Experimental Details:

General Methods. ¹H, ¹³C, NMR spectra were recorded on a Bruker instrument. Chemical shifts (δ) 400 are reported in ppm relative to residual solvent signals for ¹H and ¹³C NMR (¹H NMR: 7.26 ppm for $CDCl_3$, 3.34 ppm for CD_3OD ; ¹³C NMR: 77.0 ppm for CDCl₃, 49.00 ppm for CD₃OD. ¹³C NMR spectra were acquired with ¹H broad band decoupled mode. Mass spectra were recorded on a Micro mass LCT spectrometer using electrospray (ES) ionization techniques. Optical rotations were measured on a Perkin-Elmer 241 polarimeter. The enantiomeric excess (ee) of the products was determined by chiral stationary phase CSP-HPLC (Daicel Chiralpak AD and Chiralcel OD columns), using a UV detector operating at 254 nm. Infrared (IR) spectra were recorded as thin films between NaCl plates. Absorption maximum (v_{max}) was reported in wavenumbers (cm⁻¹) and only selected peaks are reported.

Materials. Analytical grade solvents and commercially available reagents were used as received, unless otherwise stated. Reactions were checked for completion by TLC (EM Science, silica gel 60 F254). Flash chromatography was performed using silica gel 60 (0.040-0.063 mm, 230-400 mesh). Racemic samples were prepared using tetrabutylammonium bromide as a catalyst at room temperature overnight. Experimental procedure for the preparation of catalyst N- (2-methoxy) benzyl quinidinium bromide (4b)

To a stirred suspension of quinidine (3.47 g, 10.7 mmol) in THF (42.0 mL), 2-(methoxy) benzyl bromide (2.80 g, 13.9 mmol) was added. The resulting mixture was heated at 60 °C and stirred for 48 h at the same temperature. After cooling to r.t., the solvent was removed *in vacuo*. The residue was purified by flash chromatography on silica gel eluting with chloroform:methanol 9:1 affording the title compound as a purple solid (6.94 g, 95% yield). (O. Marianacci, G. Micheletti, L. Bernardi, F. Fini, M. Fochi, D. Pettersen, V. Sgarzani, A. Ricci *Chemistry-A. European Journal*, 2007, 13, 29, 8338)



 $[\alpha]_{D}^{20} = +400 \ (c = 0.50 \ in \ CH_{3}Cl); \ ^{1}H-NMR \ (400 \ MHz, \ CDCl_{3}): 8.77 \ (d, J = 4.4 \ Hz, 1H), 8.12 \ (d, J = 9.6 \ Hz, 1H), 7.96 \ (dd, J = 7.6 \ Hz, 1.6 \ Hz, 1H), 7.91 \ (d, J = 4.4 \ Hz, 1H), 7.49 \ (dt, J_{d} = 8.6 \ Hz, J_{t} = 1.4, 1H), 7.40 \ (dd, J = 9.2 \ Hz, 2.4 \ Hz, 1H), 7.18 \ (d, J = 2.4 \ Hz, 1H), 7.13 \ (dt, J_{d} = 6.5 \ Hz, J_{t} = 1.4, 1H), 7.01 \ (d, J = 8.4 \ Hz, 1H), 6.96 \ (d, J = 6.4 \ Hz, 1H), 6.73 \ (d, J = 6.8 \ Hz, 1H), 6.27 \ (d, J = 12.0 \ Hz, 1H), 6.13-6.06 \ (m, 1H), 5.28-5.22 \ (m, 2H), 4.75 \ (d, J = 2.8 \ Hz, 1H), 4.73-4.69 \ (m, 1H), 4.01 \ (s, 3H), 3.93 \ (s, 3H), 3.74-3.67 \ (m, 2H), 3.61 \ (t, J = 12.4 \ Hz, 1H), 2.94-2.86 \ (m, 1H), 2.66-2.61 \ (m, 1H), 2.50-2.43 \ (m, 1H), 1.95-1.77 \ (m, 3H), 1.11-1.04 \ (m, 1H); \ ^{13}C-NMR \ (100.6 \ MHz): 158.6, 158.2, 148.0, 144.3, 143.3, 136.4, 135.8, 132.7,$

132., 125.6, 122.0, 121.6, 120.6, 118.6, 115.5, 111.4, 100.6, 69.7, 64.1, 58.6, 56.0, 55.6, 53.9, 53.6, 38.6, 24.1, 24.5, 21.3; HRMS: m/z found [M-Br]⁺ 445.2482, C₂₈H₃₃N₂O₃ requires 445.2491.

General procedure for the catalytic asymmetric addition of dimethyl bromomalonate to styrylisoxazole (Table 2)

To a test tube equipped with a magnetic stirring bar, were sequentially added the relevant styrylisoxazole **1a-k** (0.10 mmol, 1.0 equiv), toluene (5.0 mL), catalyst 4b (2.63 mg, 0.005 mmol, 0.050 equiv) and dimethyl bromomalonate 2 (27 µL, 0.20 mmol, 2.0 equiv). The test tube was placed at the stated temperature (-37° C) then K_3PO_4 50% w/w was added in one portion (0.140 mL, 0.50 mmol, 5.0 equiv). The mixture was then stirred vigorously and after the stated time the reaction was quenched with $\rm NH_4Cl$ sat. sol. (4 mL) and the product extracted with toluene (3 x 1 mL). The combined organic phases were evaporated in vacuo and the residue was purified by flash gel eluting with chromatography on silica petroleum ether: EtOAc mixtures.

(+)-Dimethyl -2-(3-methyl-4-nitroisoxazol-5-yl)-3phenylcyclopropane-1,1-dicarboxylate (7a)



Prepared following general procedure using 3-methyl-4-nitro-5styrylisoxazole **1a** (23 mg, 0.10 mmol). Reaction time: 24 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7a** as a yellow oil (33.5 mg, 93% yield).

The *ee* of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*-PrOH 90:10, flow rate 1.0 mL/min, $t_{maj} = 14.95$ min, $t_{min} = 13.86$ min, 89% *ee*); $[\alpha]_{D}^{20} = +20$ (c = 0.50 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.34-7.30 (m, 5H), 4.26 (d, J = 8.4 Hz, 1H), 3.96 (d, J = 8.4 Hz, 1H), 3.74 (s,

3H), 3.50 (s, 3H), 2.58 (s, 3H); ¹³C-NMR (100.6 MHz): 168.7, 166.4, 165.1, 156.1, 132.2, 128.7, 128.6, 128.4, 53.6, 53.2, 44.9, 36.4, 29.8, 26.4, 11.8; IR (NaCl) / cm⁻¹: 1744 s, 1515 s; HRMS: m/z found [M+H]⁺ 361.1021, C₁₇H₁₇N₂O₇ requires 361.1036.

(+)-Dimethyl -2-(4-methoxyphenyl)-3-(3-methyl-4-nitroisoxazol-5-yl)cyclopropane-1,1-dicarboxylate (7b)



Prepared following general procedure using 5-(4methoxystyryl)-3-methyl-4-nitroisoxazole **1b** (26 mg, 0.10 mmol). Reaction time: 42 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7b** as a yellow oil (38.7 mg, 99% yield).

The ee of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*PrOH 80:20, flow rate 1.0 mL/min, $t_{maj} = 18.06$ min, $t_{min} = 14.31$ min, 90% ee); $[\alpha]_{D}^{20} = +23$ (c = 0.55 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.24-7.22 (m, 2H), 6.86-6.84 (m, 2H), 4.20 (d, J = 8.4 Hz, 1H), 3.90 (d, J = 8.4 Hz, 1H), 3.79 (s, 3H), 3.73 (s, 3H), 3.53 (s, 3H), 2.57 (s, 3H); ¹³C-NMR (100.6 MHz): 168.9, 166.5, 165.2, 159.6, 156.1, 129.8, 124.0, 114.1, 55.4, 53.6, 53.2, 45.0, 36.1, 29.8, 26.6, 11.8; IR (NaCl) / cm⁻¹: 1742 s, 1518 s; HRMS: *m/z* found $[M+H]^+$ 391.1135, $C_{18}H_{19}N_2O_8$ requires 391.1141.

(+)-Dimethyl -2-(2,3-dichlorophenyl)-3-(3-methyl-4nitroisoxazol-5-yl)cyclopropane-1,1-dicarboxylate (7c)



Prepared following general procedure using 5-(2,3dichlorostyryl)-3-methyl-4-nitroisoxazole **1c** (30 mg, 0.10 mmol). Reaction time: 42 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7c** as a yellow oil (42.4 mg, 99% yield).

The ee of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*PrOH 80:20, flow rate 1.0 mL/min, $t_{maj} = 10.98$ min, $t_{min} = 8.98$ min, 91% ee); $[\alpha]_D^{20} = +20$ (c = 1.00 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.46-7.43 (m, 1H), 7.22-7.21 (m, 2H), 4.29 (d, J = 8.4 Hz, 1H), 4.00 (d, J = 8.4 Hz, 1H), 3.76 (s, 3H), 3.58 (s, 3H), 2.58 (s, 3H); ¹³C-NMR (100.6 MHz): 168.1, 165.8, 165.2, 156.2, 134.1, 133.6, 132.9, 130.6, 128.2, 127.3, 53.7, 53.5, 44.4, 35.8, 29.8, 27.2, 11.7; IR (NaCl) / cm⁻¹: 1754 s, 1518 s; HRMS: *m/z* found [M+H]⁺ 429.0266, C₁₇H₁₅N₂O₇Cl₂ requires 429.0256.

(+)-Dimethyl -2-(2-chlorophenyl)-3-(3-methyl-4-nitroisoxazol-5-yl)cyclopropane-1,1-dicarboxylate (7d)



Prepared following general procedure using 5-(2-chlorostyryl)-3-methyl-4-nitroisoxazole **1d** (27 mg, 0.10 mmol). Reaction time: 48 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7d** as a yellow oil (35.8 mg, 91% yield). The ee of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*PrOH 90:10, flow rate 1.0 mL/min, $t_{maj} = 14.50$ min, $t_{min} = 12.97$ min, 92% ee); $[\alpha]_{D}^{20} = +50$ (c = 0.65 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.41-7.39 (m, 1H), 7.31-7.27 (m, 3H), 4.31 (d, J = 8.0 Hz, 1H), 4.01 (d, J = 8.4, 1H), 3.76 (s, 3H), 3.55 (s, 3H), 2.58 (s, 3H); ¹³C-NMR (100.6 MHz): 168.5, 166.0, 165.3, 156.2, 135.8, 130.6, 129.9, 129.8, 129.7, 126.9, 53.6, 53.3, 44.4, 35.4, 29.8, 26.9, 11.8; IR (NaCl) / cm⁻¹: 1730 s, 1533 s; HRMS: *m/z* found [M+H]⁺ 395.0636, C₁₇H₁₆N₂O₇Cl requires 395.0646.

(+)-Dimethyl 2-(4-fluorophenyl)-3-(3-methyl-4-nitroisoxazol-5yl)cyclopropane-1,1-dicarboxylate (7e)



Prepared following general procedure using 5-(4-fluorostyryl)-3-methyl-4-nitroisoxazole **1e** (25 mg, 0.10 mmol). Reaction time: 24 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7e** as a yellow oil (37.4 mg, 99% yield).

The ee of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*PrOH 80:20, flow rate 1.0 mL/min, $t_{maj} = 12.32$ min, $t_{min} = 10.46$ min, 87% ee); $[\alpha]_{D}^{20} = +10$ (c = 0.72 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.32-7.29 (m, 2H), 7.05-7.01 (m, 2H), 4.22 (d, J = 8.4 Hz, 1H), 3.91 (d, J = 8.4 Hz, 1H), 3.74 (s, 3H), 3.53 (s, 3H), 2.57 (s, 3H); ¹³C-NMR (100.6 MHz): 168.5, 166.3, 165.0, 162.7 (d, J = 247 Hz), 156.2, 130.4 (d, J = 8.0 Hz), 128.0 (d, J = 3.0 Hz), 115.8 (d, J = 21 Hz), 53.7, 53.3, 44.9, 35.7, 31.7, 29.8, 11.7; IR

(NaCl) / cm⁻¹: 1754 s, 1526 s; HRMS: m/z found [M+H]⁺ 379.0936, C₁₇H₁₆N₂O₇F requires 379.0942.

(+)-Dimethyl 2-(3-methyl-4-nitroisoxazol-5-yl)-3-(thiophen-2yl)cyclopropane-1,1-dicarboxylate (7f)



Prepared following general procedure using 3-methyl-4-nitro-5-(2-(thiophen-2-yl)vinyl)isoxazole **1f** (24 mg, 0.10 mmol). Reaction time: 42 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7f** as a yellow oil (35.8 mg, 98% yield).

The ee of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*PrOH 90:10, flow rate 1.0 mL/min, $t_{maj} = 16.38$ min, $t_{min} = 14.81$ min, 87% ee); $[\alpha]_{D}^{20} = +13$ (c = 0.58 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.24 (d, J = 0.8 Hz, 1H), 7.01-7.00 (m, 1H), 6.97-6.95 (m, 1H), 4.18 (d, J = 8.0 Hz, 1H), 3.99 (d, J = 8.0 Hz, 1H), 3.73 (s, 3H), 3.61 (s, 3H), 2.57 (s, 3H); ¹³C-NMR (100.6 MHz): 168.0, 166.1, 164.8, 156.1, 134.8, 127.5, 127.1, 126.3, 53.7, 53.4, 45.3, 31.3, 29.8, 28.2, 11.7; IR (NaCl) / cm⁻¹: 1734 s, 1549 s; HRMS: *m/z* found $[M+H]^+$ 367.0582, C₁₅H₁₅N₂O₇S requires 367.0600.

(+)-Dimethyl 2-(furan-2-yl)-3-(3-methyl-4-nitroisoxazol-5yl)cyclopropane-1,1-dicarboxylate (7g)



Prepared following general procedure using 5-(2-(furan-2yl)vinyl)-3-methyl-4-nitroisoxazole **1g** (22 mg, 0.10 mmol). Reaction time: 42 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7g** as a yellow oil (34.8 mg, 99% yield).

The ee of the product was determined by CSP-HPLC using a Chiralcel OD column (*n*-hexane/*i*PrOH 90:10, flow rate 1.0 mL/min, $t_{maj} = 23.55$ min, $t_{min} = 15.32$ min, 86% ee); $[\alpha]_D^{20} = +24$ (c = 0.53 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.35-7.34 (m, 1H), 6.35-6.33 (m, 2H), 4.11 (d, J = 8.0 Hz, 1H), 3.84 (d, J = 7.6 Hz, 1H), 3.71 (s, 3H), 3.68 (s, 3H), 2.57 (s, 3H); ¹³C-NMR (100.6 MHz): 167.8, 166.0, 165.0, 156.1, 146.6, 143.0, 111.0, 109.5, 53.7, 53.5, 43.7, 29.8, 29.3, 26.5, 11.7; IR (NaCl) / cm⁻¹: 1734 s, 1518 s; HRMS: *m/z* found [M+H]⁺ 351.0820, C₁₅H₁₅N₂O₈ requires 351.0828.

(+)-Dimethyl 2-(2-methoxyphenyl)-3-(3-methyl-4-nitroisoxazol-5-yl)cyclopropane-1,1-dicarboxylate (7h)



Prepared following general procedure using 5-(2methoxystyryl)-3-methyl-4-nitroisoxazole **1h** (26 mg, 0.10 mmol). Reaction time: 72 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7h** as a yellow oil (37.8 mg, 97% yield).

The ee of the product was determined by CSP-HPLC using a Chiralcel OD column (*n*-hexane/*i*-PrOH 95:5, flow rate 0.50 mL/min, $t_{maj} = 39.46$ min, $t_{min} = 29.21$ min, 96% ee); $[\alpha]_D^{20} = +5.0$ (c = 0.31 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.31-7.27 (m, 1H), 7.18-7.16 (m, 1H), 6.94-6.90 (m, 1H), 6.87 (d, J = 8.4 Hz, 1H), 4.23 (d, J = 8.4 Hz, 1H), 3.94 (d, J = 8.4 Hz, 1H), 3.83 (s, 3H), 3.73 (s, 3H), 3.51 (s, 3H), 2.58 (s, 3H); ¹³C-NMR (100.6 MHz): 169.3, 166.6, 165.6, 158.7, 156.1, 129.7, 129.2, 129.0, 128.4, 120.9, 110.5, 55.7, 53.5, 53.0, 44.4, 32.9, 26.7, 11.8; IR (NaCl) / cm⁻¹: 1734 s, 1518 s; HRMS: *m/z* found [M-H]⁻ 389.0966, C₁₈H₁₇N₂O₈ requires 389.0985.

(+)-Dimethyl 2-(2-bromophenyl)-3-(3-methyl-4-nitroisoxazol-5yl)cyclopropane-1,1-dicarboxylate (7i)



Prepared following general procedure using 5-(2-bromostyryl)-3-methyl-4-nitroisoxazole **1i** (31 mg, 0.10 mmol). Reaction time: 45 h. Column chromatography (Solvents petroleum ether:EtOAc 9:1) afforded **7i** as a yellow oil (43.4 mg, 99% yield).

The *ee* of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*-PrOH 90:10, flow rate 1.0 mL/min, $t_{maj} = 16.78$ min, $t_{min} = 15.22$ min, 93% *ee*); $[\alpha]_{D}^{20} = +1.0$ (c = 0.62 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.60-7.58 (m, 1H), 7.33-7.26 (m, 2H), 7.23-7.18 (m, 1H), 4.31 (d, J = 8.4 Hz, 1H), 3.99 (d, J = 8.6 Hz, 1H), 3.76 (s, 3H), 3.55 (s,

3H), 2.58 (s, 3H); ¹³C-NMR (100.6 MHz): 168.4, 165.9, 165.2, 156.2, 133.0, 132.3, 130.0, 130.0, 127.5, 125.8, 53.6, 53.3, 44.6, 37.6, 27.2, 11.8; IR (NaCl) / cm⁻¹: 1738 s, 1522 s; HRMS: m/z found [M-H]⁻ 436.9993, C₁₇H₁₄N₂O₇Br requires 436.9984.

(+)-Dimethyl 2-(2,4-dimethoxyphenyl)-3-(3-methyl-4nitroisoxazol-5-yl)cyclopropane-1,1-dicarboxylate (7j)



Prepared following general procedure using 5-(2,4dimethoxystyryl)-3-methyl-4-nitroisoxazole **1j** (29 mg, 0.10 mmol). Reaction time: 72 h. Column chromatography (Solvents petroleum ether:EtOAc 85:15) afforded **7j** as a yellow oil (39.1 mg, 93% yield).

The *ee* of the product was determined by CSP-HPLC using a Chiralcel OD column (*n*-hexane/*i*-PrOH 80:20, flow rate 0.75 mL/min, $t_{maj} = 23.57$ min, $t_{min} = 20.01$ min, 94% *ee*); $[\alpha]_{D}^{20} = +4.0$ (c = 0.36 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 7.08-7.05 (m, 1H), 6.44-6.42 (m, 2H), 4.18 (d, J = 8.4 Hz, 1H), 3.87 (d, J = 8.4 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.72 (s, 3H), 3.54 (s, 3H), 2.57 (s, 3H); ¹³C-NMR (100.6 MHz): 169.4, 166.7, 165.6, 161.1, 159.7, 156.1, 129.5, 113.2, 104.0, 98.6, 55.7, 55.5, 53.4, 53.1, 44.4, 32.7, 29.8, 26.7, 11.8; IR (NaCl) / cm⁻¹: 1734 s, 1510 s; HRMS: *m/z* found [M-H]⁻ 419.1109, C₁₉H₁₉N₂O₉ requires 419.1091.

(+)-Dimethyl 2-hexyl-3-(3-methyl-4-nitroisoxazol-5yl)cyclopropane-1,1-dicarboxylate (7k)



Prepared following general procedure using 3-methyl-4-nitro-5-(oct-1-en-1-yl)isoxazole **1k** (23 mg, 0.10 mmol). Reaction time: 60 h. Column chromatography (Solvents petroleum ether:EtOAc 95:5) afforded **7k** as a colourless oil (36.4 mg, 99% yield). The *ee* of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*-PrOH 95:5, flow rate 1.0 mL/min, $t_{maj} = 6.26$ min, $t_{min} = 7.49$ min, 84% *ee*); $[\alpha]_D^{20} = +7.0$ (c = 0.32 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 3.83-3.82 (m, 4H), 3.65 (s, 3H), 3.55 (d, J = 7.6 Hz, 1H), 2.53 (s, 3H), 1.64-1.58 (m, 2H), 1.49-1.40 (m, 2H), 1.34-1.24 (m, 6H), 0.89-0.85 (m, 3H); ¹³C-NMR (100.6 MHz): 169.4, 166.8, 166.5, 165.1, 156.0, 54.1, 53.4, 43.2, 41.7, 33.1, 31.7, 28.8, 28.1, 27.2, 22.6, 14.1, 11.7; IR (NaCl) / cm⁻¹: 1750 s, 1526 s; HRMS: *m/z* found [M-H]⁻ 367.1512, C₁₇H₂₃N₂O₇ requires 367.1505.

(+)-Dimethyl 2-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-3-(3methyl-4-nitroisoxazol-5-yl)cyclopropane-1,1-dicarboxylate (71)



Prepared following general procedure using 5-(2-(2,3dihydrobenzo[b][1,4]dioxin-5-yl)vinyl)-3-methyl-4nitroisoxazole **11** (29 mg, 0.10 mmol). Reaction time: 48 h. Column chromatography (Solvents petroleum ether:EtOAc 8:2) afforded **71** as a yellow oil (39.8 mg, 95% yield). The ee of the product was determined by CSP-HPLC using a Chiralpak AD column (*n*-hexane/*i*PrOH 80:20, flow rate 1.0 mL/min, $t_{maj} = 18.58$ min, $t_{min} = 23.14$ min, 90% ee); $[\alpha]_{D}^{20} = -23$ (c = 0.88 in CHCl₃); ¹H-NMR (400 MHz, CDCl₃): 6.82-6.75 (m, 3H), 4.23 (s, 4H), 4.15 (d, J = 8.0 Hz, 1H), 3.84 (d, J = 8.0 Hz, 1H), 3.72 (s, 3H), 3.58 (s, 3H), 2.56 (s, 3H); ¹³C-NMR (100.6 MHz): 168.8, 166.4, 165.2, 156.1, 143.7, 143.6, 125.4, 125.2, 121.5, 117.6, 117.5, 64.4, 64.4, 53.6, 53.3, 44.9, 36.0, 26.7, 11.7; IR (NaCl) / cm⁻¹: 1742 s, 1522 s; HRMS: *m/z* found [M+H]⁺ 419.1078, C₁₉H₁₉N₂O₉ requires 419.1091.



























General procedure for the oxidation and successive methylation with trimethylsilyl diazomethane of cyclopropanes 7a and 7b.

To a solution of cyclopropane 7 (a, b) (0.1 mmol) in THF (1.0 mL) was added dropwise a solution of KMnO₄ in H₂O : Acetone (3.5 :1). The reaction mixture was stirred for 1 h at room temperature and then a Na_2SO_3 saturated solution (10 mL) was added to destroy the excess of $KMnO_4$: the formation of a brown precipitate was observed (MnO₂). The mixture was then acidified with HCl 6 M until pH = 3. At this point it was noted that the solution became clear. The mixture was then extracted with DCM (3 x 1mL) and the combined organic phases were evaporated. The crude (assumed 0.1 mmol) was then dissolved in diethyl ether : MeOH (9 : 1, 1 mL) and treated with trimethylsilyl diazomethane (0.6 mmol, 95 µl) added dropwise until the formation of bubbles ceased. The mixture was filtered through a small silica plug end evaporated. The product was then purified by chromatography on silica gel using dichloromethane as the eluent.

(+)-Trimethyl 3-phenylcyclopropane-1,1,2-tricarboxylate 8a.



Following the general procedure compound **8a** was obtained as a pale yellow oil (18 mg, 60% for two steps). The *ee* of the product was determined by HPLC using a Chiralpak AD column (*n*-hexane/*i*PrOH 80:20, flow rate 1.0 mL/min, $t_{maj} = 8.76$ min, $t_{min} = 5.77$ min, 85% *ee*); ¹H-NMR (400 MHz, CDCl3): 7.18 (m, 5H), 3.71 (s, 3H), 3.66 (s, 3H), 3.54 (d, J = 7.6 Hz, 1H), 3.38 (s, 3H), 3.15 (d, J = 7.6 Hz, 1H); ¹³C-NMR (100.6 MHz): 169.68, 166.58, 165.75, 132.92, 128.67, 128.49, 127.93, 53.32, 53.02,

52.75, 44.18, 36.22, 31.05; m/z found $[M+H]^+$ 293.112, $C_{15}H_{17}O_6$ requires 293.1025.

(+)-trimethyl 3-(4-methoxyphenyl)cyclopropane-1,1,2-tricarboxylate 8b.



Following the general procedure compound **8b** was obtained as a pale yellow oil (20 mg, 62% for two steps). The *ee* of the product was determined by HPLC using a Chiralpak AD column (*n*-hexane/*i*PrOH 80:20, flow rate 1.0 mL/min, $t_{maj} = 20.64$ min, $t_{min} = 8.66$ min, 87% *ee*); ¹H-NMR (400 MHz, CDCl3): 7.17 (d, J = 8.4 Hz, 2H), 6.8 (d, J = 8.4 Hz, 2H), 3.81 (s, 3H), 3.78 (s, 3H), 3.75 (s, 3H), 3.58 (d, J = 7.6 Hz, 1H), 3.50 (s, 3H), 3.21 (d, J = 7.6 Hz, 1H); ¹³C-NMR (100.6 MHz): 169.74, 166.66, 165.82, 159.21, 129.77, 124.77, 113.86, 55.34, 53.28, 53.05, 52.72, 44.21, 35.74, 31.20; *m/z* found [M+H]⁺ 323.1102, C₁₆H₁₉O₇ requires 323.1131.

(+)-3-Phenyl-cyclopropane-1,1,2-tricarboxylic acid dimethyl ester 10.



¹H-NMR (400 MHz, CDCl3): 7.33-7.25 (m, 5H), 3.81 (s, 3H), 3.66 (d, J = 7.2, 1H), 3.50 (s, 3H), 3.25 (d, J = 7.2, 1H), ¹³C-NMR (100.6 MHz): 174.9, 166.3, 165.5, 132.6, 128.7, 128.6, 128.1, 53.4, 53.1, 44.7, 36.6, 30.8; m/z found [M+H]⁺ 279.0894, C₁₄H₁₅O₆ requires 279.0869.



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm





HPLC Data



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Software Version	6.3.1.0504	Date	: 14/04/2011 16:03:19
Operator	manager	Sample Name	: CD57
Sample Number	SER200	Study	:
AutoSampler	Backin Elmost I.C.	Rack/Vial	: 0/1
Instrument Name Instrument Serial # : Delay Time Sampling Rate :	None 0.00 min 2.2727 pts/s	A/D mV Range End Time	: 1000 : 40.00 min
Sample Volume :	1.00000 ul	Area Reject	: 0.000000
Sample Amount :	1.0000	Dilution Factor	: 1.00
Data Acquisition Time :	05/02/2011 12:12:32	Cycle	: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD57CD57B10%.1ml.40minB.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia\CD57CD57B10%.1ml.40minB.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia\CD57CD57B10%.1ml.40minB.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA/Results/Claudia/CD57CD57B10%.1ml.40minB.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia\CD57CD57B10%.1ml.40minB.001.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver8.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD57-B10%.1ml.40min-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1 2		13.860 14.945	756307.00 12775120.70	32729.20 466119.54	5.59 94.41	5.59 94.41			*MM *MM	0.7563 12.7751	0.7563 12.7751
			13531427.70	498848.74	100.00	100.00				13.5314	13.5314

Missing Component Report

Component Expected Retention (Calibration File)

All components were found

Electronic Supplementary Material (ESI) for Chemical Communications This journal is The Royal Society of Chemistry 2012



Software Version Operator Sample Number AutoSampler Instrument Name Instrument Serial # Delay Time Sampling Rate Sample Volume Sample Amount	: 6.3.1.0504 : manager : : SER200 : PerkinElmer LC : None : 0.00 min : 2.2727 pts/s : 1.00000 ul : 1.000	Date Sample Name Study Rack/Vial Channel A/D mV Range End Time Area Reject	: 14/04/2011 15:59:04 : CD57 Racemate : : 0/3 : A : 1000 : 18.57 min : 0.000000
Sample Amount Data Acquisition Time	: 1.0000 : 04/12/2010 17:57:16	Dilution Factor	: 1.00
Raw Data File : C:\TO	ALCHROM DATA\Results\Claudia\CD57 Rad	emate.ad.B10%.	.1ml.A.003.raw

Result File : C:\TOTALCHROM DATA\Results\LClaudia\CD57 Racemate.ad.B10%.1ml.A.003.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD57 Racemate.ad.B10%.1ml.A.003.raw Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD57 Racemate ad.B10%.1ml.A.003.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD57 Racemate.ad.B10%.1ml.A.003.rst [Editing in Progress] Report Format File: C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD57 Racemate.ad.B10%.1ml.A.003.rst [Editing in Progress] Report Format File: C:\TOTALCHROM DATA\Sequences\CD57 racemate ad.B10%.1ml.-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1 2		13.112 14.439	1946287.12 1969012.57	84065.70 76093.49	49.71 50.29	49.71 50.29			*MM *MM	1.9463 1.9690	1.9463 1.9690
			3915299.69	160159.19	100.00	100.00				3.9153	3.9153

Missing Component Report

Component Expected Retention (Calibration File)

All components were found



Electronic Supplementary Material (ESI) for Chemical Communications This journal is The Royal Society of Chemistry 2012
Software Version	: 6.3.1.0504	Date	: 14/04/2011 16:33:46
Operator	: manager	Sample Name	: CD60 second
Sample Number	:	Study	:
AutoSampler	: SER200	Rack/Vial	: 0/1
Instrument Name	: PerkinElmer LC	Channel	: B
Instrument Serial #	: None	A/D mV Range	: 1000
Delay Time Sampling Rate Sample Volume Sample Amount Data Acquisition Time	: 0.00 min : 2.2727 pts/s : 1.000000 ul : 1.0000 : 12/04/2011 17:52:14	End Time Area Reject Dilution Factor Cycle	: 29.99 min : 0.000000 : 1.00 : 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD60 secondCD60 second.ad.B20%.1ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD60 secondCD60 second.ad.B20%.1ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD60 secondCD60 second.ad.B20%.1ml.B.001.raw

Proc Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia results\CD60 second.ad.B20%.1ml.B.001.rst [Editing in Progress]

Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia results\CD60 second.ad.B20%.1ml.B.001.rst [Editing in Progress]

Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt

Sequence File : C:\TOTALCHROM DATA\Sequences\CD60 second-.ad.B20%.1ml.-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV"sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1		14.307 18.062	806631.17 14753116.60	27698.33 398002.78	5.18 94.82	5.18 94.82			*MM *MM	0.8066 14.7531	0.8066 14.7531
			15559747.77	425701.12	100.00	100.00				15.5597	15.5597

Missing Component Report

Component Expected Retention (Calibration File)



Software Version Operator Sample Number AutoSampler		6.3.1.0504 manager SER200	Date Sample Name Study Rack/Vial		20/04/2011 12:26:39 CD100Asecond 0/1
Instrument Name	:	PerkinElmer LC	Channel	:	В
Instrument Serial #	:	None	A/D mV Range	:	1000
Delay Time	:	0.00 min	End Time	:	29.99 min
Sampling Rate	:	2.2727 pts/s			
Sample Volume	:	1.000000 ul			
Sample Amount Data Acquisition Time	:	1.0000 13/04/2011 10:27:01	Area Reject Dilution Factor Cycle	-	1.00

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD100AsecondCD100Asecond.ad.B20%.1ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD100AsecondCD100Asecond.ad.B20%.1ml.B.001.rst [Editing in Progress]

Inst Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM

DATA\Results\Claudia\CD100AsecondCD100Asecond.ad.B20%.1ml.B.001.raw

Proc Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia

results\CD100AsecondCD100Asecond.ad.B20%.1ml.B.001.rst [Editing in Progress]

Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia

results\CD100AsecondCD100Asecond.ad.B20%.1ml.B.001.rst [Editing in Progress]

Report Format File: C:\PenExe\TcWS\Ver8.3.1\Config\User\manager\Default.rpt

Sequence File : C:\TOTALCHROM DATA\Sequences\CD100Asecond-.ad.B20%.1ml.-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV"sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1		13.493	2928873.27	108961.91	50.44	50.44			*MM	2.9289	2.9289
2		16.874	2877244.27	84670.65	49.56	49.56			*MM	2.8772	2.8772
			5806117.54	193632.56	100.00	100.00				5.8061	5.8061

Missing Component Report

Component Expected Retention (Calibration File)





Software Version		6.3.1.0504	Date		14/04/2011 16:37:02
Operator	÷	manager	Sample Name	÷	CD61
Sample Number	:		Study	÷	
AutoSampler	:	SER200	Rack/Vial	÷	0/1
Instrument Name	:	PerkinElmer LC	Channel	:	в
Instrument Serial #	:	None	A/D mV Range	:	1000
Delay Time	:	0.00 min	End Time	:	29.99 min
Sampling Rate	:	2.2727 pts/s			
Sample Volume	:	1.000000 ul			
Sample Amount	:	1.0000	Area Reject	÷	0.000000
Data Acquisition Time	:	07/02/2011 17:52:23	Cycle	:	1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD61CD61.ad.B20%.1ml.30minB.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia\CD61CD61.ad.B20%.1ml.30minB.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD61CD61.ad.B20%.1ml.30minB.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD61CD61.ad.B20%.1ml.30minB.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD61CD61.ad.B20%.1ml.30minB.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD61CD61.ad.B20%.1ml.30minB.001.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver8.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD61-.ad.B20%.1ml.30min-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1 2		8.976 10.978	342538.49 7105561.83	20994.23 329210.98	4.60 95.40	4.60 95.40			*MM *MM	0.3425 7.1056	0.3425 7.1056
			7448100.32	350205.21	100.00	100.00				7.4481	7.4481

Missing Component Report

Component Expected Retention (Calibration File)

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Page 1 of 1

Software Version	:	6.3.1.0504	Date	:	14/04/2011 16:38:39
Operator	:	manager	Sample Name	:	CD 61 Racemate
Sample Number	- 1		Study	:	
AutoSampler	- 1	SER200	Rack/Vial	:	0/3
Instrument Name	:	PerkinElmer LC	Channel	:	A
Instrument Serial #	- 1	None	A/D mV Range	:	1000
Delay Time	- 1	0.00 min	End Time	:	24.60 min
Sampling Rate	- 1	2.2727 pts/s			
Sample Volume	- 1	1.000000 ul			
Sample Amount	:	1.0000	Area Reject	÷	0.000000
Data Acquisition Tir	me :	23/01/2011 16:48:21	Dilution Factor	÷	1.00
			Cycle	-	1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD61 Racemate.ad.B20%.1ml.A.003.raw Result File : C:\TOTALCHROM DATA\Results\Claudia\CD61 Racemate.ad.B20%.1ml.A.003.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B20%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD61 Racemate.ad.B20%.1ml.A.003.raw Proc Method : C:\TOTALCHROM DATA\Methods\B20%-1mL-120min.mth from C:\TOTALCHROM DATA\Results\Claudia\CD61 Racemate.ad.B20%.1ml.A.003.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1mL-120min.mth from C:\TOTALCHROM DATA\Results\Claudia\CD61 Racemate.ad.B20%.1ml.A.003.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1mL-120min.mth from C:\TOTALCHROM DATA\Results\Claudia\CD61 Racemate.ad.B20%.1ml.A.003.rst [Editing in Progress] Report Format File: C:\TOTALCHROM DATA\Methods\default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD61 Racemate.ad.B20%.1ml.-..seq

DEFAULT REPORT

Peak	Time	Area	Height	Area	Norm. Area	BL	Area/Height
#	[min]	[µV·s]	[µV]	[%]	[%]		[s]
1	8.353	6546068.10	415162.25	50.48	50.48	*MM	15.7675
	10.076	6422218.06	336283.39	49.52	49.52	*MM	19.0976
		12968286.16	751445.64	100.00	100.00		

Missing Component Report Component Expected Retention (Calibration File)

Electronic Supplementary Material (ESI) for Chemical Communications This journal is C The Royal Society of Chemistry 2012



Software Version Operator Sample Number AutoSampler Instrument Name Instrument Serial # Delay Time Sampling Rate	: 6.3.1.0504 : manager : : SER200 : PerkinElmer LC : None : 0.00 min : 2.2727 pts/s	Date Sample Name Study Rack/Vial Channel A/D mV Range End Time	: 14/04/2011 16:41:48 : CD63 : : 0/1 : B : 1000 : 40.00 min
Sample Volume	: 1.000000 ul	Area Reject	: 0.000000
Sample Amount	: 1.0000	Dilution Factor	: 1.00
Data Acquisition Time	: 11/02/2011 11:41:58	Cvcle	: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD63CD63.ad.B10%.1ml.40minB.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD63CD63.ad.B10%.1ml.40minB.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia\CD63CD63.ad.B10%.1ml.40minB.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD63CD63.ad.B10%.1ml.40minB.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD63CD63.ad.B10%.1ml.40minB.001.rst [Editing in Progress] Report Format File: C:\TOTALCHROM DATA\Sequences\blank-.ad.B10%.1ml.40min-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV"sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1 2		12.973 14.498	699919.77 16430668.01	30818.51 590314.32	4.09 95.91	4.09 95.91			*MM *MM	0.6999 16.4307	0.6999 16.4307
			17130587.78	621132.83	100.00	100.00				17.1306	17.1306

Missing Component Report

Component Expected Retention (Calibration File)



Software Version	: 6.3.1.0504	Date	: 14/04/2011 16:43:09
Operator	: manager	Sample Name	: CD63 Racemate
Sample Number	1	Study	1
AutoSampler	: SER200	Rack/Vial	: 0/1
Instrument Name	: PerkinElmer LC	Channel	: B
Instrument Serial #	: None	A/D mV Range	: 1000
Delay Time	: 0.00 min	End Time	: 31.86 min
Sampling Rate	: 2.2727 pts/s		
Sample Volume	: 1.000000 ul	1200 - <u>-</u> 0202000 - 1	
Sample Amount	: 1.0000	Area Reject	: 0.000000
Data Acquisition Time	: 17/12/2010 16:48:03	Dilution Factor	: 1.00
		Cycle	: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD63 Racemate.ad.B10%.1ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia\CD63 Racemate.ad.B10%.1ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD63 Racemate.ad.B10%.1ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD63 Racemate.ad.B10%.1ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD63 Racemate.ad.B10%.1ml.B.001.rst [Editing in Progress] Report Format File: C:\PenExe\ToW S\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD63 Racemate.ad.B10%.1ml.-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV"sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1 2		12.489	1247421.65 1212189.21	54173.93 47759.79	50.72 49.28	50.72 49.28			*MM *MM	1.2474	1.2474
			2459610.87	101933.73	100.00	100.00				2.4596	2.4596

Missing Component Report

Component Expected Retention (Calibration File)

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Software Version	:	6.3.1.0504
Operator	:	manager
Sample Number	:	
AutoSampler	:	SER200
Instrument Name	:	PerkinElmer LC
Instrument Serial #	:	None
Delay Time	:	0.00 min
Sampling Rate	:	2.2727 pts/s
Sample Volume	:	1.000000 ul
Sample Amount	:	1.0000
Data Acquisition Time	:	11/02/2011 14:08:34

 Date
 : 14/04/2011 16:46:51

 Sample Name
 : CD64

 Study
 :

 Rack/Vial
 : 0/1

 Channel
 : B

 A/D mV Range
 : 1000

 End Time
 : 29.99 min

Area Reject: 0.000000 Dilution Factor : 1.00 Cycle: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD64CD64.ad.B20%.1ml.30minB.001-20110211-140844.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD64CD64.ad.B20%.1ml.30minB.001-20110211-144342.rst [Editing in Progress]

Inst Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD64CD64.ad.B20%.1ml.30minB.001-20110211-140844.raw Proc Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia results\CD64CD64.ad.B20%.1ml.30minB.001-20110211-144342.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia results\CD64CD64.ad.B20%.1ml.30minB.001-20110211-144342.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD64-.ad.B20%.1ml.30min-..seq

DEFAULT REPORT

Peak Component #Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range	Raw Adjusted Amount Amount
1	10.450	918828.39	49186.42	6.62	6.62	*MM 0.9188 0.9188
2	12.320	12956534.55	540228.36	93.38	93.38	*MM 12.9565 12.9565
		13875362.94	589414.78	100.00	100.00	13.8754 13.8754

Missing Component Report

Component Expected Retention (Calibration File)



Software Version	: 6.3.1.0504	Date	: 14/04/2011 16:48:55
Operator	: manager	Sample Name	: CD64 Racemate
Sample Number		Study	1.000
AutoSampler	: SER200	Rack/Vial	: 0/4
Instrument Name	: PerkinElmer LC	Channel	: A
Instrument Serial #	: None	A/D mV Range	: 1000
Delay Time	: 0.00 min	End Time	: 15.33 min
Sampling Rate	: 2.2727 pts/s		
Sample Volume	: 1.000000 ul	0000320000372	
Sample Amount	: 1.0000	Area Reject: 0.0	000000
Data Acquisition Tim	TALCHROM DATA Results Clau	Dilution Factor: Idia\CD64 Rac €nate:.a d.B20%	: 1.00 .1ml.A.004.raw
Result File : C:\TOT	ALCHROM DATA\Results\Claudia	CD64 Racemate.ad.B20%.1m	1.A.004.rst
Inst Method : C:\TO	TALCHROM DATA\Methods\B20%	-1mL-120min from C:\TOTAL	CHROM
DATA\Results\Clau	dia\CD64 Racemate.ad.B20%.1ml	.A.004.raw	
Proc Method : C:\TC	TALCHROM DATA\Methods\B20	%-1mL-120min.mth from C:\TC	DTALCHROM
DATA\Results\Clau	dia\CD64 Racemate.ad.B20%.1ml	A.004.rst [Editing in Progress]	
Calib Method : C:\T	OTALCHROM DATA\Methods\B20	%-1mL-120min.mth from C:\T(OTALCHROM
DATA\Results\Clau	dia\CD64 Racemate.ad.B20%.1ml	A.004.rst [Editing in Progress]	1
Report Format File:	C:\TOTALCHROM DATA\Methods	\default.rpt	
Sequence File : C:\]	TOTAL CHROM DATA\Sequences\	CD64 Racemate ad B20% 1m	- sea

DEFAULT REPORT

Peak #	Time [min]	Area [µV·s]	Height [µV]	Area [%]	Norm. Area [%]	BL	Area/Height [5]
1	10.179	4816175.88	256414.38	49.79	49.79	*MM	18.7828
2	11.917	4856298.93	218456.69	50.21	50.21	*MM	22.2300

9672474.81 474871.07 100.00 100.00

Missing Component Report Component Expected Retention (Calibration File)



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Software Version	: 6.3.1.0504	Date : 15/04/2011 12:30:24
Operator	: manager	Sample Name : CD68
Sample Number		Study :
AutoSampler	: SER200	Rack/Vial : 0/1
Instrument Name	: PerkinElmer LC	Channel : B
Instrument Serial #	: None	A/D mV Range : 1000
Delay Time	: 0.00 min	End Time : 40.00 min
Sampling Rate	: 2.2727 pts/s	
Sample Volume	: 1.000000 ul	
Sample Amount	: 1.0000	Area Reject: 0.000000
Data Acquisition Time	: 17/02/2011 11:10:27	Dilution Factor : 1.00 Cycle: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD68CD68B10%.1.0ml.40minB.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD68CD68B10%.1.0ml.40minB.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia\CD68CD68B10%.1.0ml.40minB.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD68CD68B10%.1.0ml.40minB.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD68CD68B10%.1.0ml.40minB.001.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver8.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD68-B10%.1.0ml.40min-..seq

			DE	FAL	JLT REPO	RT
Peak Component #Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range	Raw Adjusted Amount Amount
1	16.383	28380202.40	912851.83	6.72	6.72	*MM 2.0435 2.0435
2				93.28	93.28	*MM 28.3802 28.3802
		30423661.34	985815.19	100.00	100.00	30.4237 30.4237

Missing Component Report Component Expected Retention (Calibration File)

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Software Version	: 6.3.1.0504	Date	: 15/04/2011 12:32:38		
Operator	: manager	Sample Name	: CD68 Racemate		
Sample Number	1	Study	1		
AutoSampler	: SER200	Rack/Vial	: 0/3		
Instrument Name	: PerkinElmer LC	Channel	: B		
Instrument Serial #	: None	A/D mV Range	: 1000		
Delay Time	: 0.00 min	End Time	: 16.57 min		
Sampling Rate	: 2.2727 pts/s				
Sample Volume	: 1.000000 ul				
Sample Amount	: 1.0000	Area Reject: 0.0	000000		
Data Acquisition Time	: 17/12/2010 17:57:16	Dilution Factor : 1.00 Cycle: 3			
Raw Data File : C:\TO	TALCHROM DATA\Results\Claudia	CD68 Racemate.ad.B10%.	1ml.B.003.raw		

Result File : C:\TOTALCHROM DATA\Results\Claudia\CD68 Racemate.ad.B10%.1ml.B.003.rst Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD68 Racemate.ad.B10%.1ml.B.003.raw Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD68 Racemate.ad.B10%.1ml.B.003.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD68 Racemate.ad.B10%.1ml.B.003.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD68 Racemate.ad.B10%.1ml.-..seq

DEFAULT REPORT

Peak Componen #Name[min]	nt Time	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range		Raw Adj Amount A	usted Amount
1	13.112	1432427.08	61795.88	49.83	49.83	"MM	1.4324	1.4324
2	14.439	1442196.21	55915.41	50.17	50.17	*MM	1.4422	1.4422
		2874623.29	117711.29	100.00	100.00		2.8746	2.8746

Missing Component Report

Component Expected Retention (Calibration File)





Software Version	: 6.3.1.0504	Date : 15/04/2011 12:40:4
Operator	: manager	Sample Name : CD69ChiralcellOD
Sample Number		Study :
AutoSampler	: SER200	Rack/Vial : 0/1
Instrument Name	: PerkinElmer LC	Channel : B
Instrument Serial #	: None	A/D mV Range : 1000
Delay Time	: 0.00 min	End Time : 59.99 min
Sampling Rate	: 2.2727 pts/s	
Sample Volume	: 1.000000 ul	
Sample Amount	: 1.0000	Area Reject: 0.000000
Data Acquisition Time	: 25/03/2011 12:57:32	Cycle: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD69ChiralcellODCD69ChiralcellOD.ad.B10%.1.0ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD69ChiralcellODCD69ChiralcellOD.ad.B10%.1.0ml.B.001.rst [Editing in Progress]

Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-60min from C:\TOTALCHROM DATA\Results\Claudia\CD69ChiralcelIODCD69ChiralcelIOD.ad.B10%.1.0ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-60min from C:\TOTALCHROM DATA\Results\Claudia results\CD69ChiralcelIODCD69ChiralcelIOD.ad.B10%.1.0ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-60min from C:\TOTALCHROM DATA\Results\Claudia results\CD69ChiralcelIODCD69ChiralcelIOD.ad.B10%.1.0ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-60min from C:\TOTALCHROM DATA\Results\Claudia results\CD69ChiralcelIODCD69ChiralcelIOD.ad.B10%.1.0ml.B.001.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD69ChiralcelIOD.-ad.B10%.1.0ml.-..seq

DEFAULT REPORT

Peak Component	Time	Area	Height	Area	Norm. Area Cal.VoltBL		Raw Adj	usted
#Name	[min]	[uV*sec]	[uV]	[%]	[%]Range Range		Amount A	Amount
1 2	15.319	327538.04	7263.67	7.07	7.07	*MM	0.3275	0.3275
	23.547	4302042.55	59652.43	92.93	92.93	*MM	4.3020	4.3020
		4629580.59	66916.10	100.00	100.00		4.6296	4.6296

Missing Component Report Component Expected Retention (Calibration File)

Electronic Supplementary Material (ESI) for Chemical Communications This journal is The Royal Society of Chemistry 2012



Software Version Operator Sample Number AutoSampler Instrument Name Instrument Serial # Delay Time Sampling Rate Sample Volume Sample Amount Data Acquisition Time	: 6.3.1.0504 : manager : : SER200 : PerkinElmer LC : None : 0.00 min : 2.2727 pts/s : 1.000000 ul : 1.0000 : 29/04/2011 14:21:37	Date : Sample Name : Study : Rack/Vial : Channel : A/D mV Range : End Time : Area Reject : Dilution Factor :	29/04/2011 15:04:44 CD69-A Racemate 0/1 B 1000 40.00 min 0.000000 1.00
Data Acquisition Time	: 29/04/2011 14:21:37	Cycle :	: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD69-A RacemateCD69-A Racemate.ad.B10%.1ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD69-A RacemateCD69-A Racemate.ad.B10%.1ml.B.001.rst [Editing in Progress]

Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia\CD69-A RacemateCD69-A Racemate.ad.B10%.1ml.B.001.raw

Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD69-A RacemateCD69-A Racemate.ad.B10%.1ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD69-A

Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD69-A RacemateCD69-A Racemate.ad.B10%.1ml.B.001.rst [Editing in Progress]

Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt

Sequence File : C:\TOTALCHROM DATA\Sequences\Blank-.ad.B10%.1ml.-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1		14.564 23.115	14271944.53 14259224.82	286916.46 197132.92	50.02 49.98	50.02 49.98			*MM *MM	14.2719 14.2592	14.2719 14.2592
			28531169.35	484049.38	100.00	100.00				28.5312	28.5312

Missing Component Report

Component Expected Retention (Calibration File)



Software Version	: 6.3.1.0504	Date : 15/04/2011 14:55:38
Operator	: manager	Sample Name : CD75BestOD
Sample Number	1	Study :
AutoSampler	: SER200	Rack/Vial : 0/1
Instrument Name	: PerkinElmer LC	Channel : B
Instrument Serial #	: None	A/D mV Range : 1000
Delay Time	: 0.00 min	End Time : 59.99 min
Sampling Rate	: 2.2727 pts/s	
Sample Volume	: 1.000000 ul	and the second second second second second second
Sample Amount	: 1.0000	Area Reject: 0.000000
Data Acquisition Time	: 05/04/2011 18:25:23	Dilution Factor : 1.00 Cycle: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD75BestODCD75BestOD.ad.B5%.0.50ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD75BestODCD75BestOD.ad.B5%.0.50ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B5%-0.5mL-80min from C:\TOTALCHROM DATA\Results\Claudia\CD75BestODCD75BestOD.ad.B5%.0.50ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B5%-0.5mL-80min from C:\TOTALCHROM DATA\Results\Claudia results\CD75BestODCD75BestOD.ad.B5%.0.50ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B5%-0.5mL-80min from C:\TOTALCHROM DATA\Results\Claudia results\CD75BestODCD75BestOD.ad.B5%.0.50ml.B.001.rst [Editing in Progress] Report Format File: C:\TOTALCHROM DATA\Sequences\CD91OD-.ad.B5%.0.50ml.-.seq

DEFAULT REPORT

Peak Component #Name	Time [min]	Area [uV"sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range		Raw Adjusted Amount Amount
1	29.135	213070.47	3498.73	2.00	2.00	"MM	0.2131 0.2131
2	39.461	10456185.32 10669255.79	89610.60 93109.33	98.00	98.00	*MM	10.4562 10.4562
					100.00		10.6693 10.6693

Missing Component Report Component Expected Retention (Calibration File)



Software Version Operator Sample Number AutoSampler Instrument Name	: 6.3.1.0504 : manager : : SER200 : PerkinElmer LC	Date : 15/04/2011 15:00:52 Sample Name : CD910D Study : Rack/Vial : 0/1 Channel : B AD cm/0 Rames : 1000
Delay Time	: 0.00 min	A/D mV Range : 1000 End Time : 59.99 min
Sampling Rate Sample Volume Sample Amount Data Acquisition Time	: 2.2727 pts/s : 1.00000 ul : 1.0000 : 05/04/2011 15:22:02	Area Reject: 0.000000 Dilution Factor : 1.00 Cycle: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD910DCD910D.ad.B5%.0.50ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD910DCD910D.ad.B5%.0.50ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B5%-0.5ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B5%-0.5ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B5%-0.5ml.B.001.raw Calib Method : C:\TOTALCHROM DATA\Methods\B5%-0.5mL-60min from C:\TOTALCHROM DATA\Results\Claudia results\CD910DCD910D.ad.B5%.0.50ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B5%-0.5mL-60min from C:\TOTALCHROM DATA\Results\Claudia results\CD910DCD910D.ad.B5%.0.50ml.B.001.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD910D-.ad.B5%.0.50ml.-.seq

DEFAULT REPORT

Peak Component #Name	[min]	[min]	Area [uV"sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range		Raw Adj Amount A	usted Amount
1	28.842	6734901.13	73626.80	50.16	50.16	*MM	6.7349	6.7349	
2	39.864	6690779.14	57245.53	49.84	49.84	*MM	6.6908	6.6908	
		13425680.26	130872.33	100.00	100.00		13.4257	13.4257	

Missing Component Report

Component Expected Retention (Calibration File)

Electronic Supplementary Material (ESI) for Chemical Communications This journal is The Royal Society of Chemistry 2012



Software Version	: 6.3.1.0504	Date : 1	5/04/2011 15:03:23			
Operator	: manager	Sample Name : C	D76			
Sample Number	1	Study :				
AutoSampler	: SER200	Rack/Vial : 0	/1			
Instrument Name	: PerkinElmer LC	Channel : B	1			
Instrument Serial #	: None	A/D mV Range : 1	000			
Delay Time	: 0.00 min	End Time : 4	0.00 min			
Sampling Rate	: 2.2727 pts/s					
Sample Volume	: 1.000000 ul					
Sample Amount	: 1.0000	Area Reject: 0.0000	00			
Data Acquisition Time	: 24/02/2011 15:07:32	Dilution Factor : 1.00 Cycle: 1				

Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD76CD76.ad.B10%.1ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Results\Claudia results\CD76CD76.ad.B10%.1ml.B.001.rst [Editing in Progress] DATA\Results\Claudia\CD76CD76.ad.B10%.1ml.B.001.raw

Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD76CD76.ad.B10%.1ml.B.001.rst [Editing in Progress]

Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD76CD76.ad.B10%.1ml.B.001.rst [Editing in Progress]

Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt

Sequence File : C:\TOTALCHROM DATA\Sequences\CD76-.ad.B10%.1ml.-..seq

DEFAULT REPORT

Peak Component #Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range		Raw Adjusted Amount Amount
1	15.217	472008.21	18308.40	3.28	3.28	*MM	0.4720 0.4720
2	16.779	13902224.40	444960.11	96.72	96.72	*MM	13.9022 13.9022
					100.00		14.3742 14.3742

Missing Component Report

Component Expected Retention (Calibration File)





Software Version	: 6.3.1.0504	Date : 15/04/2011 15:05:25
Operator	: manager	Sample Name : CD92
Sample Number		Study :
AutoSampler	: SER200	Rack/Vial : 0/1
Instrument Name	: PerkinElmer LC	Channel : B
Instrument Serial #	: None	A/D mV Range : 1000
Delay Time	: 0.00 min	End Time : 40.00 min
Sampling Rate	: 2.2727 pts/s	
Sample Volume	: 1.000000 ul	
Sample Amount	: 1.0000	Area Reject: 0.000000
Data Acquisition Time	: 30/03/2011 11:11:32	Dilution Factor: 1.00 Cycle: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD92CD92.ad.B10%.1ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD92CD92.ad.B10%.1ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia\CD92CD92.ad.B10%.1ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD92CD92.ad.B10%.1ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B10%-1mL-40min from C:\TOTALCHROM DATA\Results\Claudia

results\CD92CD92.ad.B10%.1ml.B.001.rst [Editing in Progress]

Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt

Sequence File : C:\TOTALCHROM DATA\Sequences\Blank-.ad.B10%.1ml.-..seq

DEFAULT REPORT

Peak Component #Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range		Raw Adjusted Amount Amount
1	13.156	15129904.88	564799.47	50.08	50.08	*MM	15.1299 15.1299
2	14.395	15079482.20	519665.54	49.92	49.92	*MM	15.0795 15.0795
		30209387.08	1.08e+06	100.00	100.00		30,2094 30,2094

Missing Component Report

Component Expected Retention (Calibration File)

Electronic Supplementary Material (ESI) for Chemical Communications This journal is The Royal Society of Chemistry 2012

Software Version	: 6.3.1.0504	Date	: 15/04/2011 15:08:22
Operator	: manager	Sample Name	: CD77Best
Sample Number	1	Study	:
AutoSampler	: SER200	Rack/Vial	: 0/1
Instrument Name	: PerkinElmer LC	Channel	: B
Instrument Serial #	: None	A/D mV Range	: 1000
Delay Time	: 0.00 min	End Time	: 40.00 min
Sampling Rate	: 2.2727 pts/s		
Sample Volume	: 1.000000 ul		
Sample Amount	: 1.0000	Area Reject: 0.0	000000
Data Acquisition Time	: 25/03/2011 12:12:51	Cycle: 1	1.00

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD77BestCD77Best.ad.B20%.0.75ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD77BestCD77Best.ad.B20%.0.75ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B20%-0.75mL-40min from C:\TOTALCHROM DATA\Results\Claudia\CD77BestCD77Best.ad.B20%.0.75ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B20%-0.75mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD77Best.ad.B20%.0.75ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-0.75mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD77BestCD77Best.ad.B20%.0.75ml.B.001.rst [Editing in Progress] Report Format File: C:\TOTALCHROM DATA\Sequences\CD77Best-, ad.B20%.0.75ml.-..seq

DEFAULT REPORT

Peak Component #Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range		Raw Adjusted	
1	20.013	166014.38	1976.39	2.87	2.87	"MM	0.1660	0.1660
2	23.569	5609374.76	69153.20	97.13	97.13	*MM	5.6094	5.6094
		5775389.15	71129.60	100.00	100.00		5.7754	5.7754

Missing Component Report

Component Expected Retention (Calibration File)



Software Version	: 6.3.1.0504	Date : 15/04/2011 15:10:36	1
Operator	: manager	Sample Name : CD93ChiralcelIOD	
Sample Number	1	Study :	
AutoSampler	: SER200	Rack/Vial : 0/1	
Instrument Name	: PerkinElmer LC	Channel : B	
Instrument Serial #	: None	A/D mV Range : 1000	
Delay Time	: 0.00 min	End Time : 40.00 min	
Sampling Rate	: 2.2727 pts/s		
Sample Volume	: 1.000000 ul		
Sample Amount	: 1.0000	Area Reject: 0.000000	
Data Acquisition Time	: 05/04/2011 17:30:34	Dilution Factor : 1.00 Cycle: 1	

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD93ChiralcellODCD93ChiralcellOD.ad.B20%.0.75ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD93ChiralcellODCD93ChiralcellOD.ad.B20%.0.75ml.B.001.rst [Editing in Progress]

Inst Method : C:\TOTALCHROM DATA\Methods\B20%-0.75mL-40min from C:\TOTALCHROM DATA\Results\Claudia\CD93ChiralcellODCD93ChiralcellOD.ad.B20%.0.75ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B20%-0.75mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD93ChiralcellODCD93ChiralcellOD.ad.B20%.0.75ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-0.75mL-40min from C:\TOTALCHROM DATA\Results\Claudia results\CD93ChiralcellODCD93ChiralcellOD.ad.B20%.0.75ml.B.001.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD93ChiralcellOD.ad.B20%.0.75ml.-..seq

DEFAULT REPORT

Peak Component #Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range		Raw Adjusted Amount Amount	
1	18.517	3805366.87	46415.32	47.70	47.70	"MM	3.8054	3.8054
2	21.963	4172767.99	57112.58	52.30	52.30	"MM	4.1728	4.1728
		7978134.87	103527.90	100.00	100.00		7.9781	7.9781

Missing Component Report

Component Expected Retention (Calibration File)

Electronic Supplementary Material (ESI) for Chemical Communications This journal is C The Royal Society of Chemistry 2012


Software Version		6.3.1.0504	Date	:	20/04/2011 14:49:28
Operator	-	manager	Sample Name	÷	CD88-C
Sample Number	:		Study	:	
AutoSampler	:	SER200	Rack/Vial	:	0/1
Instrument Name	:	PerkinElmer LC	Channel	:	в
Instrument Serial #	:	None	A/D mV Range	:	1000
Delay Time	:	0.00 min	End Time	:	15.00 min
Sampling Rate	:	2.2727 pts/s			
Sample Volume	:	1.000000 ul			
Sample Amount	:	1.0000	Area Reject	÷	0.000000
Data Acquisition Time	1	20/04/2011 12:38:43	Dilution Factor	ŝ	1.00
			Cycle	•	

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD88-CCD88-C.ad.B5%.1ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD88-CCD88-C.ad.B5%.1ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B5%-1mL-15min from C:\TOTALCHROM DATA\Results\Claudia\CD88-CCD88-C.ad.B5%.1ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B5%-1mL-15min from C:\TOTALCHROM DATA\Results\Claudia results\CD88-CCD88-C.ad.B5%.1ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B5%-1mL-15min from C:\TOTALCHROM DATA\Results\Claudia results\CD88-CCD88-C.ad.B5%.1ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B5%-1mL-15min from C:\TOTALCHROM DATA\Results\Claudia results\CD88-CCD88-C.ad.B5%.1ml.B.001.rst [Editing in Progress] Report Format File: C:\TOTALCHROM DATA\Sequences\Blank-.ad.B5%.1ml.-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1		8 283	10470752 70	001383.87	01 30	01.30			*MM	10 4708	10 4708
2		7 4 9 5	997870 53	73822.33	8.69	8 69			*MM	0.9979	0.9979
3		13.662	478.27	52.05	0.00	0.00			*MM	0.0005	0.0005
4		14.696	334.97	54.06	0.00	0.00			*MM	0.0003	0.0003
			11478436.57	975292.11	100.00	100.00				11.4784	11.4784

Missing Component Report

Component Expected Retention (Calibration File)



Software Version Operator Sample Number AutoSampler Instrument Name Instrument Serial # Delay Time Sampling Rate Sample Volume Sample Amount		6.3.1.0504 manager SER200 PerkinElmer LC None 0.00 min 2.2727 pts/s 1.000000 ul 1.0000	Date Sample Name Study Rack/Vial Channel A/D mV Range End Time Area Reject 0.0 Dilution Factor :	: : : : :	15/04/2011 15:13:14 CD-97 0/1 B 1000 29.99 min
Data Acquisition Time	1	30/03/2011 15:25:19	Cycle: 1		

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD97CD-97.ad.B5%.1.0ml.B.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD97CD-97.ad.B5%.1.0ml.B.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B5%-1mL-30min from C:\TOTALCHROM DATA\Results\Claudia\CD97CD-97.ad.B5%.1.0ml.B.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B5%-1mL-30min from C:\TOTALCHROM DATA\Results\Claudia results\CD97CD-97.ad.B5%.1.0ml.B.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B5%-1mL-30min from C:\TOTALCHROM DATA\Results\Claudia results\CD97CD-97.ad.B5%.1.0ml.B.001.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD97-.ad.B5%.1.0ml.-..seq

DEFAULT REPORT

Peak Component #Name	Time [min]	Area [uV"sec]	Height [uV]	Area [%]	Norm. Area Cal.VoltBL [%]Range Range		Raw Adjusted Amount Amount	
1	6.747	5621722.72	441060.84	49.66	49.66	*MM	5.6217	5.6217
2	8.118	5697925.19	373365.25	50.34	50.34	*MM	5.6979	5.6979
		11319647.91	814426.09	100.00	100.00		11.3196	11.3196

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Component Expected Retention (Calibration File)

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Software Version	: 6.3.1.0504	Date : 14/04/2011 16:55:24
Operator	: manager	Sample Name : CD65
Sample Number	:	Study :
AutoSampler	: SER200	Rack/Vial : 0/1
Instrument Name	: PerkinElmer LC	Channel : B
Instrument Serial #	: None	A/D mV Range : 1000
Delay Time	: 0.00 min	End Time : 29.99 min
Sampling Rate	: 2.2727 pts/s	
Sample Volume	: 1.000000 ul	
Sample Amount	: 1.0000	Area Reject: 0.000000
Data Acquisition Time	: 11/02/2011 14:57:42	Dilution Factor : 1.00
		Cycle: 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD65CD65.ad.B20%.1ml.30minB.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia results\CD65CD65.ad.B20%.1ml.30minB.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD65CD65.ad.B20%.1ml.30minB.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia results\CD65CD65.ad.B20%.1ml.30minB.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia results\CD65CD65.ad.B20%.1ml.30minB.001.rst [Editing in Progress] Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt

Sequence File : C:\TOTALCHROM DATA\Sequences\CD64-.ad.B20%.1ml.30min-..seq

	DEFAULT REPORT								
Peak Component #Name	Component Time Area Height Area me [min] [uV*sec] [uV] [%]		Intea Norm. Area Cal.VoltBL [%]Range Range			Raw Adjusted Amount Amount			
1	18.575	7974959.83	202182.09	95.05	95.05	*MM	7.9750	7.9750	
2	23.144	415397.11	9722.32	4.95	4.95	*MM	0.4154	0.4154	
		8390356.94	211904.41	100.00	100.00		8.3904	8.3904	

Missing Component Report Component Expected Retention (Calibration File)

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: CD65 Racemate : : 0/12 : B : 1000
: : 0/12 : B : 1000
: 0/12 : B : 1000
: B : 1000
: 1000
: 32.35 min
00000
1.00
0

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD65 Racemate.ad.B20%.1ml.B.007.raw Result File : C:\TOTALCHROM DATA\Results\Claudia\CD65 Racemate.ad.B20%.1ml.B.007.rst Inst Method : C:\TOTALCHROM DATA\Methods\B20%-1mL-120min from C:\TOTALCHROM DATA\Results\Claudia\CD65 Racemate.ad.B20%.1ml.B.007.raw Proc Method : C:\TOTALCHROM DATA\Methods\B20%-1mL-120min.mth from C:\TOTALCHROM DATA\Results\Claudia\CD65 Racemate.ad.B20%.1ml.B.007.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1mL-120min.mth from C:\TOTALCHROM DATA\Results\Claudia\CD65 Racemate.ad.B20%.1ml.B.007.rst [Editing in Progress] Report Format File: C:\TOTALCHROM DATA\Methods\default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD65 Racemate.ad.B20%.1ml.-..seq

					DEF	AL	ILT RI	EPORT
Peak #	Time [min]	Area [u]/.s]	Height	Area	Norm. Area	BL	Area/Height	
				[70]			[0]	
1	18.304	412861.13	9746.55	52.61	52.61	*MM *N4N4	42.3597	
2	22.991			47.59	47.59	IVIIVI	40.0049	
		784763.13	17816.48	100.00	100.00			

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Software Version Operator Sample Number	: 6.3.1.0504 : manager	Date : 02/06/2011 16:18:54 Sample Name : CD56 Study :
AutoSampler Instrument Name	: SER200 : PerkinElmer LC	Rack/Vial : 0/1 Channel : A
Instrument Serial # Delay Time	: None : 0.00 min	A/D mV Range : 1000 End Time : 29.99 min
Sampling Rate Sample Volume Sample Amount Data Acquisition Time	: 2.2727 pts/s : 1.00000 ul : 1.0000 : 04/02/2011 13:14:20	Area Reject : 0.000000 Dilution Factor : 1.00 Cycle : 1

Raw Data File : C:\TOTALCHROM DATA\Results\Claudia\CD56CD56B20%.1ml.30minA.001.raw Result File : C:\TOTALCHROM DATA\Results\Claudia\CD56CD56B20%.1ml.30minA.001.rst [Editing in Progress] Inst Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD56CD56B20%. 1ml.30minA.001.raw Proc Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD56CD56B20%. 1ml.30minA.001.rst [Editing in Progress] Calib Method : C:\TOTALCHROM DATA\Methods\B20%-1.0mL.30min from C:\TOTALCHROM DATA\Results\Claudia\CD56CD56B20%. 1ml.30minA.001.rst [Editing in Progress] Report Format File: C:\PenExe\ToWS\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\CD56-B20%.1ml.30min-.seq



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Report Format File: C:\PenExe\Tc\WS\Ver6.3.1\Config\User\manager\Default.rpt Sequence File : C:\TOTALCHROM DATA\Sequences\PRS-.ad.B20%.1ml.30min.-..seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1		9.064 22.103	1609535.81 23689544.13	95525.18 529096.62	6.36 93.64	6.36 93.64			*MM *MM	1.6095 23.6895	1.6095 23.6895
			25299079.94	624621.79	100.00	100.00				25.2991	25.2991

Missing Component Report

Component Expected Retention (Calibration File)