Supplementary Material (ESI) for Chemical Communications

Supporting Information

Confirmation by IR of the Preferred Conformations of CFTA Esters in Solution: A Highly Reliable Criterion for the Stereochemistry Assignment of Chiral Alcohols

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CONTENTS

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S-1. Typical Procedure for Preparation of α-Cyano-α-fluoro-p-tolylacetic Acid Derivatives

In a 10 ml flask, (1*R*, 2*S*, 5*R*)-(-)-menthol (15.6 mg, 0.10 mmol) and pyridine (16.3 μl, 0.20 mmol) were dissolved in dry dichloromethane (1 ml). To this solution, CFTA-Cl (19.6 μl, 0.12 mmol) was added and the mixture was stirred for 2 h at ambient temperature. Aqueous solution of 10% HCl was added and dichloromethane was removed under reduced pressure. The residual solution was extracted with AcOEt twice and the combined extract was then washed with brine. The organic layer was dried over $MgSO_4$ and the solvent was evaporated. The residue was column-chromatographed on SiO_2 (eluent, Hex:AcOEt = 10:1) to afford the product as colorless oil (26 mg, 78%).

(R)-CFTA ester of (S)-1-phenylethanol (CAS: 278181-81-0)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 1.61 (3H, d, *J* = 6.6 Hz), 2.38 (3H, brs), 5.96 (1H, q, *J* = 6.6 Hz), 7.13(2H, m), 7.21 (2H, brd, *J* = 8.8 Hz), 7.22-7.30 (3H), 7.41 (2H, brd, *J* = 7.9 Hz).

(R)-CFTA ester of (R)-1-phenylethanol (CAS: 278181-67-2)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 1.51 (3H, d, *J* = 6.6 Hz), 2.39 (3H, s), 5.96 (1H, q, *J* = 6.6 Hz), 7.27 (2H, brd, *J* = 8.6 Hz), 7.29-7.39 (5H), 7.49 (2H, brd, *J* = 8.3 Hz).

(S)-CFTA ester of (S)-1-phenylpropanol

Colorless oil, $[\alpha]_D^{25}$ –45.7 (*c* 0.96, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.71 (3H, t, *J* = 7.5 Hz), 1.81 (1H, ddq, *J* = 15.4, 7.5, 6.1 Hz), 1.88 (1H, ddq, *J* = 15.4, 7.6, 7.6 Hz), 2.40 (3H, s), 5.73 (1H, dd, *J* = 7.6, 6.1 Hz), 7.24-7.38 (7H, m), 7.52 (2H, brd, *J* = 8.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.7, 21.3, 29.2, 81.8, 87.1 (d, *J* = 196.9 Hz), 114.1 (d, *J* = 33.7 Hz), 125.7 (d, *J* = 4.4 Hz), 126.2, 128.36, 128.39, 128.4 (d, *J* = 23.4 Hz), 129.7, 138.2, 141.5 (d, *J* = 2.2 Hz), 162.2 (d, *J* = 30.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –144.6 ppm; IR (*ν*, neat) 1773, 1248, 1055 cm^{-1}; MS (EI), *m/z*: 311 (M^+), 149 (*p*-tolC(CN)FH^+), 121 ($C_9H_{13}^+$), 120 ($C_9H_{12}^+$); HRMS (ESI) Calcd for $C_{19}H_{18}FNNaO_2$ (M + Na): 314.1219, Found: 334.1213.

(R)-CFTA ester of (S)-1-phenylpropanol

Colorless oil, $[\alpha]_D^{26}$ –13.3 (*c* 1.20, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.92 (3H, t, *J* = 7.5 Hz), 1.87 (1H, ddq, *J* = 14.5, 7.5, 6.1 Hz), 1.98 (1H, ddq, *J* = 14.5, 7.8, 7.5 Hz), 2.38 (3H, s), 5.74 (1H, dd, *J* = 7.8, 6.1 Hz), 7.27 (2H, brd, *J* = 10 Hz), 7.18-7.27 (3H), 7.24 (2H, d, *J* = 6.1 Hz), 7.51 (2H, brd, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.5, 21.3, 29.2, 81.7, 87.1 (d, *J* = 196.9 Hz), 114.0 (d, *J* = 32.7 Hz), 125.5 (d, *J*= 5.1 Hz), 126.3, 128.5, 128.6, 128.7 (d, *J* = 23.4 Hz), 129.8, 138.4, 141.6 (d, *J* = 2.2 Hz), 162.4 (d, *J* = 30.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –143.7 ppm; IR (*ν*, neat) 1773, 1250, 1055 cm^{-1}; MS (EI), *m/z*: 311 (M^+), 148 (*p*-tolC(CN)F^+), 120 ($C_9H_{12}^+$); HRMS (ESI) Calcd for $C_{19}H_{18}FNNaO_2$ (M + Na): 314.1219, Found: 334.1213.

(S)-CFTA ester of (R)-4-methylpentan-2-ol

Colorless oil, $[\alpha]_D^{27}$ –31.2 (*c* 0.67, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.73 (3H, d, *J* = 6.1 Hz), 0.76 (3H, d, *J* = 6.6 Hz), 1.21-1.35 (2H), 1.30 (3H, d, *J* = 6.4 Hz), 1.54 (1H, m), 2.40 (3H, s), 5.13 (1H, m), 7.27 (2H, brd, *J* = 8.0 Hz), 7.51 (2H, brd, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.0, 21.3, 21.9, 22.7, 24.4, 44.5, 74.7, 87.2 (d, *J* = 96.5 Hz), 114.2 (d, *J* = 33.5 Hz), 125.5 (d, *J* = 4.7 Hz), 128.8 (d, *J* = 24.0 Hz), 129.7, 141.5 (d, *J* = 1.9 Hz), 162.7 (d, *J* = 29.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –144.5 ppm; IR (*ν*, neat) 1771, 1258, 1059 cm^{-1}; MS (EI), *m/z*: 277 (M^+), 149

(*p*-tolC(CN)FH$^+$), 101 ($C_6H_{14}O^+$); HRMS Calcd for $C_{16}H_{20}O_2FN$: 277.1478, Found: 277.1480.

(R)-CFTA ester of (R)-4-methylpentan-2-ol

Colorless oil, $[\alpha]_D^{28}$ –29.4 (*c* 0.48, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.87 (3H, d, *J* = 6.4 Hz), 0.90 (3H, d, *J* = 6.4 Hz), 1.16 (3H, d, *J* = 6.4 Hz), 1.34 (1H, m), 1.62 (1H, m), 1.66 (1H, m), 2.40 (3H, s), 5.09 (1H, m), 7.26 (2H, brd, *J* = 8.1 Hz), 7.50 (2H, brd, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.8, 21.2, 22.1, 22.8, 24.6, 44.5 74.7, 87.1 (d, *J* = 196.5 Hz), 114.2 (d, *J* = 34.5 Hz), 125.5 (d, *J* = 4.8 Hz), 128.8, 129.3 (d, *J* = 97.5 Hz), 141.5 (d, *J* = 3.9 Hz), 162.7 (d, *J* = 29.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –144.6 ppm; IR (ν, neat) 1771, 1258, 1059 cm^{-1}, MS (EI), *m/z*: 278 (M+H$^+$), 277 (M$^+$), 149 (*p*-tolC(CN)FH$^+$), 101 ($C_6H_{14}O^+$); HRMS Calcd for $C_{16}H_{20}O_2FN$: 277.1478, Found: 277.1480.

(S)-CFTA ester of (R)-2-octanol (CAS: 278181-80-9)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.87 (3H, t, *J* = 6.9 Hz), 1.17 (3H, d, *J* = 6.1 Hz), 1.20-1.30 (8H), 1.55 (1H, m), 1.65 (1H, m), 2.39 (3H, s), 5.03 (1H, qdd, *J* = 6.1, 4.4, 3.1 Hz), 7.27 (2H, brd, *J* = 8.8 Hz), 7.51 (2H, brd, *J* = 8.3 Hz).

(R)-CFTA ester of (R)-2-octanol (CAS: 278181-66-1)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.84 (3H, t, *J* = 7.3 Hz), 0.89 (1H, m), 1.01 (1H, m), 1.04-1.13 (3H), 1.13 (1H, m), 1.14-1.23 (2H, m), 1.31 (3H, d, *J* = 6.1 Hz), 1.46 (1H, qdd, *J* = 9.1, 6.8, 5.1 Hz), 1.53 (1H, ddq, *J* = 7.6, 7.6, 6.9 Hz), 2.39 (3H, s), 5.02 (1H, dqd, *J* = 7.8, 6.1, 5.1 Hz), 7.27 (2H, brd, *J* = 8.8 Hz), 7.52 (2H, brd, *J* = 8.3 Hz).

(S)-CFTA ester of (R)-2-methyl-1-phenylpropan-1-ol

Colorless glassy solid, $[\alpha]_D^{25}$ –1.4 (*c* 1.11), ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.82 (3H, d, *J* = 6.9 Hz), 1.00 (3H, d, *J* = 6.9 Hz), 2.14 (1H, dsept, *J* = 7.6, 6.9 Hz), 2.39 (3H, s), 5.52 (1H, d, *J* = 7.6 Hz), 6.98 (2H, brd, *J* = 7.6 Hz), 7.16-7.23 (5H, m), 7.38 (2H, brd, *J* = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.1, 18.5, 21.3, 33.6, 85.4, 86.9 (d, *J* = 96.1 Hz), 114.1 (d, *J* = 33.7 Hz), 125.7 (d, *J* = 5.1 Hz), 126.6, 128.22, 128.26, 129.1 (d, *J* = 23.4 Hz), 129.7, 137.4, 141.5 (d, *J* = 2.2 Hz), 162.0 (d, *J* = 30.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –143.7 ppm; IR (ν, neat) 1775, 1246, 1055 cm^{-1}; MS (ESI), *m/z*: 324 (M – 1), 348 (M + Na), 673 (2M + Na); HRMS (ESI) Calcd for $C_{20}H_{20}FNNaO_2$ (M + Na): 348.1376, Found: 348.1368.

(R)-CFTA ester of (R)-2-methyl-1-phenylpropan-1-ol

Colorless oil, $[\alpha]_D^{24}$ +47.0 (*c* 1.19, $CHCl_3$), ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.68 (3H, d, *J* = 6.9 Hz), 0.76 (3H, d, *J* = 6.6 Hz), 2.07 (1H, m), 2.40 (3H, s), 5.51 (1H, d, *J* = 7.6 Hz), 7.26-7.38 (7H), 7.53 (2H, brd, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.9, 18.4, 21.3, 85.3, 87.2 (196.9 Hz), 114.0 (d, *J* = 32.9 Hz), 125.6 (d, *J* = 5.1 Hz), 126.7, 128.43, 128.45, 128.7 (d, *J* = 24.1 Hz), 129.8, 137.7, 141.6 (d, *J* = 2.2 Hz), 162.0 (d, *J* = 30.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –144.4 ppm; IR (ν, neat) 1774, 1248, 1055 cm^{-1}; MS (ESI), *m/z*: 324 (M – 1), 348 (M + Na), 673 (2M + Na); HRMS (ESI) Calcd for $C_{20}H_{20}FNNaO_2$ (M + Na): 348.1376, Found: 348.1369.

(S)-CFTA ester of (1S,2S,5R)-menthol (CAS: 278181-87-6)

^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 0.49 (3H, d, *J* = 7.1 Hz), 0.68 (3H, d, *J* = 7.1 Hz), 0.87 (1H, m), 0.93 (3H, d, *J* = 6.6 Hz), 0.97 (1H, d, qd, *J* = 13.1, 3.3 Hz), 1.12 (q, *J* = 11.5 Hz), 1.21 (1H, qdd, *J* = 6.9, 6.9, 3.3 Hz), 1.38 (1H, dddd, *J* = 11.6, 11.6, 2.9, 2.9 Hz), 1.48 (1H, m), 1.63 (1H, m), 1.67 (brd, *J* = 15.6), 2.04 (1H, brd, *J* = 12.0 Hz), 2.40 (3H, s), 4.75 (1H, ddd, *J* = 12.0, 12.0, 4.1 Hz), 7.27 (2H, brd, *J* = 7.0 Hz), 7.51 (2H, brd, *J* = 8.1 Hz).

(R)-CFTA ester of (1S,2S,5R)-menthol (CAS: 278181-73-0)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.75 (3H, d, *J* = 6.8 Hz), 0.82 (1H, m), 0.87 (3H, d, *J* = 6.6 Hz), 0.89 (3H, d, *J* = 7.1 H), 0.92 (1H, m), 1.04 (1H, ddd, *J* = 13.9, 11.6, 3.9 Hz), 1.45 (1H, m), 1.47 (1H, dddd, *J* = 11.3, 11.3, 3.2, 3.2 Hz), 1.67 (1H, m), 1.69 (1H, dq, *J* = 13.9, 3.6 Hz), 1.84 (1H, m), 1.87 (1H. dddd, *J* = 8.1, 7.1, 7.1, 2.9 H), 2.40 (3H, brs), 4.82 (1H, td, *J* = 11.0, 4.4 Hz), 7.28 (2H, brd, *J* = 7.7 Hz), 7.50 (2H, brd, *J* = 7.7 Hz).

(S)-CFTA ester of (1S,2R,5R)-isomenthol (CAS: 278181-86-5)

^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 0.84 (3H, d, *J* = 6.8 Hz), 0.86 (3H, d, *J* = 6.8 Hz), 0.94 (3H, d, *J* = 6.7 Hz), 1.17 (1H, dddd, *J* = 12.8, 7.7, 6.8, 3.6 Hz), 1.38 (1H, ddd, *J* = 13.7, 8.6, 3.2 Hz), 1.42-1.53 (3H), 1.53 (1H, m), 1.64 (1H, m), 1.72 (1H, dsept, *J* = 7.1, 7.1 Hz), 2.40 (3H, s), 4.82 (1H, ddd, *J* = 6.2, 6.2, 3.4 Hz), 7.27 (2H, brd, *J* = 8.9 Hz), 7.52 (2H, brd, *J* = 8.3 Hz).

(R)-CFTA ester of (1S,2R,5R)-isomenthol (CAS: 278181-72-9)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.73 (3H, d, *J* = 6.6 Hz), 0.83 (3H, d, *J* = 6.6 Hz), 0.92 (3H, d, *J* = 7.1 Hz), 1.18 (1H, m), 1.25 (1H, m), 1.42 (1H, m), 1.41 (2H, m), 1.46 (1H, dd, *J* = 14.1, 7.1), 1.52 (1H, ddd, *J* = 13.2, 8.5, 3.5 Hz), 1.71 (1H, ddd, *J* = 13.3, 6.6, 4.7 Hz), 1.88 (1H, m), 2.40 (3H, s), 5.14 (1H, ddd, *J* = 6.6, 6.6, 3.5 Hz), 7.28 (2H, brd, *J* = 8.6 Hz), 7.52 (2H, brd, *J* = 7.8 Hz).

(S)-CFTA ester of (1S,2S,5R)-neomenthol (CAS: 278181-85-4)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.67 (3H, d, *J* = 6.1 Hz), 0.86 (3H, d, *J* = 6.8 Hz), 0.89 (3H, d, *J* = 6.6 Hz), 0.93-1.05 (3H), 1.24 (1H, dd, *J* = 13.2, 3.7 Hz), 1.26 (1H, td, *J* = 13.2, 3.7 Hz), 1.46 (1H, ddq, *J* = 10.0, 10.0, 6.6 Hz), 1.64 (1H, brd, *J* = 6.2 Hz), 1.68-1.80 (2H), 2.40 (3H, s), 5.32 (1H, brs), 7.27 (2H, brd, *J* = 8.1 Hz), 7.50 (2H, brd, *J* = 8.1 Hz).

(R)-CFTA ester of (1S,2S,5R)-neomenthol (CAS: 278181-71-8)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.53 (3H, d, *J* = 6.6 Hz), 0.71 (3H, d, *J* = 6.8 Hz), 0.83 (1H, m), 0.87 (3H, d, *J* = 6.4 Hz), 0.92 (1H, brd, *J* = 10.4 Hz), 0.93 (1H, m), 1.10 (1H, ddd, *J* = 14.4, 12.5, 2.2 Hz), 1.24 (1H, dddd, *J* = 13.3, 12.5, 12.5, 3.4 Hz), 1.65 (1H, m), 1.69 (1H, m), 1.76 (1H, m), 2.05 (1H, dddd, *J* = 14.6, 5.8, 5.8, 2.4 Hz), 2.40 (3H, brs), 5.25 (1H, brd, *J* = 1.8 Hz), 7.27 (2H, brd, *J* = 7.9 Hz), 7.51 (2H, brd, *J* = 7.6 Hz).

(S)-CFTA ester of (1R,2R)-exo-borneol

Colorless oil, $[\alpha]_D^{27}$ –55.6 (*c* 1.30, $CHCl_3$), ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm), 0.52 (3H, s), 0.79 (3H, s), 0.91 (3H, s), 1.07 (1H, ddd, *J* = Hz), 1.08 (1H, ddd, *J* = Hz), 1.52 (1H, dd, *J* = Hz), 1.68 (1H, m), 1.77 (1H, dd, *J* = Hz), 1.83 (1H, dd, *J* = Hz), 1.87 (1H, dq, *J* = Hz), 2.40 (3H, s), 4.77 (1H, dd, *J* = Hz), 7.28 (1H, brd, *J* = Hz), 7.50 (2H, brd, *J* = Hz), ^{13}C NMR (376 MHz, $CDCl_3$) δ 10.8, 19.6, 19.9, 21.3, 26.8, 33.3, 38.1, 44.9, 47.0, 49.2, 84.2, 87.2 (d, *J* = 196.5 Hz), 114.1 (d, *J* = 32.6 Hz), 125.4 (d, *J* = 4.8 Hz), 128.8 (d, *J* = 23.9 Hz), 129.7, 141.5, (d, *J* = 2.9 Hz), 162.6 (d, *J* = 30.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -146.0 ppm, IR (*ν*, neat) 177.1, 1250, 1059 cm^{-1}; MS (EI), *m/z*: 329 (m^+), 314 (M – Me^+), 148 (*p*-tolC(CN)F^+), 138 (M – CFTA-O^+); HRMS Calcd for $C_{20}H_{24}O_2FN$: 329.1791, Found: 329.1796.

(R)-CFTA ester of (1R,2R)-exo-borneol

Colorless oil, $[\alpha]_D^{27}$ –37.9 (*c* 1.55, $CHCl_3$), ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.81 (3H, s), 0.82 (3H, s), 0.89 (3H, s),

1.04 (1H, m), 1.13 (1H, dd, *J* = 14.0, 3.4 Hz), 1.54 (1H, ddd, *J* = Hz), 1.58 (1H, ddd, *J* = Hz), 1.66 (1H, m), 1.71 (1H, m), 1.73 (1H, m), 2.39 (3H, s), 4.78 (1H, dd, *J* = Hz), 7.26 (1H, brd, *J* = Hz), 7.48 (2H, brd, *J* = Hz)), ^{13}C NMR (376 MHz, $CDCl_3$) δ 11.2, 19.5, 19.9, 21.3, 26.8, 33.3, 38.0, 44.8, 47.0, 49.3, 85.3, 87.1, (d, *J* = 196.4 Hz), 114.1 (d, *J* = 33.5 Hz), 125.4 (d, *J* = 3.7 Hz), 128.6 (d, *J* = 24.0 Hz), 129.8, 141.5, 162.6 (d, *J* = 20.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -145.5 ppm, IR (*ν*, neat) 1771, 1250, 1059 cm^{-1}; MS (EI), *m*/*z*: 329 (M^+), 314 (M – Me^+), 149 (*p*-tolC(CN)FH^+), 138 (M – CFTA-O^+); HRMS Calcd for $C_{20}H_{24}O_2FN$: 329.1791, Found: 329.1794.

(S)-CFTA ester of (1S,2R)-endo-borneol (CAS: 278181-84-3)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 0.66 (3H, s), 0.85 (3H, s), 0.86 (1H, m), 0.87 (3H, s), 1.09 (1H, dd, *J* = 14.0, 3.4 Hz), 1.24 (1H, m), 1.26 (1H, m), 1.72 (1H, m), 1.77 (1H, m), 2.38 (1H, m), 2.40 (3H, s), 4.98 (1H, ddd, *J* = 10.0, 3.4, 2.0 Hz), 7.28 (1H, brd, *J* = 8.6 Hz), 7.54 (2H, brd, *J* = 7.8 Hz).

(R)-CFTA ester of (1S,2R)-endo-borneol (CAS: 278181-70-7)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm), 0.77 (1H, dd, *J* = 13.9, 3.2 Hz), 0.87 (6H, brs), 0.88 (3H, s), 1.05 (1H, ddd, *J* = 12.5, 9.5, 4.4 Hz), 1.34 (1H, m), 1.66 (1H, dd, *J* = 5.0, 4.4 Hz), 1.72 (1H, ddddd, *J* = 12.2, 12.2, 3.9, 3.9, 3.9 Hz), 1.86 (1H, ddd, *J* = 13.4, 9.5, 4.4 Hz), 2.29 (1H, dddd, *J* = 9.9, 9.9, 4.3, 3.9 Hz), 2.40 (3H, s), 5.03 (1H, ddd, *J* = 9.8, 2.5, 2.5 Hz), 7.29 (2H, brd, *J* = 8.1 Hz), 7.52 (2H, brd, *J* = 8.3 Hz).

(S)-CFTA ester of 3β-chorestanol

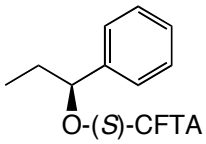
Colorless micro-crystals; mp = 95-97 °C (EtOH); $[\alpha]_D^{24}$ +1.7 (*c* 1.25, $CHCl_3$); ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 0.62 (1H, ddd, *J* = 12.9, 11.0, 4.0 Hz), 0.64 (3H, s), 0.81 (3H, s), 0.85 (1H, m), 0.856 (3H, d, *J* = 6.9 Hz), 0.863 (3H, d, *J* = 6.9 Hz), 0.89 (3H, d, *J* = 6.5 Hz), 0.94-1.03 (5H), 1.04-1.20 (6H), 1.21-1.38 (7H), 1.44 (1H, m), 1.45-1.57 (4H), 1.65 (1H), 1.66 (1H), 1.70 (1H), 1.71 (1H), 1.80 (1H, m), 1.95 (1H, ddd, *J* = 12.8, 4.0, 3.0 Hz), 2.40 (3H, s), 4.84 (1H, dddd, *J* = 11.6, 11.6, 4.7, 4.7 Hz), 7.27 (2H, brd, *J* = 8.6 Hz), 7.50 (2H, brd, *J* = 8.0 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 12.6, 12.2, 18.7, 21.2, 21.3, 22.6, 22.8, 23.8, 24.2, 26.9, 28.1, 28.2, 28.5, 31.9, 33.4, 35.39, 35.42, 35.8, 36.2, 36.5, 39.5, 39.9, 42.6, 44.6, 54.1, 56.3, 56.4, 78.5, 87.3 (d, *J* = 196.5 Hz), 114.2 (d, *J* = 33.0 Hz), 125.5 (d, *J* = 4.3 Hz), 128.8 (d, *J* = 23.6 Hz), 129.8, 141.5, 162.6 (d, *J* = 30.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –144.2 ppm; HRMS (EI) Calcd for $C_{37}H_{54}O_2FN$: 563.4139, Found: 563.4138.

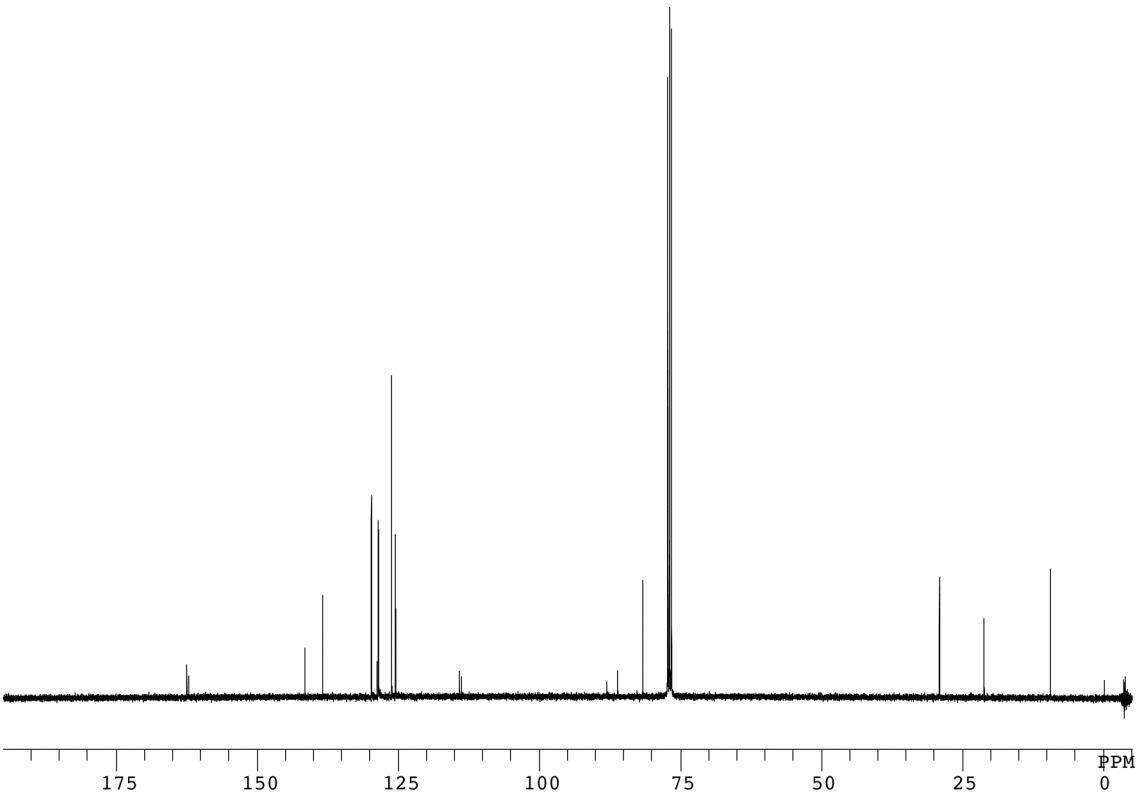
(R)-CFTA ester of 3β-chorestanol

Colorless micro-crystals; mp = 113-114 °C (EtOH); $[\alpha]_D^{24}$ +20.4 (*c* 1.34, $CHCl_3$); ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 0.63 (1H, ddd, *J* = 12.9, 11.6, 4.2 Hz), 0.64 (3H, s), 0.857 (3H, d, *J* = 6.8 Hz), 0.861 (3H, d, *J* = 6.8 Hz), 0.89 (3H, d, *J* = 6.7 Hz), 0.97 (1H, m), 0.99 (2H), 1.05-1.15 (6H), 1.45 (1H), 1.51 (1H), 1.53 (2H), 1.60 (1H, brd, *J* = 12.9), 1.64 (1H, dddd, *J* = 11.1, 11.1, 3.6, 3.6 Hz), 1.76 (1H, ddd, *J* = 13.4, 3.7, 3.7 Hz), 1.80 (1H, m), 1.88 (1H, brd, *J* = 12.9), 1.96 (1H, ddd, *J* = 12.7, 3.3, 3.3 Hz), 2.40 (3H, s), 4.84 (1H, dddd, *J* = 11.4, 11.4, 4.8, 4.8 Hz), 7.27 (2H, brd, *J* = 7.8Hz), 7.50 (2H, brd, *J* = 8.0 Hz), ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 12.0, 12.2, 18.6, 21.2, 21.3, 22.5, 22.8, 23.8, 24.2, 27.0, 28.0, 28.2, 28.5, 31.9, 33.3, 35.37, 35.39, 35.8, 36.2, 36.5, 39.5, 39.9, 42.6, 44.6, 54.1, 56.2, 56.3, 78.5, 87.1 (d, *J* = 195.0 Hz), 114.2 (d, *J* = 33.0 Hz), 125.5 (d, *J* = 4.3 Hz), 128.8 (d, *J* = 22.9 Hz), 129.8, 141.5, 162.6 (d, *J* = 30.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -144.2 ppm; HRMS (EI) Calcd for $C_{37}H_{54}O_2FN$: 563.4139, Found: 563.4153.

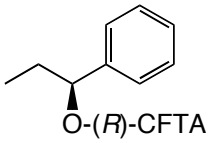
S-2. ^{1}H and ^{13}C NMR Spectra of New Compounds

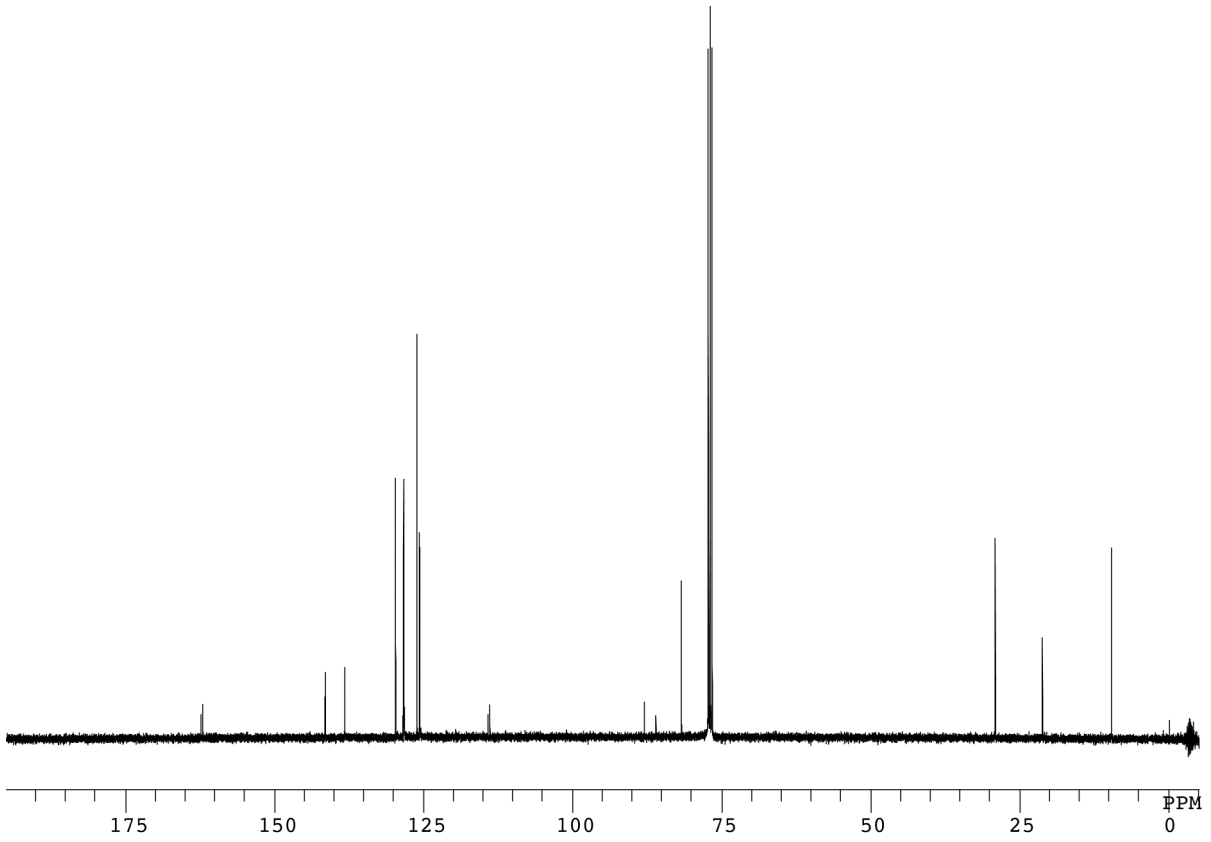
(S)-CFTA ester of (S)-1-phenylpropan-1-ol



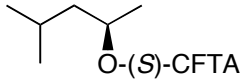


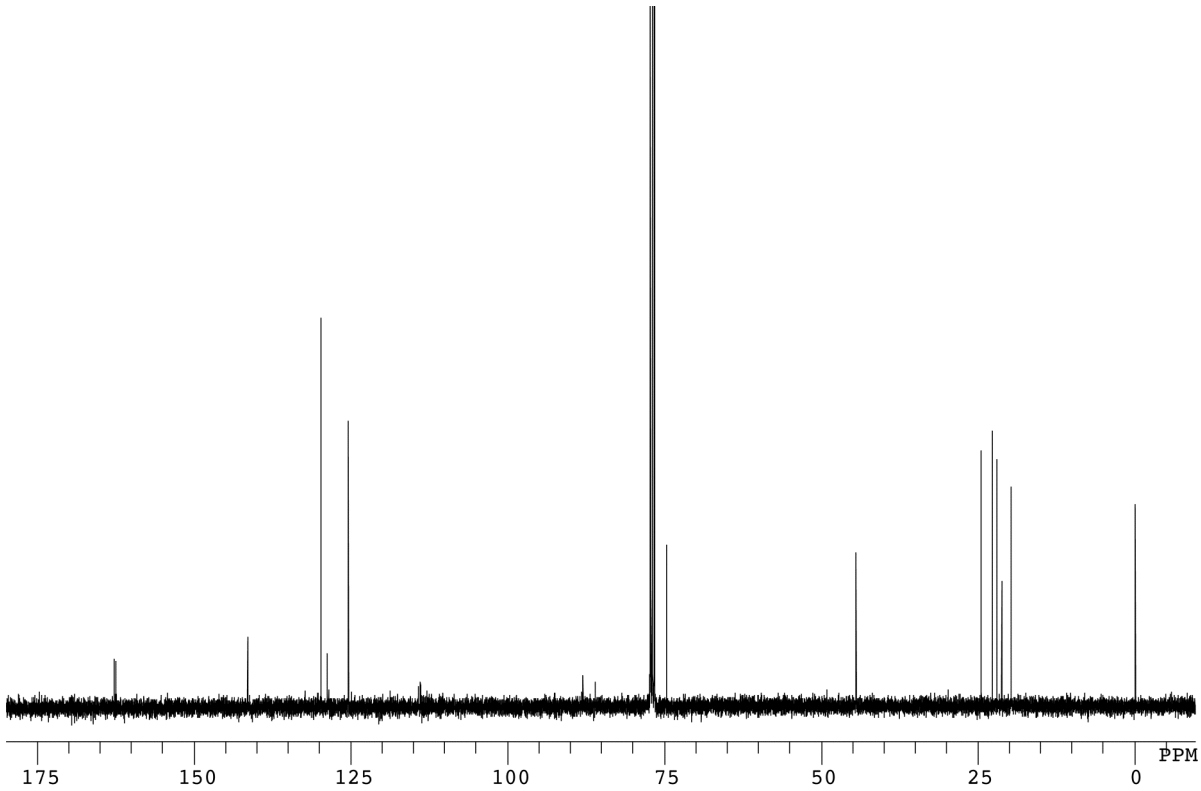
(R)-CFTA ester of (S)-1-phenylpropan-1-ol



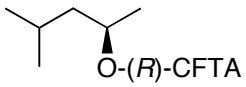


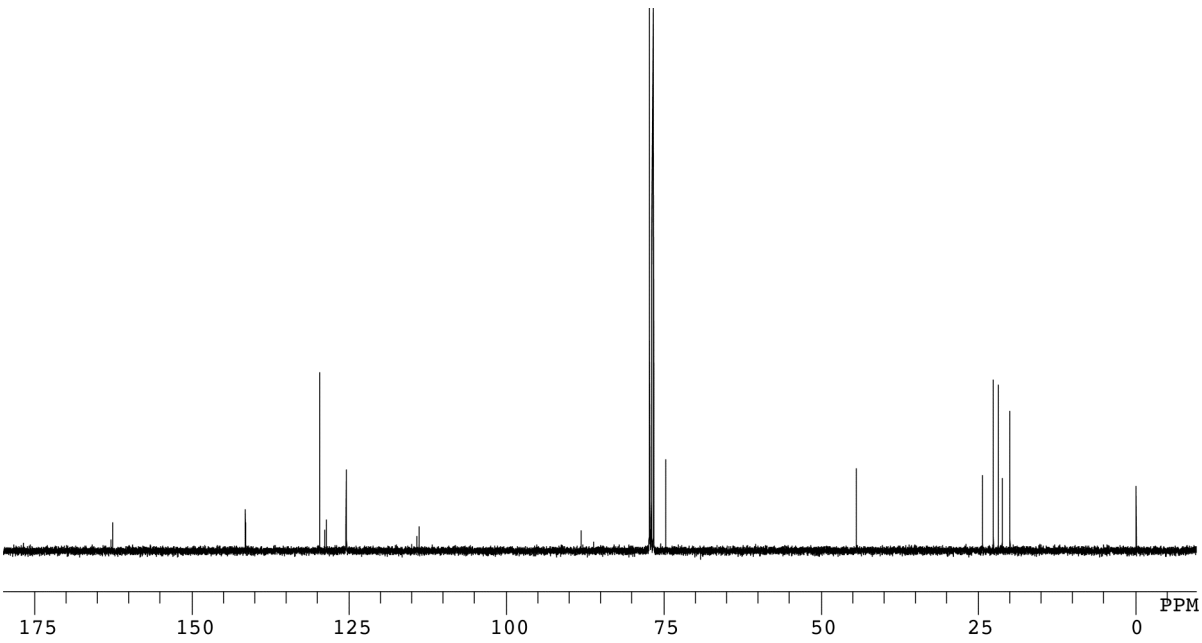
(S)-CFTA ester of (R)-4-methylpentan-2-ol



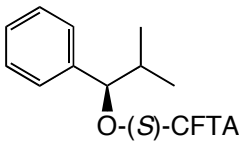


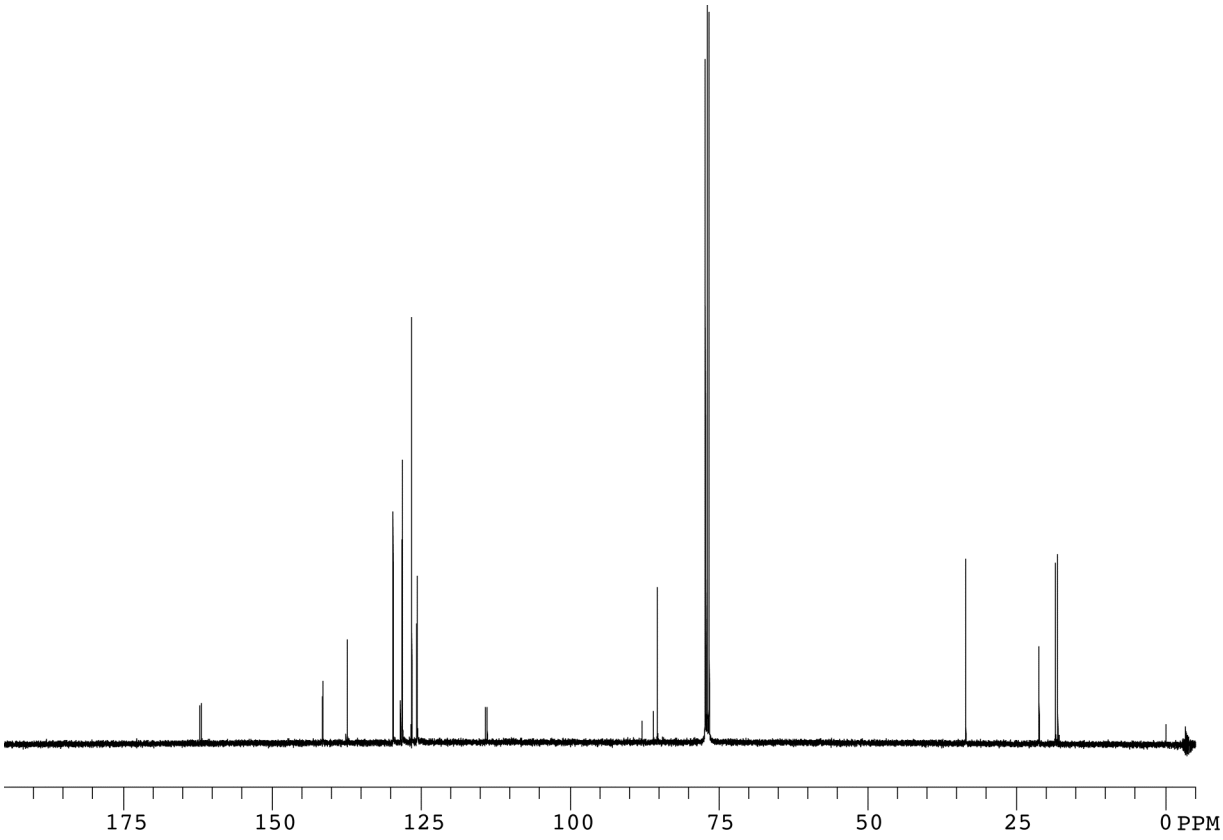
(R)-CFTA ester of (R)-4-methylpentan-2-ol



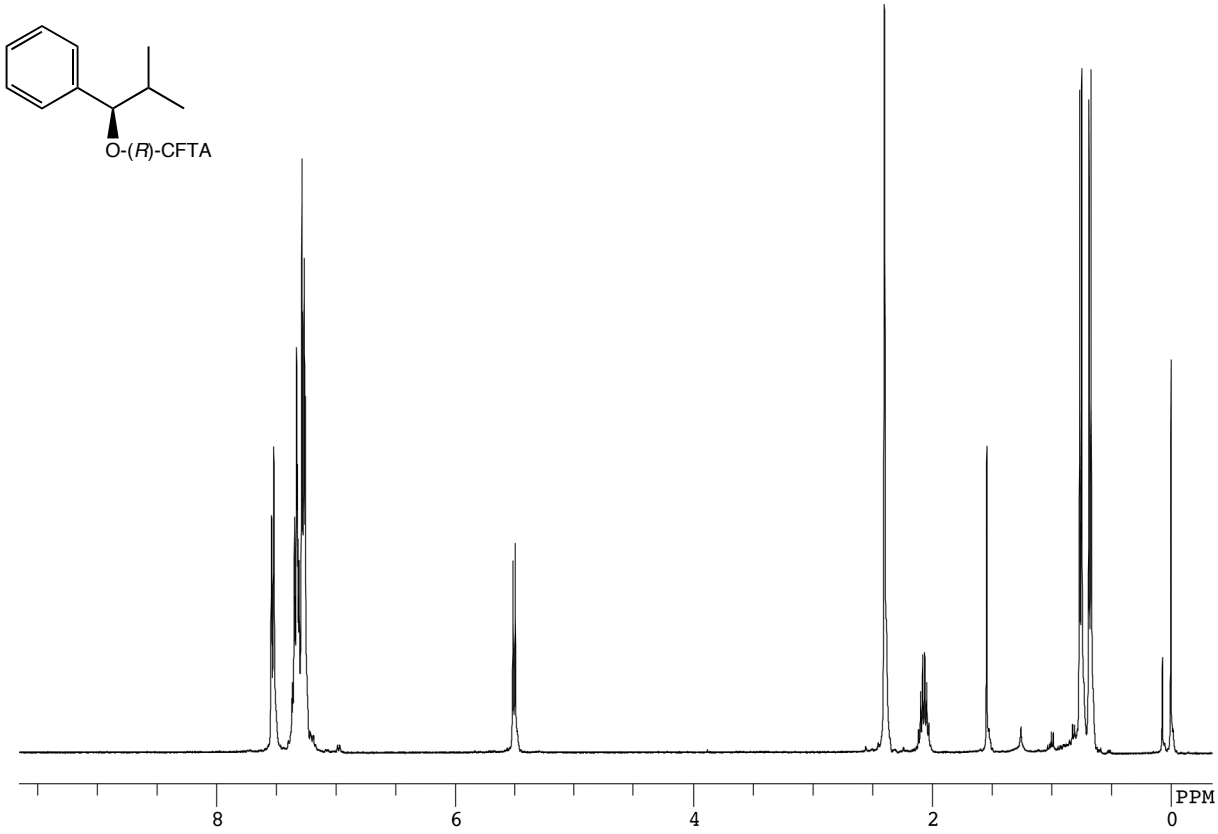


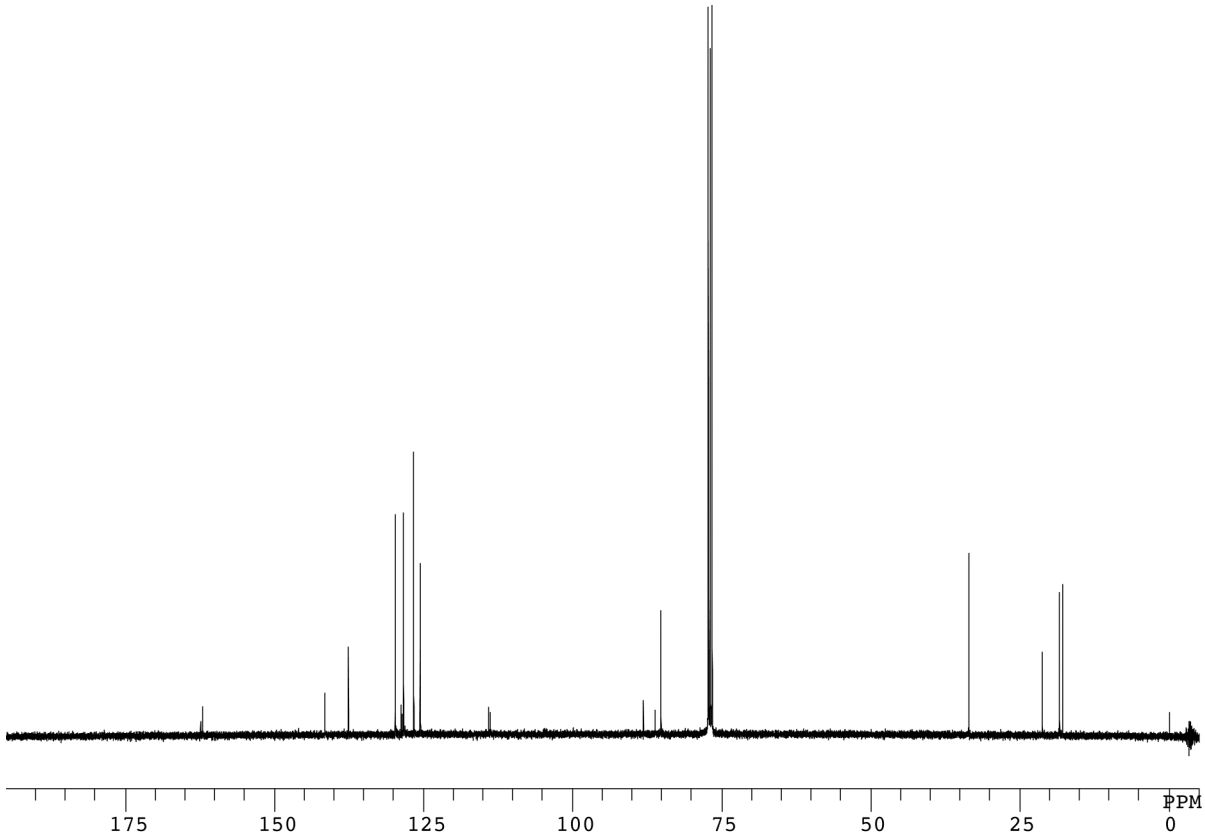
(S)-CFTA ester of (R)-2-methyl-1-phenylpropanol



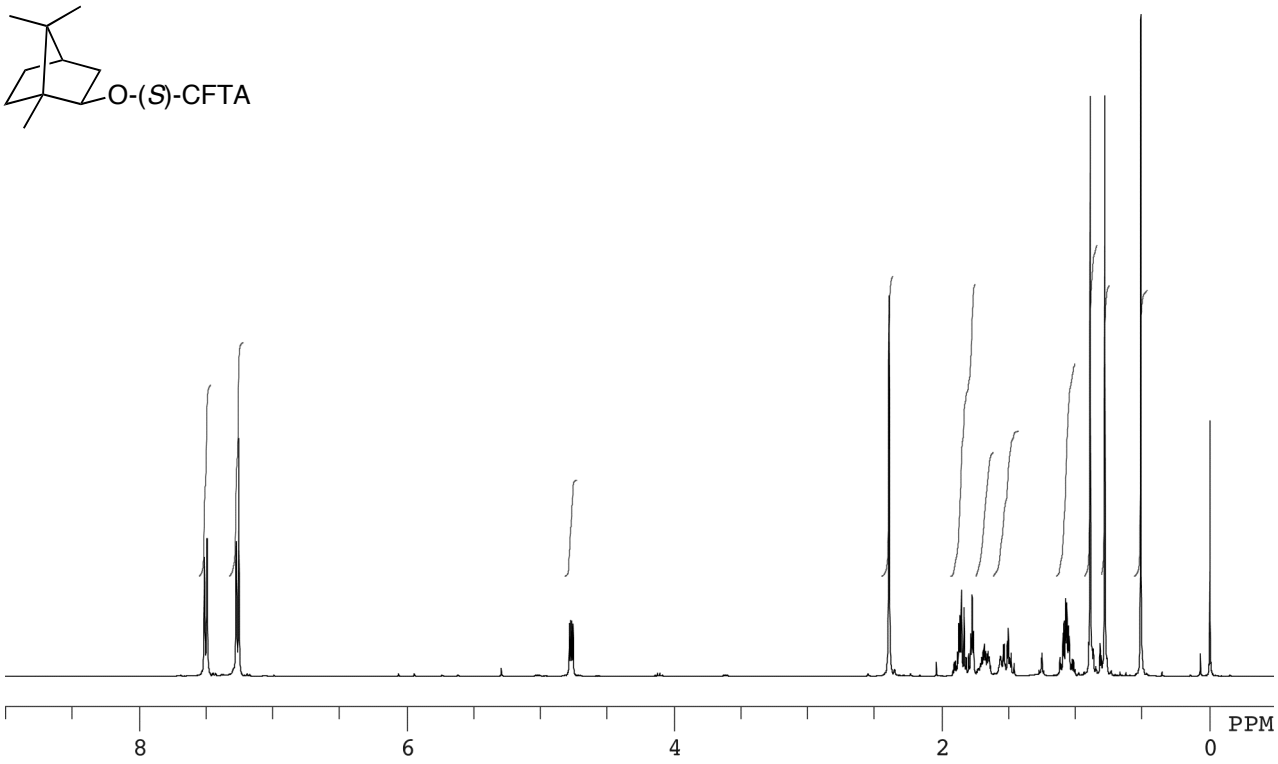


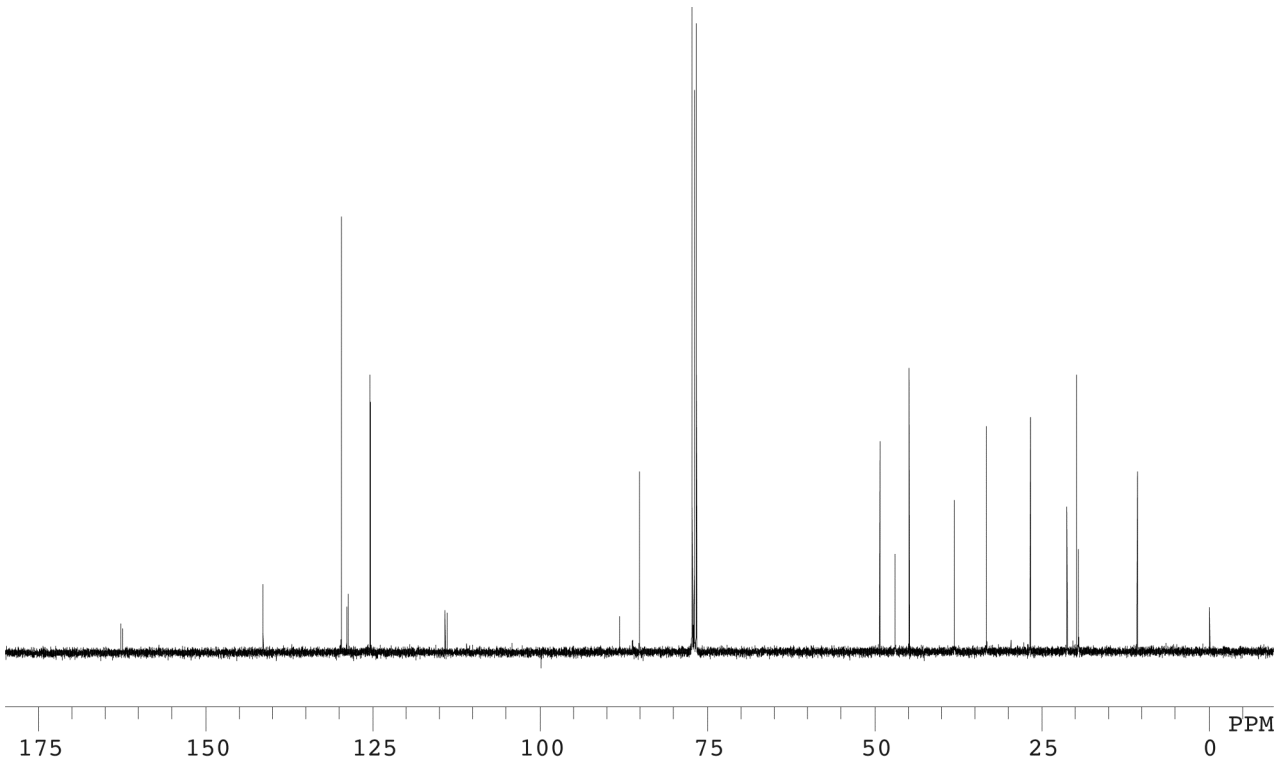
(R)-CFTA ester of (R)-2-methyl-1-phenylpropanol



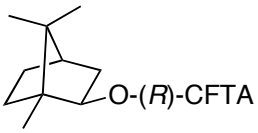


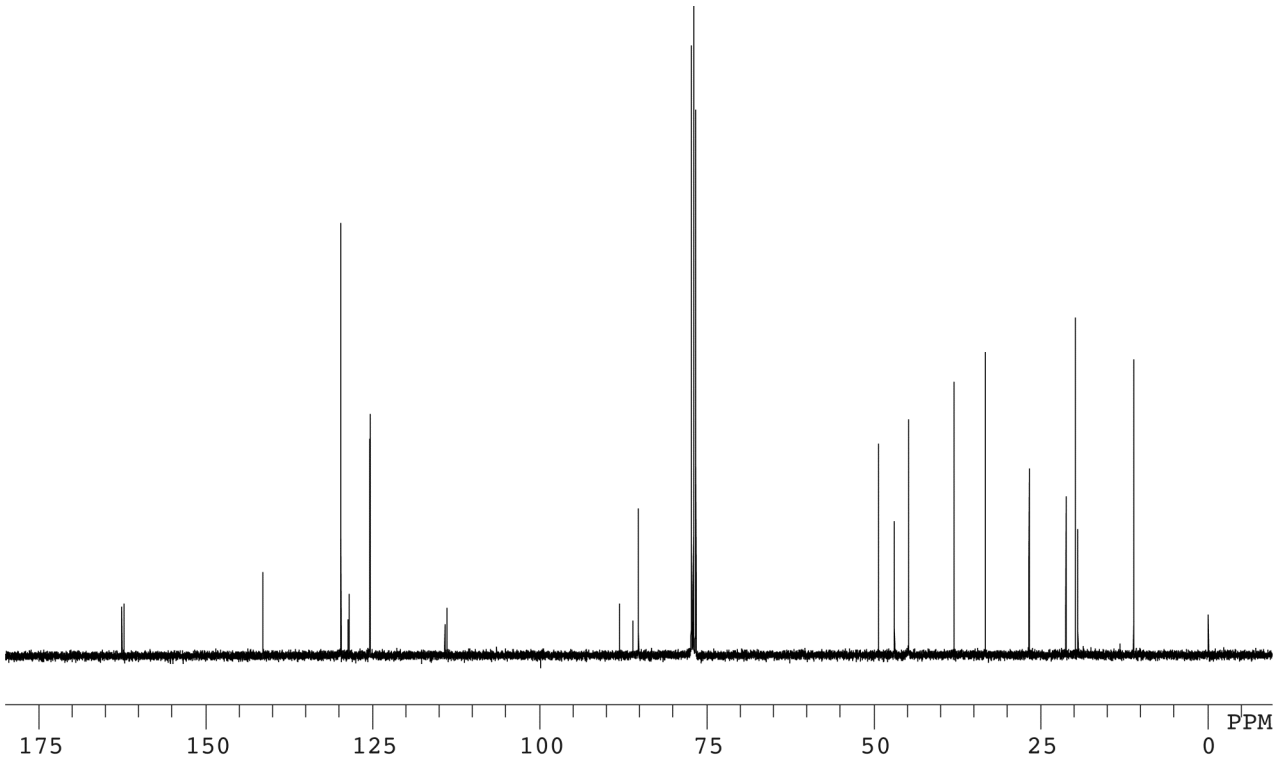
(S)-CFTA ester of (1R,2R)-exo-borneol



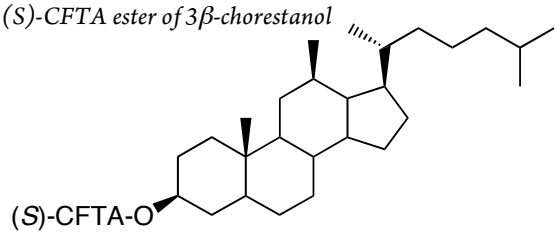


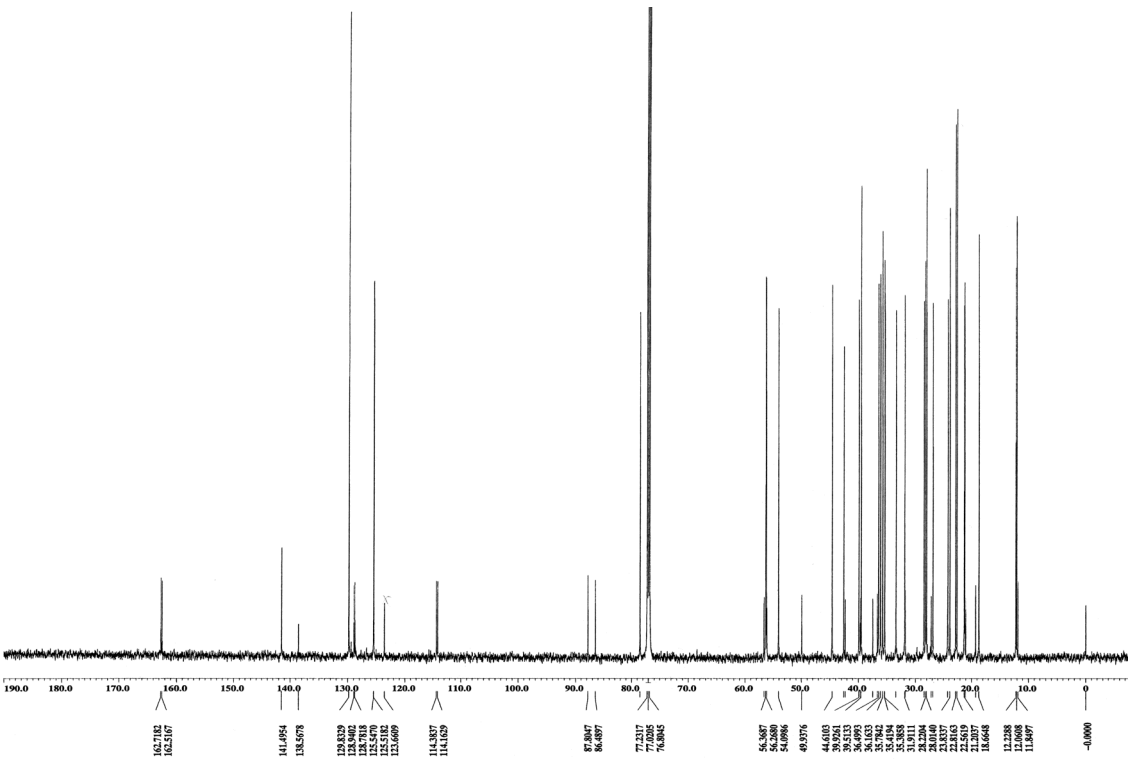
(R)-CFTA ester of (1R,2R)-exo-borneol



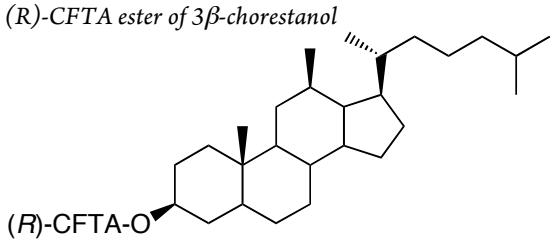


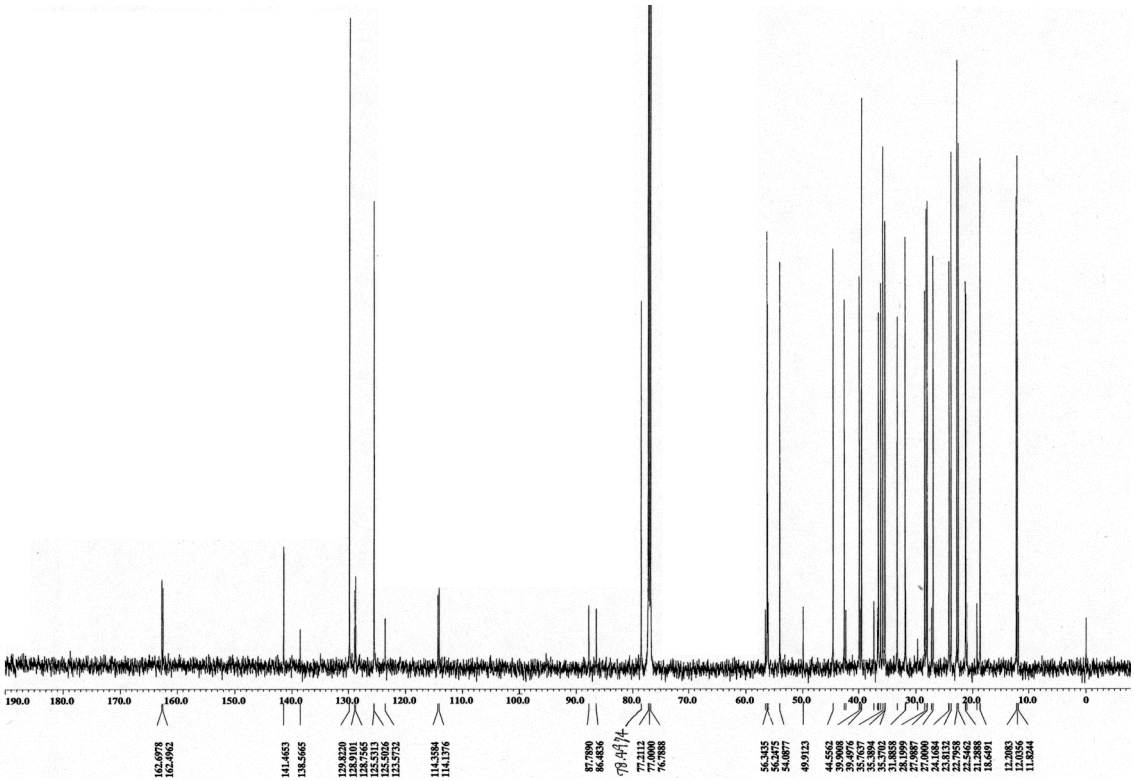
(S)-CFTA ester of 3β-chorestanol





(R)-CFTA ester of 3β-chorestanol





S-3. Structures of the CFTA esters examined and their ^{1}H chemical shift difference values

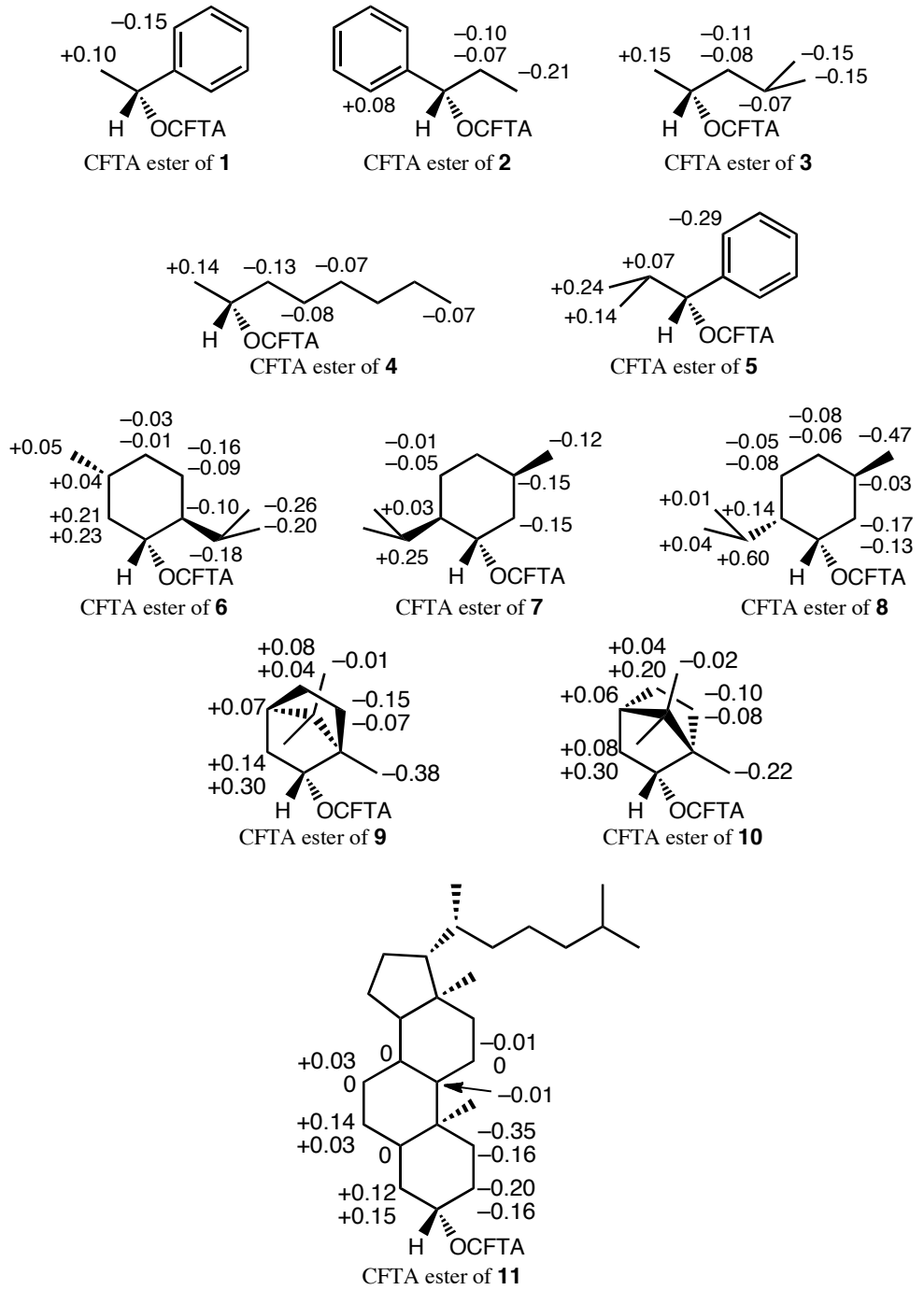
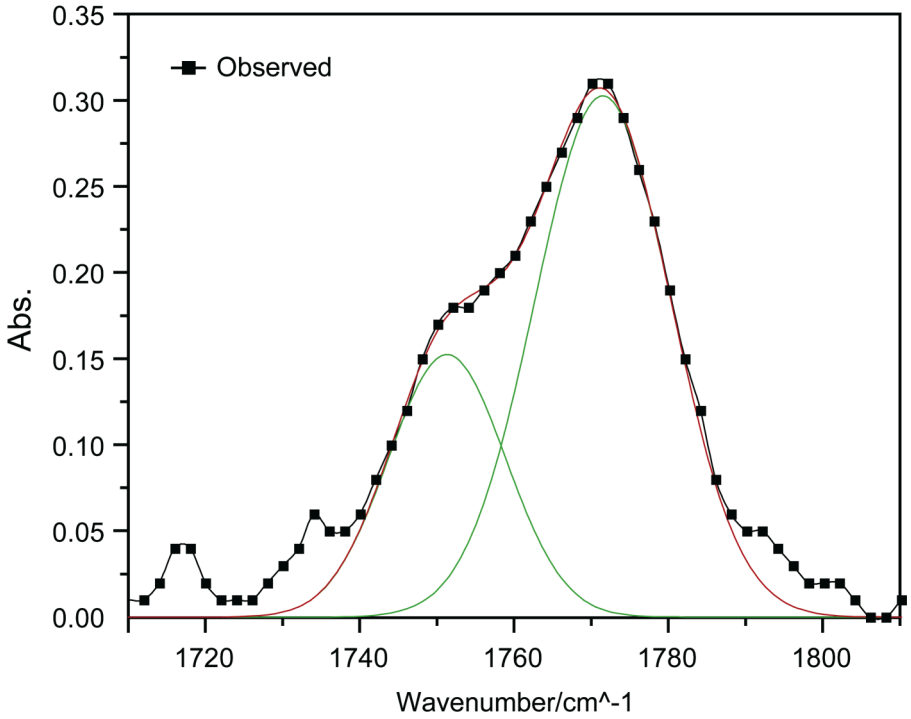


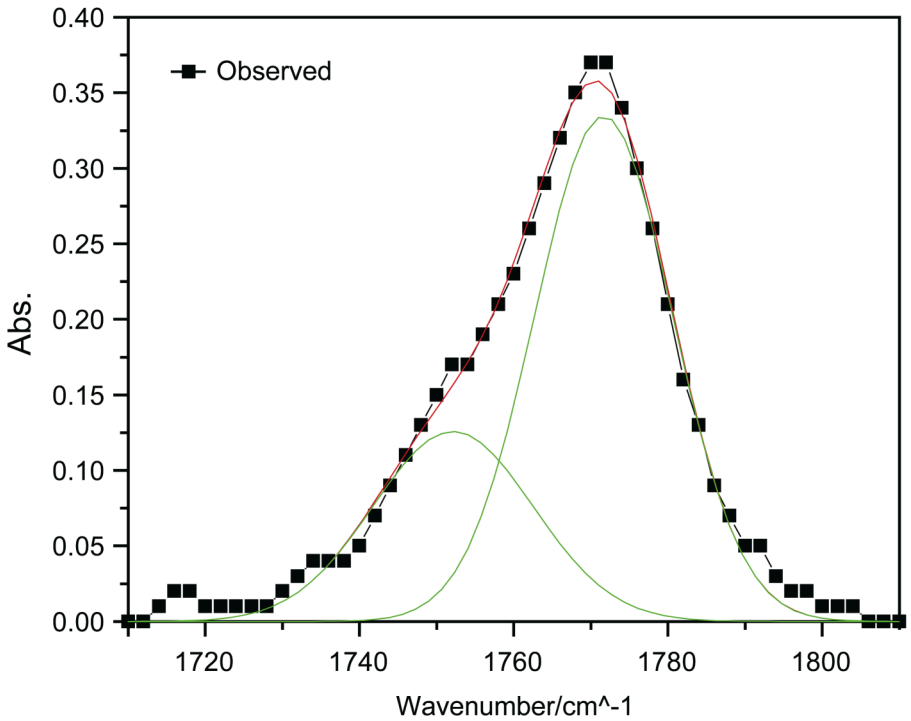
Figure S1. Chemical shift differences ($\Delta\delta = \delta_{S\text{-CFTAester}} - \delta_{R\text{-CFTAester}}$) observed for the CFTA esters of chiral secondary alcohols **1**–**11** used in the IR study.

S-4. IR measurement and curve-fitting. Each solution used for the IR measurement was prepared by dissolving the CFTA esters of **1**-**11** in chloroform (0.1 M). IR spectra were recorded on a Shimadzu FTIR-8100M using a liquid cell (thickness: 0.1 mm, KBr window) at room temperature. Deconvolution of the carbonyl absorption signals were carried out by using the Origin 7 program with Gauss function.

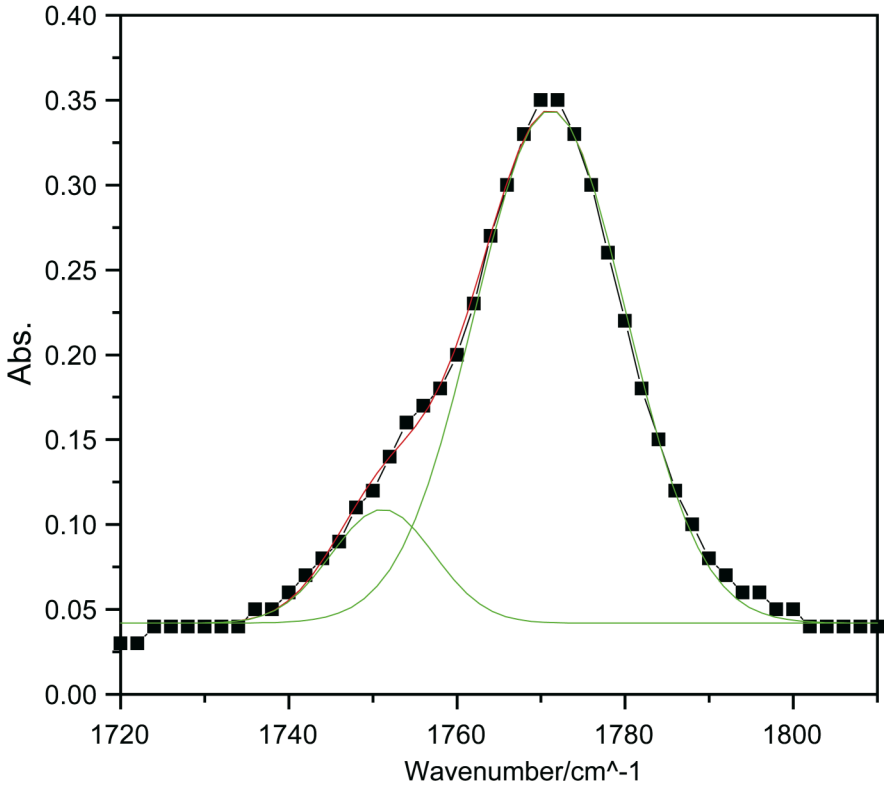
(*S*)-CFTA ester of **1**



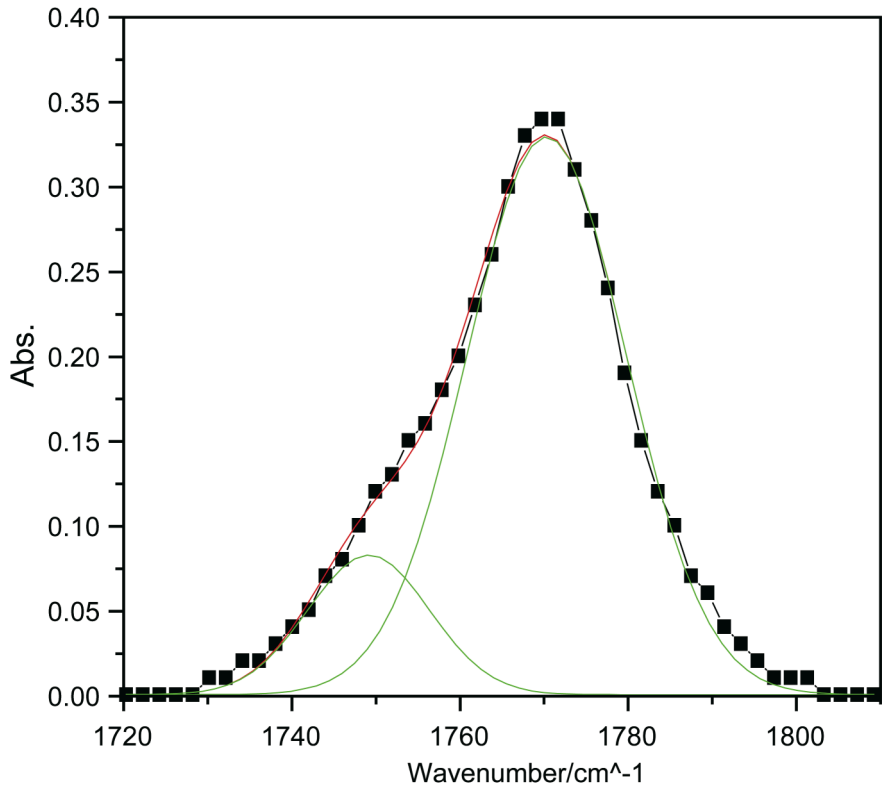
(*R*)-CFTA ester of **1**



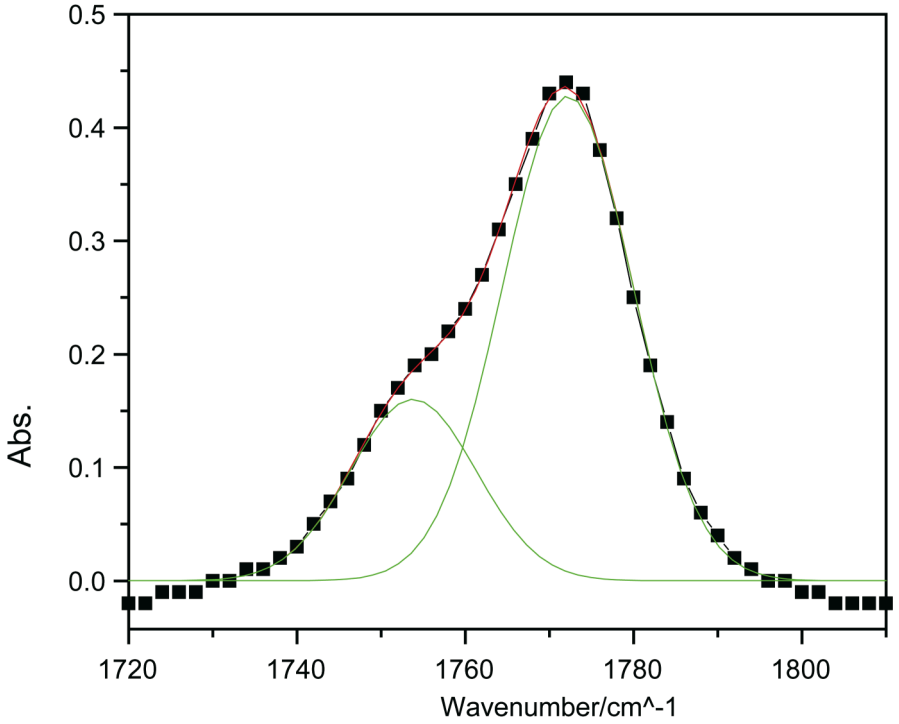
(*S*)-CFTA ester of **2**



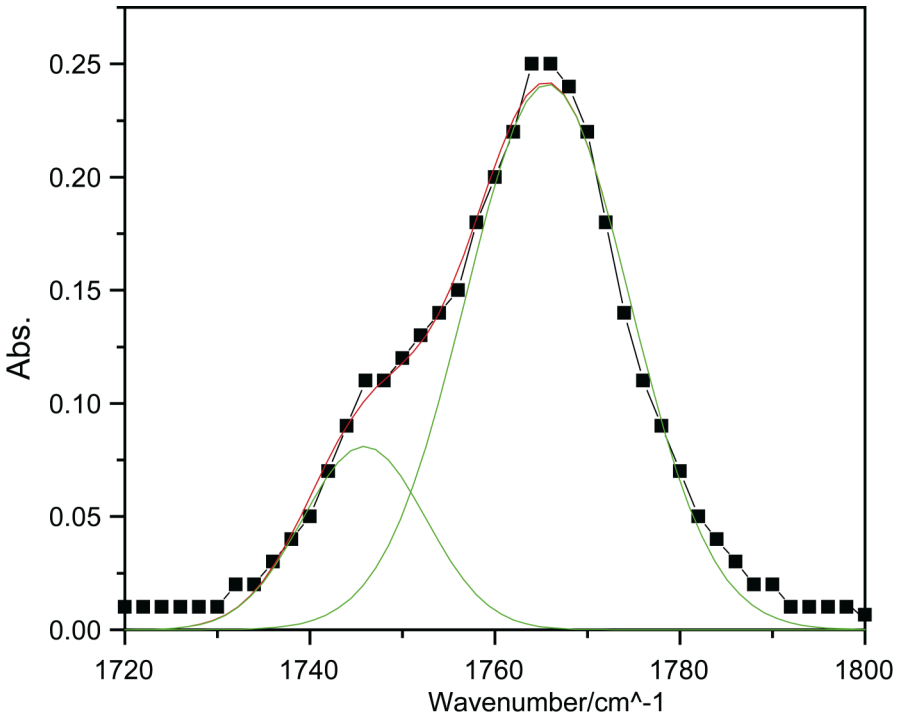
(*R*)-CFTA ester of **2**



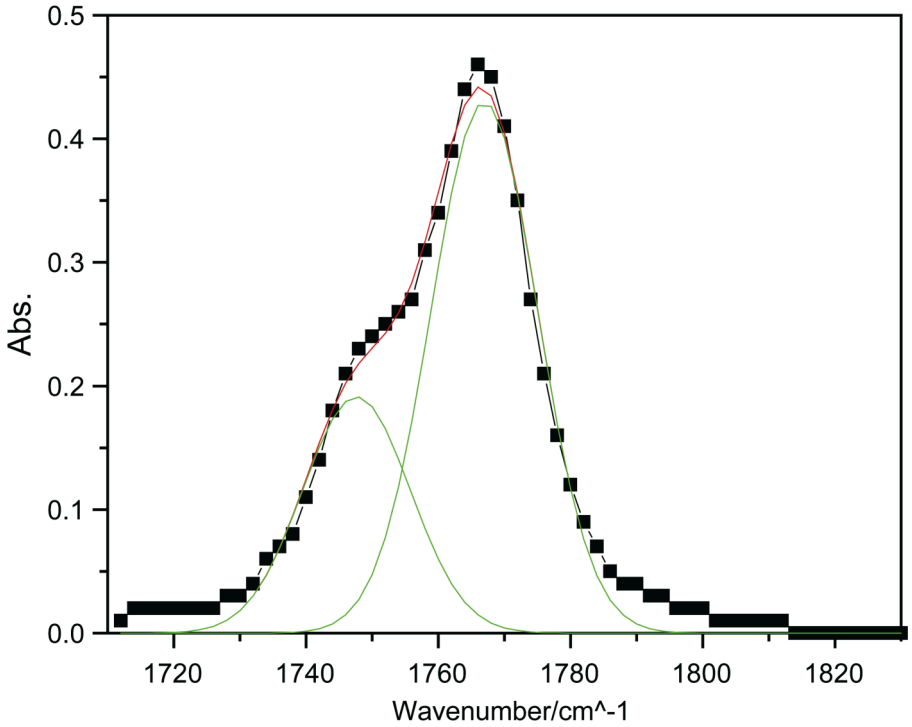
(*S*)-CFTA ester of **3**



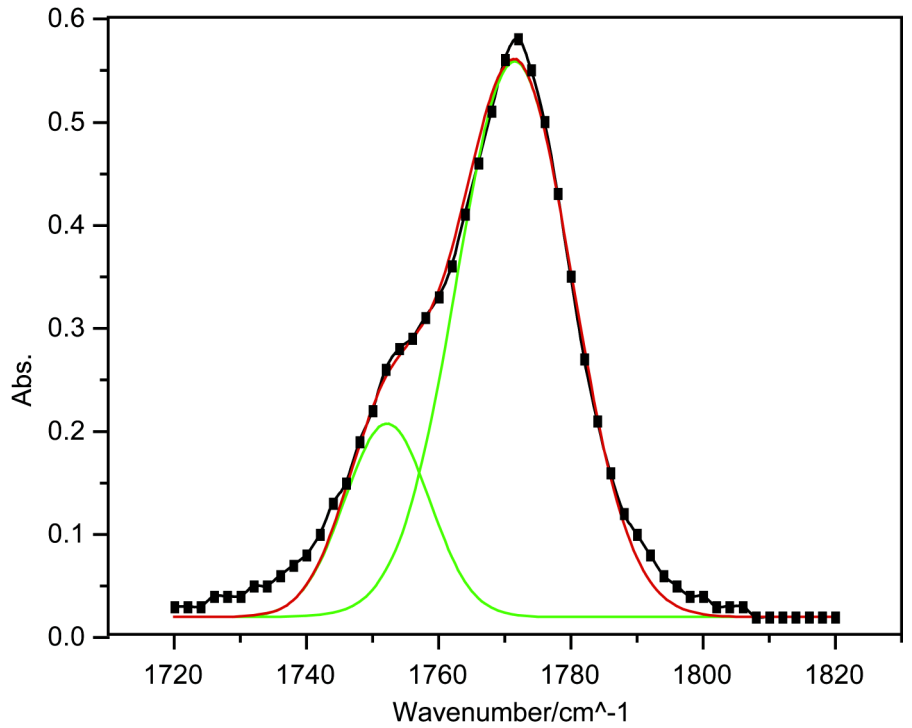
(*R*)-CFTA ester of **3**



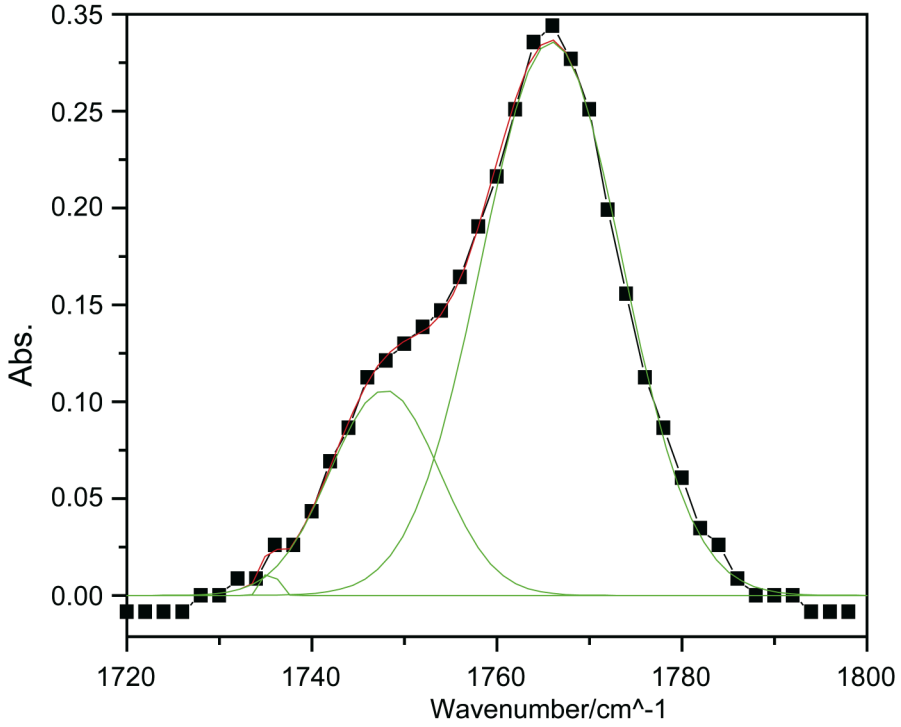
(*S*)-CFTA ester of **4**



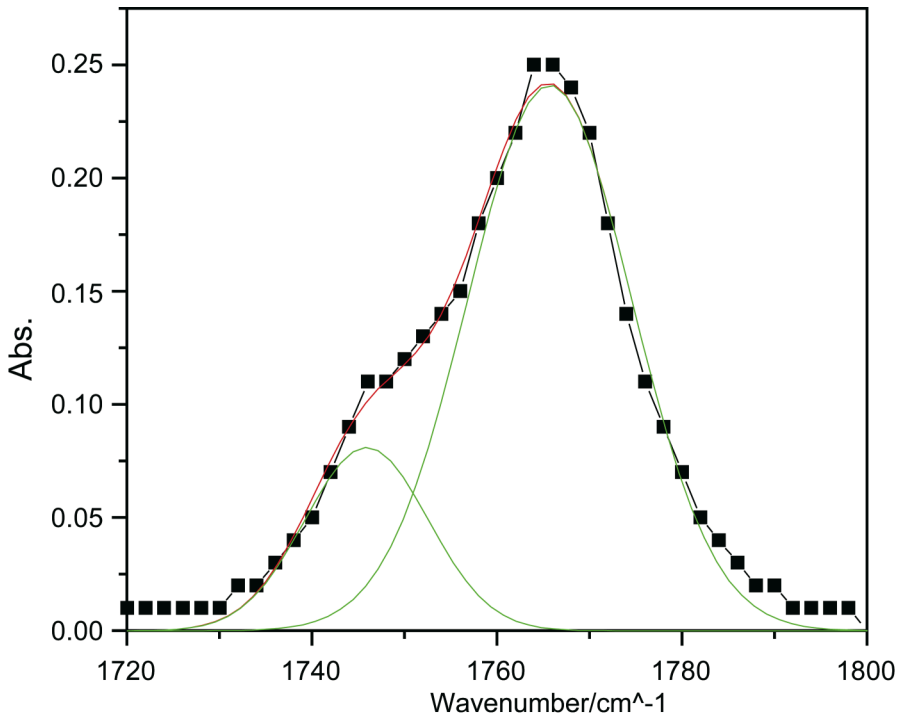
(*R*)-CFTA ester of **4**



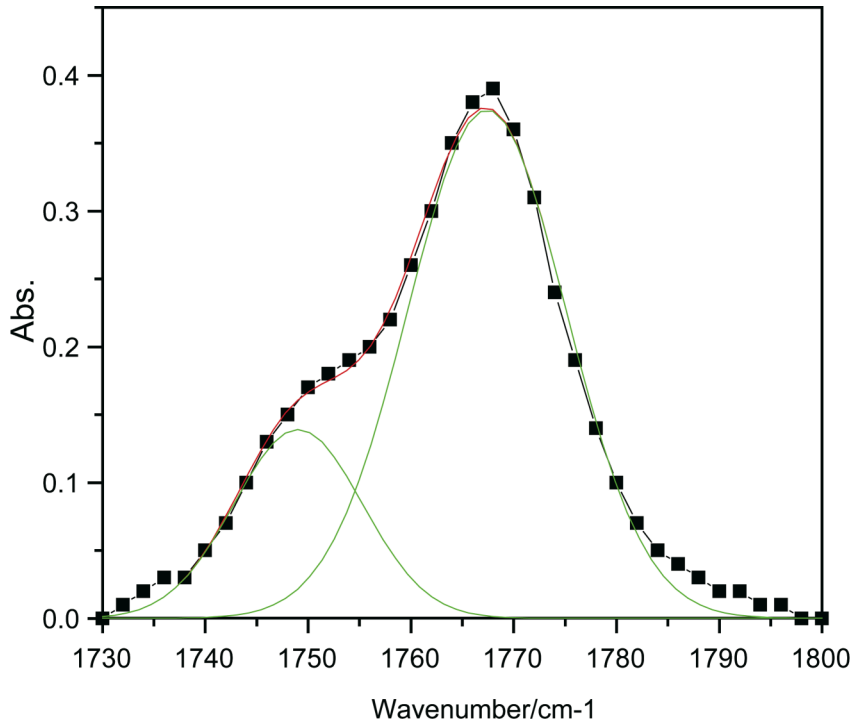
(*S*)-CFTA ester of **5**



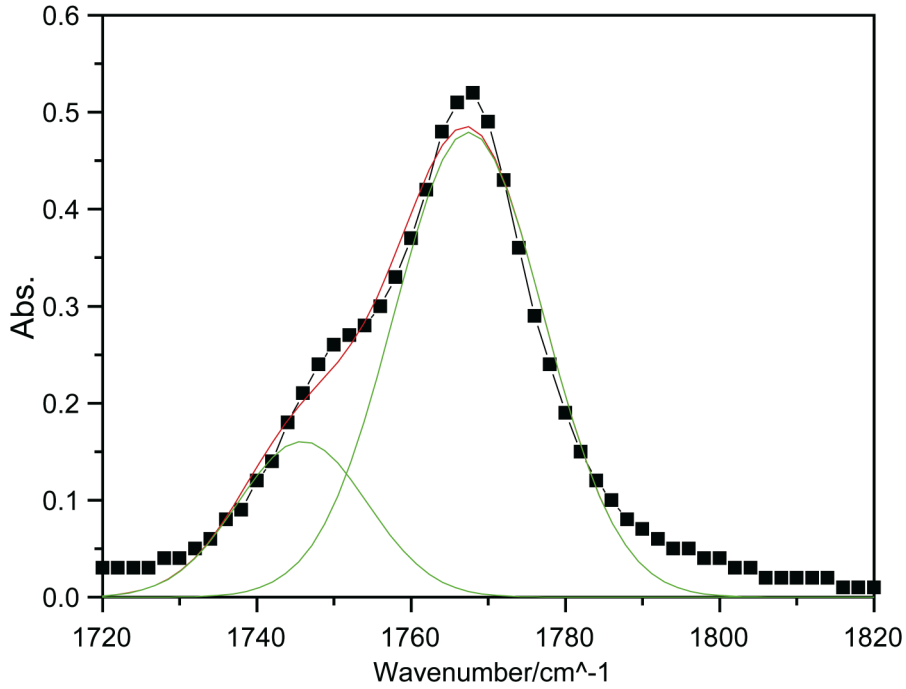
(*R*)-CFTA ester of **5**



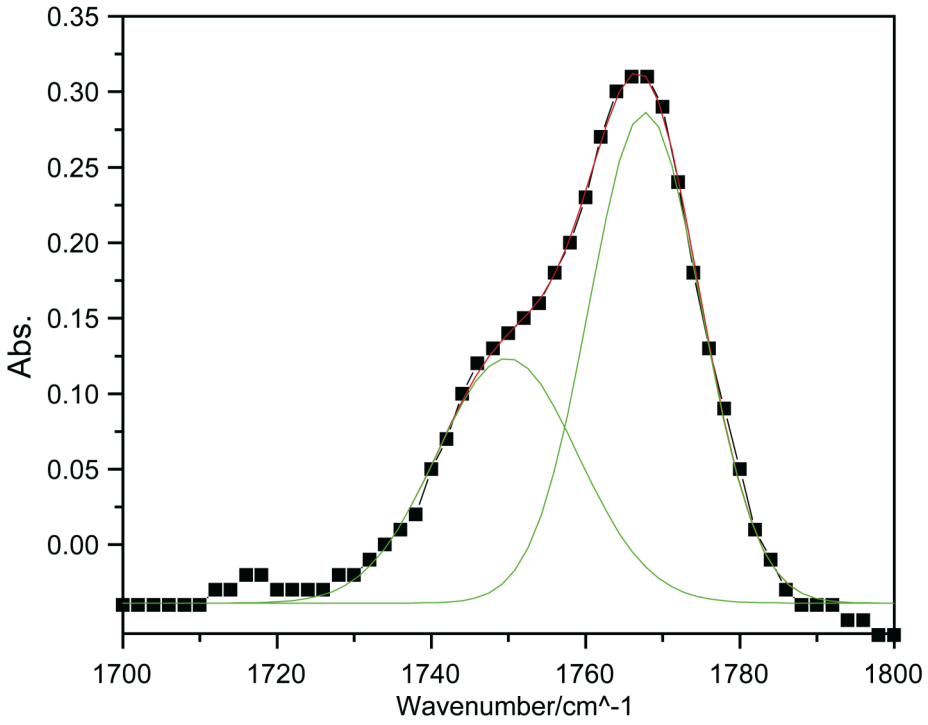
(*S*)-CFTA ester of **6**



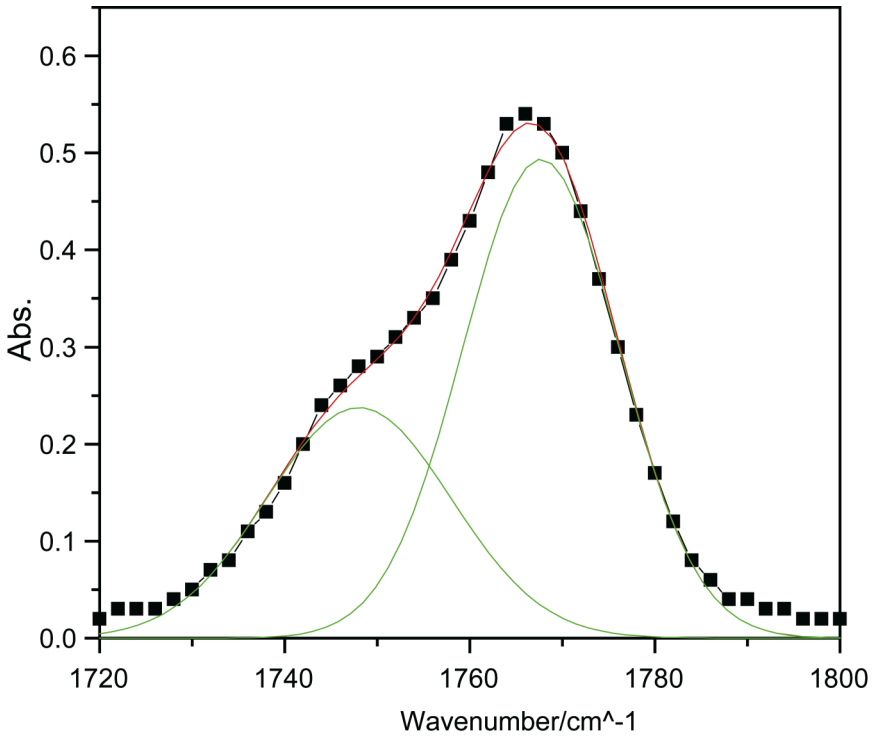
(*R*)-CFTA ester of **6**



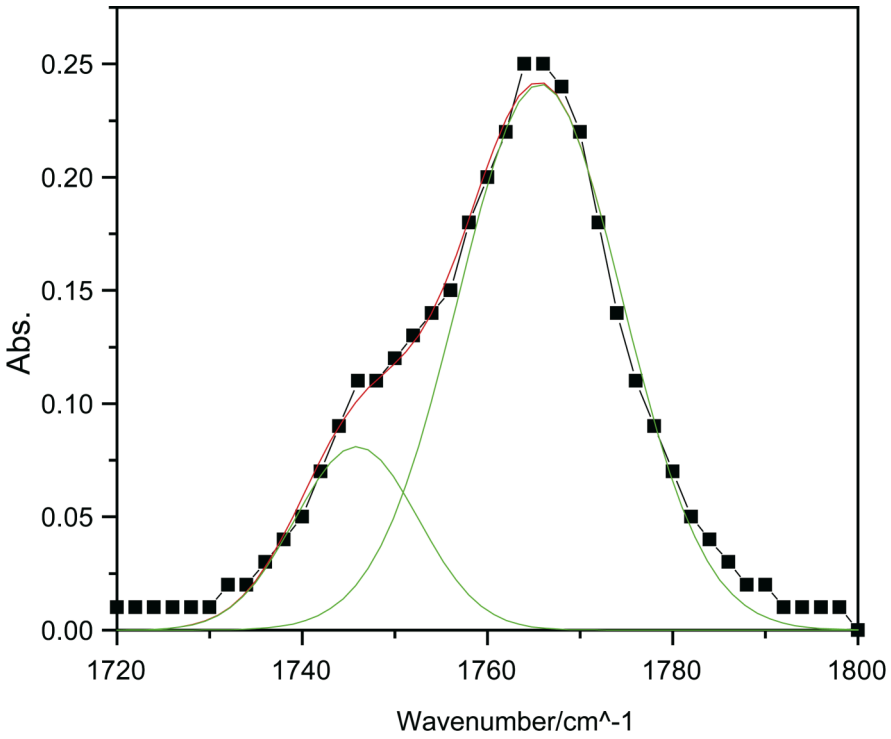
(*S*)-CFTA ester of **7**



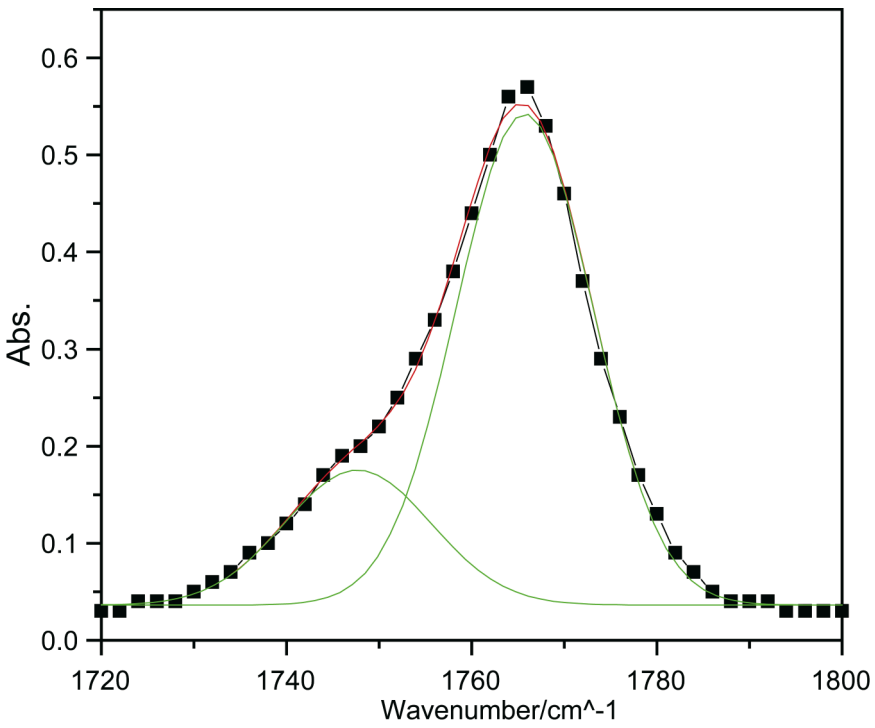
(*R*)-CFTA ester of **7**



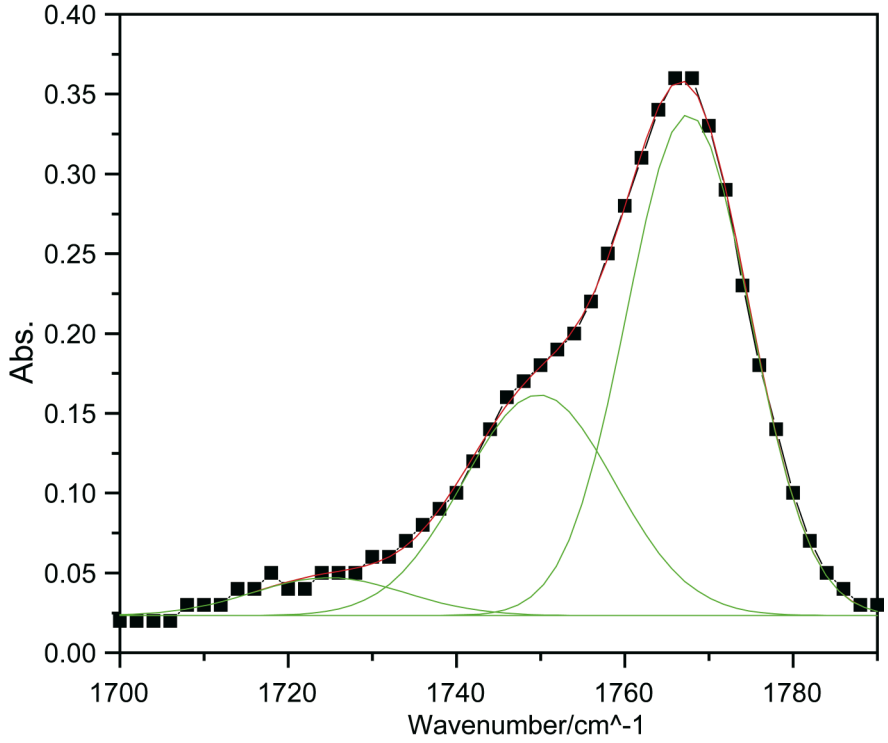
(*S*)-CFTA ester of **8**



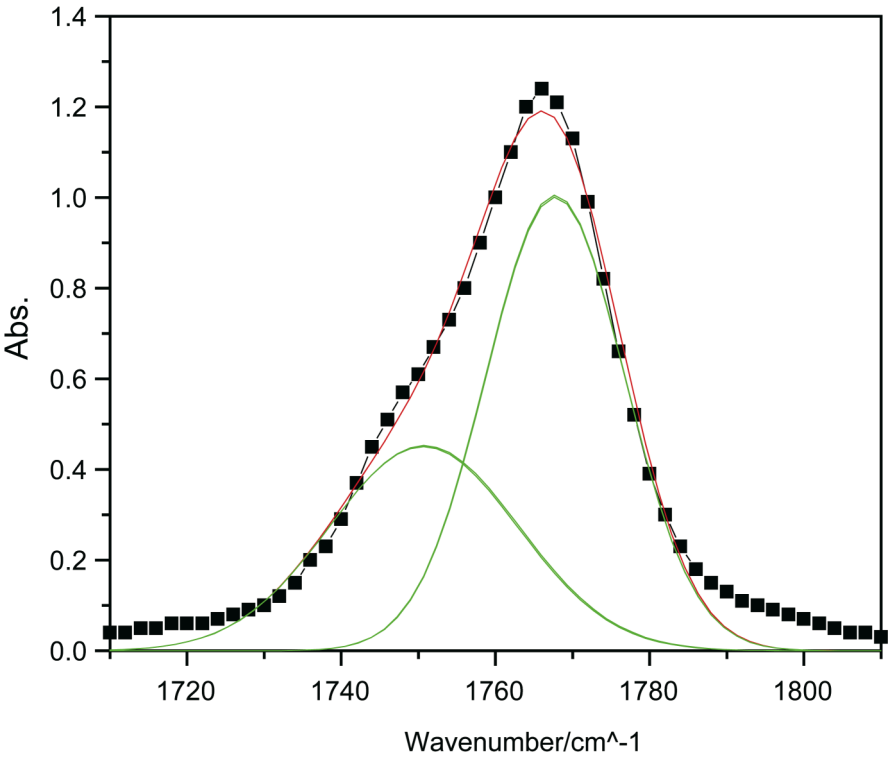
(*R*)-CFTA ester of **8**



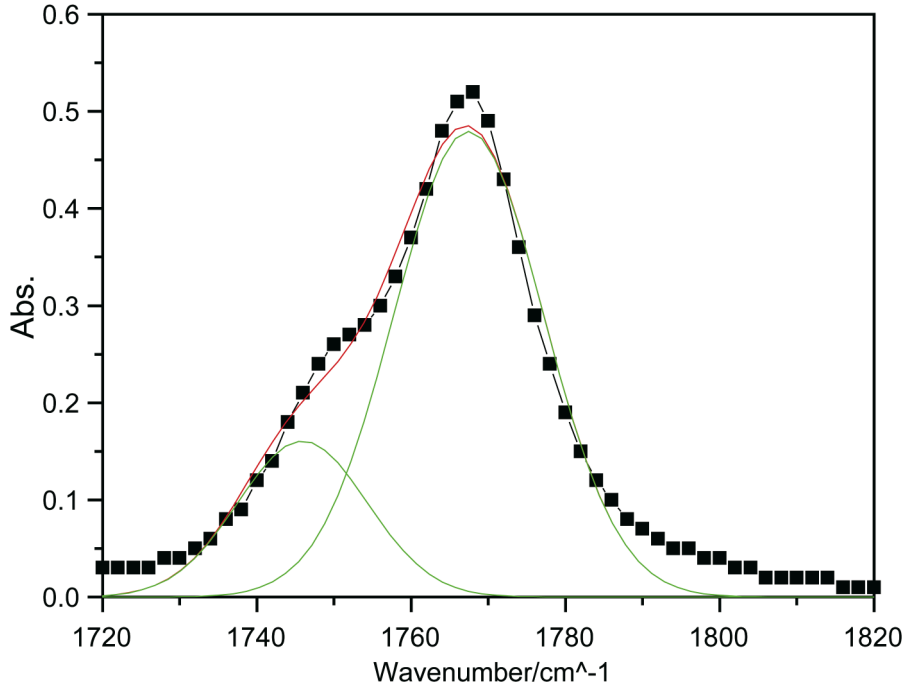
(*S*)-CFTA ester of **9**



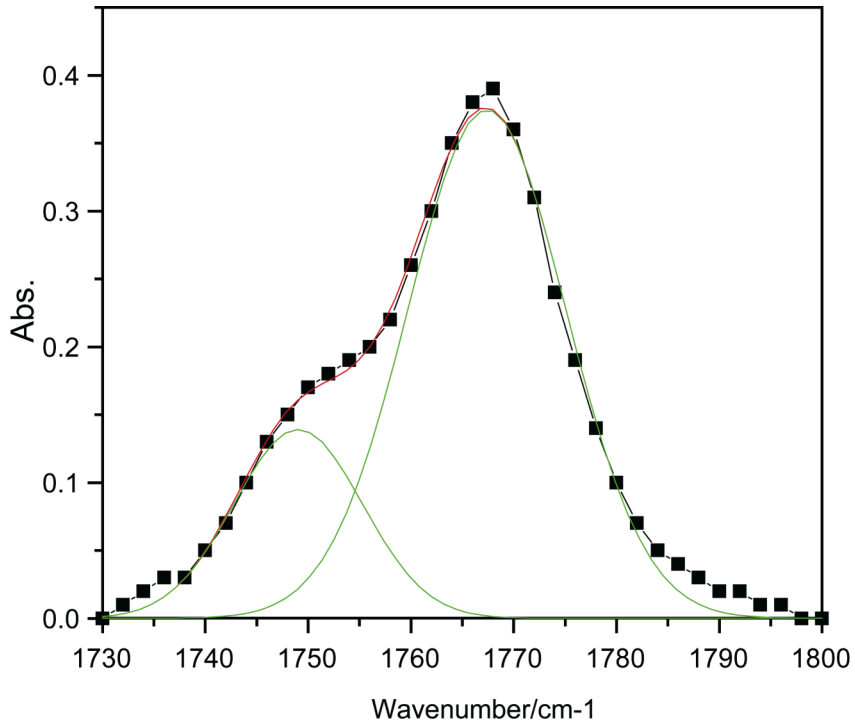
(*R*)-CFTA ester of **9**



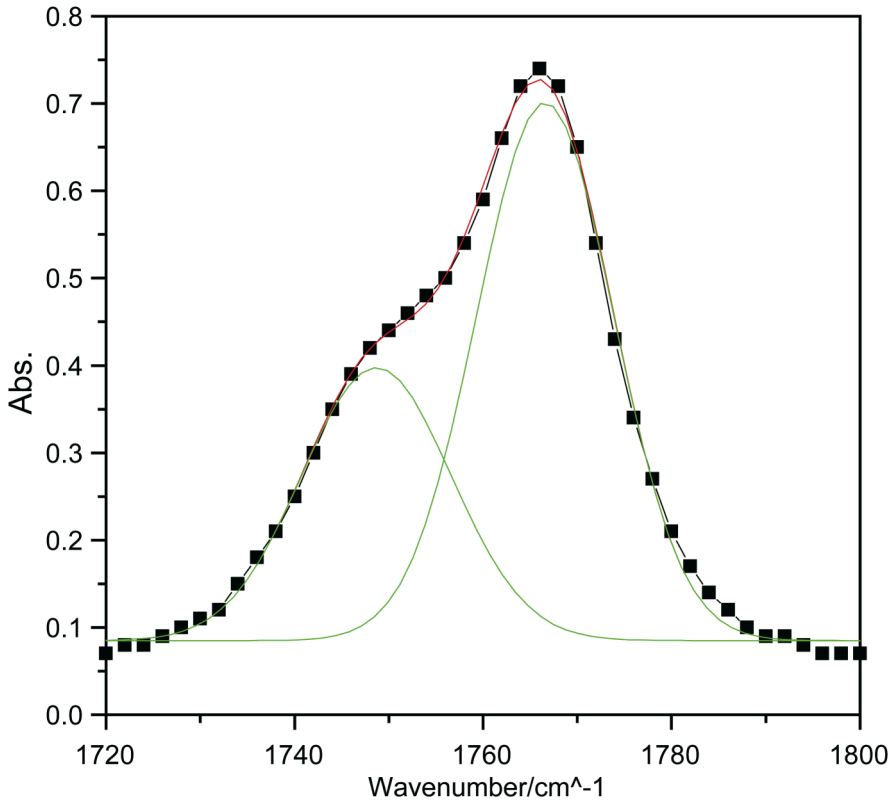
(*S*)-CFTA ester of **10**



(*R*)-CFTA ester of **10**



(*S*)-CFTA ester of **11**



(*R*)-CFTA ester of **11**

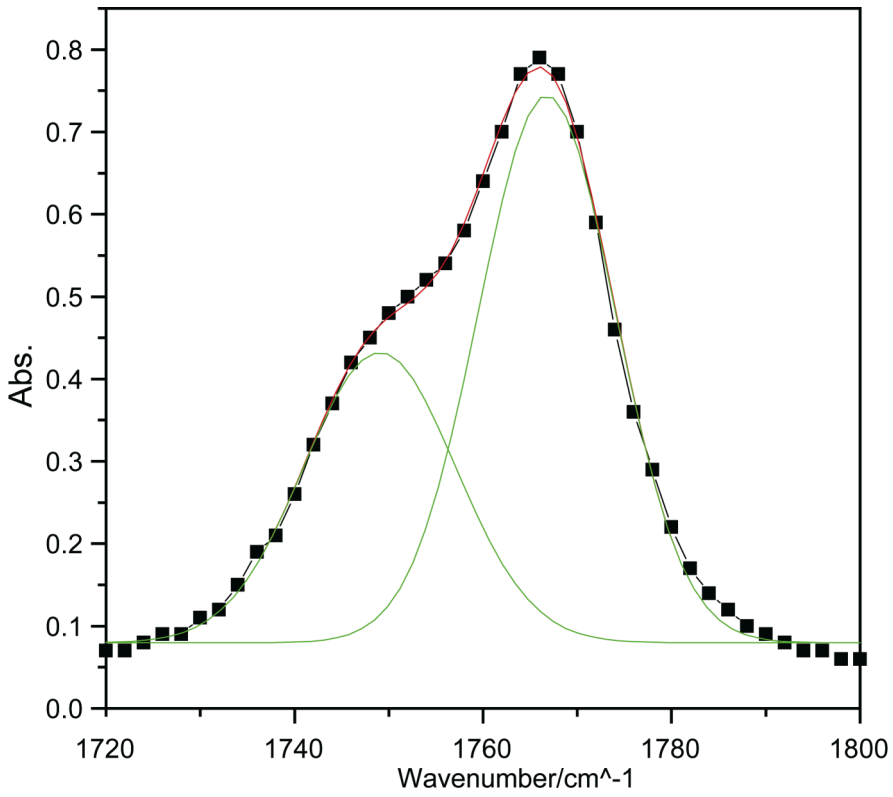


Table S1. Absorptions of C=O stretching bands observed for CFTA esters in $CHCl_3$ solutions.

Alcohol moiety	(*R*)/(*S*) [a]	$\nu_{C=O}$ / cm^{-1} (A_{max})		A_I/A_{II} [b]
		Band **I**	Band **II**	
1	*S*	1772 (0.33)	1752 (0.13)	2.3
	R	1771 (0.30)	1751 (0.15)	2.3
2	*S*	1771 (0.27)	1750 (0.08)	4.8
	R	1771 (0.30)	1749 (0.07)	6.6
3	*S*	1766 (0.33)	1748 (0.12)	3.5
	R	1755 (0.24)	1746 (0.08)	4.0
4	*S*	1772 (0.30)	1754 (0.07)	6.6
	R	1771 (0.43)	1751 (0.19)	2.2
5	*S*	1771 (0.33)	1754 (0.08)	5.3
	R	1772 (0.33)	1752 (0.11)	2.8
6	*S*	1766 (0.39)	1748 (0.15)	2.2
	R	1766 (0.39)	1747 (0.16)	2.3
7	*S*	1768 (0.32)	1750 (0.16)	1.6
	R	1768 (0.49)	1748 (0.24)	1.9
8	*S*	1766 (0.32)	1756 (0.07)	3.7
	R	1766 (0.50)	1748 (0.14)	3.4
9	*S*	1767 (0.31)	1751 (0.14)	1.8
	R	1768 (1.00)	1751 (0.45)	1.6
10	*S*	1767 (0.37)	1749 (0.14)	3.3
	R	1767 (0.48)	1746 (0.16)	3.5
11	*S*	1767 (0.74)	1749 (0.43)	2.4
	R	1767 (0.70)	1749 (0.40)	1.8

[a] Absolute configuration of CFTA moiety.

[b] Ratio of areas of Band **I** and Band **II** absorptions.

S-5. Calclations.

Full structure optimizations and vibrational analysis were conducted on Gaussian 03 program suite[1] using density fractional theory (B3LYP/6-31G(d)).

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1) Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Wallingford, CT, **2004**.

cartesian coordinates of the optimized structures.

(*S*)-CFTA ester of **1**

sp conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.902499	-0.478853	-1.255689
2	6	0	-4.682072	-0.775532	-0.131088
3	6	0	-4.210975	-0.365580	1.124509
4	6	0	-6.004927	-1.491620	-0.266039
5	6	0	-3.007244	0.321114	1.255042
6	6	0	-2.246539	0.617897	0.118271
7	6	0	-2.696088	0.211026	-1.139318
8	6	0	-0.915100	1.333347	0.316876
9	6	0	0.159882	0.304368	0.778162
10	9	0	-1.031507	2.262596	1.337605
11	6	0	-0.461145	2.049835	-0.891953
12	8	0	0.471739	0.161966	1.931841
13	7	0	-0.100742	2.617817	-1.836730
14	8	0	0.596734	-0.398684	-0.271912
15	6	0	1.622129	-1.417751	-0.020722
16	6	0	1.438179	-2.458566	-1.120038
17	6	0	2.996684	-0.780634	-0.012442
18	6	0	3.936949	-1.166949	0.948148
19	6	0	5.225230	-0.630241	0.934383
20	6	0	5.579950	0.308554	-0.035070
21	6	0	4.641966	0.707490	-0.990164
22	6	0	3.358151	0.163072	-0.983095
23	1	0	-4.244578	-0.786595	-2.240825
24	1	0	-4.795453	-0.587115	2.014405
25	1	0	-6.182219	-2.168279	0.576913
26	1	0	-6.051054	-2.078577	-1.188914
27	1	0	-6.839344	-0.778219	-0.289579
28	1	0	-2.655733	0.632245	2.233114
29	1	0	-2.113360	0.434901	-2.027904
30	1	0	1.412691	-1.851677	0.960333
31	1	0	1.602789	-2.013523	-2.106330
32	1	0	0.428522	-2.880445	-1.086800
33	1	0	2.163092	-3.267231	-0.983894
34	1	0	3.657856	-1.885385	1.715535
35	1	0	5.945744	-0.936586	1.687932
36	1	0	6.579997	0.733635	-0.042425
37	1	0	4.908974	1.445782	-1.741395
38	1	0	2.627856	0.486862	-1.719574

(*S*)-CFTA ester of **1**

ap conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.628862	1.070257	-1.184226
2	6	0	3.727042	2.115642	-0.252832
3	6	0	3.027454	1.989941	0.951453
4	6	0	4.563407	3.337188	-0.552233
5	6	0	2.252228	0.862280	1.227710
6	6	0	2.169534	-0.166263	0.289705
7	6	0	2.861197	-0.059916	-0.923132
8	6	0	1.309388	-1.397300	0.584215
9	6	0	0.141170	-1.471065	-0.436900
10	9	0	0.800225	-1.324769	1.871298
11	6	0	2.101404	-2.643622	0.497308
12	8	0	0.305703	-1.870839	-1.567126
13	7	0	2.734030	-3.614610	0.459224
14	8	0	-0.983486	-0.997481	0.089288
15	6	0	-2.163967	-0.956055	-0.786079
16	6	0	-2.854999	-2.317574	-0.729450
17	6	0	-3.031666	0.185813	-0.308193
18	6	0	-3.636657	1.033024	-1.242458
19	6	0	-4.489377	2.056513	-0.825121
20	6	0	-4.735146	2.248885	0.534613
21	6	0	-4.126273	1.412775	1.473756
22	6	0	-3.282947	0.384245	1.055838
23	1	0	4.163850	1.141090	-2.128420
24	1	0	3.087069	2.784997	1.690665
25	1	0	4.570222	4.034490	0.291085
26	1	0	4.181501	3.875796	-1.428452
27	1	0	5.602947	3.064559	-0.770973
28	1	0	1.718092	0.783226	2.167182
29	1	0	2.793501	-0.855218	-1.659023
30	1	0	-1.806236	-0.764780	-1.800809
31	1	0	-3.158446	-2.552482	0.295713
32	1	0	-2.187351	-3.102105	-1.097731
33	1	0	-3.751860	-2.300987	-1.357264
34	1	0	-3.439300	0.892752	-2.303015
35	1	0	-4.952678	2.707125	-1.561903
36	1	0	-5.393402	3.048957	0.862299
37	1	0	-4.308252	1.562459	2.534634
38	1	0	-2.801550	-0.256727	1.788623

(*R*)-CFTA ester of **1**

sp conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.331617	2.031586	0.733053
2	6	0	-3.382809	2.192285	-0.180761
3	6	0	-3.792661	1.073403	-0.915801
4	6	0	-4.065817	3.529166	-0.346746
5	6	0	-3.183110	-0.168772	-0.745219
6	6	0	-2.145701	-0.311774	0.179347
7	6	0	-1.715457	0.796314	0.915857
8	6	0	-1.460492	-1.670017	0.310226
9	6	0	-0.230433	-1.719411	-0.643282
10	9	0	-2.317995	-2.674248	-0.103603
11	6	0	-1.062819	-1.967277	1.701704
12	8	0	-0.282004	-2.201643	-1.746143
13	7	0	-0.758657	-2.204664	2.795408
14	8	0	0.813194	-1.109258	-0.077064
15	6	0	2.042180	-0.989713	-0.874826
16	6	0	2.786177	0.221448	-0.360717
17	6	0	2.833034	-2.291472	-0.754428
18	6	0	2.958546	0.434448	1.013697
19	6	0	3.689082	1.530947	1.469477
20	6	0	4.263585	2.421380	0.558778
21	6	0	4.096739	2.214295	-0.810651
22	6	0	3.356213	1.121998	-1.266384
23	1	0	-1.990240	2.885605	1.313264
24	1	0	-4.602355	1.172585	-1.634787
25	1	0	-4.597593	3.591474	-1.301554
26	1	0	-3.346912	4.354755	-0.303566
27	1	0	-4.801573	3.698726	0.450550
28	1	0	-3.512114	-1.025178	-1.322805
29	1	0	-0.903742	0.697095	1.630227
30	1	0	1.735312	-0.837260	-1.912828
31	1	0	3.764363	-2.208575	-1.324384
32	1	0	2.254712	-3.129997	-1.153033
33	1	0	3.087608	-2.491654	0.291193
34	1	0	2.507262	-0.251774	1.724800
35	1	0	3.811325	1.690174	2.537525
36	1	0	4.834780	3.274004	0.916074
37	1	0	4.534548	2.905730	-1.525593
38	1	0	3.219813	0.969363	-2.334811

(*R*)-CFTA ester of **1**

ap conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.081108	-0.141777	-1.294924
2	6	0	-4.805297	-0.713978	-0.237757
3	6	0	-4.235400	-0.687270	1.039194
4	6	0	-6.165334	-1.325844	-0.477512
5	6	0	-2.986352	-0.106478	1.265641
6	6	0	-2.285165	0.461644	0.202375
7	6	0	-2.835554	0.441262	-1.084809
8	6	0	-0.909581	1.087456	0.444672
9	6	0	0.167441	0.287163	-0.337168
10	9	0	-0.612500	1.070175	1.798718
11	6	0	-0.875890	2.499641	0.006716
12	8	0	0.349630	0.448181	-1.521197
13	7	0	-0.870444	3.615701	-0.307535
14	8	0	0.766096	-0.600467	0.454074
15	6	0	1.795340	-1.450494	-0.162584
16	6	0	3.131444	-0.738091	-0.143695
17	6	0	1.778109	-2.749582	0.635040
18	6	0	3.611080	-0.144950	1.031859
19	6	0	4.859562	0.474893	1.049497
20	6	0	5.645824	0.502490	-0.105104
21	6	0	5.172989	-0.083756	-1.279416
22	6	0	3.918321	-0.695430	-1.298879
23	1	0	-4.499841	-0.151394	-2.298532
24	1	0	-4.774773	-1.126007	1.875185
25	1	0	-6.523956	-1.863553	0.405586
26	1	0	-6.144807	-2.030697	-1.316990
27	1	0	-6.908677	-0.556330	-0.722057
28	1	0	-2.561801	-0.093681	2.262569
29	1	0	-2.287980	0.873727	-1.916667
30	1	0	1.490048	-1.628243	-1.196495
31	1	0	2.512087	-3.445601	0.216747
32	1	0	0.787930	-3.214436	0.592973
33	1	0	2.036681	-2.567794	1.682801
34	1	0	2.996263	-0.153371	1.927871
35	1	0	5.218723	0.938553	1.964306
36	1	0	6.619016	0.985648	-0.090232
37	1	0	5.773757	-0.055765	-2.184399
38	1	0	3.544564	-1.135643	-2.220274

(*S*)-CFTA ester of **9**

sp conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.796595	0.018309	0.798266
2	6	0	4.615741	0.215677	-0.498124
3	6	0	2.972623	-1.278466	0.613775
4	6	0	2.709626	1.134466	0.697903
5	6	0	3.520006	0.616899	-1.533821
6	6	0	2.196833	0.631460	-0.706547
7	6	0	1.926653	-0.879368	-0.457302
8	6	0	1.669122	1.101006	1.833655
9	8	0	0.584999	-1.143775	0.069741
10	6	0	1.055531	1.386421	-1.375166
11	6	0	3.284630	2.564374	0.676669
12	6	0	-0.327998	-1.661646	-0.754878
13	6	0	-1.679734	-1.852026	-0.003394
14	8	0	-0.200945	-1.921324	-1.925021
15	9	0	-2.414416	-2.763347	-0.747320
16	6	0	-2.420384	-0.521125	0.046632
17	6	0	-1.459724	-2.441466	1.331871
18	7	0	-1.296792	-2.915316	2.377736
19	6	0	-2.995401	-0.052423	-1.141690
20	6	0	-2.513464	0.247735	1.207879
21	6	0	-3.180544	1.473112	1.178412
22	6	0	-3.767850	1.953149	0.002282
23	6	0	-4.517730	3.263877	-0.018335
24	6	0	-3.660923	1.169135	-1.156543
25	1	0	4.396141	0.026469	1.714205
26	1	0	5.147566	-0.698743	-0.782247
27	1	0	5.370529	0.999891	-0.385205
28	1	0	2.465499	-1.583991	1.532484
29	1	0	3.591132	-2.121466	0.288458
30	1	0	3.456096	-0.080434	-2.376682
31	1	0	3.709243	1.605820	-1.962570
32	1	0	2.002824	-1.449508	-1.383449
33	1	0	0.875662	1.835350	1.649607
34	1	0	2.148201	1.373580	2.782429
35	1	0	1.187319	0.132808	1.969155
36	1	0	0.152543	1.392133	-0.755969
37	1	0	0.795664	0.930474	-2.337709
38	1	0	1.337909	2.428079	-1.566443
39	1	0	2.481361	3.298344	0.541550
40	1	0	4.022933	2.738578	-0.109373
41	1	0	3.766976	2.787899	1.636063
42	1	0	-2.920012	-0.648155	-2.045589
43	1	0	-2.074683	-0.106167	2.135880
44	1	0	-3.249614	2.061092	2.090279
45	1	0	-4.312391	3.828544	-0.934552
46	1	0	-4.249500	3.893224	0.836043
47	1	0	-5.602394	3.098751	0.022752
48	1	0	-4.105789	1.520958	-2.084418

(*S*)-CFTA ester of **9**

ap conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.798822	2.661268	0.071936
2	6	0	-1.479593	1.249932	0.378536
3	6	0	-2.709518	0.352753	0.223402
4	6	0	-0.355843	0.768086	-0.581162
5	9	0	-1.024790	1.209551	1.688275
6	8	0	-0.384073	1.012589	-1.765719
7	8	0	0.543735	0.044385	0.076348
8	6	0	1.978262	-1.930709	-0.097047
9	6	0	3.482112	-1.826062	0.247429
10	6	0	4.245989	-1.765253	-1.097080
11	6	0	3.896232	-0.337667	-1.621926
12	6	0	2.982137	0.264783	-0.511164
13	6	0	3.609111	-0.368692	0.790335
14	6	0	1.656363	-0.532668	-0.680868
15	6	0	2.825311	-0.108271	2.092529
16	6	0	5.062328	0.064858	1.064818
17	7	0	-2.061733	3.770816	-0.138617
18	6	0	-3.392071	0.292118	-0.997208
19	6	0	-4.500884	-0.538274	-1.128698
20	6	0	-4.956205	-1.321075	-0.057230
21	6	0	2.834597	1.778965	-0.577022
22	6	0	-6.178637	-2.195908	-0.204526
23	6	0	-4.256746	-1.249831	1.152292
24	6	0	-3.142551	-0.422448	1.299331
25	1	0	1.363366	-2.112347	0.788517
26	1	0	1.767713	-2.733205	-0.811726
27	1	0	3.828892	-2.612224	0.925894
28	1	0	3.919758	-2.555884	-1.781562
29	1	0	5.324008	-1.891382	-0.958182
30	1	0	4.791784	0.278475	-1.748348
31	1	0	3.388985	-0.353749	-2.593144
32	1	0	1.338059	-0.549377	-1.723742
33	1	0	2.940829	0.937090	2.402573
34	1	0	3.231277	-0.729868	2.900617
35	1	0	1.754975	-0.301500	2.020630
36	1	0	5.101022	1.122667	1.350292
37	1	0	5.738048	-0.071528	0.217612
38	1	0	5.470225	-0.510295	1.905037
39	1	0	-3.050945	0.884615	-1.840423
40	1	0	-5.023239	-0.578264	-2.081620
41	1	0	2.205645	2.160686	0.234490
42	1	0	2.381066	2.090775	-1.524795
43	1	0	3.812061	2.268199	-0.498798
44	1	0	-6.184955	-2.716517	-1.168666
45	1	0	-7.099570	-1.600361	-0.153485
46	1	0	-6.230425	-2.949016	0.588016
47	1	0	-4.586010	-1.849929	1.997199
48	1	0	-2.614065	-0.379941	2.244362

(*R*)-CFTA ester of **9**

sp conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.779569	-0.274113	1.197401
2	6	0	-3.754284	-1.271705	1.196210
3	6	0	-4.584793	-1.475343	0.087615
4	6	0	-4.404148	-0.650541	-1.032135
5	6	0	-5.663299	-2.532434	0.105224
6	6	0	-3.433421	0.346719	-1.044878
7	6	0	-2.618101	0.541874	0.076272
8	6	0	-1.548414	1.623868	-0.004269
9	6	0	-1.055538	2.051469	1.320255
10	6	0	-0.366326	1.122060	-0.887395
11	9	0	-2.064384	2.742624	-0.639248
12	8	0	-0.234447	1.454898	-2.037977
13	8	0	0.385019	0.263914	-0.193411
14	7	0	-0.664563	2.400931	2.354826
15	6	0	1.622131	-1.844785	-0.445534
16	6	0	3.064983	-1.960998	0.101253
17	6	0	4.016070	-1.828757	-1.111099
18	6	0	3.884951	-0.319092	-1.483188
19	6	0	2.889485	0.250325	-0.425002
20	6	0	3.260333	-0.604239	0.848058
21	6	0	1.527765	-0.357198	-0.867343
22	6	0	2.332988	-0.415465	2.064107
23	6	0	4.697154	-0.375556	1.357273
24	6	0	2.905624	1.768494	-0.305578
25	1	0	-2.153750	-0.131203	2.073313
26	1	0	-3.872869	-1.898449	2.076763
27	1	0	-5.033902	-0.790754	-1.907501
28	1	0	-6.628143	-2.106526	0.410973
29	1	0	-5.425085	-3.337432	0.807861
30	1	0	-5.805461	-2.976695	-0.885769
31	1	0	-3.306412	0.978456	-1.917980
32	1	0	0.870130	-2.064642	0.316568
33	1	0	1.439933	-2.521251	-1.287167
34	1	0	3.230586	-2.858761	0.705569
35	1	0	3.719809	-2.491371	-1.931587
36	1	0	5.045001	-2.090925	-0.846778
37	1	0	4.845813	0.200456	-1.417719
38	1	0	3.516381	-0.163734	-2.503474
39	1	0	1.361590	-0.212588	-1.935140
40	1	0	2.439170	0.593733	2.478222
41	1	0	2.612979	-1.121596	2.855972
42	1	0	1.274920	-0.559170	1.846003
43	1	0	4.787654	0.615983	1.816152
44	1	0	5.463711	-0.449259	0.582532
45	1	0	4.941127	-1.112570	2.132077
46	1	0	2.218739	2.122015	0.470721
47	1	0	2.614034	2.240601	-1.251221
48	1	0	3.909319	2.127564	-0.051339

(*R*)-CFTA ester of **9**

ap conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.068642	0.140868	-1.016594
2	6	0	3.880708	-0.973271	-1.201160
3	6	0	4.126624	-1.877713	-0.156350
4	6	0	3.526070	-1.629542	1.081881
5	6	0	5.020557	-3.076283	-0.370083
6	6	0	2.708713	-0.515494	1.282879
7	6	0	2.479805	0.373425	0.232490
8	6	0	1.576747	1.590364	0.450400
9	6	0	2.287321	2.850564	0.143021
10	6	0	0.324872	1.481213	-0.464605
11	9	0	1.184289	1.654584	1.778712
12	8	0	0.384269	1.714344	-1.650267
13	8	0	-0.730634	1.070596	0.230013
14	7	0	2.858663	3.836816	-0.070123
15	6	0	-3.154265	1.405608	0.380013
16	6	0	-4.085452	0.180084	0.533653
17	6	0	-4.712905	-0.080682	-0.856198
18	6	0	-3.507117	-0.639897	-1.673286
19	6	0	-2.327110	-0.655061	-0.653227
20	6	0	-3.077420	-1.001323	0.690578
21	6	0	-1.991717	0.854073	-0.483227
22	6	0	-2.214728	-0.930016	1.966257
23	6	0	-3.745562	-2.390193	0.695169
24	6	0	-1.153144	-1.529217	-1.073686
25	1	0	2.885542	0.825191	-1.839072
26	1	0	4.334145	-1.143276	-2.174923
27	1	0	3.699265	-2.315028	1.907917
28	1	0	6.051404	-2.769199	-0.586807
29	1	0	4.680954	-3.681712	-1.219100
30	1	0	5.044540	-3.720997	0.513832
31	1	0	2.255223	-0.337454	2.250725
32	1	0	-2.768303	1.755776	1.340880
33	1	0	-3.655568	2.253059	-0.099113
34	1	0	-4.814939	0.285667	1.343061
35	1	0	-5.125467	0.836432	-1.290396
36	1	0	-5.533242	-0.802750	-0.801910
37	1	0	-3.701347	-1.651981	-2.042045
38	1	0	-3.269238	-0.028949	-2.551413
39	1	0	-1.883978	1.346977	-1.449715
40	1	0	-1.490437	-1.753387	1.981460
41	1	0	-2.852657	-1.046271	2.851493
42	1	0	-1.649841	-0.004332	2.076013
43	1	0	-2.987032	-3.181485	0.721875
44	1	0	-4.387459	-2.581236	-0.167705
45	1	0	-4.362382	-2.505012	1.594857
46	1	0	-0.354669	-1.526746	-0.324501
47	1	0	-0.722494	-1.179821	-2.019576
48	1	0	-1.474203	-2.566981	-1.218906

(*S*)-CFTA ester of **10**

sp conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.207988	0.945801	-1.073406
2	6	0	-3.385647	-0.176723	-1.096242
3	6	0	-4.307498	1.751701	0.070123
4	6	0	-2.643062	-0.521101	0.039437
5	6	0	-2.725458	0.272468	1.185197
6	6	0	-1.720468	-1.731404	-0.052785
7	6	0	-3.550691	1.397122	1.193294
8	6	0	-0.441507	-1.330764	-0.845041
9	9	0	-2.337102	-2.735608	-0.782419
10	6	0	-5.224603	2.951472	0.093753
11	6	0	-1.368799	-2.289491	1.267887
12	7	0	-1.096842	-2.736451	2.302944
13	8	0	0.409499	-0.681992	-0.049258
14	6	0	1.608122	-0.131391	-0.674158
15	6	0	2.722684	-1.188733	-0.898878
16	6	0	3.918966	-0.588942	-0.121378
17	6	0	3.624685	-0.788502	1.383003
18	6	0	2.464406	0.220115	1.644203
19	6	0	2.247275	0.915602	0.268495
20	6	0	1.472951	2.225959	0.342362
21	6	0	3.714894	0.948915	-0.313600
22	6	0	4.688431	1.819273	0.501811
23	6	0	3.830201	1.415564	-1.778685
24	8	0	-0.314955	-1.544684	-2.024375
25	1	0	-4.782507	1.201609	-1.960612
26	1	0	-3.316536	-0.789069	-1.989198
27	1	0	-2.155591	0.013977	2.072769
28	1	0	-3.609837	2.005098	2.092701
29	1	0	-6.261185	2.652267	0.297762
30	1	0	-5.223289	3.475403	-0.868287
31	1	0	-4.931418	3.665242	0.870098
32	1	0	1.276375	0.317351	-1.612008
33	1	0	2.928092	-1.319275	-1.964657
34	1	0	2.425303	-2.165634	-0.504981
35	1	0	4.891412	-0.975883	-0.443197
36	1	0	4.501851	-0.564791	1.998342
37	1	0	3.336888	-1.821692	1.603328
38	1	0	2.734393	0.962411	2.402279
39	1	0	1.551425	-0.269116	1.991055
40	1	0	1.969516	2.943686	1.005160
41	1	0	0.462484	2.057961	0.733299
42	1	0	1.370959	2.692493	-0.645112
43	1	0	4.448768	2.882620	0.381843
44	1	0	5.713110	1.675686	0.137577
45	1	0	4.687607	1.601330	1.571971
46	1	0	3.570428	2.477005	-1.871221
47	1	0	3.199791	0.862177	-2.479096
48	1	0	4.866061	1.306525	-2.121941

(*S*)-CFTA ester of **10**

ap conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.985549	-0.426427	-1.300315
2	6	0	3.892439	-1.475474	-1.139195
3	6	0	4.483445	-1.743388	0.099661
4	6	0	4.134807	-0.926816	1.186551
5	6	0	5.476303	-2.868952	0.269229
6	6	0	3.232557	0.122106	1.041812
7	6	0	2.655317	0.376005	-0.208494
8	6	0	1.654656	1.521644	-0.380474
9	9	0	1.273741	1.621426	-1.709993
10	6	0	0.406169	1.256140	0.503575
11	6	0	2.250784	2.819653	0.003193
12	7	0	2.734647	3.837733	0.274992
13	8	0	0.408880	1.469767	1.694539
14	8	0	-0.583298	0.733968	-0.212259
15	6	0	-1.803813	0.391767	0.512974
16	6	0	-2.974014	0.241246	-0.487664
17	6	0	-3.483796	1.567678	-1.037694
18	6	0	-2.516847	-0.771188	-1.577183
19	6	0	-2.486015	-2.142302	-0.834155
20	6	0	-2.901289	-1.761634	0.605976
21	6	0	-3.962061	-0.637326	0.376284
22	6	0	-1.716531	-0.984387	1.226774
23	6	0	-4.463344	0.027670	1.674068
24	6	0	-5.214508	-1.101039	-0.389905
25	1	0	2.540979	-0.232279	-2.269245
26	1	0	4.144119	-2.094137	-1.997186
27	1	0	4.578043	-1.114225	2.161786
28	1	0	6.478490	-2.483210	0.495079
29	1	0	5.551261	-3.476933	-0.637543
30	1	0	5.193190	-3.530664	1.096444
31	1	0	2.970794	0.738808	1.896113
32	1	0	-1.975493	1.207124	1.216935
33	1	0	-4.328009	1.417243	-1.720087
34	1	0	-2.694711	2.082916	-1.597705
35	1	0	-3.813491	2.239712	-0.235992
36	1	0	-1.545976	-0.491420	-1.992443
37	1	0	-3.228948	-0.775615	-2.408546
38	1	0	-3.183434	-2.859413	-1.278516
39	1	0	-1.494859	-2.607694	-0.855875
40	1	0	-3.240104	-2.607468	1.213146
41	1	0	-1.804506	-0.868295	2.310317
42	1	0	-0.755748	-1.471019	1.030257
43	1	0	-5.071774	-0.683467	2.245872
44	1	0	-5.103037	0.888356	1.445287
45	1	0	-3.669622	0.378112	2.338758
46	1	0	-5.770781	-1.831919	0.209759
47	1	0	-4.998063	-1.565298	-1.354605
48	1	0	-5.888031	-0.255921	-0.575368

(*R*)-CFTA ester of **10**

sp conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.440439	1.384397	1.238613
2	6	0	2.702490	0.200558	1.216686
3	6	0	4.068584	1.871034	0.086442
4	6	0	2.578429	-0.519625	0.027598
5	6	0	3.194296	-0.043891	-1.136958
6	6	0	1.754245	-1.796966	-0.078762
7	6	0	3.930137	1.136391	-1.100821
8	6	0	0.425360	-1.486973	-0.829372
9	6	0	1.476435	-2.418627	1.231046
10	6	0	4.892877	3.136102	0.120675
11	9	0	2.433039	-2.727374	-0.850074
12	7	0	1.261171	-2.918864	2.254989
13	8	0	-0.429210	-0.868862	-0.013396
14	6	0	-1.715243	-0.477053	-0.582038
15	6	0	-1.638211	0.823790	-1.426475
16	6	0	-2.669703	1.742263	-0.727745
17	6	0	-2.023949	2.218392	0.593403
18	6	0	-2.020891	0.922573	1.461992
19	6	0	-2.706308	-0.143881	0.558409
20	6	0	-3.211983	-1.369996	1.309110
21	6	0	-3.753786	0.729480	-0.237402
22	6	0	-4.844851	1.354276	0.650985
23	6	0	-4.484567	-0.009144	-1.376418
24	8	0	0.261226	-1.741994	-1.995799
25	1	0	3.532172	1.934830	2.171710
26	1	0	2.231921	-0.159652	2.126656
27	1	0	3.096356	-0.601864	-2.062691
28	1	0	4.406006	1.494280	-2.010835
29	1	0	4.747165	3.733483	-0.786035
30	1	0	5.964633	2.907422	0.188134
31	1	0	4.636136	3.759181	0.983189
32	1	0	-2.052273	-1.328983	-1.174834
33	1	0	-1.881786	0.625589	-2.473649
34	1	0	-0.629496	1.248301	-1.403615
35	1	0	-3.039862	2.553040	-1.363814
36	1	0	-2.606436	3.018353	1.061234
37	1	0	-1.016006	2.613623	0.428083
38	1	0	-2.588557	1.051850	2.388895
39	1	0	-1.014967	0.608833	1.749558
40	1	0	-3.926620	-1.089704	2.091229
41	1	0	-2.381899	-1.897161	1.793487
42	1	0	-3.708840	-2.080852	0.637476
43	1	0	-5.539308	0.584248	1.007213
44	1	0	-5.432654	2.076384	0.070996
45	1	0	-4.457231	1.876931	1.528142
46	1	0	-5.124921	-0.802766	-0.973756
47	1	0	-3.821807	-0.467120	-2.115028
48	1	0	-5.136188	0.688413	-1.916249

(*R*)-CFTA ester of **10**

ap conformer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.315899	0.154475	1.033243
2	6	0	-4.263195	-0.855072	1.174694
3	6	0	-4.615495	-1.679818	0.095778
4	6	0	-3.979218	-1.464046	-1.131374
5	6	0	-5.666489	-2.752810	0.254786
6	6	0	-3.027069	-0.455895	-1.288690
7	6	0	-2.695886	0.357857	-0.205097
8	6	0	-1.641927	1.454819	-0.371464
9	6	0	-2.182851	2.782945	-0.010265
10	6	0	-0.419051	1.140414	0.532781
11	9	0	-1.235473	1.524373	-1.695909
12	8	0	-0.417864	1.382174	1.718152
13	8	0	0.541096	0.542331	-0.162903
14	7	0	-2.623950	3.825208	0.241850
15	6	0	1.728677	0.123279	0.575607
16	6	0	2.504280	-0.924982	-0.257641
17	6	0	1.844954	-2.298308	-0.279706
18	6	0	2.743434	-0.301523	-1.663149
19	6	0	3.799988	0.817581	-1.407868
20	6	0	4.024882	0.735131	0.119892
21	6	0	3.933819	-0.798770	0.401597
22	6	0	2.742707	1.279185	0.794305
23	6	0	3.996171	-1.167049	1.897937
24	6	0	5.020755	-1.632561	-0.300938
25	1	0	-3.051891	0.777942	1.882049
26	1	0	-4.738513	-1.004555	2.141255
27	1	0	-4.230563	-2.092433	-1.982453
28	1	0	-6.675800	-2.320797	0.253805
29	1	0	-5.548222	-3.292644	1.200950
30	1	0	-5.620921	-3.482459	-0.559783
31	1	0	-2.546226	-0.302526	-2.247578
32	1	0	1.369754	-0.289986	1.519460
33	1	0	2.428173	-3.010078	-0.874961
34	1	0	0.843094	-2.240798	-0.721127
35	1	0	1.738494	-2.711323	0.730757
36	1	0	1.814094	0.084170	-2.088079
37	1	0	3.117914	-1.063936	-2.353723
38	1	0	4.725714	0.635036	-1.962722
39	1	0	3.440297	1.807798	-1.706770
40	1	0	4.943537	1.221106	0.464512
41	1	0	2.875697	1.486072	1.859530
42	1	0	2.393829	2.204995	0.326222
43	1	0	5.002633	-0.972734	2.287613
44	1	0	3.794599	-2.235220	2.042765
45	1	0	3.295396	-0.613342	2.527797
46	1	0	6.008665	-1.369729	0.096690
47	1	0	5.055773	-1.493589	-1.383594
48	1	0	4.870017	-2.701943	-0.110957