Supporting Information for

Highly Enantioselective Organocatalytic Biginelli Reaction

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Table S1. A Survey of Solvents.^a

Entry	Solvent	Catalyst (mol%)	Time (d)	Yield (%) ^b	Ee (%)
1	CH ₂ Cl ₂	20	4	91	85
2	THF	20	4	63	61
3	PhCH ₃	20	4	86	79
4	CHCl ₃	20	4	89	79
5	Et ₂ O	20	4	66	66
6	PhCH ₃	20	4	92	80
7	CH ₂ Cl ₂	10	4	75	82 ^d
8	CH ₂ Cl ₂	10	4	84	85
9	CH ₂ Cl ₂	10	6	94	85

^a The reaction was carried out in a 0.2 mmol scale and the ratio of **1a**/ **2**/ **3a** is 1/ 1.2/ 3. ^b Isolated yield based on aldehyde and analytically pure **4aa**. ^c Determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 70 : 30, flow rate 1.0 mL/min). ^d Addition of 5A MS (500mg).

Scheme S1. Scalemic Preparation of Optically Active Monastrol.

General data: NMR spectra were recorded on a Bruker-300 MHz spectrometer. Optical rotations were measured on a Perkin-Elmer 241 Polarimeter at $\lambda = 589$ nm. FT-ICRMS spectra were recorded on P-SIMS-Gly of Bruker Daltonics Inc. Infrared spectra were recorded on a Nicolet MX-1E FT-IR spectrometer. HPLC analysis was performed on Waters-Breeze (2487 Dual λ Absorbance Detector and 1525 Binary HPLC Pump). Chiralpak AS and AD columns were purchased from Daicel Chemical Industries, LTD. Solvents for the column chromatography were distilled before use.

Materials: All starting materials were purchased from Acros or Aldrich and used directly.

Experimental Section:

The preparation of catalysts: Chiral catalysts **7a-d** were prepared on the base of the literature procedures.¹⁻³

(R)-2,6-Bis-(4-fluoro-phenyl)-4-oxo-3,5-dioxo-4 λ 5-phospha-cyclohepta[2,1-a;3,4-a']dinaphthalen-4-ol (7b**):** $[\alpha]_{\text{D}}^{28} = -117.3^\circ$ ($c = 0.4$, CHCl_3); white solid; mp 252-254 °C; ^1H NMR (DMSO, 300 MHz) δ (ppm) 7.10 (d, $J = 8.6$ Hz, 2H), 7.28-7.34 (m, 6H), 7.50 (t, $J = 7.7$ Hz, 2H), 7.93-7.98 (m, 4H), 8.10 (d, $J = 7.9$ Hz, 2H), 8.15 (s, 2H); ^{13}C NMR (DMSO, 300 MHz) δ (ppm) 114.49, 122.33, 125.44, 126.01, 126.62, 128.59, 130.49, 130.83, 131.57, 132.04, 132.14, 132.86, 133.75, 145.82, 145.94, 160.20, 163.44; IR (KBr): γ 3455, 1736, 1596, 1509, 1246, 1153, 833 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{32}\text{H}_{18}\text{F}_2\text{O}_4\text{P}_1 + \text{Na}_2)^+$ requires m/z 581.0701, found m/z 581.0706.

The synthesis of chiral catalysts **8a-8c**:

(R)-4-Oxo-2,6-diphenyl--3,5-dioxo-4 λ 5-phospha-cyclohepta[2,1-a;3,4-a']dinaphthalen-4-ol (8a**):** Compound **A** was prepared by following the procedure described by Schaus.⁴ To a solution of

A (2 mmol) in pyridine (5 mL) was added phosphorus oxychloride (4.0 mmol) at room temperature under N₂ and the reaction mixture was stirred at 70 °C for 3 h. Then water (3 mL) was added and the resulting suspension was stirred for the additional 2 h. Dichloromethane was added and pyridine was removed by the reverse extraction with aqueous HCl (6.0 M). The organic phase was dried over Na₂SO₄ and purified by column chromatography on silica gel (2% MeOH in CH₂Cl₂) to yield **8a** as a white solid (864 mg, 85% yield). $[\alpha]_D^{28} = -241.5^\circ$ (c = 0.4, CHCl₃); m.p. 286-288 °C; ¹H NMR (DMSO, 300 MHz) δ (ppm) 1.54-1.61 (m, 3H), 1.77 (m, 3H), 2.16-2.24 (m, 1H), 2.610-2.69 (m, 1H), 2.84-2.86 (m, 2H), 7.20 (s, 1H), 7.31-7.44 (m, 3H), 7.612-7.65 (m, 2H); ¹³C NMR (DMSO, 75 MHz) δ (ppm) 22.12, 27.33, 28.47, 127.08, 127.15, 128.06, 129.35, 130.85, 134.35, 136.59, 137.14, 143.16, 143.29; IR (KBr): γ 3422, 2931, 2856, 1447, 1253, 1219, 1019, 767, 697 cm⁻¹; HRMS (FT-ICRMS) exact mass calcd for (C₃₂H₂₈O₄P₁+Na₂)⁺ requires m/z 553.1515, found m/z 553.1508.

(R)-2,6-Bis-(4-fluoro-phenyl)-4-oxo--3,5-dioxa-4I5-phospha-cyclohepta[2,1-a;3,4-a']dinaphthalen-4-ol (8b): $[\alpha]_D^{28} = -166.8^\circ$ (c = 0.41, CHCl₃); white solid; mp 265-268 °C; ¹H NMR (DMSO, 300 MHz) δ (ppm) 1.50-1.57 (m, 1H), 1.74 (m, 3H), 2.11-2.19 (m, 1H), 2.57-2.65 (m, 1H), 2.79-2.82 (m, 2H), 7.13-7.23 (m, 3H), 7.73-7.78 (m, 2H); ¹³C NMR (DMSO, 75 MHz) δ (ppm) 22.23, 27.40, 28.51, 127.77, 128.11, 129.59, 130.18, 131.59, 132.66, 136.34, 136.87, 145.17, 145.29; IR (KBr) γ 3415, 2933, 2857, 1602, 1511, 1229, 1193, 835 cm⁻¹; HRMS (FT-ICRMS) exact mass calcd for (C₃₂H₂₆F₂O₄P₁+Na₂)⁺ requires m/z 589.1327, found m/z 589.1352.

(R)-2,6-Bis-(4-chloro-phenyl)-4-oxo--3,5-dioxa-4I5-phospha-cyclohepta[2,1-a;3,4-a']dinaphthalen-4-ol (8c): $[\alpha]_D^{28} = -137.1^\circ$ (c = 0.21, CHCl₃); white solid; mp 252-254 °C; ¹H NMR (DMSO, 300 MHz) δ (ppm) 1.49-1.52 (m, 1H), 1.73 (m, 3H), 2.10-2.15 (m, 1H), 2.55-2.62 (m, 1H), 2.78-2.82 (m, 2H), 7.09 (s, 1H), 7.42 (d, *J* = 8.5 Hz, 2H,), 7.84-7.87 (d, *J* = 8.4 Hz, 2H); ¹³C NMR (DMSO, 75 MHz) δ (ppm) 22.28, 27.42, 28.47, 127.77, 128.11, 129.59, 130.18, 131.59, 132.66, 136.34, 136.87, 145.17, 145.29; IR (KBr): γ 3409, 2931, 2856, 1633, 1494, 1245, 1197, 1097, 826 cm⁻¹; HRMS (FT-ICRMS) exact mass calcd for (C₃₂H₂₆Cl₂O₄P₁+Na₂)⁺ requires m/z 621.0736, found m/z 621.0753.

General Procedure for the organocatalytic Biginelli reaction:

After a solution of aldehyde (0.2 mmol), thiourea (0.24 mmol) and a chiral phosphoric acid (0.02 mmol) in CH₂Cl₂ (3ml) was stirred at 25 °C for 2h, a β -keto ester (0.6 mmol) was added. The resulting reaction mixture was stirred at 25 °C for 6 days (monitored by TLC) and then EtOAc (3 mL) and some silica gel were added. After removal of solvent, the residue was purified through

flash column chromatography on a silica gel (eluent: petroleum ether: ethyl acetate = 6:1- 3:1) to yield pure products.

6-Methyl-4-(4-nitro-phenyl)-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4aa): $[\alpha]_D^{28} = -158.2^\circ$ ($c = 0.5$, EtOAc); white solid; mp 178-180 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.19 (t, $J = 7.1$ Hz, 3H), 2.37 (s, 3H), 4.07-4.14 (q, 2H), 5.50 (s, 1H), 7.46 (d, $J = 8.3$ Hz, 2H), 7.99 (brs, 1H), 8.16 (d, $J = 8.3$ Hz, 2H), 8.35 (brs, 1H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 14.10, 18.46, 55.37, 60.85, 102.08, 124.16, 127.74, 143.77, 147.68, 148.89, 164.79, 174.04.; IR (KBr) γ 3299, 3171, 2981, 1708, 1685, 1663, 1564, 1521, 1346, 1193, 1174, 1108, 855 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{16}\text{N}_3\text{O}_4\text{S}_1)^+$ requires m/z 322.0856, found m/z 322.0871; Enantiomeric excess: 85%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 70: 30, flow rate 1.0 mL/min): $t_R = 14.68$ min (major), $t_R = 19.66$ min (minor).

4-(3-Fluoro-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ba): $[\alpha]_D^{28} = -85.8^\circ$ ($c = 0.41$, EtOAc); white solid; mp 188-190 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 0.82 (t, $J = 7.1$ Hz, 3H), 2.00 (s, 3H), 3.68-.375 (m, 2H), 4.96 (d, $J = 3.5$ Hz, 1H), 6.55-6.67 (m, 2H), 6.73-6.76 (m, 1H), 6.89-6.96 (m, 1H), 8.98 (brs, 1H), 9.59 (brs, 1H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 13.69, 17.24, 53.89, 59.45, 100.54, 113.21, 114.01, 122.02, 129.60, 144.86, 145.69, 163.78, 165.01, 174.420; IR (KBr) γ 3294, 3182, 2984, 2936, 1681, 1640, 1561, 1453, 1187, 1112, 782, 694 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{15}\text{F}_1\text{N}_2\text{O}_2\text{S}_1 + \text{Na})^+$ requires m/z 317.0730, found m/z 317.0746; Enantiomeric excess: 91%, determined by HPLC (Daicel Chirapak AD-H, hexane/ isopropanol = 80: 20, flow rate 1.0 mL/min): $t_R = 7.08$ min (minor), $t_R = 8.15$ min (major).

6-Methyl-4-(3-nitro-phenyl)-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ca): $[\alpha]_D^{28} = -100.5^\circ$ ($c = 0.38$, EtOAc); white solid; mp 203-205 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.01 (t, $J = 7.1$ Hz, 3H,), 2.29 (s, 3H), 3.95-4.03 (m, 2H), 5.35 (d, $J = 3.7$ Hz, 1H), 7.43-7.59 (m, 2H,), 8.00-8.04 (m, 1H), 8.08-8.10 (m, 1H); 9.43 (brs, 1H), 10.02 (brs, 1H), ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 13.61, 17.29, 53.70, 59.59, 99.95, 121.37, 122.05, 129.16, 132.53, 145.05, 145.52, 147.63, 164.811, 174.59; IR (KBr): γ 3432, 3181, 2930, 1713, 1658, 1593, 1531, 1344, 1189, 1102, 735, 688 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{15}\text{N}_3\text{O}_4\text{S}_1 + \text{Na})^+$ requires m/z 344.0675, found m/z 344.0665; Enantiomeric excess: 88%, determined by HPLC (Daicel Chirapak AD-H, hexane/ iso-propanol = 80: 20, flow rate 1.0 mL/min): $t_R = 12.58$ min (major), $t_R = 14.87$ min (minor).

4-(2-Chloro-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4da): $[\alpha]_{\text{D}}^{28} = -47.8^{\circ}$ ($c = 0.28$, EtOAc); white solid; mp 148-150 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.05 (t, $J = 7.1$ Hz, 3H), 2.45 (s, 3H), 3.98-4.10 (m, 2H), 5.90 (d, $J = 2.7$ Hz, 1H), 7.20-7.25 (m, 4H), 7.36-7.40 (m, 1H), 7.98 (brs, 1H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 13.88, 18.15, 52.76, 60.40, 100.71, 127.73, 128.33, 129.77, 129.95, 132.61, 138.29, 144.36, 164.82, 174.46; IR (KBr) γ 3422, 3215, 2980, 2928, 1707, 1652, 1570, 1465, 1194, 1179, 1099, 748 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{15}\text{Cl}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 333.0435, found m/z 333.0427; Enantiomeric excess: 91%, determined by HPLC (Daicel Chirapak AS-H, hexane/isopropanol = 90: 10, flow rate 1.0 mL/min): $t_{\text{R}} = 12.43$ min (minor), $t_{\text{R}} = 14.70$ min (major).

4-(3-Chloro-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ea): $[\alpha]_{\text{D}}^{28} = -102.6^{\circ}$ ($c = 0.5$, EtOAc); white solid; mp 142-144 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.09 (t, $J = 7.1$ Hz, 3H), 2.27 (s, 3H), 3.94-4.04 (m, 2H), 5.21(d, $J = 3.3$ Hz, 1H), 7.10-7.19 (m, 4H), 9.19 (brs, 1H), 9.78 (brs, 1H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 13.62, 17.28, 54.07, 59.47, 100.47, 124.61, 126.51, 127.25, 129.41, 133.46, 144.75, 145.04, 164.95, 174.34; IR (KBr) γ 3422, 3185, 2982, 1706, 1647, 1574, 1472, 1194, 1180, 1098, 775, 696 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{15}\text{Cl}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 333.0435, found m/z 333.0433; Enantiomeric excess: 90%, determined by HPLC (Daicel Chirapak AS-H, hexane/isopropanol = 70: 30, flow rate 1.0 mL/min): $t_{\text{R}} = 8.66$ min (major), $t_{\text{R}} = 10.90$ min (minor).

6-Methyl-4-(2-nitro-phenyl)-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4fa): $[\alpha]_{\text{D}}^{28} = -282.0$ ($c = 0.35$, EtOAc); white solid; mp 178-180 °C; ^1H NMR (DMSO, 300 MHz) δ (ppm) 0.93 (t, $J = 7.1$ Hz, 3H), 2.31 (s, 3H), 2.83-3.89 (m, 2H), 5.96 (d, $J = 2.9$ Hz, 1H), 7.50-7.57 (m, 2H), 7.73-7.76 (m, 1H), 7.92-7.95 (m, 1H), 9.59 (brs, 1H), 10.46 (brs, 1H); ^{13}C NMR (DMSO, 75 MHz) δ (ppm) 13.70, 17.12, 49.21, 59.56, 99.84, 124.24, 129.15, 129.49, 134.29, 138.08, 145.84, 147.24, 164.53, 174.15; IR (KBr) γ 3233, 2957, 2926, 1720, 1657, 1573, 1523, 1464, 1193, 1092, 762 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{15}\text{N}_3\text{O}_4\text{S}_1+\text{Na})^+$ requires m/z 344.0675, found m/z 344.0672; Enantiomeric excess: 90%, determined by HPLC (Daicel Chirapak AD-H, hexane/ isopropanol = 90: 10, flow rate 1.0 mL/min): $t_{\text{R}} = 20.74$ min (minor), $t_{\text{R}} = 27.86$ min (major).

4-(3-Bromo-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ga): $[\alpha]_{\text{D}}^{28} = -86.3^{\circ}$ ($c = 0.32$, MeOH); white solid; mp 149-151 °C; ^1H NMR (DMSO, 300 MHz) δ (ppm) 1.10 (t, $J = 7.0$ Hz, 3H), 2.29 (s, 3H), 4.00-4.04 (m, 2H), 5.17 (d, $J = 2.3$ Hz, 1H),

7.20-7.22 (m, 1H), 7.30-7.37 (m, 2H), 7.47-7.49 (m, 1H), 9.67 (brs, 1H), 10.40 (brs, 1H); ^{13}C NMR (DMSO, 75 MHz) δ (ppm) 13.97, 17.18, 53.56, 59.68, 100.10, 121.65, 125.37, 129.25, 130.54, 130.95, 145.54, 146.00, 164.93, 174.34; IR (KBr) γ 3304, 3186, 2981, 2926, 1663, 1576, 1460, 1193, 1115, 770, 666 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{15}\text{Br}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 376.9930, found m/z 376.9945; Enantiomeric excess: 91%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 70: 30, flow rate 1.0 mL/min): t_R = 8.80 min (major), t_R = 11.30 min (minor).

4-(3,5-Dibromo-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ha): $[\alpha]_D^{28} = -126.3^\circ$ ($c = 0.51$, EtOAc); white solid; mp 208-210 $^\circ\text{C}$; ^1H NMR (DMSO, 300 MHz) δ (ppm) 1.20 (t, $J = 7.1$ Hz, 3H), 2.38 (s, 3H), 4.12 (m, 2H), 5.34 (d, $J = 2.9$ Hz, 1H), 7.36 (d, $J = 1.7$ Hz, 2H), 7.58 (m, 1H), 7.74 (brs, 1H), 8.15 (brs, 1H); ^{13}C NMR (DMSO, 75 MHz) δ (ppm) 14.10, 18.49, 55.26, 60.74, 100.79, 123.34, 128.78, 134.03, 143.66, 145.82, 164.72, 174.45; IR (KBr) γ 3418, 3176, 2997, 2930, 1708, 1686, 1646, 1578, 1462, 1197, 1191, 1095, 853, 727 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{15}\text{Br}_2\text{N}_2\text{O}_2\text{S}_1)^+$ requires m/z 432.9216, found m/z 432.9207; Enantiomeric excess: 96%, determined by HPLC (Daicel Chirapak AD-H, hexane/ iso-propanol = 80: 20, flow rate 1.0 mL/min): t_R = 6.56 min (minor), t_R = 7.80 min (major).

4-(3,5-Bis-trifluoromethyl-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ia): (the reaction was carried out on a 0.5 mmol scale); $[\alpha]_D^{28} = -57.4^\circ$ ($c = 0.46$, EtOAc); white solid; mp 105-107 $^\circ\text{C}$; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.16 (t, $J = 7.1$ Hz, 3H), 2.38 (s, 3H), 4.10 (m, 2H), 5.55 (d, $J = 3.1$ Hz, 1H), 7.73 (s, 2H), 7.79 (s, 1H), 8.21 (brs, 1H), 8.59 (brs, 1H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 13.46, 18.24, 55.21, 60.83, 101.64, 122.28, 124.79, 131.94, 144.33, 144.82, 164.69, 174.61; IR (KBr) γ 3195, 2985, 1713, 1656, 1582, 1472, 1372, 1275, 1169, 1128, 894, 680 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{16}\text{H}_{15}\text{F}_6\text{N}_2\text{O}_2\text{S}_1)^+$ requires m/z 413.0753, found m/z 413.0730; Enantiomeric excess: 97%, determined by HPLC (Daicel Chirapak AD-H, hexane/ isopropanol = 95: 5, flow rate 1.0 mL/min): t_R = 7.28 min (minor), t_R = 14.93 min (major).

4-(4-Methoxycarbonyl-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ja): $[\alpha]_D^{28} = -165.2^\circ$ ($c = 0.31$, EtOAc); white solid; mp 168-170 $^\circ\text{C}$; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.15 (t, $J = 7.1$ Hz, 3H), 2.35 (s, 3H), 3.89 (s, 3H), 4.03 - 4.11 (m, 2H), 5.43 (d, $J = 3.0$ Hz, 1H,), 7.33-7.36 (m, 2H), 7.77 (brs, 1H), 7.95-7.98 (m, 2H), 8.28 (brs, 1H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 14.04, 18.32, 52.19, 55.76, 60.54, 102.31, 126.79, 130.05,

130.19, 143.31, 146.98, 165.00, 166.57, 174.60; IR (KBr) γ 3410, 3291, 3195, 2981, 2950, 1721, 1649, 1566, 1459, 1281, 1180, 1107, 811 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{16}\text{H}_{19}\text{N}_2\text{O}_4\text{S}_1)^+$ requires m/z 335.1060, found m/z 335.1057; Enantiomeric excess: 90%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 70 : 30, flow rate 1.0 mL/min): t_R = 10.85 min (major), t_R = 17.53 min (minor).

4-(1-Bromo-naphthalen-2-yl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ka): $[\alpha]_D^{28} = -37.5$ ($c = 0.44$, EtOAc); white solid; mp 180-182 $^{\circ}\text{C}$; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 0.99 (t, $J = 7.1$ Hz, 3H), 2.484 (s, 3H), 3.96 (m, 2H), 6.16 (d, $J = 2.7$ Hz, 1H), 7.34 (m, 2H), 7.55-7.63 (m, 2H), 7.77-7.82 (m, 2H), 8.07 (brs, 1H), 8.35 (d, $J = 8.5$ Hz, 1H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 13.92, 18.17, 56.33, 60.38, 101.30, 123.00, 124.62, 127.12, 127.92, 128.13, 129.02, 132.26, 134.33, 137.91, 144.32, 164.87, 174.18; IR (KBr) γ 3415, 3177, 2981, 2928, 1707, 1649, 1567, 1460, 1314, 1184, 1098, 755 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{18}\text{H}_{18}\text{Br}_1\text{N}_2\text{O}_2\text{S}_1)^+$ requires m/z 405.0267, found m/z 405.0268; Enantiomeric excess: 91%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 70: 30, flow rate 1.0 mL/min): t_R = 9.31 min (major), t_R = 14.40 min (minor).

4-Cyclohexyl-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4la): $[\alpha]_D^{28} = +220.6^{\circ}$ ($c = 0.31$, EtOAc); white solid; mp 196-198 $^{\circ}\text{C}$; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 8.20 (brs, 1H), 7.65 (brs, 1H), 4.12-4.21 (m, 3H), 2.30 (s, 3H), 1.49-1.72 (m, 6H), 1.27 (t, $J = 7.1$ Hz, 3H), 1.20-1.01 (m, 5H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 175.7, 165.7, 143.7, 101.6, 60.3, 57.1, 44.8, 28.5, 26.5, 26.1, 26.0, 25.8, 18.1, 14.2; IR (KBr) γ 3172, 2981, 2920, 2849, 17.3, 1640, 1468, 1272, 1189, 1094, 772 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{22}\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 305.1294, found m/z 305.1282; Enantiomeric excess: 92%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 85: 15, flow rate 1.0 mL/min): t_R = 9.199 min (minor); t_R = 10.866 min (major).

6-Methyl-4-styryl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4ma) : white solid; mp 176-178 $^{\circ}\text{C}$; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.29 (t, $J = 7.1$ Hz, 3H,), 2.32 (s, 3H), 4.16-4.25 (m, 2H), 5.02 (m, 1H), 6.11-6.53 (m, 2H,), 7.14 (brs, 1H), 7.30-7.36 (m, 5H), 7.81 (brs, 1H), ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 14.29, 18.46, 53.91, 60.52, 101.73, 126.68, 127.17, 128.15, 128.61, 131.19, 135.86, 143.08, 165.14, 175.80; IR (KBr): γ 3157, 2976, 1702, 1646, 1586, 1181, 1094, 1019, 961, 757 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{16}\text{H}_{18}\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 325.0981, found m/z 325.1006; Enantiomeric excess: 88%, determined by HPLC

(Daicel Chirapak AD-H, hexane/ iso-propanol = 85: 15, flow rate 1.0 mL/min): t_R = 10.86 min (major), t_R = 12.25 min (minor).

4-(3-Methoxy-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4na) : $[\alpha]_D^{25} = -102.9^\circ$ ($c = 0.31$, EtOAc); white solid; mp 170-172 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.18(t, $J = 7.1$ Hz, 3H,), 2.34 (s, 3H), 3.75 (s, 3H), 4.04-4.12 (m, 2H), 5.34 (d, $J = 3.1$ Hz, 1H), 6.77-6.87 (m, 3H), 7.18-7.26 (m, 1H), 7.90 (brs, 1H), 8.49 (brs, 1H), ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 14.05, 18.08, 55.18, 55.84, 60.34, 102.62, 112.64, 113.35, 118.92, 129.84, 143.07, 143.76, 159.82, 165.22, 174.21; IR (KBr): γ 3157, 2996, 1707, 1648, 1593, 1486, 1324, 1274, 1189, 1093, 755, 694 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{15}\text{H}_{19}\text{N}_2\text{O}_3\text{S}_1)^+$ requires m/z 307.1111, found m/z 307.1120; Enantiomeric excess: 90%, determined by HPLC (Daicel Chirapak AS-H, hexane/ iso-propanol = 70: 30, flow rate 1.0 mL/min): t_R = 10.87 min (major), t_R = 15.10 min (minor).

5-Methoxycarbonyl-6-methyl-4-(3-bromo-phenyl)-3,4-dihydropyrimidin-2(1H)-thione (4gb): $[\alpha]_D^{28} = -90.5^\circ$ ($c = 0.39$, EtOAc); white solid; mp 192-194 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 7.84 (brs, 1H), 7.41-7.45 (m, 2H), 7.29 (brs, 1H), 7.20-7.26 (m, 2H), 5.37 (d, $J = 3.0$ Hz, 1H), 3.66 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 174.8, 165.5, 144.3, 143.4, 131.6, 130.6, 129.8, 125.4, 123.0, 102.2, 55.6, 51.6, 18.6; IR (KBr) γ 3292, 2954, 1658, 1540, 1345, 1194, 1172, 1110, 776, 673 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{13}\text{H}_{13}\text{Br}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 362.9773, found m/z 362.9770; Enantiomeric excess: 91%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 70: 30, flow rate 1.0 mL/min): t_R = 11.429 min (major), t_R = 14.718 min (minor).

5-Methoxycarbonyl-6-methyl-4-(3,5-dibromo-phenyl)-3,4-dihydropyrimidin-2(1H)-thione (4hb): $[\alpha]_D^{28} = -108.5^\circ$ ($c = 0.26$, EtOAc); white solid; mp 194-196 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 7.94 (brs, 1H), 7.59-7.60 (m, 1H), 7.48 (brs, 1H), 7.34-7.35 (m, 2H), 5.34 (d, $J = 3.2$ Hz, 1H); 3.68 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 174.7, 165.4, 145.7, 144.1, 134.2, 128.7, 123.6, 101.7, 55.2, 51.8, 18.7; IR (KBr) γ 3181, 2949, 1697, 1651, 1558, 1430, 1177, 1112, 856, 729 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{13}\text{H}_{12}\text{Br}_2\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 440.8878, found m/z 440.8862; Enantiomeric excess: 96%, determined by HPLC (Daicel Chirapak AD-H, hexane/ isopropanol = 80: 20, flow rate 1.0 mL/min): t_R = 7.208 min (minor); t_R = 8.324 min (major).

iso-Propyl-4-(3-bromo-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

(4gc): $[\alpha]_{\text{D}}^{28} = -98.7^{\circ}$ ($c = 0.23$, EtOAc); white solid; mp 142-144 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 7.67 (brs, 1H), 7.42-7.44 (m, 2H), 7.19-7.26 (m, 2H), 7.12 (brs, 1H), 5.36 (d, $J = 1.0\text{ Hz}$, 1H), 4.96-4.99 (m, 1H), 2.37 (s, 3H), 1.24 (d, $J = 6.3\text{ Hz}$, 3H), 1.07 (d, $J = 6.2\text{ Hz}$, 3H), ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 174.7, 164.4, 144.6, 142.8, 131.5, 130.5, 130.1, 125.5, 122.8, 102.7, 68.2, 55.9, 22.0, 21.6, 18.4; IR (KBr) γ 3422, 3174, 2978, 1705, 1650, 1572, 1469, 1192, 1177, 1096, 774, 696 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{15}\text{H}_{17}\text{Br}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 391.0086, found m/z 391.0096; Enantiomeric excess: 92%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 80: 20, flow rate 1.0 mL/min): $t_{\text{R}} = 9.271\text{ min}$ (major), $t_{\text{R}} = 12.905\text{ min}$ (minor).

iso-Propyl-4-(3-fluoro-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (4bc): $[\alpha]_{\text{D}}^{28} = -68.7^{\circ}$ ($c = 0.45$, EtOAc); white solid; mp 174-176 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 7.76 (brs, 1H), 7.30-7.31 (m, 1H), 7.21 (brs, 1H), 7.08 (d, $J = 7.9\text{ Hz}$, 1H), 6.99-7.01 (m, 2H), 5.39 (d, $J = 2.8\text{ Hz}$, 1H); 4.96-4.99 (m, 1H); 2.37 (s, 3H); 1.22 (d, $J = 6.2\text{ Hz}$, 3H), 1.06 (d, $J = 6.2\text{ Hz}$, 3H); IR (KBr) γ 3430, 3160, 2987, 1703, 1649, 1595, 1485, 1276, 1195, 1094, 770, 710 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{15}\text{H}_{17}\text{F}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 331.0887, found m/z 331.0876; Enantiomeric excess: 94%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 80: 20, flow rate 1.0 mL/min): $t_{\text{R}} = 9.711\text{ min}$ (major), $t_{\text{R}} = 12.709\text{ min}$ (minor).

tert-Butyl-4-(3-bromo-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (4jd): $[\alpha]_{\text{D}}^{28} = -86.8^{\circ}$ ($c = 0.34$, EtOAc); white solid; mp 178-180 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 7.64 (brs, 1H), 7.42-7.44 (m, 2H), 7.22-7.23 (m, 2H), 7.11 (brs, 1H), 5.31 (d, $J = 2.7\text{ Hz}$, 1H); 2.34 (s, 3H), 1.36 (s, 9H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 174.6, 164.1, 144.6, 142.1, 131.5, 130.6, 130.0, 125.4, 122.8, 103.7, 81.5, 56.0, 28.1, 18.3; IR (KBr) γ 3170, 2975, 1705, 1651, 1584, 1472, 1201, 1158, 1098, 770, 695 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{16}\text{H}_{19}\text{Br}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 405.0243, found m/z 405.0235; Enantiomeric excess: 92%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 80: 20, flow rate 1.0 mL/min): $t_{\text{R}} = 8.989\text{ min}$ (major), $t_{\text{R}} = 11.590\text{ min}$ (minor).

tert-Butyl-4-(3-fluoro-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (4bd): $[\alpha]_{\text{D}}^{28} = -67.9^{\circ}$ ($c = 0.38$, EtOAc); white solid; mp 168-170 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 7.61 (brs, 1H), 7.26-7.34 (m, 1H), 7.06-7.26 (m, 2H), 6.98-7.02 (m, 2H), 5.35 (d, $J = 3.0\text{ Hz}$, 1H), 2.34 (s, 3H), 1.36 (s, 9H); IR (KBr) γ 3426, 3176, 2980, 170, 1649, 1590, 1485, 1452,

1200, 1158, 1095, 780, 695 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{16}\text{H}_{19}\text{F}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 345.1043, found m/z 345.1031; Enantiomeric excess: 94%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 80: 20, flow rate 1.0 mL/min): t_R = 9.387 min (major), t_R = 12.065 min (minor).

***iso*-Propyl-4-(2-fluoro-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (4oc):** $[\alpha]_D^{28} = -88.1^\circ$ ($c = 0.32$, EtOAc); white solid; mp 203-205 $^\circ\text{C}$; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 7.82 (brs, 1H), 7.26-7.30 (m, 1H), 7.20-7.22 (m, 1H), 7.05-7.13 (m, 3H); 5.73 (d, $J = 2.9$ Hz, 1H), 4.89-4.95 (m, 1H), 2.42 (s, 3H), 1.19 (d, $J = 6.2$ Hz, 3H), 0.93 (d, $J = 6.2$ Hz, 3H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 174.6, 164.4, 161.3, 158.9, 143.8, 130.2, 128.6, 124.6, 122.2, 100.9, 68.0, 50.0, 21.8, 21.3, 18.1; IR (KBr) γ 3443, 3171, 2981, 1703, 1652, 1591, 1198, 1097, 756 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{15}\text{H}_{17}\text{F}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 331.0887, found m/z 331.0876; Enantiomeric excess: 91%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 80: 20, flow rate 1.0 mL/min): t_R = 9.056 min (major), t_R = 11.937 min (minor).

***tert*-Butyl-4-(2-fluoro-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (4od):** $[\alpha]_D^{28} = -86.9^\circ$ ($c = 0.49$, EtOAc); white solid; mp 208-210 $^\circ\text{C}$; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 7.63 (brs, 1H), 7.26-7.30 (m, 1H), 7.19-7.21 (m, 1H), 7.12-7.14 (m, 1H), 7.07-7.09 (m, 1H), 7.06 (brs, 1H), 5.70 (d, $J = 2.4$ Hz, 1H), 2.40 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 174.5, 164.1, 161.3, 158.8, 143.2, 130.1, 124.6, 122.2, 101.8, 81.2, 50.1, 28.0, 18.1; IR (KBr) γ 3420, 3177, 3001, 2930, 1710, 1657, 1585, 1320, 1257, 1201, 1160, 1099, 758 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{16}\text{H}_{19}\text{F}_1\text{N}_2\text{O}_2\text{S}_1+\text{Na})^+$ requires m/z 345.1043, found m/z 345.1026; Enantiomeric excess: 92%, determined by HPLC (Daicel Chirapak AS-H, hexane/ isopropanol = 80: 20, flow rate 1.0 mL/min): t_R = 8.236 min (major), t_R = 10.184 min (minor).

4-(3-Hydroxy-phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (Monastrol): $[\alpha]_D^{28} = -63.3^\circ$ ($c = 0.2$, MeOH); white solid; mp 160-162 $^\circ\text{C}$; ^1H NMR (DMSO, 300 MHz) δ (ppm) 1.11 (t, $J = 7.1$ Hz, 3H), 2.27 (s, 3H), 3.98-4.05 (m, 2H), 5.09 (d, $J = 2.9$ Hz, 1H), 6.63-6.65 (m, 3H), 7.09-7.14 (m, 1H), 9.44 (brs, 1H), 9.60 (brs, 1H), 10.29 (brs, 1H); ^{13}C NMR (DMSO, 75 MHz) δ (ppm) 13.74, 17.32, 54.60, 59.44, 101.27, 113.50, 114.59, 117.35, 128.95, 144.04, 144.28, 157.10, 165.24, 174.13; IR (KBr) γ 3272, 2981, 2934, 1687, 1656, 1567, 1460, 1274, 1188, 1106, 782, 698 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}_3\text{S}_1+\text{Na})^+$ requires m/z 315.0774, found m/z 315.0777; Enantiomeric excess: 91%,

determined by HPLC (Daicel Chirapak AD-H, hexane/ isopropanol = 70: 30, flow rate 1.0 mL/min): t_R = 8.236 min (major), t_R = 10.184 min (minor).

General Procedure for the organocatalytic Biginelli reactions of urea:

After a solution of aldehyde (0.2 mmol), urea (0.24 mmol) and a chiral phosphoric acid (0.02 mmol) in CH_2Cl_2 (3ml) was stirred at 25 °C for 2h, a β -keto ester (1.0 mmol) was added. The resulting reaction mixture was stirred at 25 °C for 8 days (monitored by TLC) and then EtOAc (3 mL) and some silica gel were added. After removal of solvent, the residue was purified through flash column chromatography on a silica gel (eluent: DCM: ethyl acetate = 3:1- 2:1) to yield pure products.

6-Methyl-4-(3-nitro-phenyl)-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid propyl ester (4cb): $[\alpha]_D^{28} = -70.7^\circ$ ($c = 0.14$, MeOH); white solid; mp 207-209 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.03 (d, $J = 6.2$ Hz, 3H), 1.21 (d, $J = 6.2$ Hz, 3H), 2.35 (s, 3H), 4.91-4.99 (m, 1H), 5.49 (d, $J = 2.6$ Hz, 1H), 6.37 (s, 1H), 7.47-7.71 (m, 2H,), 8.11-8.17 (m, 2H), 8.44 (brs, 1H), ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 18.65, 21.67, 21.98, 55.11, 67.87, 100.68, 121.86, 122.89, 129.77, 132.75, 145.83, 147.13, 148.26, 153.29, 164.59; IR (KBr): γ 3234, 2977, 2932, 1705, 1635, 1530, 1348, 1287, 1218, 1078, 803, 686 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{15}\text{H}_{17}\text{N}_3\text{O}_5+\text{Na})^+$ requires m/z 342.1060, found m/z 342.1058; Enantiomeric excess: 90%, determined by HPLC (Daicel Chirapak AD-H, hexane/ iso-propanol = 80: 20, flow rate 1.0 mL/min): t_R = 8.44 min (major), t_R = 10.91 min (minor).

4-(3,5-Dibromo-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid ethyl ester (4hc): $[\alpha]_D^{28} = -75.0^\circ$ ($c = 0.20$, MeOH); white solid; mp 181-183 °C; ^1H NMR (CDCl_3 , 300 MHz) δ (ppm) 1.20 (t, $J = 7.1$ Hz, 3H), 2.35 (s, 3H), 4.04-4.16 (m, 2H), 5.33 (d, $J = 2.5$ Hz, 1H), 6.02 (brs, 1H), 7.37-7.38 (d, $J = 1.2$ Hz, 2H,), 7.56 (s, 1H), 8.23 (brs, 1H), ^{13}C NMR (CDCl_3 , 75 MHz) δ (ppm) 14.15, 18.80, 55.01, 60.32, 100.24, 123.15, 128.66, 133.62, 147.19, 147.28, 152.91, 165.10; IR (KBr): γ 3425, 3256, 2976, 1695, 1641, 1230, 1219, 1092, 850, 729 cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{14}\text{H}_{14}\text{Br}_2\text{N}_2\text{O}_3+\text{Na})^+$ requires m/z 438.9263, found m/z 438.6268; Enantiomeric excess: 97%, determined by HPLC (Daicel Chirapak AD-H, hexane/ iso-propanol = 95: 5, flow rate 1.0 mL/min): t_R = 27.97 min (major), t_R = 31.98 min (minor).

4-(3,5-Difluoro-phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid methyl ester(4pb): $[\alpha]_D^{28} = -28.3^\circ$ ($c = 0.12$, MeOH); white solid; mp 252-254 °C; ^1H NMR

(DMSO, 300 MHz) δ (ppm) 2.26 (s, 3H), 3.55 (s, 3H), 5.17 (m, 1H), 6.88-6.90 (m, 2H), 7.10-7.16 (m, 1H), 7.85 (brs, 1H), 8.23 (brs, 1H), ^{13}C NMR (DMSO, 75 MHz) δ (ppm) 17.90, 50.93, 53.16, 97.79, 102.86, 109.07, 109.40, 149.07, 151.86, 160.65, 165.63; IR (KBr): γ 3307, 2951, 1664, 1638, 1596, 1434, 1343, 1237, 1092, 861, 701; cm^{-1} ; HRMS (FT-ICRMS) exact mass calcd for $(\text{C}_{13}\text{H}_{12}\text{F}_2\text{N}_2\text{O}_3+\text{Na})^+$ requires m/z 305.0708, found m/z 305.0700; Enantiomeric excess: 93%, determined by HPLC (Daicel Chirapak OD-H, hexane/ iso-propanol = 85: 15, flow rate 1.0 mL/min): t_R = 8.23 min (major), t_R = 6.87 min (minor).

References:

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- (4) McDougal, N. T.; Schaus, S. E. *J. Am. Chem. Soc.* **2003**, *125*, 12094.

Selected HPLC

USTC

Project Name: xxy
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-0606171-0	Acquired By: System
Sample Type: Unknown	Date Acquired: 6/21/2006 2:57:06 PM
Vial: 1	Acq. Method: XXY
Injection #: 3	Date Processed: 6/21/2006 3:17:14 PM
Injection Volume: 20.00 ul	Channel Name: 2487Channel 1
Run Time: 60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.484	10732048	50.03	268215	58.11
2	14.560	10717114	49.97	193387	41.89

USTC

Project Name: xxy
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-0606171-1	Acquired By: System
Sample Type: Unknown	Date Acquired: 6/23/2006 4:01:26 PM
Vial: 1	Acq. Method: xxy280254
Injection #: 2	Date Processed: 6/23/2006 4:24:12 PM
Injection Volume: 20.00 ul	Channel Name: 2487Channel 1
Run Time: 60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.429	9725478	95.51	247192	96.34
2	14.718	457139	4.49	9385	3.66

USTC

Project Name: xxy
Reported by User: System*Breeze*

SAMPLE INFORMATION

Sample Name: cxh-0606162-0
Sample Type: Unknown
Vial: 1
Injection #: 7
Injection Volume: 20.00 ul
Run Time: 60.00 MinutesAcquired By: System
Date Acquired: 6/23/2006 11:20:22 AM
Acq. Method: xxy280254
Date Processed: 6/23/2006 11:42:10 AM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.261	3704864	50.06	122056	60.78
2	12.710	3695999	49.94	78757	39.22

USTC

Project Name: xxy
Reported by User: System*Breeze*

SAMPLE INFORMATION

Sample Name: cxh-0606162-1
Sample Type: Unknown
Vial: 1
Injection #: 6
Injection Volume: 20.00 ul
Run Time: 60.00 MinutesAcquired By: System
Date Acquired: 6/23/2006 10:54:20 AM
Acq. Method: xxy280254
Date Processed: 6/23/2006 11:14:01 AM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.271	17413062	95.90	539355	97.16
2	12.905	744037	4.10	15774	2.84

SAMPLE INFORMATION

Sample Name:	cxh-0606222-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/29/2006 10:52:15 AM
Vial:	1	Acq. Method:	XXY
Injection #:	6	Date Processed:	6/29/2006 11:14:33 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.790	10682519	49.83	300215	60.25
2	12.631	10757320	50.17	198093	39.75

SAMPLE INFORMATION

Sample Name:	cxh-0606222-1	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/29/2006 10:33:13 AM
Vial:	1	Acq. Method:	XXY
Injection #:	5	Date Processed:	6/29/2006 10:52:57 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.711	12818844	97.00	366120	97.69
2	12.709	396378	3.00	8662	2.31

USTC

Project Name: xxy
Reported by User: System*Breeze*

SAMPLE INFORMATION

Sample Name:	cxh-0606221-1	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/29/2006 9:23:13 AM
Vial:	1	Acq. Method:	XXYa
Injection #:	1	Date Processed:	6/29/2006 9:46:53 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.387	3131611	96.91	95404	97.74
2	12.065	99757	3.09	2205	2.26

USTC

Project Name: xxy
Reported by User: System*Breeze*

SAMPLE INFORMATION

Sample Name:	cxh-0606221-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/29/2006 10:02:09 AM
Vial:	1	Acq. Method:	XXY
Injection #:	3	Date Processed:	6/29/2006 10:18:32 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.046	15175436	49.93	472307	59.29
2	11.225	15220682	50.07	324246	40.71

USTC

Project Name: xxy
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	cxh-0606132-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/19/2006 8:32:07 PM
Vial:	1	Acq. Method:	xyy280254
Injection #:	3	Date Processed:	6/19/2006 8:45:24 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1 8.153	1532024	50.21	65043	57.35
2 9.994	1519146	49.79	48373	42.65

USTC

Project Name: xxy
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	cxh-0606132-1	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/19/2006 8:13:43 PM
Vial:	1	Acq. Method:	XXY
Injection #:	2	Date Processed:	6/19/2006 8:27:49 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1 8.236	25734694	95.83	980676	96.31
2 10.184	1119057	4.17	37564	3.69

USTC

Project Name: xxy
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	cxh-0606133-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/19/2006 12:41:34 PM
Vial:	1	Acq. Method:	XXY
Injection #:	2	Date Processed:	6/19/2006 1:08:06 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.387	1979219	50.01	71045	58.77
2	12.239	1978378	49.99	49836	41.23

USTC

Project Name: xxy
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	cxh-0606133-1	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/19/2006 9:13:05 PM
Vial:	1	Acq. Method:	xy280254
Injection #:	4	Date Processed:	6/19/2006 9:29:55 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.056	4268431	95.49	147789	96.52
2	11.937	201741	4.51	5330	3.48

USTC

Project Name: xxy
Reported by User: System*Breeze*

SAMPLE INFORMATION

Sample Name:	cxh-3-oh-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/12/2006 6:53:31 PM
Vial:	1	Acq. Method:	XXYa
Injection #:	1	Date Processed:	7/12/2006 7:08:29 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.181	1691871	50.44	104068	57.00
2	8.926	1662504	49.56	78502	43.00

USTC

Project Name: xxy
Reported by User: System*Breeze*

SAMPLE INFORMATION

Sample Name:	cxh-3-oh-1	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/12/2006 7:19:01 PM
Vial:	1	Acq. Method:	XXYa
Injection #:	2	Date Processed:	7/12/2006 7:31:46 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.050	7061170	95.54	448499	96.36
2	8.728	330006	4.46	16946	3.64

USTC

Project Name: xxy
Reported by User: System*Breeze*

SAMPLE INFORMATION

Sample Name: cxh-0606233-0
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 20.00 ul
Run Time: 60.00 Minutes

Acquired By: System
Date Acquired: 6/30/2006 5:13:01 PM
Acq. Method: XXY
Date Processed: 6/30/2006 5:26:27 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.212	2940721	49.99	206623	54.18
2	8.349	2941412	50.01	174770	45.82

USTC

Project Name: xxy
Reported by User: System*Breeze*

SAMPLE INFORMATION

Sample Name: cxh-0606233-1
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 20.00 ul
Run Time: 60.00 Minutes

Acquired By: System
Date Acquired: 6/30/2006 5:32:11 PM
Acq. Method: XXY
Date Processed: 6/30/2006 5:50:50 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.208	242627	1.78	16910	2.11
2	8.324	13412614	98.22	785548	97.89

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-83-0
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 20.00 ul
Run Time: 60.00 Minutes

Acquired By: System
Date Acquired: 6/1/06 12:38:11 PM
Acq. Method: 100A
Date Processed: 6/1/06 12:56:35 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	3.363	399703	1.43	43529	4.79
2	12.677	13772967	49.32	477058	52.55
3	14.970	13750953	49.24	387281	42.66

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-83
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 20.00 ul
Run Time: 25.00 Minutes

Acquired By: System
Date Acquired: 6/1/06 12:57:24 PM
Acq. Method: 100A
Date Processed: 6/1/06 1:27:29 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	3.328	832966	5.21	129470	19.55
2	7.331	226566	1.42	14568	2.20
3	12.587	14048004	87.80	492465	74.36
4	14.870	892485	5.58	25800	3.90

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION			
Sample Name:	cxh-0 82 #	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/31/06 5:45:39 PM
Vial:	1	Acq. Method:	100B 254
Injection #:	3	Date Processed:	5/31/06 6:15:09 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	3.002	110823	1.70	13850	7.73
2	3.647	213748	3.27	28348	15.82
3	18.864	3114031	47.63	77508	43.24
4	24.448	3099436	47.41	59530	33.21

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION			
Sample Name:	cxh 82 #	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/1/06 9:52:46 AM
Vial:	1	Acq. Method:	100B 254
Injection #:	1	Date Processed:	6/1/06 10:36:33 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	3.024	118534	3.51	10322	10.10
2	3.320	45439	1.34	5971	5.84
3	3.697	277725	8.22	36581	35.78
4	20.742	146332	4.33	3798	3.71
5	27.865	2790589	82.60	45573	44.57

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-0 84#
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 20.00 ul
Run Time: 60.00 Minutes
Acquired By: System
Date Acquired: 5/31/06 5:01:41 PM
Acq. Method: 100B 254
Date Processed: 5/31/06 5:22:45 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	3.021	108785	1.13	11392	3.01
2	3.301	46406	0.48	6310	1.67
3	3.678	332165	3.46	42673	11.29
4	12.515	4458426	46.48	168694	44.64
5	14.773	4449992	46.39	143695	38.03
6	19.645	195975	2.04	5128	1.36

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh 84#
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 20.00 ul
Run Time: 60.00 Minutes
Acquired By: System
Date Acquired: 5/31/06 5:23:22 PM
Acq. Method: 100B 254
Date Processed: 6/1/06 10:14:31 AM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	3.002	31310	0.85	6044	3.81
2	3.295	33019	0.90	5957	3.76
3	3.672	355239	9.69	44564	28.11
4	12.431	154060	4.20	5942	3.75
5	14.703	3092850	84.35	96005	60.57

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-85-0
Sample Type: Unknown
Vial: 1
Injection #: 3
Injection Volume: 20.00 ul
Run Time: 30.00 Minutes

Acquired By: System
Date Acquired: 6/1/06 1:29:25 PM
Acq. Method: 100A
Date Processed: 6/1/06 3:01:44 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	3.335	279641	14.72	38061	27.71
2	7.252	817864	43.06	53188	38.73
3	8.274	801806	42.22	46098	33.56

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-85
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 20.00 ul
Run Time: 30.00 Minutes

Acquired By: System
Date Acquired: 6/1/06 3:03:43 PM
Acq. Method: 100A
Date Processed: 6/1/06 3:15:03 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	3.287	1900699	10.85	121716	13.77
2	4.083	79986	0.45	8403	0.95
3	7.088	695584	3.90	30038	3.40
4	8.157	15178176	85.01	723705	81.88

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-0
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 20.00 ul
Run Time: 40.00 Minutes
Acquired By: System
Date Acquired: 7/11/06 10:34:35 AM
Acq. Method: 100A
Date Processed: 7/11/06 10:53:50 AM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	7.275	7844957	50.11	330020	61.98
2	15.137	7811729	49.89	202433	38.02

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-107
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 20.00 ul
Run Time: 40.00 Minutes
Acquired By: System
Date Acquired: 7/11/06 10:54:31 AM
Acq. Method: 100A
Date Processed: 7/11/06 11:13:43 AM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	7.283	241823	1.67	10237	3.31
2	14.935	14227841	98.33	299265	96.69

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION			
Sample Name:	cxh-119-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/23/06 10:03:13 AM
Vial:	1	Acq. Method:	100A
Injection #:	1	Date Processed:	6/23/06 10:19:31 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	3.546	388113	9.38	17550	11.84
2	8.715	1882490	45.49	75461	50.90
3	10.827	1867608	45.13	55229	37.26

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION			
Sample Name:	cxh-119	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/23/06 10:21:01 AM
Vial:	1	Acq. Method:	100A
Injection #:	2	Date Processed:	6/23/06 10:34:11 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	3.360	295724	5.17	20560	8.56
2	3.490	189680	3.32	20773	8.65
3	8.665	4967143	86.92	192342	80.06
4	10.904	262108	4.59	6561	2.73

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION			
Sample Name:	cxh-120-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/23/06 10:34:55 AM
Vial:	1	Acq. Method:	100A
Injection #:	3	Date Processed:	6/23/06 10:54:59 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	3.319	385903	2.03	25710	4.16
2	3.483	220773	1.16	23290	3.77
3	4.599	270448	1.43	7642	1.24
4	5.767	289557	1.53	5958	0.96
5	8.856	8907900	46.94	325074	52.57
6	11.219	8900752	46.91	230673	37.30

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION			
Sample Name:	cxh-120	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	6/23/06 11:01:32 AM
Vial:	1	Acq. Method:	100A
Injection #:	4	Date Processed:	6/23/06 3:25:35 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	3.472	399802	7.78	19656	9.80
2	8.808	4524509	88.03	174979	87.21
3	11.308	215323	4.19	6004	2.99

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-131-0
Sample Type: Unknown
Vial: 1
Injection #: 5
Injection Volume: 20.00 ul
Run Time: 20.00 Minutes

Acquired By: System
Date Acquired: 6/26/06 5:43:09 PM
Acq. Method: 100A
Date Processed: 6/26/06 6:21:15 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	3.383	160445	1.73	14716	4.76
2	3.456	128551	1.39	15077	4.88
3	4.022	160502	1.73	11067	3.58
4	4.744	165050	1.78	15127	4.90
5	5.111	191907	2.07	6948	2.25
6	5.721	178148	1.92	13991	4.53
7	6.301	100336	1.08	9391	3.04
8	9.389	4131614	44.60	142598	46.17
9	14.392	4047667	43.69	79921	25.88

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-131
Sample Type: Unknown
Vial: 1
Injection #: 4
Injection Volume: 20.00 ul
Run Time: 40.00 Minutes

Acquired By: System
Date Acquired: 6/26/06 5:16:00 PM
Acq. Method: 100A
Date Processed: 6/26/06 5:34:25 PM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	3.350	357525	1.57	24194	3.05
2	3.437	263584	1.16	23534	2.97
3	4.045	82797	0.36	5620	0.71
4	4.736	98492	0.43	5374	0.68
5	9.312	20880764	91.95	713005	89.98
6	14.405	1026814	4.52	20650	2.61

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-133-0
Sample Type: Unknown
Vial: 1
Injection #: 1
Injection Volume: 20.00 ul
Run Time: 40.00 Minutes

Acquired By: System
Date Acquired: 7/19/06 10:21:25 AM
Acq. Method: 100A
Date Processed: 7/19/06 10:39:21 AM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	9.196	1062329	50.16	48776	56.68
2	11.027	1055587	49.84	37278	43.32

ulas

Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name: cxh-133
Sample Type: Unknown
Vial: 1
Injection #: 2
Injection Volume: 20.00 ul
Run Time: 40.00 Minutes

Acquired By: System
Date Acquired: 7/19/06 10:41:14 AM
Acq. Method: 100A
Date Processed: 7/19/06 11:18:48 AM
Channel Name: 2487Channel 1
Sample Set Name:

	RT (min)	Area ($\mu V \cdot sec$)	% Area	Height (μV)	% Height
1	8.710	99800	0.66	5470	1.13
2	9.199	592356	3.94	24728	5.10
3	10.866	14356950	95.40	454965	93.78

Selected NMR spectra