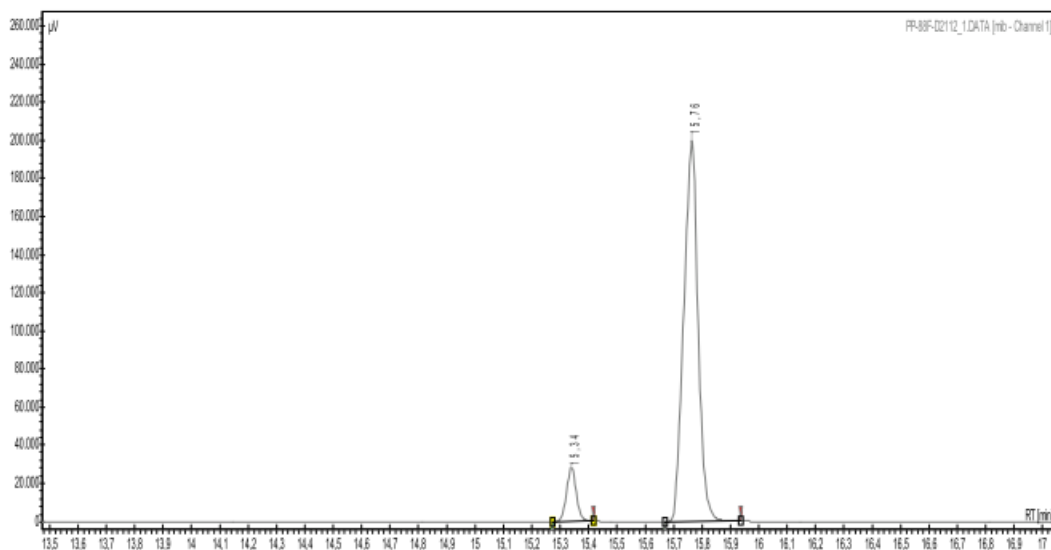
Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	21,136	22,158	24,112	0,000	94,22	182766,0	140173,7	94,222
2	UNKNOWN	30,930	32,692	34,091	0,000	5,78	9637,9	8595,2	5,778
Total						100,00	192403,9	148768,8	100,000



Peak results :

PP-88-F-rac9876571.D\\DATA [mib - Channel 1]

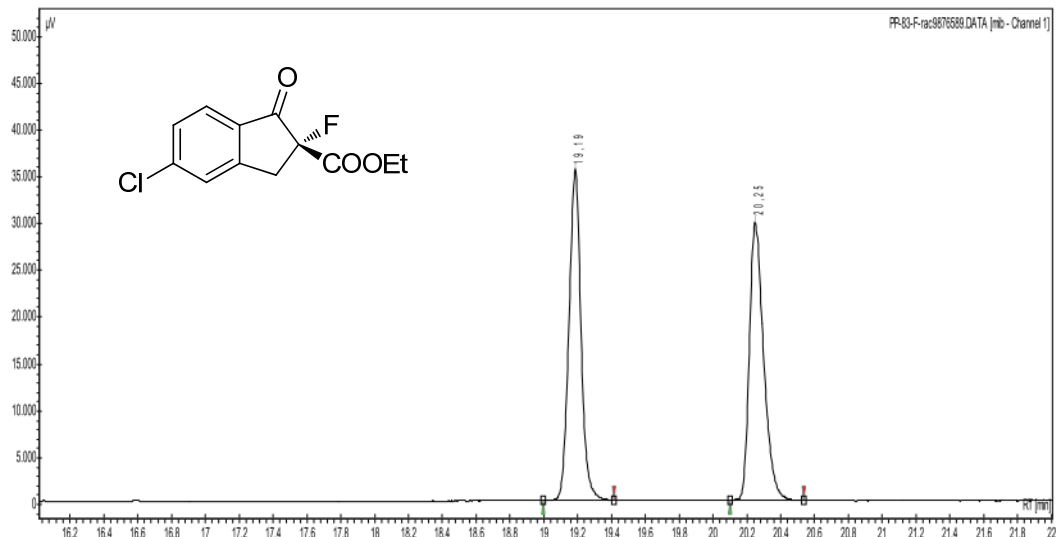
Index	Name	Time [Min]	Quantity [% Area]	Height [µV]	Area [µV.Min]	Area % [%]
1	UNKNOWN	15.29	49.95	77808.9	4104.6	49.951
2	UNKNOWN	15.70	50.05	76365.0	4112.6	50.049
Total			100.00	154173.8	8217.2	100.000



Peak results :

PP-88F-D2112_1.D\\DATA [mib - Channel 1]

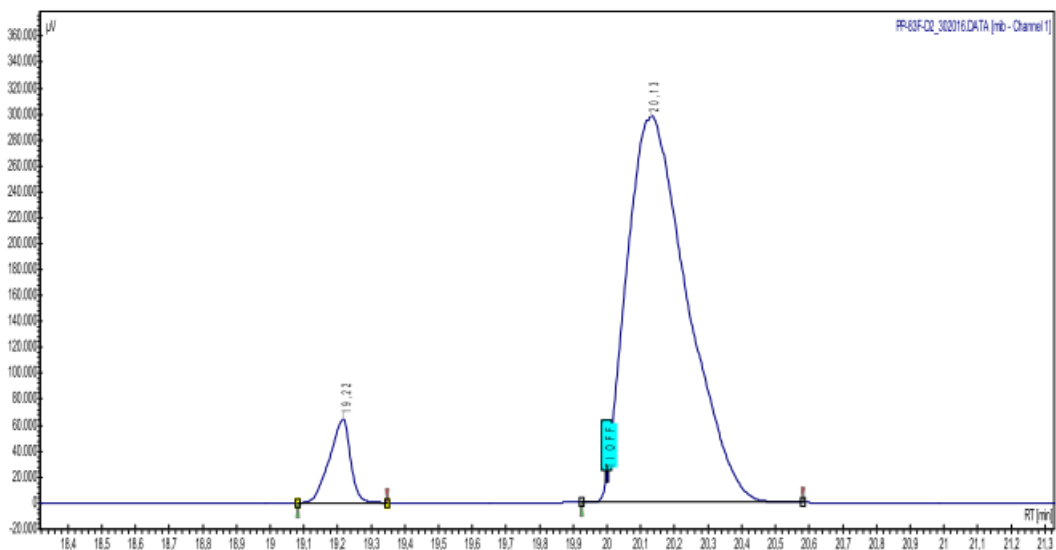
Index	Name	Time [Min]	Quantity [% Area]	Height [µV]	Area [µV.Min]	Area % [%]
1	UNKNOWN	15.34	8.91	28497.8	1138.2	8.910
2	UNKNOWN	15.76	91.09	200248.4	11637.1	91.090
Total			100.00	228746.2	12775.4	100.000



Peak results :

PP-83-F-rac9876589.DAT [mib - Channel 1]

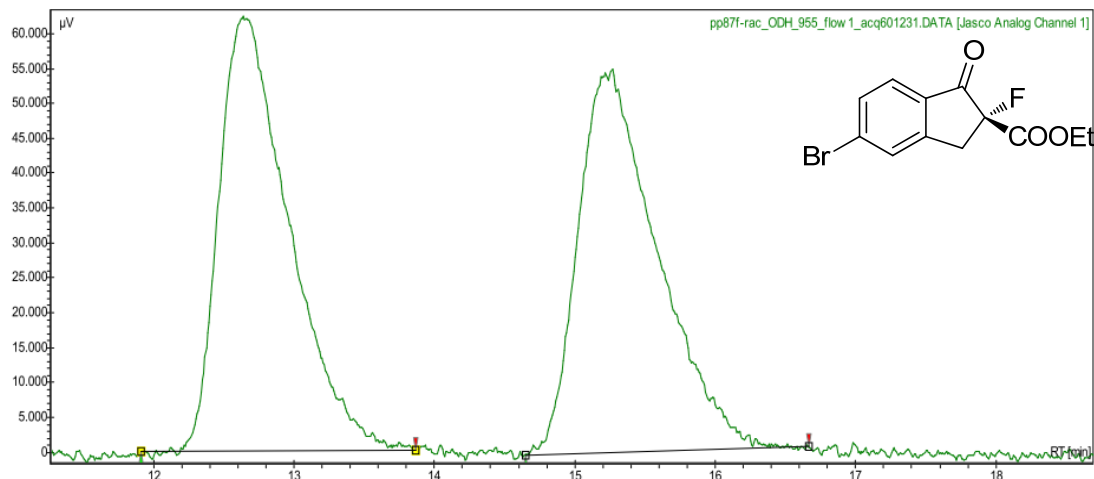
Index	Name	Time [Min]	Quantity [% Area]	Height [μV]	Area [$\mu V \cdot \text{Min}$]	Area % [%]
1	UNKNOWN	19.19	50.05	35444.2	2904.2	50.049
2	UNKNOWN	20.25	49.95	29695.0	2898.6	49.951
Total			100.00	65139.2	5802.8	100.000



Peak results :

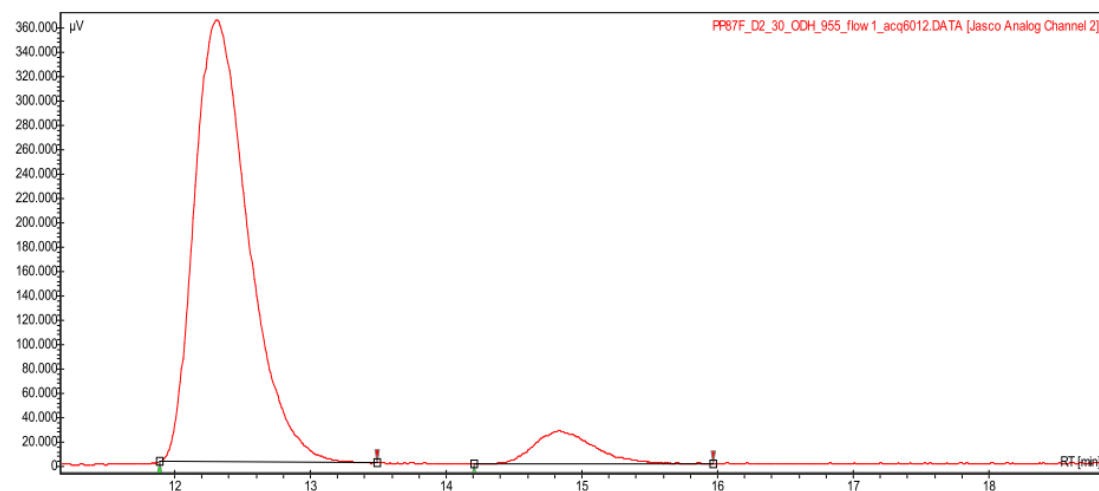
PP-83F-D2_302016.DAT [mib - Channel 1]

Index	Name	Time [Min]	Quantity [% Area]	Height [μV]	Area [$\mu V \cdot \text{Min}$]	Area % [%]
1	UNKNOWN	19.22	6.89	64810.9	4603.5	6.885
2	UNKNOWN	20.13	93.11	298570.2	62254.7	93.115
Total			100.00	363381.1	66858.2	100.000



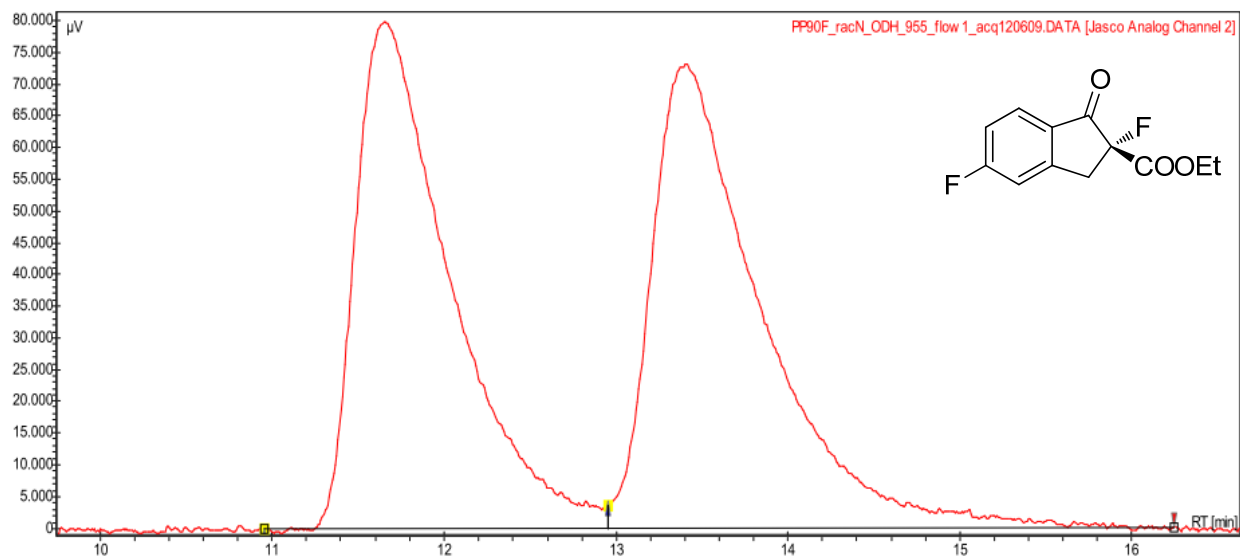
pp87f-rac_ODH_955_flow1_acq601231.D [Jasco Analog Channel 1]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	11,911	12,650	13,867	0,000	50,15	61890,1	36128,8	50,146
2	UNKNOWN	14,648	15,258	16,663	0,000	49,85	54561,1	35918,9	49,854
Total						100,00	116451,1	72047,7	100,000



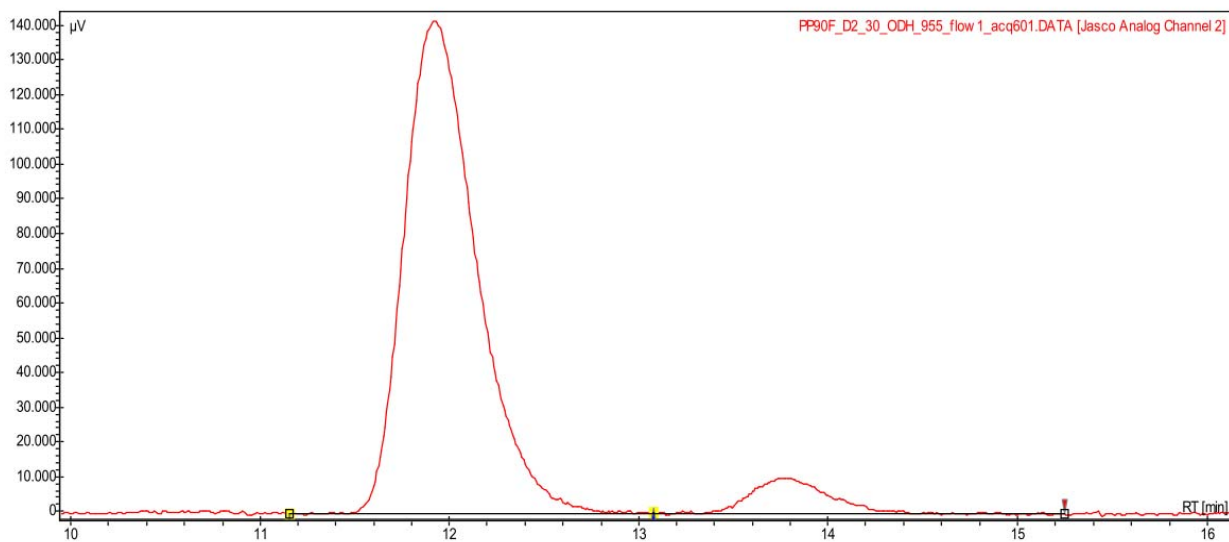
PP87F_D2_30_ODH_955_flow1_acq6012.D [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	11,888	12,308	13,491	0,000	92,42	362818,0	167517,0	92,421
2	UNKNOWN	14,206	14,833	15,969	0,000	7,58	26954,6	13737,1	7,579
Total						100,00	389772,6	181254,2	100,000



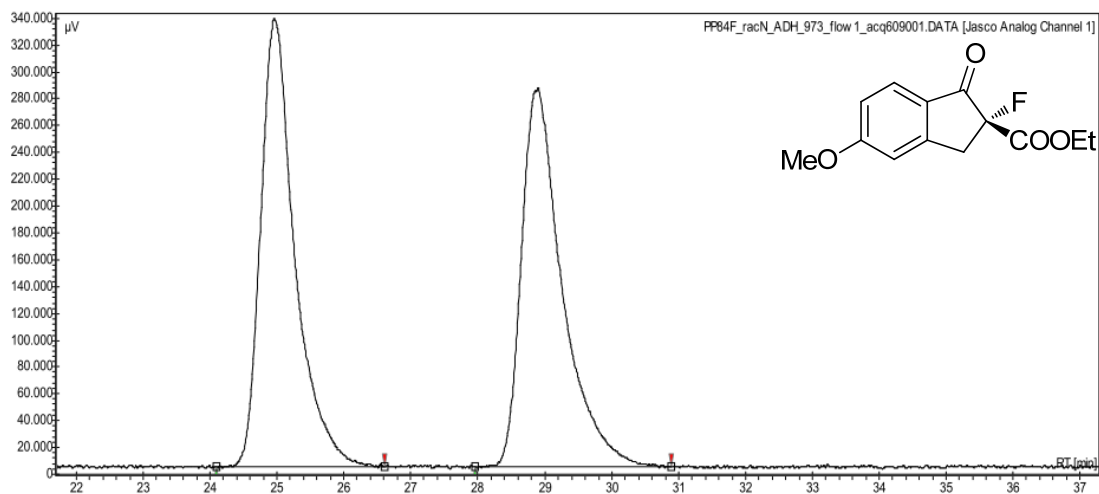
PP90F_racN_ODH_955_flow1_acq120609.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	10,953	11,658	12,952	0,000	48,63	79894,9	51000,1	48,629
2	UNKNOWN	12,952	13,400	16,246	0,000	51,37	73060,7	53876,0	51,371
Total						100,00	152955,6	104876,1	100,000



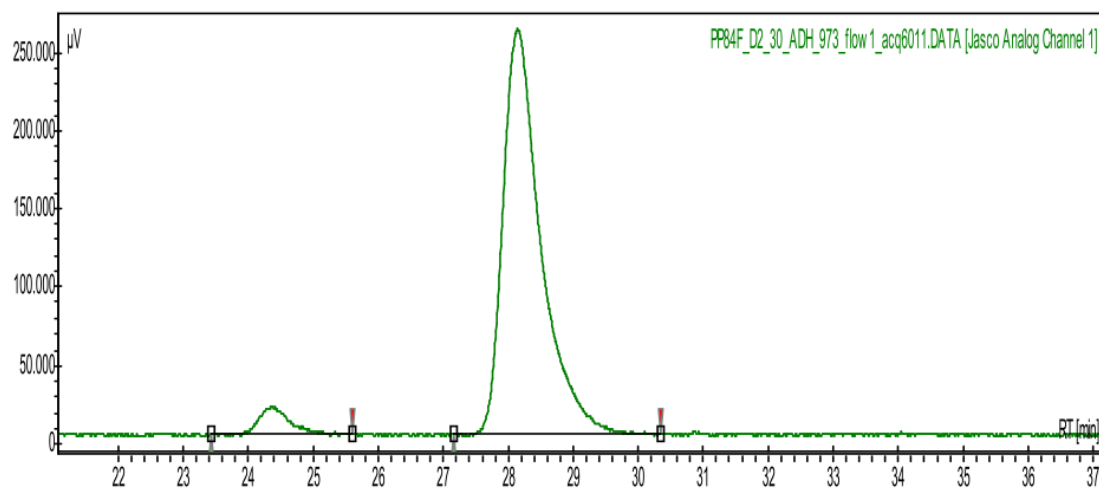
PP90F_D2_30_ODH_955_flow1_acq601.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	11,157	11,917	13,079	0,000	92,37	141756,5	62867,1	92,369
2	UNKNOWN	13,079	13,775	15,248	0,000	7,63	10196,9	5193,7	7,631
Total						100,00	151953,3	68060,7	100,000



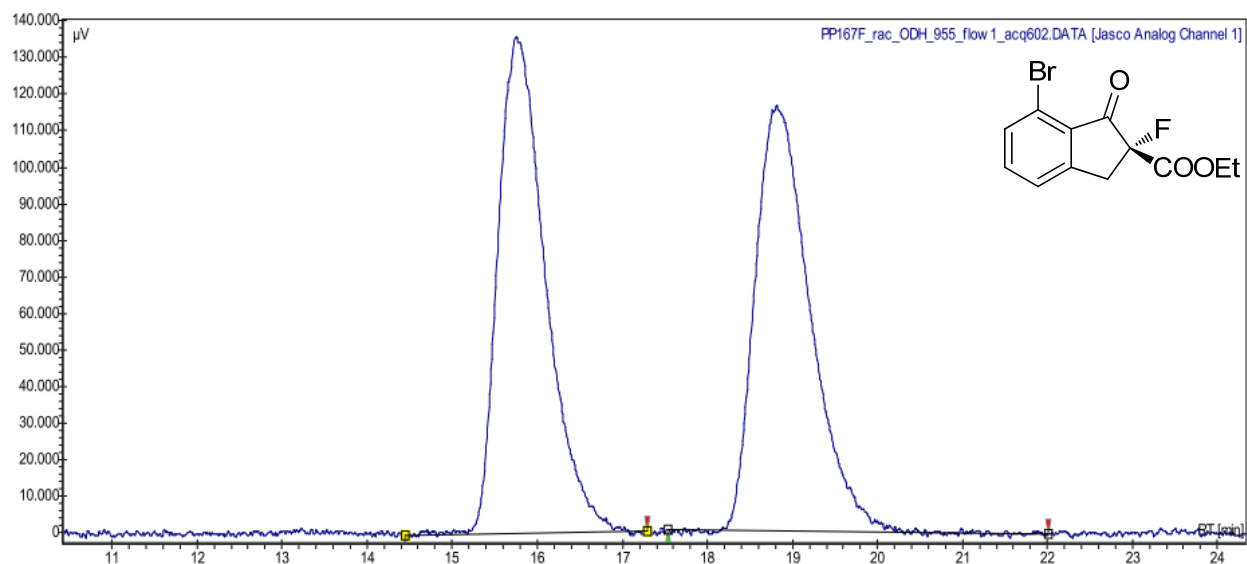
PP84F_racN_ADH_973_flow1_acq609001.DATA [Jasco Analog Channel 1]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	24,096	24,967	26,612	0,000	49,75	333808,4	197349,9	49,748
2	UNKNOWN	27,969	28,900	30,898	0,000	50,25	282291,8	199347,6	50,252
Total						100,00	616100,2	396697,5	100,000



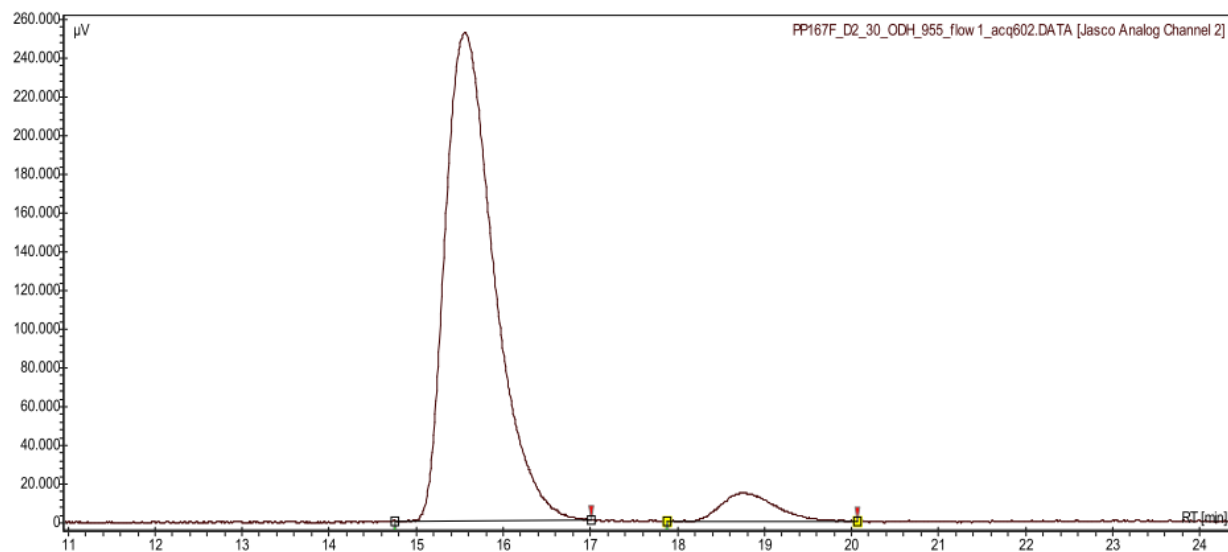
PP84F_D2_30_ADH_973_flow1_acq60111.DATA [Jasco Analog Channel 1]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	23,430	24,367	25,599	0,000	4,75	17319,3	8715,8	4,748
2	UNKNOWN	27,161	28,142	30,345	0,000	95,25	260111,8	174836,7	95,252
Total						100,00	277431,1	183552,5	100,000



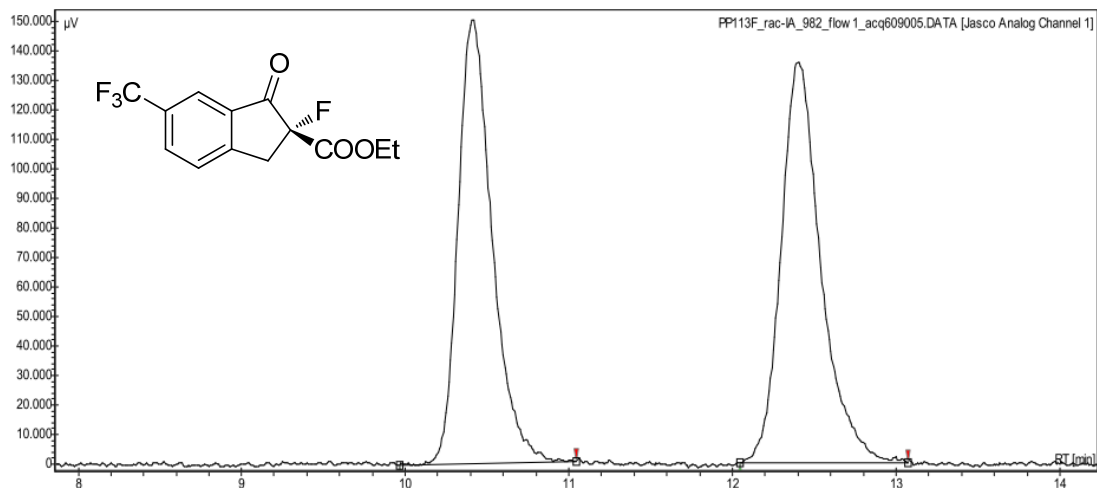
PP167F_rac_ODH_955_flow1_acq602.DATA [Jasco Analog Channel 1]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	14,442	15,750	17,293	0,000	50,37	135847,6	88070,1	50,370
2	UNKNOWN	17,541	18,817	22,004	0,000	49,63	115968,0	86777,2	49,630
Total						100,00	251815,7	174847,3	100,000



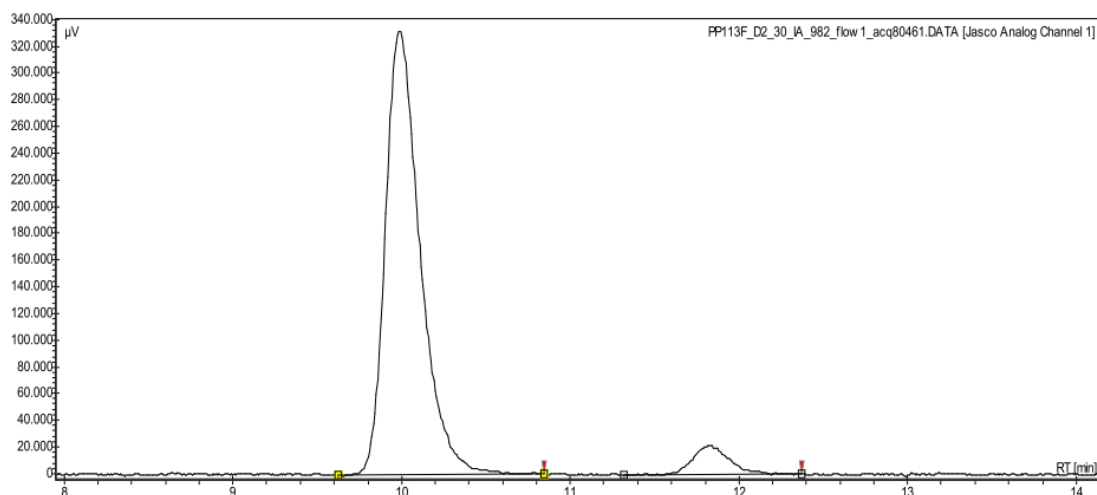
PP167F_D2_30_ODH_955_flow1_acq602.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	14,754	15,558	17,004	0,000	93,88	251784,3	162684,8	93,882
2	UNKNOWN	17,875	18,742	20,067	0,000	6,12	14775,1	10602,2	6,118
Total						100,00	266559,4	173287,0	100,000



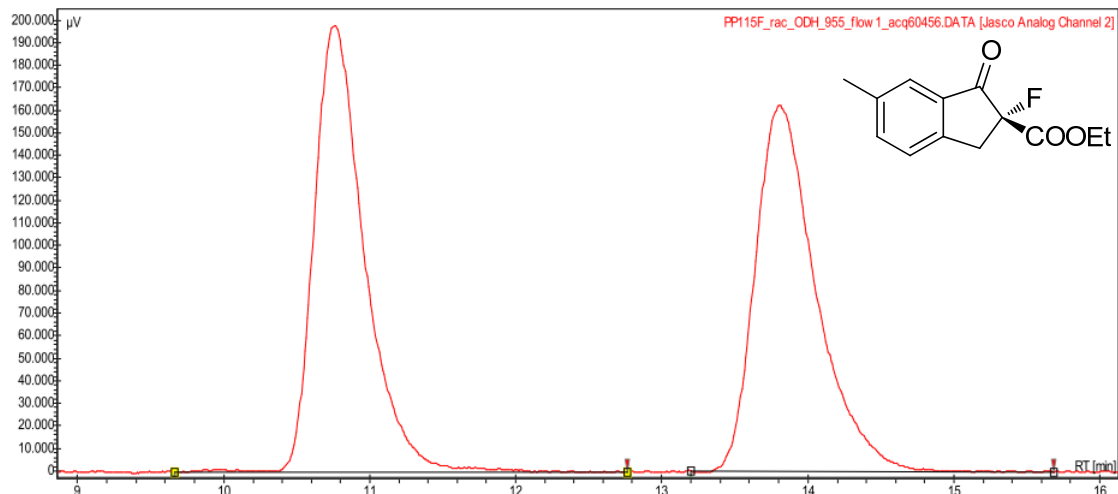
PP113F_rac-IA_982_flow1_acq609005.D [Jasco Analog Channel 1]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	9,965	10,408	11,045	0,000	48,64	150211,0	36264,9	48,638
2	UNKNOWN	12,046	12,400	13,074	0,000	51,36	135895,0	38296,3	51,362
Total						100,00	286105,9	74561,3	100,000



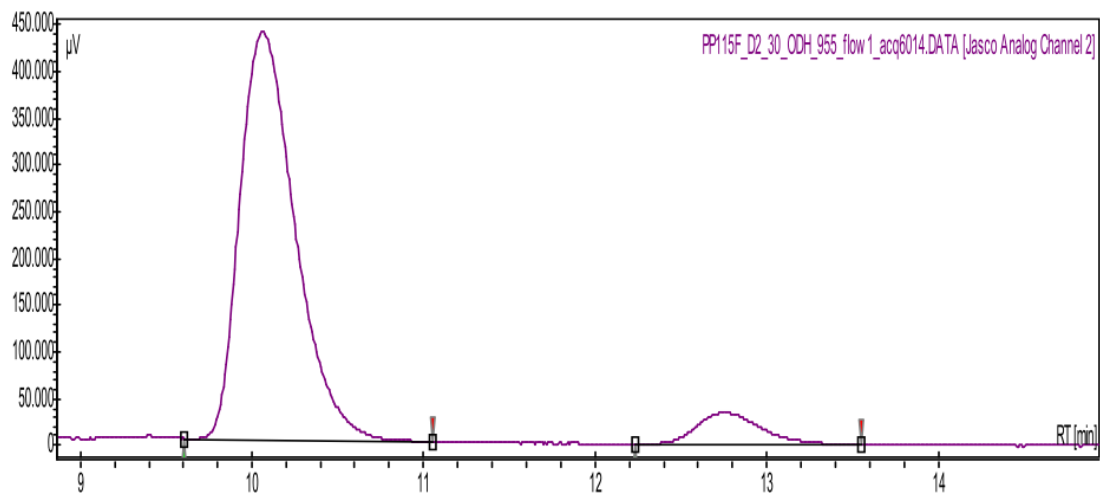
PP113F_D2_30_IA_982_flow1_acq80461.D [Jasco Analog Channel 1]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	9,626	9,983	10,842	0,000	93,51	331644,0	79156,4	93,515
2	UNKNOWN	11,315	11,833	12,369	0,000	6,49	21784,3	5489,3	6,485
Total						100,00	353428,3	84645,7	100,000



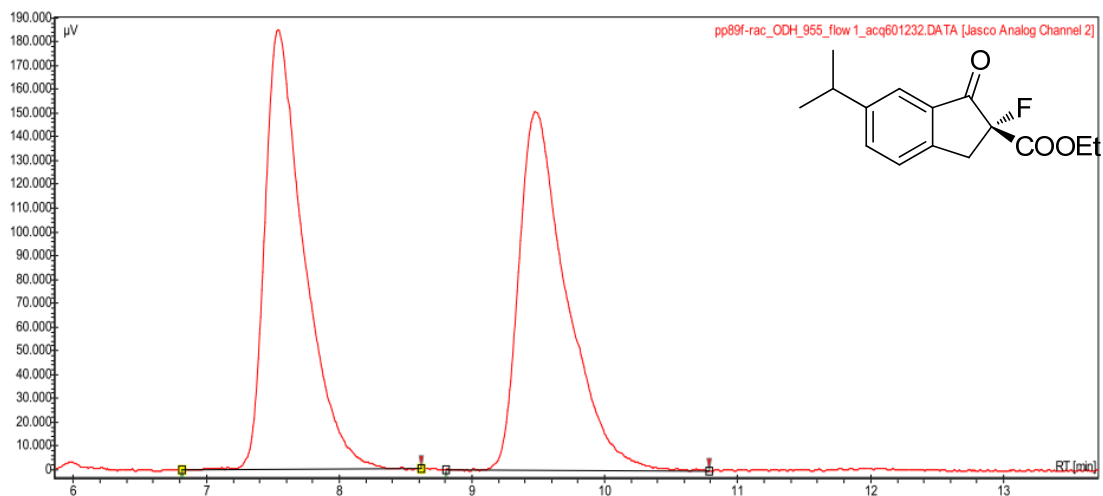
PP115F_rac_ODH_955_flow1_acq60456.D [Jasco Analog Channel 2]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	9,669	10,767	12,769	0,000	50,30	197891,6	79288,5	50,305
2	UNKNOWN	13,202	13,817	15,682	0,000	49,70	162388,7	78327,7	49,695
Total						100,00	360280,3	157616,2	100,000



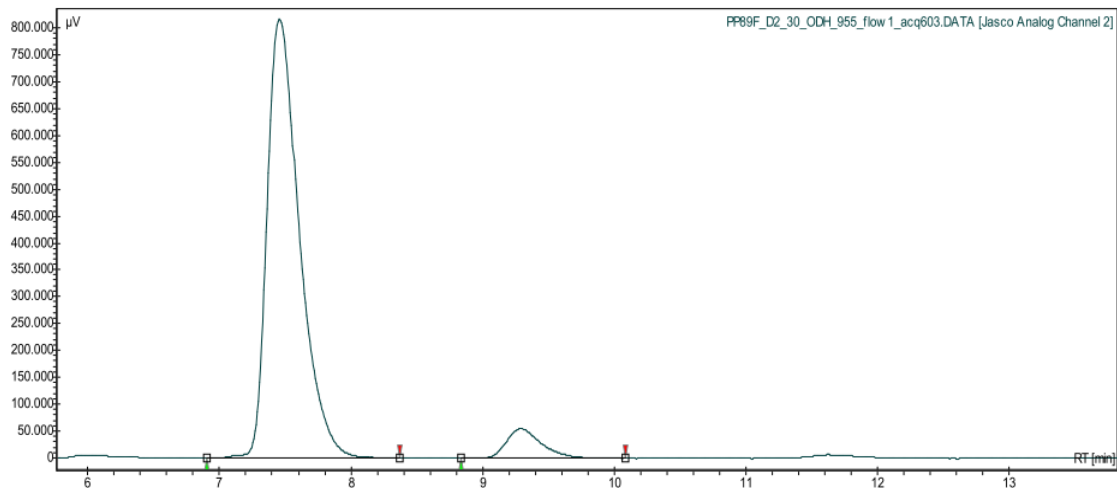
PP115F_D2_30_ODH_955_flow1_acq6014.D [Jasco Analog Channel 2]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	9,604	10,058	11,054	0,000	91,74	435884,2	162393,6	91,736
2	UNKNOWN	12,233	12,758	13,551	0,000	8,26	33984,8	14629,7	8,264
Total						100,00	469869,0	177023,3	100,000



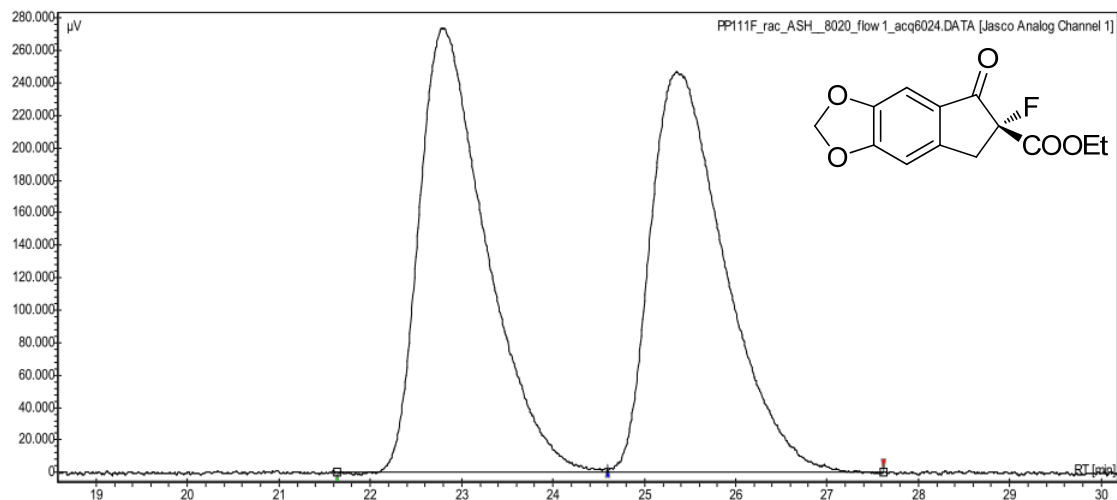
pp89f-rac_ODH_955_flow1_acq601232.D [Jasco Analog Channel 2]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	6,818	7,542	8,616	0,000	50,17	184715,6	63030,8	50,169
2	UNKNOWN	8,802	9,483	10,785	0,000	49,83	150423,4	62605,7	49,831
Total						100,00	335139,0	125636,5	100,000



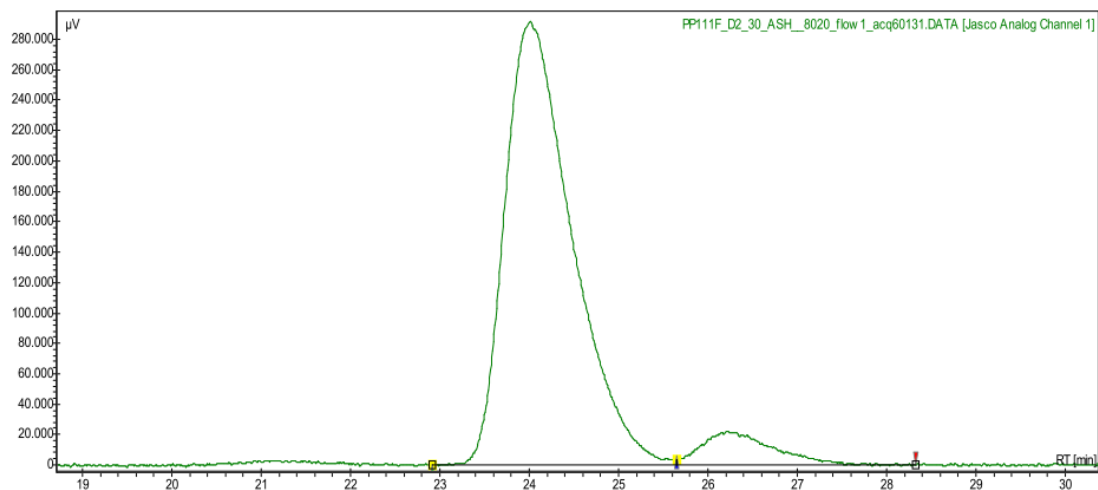
PP89F_D2_30_ODH_955_flow1_acq603.D [Jasco Analog Channel 2]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	6,905	7,458	8,370	0,000	93,02	816359,5	227132,7	93,017
2	UNKNOWN	8,836	9,292	10,085	0,000	6,98	55032,7	17050,8	6,983
Total						100,00	871392,2	244183,6	100,000



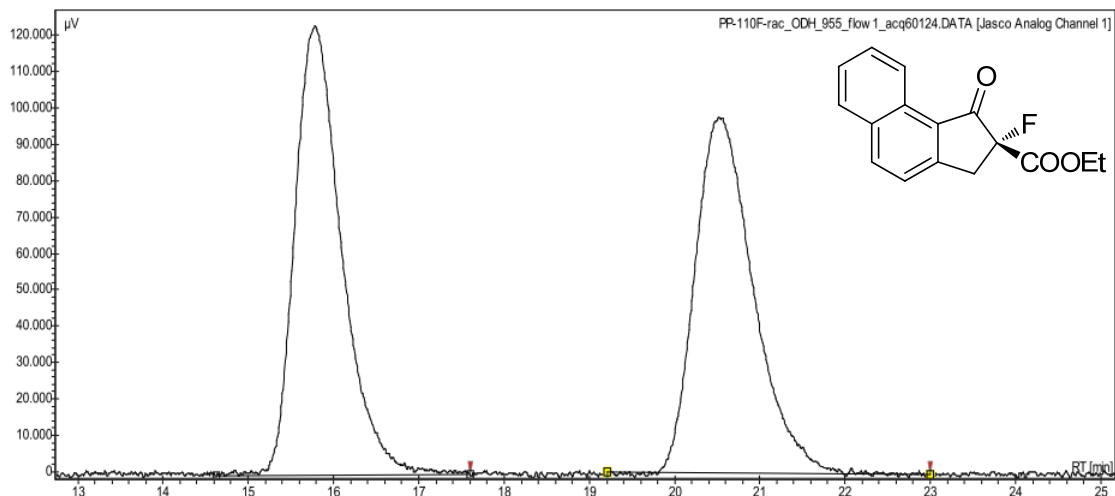
PP111F_rac_ASH_8020_flow1_acq6024.DATA [Jasco Analog Channel 1]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	21,638	22,800	24,598	0,000	49,84	273180,6	231258,4	49,837
2	UNKNOWN	24,598	25,358	27,618	0,000	50,16	246732,8	232772,8	50,163
Total						100,00	519913,4	464031,1	100,000



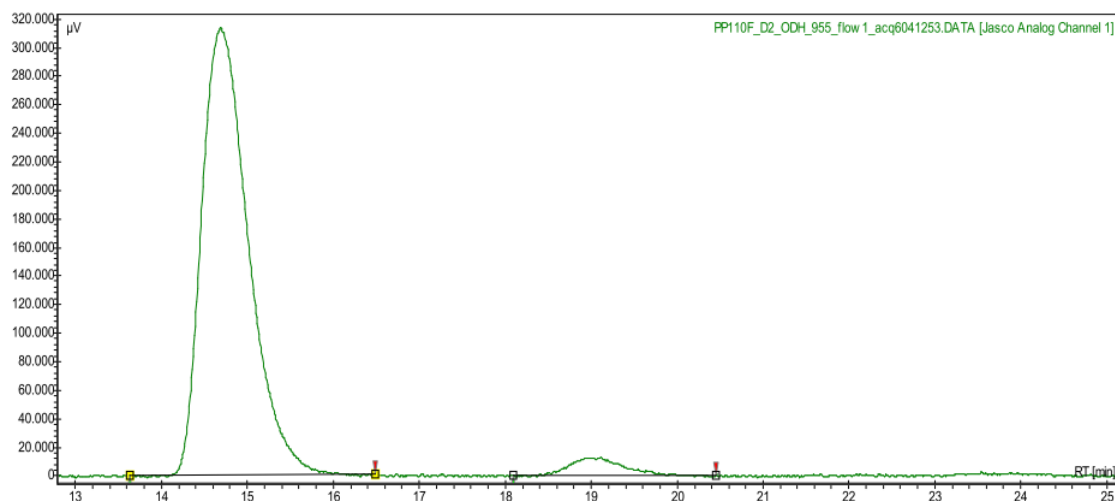
PP111F_D2_30_ASH_8020_flow1_acq60131.DATA [Jasco Analog Channel 1]

Index	Name	Start [Min]	Time [Min]	End [Min]	Ret. time Offset [Min]	Quantity [% Area]	Height [μV]	Area [μV.Min]	Area % [%]
1	UNKNOWN	22,921	24,017	25,646	0,000	92,68	291606,3	254231,6	92,684
2	UNKNOWN	25,646	26,225	28,326	0,000	7,32	21635,6	20066,5	7,316
Total						100,00	313241,9	274298,1	100,000



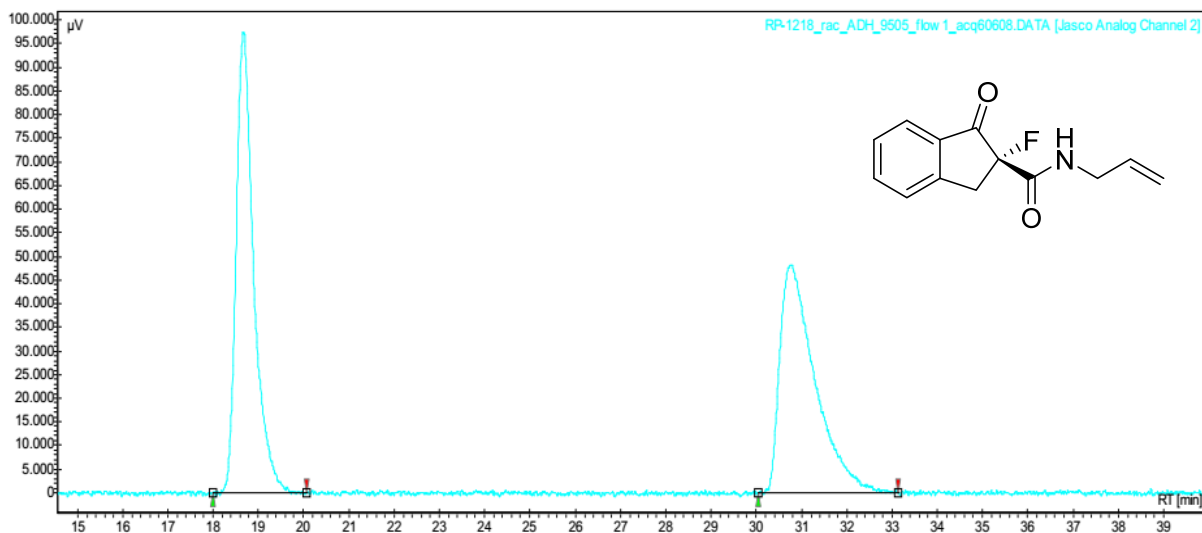
PP-110F-rac_ODH_955_flow1_acq60124.DATA [Jasco Analog Channel 1]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
2	UNKNOWN	14,628	15,775	17,603	0,000	50,62	123180,8	79222,6	50,622
1	UNKNOWN	19,215	20,525	22,996	0,000	49,38	97853,4	77277,3	49,378
Total						100,00	221034,3	156499,9	100,000



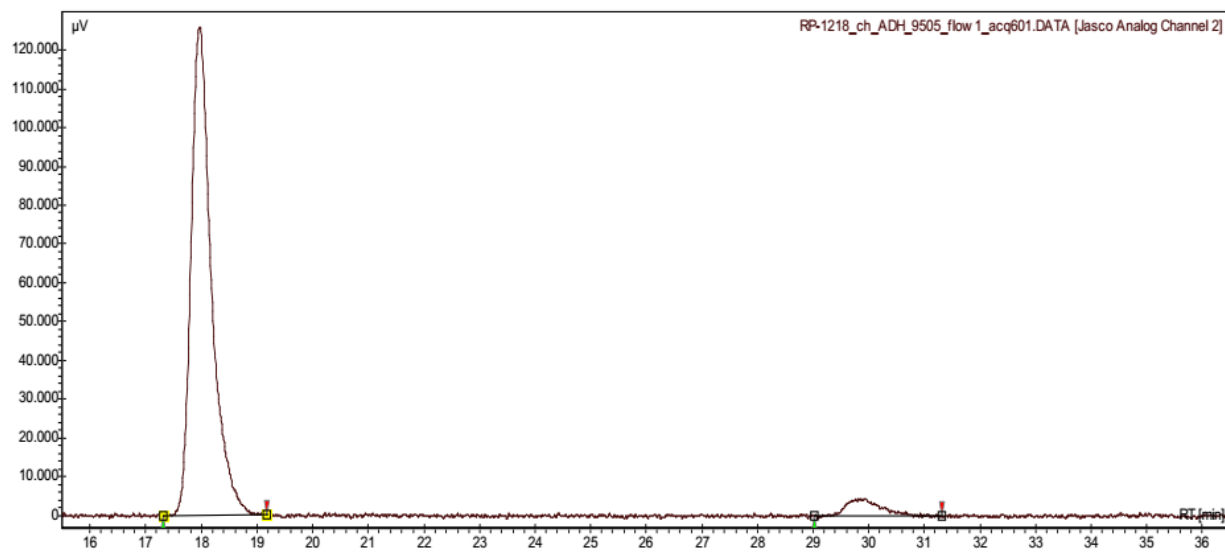
PP110F_D2_ODH_955_flow1_acq6041253.DATA [Jasco Analog Channel 1]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	13,636	14,692	16,488	0,000	95,91	313726,4	196174,3	95,915
2	UNKNOWN	18,099	19,108	20,455	0,000	4,09	12621,3	8355,8	4,085
Total						100,00	326347,7	204530,0	100,000



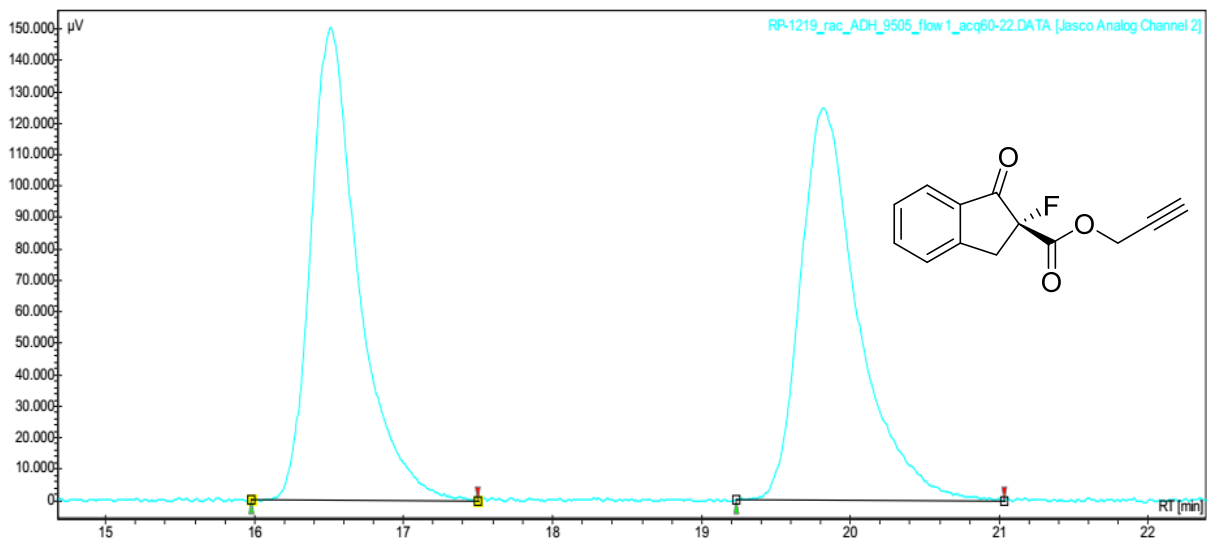
RP-1218_rac_ADH_9505_flow1_acq60608.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	17,999	18,667	20,079	0,000	50,10	97313,9	43631,7	50,097
2	UNKNOWN	30,047	30,758	33,131	0,000	49,90	48126,1	43463,4	49,903
Total						100,00	145440,1	87095,1	100,000



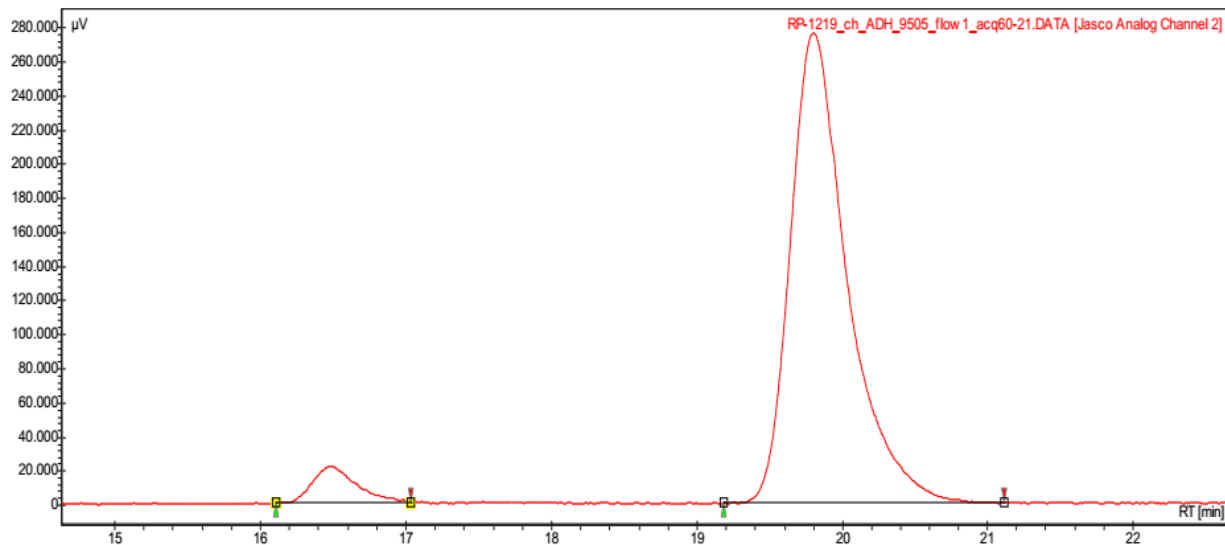
RP-1218_ch_ADH_9505_flow1_acq601.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	17,314	17,967	19,175	0,000	94,69	126118,7	53578,5	94,694
2	UNKNOWN	29,023	29,925	31,317	0,000	5,31	4290,4	3001,9	5,306
Total						100,00	130409,1	56580,4	100,000



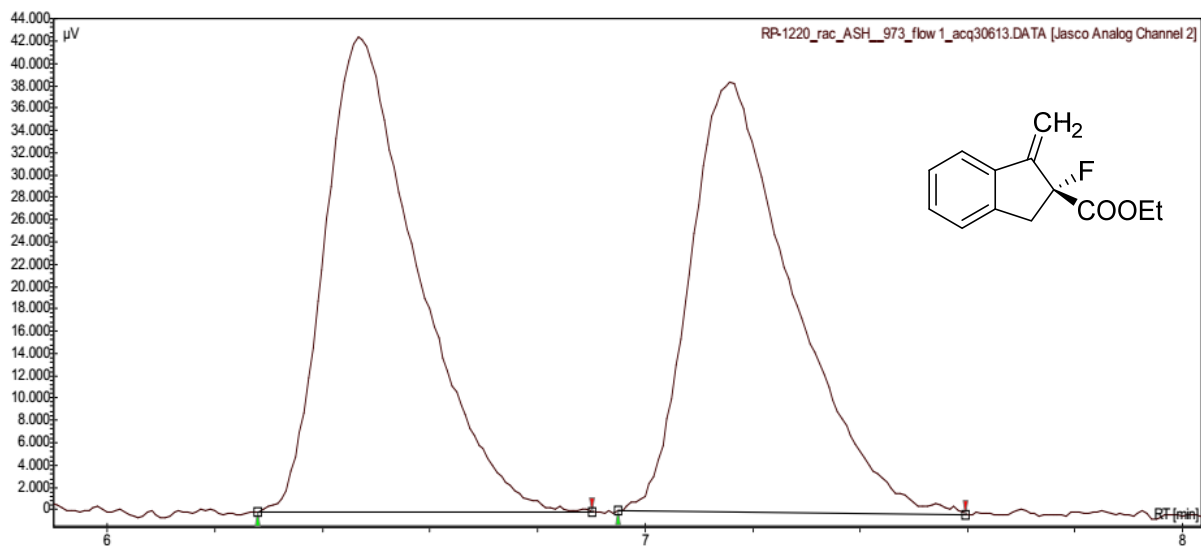
RP-1219_rac_ADH_9505_flow1_acq60-22.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time	Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]		[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	15,975	16,508	17,496		0,000	49,90	150532,2	55602,8	49,904
2	UNKNOWN	19,232	19,817	21,035		0,000	50,10	124609,1	55817,7	50,096
Total							100,00	275141,2	111420,4	100,000



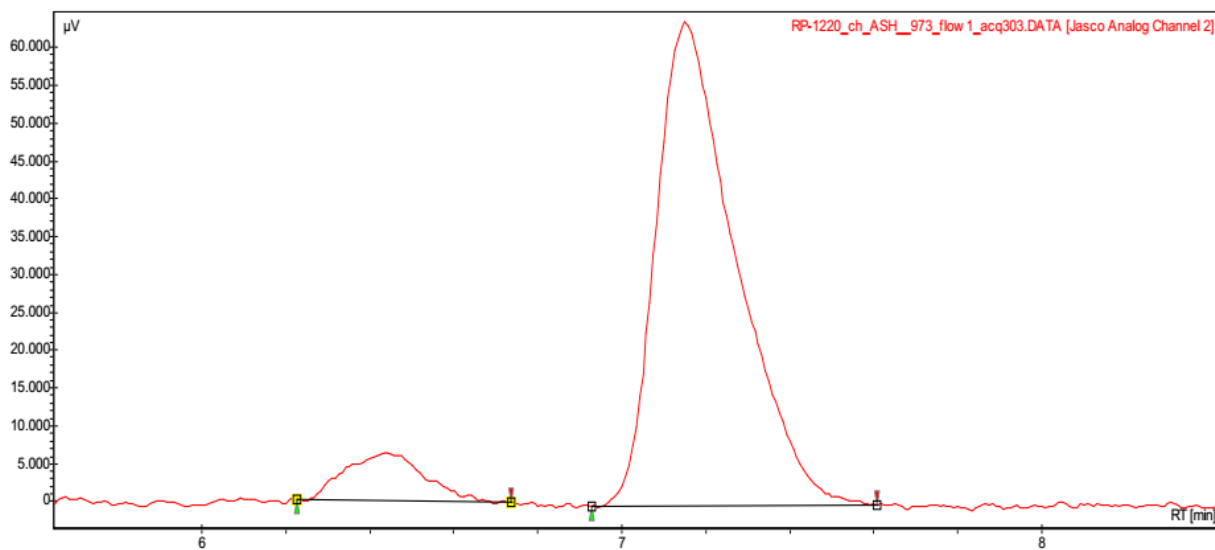
RP-1219_ch_ADH_9505_flow1_acq60-21.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time	Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]		[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	16,106	16,483	17,031		0,000	5,56	21274,8	7285,2	5,562
2	UNKNOWN	19,187	19,800	21,113		0,000	94,44	275396,7	123685,5	94,438
Total							100,00	296671,6	130970,7	100,000



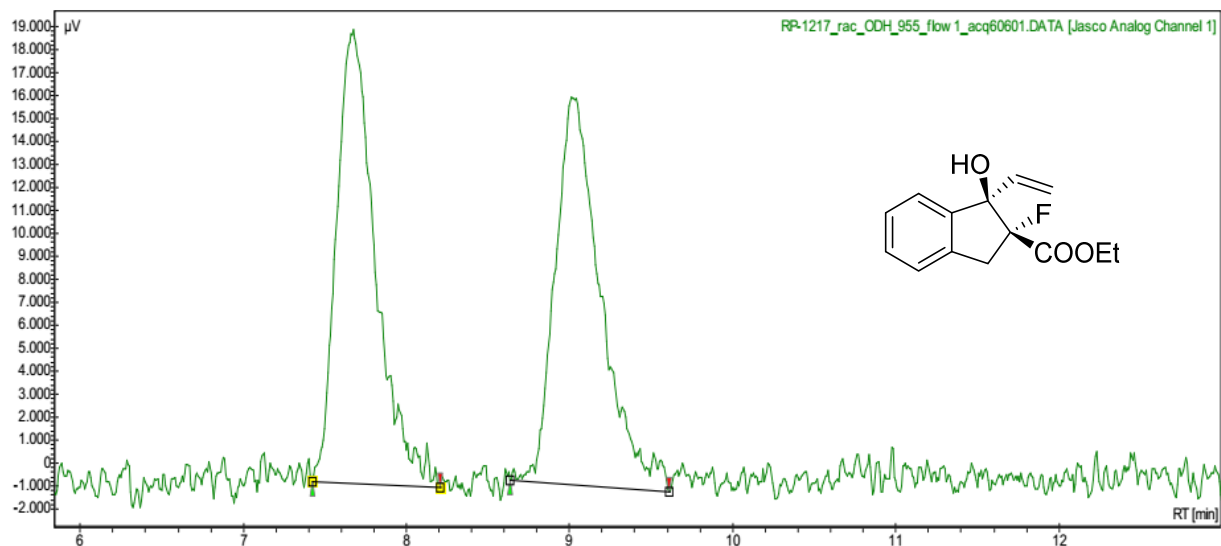
RP-1220_rac_ASH_973_flow1_acq30613.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	6,280	6,467	6,903	0,000	49,89	42560,0	8535,8	49,887
2	UNKNOWN	6,951	7,158	7,597	0,000	50,11	38480,1	8574,6	50,113
Total						100,00	81040,1	17110,4	100,000



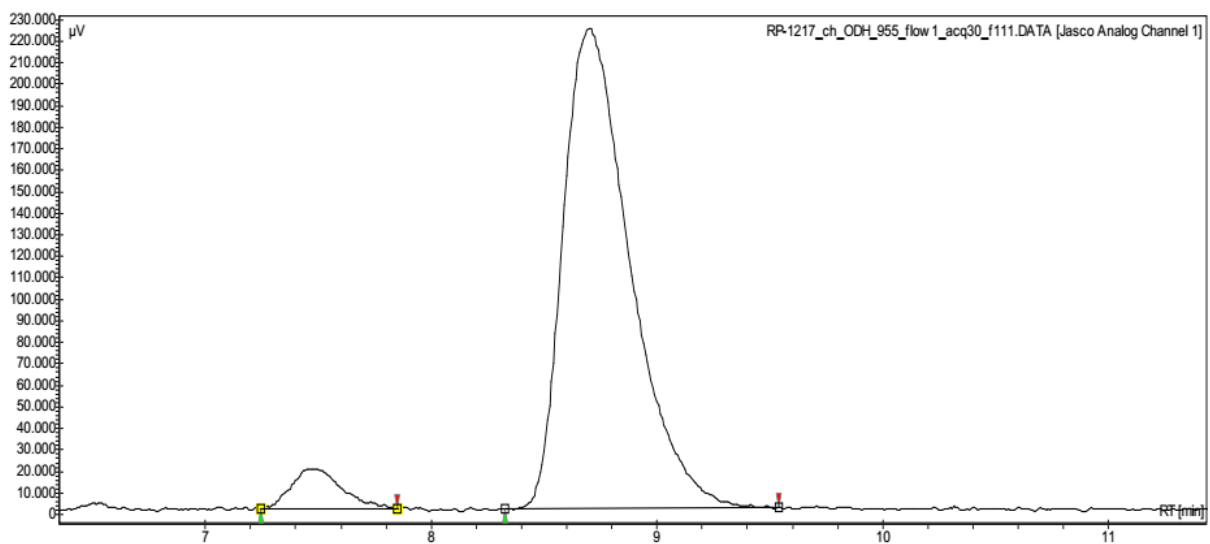
RP-1220_ch_ASH_973_flow1_acq303.DATA [Jasco Analog Channel 2]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	6,224	6,433	6,736	0,000	8,99	6397,3	1387,6	8,994
2	UNKNOWN	6,928	7,150	7,606	0,000	91,01	63978,8	14040,9	91,006
Total						100,00	70376,0	15428,5	100,000



RP-1217_rac_ODH_955_flow1_acq60601.DATA [Jasco Analog Channel 1]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	7,422	7,667	8,205	0,000	50,02	19500,5	5465,3	50,019
2	UNKNOWN	8,637	9,033	9,610	0,000	49,98	16746,2	5461,2	49,981
Total						100,00	36246,7	10926,4	100,000



RP-1217_ch_ODH_955_flow1_acq30_f111.DATA [Jasco Analog Channel 1]

Index	Name	Start	Time	End	Ret. time Offset	Quantity	Height	Area	Area %
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	7,246	7,458	7,850	0,000	5,77	18103,1	4670,0	5,768
2	UNKNOWN	8,328	8,700	9,540	0,000	94,23	222970,6	76295,7	94,232
Total						100,00	241073,7	80965,7	100,000

