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Supporting Information for

Synergistic Cu/Pd-Catalyzed Asymmetric Allylation: A Facile Access to α-Quaternary

Cysteine Derivatives

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Contents

I. General remarks	2
II. General procedure for dual Cu/Pd Catalyzed allylic alkylation reaction of cyclic imino esters	2
III. General procedures for gram-scale reaction and synthetic transformation	12
IV. Absolute configuration determination of (<i>S</i> , <i>E</i>)- 5 e	17
V. Reference	18
VI. ¹ H NMR and ¹³ C NMR spectra	19
VII. HPLC spectra	45

I. General remarks

¹H NMR spectra were recorded on a Bruker 400 MHz spectrometer in CDCl₃. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data are reported as (s = single, d = double, t = triple, q = quarte, m = multiple or unresolved, brs = broad single, coupling constant(s) in Hz, integration). ¹³C NMR spectra were recorded on a Bruker 100 MHz spectrometer in CDCl₃. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard. Commercially obtained reagents were used without further purification. Solvents were purified prior to use according to the standard methods. Unless otherwise noted, all reactions were carried out under nitrogen atmosphere. All reactions were monitored by TLC with silica gelcoated plates. Enantiomeric ratios were determined by chiral-phase HPLC analysis in comparison with authentic racemic materials using a chiralpak AD-H, chiralcel OD-H and IE column with hexane and *i*-PrOH as solvents. Cyclic imino ester,¹ allylcarbonates,² L1-L4³ were prepared according to the literature procedure. The absolute configuration of **5e** was determined by X-ray analysis, and those of other adducts were deduced on the basis of this result.⁴ The racemic products were obtained by running reactions with a racemic catalyst or blending equal amount of two enantiomers.

II. General procedure for dual Cu/Pd-catalyzed allylic alkylation reaction of cyclic imino esters

The preparation of Cu catalyst: A flame dried Schlenk tube was cooled to rt and filled with N₂. To this flask were added (S,S_p) -^{*t*}Bu-Phosferrox **L2** (0.01 mmol, 5 mol %) and Cu(OTf)₂ (0.01 mmol, 5 mol %) were dissolved in 0.5 mL of THF, and stirred at room temperature for about 0.5 h.

The preparation of Pd catalyst: A flame dried Schlenk tube was cooled to rt and filled with N₂. To this flask were added (*S*,*S_p*)-*^t*Bu-Phosferrox **L2** (0.01 mmol, 5 mol %) and [Pd(η^3 -allyl)Cl]₂ (0.005 mmol, 2.5 mol %) were dissolved in 0.5 mL of THF, and stirred at room temperature for about 0.5 h.

A flame dried Schlenk tube was cooled to rt and filled with N₂. To this flask were added cyclic imino esters (0.20 mmol, 1.0 equiv), base (0.20 mmol, 1.0 equiv), Cu catalyst (5 mol %), Pd catalyst (5 mol %). The methyl cinnamyl carbonate (0.30 mmol, 1.5 equiv) was then added. The reaction mixture was stirred at room temperature for 24 h. The organic solvent was removed by rotary evaporation. The dr value was determined by ¹H NMR analysis of the crude mixture and the residue was purified by column chromatography on silica gel to give the allylation product, which was then directly analyzed by chiral HPLC to determine the enantiomeric excess.

Methyl (*S*, *E*)-4-cinnamyl-2-phenyl-4,5-dihydrothiazole-4-carboxylate (5a):



Yield (98%); 66.1 mg; yellow solid; m.p. 78-80 °C; $[\alpha]_D^{20} = -38.7$ (*c* 1.0, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.88 – 7.86 (m, 2H), 7.47 (t, *J* = 7.3 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.32 – 7.25 (m, 4H), 7.21 (t, *J* = 7.1 Hz, 1H), 6.52 (d, *J* = 15.8 Hz, 1H), 6.20 – 6.12 (m, 1H), 3.89 (d, *J* = 11.5 Hz, 1H), 3.81 (s, 3H), 3.45 (d, *J* = 11.5 Hz, 1H), 2.92 (dd, *J* = 7.3, 1.7 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 169.1, 137.0, 134.4, 132.8, 131.6, 128.55, 128.46, 128.45, 127.4, 126.3, 123.6, 88.3, 52.9, 41.3, 38.8. HRMS (ESI-TOF) Calcd. For C₂₀H₂₀N₂S⁺ ([M+H]⁺): 338.1209, found: 338.1195. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 10.3 and 11.6 min.

Methyl (S, E)-2-phenyl-4-(3-(p-tolyl) allyl)-4,5-dihydrothiazole-4-carboxylate (5b):



Yield (96%); 67.5 mg; yellow oil; $[α]_D^{20} = -40.4$ (*c* 1.0, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 7.3 Hz, 2H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.29 – 7.18 (m, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.49 (d, *J* = 15.7 Hz, 1H), 6.14 – 6.06 (m, 1H), 3.89 (d, *J* = 11.5 Hz, 1H), 3.81 (s, 3H), 3.45 (d, *J* = 11.5 Hz, 1H), 2.93 – 2.87 (m, 2H), 2.31 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 169.1, 137.2, 134.2, 134.1, 132.8, 131.5, 129.1, 128.5, 128.4, 126.1, 122.4, 88.3, 52.9, 41.3, 38.6, 21.1. HRMS (ESI-TOF) Calcd. For C₂₁H₂₂NO₂S⁺ ([M+H]⁺): 352.1366, found: 352.1358. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol /hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 9.6 and 10.8 min.

Methyl (*S*, *E*)-4-(3-(4-methoxyphenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-Carboxylate (5c):



Yield (75%); 55.3 mg; brown solid; m.p. 60-62 °C; $[α]_D^{20} = -23.3$ (*c* 1.0, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.88 – 7.86 (m, 2H), 7.51 – 7.45 (m, 1H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.28 – 7.25 (m, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 6.46 (d, *J* = 15.7 Hz, 1H), 6.05 – 5.97 (m, 1H), 3.89 (d, *J* = 11.5 Hz, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 3.45 (d, *J* = 11.5 Hz, 1H), 2.94 – 2.84 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 173.0, 169.1, 159.0, 133.8, 132.8, 131.5, 129.8, 128.5, 128.4, 127.4, 121.1, 113.8, 88.4, 55.2, 52.9, 41.3, 38.6. HRMS (ESI-TOF) Calcd. For C₂₁H₂₂NO₃S⁺ ([M+H]⁺): 368.1315, found: 368.1308. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 20.4 and 23.1 min.

Methyl (S, E)-4-(3-(4-chlorophenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-Carboxylate (5d):



Yield (90%); 66.9 mg; yellow solid; m.p. 42-44 °C; $[\alpha]_D^{20} = -28.5$ (*c* 0.8, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.88 (d, *J* = 7.3 Hz, 2H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 4.0 Hz, 4H), 6.47 (d, *J* = 15.8 Hz, 1H), 6.19 – 6.11 (m, 1H), 3.89 (d, *J* = 11.5 Hz, 1H), 3.81 (s, 3H), 3.43 (d, *J* = 11.5 Hz, 1H), 2.91 (d, *J* = 7.2 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 169.3, 135.4, 133.1, 133.0, 132.7, 131.6, 128.6, 128.51, 128.46, 127.4, 124.3, 88.1, 52.9, 41.3, 38.9. HRMS (ESI-TOF) Calcd. For C₂₀H₁₉ClNO₂S⁺ ([M+H]⁺): 372.0820, found: 372.0813. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 9.7 and 10.7 min.

Methyl (S, E)-4-(3-(4-bromophenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-Carboxylate (5e):



Yield (92%); 76.6 mg; white solid; m.p. 74-76 °C; $[\alpha]_D^{20} = -24.3$ (*c* 1.1, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 7.4 Hz, 2H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 8.7 Hz, 4H), 7.19 (d, *J* = 8.3 Hz, 2H), 6.45 (d, *J* = 15.8 Hz, 1H), 6.21 – 6.13 (m, 1H), 3.89 (d, *J* = 11.5 Hz, 1H), 3.82 (s, 3H), 3.43 (d, *J* = 11.5 Hz, 1H), 2.90 (d, *J* = 7.3 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 169.3, 135.8, 133.1, 132.7, 131.7, 131.5, 128.53, 128.48, 127.8, 124.4, 121.2, 88.1, 53.0, 41.3, 38.9. HRMS (ESI-TOF) Calcd. For C₂₀H₁₉BrNO₂S ([M+H]⁺): 416.0314, found: 416.0310. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 97% ee (Chiralpak IE, *i*-propanol / hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 10.5 and 11.6 min.

Methyl (S, E)-2-phenyl-4-(3-(m-tolyl) allyl)-4,5-dihydrothiazole-4-carboxylate (5f):



Yield (90%); 63.3 mg; white oil; $[α]_D^{20} = -43.4$ (*c* 0.53, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.90 – 7.88 (m, 2H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.4 Hz, 2H), 7.19 – 7.16 (m, 3H), 7.04 (d, *J* = 7.1 Hz, 1H), 6.50 (d, *J* = 15.7 Hz, 1H), 6.20 – 6.12 (m, 1H), 3.91 (d, *J* = 11.5 Hz, 1H), 3.83 (s, 3H), 3.46 (d, *J* = 11.5 Hz, 1H), 2.98 – 2.89 (m, 2H), 2.34 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 173.0, 169.2, 138.1, 137.0, 134.6, 132.9, 131.6, 128.6, 128.5, 128.4, 128.3, 127.1, 123.5, 123.4, 88.4, 53.0, 41.4, 38.8, 21.4. HRMS (ESI-TOF) Calcd. For C₂₁H₂₂NO₂S⁺ ([M+H]⁺): 352.1366, found: 352.1359. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 9.3 and 10.6 min.

Methyl (S, E)-4-(3-(3-methoxyphenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-Carboxylate (5g):



Yield (82%); 60.3 mg; white oil; $[α]_D^{20} = -34.7$ (*c* 0.5, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) ¹H NMR (400 MHz, CDCl₃) δ 7.89 – 7.86 (m, 2H), 7.52 – 7.45 (m, 1H), 7.43 – 7.40 (m, 2H), 7.22 (t, *J* = 7.9 Hz, 1H), 6.94 (d, *J* = 7.7 Hz, 1H), 6.87 – 6.86 (m, 1H), 6.78 (dd, *J* = 8.1, 2.4 Hz, 1H), 6.50 (d, *J* = 15.7 Hz, 1H), 6.18 – 6.14 (m, 1H), 3.90 (d, *J* = 11.5 Hz, 1H), 3.82 (s, 3H), 3.79 (s, 3H), 3.45 (d, *J* = 11.5 Hz, 1H), 2.93-2.91 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 169.2, 159.7, 138.5, 134.3, 132.8, 131.6, 129.4, 128.6, 128.5, 124.0, 119.0, 113.0, 111.7, 88.3, 55.2, 52.9, 41.3, 38.8. HRMS (ESI-TOF) Calcd. For C₂₁H₂₂NO₃S⁺ ([M+H]⁺): 368.1315, found: 368.1309. The product was analyzed by chiral HPLC to determine the enantiomeric excess: >99% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 15.3 and 18.2 min.

Methyl (*S*, *E*)-4-(3-(3-chlorophenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-Carboxylate (5h):



Yield (97%); 72.1 mg; white oil; $[α]_D^{20} = -21.3$ (*c* 0.4, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.89 – 7.86 (m, 2H), 7.52 – 7.46 (m, 1H), 7.43 – 7.41 (m, 2H), 7.31 (s, 1H), 7.20 – 7.19 (m, 3H), 6.46 (d, *J* = 15.8 Hz, 1H), 6.23 – 6.16 (m, 1H), 3.89 (d, *J* = 11.5 Hz, 1H), 3.82 (s, 3H), 3.42 (d, *J* = 11.5 Hz, 1H), 2.93 – 2.90 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 169.3, 138.8, 134.4, 133.0, 132.8, 131.7, 129.7, 128.6, 128.5, 127.4, 126.2, 125.3, 124.5, 88.2, 53.0, 41.3, 39.0. HRMS (ESI-TOF) Calcd. For C₂₀H₁₉ClNO₂S⁺ ([M+H]⁺): 372.0820, found: 372.0813. The product was analyzed by chiral HPLC to determine the enantiomeric excess: >99% ee (Chiralpak IE, *i*-propanol/ hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 9.6 and 10.5 min.

Methyl (S, E)-4-(3-(2-fluorophenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-Carboxylate (5i):



Yield (85%); 60.4 mg; brown oil; $[α]_D^{20} = -18.0$ (*c* 0.3, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.89 – 7.87 (m, 2H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 3H), 7.24-7.12 (m, 1H), 7.06-7.03 (m, 2H), 6.70 (d, *J* = 15.9 Hz, 1H), 6.29 – 6.21 (m, 1H), 3.91 (d, *J* = 11.5 Hz, 1H), 3.83 (s, 3H), 3.46 (d, *J* = 11.5 Hz, 1H), 2.95 (d, *J* = 7.4 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.8, 169.2, 159.9 (d, *J* = 249.9 Hz), 132.7, 131.6, 128.7 (d, *J* = 8.4 Hz), 128.5, 128.4, 127.2 (d, *J* = 3.7 Hz), 126.6 (d, *J* = 3.8 Hz), 126.2 (d, *J* = 4.2 Hz), 124.8 (d, *J* = 12.4 Hz), 124.0 (d, *J* = 3.5 Hz), 115.5 (d, *J* = 22.1 Hz), 88.2, 52.9, 41.6, 38.8. ¹⁹F NMR (376 MHz, CDCl₃) δ -118.64 (s). HRMS (ESI-TOF) Calcd. For C₂₀H₁₉FNO₂S⁺ ([M+H]⁺): 356.1115, found: 356.1111. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 98% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 9.9 and 12.2 min.

Methyl (S, E)-4-(3-(3,4-dichlorophenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-Carboxylate (5j):



Yield (95%); 77.2 mg; white oil; $[\alpha]_{D}^{20} = -15.6$ (*c* 0.7, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.89 – 7.86 (m, 2H), 7.52 – 7.46 (m, 1H), 7.42 – 7.38 (m, 3H), 7.36 – 7.32 (m, 1H), 7.14 (dd, J = 8.3, 2.0 Hz, 1H), 6.41 (d, J = 15.8 Hz, 1H), 6.23 – 6.15 (m, 1H), 3.88 (d, J = 11.5 Hz, 1H), 3.82 (s, 3H), 3.41 (d, J = 11.5 Hz, 1H), 2.92-2.90 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.8, 169.4, 137.1, 132.7, 132.6, 132.0, 131.7, 131.1, 130.4, 128.6, 128.5, 128.0, 125.9, 125.4, 88.1, 53.0, 41.3, 39.1. HRMS (ESI-TOF) Calcd. For C₂₀H₁₈Cl₂NO₂S ([M+H]⁺): 406.0430, found: 406.0424. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 97% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 11.0 and 12.3 min.

Methyl (S, E)-4-(3-(3,5-bis(trifluoromethyl) phenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-

carboxylate (5k):



Yield (94%); 89.0 mg; brown soild; m.p. 50-52 °C; $[\alpha]_D^{20} = +9.4$ (*c* 1.2, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.89 – 7.86 (m, 2H), 7.72 (d, *J* = 8.9 Hz, 3H), 7.51 – 7.47 (m, 1H), 7.42 (t, *J* = 7.4 Hz, 2H), 6.60 – 6.56 (m, 1H), 6.43 – 6.36 (m, 1H), 3.90 (d, *J* = 11.5 Hz, 1H), 3.83 (s, 3H), 3.43 (d, *J* = 11.6 Hz, 1H), 2.96 (d, *J* = 7.3 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.7, 169.6, 139.0, 132.6, 131.8 (q, *J* = 33.3 Hz), 131.7, 131.6, 128.5, 128.3, 126.1 (d, *J* = 2.7 Hz), 123.3 (q, *J* = 273.8 Hz), 120.83, 120.80, 120.76, 120.7, 87.9, 53.0, 41.3, 39.4. ¹⁹F NMR (376 MHz, CDCl₃) δ -62.98 (s). HRMS (ESI-TOF) Calcd. For C₂₂H₁₈F₆NO₂S⁺ ([M+H]⁺): 474.0957, found: 474.0951. The product was analyzed by chiral HPLC to determine the enantiomeric excess: >99% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.4 and 5.0 min.

Methyl (S, E)-4-(3-(3,5-dimethoxyphenyl) allyl)-2-phenyl-4,5-dihydrothiazole-4-carboxylate (51):



Yield (98%); 77.9 mg; brown oil; $[\alpha]_D^{20} = -27.6$ (*c* 1.4, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.88 – 7.86 (m, 2H), 7.52 – 7.44 (m, 1H), 7.41 (t, *J* = 7.4 Hz, 2H), 6.49-6.44 (m, 3H), 6.35 (t, *J* = 2.2 Hz, 1H), 6.19 – 6.12 (m, 1H), 3.89 (d, *J* = 11.5 Hz, 1H), 3.82 (s, 3H), 3.77 (s, 6H), 3.44 (d, *J* = 11.5 Hz, 1H), 2.92-2.90 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.9, 169.3, 160.9, 139.1, 134.4, 132.9, 131.7, 128.6, 128.5, 124.2, 104.5, 99.7, 88.3, 55.3, 53.0, 41.3, 38.9. HRMS (ESI-TOF) Calcd. For C₂₂H₂₄NO₄S⁺ ([M+H]⁺): 398.1421, found: 398.1416. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 30.8 and 40.9 min.

Methyl (*S*, *E*)-4-(3-(naphthalen-2-yl) allyl)-2-phenyl-4,5-dihydrothiazole-4-carboxylate (5m):



Yield (88%); 68.2 mg; brown soild; m.p. 98-100 °C; $[α]_D^{20} = -41.8$ (*c* 1.3, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.90 – 7.87 (m, 2H), 7.76 (dd, *J* = 13.9, 5.4 Hz, 3H), 7.67 (s, 1H), 7.54 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.47 – 7.38 (m, 5H), 6.67 (d, *J* = 15.8 Hz, 1H), 6.33 – 6.26 (m, 1H), 3.91 (d, *J* = 11.5 Hz, 1H), 3.82 (s, 3H), 3.47 (d, *J* = 11.5 Hz, 1H), 3.02 – 2.92 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 173.0, 169.3, 134.6, 134.5, 133.6, 133.0, 132.9, 131.7, 128.7, 128.6, 128.2, 128.1, 128.0, 127.7, 126.3, 126.1, 125.8, 124.1, 123.7, 88.5, 53.0, 41.6, 39.0. HRMS (ESI-TOF) Calcd. For C₂₄H₂₂NO₂S⁺ ([M+H]⁺): 388.1366, found: 388.1363. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 13.8 and 16.5 min.

Methyl (S, E)-4-(3-(furan-2-yl) allyl)-2-phenyl-4,5-dihydrothiazole-4-Carboxylate (5n):



Yield (83%); 54.3 mg; white oil; $[\alpha]_D^{20} = -12.0$ (*c* 0.7, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, CDCl₃) δ 7.88 – 7.86 (m, 2H), 7.51 – 7.45 (m, 1H), 7.43 – 7.41 (m, 2H), 7.31 (d, *J* = 1.4 Hz, 1H), 6.35 – 6.31 (m, 2H), 6.18 (d, *J* = 3.2 Hz, 1H), 6.14 – 6.06 (m, 1H), 3.90 (d, *J* = 11.5 Hz, 1H), 3.82 (s, 3H), 3.43 (d, *J* = 11.5 Hz, 1H), 2.95 – 2.82 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 172.8, 169.2, 152.5, 141.8, 132.9, 131.6, 128.6, 128.5, 122.8, 122.3, 111.2, 107.4, 88.4, 53.0, 41.1, 38.8. HRMS (ESI-TOF) Calcd. For C₁₈H₁₈NO₃S⁺ ([M+H]⁺): 328.1002, found: 328.0997. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 96% ee (Chiralpak IE, *i*-propanol/ hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 10.7 and 12.3 min.

Methyl (S, E)-4-(but-2-en-1-yl)-2-phenyl-4,5-dihydrothiazole-4-carboxylate (50):



Yield (80%); 44.0 mg; white soild; m.p. 36-38 °C; $[α]_D^{20} = -32.3$ (*c* 1.1, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20/1). ¹H NMR (400 MHz, CDCl₃) δ 7.86 – 7.84 (m, 2H), 7.46 (t, *J* = 7.3 Hz, 1H), 7.39 (t, *J* = 7.4 Hz, 2H), 5.64-5.56 (m, 1H), 5.44 - 5.36 (m, 1H), 3.85 (d, *J* = 11.5 Hz, 1H), 3.80 (s, 3H), 3.38 (d, *J* = 11.4 Hz, 1H), 2.82 – 2.59 (m, 2H), 1.68 – 1.66 (m, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 173.1, 168.7, 133.0, 131.5, 130.4, 128.6, 128.5, 124.5, 88.6, 52.8, 41.0, 38.5, 18.1. HRMS (ESI-TOF) Calcd. For C₁₅H₁₈NO₂S⁺ ([M+H]⁺): 276.1053, found: 276.1049. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 84% ee (Chiralpak ID, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 220 nm); t_r = 6.5 and 7.0 min.

Methyl (S, E)-4-(hex-2-en-1-yl)-2-phenyl-4,5-dihydrothiazole-4-carboxylate (5q):



Yield (45%); 27.2 mg; white oil; $[α]_D^{20} = -13.9$ (*c* 0.6, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20/1). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 – 7.78 (m, 2H), 7.50 – 7.44 (m, 1H), 7.42-7.38 (m, 2H), 5.60-5.55 (m, 1H), 5.41 – 5.36 (m, 1H), 3.87 (d, *J* = 11.5 Hz, 1H), 3.80 (s, 3H), 3.40 (d, *J* = 11.4 Hz, 1H), 2.75 – 2.67 (m, 2H), 2.01 – 1.95 (m, 2H), 1.38-1.33 (m, 2H), 0.86 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 173.1, 168.7, 136.0, 133.0, 131.5, 128.6, 128.4, 123.4, 88.6, 52.8, 41.0, 38.5, 34.7, 22.5, 13.6. HRMS (ESI-TOF) Calcd. For C₁₇H₂₂NO₂S⁺ ([M+H]⁺): 304.1366, found: 304.1363. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 83% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.5 and 7.4 min.

Methyl (S, E)-4-(3-cyclohexylallyl)-2-phenyl-4,5-dihydrothiazole-4-carboxylate (5r):



Yield (48%); 32.9 mg; white oil; $[α]_D^{20} = -16.3$ (*c* 0.8, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20/1).¹H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.84 (m, 2H), 7.47 – 7.45 (m, 1H), 7.42 – 7.38 (m, 2H), 5.52-5.49 (m, 1H), 5.35-5.33 (m, 1H), 3.86 (d, *J* = 11.5 Hz, 1H), 3.79 (s, 3H), 3.39 (d, *J* = 11.4 Hz, 1H), 2.70-2.64 (m, 2H), 1.93-1.90 (m, 1H), 1.70 – 1.63 (m, 5H), 1.26 – 1.01 (m, 5H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 173.1, 168.7, 142.1, 133.0, 131.5, 128.6, 128.4, 120.6, 88.7, 52.8, 41.1, 40.8, 38.3, 32.94, 32.93, 26.1, 25.9. HRMS (ESI-TOF) Calcd. For C₂₀H₂₆NO₂S⁺ ([M+H]⁺): 344.1679, found: 344.1678. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 69% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 220 nm); t_r = 6.8 and 8.2 min.

Methyl (S, E)-2-(4-chlorophenyl)-4-cinnamyl-4,5-dihydrothiazole-4-carboxylate (5s):



Yield (86%); 64.3 mg; yellow oil; $[α]_D^{20} = -51.5$ (*c* 0.8, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1). ¹H NMR (400 MHz, Chloroform-d) δ 7.83 – 7.80 (m, 2H), 7.41 – 7.37 (m, 2H), 7.34 – 7.27 (m, 4H), 7.25 – 7.20 (m, 1H), 6.52 (dd, *J* = 15.7, 1.4 Hz, 1H), 6.18-6.10 (m, 1H), 3.91 (d, *J* = 11.5 Hz, 1H), 3.82 (s, 3H), 3.47 (d, *J* = 11.5 Hz, 1H), 2.93-2.90 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 172.8, 168.0, 137.8, 137.0, 134.6, 131.3, 129.9, 128.8, 128.5, 127.5, 126.3, 123.4, 88.4, 53.0, 41.4, 39.1. HRMS (ESI-TOF) Calcd. For C₂₀H₁₉ClNO₂S⁺ ([M+H]⁺): 372.0820, found: 372.0820. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 97% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 8.5 and 9.1 min.

Methyl (S, E)-4-cinnamyl-2-(p-tolyl)-4,5-dihydrothiazole-4-carboxylate (5t):



Yield (96%); 67.5 mg; yellow oil; $[α]_D^{20} = -41.2$ (*c* 1.0, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20/1). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.77 – 7.75 (m, 2H), 7.34 – 7.26 (m, 4H), 7.23 – 7.18 (m, 3H), 6.54 – 6.49 (m, 1H), 6.19 – 6.12 (m, 1H), 3.87 (d, *J* = 11.5 Hz, 1H), 3.81 (s, 3H), 3.43 (d, *J* = 11.4 Hz, 1H), 2.93-2.90 (m, 2H), 2.39 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 173.1, 169.1, 142.1, 137.1, 134.4, 130.2, 129.2, 128.6, 128.5, 127.5, 126.3, 123.7, 88.3, 52.9, 41.4, 38.7, 21.5. HRMS (ESI-TOF) Calcd. For C₂₀H₁₉ClNO₂S⁺ ([M+H]⁺): 352.1366, found: 352.1374. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 98% ee (Chiralpak IE, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 10.4 and 11.6 min.

III. General procedures for gram-scale reaction and synthetic transformation



The preparation of Cu catalyst: A flame dried Schlenk tube was cooled to rt and filled with N₂. To this flask were added (S, S_p)- t Bu-Phosferrox **L2** (0.25 mmol, 5 mol %) and Cu(OTf)₂ (0.25 mmol, 5 mol %) were dissolved in 5 mL THF, and stirred at room temperature for about 0.5 h.

The preparation of Pd catalyst: A flame dried Schlenk tube was cooled to rt and filled with N₂. To this flask were added (*S*,*S_p*)-^{*t*}Bu-Phosferrox **L2** (0.25 mmol, 5 mol %) and [Pd(η^3 -allyl)Cl]₂ (0.125 mmol, 2.5 mol %), which were dissolved in 5 mL THF, and stirred at room temperature for about 0.5 h.

A flame dried Schlenk tube was cooled to rt and filled with N_2 . To this flask were added methyl 2-phenyl-4,5-dihydrothiazole-4-carboxylate (5.0 mmol, 1.0 equiv), K_2CO_3 (5.0 mmol, 1.0 equiv), Cu catalyst (5 mol %) and Pd catalyst (5 mol %). The methyl cinnamyl carbonate (7.5 mmol, 1.5 equiv)

was then added. The reaction mixture was stirred at room temperature for 24 h. The organic solvent was removed by rotary evaporation. The dr value was determined by ¹H NMR analysis of the crude mixture and the residue was purified by column chromatography on silica gel to give the allylation product **5e**, which was then directly analyzed by chiral HPLC to determine the enantiomeric excess.



LiAlH₄ (52.8 mg, 1.4 mmol) was added slowly in parts to a stirred solution of **5a** (1 mmol) in Et₂O (10 mL). After 3 h, the reaction was completed (checked by TLC). Ethyl acetate was added, and then the mixture was washed with saturated aq. NaHCO₃ (2×5 mL), H₂O (2×5 mL), saturated aq. NaCl (2×5 mL), and dried with anhydrous Na₂SO₄. The residue was purified by column chromatography (eluent: petroleum ether/ethyl acetate = 10/1) to give the product **6** (282.0 mg, 91 %), as a yellow oil.⁵

To a solution of compound **6** (76.4 mg, 0.247 mmol) in dry THF (20 mL) at 0 °C was added NIS (56 mg, 0.247 mmol) and I₂ (63 mg, 0.247 mmol) in four portions during 30 min. After stirring for an additional 24 h at room temperature, the reaction was completed (checked by TLC). 10% aqueous Na₂S₂O₃ (10 mL) was added to the reaction mixture and extracted with EtOAc (3×20 mL). The combined organic layer was dried over Na₂SO₄ and concentrated under reduced pressure to obtain a residue that was subjected to column chromatography (eluent: petroleum ether/ethyl acetate = 30/1) to afford compound **7** (38.7 mg, 36%) as a yellow solid.⁶

(S)-(4-cinnamyl-2-phenyl-4,5-dihydrothiazol-4-yl)methanol (6):



Yield (91%); 282 mg; yellow oil; $[\alpha]_{D}^{20} = -55.6$ (*c* 0.5, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether: ethyl acetate = 10:1). ¹H NMR (400 MHz, CDCl₃) δ 7.82 – 7.80 (m, 2H), 7.50 – 7.45 (m, 1H), 7.42 – 7.38 (m, 2H), 7.35 - 7.27 (m, 4H), 7.23 – 7.19 (m, 1H), 6.52 (d, *J* = 15.8 Hz, 1H), 6.25 – 6.17 (m, 1H), 3.97 (d, *J* = 11.1 Hz, 1H), 3.68 (d, *J* =

11.1 Hz, 1H), 3.42 (d, J = 11.0 Hz, 1H), 3.28 (d, J = 11.0 Hz, 1H), 2.72-2.59 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 168.7, 137.3, 133.8, 133.0, 131.4, 128.54, 128.50, 128.4, 127.3, 126.2, 124.6, 86.6, 67.9, 39.6, 37.2. HRMS (ESI-TOF) Calcd. For C₁₉H₂₀NOS⁺ ([M+H]⁺): 310.1260, found: 310.1255. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak ID, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 15.2 and 24.1 min.

(S)-8-(iodo(phenyl)methyl)-2-phenyl-7-oxa-3-thia-1-azaspiro[4.4]non-1-ene (7):



Yield (36%); 38.7 mg; yellow solid; m.p. 42-44 °C; $[\alpha]_D^{20} = +14.0$ (*c* 0.9, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 30/1). ¹H NMR (400 MHz, CDCl₃) δ 8.04 – 8.02 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.47 -7.41 (m, 4H), 7.34 – 7.32 (m, 3H), 4.45 – 4.32 (m, 3H), 4.02 (dd, *J* = 9.9, 1.6 Hz, 1H), 3.39 (d, *J* = 13.2 Hz, 1H), 3.09 (d, *J* = 13.2 Hz, 1H), 2.80 – 2.78 (m, 1H), 2.38 (dd, *J* = 13.9, 10.3 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 166.2, 138.8, 133.4, 129.6, 129.5, 128.54, 128.52, 128.4, 127.4, 71.6, 68.9, 64.0, 49.9, 46.1, 27.1. HRMS (ESI-TOF) Calcd. For C₁₉H₁₈NOS⁺ ([M-I]⁺): 309.1181, found: 309.1149.



The preparation of Cu catalyst: A flame dried Schlenk tube was cooled to rt and filled with N₂. To this flask were added (S, S_p)- t Bu-Phosferrox **L2** (0.05 mmol, 5 mol %) and Cu(OTf)₂ (0.05 mmol, 5 mol %) were dissolved in 5 mL THF, and stirred at room temperature for about 0.5 h.

The preparation of Pd catalyst: A flame dried Schlenk tube was cooled to rt and filled with N₂. To

this flask were added (S,S_p) -^{*t*}Bu-Phosferrox **L2** (0.05 mmol, 5 mol %) and $[Pd(\eta^3-allyl)Cl]_2$ (0.025 mmol, 2.5 mol %), which were dissolved in 5 mL THF, and stirred at room temperature for about 0.5 h.

A flame dried Schlenk tube was cooled to rt and filled with N₂. To this flask were added **1b** (1.0 mmol, 1.0 equiv), K₂CO₃ (1.0 mmol, 1.0 equiv), Cu catalyst (5 mol %) and Pd catalyst (5 mol %). The methyl cinnamyl carbonate (1.5 mmol, 1.5 equiv) was then added. The reaction mixture was stirred at room temperature for 24 h. The organic solvent was removed by rotary evaporation. The dr value was determined by ¹H NMR analysis of the crude mixture and the residue was purified by column chromatography to give the allylation product **5p** (246.0 mg, 65%), which was then directly analyzed by HPLC to determine the enantiomeric excess.

5p (246 mg, 0.65 mmol, 1.0 equiv) was dissolved in DCM and TFA was added (3:1 v/v, 0.2 M). The reaction was stirred at 25 °C for 2 hours and concentrated under reduced pressure to obtain crude residue **8**, it was used in the next reaction without further purification.⁷

To a solution of **8** (0.65 mmol, 1.0 equiv) in MeCN (15 mL), were added NaHCO₃ (0.78 mmol, 1.2 equiv), I₂ (0.78 mmol, 1.2 equiv), KI (0.78 mmol, 1.2 equiv) at 0 °C, after stirring for 2 h, the reaction mixture was allowed to warm to room temperature and stirred for 10 h. The reaction was quenched with saturated aqueous Na₂S₂O₃ solution (20 mL) and diluted with EtOAc (25 mL). The organic layer was separated and the aqueous layer extracted with EtOAc (2×25 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude residue was purified by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 40/1) to obtain the **9** (113.0mg, 39%, dr = 16:1) and **10** (102.0 mg, 36%, dr = 16:1) as a yellow solid.⁸

Tert-butyl (S)-4-cinnamyl-2-phenyl-4,5-dihydrothiazole-4-carboxylate (5p):



Yield (65%); 246.0 mg; yellow oil; $[\alpha]_D^{20} = -13.4$ (*c* 1.4, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 50/1). ¹H NMR (400 MHz, CDCl₃) δ 7.89 – 7.87 (m, 2H), 7.48 – 7.42 (m, 1H), 7.41 – 7.36 (m, 2H), 7.35 – 7.30 (m, 2H), 7.30 – 7.25 (m, 2H), 7.22 – 7.15 (m, 1H), 6.52 (d, *J* = 15.8 Hz, 1H), 6.26 – 6.18 (m, 1H), 3.82 (d, *J* = 11.4 Hz,

1H), 3.39 (d, J = 11.4 Hz, 1H), 2.93 – 2.84 (m, 2H), 1.49 (s, 9H). ¹³C NMR (100 MHz, CDCl₃) δ 171.3, 168.5, 137.2, 134.0, 133.1, 131.4, 128.6, 128.5, 128.4, 127.4, 126.3, 124.3, 88.7, 82.2, 41.4, 39.1, 28.1. HRMS (ESI-TOF) Calcd. For C₂₃H₂₆NO₂S⁺ ([M+H]⁺): 380.1679, found: 380.1672. The product was analyzed by chiral HPLC to determine the enantiomeric excess: 99% ee (Chiralpak ID, *i*-propanol/hexane = 1/99, flow rate 1.0 mL/min, $\lambda = 254$ nm); t_r = 5.8 and 6.8 min.

(S)-8-(iodo(phenyl)methyl)-2-phenyl-7-oxa-3-thia-1-azaspiro[4.4]non-1-en-6-one (9):



Yield (39%); 113.0 mg; yellow solid; m.p. 110-112 °C; $[\alpha]_D^{20} = +38.4$ (*c* 0.8, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 40/1). ¹H NMR (400 MHz, CDCl₃) δ 7.84 – 7.82 (m, 2H), 7.50 – 7.46 (m, 3H), 7.43 -7.40 (m, 2H), 7.36 – 7.29 (m, 3H), 5.24 – 5.16 (m, 2H), 4.01 (d, *J* = 11.2 Hz, 1H), 3.34 (d, *J* = 11.2 Hz, 1H), 2.98 – 2.94 (m, 1H), 2.20 – 2.15 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 174.4, 170.7, 139.2, 132.2, 132.0, 129.0, 128.8, 128.7, 128.6, 128.2, 85.9, 80.6, 45.0, 38.4, 33.5. HRMS (ESI-TOF) Calcd. For C₁₉H₁₇INO₂S⁺ ([M+H]⁺): 450.0019, found: 450.0011.

(S)-9-iodo-2,8-diphenyl-7-oxa-3-thia-1-azaspiro[4.5]dec-1-en-6-one (10):



Yield (35%); 102.0 mg; yellow solid; m.p. 110-112 °C; $[\alpha]_D^{20} = -94.4$ (*c* 0.5, CHCl₃); it was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 40/1). ¹H NMR (400 MHz, CDCl₃) δ 7.88 – 7.86 (m, 2H), 7.53 – 7.51 (m, 1H), 7.49 – 7.45 (m, 4H), 7.35 – 7.29 (m, 3H), 5.52 (d, *J* = 10.0 Hz, 1H), 5.17 – 5.12 (m, 1H), 3.87 (d, *J* = 11.2 Hz, 1H), 3.44 (d, *J* = 11.6 Hz, 1H), 2.90 – 2.76 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 175.2, 171.4, 139.5, 132.1, 128.9, 128.8, 128.7, 128.2, 84.2, 80.3, 42.2, 40.0, 33.8. HRMS (ESI-TOF) Calcd. For C₁₉H₁₇INO₂S⁺ ([M+H]⁺): 450.0019, found: 450.0014.

IV. Absolute configuration determination of (S, E)-5e



In a 10 mL oven-dried glass sample vial, 10 mg pure 5e and 0.1 mL CH₃OH were added, and then 4 mL *n*-hexane was slowly added to the solution, which was sealed with perforated paper at room temperature to grow crystals.

Bond precision:	C-C = 0.0041	l A	Wavelength $= 1.54184$				
Cell:	a = 7.6819 (1) 1	b = 5.8950(1)		c = 20.1743 (1)		
;	alpha = 90	beta	= 91.416 (1)		gamma	a = 90	
Temperature:	100 K						
		Ca	lculated		Report	ed	
Volume		91.	3.31 (2)		913.31	(2)	
Space group		P 21			P 1 21 1		
Hall group		P 2yb			P 2yb		
Moiety formula		C20 H18 Br N O2 S			C20 H18 Br N O2 S		
Sum formula		C20 H18 Br N O2 S			C20 H18 Br N O2 S		
Mr		416	.31	4	416.32		
Dx, g cm ⁻³		1.514		1.514			
Z		2			2		
Mu (mm ⁻¹)		4.2	40	4.240			
F000		424.0		424.0			
F000'		42	4.26				
h,k,lmax		9,7,25			9,7,25		
Nref		3699[2039]			3585		
Tmin,Tmax		0.489,0.809			0.548,1.000		
Tmin'		0.	267				
Correction method =	# Reported	Т	T Limits: Tmin = 0.548 Tmax = 1.000				

AbsCorr = MULTI-SCAN Data completeness = 1.76/0.97

R(reflections) = 0.0213(3567)S = 1.080 Theta(max) = 73.736 wR2(reflections) = 0.0579(3585) Npar= 227

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VI. ¹H NMR and ¹³C NMR spectra







¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)







¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)





¹⁹**F NMR** (376 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)





¹⁹**F NMR** (376 MHz, CDCl₃)







¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)


¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)





¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)

VII. HPLC spectra



Data File E:\DATA\WHM-2\WHM-3-126-PH-RAC 2019-11-27 11-27-40\WHM-3-126-Ph-RAC-2.D Sample Name: WHM-3-126-Ph-rac-2

Acq. Operator	: SYSTE	EM		Seq. Line :	1			
Acq. Instrument	: 1260			Location :	3			
Injection Date	: 11/27	/2019 11:29:05	AM	Inj :	1			
				Inj Volume :	5.000 µl			
Acq. Method	: E:\DA M	\TA\WHM-2\WHM-3-	126-PH-RAC	2019-11-27 1	1-27-40\1	EH-98-21ML	L-20MIN-5U	
Last changed	: 11/27 (modi	/2019 11:44:31 fied after load	AM by SYST ling)	EM				
Analysis Method	: E:\DA	TA\WHM-2\WHM-3-	126-PH-RAC	2019-11-27 1	1-27-40\1	EH-98-21MU	L-20MIN-5U	L.
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Peak RetTime Typ	e Widt	h Area	Height	Area				
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1 11.842 BB	0.28	321 5760.70996	310,93454	50.2634				
2 13.629 BB	0.37	33 5700.32324	229.88614	49.7366				
Totals :		1.14610e4	540.82068					
		+++ End of F	eport ***					
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12/2//2020 8:49	:19 PM	SYSTEM					Fage	1 01 1



Data File E:\DATA\WHM-2\WHM-3-144-THFET20 2019-12-12 18-05-56\WHM-3-144-THFET201.D Sample Name: WHM-3-144-THF



1260 1/6/2020 4:47:26 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\WHM-3-149-P-ME-RAC1.D Sample Name: WHM-3-149-P-ME-RAC

Acq. Operator	: SYSTEM	Seq. Line	: 2		
Acq. Instrument	: 1260	Location	: 1		
Injection Date	: 12/16/2019 7:44:33 P	M Inj	: 1		
		Inj Volume	: 5.000 µl		
Acq. Method	: E:\DATA\WHM-2\WHM-3-:	149-P-ME-RAC 2019-12	-16 19-38-11	\IEH-98-21ML-20MIN-	
Last changed	12/16/2010 7:57:07 0	he everen			
Last changed	(modified after load	ing)			
Analysis Method	: E:\DATA\WHM-2\WHM-3-	149-P-ME-RAC 2019-12	-16 19-38-11	\IEH-98-21ML-20MIN-	
-	5UL.M (Sequence Meth	od)			
Last changed	: 12/27/2020 8:53:41 P	M by SYSTEM			
	(modified after load:	ing)			
Additional Info	: Peak(s) manually into	egrated			
DAD1 A, SI	g=254,4 Ref=360,100 (E:\DATA\WH	IWHM-3-149-P-ME-RAC 2019	-12-16 19-38-11W	VHM-3-149-P-ME-RAC1.D)	
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#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.741	вв	0.2212	3137.48145	215.00465	50.1616
2	10.880	BB	0.2892	3117.26099	162.18855	49.8384

6254.74243 377.19321

1260 12/27/2020 8:53:44 PM SYSTEM

Totals :



Data File E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\WHM-3-149-P-ME-RAC5.D Sample Name: WHM-3-148-P-ME

Acq. Operator :: VSTEM Seq. Line :: 6 Acq. Instrument :: 126 Location :: 5 Injection Date :: 12/16/2019 9:84:06 PM Inj :: 1 Inj Volume :: 5.000 µl Acq. Method :: E:\DATA\WHM-2\WHM-3-149-P-ME-MAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SUL.M Last changed :: 12/16/2019 8:00:08 PM by SYSTEM Analysis Method :: E:\DATA\WHM-2\WHM-3-149-P-ME-MAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SUL.M Last changed :: 12/6/2019 4:57:58 PM by SYSTEM (modified after loading) Additional Info :: Peak(s) manually integrated Dot A Sup-54.4 Mer-50(100 (ECATAWIM-WHMA-148-AME-6AC 2019-12-18 1958-11W/MAA-148-AME-6ACSD) mU mU mU mU mu area Percent Report Area Percent Report Area Percent Report Area Percent with ISTDs Signal 1: DADI A, Sig=254.4 Ref=360,100 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DADI A, Sig=254.4 Ref=366,100 Peak RetTime Type Width Area Height Area # [mi] [mi] [mi] [mi] [mi] [mi] [mi] 1 9.6148 8 0.2129 9903.38316 665.14752 93.9555 2 10.774 88 0.2249 60.75577 3.29874 0.6045 Totals : 1.005014 689.44626 		
Acq. Instrument : 1209 Location : 5 Injection Date : 12/16/2019 9:00:00 FM Inj : 1 Inj Volume : 5.000 µl Acq. Method : E:\DATA\WMM-2\WMM-3:49-P-ME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SUL.M (Sequence Method) Last changed : 12/06/2019 8:00:00 FS VSTEM (modified after Loading) Additional Trois : Peak(5 amoully integrated DADIA Sep-564 Ame-500.00 (ESDATAWH-WMM-5-180-AME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SUL.M (Sequence Method) additional Trois : Peak(5 amoully integrated DADIA Sep-564 Ame-500.00 (ESDATAWH-WMM-5-180-AME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- Solution : Peak(5 amoully integrated DADIA Sep-564 Ame-500.00 (ESDATAWH-WMM-5-180-AME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- Solution : Second :	Acg. Operator : SYSTEM Seg. Line : 6	
Injection Date : 12/16/2019 9:04:06 PM Inj : 1 Inj Volume : 5.000 µl Acq. Method :: E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SUL.M Last changed :: 12/16/2019 8:00:08 PM by SYSTEM Analysis Method :: E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SUL.M (Sequence Method) Last changed :: 12/6/2029 4:57:58 PM by SYSTEM (modified after loading) Additional Info :: Peak(s) manually integrated Modified after loading) Additional Info :: Signal Multiplier :: 1.0000 Dilution :: 1.0000 Dilution :: 1.0000 Peak RetTime Type Midth Area Height Area # [min] [mul*] [mul*] [mul*] X 	Acq. Instrument : 1260 Location : 5	
Inj Volume: 5.000 µl Acq. Method :: E:\UTATAUHH-2\WH-3.149-P-ME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SULM Last changed :: 12/16/2019 8:00:00 ECOMMUNE-XMAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SULM (Sequence Method) Last changed :: 16/2020 457:58 PM by SYSTEM (modified after loading) Additional Thro: Peak(5) smaxully integrated DACIA Seg-564 Ref-300.00 (ECOMMUNE WHAS-168-ME-RAC 2019-12-16 19-38-11WHAS-168-ME-RAC 50) 	Injection Date : 12/16/2019 9:04:06 PM Inj : 1	
Acq. Method :: [:\DATA\UMEN-2.149-P-ME-RAC 2019-12-15 19-38-11\[EH-98-2]ML-20MIN- SU.M (Sequence Method) Last changed :: 1/2/16/2019 8:00:00 PM by SYSTEM Analysis Method :: [DATA\UMEN-2.149-P-ME-RAC 2019-12-16 19-38-11\[EH-98-2]ML-20MIN- SU.M (Sequence Method) Last changed :: 1/6/2020 4:57:158 PM by SYSTEM (mdified after loading) Additional Info: Peak(s) manually integrated DUALA Sep254 Met300.00 (ECOTATAWH-WHMS-5:68-ME-RAC 2019-12-16 19-38-11\[EH-98-2]ML-20MIN- 500 00 00 00 00 00 (ECOTATAWH-WHMS-5:68-ME-RAC 2019-12-16 19-38-11\[EH-98-2]ML-20MIN- 100 00 00 00 00 00 (ECOTATAWH-WHMS-5:68-ME-RAC 2019-12-16 19-38-11\]EH-98-2]ML-20MIN- MUT 00 00 00 00 00 (ECOTATAWH-WHMS-5:68-ME-RAC 2019-12-16 19-38-11\]EH-98-2]ML-20MIN- Metabolic Content of the second of	Inj Volume : 5.000 µl	
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Last changed : 12/16/2019 8:00:00 PM by SYSTEM Analysis Method : E:\ultimatureHetaues. 1-109-PME.RAC 2019-12-16 19-38-11\lEH-98-21ML-20MIN- SuL.M (Sequence Method) Last changed : 1/6/2020 4:57:58 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated DUALA Seg-254.8 Rel-300,000 (ECD/MANN-L.WHAS-168-PAME.RAC 2016-12-16 19-38-11WHRAS-168-PAME.PAAC.50.0) mu and a seg-254.9 Rel-300,000 (ECD/MANN-L.WHAS-168-PAME.PAAC.2016-12-16 19-38-11WHRAS-168-PAME.PAAC.50.0) Area Percent Report 	SUL.M	
Analysis Method : E:\DATAWHM-2:L49-PME-RAC 2019-12-16 19-38-11\TEH-98-2:-1ML-20MTN- S.U. M. (Sequence Method) Last changed : 1/6/2020 4:57:58 PM by SYSTEM (modified after loading) Additional Info: Peak(s) manually integrated DADIA_Sep254.4 Mer-300_000 (E:DATAWHWHM-3-169-PME-RAC 2019-12-16 19-38-11WHM-3-169-PME-RAC 5D)	Last changed : 12/16/2019 8:00:08 PM by SYSTEM	
SUL M (Sequence Method) Last changed : 1/6/2020 4:57:58 M by SYSTEM (modified after loading) Additional Info : Peak(3) manually integrated	Analysis Method : E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN-	
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(modified after loading) Additional Info : Peak(s) manually integrated DND1A Sup254.4 Ref-300,00 (E:DATAWHL WHB.3-168-PAME-RAC 2019-12-16 19-36-110WHB.3-168-PAME-RAC 2019 mAU additional transmission of the state of the s	Last changed : 1/6/2020 4:57:58 PM by SYSTEM	
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Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] % 		
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] % 		
Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %	Signal 1: DAD1 A, Sig=254,4 Ref=360,100	
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	# [min] [mAU*s] [mAU] %	
1 9.614 BB 0.2189 9989.36816 686.14752 99.3955 2 10.774 BB 0.2249 60.75687 3.29874 0.6045 Totals : 1.00501e4 689.44626 **** End of Report ***		
2 10.774 BB 0.2249 60.75687 3.29874 0.6045 Totals : 1.00501e4 689.44626 	1 9.614 BB 0.2189 9989.36816 686.14752 99.3955	
Totals : 1.00501e4 689.44626	2 10.774 BB 0.2249 60.75687 3.29874 0.6045	
Totals : 1.00501e4 689.44626		
*** End of Report ***	Totals : 1.00501e4 689.44626	
*** End of Report ***		
*** End of Report ***		
*** End of Report ***		

1260 1/6/2020 4:58:02 PM SYSTEM



Data File E:\DATA\wHM-2\WHM-3-151-M-OME 2019-12-20 14-52-47\WHM-3-151-M-OME3.D Sample Name: WHM-3-149-P-OME-RAC

Acq. Operator : SYSTEM Seq. Line : 4 Location : 5 Acq. Instrument : 1260 Injection Date : 12/20/2019 3:37:57 PM Inj : 1 Inj Volume : 5.000 µl Acq. Method : E:\DATA\WHM-2\WHM-3-151-M-OME 2019-12-20 14-52-47\AD-95-5-30min-5UL-0.5ML.M Last changed : 12/20/2019 2:55:57 PM by SYSTEM Analysis Method : E:\DATA\WHM-2\WHM-3-151-M-OME 2019-12-20 14-52-47\AD-95-5-30min-5UL-0.5ML.M (Sequence Method) Last changed : 1/6/2020 5:11:59 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated DAD1 B, Sig=254,4 Ref=360,100 (E:\DATA\WHM-2WHM-3-151-M-OME 2019-12-20 14-52-47\WHM-3-151-M-OME3.D) mAU -200 -8 175 ä 150 -125-100 -75-50 -25 0 15 10 20 ----------Area Percent Report _____ Sorted By : Signal Multiplier 1.0000 : Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 B, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] % 1 20.393 VB 0.5243 6505.52002 175.98625 50.8618 2 23.130 BB 0.5552 6285.05176 164.33684 49.1382 Totals : 1.27906e4 340.32309 -----*** End of Report ***

1260 1/6/2020 5:12:17 PM SYSTEM



Data File E:\DATA\WHM-2\whm-3-148-p-ome-s 2019-12-20 21-43-40\whm-3-148-p-ome-s1.D Sample Name: whm-3-148-p-ome-s

Acg. Operator : SYSTEM Seg. Line : 2
Acg. Instrument : 1260 Location : 6
Injection Date : 12/20/2019 9:56:18 PM Inj : 1
Ini Volume : 5,000 ul
Acq. Method : E:\DATA\WHM-2\whm-3-148-p-ome-s 2019-12-20 21-43-40\AD-95-5-30min-5UL-0.5ML
Last changed : 12/20/2019 9:43:40 PM by SYSTEM
Analysis Method : E:\DATA\WHM-2\whm-3-148-p-ome-s 2019-12-20 21-43-40\AD-95-5-30min-5UL-0.5ML
.M (Sequence Method)
Last changed : 1/6/2020 5:17:10 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated
DAD1 B, Sig=254,4 Ref=360,100 (E:DATAWHM-2whm-3-148-p-ome-s 2019-12-20 21-43-40whm-3-148-p-ome-s 1.D)
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100 10 15 20 25 m Area Percent Report Area Percent Report Sorted By :: Signal Multiplier :: 1.0000 10000 10000 10000 10000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 8, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] % % 1 20.408 BB 0.3746 175.36024 5.59551 0.6162 2 23.131 BB 0.5618 2.82832e4 735.26331 99.3838 Totals : 2.84585e4 740.85882
100 0 5 10 15 20 25 m Area Percent Report
100 0

1260 1/6/2020 5:17:13 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\WHM-3-149-P-ME-RAC3.D Sample Name: WHM-3-149-P-CL-RAC

Acq. Operator	: SYSTEM Seq. Line : 4
Acq. Instrument	: 1260 Location : 3
Injection Date	: 12/16/2019 8:21:19 PM Inj: 1
-	Inj Volume : 5.000 µl
Acq. Method	: E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN- SUL.M
Last changed	: 12/16/2019 8:00:08 PM by SYSTEM
Analysis Method	: E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN-
	5UL.M (Sequence Method)
Last changed	: 1/6/2020 5:00:49 PM by SYSTEM
	(modified after loading)
DAD1 A, S	Sig=254,4 Ref=360,100 (E:\DATA\WHWHM-3-149-P-ME-RAC 2019-12-16 19-38-11\WHM-3-149-P-ME-RAC3.D)
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	Area Percent Report
Sorted By	: Signal
Multiplier	: 1.0000
Dilution	: 1.0000
Do not use Mult	tiplier & Dilution Factor with ISTDs
Signal 1: DAD1	A, Sig=254,4 Ref=360,100
Peak RetTime Ty	/pe Width Area Height Area
# [min]	[min] [mAU*s] [mAU] %
1 9.792 BV	0.2270 1718.11230 113.86243 50.1000
2 10.686 VB	3 0.2946 1711.25476 86.93739 49.9000
Totals :	3429.36707 200.79982
	*** End of Report ***

1260 1/6/2020 5:01:07 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\WHM-3-149-P-ME-RAC7.D Sample Name: WHM-3-148-P-CL

Acq. Operator : SYSTEM	Seq. Line : 8
Acq. Instrument : 1260	Location : 7
Injection Date : 12/16/2010 0:51:54 DM	Ini : 1
Injection bate : 12/10/2019 9.51.54 Ph	Inj. I Taj Valuma : E 000 ul
Acq. Method : E:\DATA\WHM-2\WHM-3-149-P-M	E-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN-
SUL.M	
Last changed : 12/16/2019 9:53:01 PM by SY	STEM
(modified after loading)	
Analysis Method : E:\DATA\WHM-2\WHM-3-149-P-M	E-RAC 2019-12-16 19-38-11\IEH-98-21ML-20MIN-
5UL M (Sequence Method)	
Last changed : 1/6/2020 5:02:25 DM by SVST	EM
Last changed . 1/0/2020 5.02.25 PH by 5151	
(modified after loading)	
DADT A, Sig=204,4 Rel=300,100 (EXDATAWHIWHMA3	149+P*ME*RAC 2019+12+10 19+30+11W/PMP3+149+P*ME*RAC7.D)
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Area Percent Report	6 8 10 12 14 min
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Area Percent Report Sorted By : Signal Multiplier : 1.0000	8 8 10 12 14 mir
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000	
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with	6 8 10 12 14 min
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with	6 8 10 12 14 min
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with	6 8 10 12 14 min
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with	8 8 10 12 14 min
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100	10 12 14 min
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100	6 8 10 12 14 min
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height	6 8 10 12 14 min
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height # [min] [mAU*s] [mAU]	6 8 10 12 14 min
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height # [min] [min] [mAU*s] [mAU]	ISTDs
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height # [min] [min] [mAU*s] [mAU] 	Area X
0 2 4 Area Percent Report Sorted By : Signal Multiplier 1.0000 Dilution 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [min] 1 9.739 BB 0.2246 3862.45410 258.154 2 10.653 BB 0.1998 19.45106 1.152	Area %
0 2 4 Area Percent Report Area Percent Report Sorted By : Signal Multiplier 1.0000 Dilution 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [min] [mAU*s]	Area X
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0 2 4 Area Percent Report Area Percent Report Sorted By : Signal Multiplier 1.0000 Dilution 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [min] [mAU*s] 1 9.739 BB 0.2246 3862.45410 258.154 2 10.653 BB 0.1998 19.46106 1.153 Totals : 3881.91516 259.308	Area x
0 2 4 Area Percent Report Area Percent Report Sorted By : Signal Multiplier 1.0000 Dilution 1.0000 Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [min] [mAU*s] 1 9.739 BB 0.2246 3862.45410 258.154 2 10.653 BB 0.1998 19.46106 1.153 Totals : 3881.91516 259.308 **** End of Report *	Area %

1260 1/6/2020 5:02:35 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\WHM-3-149-P-ME-RAC4.D Sample Name: WHM-3-149-P-BR-RAC

_____ Seq. Line : 5 Location : 4 Acq. Operator : SYSTEM Acq. Instrument : 1260 Inj: 1 Injection Date : 12/16/2019 8:42:43 PM Inj Volume : 5.000 µl : E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\IEH-98-2--1ML-20MIN-Acq. Method 5UL.M Last changed : 12/16/2019 8:00:08 PM by SYSTEM Analysis Method : E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\IEH-98-2--1ML-20MIN-5UL.M (Sequence Method) Last changed : 1/6/2020 5:04:45 PM by SYSTEM (modified after loading) DAD1 A, Sig=254,4 Ref=360,100 (E:\DATA\WH...WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\WHM-3-149-P-ME-RAC4.D) mAU 200 10.498 150-553 100 50 0 10 _____ Area Percent Report _____ Sorted By : Signal 1.0000 Multiplier : 1.0000 Dilution . Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Height Area Area [min] [mAU*s] # [min] [mAU] % 1 10.498 BB 0.2474 2140.94800 129.81493 50.6023 2 11.593 BB 0.3459 2089.98291 89.67770 49.3977 4230.93091 219.49262 Totals : -----*** End of Report ***

1260 1/6/2020 5:04:53 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-149-P-ME-RAC 2019-12-16 19-38-11\WHM-3-149-P-ME-RAC8.D Sample Name: WHM-3-148-P-BR

Acc. Operator	: SYSTEM	Seq. Line :	9		
Acq. Instrument	: 1260	Location :	8		
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injection bate	. 12/10/2019 10.13.25 PM	Inj Volumo :	5 000 11		
Aca Mathad	- E-\DATA\UUM-2\UUM-2-140-1	ME-DAC 2010-12-16	10-39-11\ TEU-0	0.0.1ML.00MTN	
Acq. Method	: E:\DATA\WHM-2\WHM-3-149-0	-ME-KAC 2019-12-16	19-39-11/160-9	8-2IML-20MIN-	
Last shared	50L.M	OVETEN			
Last changed	: 12/16/2019 9:53:01 PM by	SYSTEM	10 30 113 750 0		
Analysis Method	: E:\DATA\WHM-2\WHM-3-149-P	-ME-KAC 2019-12-16	19-38-11/1EH-9	8-21ML-20M1N-	
	SUL.M (Sequence Method)				
Last changed	: 1/6/2020 5:04:45 PM by S	STEM			
DADI A R	(modified after loading)				
	Ig=254,4 Ref=360,100 (E:\DATAWHWH	W+3+149+P+ME+RAC 2019+12+	10 19-30-11 W/PMM-3-14	9+P+ME+RAU8.D)	
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Sorted By Multiplier Dilution Do not use Mult	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor wit	rt th ISTDs	<u>10</u>	209:1- 	14 mi
Sorted By Multiplier Dilution Do not use Mult	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor wit	th ISTDs	<u>10</u> .	209-1 	14 mi
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Sorted By Multiplier Dilution Do not use Mult Signal 1: DAD1 A Peak RetTime Ty # [min] 1 10.472 BB	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heig [min] [mAU*s] [mAU 	th ISTDs	<u>10</u>	209-1	14 mi
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Sorted By Multiplier Dilution Do not use Mult Signal 1: DAD1 A Peak RetTime Ty # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heig [min] [mAU*s] [mAU 	th ISTDs			14 mi
Sorted By Multiplier Dilution Do not use Mult Signal 1: DAD1 // Peak RetTime Ty # [min] 1 10.472 BB 2 11.635 BB Totals :	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Hein [min] [mAU*s] [mAU 	th ISTDs	<u>10</u>	12	14 mi
Sorted By Multiplier Dilution Do not use Mult Signal 1: DAD1 A Peak RetTime Ty # [min] 1 10.472 BB 2 11.635 BB Totals :	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heig [min] [mAU*s] [mAU 	th ISTDs	<u>10</u>	12	14 mi
Sorted By Multiplier Dilution Do not use Mult Signal 1: DAD1 A Peak RetTime Ty # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heig [min] [mAU*5] [mAL 	th ISTDs			14 mi
o o Sorted By Multiplier Dilution Do not use Mult Signal 1: DAD1 A Peak RetTime Ty # [min] 1 10.472 BB 2 11.635 BB Totals :	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heig [min] [mAU*s] [mAU 	th ISTDs			14 mi
Sorted By Multiplier Dilution Do not use Mult Signal 1: DAD1 J Peak RetTime Ty # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heig [min] [mAU*s] [mAU 	th ISTDs	<u>10</u>	12	14 mi
o o o Sorted By Multiplier Dilution Do not use Mult Signal 1: DAD1 of Peak RetTime Ty # [min] 1 10.472 BB 2 11.635 BB Totals :	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heig [min] [mAU*s] [mAU 	th ISTDs	<u>10</u>		14 mi

1260 1/6/2020 5:05:45 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\WHM-3-150-M-ME-RAC1.D Sample Name: WHM-3-150-M-ME-RAC

Acq. Operator : SYSTEM Seq. Line : 2	
Acq. Instrument : 1260 Location : 1	
Injection Date : 12/17/2019 7:34:47 PM Inj : 1	
Inj Volume : 5.000 µl	
Acq. Method : E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\IEH-98-21ML-20MIN -5UL.M	
Last changed : 12/17/2019 7:22:09 PM by SYSTEM	
Analysis Method : E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\IEH-98-21ML-20MIN	
-SUL.M (Sequence Method)	
Last changed : 12/27/2020 8:57:33 PM by SYSTEM	
(modified after loading)	
Additional Info : Peak(s) manually integrated DAD1 A, SIg=254,4 Ref=360,100 (E:\DATA\WH3-150-M-ME-CL-RAC 2019-12-17 19-22-09\WHM-3-150-M-ME-RAC1.D)	
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Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS	min
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS	min
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS	min
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS	min
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS	min
Sorted By : Signal Multiplier : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS	min
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area	min
Sorted By : Signal Multiplier : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %	min
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] % 	min
50 0 2 4 6 8 10 12 14 16 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 10000 10000 10000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] % # [min] [min] [mAU*s] [mAU] % 1 9.318 BB 0.2139 3802.40796 267.43774 50.2975	min
50- -	nim
50 0 1	nim
50 6 6 6 10 12 14 16 Area Percent Report Area Percent Report Sorted By :: Signal Multiplier :: 1.0000 10 12 14 16 Do not use Multiplier & Dilution Factor with ISTDs 5 5 5 5 5 Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*5] [mAU] % %	min
50 0 1	min
so	min
50 0 1	min
30 30 4 6 8 10 12 14 16	min

1260 12/27/2020 8:57:41 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\WHM-3-151-M-ME-CL-OME3.D Sample Name: WHM-3-151-M-ME-S

_____ Acq. Operator : SYSTEM Seq. Line : 4 Acq. Instrument : 1260 Location : 3 Injection Date : 12/18/2019 10:46:50 PM Inj : 1 Inj Volume : 5.000 µl Acq. Method : E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\IEH-98-2--1ML-20MIN-5UL . M Last changed : 12/18/2019 9:51:22 PM by SYSTEM Analysis Method : E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\IEH-98-2--1ML-20MIN-5UL.M (Sequence Method) Last changed : 1/6/2020 7:57:27 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated DAD1 A. Sig=254,4 Ref=360,100 (E:DATAIWH...-3-151-M-ME-CL- 2019-12-18 21-51-22WHM-3-151-M-ME-CL-OME3.D) mAU 1750 -1500 ŝ 1250 -1000 -750 -500 -250 -0220 0 12 10 -----------Area Percent Report _____ Sorted By Signal : Multiplier : 1.0000 1.0000 Dilution . Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] % 1 9.251 BB 0.2158 1.78877e4 1243.89124 99.2534 2 10.590 BB 0.2654 134.55562 6.81284 0.7466 Totals : 1.80223e4 1250.70408 ----------*** End of Report ***

1260 1/6/2020 7:57:35 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\WHM-3-150-M-ME-RAC10.D Sample Name: WHM-3-150-M-ME-RAC

_____ Acq. Operator : SYSTEM Seq. Line : 11 Acq. Instrument : 1260 Location : 6 Injection Date : 12/17/2019 10:26:18 PM Inj : 1 Inj Volume : 5.000 µl : E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\IEH-98-2--1ML-20MIN Acq. Method -5UL.M Last changed : 12/17/2019 10:54:25 PM by SYSTEM (modified after loading) Analysis Method : E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\IEH-98-2--1ML-20MIN -5UL.M (Sequence Method) : 12/27/2020 9:36:23 PM by SYSTEM Last changed (modified after loading) Additional Info : Peak(s) manually integrated "DAD1, Sig-262,4 Ref-355,90, EXT of WHM-3-150-M-ME-RAC10.D n AU] 80 15.347 60 8.236 40 20 0 17.5 22.5 15 20 10 12.5 Area Percent Report Sorted By Signal : Multiplier 1.0000 . Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1, Sig=262,4 Ref=355,90, EXT Signal has been modified after loading from rawdata file! Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] % 1 15.347 BB 0.3573 1524.78882 64.62830 49.1873 2 18.236 BB 0.4712 1575.17395 45.91649 50.8127 Totals : 3099,96277 110,54479 _____ *** End of Report *** 1260 12/27/2020 9:36:26 PM SYSTEM Page 1 of 1



Data File E:\DATA\WHM-2\WHM-3-151-M-OME 2019-12-20 14-52-47\WHM-3-151-M-OME1.D Sample Name: WHM-3-151-M-OME-S

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 4
Injection Date : 12/20/2019 3:05:28 PM Inj : 1
Inj Volume : 5.000 µl
Acq. Method : E:\DATA\WHM-2\WHM-3-151-M-OME 2019-12-20 14-52-47\IEH-98-21ML-20MIN-5UL.M
Last changed : 12/20/2019 2:52:47 PM by SYSTEM
Analysis Method : E:\DATA\WHM-2\WHM-3-151-M-OME 2019-12-20 14-52-47\IEH-98-21ML-20MIN-5UL.M
(Sequence Method)
Last changed : 1/6/2020 7:59:39 PM by SYSTEM
(modified after loading) Dabia Server A server in the control of t
DADTA, SIG-204,4 REF-300,100 (E:DATAWHM-2WHM-310 HW-OME 2019-1240 H4-0244/WHM-3-10 HW-OME 1.D)
350 -
Ener
250
200 -
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50
50 0 0 2 4 6 8 10 12 14 16 18 mi
50 50 0 0 2 4 6 8 10 12 14 16 18 mi
50 0 0 2 4 6 8 10 12 14 16 18 mi
50 50 0 2 4 6 8 10 12 14 16 18 mi Area Percent Report
50 50 0 2 4 6 8 10 12 14 16 18 mi Area Percent Report
50 50 0 2 4 6 8 10 12 14 16 18 mi
50 6 8 10 12 14 16 18 mi Area Percent Report Sorted By : Signal hubicities
50 50 0 2 4 6 8 10 12 14 16 18 mi Area Percent Report Sorted By I Signal Multiplier I 1.0000 Dilution
50
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
Area Percent Report
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peach PetTime Tume Width Area Height Area
Area Percent Report Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area 4 for final for the factor with Structure and for the factor and factor and for the factor and factor
Area Percent Report Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] X
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] X
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU*s] :
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU*s] [mAU] 1 15.712 BB 0.3644 8135.17773 334.85144 100.0000
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU] %
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] %
50 6 6 8 10 12 14 16 18 mi Area Percent Report Area Percent Report Sorted By :: Signal Multiplier :: 1.0000 10 12 14 16 18 mi Multiplier :: 1.0000 10 1.0000 1000
50 6 6 6 10 12 14 16 18 mi Area Percent Report Area Percent Report Sorted By :: Signal Multiplier 1.0000 Dilution :: 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] %
Image: Signal isolation in the image: Signal isolation
Image: state of the state

1260 1/6/2020 7:59:42 PM SYSTEM



Data File E:\DATA\wHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\WHM-3-150-M-ME-RAC2.D Sample Name: WHM-3-150-M-CL-RAC

-----Seq. Line : 3 Acq. Operator : SYSTEM Acq. Instrument : 1260 Location : 2 Injection Date : 12/17/2019 7:56:13 PM Inj: 1 Inj Volume : 5.000 µl Acq. Method : E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\IEH-98-2--1ML-20MIN -SUL.M Last changed : 12/17/2019 8:08:39 PM by SYSTEM (modified after loading) Analysis Method : E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\IEH-98-2--1ML-20MIN -SUL.M (Sequence Method) Last changed : 12/27/2020 9:44:56 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated DAD1 A, Stg-254,4 Ref-360,100 (E:DATAWH...-3-150-M-ME-CL-RAC 2019-12-17 19-22-09WHM-3-150-M-ME-RAC2.D) 270985 mAU 7 100 heat 210343 175 -150 -125 -100-75-50 -25 -0 10 -----Area Percent Report Sorted By : Signal Multiplier 1.0000 : Dilution 1.0000 . Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Height Area Area # [min] [min] [mAU*s] [mAU] % 1 9.553 MF 0.2486 2769.64697 185.71367 49.7862 2 10.534 FM 0.3148 2793.42969 147.90947 50.2138 1 9.553 MF Totals : 5563.07666 333.62314 _____ *** End of Report ***

1260 12/27/2020 9:44:59 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\WHM-3-151-M-ME-CL-OME1.D Sample Name: WHM-3-151M--CL-S

-----Acq. Operator : SYSTEM Seq. Line : 2 Location : 1 Acq. Instrument : 1260 Injection Date : 12/18/2019 10:04:03 PM Inj: 1 Inj Volume : 5.000 µl Acq. Method : E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\IEH-98-2--1ML-20MIN-5UL.M Last changed : 12/18/2019 9:51:22 PM by SYSTEM Analysis Method : E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\IEH-98-2--1ML-20MIN-5UL.M (Sequence Method) Last changed : 12/27/2020 9:49:08 PM by SYSTEM (modified after loading) *DAD1, Slg=298,4 Ref=355,90, EXT of WHM-3-151-M-ME-CL-OME1.D mAU 7 70 -60 -9.713 50 -40 -30 -20 -10 0 14 10 12 _____ Area Percent Report -----Sorted By Signal : Multiplier . 1.0000 Dilution . 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1, Sig=298,4 Ref=355,90, EXT Signal has been modified after loading from rawdata file! Peak RetTime Type Width Height Area Area # [min] [min] [mAU*s] [mAU] % 1 9.713 BB 0.2227 735.06769 50.52641 100.0000 Totals : 735,06769 50,52641 _____ *** End of Report ***

1260 12/27/2020 9:49:10 PM SYSTEM



Data File E:\DATA\LYN\LYN-4-8285 2019-12-19 16-51-14\LYN-4-82856.D Sample Name: WHM-4-1-O-F-RAC

Acq. Operator : SYSTEM Seq. Line : 7
Acg. Instrument : 1260 Location : 1
Injection Date : 12/19/2019 8:00:40 PM Inj : 1
Aca Mathad
ALQ: HELIOU . L. (MARACINGEN-40203 2019-12-13 10-51-14(11)-50-210-20010-50-0
Analysis Method - E-1007A1/VM/VM / 000E 2010 12 10 16 E1 14/TEU 00 2 -100 -200TM EU M /
Analysis method : E:\WAIA\LTM\LTM-4-8285 2019-12-19 10-51-14\IEE-98-210L-2001N-50L.M (
Sequence Method)
Last changeu : 1/0/2020 8:11:50 Ph by StStEn
Additional Tafe - Dealing)
Auditional Into : Peak(s) manually integrateu DAD14 Simple August (s) manually integrateu DAD14 Simple August (s) manually integrateu
atil]
200 -
o
1/5
150
129
100
76
50-
25-
0 2 4 6 8 10 12 14 min
Area Percent Report
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs
Signal 1: DAD1 A, Sig=254,4 Ref=360,100
Signal 1: DAD1 A, Sig=254,4 Ref=360,100
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] % 1 9.744 BB 0.2152 2609.38867 183.20775 50.2958 2 11.972 BB 0.3430 2578.69580 113.08957 49.7042 Totals : 5188.08447 296.29732
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %

S61

1260 1/6/2020 8:11:42 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-4-2-0-F-ME 2019-12-21 12-00-19\WHM-4-2-0-F-ME.D Sample Name: WHM-4-2-0-F-S

Acq. Operator : SYSTEM Seq. Line : 1
Acg. Instrument : 1260 Location : 1
Injection Date : 12/21/2019 12:01:44 PM Inj : 1
Inj Volume : 5.000 µl
Acg. Method : E:\DATA\WHM-2\WHM-4-2-0-F-ME 2019-12-21 12-00-19\IEH-98-21ML-20MIN-5UL.M
Last changed : 12/21/2019 12:00:19 PM by SYSTEM
Analysis Method : E:\DATA\WHM-2\WHM-4-2-0-F-ME 2019-12-21 12-00-19\IEH-98-21ML-20MIN-5UL.M
(Sequence Method)
Last changed : 1/6/2020 8:16:50 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated
DAD1 A, Sig=254,4 Ref=380,100 (E:/DATAI/WHM-2/WHM-42-O-F-ME 2019-12-21 12-00-19/WHM-4-2-O-F-ME.D)
mAU]
1400 -
1200 -
1000
800
600
400 -
200- 0
200-
200
200
200 0 2 2 4 6 8 10 12 14 mir Area Percent Report
200 0 0 2 2 4 6 8 10 12 14 mir Area Percent Report
200 0 0 2 2 4 6 8 10 12 14 min Area Percent Report
200 0 2 2 4 6 8 10 12 14 min Area Percent Report
200 0 2 2 4 6 8 10 12 14 min Area Percent Report
200 0 2 2 4 6 8 10 12 14 min Area Percent Report
200 0 2 2 4 6 8 10 12 14 min Area Percent Report
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200 0 2 2 4 6 8 10 12 14 min Area Percent Report
200 0 2 2 4 6 8 10 12 14 min Area Percent Report
200 0 2 2 4 6 8 10 12 14 min Area Percent Report Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %
200 200 2 4 6 8 10 12 14 min Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
200 2 4 6 8 10 12 14 min Area Percent Report
200 2 4 6 8 10 12 14 min Area Percent Report
200 0 2 4 0 0 0 12 14 min Area Percent Report
200 2 4 6 8 10 12 14 mme Area Percent Report
200 0 2 4 6 6 10 12 14 min Area Percent Report Area Percent Report Sorted By :: Signal Multiplier :: 1.0000 1.0000 Dilution :: 1.0000 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
200 0 2
200 2 4 6 8 10 12 14 min Area Percent Report

1260 1/6/2020 8:16:54 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\WHM-3-150-M-ME-RAC3.D Sample Name: WHM-3-150-3,4-CL-RAC

Acq. Operator : SYSTEM Seq. Line : 4
Acq. Instrument : 1260 Location : 3
Injection Date : 12/17/2019 8:11:42 PM Inj : 1
Inj Volume : 5.000 µl
Acq. Method : E:\DATA\WHM-2\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\IEH-98-21ML-20MIN -5UL.M
Last changed : 12/17/2019 8:13:45 PM by SYSTEM (modified after loading)
Analysis Method : E:\DATA\WHM-3\WHM-3-150-M-ME-CL-RAC 2019-12-17 19-22-09\IEH-98-21ML-20MIN
Last changed : 1/6/2020 5:45:32 PM by SYSTEM
(modified after loading) Additional Info : Peak(s) manually integrated
DAD1 A, Sig=254,4 Ref=360,100 (E:DATA\WH3-150-M-ME-CL-RAC 2019-12-17 19-22-09\WHM-3-150-M-ME-RAC3.D)
mAU 8
300
250 - 2
200
150
100
50-
0 2 4 6 8 10 12 14 mi
Area Percent Report
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs
Signal 1: DAD1 A, Sig=254,4 Ref=360,100
Peak RetTime Type Width Area Height Area
[min] [mAU*s] [mAU] %
1 11.059 BV 0.2783 5708.60791 309.31778 49.9240
2 12.238 VB 0.3982 5725.99268 216.77391 50.0760
Totals : 1.14346e4 526.09169
*** End of Report ***

1260 1/6/2020 5:45:34 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\WHM-3-151-M-ME-CL-OME2.D Sample Name: WHM-3-151-3,4-CL-S

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 2
Injection Date : 12/18/2019 10:25:27 PM Inj : 1
Inj Volume : 5.000 µl
Acq. Method : E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\IEH-98-21ML-20MIN- 5UL.M
Last changed : 12/18/2019 9:51:22 PM by SYSTEM
Analysis Method : E:\DATA\WHM-2\WHM-3-151-M-ME-CL- 2019-12-18 21-51-22\IEH-98-21ML-20MIN-
5UL.M (Sequence Method)
Last changed : 1/6/2020 7:56:20 PM by SYSTEM
(modified after loading)
DAD1 A, Sig=254,4 Ref=360,100 (E:\DATAIWH3-151-M-ME-CL- 2019-12-18 21-51-22\WHM-3-151-M-ME-CL-OME2.D)
mAU -
1750 8
1500
100
1290
1000 -
750 -
500 -
250
Area Percent Report
Sorted By : Signal
Multiplier : 1,0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISIDS
Signal 1: DAD1 A Sig-264 4 Pof-260 100
Signal I. DWDI K, SIG-23434 NEI-5003100
Pask Rattime Type Width Area Height Area
······································
1 10.956 BV R 0.2786 2.96761e4 1590.88013 98.6672
2 12.319 VB E 0.4214 400.87311 12.13612 1.3328
Totals : 3.00769e4 1603.01625
*** End of Docent ***

1260 1/6/2020 7:56:35 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-4-3-CF3-OME-2 2019-12-23 22-35-25\WHM-4-3-CF3-OME-21.D Sample Name: WHM-4-3-CF3-RAC

Acq. Operator : SYSTEM Seq. Line : 2
Ara Instrument : 1260 Location : 3
Televise Determine 12/02/2010 10.45.22 DN Televise 1
Injection bate : 12/25/2019 10:45:25 PM Inj : 1
Acq. Method : E:\DATA\WHM-2\WHM-4-3-CF3-OME-2 2019-12-23 22-35-25\ASH-98-2-1ML-ALL-20MIN- 5UL.M
Last changed : 12/23/2019 10:41:12 PM by SYSTEM
Analysis Method : F:\DATA\WHM-2\WHM-4.3-CF2-20MF-2 2019-12-23 22-35-25\ASH-98-2-1MI-AII-20MTN-
SILL M (Sequence Method)
Last changed 1/6/2020 g-21-37 DM by SYSTEM
Last changed . 1/0/2020 0.51.3/ PH by STSTEN
(modified after loading)
Additional Info : Peak(s) manually integrated
DID11B; Sig=204,4 Rel=300,100 (E:DATAWHM-2WHM-43-CF-3-OME-2 2019-12-23 22-33-20WHM-4-3-CF-3-OME-21.0)
mAU :
2000 -
1750
1500 -
1260
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E 061
500 -
250
250
250 0 0 0 1 2 250 0 0 1 2 2 5 6 7 8 9 mi
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250 0 0 1 2 3 4 5 6 7 8 9 mi Area Percent Report
250 0 0 1 2 3 4 5 6 7 8 9 mi Area Percent Report
250 0 0
250 0 0
250 0 0 0 1 2 3 4 5 6 7 8 9 mi
250 0 1 2 Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
250 0 1 2 Area Percent Report
250 0
250 0 1 2 3 4 5 6 7 8 9 mi Area Percent Report Sorted By :: Signal Multiplier :: 1.0000 1 0000 00 0000 00 0000 00 0000 00 0000 00 0000 00 0000 00 0000 00 0000 00 0000 00 0000 00 0000 00 0000 00 00000 00000 0000
250
250
250 4 5 6 7 8 9 mi Area Percent Report
250 2 3 4 5 6 7 8 9 mil Area Percent Report
250 4 5 6 7 8 9 mi Area Percent Report
250 200 2
250 2 3 4 5 6 7 8 9 m Area Percent Report Area Percent Report Sorted By :: Signal Multiplier :: 1.0000 10000 0
250 250 0 - - - Area Percent Report - - Sorted By : Signal Multiplier : 1 0.000 Do not use Multiplier - 1 4.438 WV R 0 - 1 4.438 WV R 2 5.020 VV R 0 - - -

1260 1/6/2020 8:31:40 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-4-3-CF3-S 2019-12-24 08-42-29\WHM-4-3-CF3-S1.D Sample Name: WHM-4-3-CF3-S

-----Seq. Line : 2 Acq. Operator : SYSTEM Acq. Instrument : 1260 Location : 5 Inj: 1 Injection Date : 12/24/2019 8:54:24 AM Inj Volume : 5.000 μl Acq. Method : E:\DATA\WHM-2\WHM-4-3-CF3-S 2019-12-24 08-42-29\ASH-98-2-1ML-ALL-10MIN-5UL. M Last changed : 12/24/2019 8:42:29 AM by SYSTEM Analysis Method : E:\DATA\WHM-2\WHM-4-3-CF3-5 2019-12-24 08-42-29\ASH-98-2-1ML-ALL-10MIN-5UL. M (Sequence Method) Last changed : 12/27/2020 9:52:13 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated DAD1 B, SIg-254.4 Ref-360,100 (E:\DATA\WHM-2\WHM-2\WHM-2WHM-4-3-CF3-S 2019-12-24 08-42-29WHM-4-3-CF3-S1.D) mAU⁻ 2000 1500 1000-500 0 6 _____ Area Percent Report _____ Sorted By Signal . Multiplier : 1.0000 Dilution . 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 B, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] % 1 4.218 BV R 0.1341 2.19910e4 2433.72241 100.0000 Totals : 2.19910e4 2433.72241 *** End of Report ***

1260 12/27/2020 9:52:17 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-4-3-CF3-OME-RAC 2019-12-23 19-55-46\WHM-4-3-CF3-OME2.D Sample Name: WHM-4-3-OME-RAC

Acq. Operator : SYSTEM Seq. Line : 3	
Acg. Instrument : 1260 Location : 4	
Thiertion Date : 12/23/2019 8:30:03 PM Thi: 1	
Ini Volume : 10.000 ul	
Acg. Method : E:\DATA\WHM-2\WHM-4-3-CF3-OME-RAC 2019-12-23 19-55-46\IE-98-2-1.0ML-5UL-	
40MIN.M	
Last changed : 12/23/2019 9:07:44 PM by SYSTEM	
(modified after loading)	
Analysis Method : E:\DATA\WHM-2\WHM-4-3-CF3-OME-RAC 2019-12-23 19-55-46\IE-98-2-1.0ML-5UL-	
49MIN.M (Sequence Method)	
Last changed : 1/6/2020 8:29:04 PM by SYSTEM	
(modified after loading)	
Additional Info : Peak(s) manually integrated	
DAD1 A, Stg=242,4 Ref=360,100 (E/DATAIWHM-2/WHM-4-3-CF3-OME-RAC 2019-12-23 19-55-46/WHM-4-3-CF3-OME2.D)	
mAU]	
80 -	
952	
60 - A	
40 -	
20 -	
	-
0 5 10 15 20 25 30 35 40	mir
0 5 10 15 20 25 30 35 40	mir
	mir
0 5 10 15 20 25 30 35 40	mir
0 5 10 15 20 25 30 35 40 Area Percent Report	mir
0 5 10 15 20 25 30 35 40 Area Percent Report	mir
0 5 10 15 20 25 30 35 40 Area Percent Report Sorted By : Signal	mir
0 5 10 15 20 25 30 35 40 Area Percent Report Sorted By : Signal Multiplier : 1.0000	mir
O 5 10 15 20 25 30 35 40 Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000	mir
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs	mir
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs	mir
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs	mir
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=242,4 Ref=360,100	mir
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=242,4 Ref=360,100	mir
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=242,4 Ref=360,100 Peak RetTime Type Width Area Height Area	mir
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=242,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %	mir
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=242,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %	mir
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=242,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] ** 1 30.756 BB 0.8211 3732.42529	mir
0 5 10 15 20 25 30 35 40 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=242,4 Ref=360,100 Peak RetTime Type Width Area Height Area # immail [min] [mAU*s] [mAU] % * 1 30.756 BB 0.8211 3732.42529 62.73220 51.9002 2 40.862 BB 1.2382 3459.11475 32.75167 48.0998	mir
0 5 10 15 20 25 30 35 40 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=242,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %	mir
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1260 1/6/2020 8:29:07 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-4-3-15-BR-2-OME 2020-01-08 15-13-34\WHM-4-15-3-BR-2-OME2.D Sample Name: WHM-4-3-2-OME-S

Aca. Operator: SVSTEM Sea Line: 3	
Acq. Instrument : 1260 Location : 2	
Acq. Method : E:\DATA\WHM-2\WHM-4-3-15-BR-2-OME 2020-01-08 15-13-34\IE-98-2-1ML-5UL-45MIN	
Last changed - 1/8/2020 2:12:35 DM by SVCTEM	
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1260 1/8/2020 6:11:14 PM SYSTEM



Data File E:\DATA\LYN\LYN-4-8285 2019-12-19 16-51-14\LYN-4-82857.D Sample Name: WHM-4-1-2-NA-RAC

cq. Operator : SYSTEM Seq. Line : 8
cq. Instrument : 1260 Location : 2
njection Date : 12/19/2019 8:21:58 PM Inj : 1
Inj Volume : 5.000 µl
cq. Method : E:\DATA\LYN\LYN-4-8285 2019-12-19 16-51-14\IEH-98-21ML-20MIN-5UL.M
ast changed : 12/19/2019 5:26:48 PM by SYSTEM
nalysis Method : E:\DATA\LYN\LYN-4-8285 2019-12-19 16-51-14\IEH-98-21ML-20MIN-5UL.M (
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1260 1/6/2020 8:13:30 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-4-2-FUR-2-NA-S 2019-12-21 18-00-39\WHM-4-2-FUR-2-NA-S1.D Sample Name: WHM-4-2-2-NA-S

Acq. Operator : SYSTEM	Seq. Line : 2	
Acq. Instrument : 1260	Location : 2	
Injection Date : 12/21/2019 6:23:21 PM	Inj: 1	
-	Inj Volume : 5.000 µl	
Acq. Method : E:\DATA\WHM-2\WHM-4-2-FUR-2 SUL.M	-NA-S 2019-12-21 18-00-39\IEH-98-21ML-20MI	N-
Last changed : 12/21/2019 6:00:39 PM by SY	STEM	
Analysis Method : E:\DATA\WHM-2\WHM-4-2-FUR-2	-NA-S 2019-12-21 18-00-39\IEH-98-21ML-20MI	N-
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Last changed : 1/6/2020 8:19:45 PM by SYST	'EM	
(modified after loading)		
DAD1 A, Sig=254,4 Ref=360,100 (E:\DATA\WHWHM-4	-2-FUR-2-NA-S 2019-12-21 18-00-39\WHM-4-2-FUR-2-NA-S1.D)	
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1260 1/6/2020 8:20:01 PM SYSTEM



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Data File E:\DATA\LYN\LYN-4-8285 2019-12-19 16-51-14\LYN-4-82858.D Sample Name: WHM-4-1-FUR-RAC

-----Acq. Operator : SYSTEM Seq. Line : 9 Acq. Instrument : 1260 Location : 3 Injection Date : 12/19/2019 8:43:22 PM Inj ; _ Inj Volume : 5.000 μl Acq. Method : E:\DATA\LYN\LYN-4-8285 2019-12-19 16-51-14\IEH-98-2--1ML-20MIN-5UL.M Last changed : 12/19/2019 5:26:48 PM by SYSTEM Analysis Method : E:\DATA\LYN\LYN-4-8285 2019-12-19 16-51-14\IEH-98-2--1ML-20MIN-5UL.M (Sequence Method) Last changed : 12/27/2020 10:01:15 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated "DAD1, SIg-292,4 Ref-355,90, EXT of LYN-4-82858.D mAU 485.531 40 -555 30 8 2 20 10 0 18 12 14 16 10 -----Area Percent Report _____ Sorted By : Signal : 1.0000 Multiplier Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1, Sig=292,4 Ref=355,90, EXT Signal has been modified after loading from rawdata file! 1 10.655 FM 0.2674 485.53683 30.25993 51.4546 2 12.199 BB 0.3020 458.08582 21.46368 48.5454 943.62265 51.72361 Totals : _____ *** End of Report *** Page 1 of 1 1260 12/27/2020 10:01:18 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-4-2-FUR-2-NA-S 2019-12-21 18-00-39\WHM-4-2-FUR-2-NA-S.D Sample Name: WHM-4-2-FUR-S

Acq. Operator : SYSTEM	Seq. Line : 1
Acq. Instrument : 1260	Location : 1
Injection Date : 12/21/2019 6:01:59 PM	Inj: 1
	Inj Volume : 5.000 µl
Acq. Method : E:\DATA\WHM-2\WHM-4-2-FUR-2	-NA-S 2019-12-21 18-00-39\IEH-98-21ML-20MIN-
5UL .M	
Last changed : 12/21/2019 6:00:39 PM by SY	STEM
Analysis Method : E:\DATA\WHM-2\WHM-4-2-FUR-2	-NA-S 2019-12-21 18-00-39\IEH-98-21ML-20MIN-
5UL.M (Sequence Method)	
Last changed : 1/6/2020 8:18:38 PM by SYST	EM
(modified after loading)	
Additional Info : Peak(s) manually integrated	
DAD1 A, Sig=254,4 Ref=360,100 (E:\DATA\WHWHM-4	-2-FUR-2-NA-S 2019-12-21 18-00-39W/HM-4-2-FUR-2-NA-S.D)
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Area Percent Report	6 8 10 12 14 min
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Area Percent Report	8 8 10 12 14 min
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Area Percent Report Area Percent Report Sorted By : Sorted By : Sorted By : Sorted By : Signal : Multiplier : 1.0000 Dilution Do not use Multiplier & Dilution Factor with Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width # [min] [min] 1.0682 BB 0.2351 8106.73047 1.10.682 BB 0.2873 146.31215 6.903	Area %
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1260 1/6/2020 8:18:47 PM SYSTEM


Data File E:\DATA\WHM-2\WHM-4-1-ME-RAC-5 2019-12-22 21-43-54\WHM-4-1-ME-RAC-51.D Sample Name: WHM-4-1-ME-RAC-4

Acq. Operator : SYSTEM Seq. Line : 2 Acq. Instrument : 1260 Location : 1 Injection Date : 12/22/2019 9:56:12 PM Inj : 1 Inj Volume : 5.000 µl Acq. Method : E:\DATA\WHM-2\WHM-4-1-ME-RAC-5 2019-12-22 21-43-54\IDH-98-2--1ML-20MIN-5UL. М Last changed : 12/22/2019 9:43:55 PM by SYSTEM Analysis Method : E:\DATA\WHM-2\WHM-4-1-ME-RAC-5 2019-12-22 21-43-54\IDH-98-2--1ML-20MIN-5UL. M (Sequence Method) Last changed : 1/6/2020 8:06:35 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated DAD1 A, Sig=254,4 Ref=360,100 (E:\DATA\WHM-2\WHM WHM-4-1-ME-RAC-5 2019-12-22 21-43-54/WHM-4-1-ME-RAC-51.D) mAU -852.40 .oan.n 350 -300 -250-200 -150 -100 -50 -0 _____ -----Area Percent Report _____ Sorted By Signal : Multiplier : 1.0000 1.0000 Dilution . Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] % 1 6.303 MM 0.3408 6622.45703 323.86935 50.5525 2 7.197 MM 0.3573 6477.71240 302.13586 49.4475 1.31002e4 626.00522 Totals : -----*** End of Report ***

1260 1/6/2020 8:06:39 PM SYSTEM



Data File E:\DATA\wHM-2\WHM-4-3-CF3-OME-2 2019-12-23 22-35-25\WHM-4-3-CF3-OME-23.D Sample Name: WHM-4-2-ME-S

Acq. Operator : SYSTEM Seq. Line : 4 Acq. Instrument : 1260 Location : 2 Injection Date : 12/23/2019 11:18:01 PM Inj : 1 Inj Volume : 5.000 µl Acq. Method : E:\DATA\WHM-2\WHM-4-3-CF3-OME-2 2019-12-23 22-35-25\IDH-98-2-5UL-10MIN-1ML. М Last changed : 12/23/2019 10:42:19 PM by SYSTEM Analysis Method : E:\DATA\WHM-2\WHM-4-3-CF3-OME-2 2019-12-23 22-35-25\IDH-98-2-5UL-10MIN-1ML. M (Sequence Method) Last changed : 1/6/2020 8:24:40 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated DAD1 A, Sig=220,4 Ref=360,100 (E:/DATA/WHM-2/WHM-ZWHM-4-3-CF3-OME-2 2019-12-23 22-35-25WHM-4-3-CF3-OME-23.D) mAU g 140 -120 100-80 -60 -40 -3.482 20-0 7 _____ -----Area Percent Report _____ Sorted By Signal : Multiplier : 1.0000 1.0000 Dilution . Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=220,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] % 1 6.482 BV E 0.2955 254.22264 11.47256 7.8343 2 7.037 VB R 0.3528 2990.76416 137.47588 92.1657 3244.98680 148.94844 Totals : -----*** End of Report ***

1260 1/6/2020 8:24:45 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-4-78-88-85-RAC-2 2020-08-14 08-35-29\WHM-4-78-88-85-RAC.D Sample Name: WHM-4-78-T-BU-RAC

Acq. Operator	: SYSTEM	Seq. Line : 1
Acq. Instrumen	nt : 1260	Location : 41
injection bate	2 : 8/14/2020 8:3/:00 AM	IN]: I Toj Volume : 5 888 ul
Acq. Method	: E:\DATA\WHM-2\WHM-4-78-88-8	5-RAC-2 2020-08-14 08-35-29\IDH-99-11ML-40MIN-
Last changed	• 8/14/2020 8:35:20 AM by SVS	TEN
Analysis Metho	d : E:\DATA\WHM-2\WHM-4-78-88-8	5-RAC-2 2020-08-14 08-35-29\TDH-99-11ML-40MTN-
	5UL.M (Sequence Method)	
Last changed	: 12/27/2020 10:09:42 PM by S	YSTEM
	(modified after loading)	
Additional Inf	fo : Peak(s) manually integrated	
"DAD1, S	Sig=280,4 Ref=355,90, EXT of WHM-4-78-88-85-R	AC.D
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Sorted By Multiplier Dilution Do not use Mul Signal 1: DAD1 Signal has be	Area Percent Report : Signal : 1.0000 : 1.0000 ltiplier & Dilution Factor with : 1, Sig=280,4 Ref=355,90, EXT een modified after loading from	4 5 6 7 8 9 mi
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Sorted By Multiplier Dilution Do not use Mul Signal 1: DAD1 Signal has be Peak RetTime T # [min]	Area Percent Report : Signal : 1.0000 : 1.0000 : 1.0000 ltiplier & Dilution Factor with : 1, Sig=280,4 Ref=355,90, EXT een modified after loading from : Type Width Area Height [min] [mAU*s] [mAU]	4 5 6 7 8 9 mi
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Sorted By Multiplier Dilution Do not use Mul Signal 1: DADI Signal has be Peak RetTime T # [min] - 1 5.638 B 2 6.613 B Totals :	Area Percent Report : Signal : 1.0000 : 1.0000 : 1.0000 ltiplier & Dilution Factor with : 1, Sig=280,4 Ref=355,90, EXT teen modified after loading from in Type Width Area Height [min] [mAU*s] [mAU] 	4 5 6 7 8 9 mi

1260 12/27/2020 10:09:45 PM SYSTEM



Data File E:\DATA\WHM-2\XL-7-93RAC 2020-08-28 16-24-09\WHM-4-106-T-BU-R1.D Sample Name: WHM-4-106-T-BU-R

Acq. Operator	: SYSTEM	Seq. Line : 2	
Acq. Instrument	: 1260	Location : 41	
injection Date	: 8/28/2020 4:36:33 PM	Inj: 1 Inj Volume : 5 868 vl	
Aca. Method	: F:\DATA\WHM-2\YL-7-030AC 20	10 VOIUME : 5.000 HI 20-08-28 16-24-00\TDH-00-1-4	1.0MI -254NM-10MTN M
Last changed	: 8/28/2020 4:24:09 PM hv SV	TEM	1.000 - 2.3400 - 100110.01
Analysis Method	: E:\DATA\WHM-2\XL-7-938AC 26	20-08-28 16-24-09\TDH-99-1-	1.0ML-254NM-10MIN.M (
	Sequence Method)		
Last changed	: 12/27/2020 10:13:18 PM by 9	SYSTEM	
	(modified after loading)		
Additional Info	: Peak(s) manually integrated		PILPI DI
mAU -	g=284,4 Ref=360,100 (E:VDATAW/HM-20XL-7	SORAC 2020-06-26 16-24-09W/HM-4-106-1	-00-11.0)
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Signal 1: DAD1	B, Sig=254,4 Ref=360,100		
Peak RetTime Ty	pe width Area Height	Area	
# [min]	[min] [mAU*S] [mAU]	70 	
1 5.803 VB	0.2487 85.60625 5.084	74 0.4077	
2 6.774 BB	0,3029 2,09317e4 1071.44	300 99,5923	
2 31774 00			
Totals :	2.10174e4 1076.529	974	
	*** End of Report *	•••	
12/27/2020 10-1	2,21 DM CVCTEM		Page 1 of 1
12/2//2020 10:1	DIZI MU SYSTEM		Fage IOII



Data File E:\DATA\WHM-2\WHM-5-70-H-TRAC 2021-04-25 10-04-57\WHM-5-70-HRAC-TRAC5.D Sample Name: WHM-5-70-H-RAC

Aco. Operator : SYSTEM Seg. Line : 6	
Acq. Instrument : 1260	
The Volume - F and wi	
Acq. Method : E:/UAIA/WHM-2/WHM-5//0-H-TRAC 2021-04-25 10-04-5//1EH-98-21ML-20MIN-SUL.M	
Last changed : 4/25/2021 10:34:41 AM by SYSTEM	
Analysis Method : E:\DATA\WHM-2\WHM-5-70-H-TRAC 2021-04-25 10-04-57\IEH-98-21ML-20MIN-5UL.M	
(Sequence Method)	
Last changed : 4/25/2021 12:20:28 PM by SYSTEM	
(modified after loading)	
Additional Info : Peak(s) manually integrated	
DAD1 A, SIg=254,4 Ref=360,100 (E:0A1A1WHM-2/WHM-5/0H-1RAC 2021-04-5/WHM-5/0-HRAC-1RAC5.D)	
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Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS Signal 1: DAD1 A, Sig=254,4 Ref=360,100	t min
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDS Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # formal Area Height Area	t min
Area Percent Report Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %	t nsin
0 2 4 6 8 10 12 1 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] %	t min
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0 2 4 6 8 10 12 1 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU] %	i min
0 2 4 6 8 10 12 1 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 10 12 1 Multiplier : Signal Multiplier : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*5] [mAU] %	1 min
0 2 4 6 8 10 12 1 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [muin] [mAU] %	1 min
0 2 4 6 0 10 12 1 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [multis] [mAU] %	t min
0 2 4 6 6 10 12 1 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 0 0 12 1 Multiplier : 1.0000 0 0 12 1 Sorted By : Signal 1.0000 0 0 12 1 Multiplier : 1.0000 0 <t< td=""><td>1 min</td></t<>	1 min
0 2 4 6 0 10 12 1 Area Percent Report Area Percent Report Sorted By : Signal Multiplier 1.0000 Dilution 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] 1 6.668 MM 0.1840 7309.25830 662.24860 \$0.5891 2 7.606 MM 0.2293 7139.03320 518.89240 49.4109 Totals : 1.44483e4 1181.14099	t min
0 1	t nsin
0 1	4 min

1260 4/25/2021 12:20:31 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-5-70-H-T-OPT 2021-04-25 12-23-02\WHM-5-70-H-T-OPT1.D Sample Name: WHM-5-70-T-RAC

Acq. Operator : S	YSTEM	Seq. Line : 2	
Acq. Instrument : 1	260	Location : 14	
Injection Date : 4	/25/2021 12:45:48 PM	Inj : 1	
		Inj Volume : 5.000 µl	
Acq. Method : E M	:\DATA\WHM-2\WHM-5-70-H-T-OP	PT 2021-04-25 12-23-02∖IEH-98-21ML-20MI	N-SUL.
Last changed : 4	/25/2021 12:23:03 PM by SYST	TEM	
Analysis Method : E	:\DATA\WHM-2\WHM-5-70-H-T-OP	PT 2021-04-25 12-23-02\IEH-98-21ML-20MI	N-5UL.
м	(Sequence Method)		
Last changed : 4	/25/2021 1:27:21 PM by SYSTE	EM	
0	modified after loading)		
Additional Info : P	eak(s) manually integrated		
DADTA, SIG-254	1,4 Ref=360,100 (E:VDATAW/HM-2W/HM-5-	-/0-H-1-OPT 2021-04-25 12-23-02W/HM-5-/0-H-1-OPT1.D)	
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	Area Percent Report		
Sorted By	: Signal		
Dilution	: 1.0000		
Dilution	: 1.0000		
Do Not use Multipli	er & Dilution Factor with is	5105	
Signal 1: DAD1 A. S	ig=254.4 Ref=360.100		
Signer II beer A, S	1g-194)4 Mer-9009100		
Peak RetTime Type	Width Area Height	Area	
# [min]	[min] [mAU*s] [mAU]	*	
1 6.518 BV R	0.1615 8166.49414 734.77649	91.2360	
2 7,440 VB E	0,2068 784,46008 56,90783	8.7640	
Totals :	8950,95422 791,68432	2	
		-	
	*** End of Report ***	•	
	-		
4/25/2021 1:29:38	PM SYSTEM	Pa	ge lofl



Data File E:\DATA\WHM-2\WHM-5-70-H-TRAC 2021-04-25 10-04-57\WHM-5-70-HRAC-TRAC4.D Sample Name: WHM-5-70-H-RAC

Acq. Operator :	SYSTEM Seq. Line : 5
Acq. Instrument :	1260 Location : 11
Injection Date :	4/25/2021 10:59:36 AM Inj: 1
	Ini Volume : 5,000 ul
Aca. Method :	E:\DATA\WHM-2\WHM-5-70-H-TRAC 2021-04-25 10-04-57\TEH-98-21ML-20MTN-5UL.M
Last changed :	4/25/2021 10:34:41 AM by SYSTEM
Applysis Method I	E () DATA LUM 2) LUM E 70 U TRAC 2021 04 25 10 04 57 TEH 08 2, 100 200TH EU M
Analysis Hechou .	C. (DATA (MRR-2)/MRR-3-/0-R-TKAC 2021-04-23 10-04-3/(108-96-218C-2011M-30C.M
Last changed	(Sequence Rection)
Last changed :	4/23/2021 12:00:23 PM UV STSTEM
	(modified after loading)
Additional Info :	Peak(s) manually integrated
DAD1 A, SIG-	154,4 Ref=360,100 (EXDATAWHM-20WHM-5-70-H-TRAC 2021-04-25 10-04-57WHM-5-70-HRAC-TRAC4.D)
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	Area Percent Report
Sorted By	: Signal
Sorted By Multiplier	: Signal : 1.0000
Sorted By Multiplier Dilution	: Signal : 1.0000 : 1.0000
Sorted By Multiplier Dilution	: Signal : 1.0000 : 1.0000
Sorted By Multiplier Dilution Do not use Multip	: Signal : 1.0000 : 1.0000 : 1.0000 iier & Dilution Factor with ISTDs
Sorted By Multiplier Dilution Do not use Multip:	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDs
Sorted By Multiplier Dilution Do not use Multip	: Signal : 1.0000 : 1.0000 Lier & Dilution Factor with ISTDs
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A,	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDs Sig=254,4 Ref=360,100
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A,	: Signal : 1.0000 : 1.0000 Lier & Dilution Factor with ISTDs Sig=254,4 Ref=360,100
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A, Peak RetTime Type	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDS Sig=254,4 Ref=360,100 Width Area Height Area
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A, Peak RetTime Type # [min]	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDs Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A, Peak RetTime Type # [min]	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDS Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip: Signal 1: DAD1 A, Peak RetTime Type # [min] 	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDS Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A, Peak RetTime Type # [min] 1 7.653 BB 2 9.569 BB	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDs Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A, Peak RetTime Type # [min] 1 7.653 BB 2 9.569 BB	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDs Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip: Signal 1: DAD1 A, Peak RetTime Type # [min] 	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDS Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip: Signal 1: DAD1 A, Peak RetTime Type # [min] 1 7.653 BB 2 9.569 BB Totals :	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDs Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A, Peak RetTime Type # [min] 1 7.653 BB 2 9.569 BB Totals :	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDS Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip: Signal 1: DAD1 A, Peak RetTime Type # [min] 1 7.653 BB 2 9.569 BB Totals :	: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDS Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] %
Sorted By Multiplier Dilution Do not use Multip: Signal 1: DAD1 A, Peak RetTime Type # [min] 1 7.653 BB 2 9.569 BB Totals :	<pre>: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDs Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] % </pre>
Sorted By Multiplier Dilution Do not use Multip Signal 1: DAD1 A, Peak RetTime Type # [min] 1 7.653 BB 2 9.569 BB Totals :	<pre>: Signal : 1.0000 : 1.0000 lier & Dilution Factor with ISTDS Sig=254,4 Ref=360,100 Width Area Height Area [min] [mAU*s] [mAU] % </pre>

1260 4/25/2021 12:08:28 PM SYSTEM

Page lof1



Data File E:\DATA\WHM-2\WHM-5-70-H-T-OPT 2021-04-25 12-23-02\WHM-5-70-H-T-OPT.D Sample Name: WHM-5-70-H-RAC

Acq. Operator	: SYSTEM	Seq. Line :	1			
Acq. Instrument	: 1260	Location :	13			
Injection Date	: 4/25/2021 12:24:27 PM	Inj :	1			
		Inj Volume :	5.000 µl			
Acq. Method	: E:\DATA\WHM-2\WHM-5-70-H-1	T-OPT 2021-04-25 1	2-23-02\IEH	-98-21ML-20	MIN-SUL.	
	м					
Last changed	: 4/25/2021 12:23:03 PM by 9	SYSTEM				
Analysis Method	: E:\DATA\WHM-2\WHM-5-70-H-1	F-OPT 2021-04-25 1	2-23-02\IEH	-98-21ML-20	MIN-SUL.	
	M (Sequence Method)					
Last changed	: 5/3/2021 9:52:23 AM by SYS	STEM				
	(modified after loading)					
Additional Info	: Peak(s) manually integrate	ed		6 70 H T 007 0		
DADTA, SI	g=254,4 Rei=360,100 (ENDATAW/HM-200/P	1M-0-70-H-1-OP1 2021-04-	co 12-20-02WV HIV	Ho-70-H-1-OP1.D)		
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		e i				
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0	2 4			12	<u> </u>	14 min
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50 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	2 4 Area Percent Report			12	<u> </u>	14 min
sorted By Multiplier	Area Percent Report : Signal : 1.0000			12	<u> </u>	14 min
sorted By Multiplier Dilution	Area Percent Report : Signal : 1.0000 : 1.0000			12	<u></u> .	14 min
Sorted By Multiplier Dilution Do not use Multi	Area Percent Report Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with	t 1 ISTDs		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with	h ISTDs		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with	h ISTDs		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DADI 4	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100	n ISTDs		12	<u></u> .	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4	Area Percent Report Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100	t I ISTDS		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ	Area Percent Report : Signal : 1.0000 : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heigh	n ISTDs		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ # [min]	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 De Width Area Heig! [min] [mAU*s] [mAU	n ISTDs		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DADI 4 Peak RetTime Typ # [min]	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heigf [min] [mAU*s] [mAU] 	n ISTDs		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DADI A Peak RetTime Typ # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 De Width Area Heigl [min] [mAU*5] [mAU -	n ISTDs		12		14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 De Width Area Heigi [min] [mAU*s] [mAU] - R 0.1762 3687.91235 312.83 0.2691 673.59323 37.51	n ISTDS		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 De Width Area Heig! [min] [mAU*5] [mAU -[]	n ISTDs		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 De Width Area Heigf [min] [mAU*s] [mAU] 	n ISTDs		12		14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 : 1.0000 : 0.1000 A, Sig=254,4 Ref=360,100 De Width Area Heigl [min] [mAU*s] [mAU] -	n ISTDs		12		14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ # [min] 1 6.772 VB 2 8.213 BB Totals :	Area Percent Report : Signal : 1.0000 : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 pe Width Area Heigi [min] [mAU*5] [mAU] 	n ISTDs		12		14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ # [min] 	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 De Width Area Heigi [min] [mAU*5] [mAU 	n ISTDs		12	<u> </u>	14 min
Sorted By Multiplier Dilution Do not use Multi Signal 1: DAD1 4 Peak RetTime Typ # [min] 1 6.772 VB 2 8.213 BB Totals :	Area Percent Report : Signal : 1.0000 : 1.0000 iplier & Dilution Factor with A, Sig=254,4 Ref=360,100 De Width Area Heigl [min] [mAU*s] [mAU] 	h ISTDs h ISTDs h STDs h STDs		12		14 min

1260 5/3/2021 9:52:26 AM SYSTEM



Data File E:\DATA\WHM-2\WHM-5-74-P-CL 2021-05-04 14-22-10\WHM-5-74-P-CL1.D Sample Name: WHM-5-74-P-CL-RAC

-----Acq. Operator : SYSTEM Seq. Line : 2 Location : 71 Aca, Instrument : 1260 Injection Date : 5/4/2021 2:34:29 PM Inj: 1 Inj Volume : 5.000 µl : E:\DATA\WHM-2\WHM-5-74-P-CL 2021-05-04 14-22-10\IEH-98-2--1ML-20MIN-5UL.M Acq. Method : 5/4/2021 2:22:10 PM by SYSTEM Last changed Analysis Method : E:\DATA\WHM-2\WHM-5-74-P-CL 2021-05-04 14-22-10\IEH-98-2--1ML-20MIN-5UL.M (Sequence Method) Last changed : 5/7/2021 5:01:32 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated DAD1 A. Sig=254,4 Ref=360,100 (E:VDATAWHM-2:WHM-5-74-P-CL 2021-05-04 14-22-10/WHM-5-74-P-CL1.D) 3000 2500 2000 -1500 -1000 500 0 12 14 16 10 Area Percent Report _____ Sorted By . Signal Multiplier 1.0000 Dilution 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Height Peak RetTime Type Width Area Area [min] [mAU*s] # [min] [mAU] % 1 8.555 MF 0.2215 3.84699e4 2894.13574 49.0945 2 9.076 FM 0.2729 3.98889e4 2435.91846 50.9055 7.83589e4 5330.05420 Totals : _____ *** End of Report ***

1260 5/7/2021 5:01:35 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-5-74-P-CL 2021-05-04 14-22-10\WHM-5-74-P-CL2.D Sample Name: WHM-5-74-P-CL-OPT

Acq. Operator	: SYSTEM	Seq. Line	: 3	
Acq. Instrument	: 1260	Location	: 72	
Injection Date	: 5/4/2021 2:55:52 PM	Inj	: 1	
-		Inj Volume	: 5.000 µl	
Acq. Method	: E:\DATA\WHM-2\WHM-5-74-P	-CL 2021-05-04 14	-22-10\IEH-98-21M	L-20MIN-5UL.M
Last changed	: 5/4/2021 2:57:58 PM by S	YSTEM		
	(modified after loading)			
Analysis Method	: E:\DATA\WHM-2\WHM-5-74-P	-CL 2021-05-04 14	-22-10\IEH-98-21M	L-20MIN-5UL.M (
	Sequence Method)			
Last changed	: 5/7/2021 5:03:55 PM by S	YSTEM		
	(modified after loading)			
Additional Info	: Peak(s) manually integra	ted		
DAD1 B, S	lg=220,4 Ref=360,100 (E:\DATA\WHM-2\\	WHM-5-74-P-CL 2021-05-04	4 14-22-10/WHM-5-74-P-CL2.	D)
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	2 4	6 8	10	12 14 1
	Area Percent Perc			
Sorted By	: Signal			
Multiplier	: 1.0000			
Dilution	: 1.0000			
Do not use Mult	iplier & Dilution Factor wi	th ISTDs		
	-			
Signal 1: DAD1	B, Sig=220,4 Ref=360,100			
Peak RetTime Ty	pe Width Area Hei	ght Area		
# [min]	[min] [mAU*s] [mA	u] %		
1 8.469 BV	R 0.2167 4.18701e4 2912.	47876 98.4509		
2 9.119 VB	E 0.2578 658.82886 36.	81040 1.5491		
Totals :	4.25290e4 2949.	28916		
	*** End of Repor	t ***		
	SR DM SVSTEM			Page 1 of 1
5/7/2021 5:03:5	Jo Ph Staten			



Data File E:\DATA\WHM-2\WHM-5-74-P-MERACOPT 2021-05-07 14-30-58\WHM-5-74-P-ME1.D Sample Name: WHM-P-ME-5-74-RAC

Aca. Operator : SYSTEM Sea. Line : 2
Acq. Instrument: 1260 Location: 11
Thistian Date - 5/7/2021 2:43:25 DM This 1
Acq. Method : E:\DATA\WHM-2\WHM-5-74-P-MERACOPT 2021-05-07 14-30-58\IEH-98-21ML-20MIN- 5UL.M
Last changed : 5/7/2021 2:30:59 PM by SYSTEM
Analysis Method : E:\DATA\WHM-2\WHM-5-74-P-MERACOPT 2021-05-07 14-30-58\IEH-98-21ML-20MIN-
5UL.M (Sequence Method)
Last changed + 5/7/2021 A:54:48 DM by SYSTEM
(modified after loading)
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Additional into : Peak(s) manually integrated
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Area Percent Report
Sorted By : Signal
Sorted By : Signal Multiplier : 1.0000
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU*s] [mAU]
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU*s] [mAU] '
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU*s] [mAU] ** [min] [mAU*s] 1 10.495 BB 0.2266 5386.50391 355.75015 2 11.537 BB 0.2825 5258.89941 279.51376
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU+s] [mAU] %
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] 1 10.495 BB 0.2266 5386.50391 2 11.537 BB 0.2825 5258.89941 Totals : 1.06454e4 635.26392
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU]
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mau] %
Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] * [min] [mAU] 1 10.495 BB 0.2266 5386.50391 2 11.537 BB 0.2255 5258.89941 Totals : 1.06454e4 635.26392

1260 5/7/2021 4:54:52 PM SYSTEM



Data File E:\DATA\WHM-2\WHM-5-74-P-MERACOPT 2021-05-07 14-30-58\WHM-5-74-P-ME2.D Sample Name: WHM-P-ME-5-74-OPT

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 12
Thi Volume + 5,000 ul
Acq. Method : E:\DATA\WHM-2\WHM-5-74-P-MERACOPT 2021-05-07 14-30-58\IEH-98-21ML-20MIN- 5UL.M
Last changed : 5/7/2021 2:30:59 PM by SYSTEM
Analysis Method : E:\DATA\WHM-2\WHM-5-74-P-MERACOPT 2021-05-07 14-30-58\IEH-98-21ML-20MIN-
5UL.M (Sequence Method)
Last changed : 5/7/2021 4:56:50 PM by SYSTEM
(modified after loading)
Additional Tafa (modeled angully integrated
Additional into : Peak(s) manually integrated Dabia Sin=254 Aer360 100 (FVDATWHW/WHWHKS74.BMFRACODT 2021.05.07 14.30.58WHM-5.74.B-MF2 D)
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0 2 4 6 8 10 12 14 16 mmi Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 De net use Multiplier 1.0000 De net use Multiplier 1.0000
0 2 4 6 8 10 12 14 16 mmk Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
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0 2 4 6 8 10 12 14 16 mmm Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area
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0 2 4 6 8 10 12 14 16 mmm Area Percent Report Area Percent Report Sorted By : Signal Multiplier 1.0000 Dilution 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
0 2 4 6 8 10 12 14 16 mmk Area Percent Report Area Percent Report Sorted By : Signal Multiplier 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] %
0 2 4 6 8 10 12 14 16 mmm Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 10 </td
0 2 4 6 8 10 12 14 16 mmi Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 10 10 12 14 16 mmi Sorted By : Signal Multiplier : 1.0000 100 10
0 2 4 6 8 10 12 14 16 mid Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 10 </td
0 2 4 6 8 10 12 14 16 mW Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 10 12 14 16 mW Dilution : 1.0000 10 1 1.0000 10 10 12 14 16 mW Sorted By : Signal Multiplier : 1.0000 1.0000 10

1260 5/7/2021 4:56:53 PM SYSTEM



Data File E:\DATA\WH...WHM-4-88-85-78-RRAC-3 2020-08-14 16-01-33\WHM-4--70-T-BU-R-88-852.D Sample Name: WHM-4-85-OH-RAC

Seq. Line : 3 Location : 45 Acq. Operator : SYSTEM Acq. Instrument : 1260 Injection Date : 8/14/2020 4:25:30 PM Inj: 1 Inj Volume : 5.000 µl : E:\DATA\WHM-2\WHM-4-88-85-78-RRAC-3 2020-08-14 16-01-33\IDH-98-2--1ML-40MIN Acq. Method -5UL.M Last changed : 8/14/2020 4:01:33 PM by SYSTEM Analysis Method : E:\DATA\WHM-2\WHM-4-88-85-78-RRAC-3 2020-08-14 16-01-33\IDH-98-2--1ML-40MIN -5UL.M (Sequence Method) Last changed : 12/27/2020 10:16:51 PM by SYSTEM (modified after loading) Additional Info : Peak(s) manually integrated
DAD1 A, Stg=254,4 Ref=360,100 (E:VDATAWH...8-85-78-RRAC-3 2020-08-14 16-01-33WHM-4-70-T-BU-R-88-852.D) TONZTA mAU -15.106 175 -150 -125-100 a 6914.91 75 -6 50 -25-0 10 15 -----Area Percent Report Sorted By : Signal Multiplier 1.0000 . Dilution 1.0000 . Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area [min] [mAU*s] [mAU] % # [min] 1 15.166 MM 0.6790 7042.73730 172.86771 50.6031 2 24.073 MM 2.5697 6874.87012 44.58984 49.3969 Totals : 1.39176e4 217.45755 _____ *** End of Report ***

1260 12/27/2020 10:18:08 PM SYSTEM



Data File E:\DATA\WH...WHM-4-88-85-78-RRAC-3 2020-08-14 16-01-33\WHM-4--70-T-BU-R-88-853.D Sample Name: WHM-4-84-0H-R

Acg. Operator : SYSTEM Seg. Line : 4
Acq. Instrument : 1260 Location : 46
Injection Date : 8/14/2020 5:07:00 PM Inj : 1
Ini Volume : 5.000 ul
Acq. Method : E:\DATA\WHM-2\WHM-4-88-85-78-RRAC-3 2020-08-14 16-01-33\IDH-98-21ML-40MIN -5UL.M
Last changed : 8/14/2020 4:01:33 PM by SYSTEM
Analysis Method : E:\DATA\WHM-2\WHM-4-88-85-78-RRAC-3 2020-08-14 16-01-33\IDH-98-21ML-40MIN
-5UL.M (Sequence Method)
Last changed : 12/27/2020 10:19:12 PM by SYSTEM
(modified after loading)
DAD1 A, SIg=254,4 Ref=360,100 (E:\DATA\WH8-85-78-RRAC-3 2020-08-14 16-01-33\WHM-4~70-T-BU-R-88-853.D)
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Area Percent Report
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0 5 10 15 20 25 30 7 Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs
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0 5 10 15 20 25 30 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 1.0000 Dilution : 1.0000 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area
Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [mAU*s] [mAU] %
0 5 10 15 20 25 30 7 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] %
0 5 10 15 20 25 30 Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] *
0 5 10 15 20 25 30 Area Percent Report
0 5 10 15 20 25 30 Area Percent Report
Image: Signal interface Area Percent Report Area Percent Report Image: Signal interface Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area Height Area # [min] [min] [mAU*s] [mAU] %
Image: Signal state of the
Image: Signal state of the
Image: Second
Image: Signal is the second
Area Percent Report Area Percent Report Area Percent Report Sorted By : Signal Multiplier : 1.0000 Dilution : 1.0000 Do not use Multiplier & Dilution Factor with ISTDs Signal 1: DAD1 A, Sig=254,4 Ref=360,100 Peak RetTime Type Width Area # [min] [mAU] 1 14.840 BB 0.6345 5276.73193 126.53205 100.0000 Totals : 5276.73193 126.53205 *** End of Report ***

1260 12/27/2020 10:19:17 PM SYSTEM