Supplementary information

Novel 2-phenyloxypyrimidine derivative induces apoptosis and autophagy via inhibiting PI3K pathway and activating MAPK/ERK signaling in hepatocellular carcinoma cells

Jing Wang^{1,+}, Peng Sun^{2,+}, Yijun Chen^{1*}, Hequan Yao^{2,*}, Shuzhen Wang^{1*}

Table of contents

Materials & Methods	2-26
Supplementary Table S1 PDGFR kinase inhibition of 2-phenyloxypyrimidine	
derivatives	27-28
Supplementary Table S2 Anti-proliferative activity of 2-phenyloxypyrimidine	
derivatives on HCC cell lines determined by CellTiter-Glo luminescent cell	
viability assay (IC ₅₀ , µM)	29-30
Supplementary Figure S1 Original gel images for Manuscript Fig. 5C	31-33
Supplementary Figure S2 Original gel images for Manuscript Fig. 6B	34-35
Supplementary Figure S3 Original gel images for Manuscript Fig. 6C	36
Supplementary Figure S4 Original gel images for Manuscript Fig. 6D	37
Supplementary Figure S5 Original gel images for Manuscript Fig. 6E	38
Supplementary Figure S6 Original gel images for Manuscript Fig. 7A	39-44
Supplementary Figure S7 Original gel images for Manuscript Fig. 7B	45-46
Supplementary NMR and HRMS data for all compounds	47-186

Materials & Methods

Chemical synthesis



N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)-2-phenylacetamide: A round bottom flask was charged with 0.28 g of **8**, 0.13 g of benzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.38 g of **A2** was obtained in the yield of 96%. HPLC R_t = 13.3 min, purity: 99%; ¹H NMR(300 MHz, CDCl₃) δ 9.18 (d, J = 1.8 Hz, 1H), 8.69 – 8.68 (m, 1H), 8.32 (d, J = 8.0 Hz, 1H), 7.99 (s, 1H), 7.51 (s, 1H), 7.42 – 7.38 (m, 2H), 7.36 – 7.27 (m, 5H), 7.25 – 7.16 (m, 2H), 3.64 (s, 2H), 2.12 (s, 3H) ppm; ¹³C NMR(75 MHz, CDCl₃) δ 169.2, 164.0, 165.3, 164.6, 160.6, 151.9, 151.3, 148.5, 136.9, 134.9, 134.5, 131.8, 131.2, 127.5, 126.4, 123.8, 117.0, 113.6, 111.6, 44.6, 15.9 ppm; HRMS (ESI) calcd for [C₂₄H₂₀N₄O₂+H]+ 397.1586, found 397.1465.



N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)-2-phenylacetamide: A round bottom flask was charged with 0.28 g of **8**, 0.13 g of 4-methylbenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.33 g of **A3** was obtained in the yield of 85%. HPLC R_t = 11.8 min, purity: 99%; ¹H NMR(300 MHz, CDCl₃) δ 9.20 (s, 1H), 8.70 (d, J = 3.4 Hz, 1H), 8.68 – 8.58 (m, 1H), 8.37 – 8.34 (m, 1H), 7.98 (d, J = 8.1 Hz 1H), 7.73 – 7.67 (m, 3H), 7.45 – 7.40 (m, 3H), 7.39 – 7.18 (m, 3H), 2.36 (s, 3H), 2.17 (s, 3H) ppm; ¹³C NMR(75 MHz, CDCl₃) δ 165.6, 165.4, 164.6, 160.6, 151.8, 151.4, 148.4, 142.3, 137.2, 135.0, 132.0, 131.8, 130.0, 129.4, 129.0, 127.0, 126.4, 123.9, 117.4, 114.0, 111.6, 21.5, 16.0 ppm; HRMS (ESI) calcd for $[C_{24}H_{20}N_4O_2+H]+$ 397.1586, found 397.1665.



3-methyl-N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g of 8, 0.13 g of 3-methylbenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.35 g of A4 was obtained in the yield of 90%. HPLC $R_t = 12.0$ min, purity: 99%; ¹H NMR(300 MHz, CDCl₃) δ 9.12 (d, J = 1.2 Hz 1H), 8.61 (d, J = 3.5 Hz, 1H), 8.50 (d, J = 5.2 Hz, 1H), 8.27 (d, J = 8.0 Hz, 1H), 7.98 (d, J = 8.1 Hz 1H), 7.73 – 7.67 (m, 1H), 7.45 – 7.40 (m, 1H), 8.21 (s, 1H), 7.60 – 7.50 (s, 3H), 7.37 – 7.30 (m, 3H), 7.20 – 7.14 (m, 3H), 2.26 (s, 3H), 2.09 (s, 3H) ppm; ¹³C NMR(75 MHz, CDCl₃) & 166.2, 165.3, 164.5, 160.6, 151.7, 151.4, 148.4, 138.4, 137.4, 135.0, 134.8, 132.4, 131.8, 131.3, 128.4, 127.9, 126.3, 124.2, 123.8, 117.6, 114.1, 111.6, 21.2, 15.9 ppm; HRMS (ESI) calcd for [C₂₄H₂₀N₄O₂+H]+ 397.1586, found 397.1664.



4-methoxy-N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)benzamid e: A round bottom flask was charged with 0.28 g of **8**, 0.17 g of 4-methoxybenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.37 g of **A5** was obtained in the yield of 90%. HPLC R_t = 14.2 min, purity: 99%; ¹H NMR(300 MHz, CDCl₃) δ 9.12 (d, J = 1.2 Hz 1H), 8.61 (d, J = 3.5 Hz, 1H), 8.50 (d, J = 5.2 Hz, 1H), 8.27 (d, J = 8.0 Hz, 1H), 7.98 (d, J = 8.1 Hz 1H), 7.73 – 7.67 (m, 1H), 7.45 – 7.40 (m, 1H), 8.21 (s, 1H), 7.60 – 7.50 (s, 3H), 7.37 – 7.30 (m, 3H), 7.20 – 7.14 (m, 3H), 2.26 (s, 3H), 2.09 (s, 3H) ppm; ¹³C NMR(75 MHz, CDCl₃) δ 165.4, 164.7, 162.4, 160.6, 151.9, 151.4, 148.5, 137.3, 134.9, 131.8, 129.0, 127.0, 126.3, 123.8, 117.5, 114.0, 113.8, 111.6, 55.4, 16.0 ppm; HRMS (ESI) calcd for [C₂₄H₂₀N₄O₃+H]+ 413.1535, found 413.1614.



4-chloro-N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g of **8**, 0.17 g of 4-chlorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.36 g of **A6** was obtained in the yield of 87%. HPLC R_t = 13.7 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 9.18 (s, 1H), 8.68 (d, J = 3.5 Hz, 1H), 8.57– 8.54 (m, 2H), 8.32 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 8.5 Hz, 2H), 7.65 (s, 1H), 7.44 – 7.31 (m, 5H), 7.22 (d, J = 8.0 Hz, 1H), 2.16 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.3, 164.9, 160.6, 151.9, 151.4, 148.5, 137.9, 137.0, 134.9, 133.2, 131.7, 131.4, 128.8, 128.6, 126.8, 123.8, 117.6, 114.2, 111.7, 16.0 ppm; HRMS (ESI) calcd for [C₂₃H₁₇N₄O₂Cl+H]+ 417.1040, found 417.1119.



3-chloro-N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g of **8**, 0.17 g of 3-chlorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.38 g of **A7** was obtained in the yield of 91%. HPLC R_t = 12.5 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 9.17 (s, 1H), 8.80 (s, 1H), 8.66 (d, J = 4.5 Hz, 1H), 8.55 (d, J = 5.1 Hz, 1H), 8.32 (d, J = 7.9 Hz, 2H), 7.78 (s, 1H), 7.67 (d, J = 7.9 Hz, 2H), 7.44 – 7.31 (m, 4H), 7.28 – 7.30 (m, 1H), 7.20 (d, J = 8.2 Hz, 1H), 2.14 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.3, 164.7, 164.4, 160.6, 152.0, 151.4, 148.6, 136.8, 136.7, 134.9, 134.8, 131.8, 131.4, 130.0, 127.4, 126.9, 125.2, 123.8, 117.6, 114.2, 111.7, 16.0 ppm; HRMS (ESI) calcd for [C₂₃H₁₇N₄O₂Cl+H]+ 417.1040, found 417.1119.



N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)-4-nitrobenzamide: A round bottom flask was charged with 0.28 g of **8**, 0.18 g of 4-nitrobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 50:1(v:v) as eluent. 0.32 g of **A8** was obtained in the yield of 75%. HPLC R_t = 9.8 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 9.22 (d, J = 1.7 Hz, 1H), 8.72 (dd, J = 4.8 Hz, J = 1.5 Hz, 1H), 8.33 (dt, J = 8.0 Hz, J = 1.7 Hz, 1H), 8.72 (dd, J = 4.8 Hz, J = 1.5 Hz, 1H), 8.33 (dt, J = 8.0 Hz, J = 1.7 Hz, 1H), 8.40 (d, J = 8.6 Hz, 2H), 8.14 (s, 1H), 8.01 (d, J = 8.7 Hz, 2H), 7.67 (s, 1H), 7.49 (d, J = 5.2 Hz, 1H), 7.46 - 7.39 (m, 2H), 7.30 (d, J = 8.3 Hz, 1H), 2.21 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.2, 164.6, 163.8, 160.6, 151.8, 151.4, 149.6, 148.5, 140.4, 136.4, 134.9, 131.7, 131.5, 128.4, 127.5, 123.9, 117.7, 114.4, 111.7, 16.0 ppm; HRMS (ESI) calcd for [C₂₃H₁₇N₅O₄+H]+ 427.1281, found 427.1407.



N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)-3-nitrobenzamide: A round bottom flask was charged with 0.28 g of **8**, 0.18 g of 3-nitrobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 50:1(v:v) as eluent. 0.33 g of **A9** was obtained in the yield of 77%. HPLC R_t = 8.1 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 9.27 (s, 1H), 9.16 (d, J = 1.5 Hz, 1H), 8.67 – 8.66 (m, 2H), 8.57 (d, J = 5.2Hz, 1H), 8.32 - 8.20 (m, 3H), 7.65 (d, J = 1.3 Hz, 1H), 7.57 (d, J = 8.0 Hz, 1H), 7.46 – 7.37 (m, 3H), 7.20 (d, J = 8.3 Hz, 1H), 2.13 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.2, 164.6, 163.6, 160.6, 151.9, 151.4, 148.5, 148.0, 136.6, 136.4, 134.9, 133.6, 131.7, 131.4, 129.9, 127.2,

126.2, 123.9, 122.0, 117.9, 114.5, 111.7, 16.0 ppm; HRMS (ESI) calcd for [C₂₃H₁₇N₅O₄+H]+ 427.1281, found 427.1405.



4-fluoro-N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g of **8**, 0.15 g of 4-fluorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 50:1(v:v) as eluent. 0.38 g of **A10** was obtained in the yield of 95%. HPLC R_t = 11.9 min, purity: 98%; ¹H NMR (300 MHz, CDCl₃) δ 9.11 (s, 1H), 8.60 (d, J = 3.9 Hz, 1H), 8.48 (d, J = 5.0 Hz, 1H), 8.38 (s, 1H), 8.25 (d, J = 7.8 Hz, 1H), 7.75 (dd, J = 7.8, 5.5 Hz, 2H), 7.56 (s, 1H), 7.33 (dd, J = 14.9, 6.5 Hz, 3H), 7.14 (d, J = 8.2 Hz, 1H), 6.96 (t, J = 8.4 Hz, 2H), 2.08 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 166.4, 165.3, 164.6, 160.6, 151.8, 151.4, 148.5, 137.0, 134.9, 131.8, 131.4, 129.6, 129.5, 126.7, 123.8, 117.6, 115.8, 115.5, 114.2, 111.6, 15.9 ppm; HRMS (ESI) calcd for [C₂₃H₁₇N₄O₂F+H]+ 401.1336, found 401.1414.



N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)nicotinamide: A round bottom flask was charged with 0.28 g of **8**, 0.13 g of nicotinic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 30:1(v:v) as eluent. 0.34 g of **A11** was obtained in the yield of 89%. HPLC R_t = 7.6 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 9.19 (s, 1H), 8.76 (s, 1H), 8.69 (s, 1H), 8.59 (d, J = 5.1 Hz, 1H), 8.33 (d, J = 8.0 Hz, 1H), 7.68 – 7.65 (m, 3H), 7.47 – 7.40 (m, 3H), 7.26 (d, J = 8.4 Hz, 1H), 2.18 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.3, 164.7, 163.9, 160.6, 152.0, 151.4, 150.5, 148.6, 142.1, 136.5, 134.8, 131.7, 131.5, 127.4, 123.8, 121.0, 117.7, 114.4, 111.7, 16.0 ppm; HRMS (ESI)

calcd for [C₂₂H₁₇N₅O₂+H]+ 384.1382, found 384.1463.



N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)oxy)phenyl)isonicotinamide: A round bottom flask was charged with 0.28 g of **8**, 0.13 g of isonicotinic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 30:1(v:v) as eluent. 0.31 g of A12 was obtained in the yield of 82%. HPLC R_t = 8.3 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) 9.20 (s, 1H), 9.08 (d, J = 1.4 Hz, 1H), 8.96 (s, 1H), 8.66 - 8.50 (m, 2H), 8.47 (d, J = 5.2 Hz, 1H), 8.27 - 8.16 (m, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.57 (d, J = 1.5 Hz, 1H), 7.41 - 7.26 (m, 3H), 7.22 (dd, J = 7.5, 4.6 Hz, 1H), 7.12 (d, J = 8.3 Hz, 1H), 2.06 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.2, 164.6, 164.1, 160.6, 152.0, 151.8, 151.3, 148.4, 148.0, 136.9, 135.6, 134.9, 131.7, 131.4, 130.9, 127.0, 123.9, 123.6, 117.9, 114.4, 111.7, 15.9 ppm; HRMS (ESI) calcd for [C₂₂H₁₇N₅O₂+H]+ 384.1382, found 384.1459.



N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g **8 (4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline)**, 0.13 g benzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 150:1(v:v) as eluent. 0.33 g of **B1** was obtained in the yield of 86%. HPLC R_t = 15.1 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) 8.85 (s, 1H), 8.37 (d, J = 5.2 Hz, 1H), 7.96 (d, J = 6.3 Hz, 2H), 7.74 (d, J = 7.3 Hz, 2H), 7.61 (s, 1H), 7.51 (d, J = 6.9 Hz, 1H), 7.41 – 7.30 (m, 5H), 7.24 (t, J = 7.6 Hz, 2H), 7.13 (d, J = 8.3 Hz, 1H), 2.09 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.2, 166.3, 165.2, 159.8, 151.4, 137.4, 135.8, 134.8, 131.6, 131.4, 131.3, 128.9, 128.5, 127.4, 127.2, 126.5, 117.8, 114.3, 111.7, 16.0 ppm; HRMS (ESI) calcd for [C₂₄H₁9N₃O₂+H]+



N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)-2-phenylacetamide: A round bottom flask was charged with 0.28 g 8

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.15 g 2-phenylacetic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 150:1(v:v) as eluent. 0.37 g of **B2** was obtained in the yield of 94%. HPLC R_t = 16.9 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.42 (d, J = 5.1 Hz, 1H), 7.97 (d, J = 6.5 Hz, 2H), 7.41 (d, J = 6.5 Hz, 4H), 7.34 (d, J = 5.1 Hz, 1H), 7.29 – 7.21 (m, 6H), 7.11 (d, J = 8.1 Hz, 1H), 3.61 (s, 2H), 2.09 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 169.0, 167.2, 165.3, 160.0, 151.500, 136.708, 136.0, 134.5, 131.4, 131.2, 129.5, 129.1, 128.9, 127.6, 127.4, 126.6, 117.0, 113.6, 111.6, 44.7, 16.0 ppm; HRMS (ESI) calcd for [C₂₅H₂₁N₃O₂+H]+ 396.1634, found 396.1711.



4-methyl-N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g **8**

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.13 g of 4-methylbenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 150:1(v:v) as eluent. 0.36 g of **B3** was obtained in the yield of 91%. HPLC R_t = 14.6 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.48 (d, J = 5.2 Hz, 1H), 8.22 (s, 1H), 8.03 – 8.00 (m, 2H), 7.62 – 7.56 (m, 3H), 7.51 – 7.38 (m, 5H), 7.27 – 7.20 (m, 3H), 2.33 (s, 3H), 2.15 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.2, 166.0, 165.3, 159.9, 151.5, 138.5, 137.2, 135.9, 134.9, 134.0, 132.5, 131.4, 131.3, 130.6, 128.9, 128.3, 127.4, 127.2, 126.6, 124.1, 117.5, 114.0, 111.6, 21.3, 16.0 ppm; HRMS (ESI) calcd for [C₂₅H₂₁N₃O₂+H]+ 396.1634, found 396.1714.



3-methyl-N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g **8**

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.13 g of 4-methylbenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 150:1(v:v) as eluent. 0.32 g of **B4** was obtained in the yield of 81%. HPLC R_t = 15.8 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.42 (d, J = 5.1 Hz, 1H), 7.97 – 7.94 (m, 3H), 7.64 (d, J = 8.1 Hz, 2H), 7.47 (d, J = 1.6 Hz, 1H), 7.41 (s, 1H), 7.40 – 7.32 (m, 5H), 7.18– 7.12 (m, 3H), 2.29 (s, 3H), 2.09 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.2, 165.3, 160.0, 142.3, 151.6, 142.3, 137.1, 136.0, 131.4, 128.9, 127.0, 117.4, 113.9, 111.6, 21.3, 16.0 ppm; HRMS (ESI) calcd for [C₂₅H₂₁N₃O₂+H]+ 396.1634, found 396.1713.



4-methoxy-N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g **8**

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.16 g of 4-methoxybenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 150:1(v:v) as eluent. 0.35 g of **B5** was obtained in the yield of 86%. HPLC R_t = 14.1 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.43 (d, J = 5.2 Hz, 1H), 8.37 (s, 1H), 8.00 (d, J = 7.7Hz, 2H), 7.76 (d, J = 8.7Hz, 2H), 7.55 (s, 1H), 7.49 - 7.34 (m, 5H), 7.17 (d, J = 8.2 Hz, 1H), 6.81 (d, J = 8.7 Hz, 3H), 3.75 (s, 3H), 2.13 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.1, 165.5, 165.3, 159.9, 151.5, 137.4, 135.9, 131.4, 131.3, 129.0, 128.9, 127.3, 127.0, 126.3, 117.6, 114.1, 113.8, 111.6, 55.4, 16.0 ppm; HRMS (ESI) calcd for [C₂₅H₂₁N₃O₃+H]+ 412.1583, found

412.1662.



4-chloro-N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g **8**

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.16 g of 4-chlorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 150:1(v:v) as eluent. 0.37 g of **B6** was obtained in the yield of 89%. HPLC R_t = 11.7 min, purity: 97%; ¹H NMR (300 MHz, CDCl₃) δ 8.53 (d, J = 5.2 Hz, 1H), 8.04 (dd, J = 7.3, 1.5Hz, 2H), 7.88 (s, 1H), 7.77 (d, J = 8.5 Hz, 2H), 7.53 – 7.41 (m, 8H), 7.29 – 7.26 (m, 1H), 2.19 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.2, 165.2, 164.6, 159.9, 151.6, 138.0, 136.8, 135.9, 133.3, 131.4, 128.9, 128.5, 127.3, 127.0, 117.5, 114.1, 111.7, 16.0 ppm; HRMS (ESI) calcd for [C₂₄H₁₈N₃O₂Cl+H]+ 416.1088, found 416.1665.



3-chloro-N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g **8**

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.16 g of 3-chlorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 150:1(v:v) as eluent. 0.35 g of **B7** was obtained in the yield of 84%. HPLC R_t = 13.6 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.91 (s, 1H), 8.39 (d, J = 5.2 Hz, 1H), 7.96 (d, J = 6.6 Hz, 2H), 7.71 (s, 1H), 7.61 – 7.48 (m, 3H), 7.43 – 7.34 (m, 5H), 7.18 (d, J = 8.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 2.08 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.2, 165.1, 164.9, 159.8, 151.4, 137.0, 136.6, 135.8, 134.5, 131.5, 131.3, 129.8, 127.5, 127.3, 126.8, 125.4, 117.9, 114.4, 111.8, 16.0 ppm; HRMS (ESI) calcd for $[C_{24}H_{18}N_3O_2Cl+H] + 416.1088$, found 416.1165.



N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)-4-nitrobenzamide: A round bottom flask was charged with 0.28 g 8

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.16 g of 4-nitrobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.33 g of **B8** was obtained in the yield of 77%. HPLC R_t = 11.8 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.55 (d, J = 5.1 Hz, 1H), 8.33 (d, J = 8.7 Hz, 2H), 8.14 – 7.93 (m, 4H), 7.84 (s, 1H), 7.56 (s, 1H), 7.50 – 7.44 (m, 4H), 7.32 (d, J = 8.2 Hz, 1H), 2.22 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.3, 165.1, 163.9, 159.9, 151.5, 149.5, 140.4, 136.4, 135.7, 131.5, 129.0, 128.4, 127.3, 123.8, 117.8, 114.3, 111.8, 16.0 ppm; HRMS (ESI) calcd for [C₂₄H₁₈N₄O₄+H]+ 427.1328, found 427.1403.



N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)-3-nitrobenzamide: A round bottom flask was charged with 0.28 g 8

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.16 g of 3-nitrobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.31 g of **B9** was obtained in the yield of 73%. HPLC R_t = 12.6 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.65 (t, J = 1.7 Hz, 1H), 8.58 (s, 1H), 8.49 (d, J = 5.2 Hz, 1H), 8.35 – 8.24 (m, 1H), 8.19 (d, J = 7.9 Hz, 1H), 7.99 (dd, J = 7.9, 1.6 Hz, 2H), 7.59 (t, J = 8.0 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.45 – 7.35 (m, 4H), 7.24 (dd, J = 9.7, 5.3 Hz, 1H), 2.14 (s, 3H). ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.3, 165.1, 163.5, 159.8, 151.4, 148.0, 136.5, 135.7, 133.5, 131.5, 129.9, 128.9, 127.3, 126.2, 122.0, 117.8, 114.4, 111.8, 16.0 ppm; HRMS (ESI) calcd for [C₂₄H₁₈N₄O₄+H]+ 427.1328, found 427.1407.



4-fluoro-N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)benzamide: A round bottom flask was charged with 0.28 g **8**

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.15 g of 4-fluorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.32 g of **B10** was obtained in the yield of 80%. HPLC R_t = 10.6 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.52 (d, J = 5.2 Hz, 1H), 8.04 (dd, J = 7.5, 1.7 Hz, 2H), 7.91 (s, 1H), 7.84 (dd, J = 8.7, 5.3 Hz, 2H), 7.58 – 7.37 (m, 6H), 7.27 (d, J = 6.3 Hz, 1H), 7.12 (t, J = 8.6 Hz, 2H), 2.19 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.2, 166.5, 160.0, 151.6, 136.8, 136.0, 131.4, 129.4, 129.3, 128.9, 127.3, 127.0, 117.4, 115.9, 115.6, 114.1, 111.6, 16.0 ppm; HRMS (ESI) calcd for [C₂₄H₁₈N₃O₂F+H]+ 400.1383, found 400.1463.



N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)nicotinamide: A round bottom flask was charged with 0.28 g 8

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.13 g of nicotinic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 50:1(v:v) as eluent. 0.34 g of **B11** was obtained in the yield of 89%. HPLC R_t = 10.9 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 9.38 (s, 1H), 8.55 (d, J = 4.3 Hz, 2H), 8.43 (d, J = 5.1 Hz, 1H), 7.98 (d, J = 6.9 Hz, 2H), 7.61 – 7.50 (m, 4H), 7.46 – 7.36 (m, 4H), 7.19 (d, J = 8.2 Hz, 1H), 2.13 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.2, 165.1, 164.2, 159.9, 151.5, 150.2, 142.2, 136.7, 135.7, 131.5,

131.4, 128.9, 127.3, 121.3, 117.9, 114.4, 111.8, 16.0 ppm; HRMS (ESI) calcd for [C₂₃H₁₈N₄O₂+H]+ 383.1430, found 383.1506.



N-(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)phenyl)isonicotinamide: A round bottom flask was charged with 0.28 g **8**

(4-methyl-3-((4-phenylpyrimidin-2-yl)oxy)aniline), 0.13 g of isonicotinic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 50:1(v:v) as eluent. 0.34 g of **B12** was obtained in the yield of 89%. HPLC R_t = 11.7 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 9.00 (d, J = 1.5 Hz, 1H), 8.91 (s, 1H), 8.63 (dd, J = 4.7, 1.3 Hz, 1H), 8.45 (d, J = 5.2 Hz, 1H), 8.12 (d, J = 8.0 Hz, 2H), 7.61 – 7.50 (m, 4H), 7.51 (s, 2H), 7.48 – 7.38 (m, 4H), 7.30 – 7.28 (m, 1H), 7.21 (d, J = 8.8 Hz, 1H), 2.14 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.2, 165.1, 164.0, 159.8, 152.2, 151.5, 148.0, 136.8, 135.8, 135.5, 131.4, 130.8, 128.9, 127.3, 123.6, 117.8, 114.3, 111.8, 16.0 ppm; HRMS (ESI) calcd for [C₂₃H₁₈N₄O₂+H]+ 383.1430, found 383.1507.



N-(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)phenyl)acetamide: A round bottom flask was charged with 0.32 g 8

(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)aniline), 0.07 g of acetic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 200:1(v:v) as eluent. 0.37 g of C1 was obtained in the yield of 96%. HPLC R_t = 20.7 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.49 (d, J = 5.1 Hz, 1H), 8.22 – 8.08 (m, 1H), 7.90 – 7.71 (m, 3H), 7.60 (d, J = 6.6 Hz, 1H), 7.50 – 7.34 (m, 4H), 7.23 (d, J = 5.1 Hz, 1H), 7.13 – 7.05 (m, 2H), 2.10 (s, 3H), 1.92 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 169.8, 168.4, 165.1, 159.4, 151.4, 137.3, 135.0, 133.9, 131.3, 130.8, 130.4, 128.6, 128.3, 127.1, 126.3, 126.0, 125.2, 125.0, 117.0, 116.8, 113.6, 24.4, 16.0 ppm; HRMS (ESI) calcd for $[C_{23}H_{19}N_3O_2+H]$ + 370.1477, found 370.1556.



N-(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)phenyl)propionamide: A round bottom flask was charged with 0.32 g 8

(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)aniline), 0.08 g of acetic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 200:1(v:v) as eluent. 0.36 g of C2 was obtained in the yield of 94%. HPLC R_t = 19.1 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.48 (d, J = 5.0 Hz, 1H), 8.23 – 8.10 (m, 1H), 7.91 – 7.69 (m, 3H), 7.59 (d, J = 7.0 Hz, 1H), 7.52 – 7.33 (m, 4H), 7.20 (t, J = 7.1 Hz, 1H), 7.12 (d, J = 7.9 Hz, 1H), 7.05 (d, J = 8.1 Hz, 1H), 2.21 – 2.12 (m, 2H), 2.10 (s, 3H), 1.04 (t, J = 7.5 Hz, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 172.2, 169.8, 165.1, 159.4, 151.4, 137.4, 135.0, 133.9, 131.2, 130.8, 130.4, 128.6, 128.3, 127.1, 126.3, 125.8, 125.2, 125.1, 116.9, 116.8, 113.6, 30.4, 16.0, 9.6 ppm; HRMS (ESI) calcd for [C₂₄H₂₁N₃O₂+H]+ 384.1634, found 384.1712.



N-(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)phenyl)furan-2-carboxa mide: A round bottom flask was charged with 0.32 g 8

(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)aniline), 0.12 g of furan-2-carboxylic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 200:1(v:v) as eluent. 0.35 g of C3 was obtained in the yield of 83%. HPLC R_t = 18.3 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.62 (d, J = 5.1 Hz, 1H), 8.32 – 8.22 (m, 1H), 8.13 (s, 1H), 7.94 (d, J = 8.2 Hz, 1H), 7.89 (dd, J = 6.4, 3.0 Hz, 1H), 7.77 – 7.67 (m, 2H), 7.60 – 7.43 (m, 4H), 7.42 – 7.29 (m, 2H), 7.23 (dd, J = 11.5, 5.5 Hz, 2H), 6.52 (dd, J = 3.4, 1.7 Hz, 1H), 2.24 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 169.7, 165.1, 159.6, 155.9, 151.7, 147.8, 144.2, 136.4, 135.0, 133.9, 131.4, 130.7, 130.4, 128.5, 128.3, 127.1, 126.7, 126.2, 125.2, 125.1, 117.0, 116.8, 115.3, 113.8, 112.6, 16.0 ppm; HRMS (ESI) calcd for [C₂₆H₁₉N₃O₃+H]+ 422.1426, found 422.1504.



N-(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)phenyl)furan-3-carboxa mide: A round bottom flask was charged with 0.32 g 8

(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)aniline), 0.12 g of furan-3-carboxylic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 200:1(v:v) as eluent. 0.38 g of C4 was obtained in the yield of 90%. HPLC R_t = 20.3 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.58 (d, J = 5.1 Hz, 1H), 8.29 – 8.18 (m, 1H), 7.97 (s, 1H), 7.93 (d, J = 8.2 Hz, 1H), 7.88 (dd, J = 6.1, 3.2 Hz, 1H), 7.78 (s, 1H), 7.69 (d, J = 7.1 Hz, 1H), 7.61 (s, 1H), 7.56 – 7.43 (m, 3H), 7.40 (s, 1H), 7.33 (dd, J = 11.0, 3.4 Hz, 2H), 7.27 – 7.16 (m, 1H), 6.68 (s, 1H), 2.21 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 169.8, 165.1, 160.7, 159.5, 151.6, 145.1, 143.9, 136.7, 135.0, 133.9, 131.4, 130.8, 130.4, 128.6, 128.3, 127.1, 126.7, 126.25, 125.2, 125.1, 123.0, 117.4, 116.8, 114.1, 108.4, 16.0 ppm; HRMS (ESI) calcd for [C₂₆H₁₉N₃O₃+H]+ 422.1426, found 422.1506.



N-(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)phenyl)thiophene-2-carb oxamide: A round bottom flask was charged with 0.32 g 8 (4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)aniline), 0.14 g of thiophene-2-carboxylic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 200:1(v:v) as eluent. 0.38 g of C5 was obtained in the yield of 90%. HPLC R_t = 19.7 min, purity: 98%; ¹H NMR (300 MHz, CDCl₃) δ 8.61 (d, J = 5.1 Hz, 1H), 8.32 – 8.23 (m, 1H), 7.99 – 7.85 (m, 3H), 7.78 – 7.64 (m, 3H), 7.59 – 7.42 (m, 4H), 7.35 (dd, J = 7.3, 3.9 Hz, 3H), 7.25 (d, J = 7.8 Hz, 1H), 2.24 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 169.7, 159.5, 136.8, 135.1, 133.9, 131.4, 130.7, 130.4, 128.6, 128.5, 128.3, 127.1, 126.9, 126.2, 126.1, 125.2, 125.1, 117.2, 116.8, 114.0, 16.0 ppm; HRMS (ESI) calcd for [C₂₆H₁₉N₃O₂S+H]+ 438.1198, found 438.1276.



4-chloro-N-(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)phenyl)benzami de: A round bottom flask was charged with 0.32 g **8**

(4-methyl-3-((4-(naphthalen-1-yl)pyrimidin-2-yl)oxy)aniline), 0.14 g of 4-chlorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 200:1(v:v) as eluent. 0.40 g of C6 was obtained in the yield of 86%. HPLC R_t = 9.7 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.57 – 8.44 (m, 2H), 8.21 – 8.12 (m, 1H), 7.90 – 7.76 (m, 2H), 7.67 – 7.55 (m, 4H), 7.43 (dd, J = 9.0, 5.6 Hz, 3H), 7.39 – 7.31 (m, 1H), 7.27 – 7.10 (m, 4H), 2.18 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 169.7, 165.1, 164.9, 159.5, 151.5, 137.8, 137.0, 134.8, 133.8, 133.1, 131.4, 130.8, 130.3, 128.7, 128.6, 128.2, 127.1, 126.7, 126.2, 125.1, 125.0, 117.7, 116.9, 114.3, 16.0 ppm; HRMS (ESI) calcd for [C₂₈H₂₀N₃O₂Cl+H]+ 466.1244, found 466.1313.



N-(3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)benzamide: A round bottom flask was charged with 0.26 g 8

3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.13 g of benzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced

pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.31 g of **D1** was obtained in the yield of 83%. HPLC R_t = 15.7 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.46 (d, J = 5.2 Hz, 1H), 7.99 (s, 1H), 7.82 (d, J = 7.5 Hz, 2H), 7.60 (s, 1H), 7.56 – 7.37 (m, 5H), 7.31 (t, J = 4.6 Hz, 2H), 7.25 (d, J = 8.8 Hz, 1H), 6.63 – 6.49 (m, 1H), 2.17 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 166.1, 164.9, 159.7, 158.1, 151.3, 151.1, 145.5, 137.2, 134.8, 131.6, 131.2, 128.4, 127.8, 126.5, 117.7, 114.2, 113.5, 112.7, 109.7, 15.9 ppm; HRMS (ESI) calcd for [C₂₂H₁₇N₃O₃+H]+ 372.1270, found 372.1344.



N-(3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)-2-phenylacetamide: A round bottom flask was charged with 0.26 g 8

3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.14 g of 2-phenylacetic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.36 g of **D2** was obtained in the yield of 93%. HPLC R_t = 16.5 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.40 (d, J = 5.2 Hz, 1H), 7.63 (s, 1H), 7.58 (dd, J = 1.5, 0.6 Hz, 1H), 7.39 – 7.19 (m, 10H), 7.14 (d, J = 8.2 Hz, 1H), 6.54 (dd, J = 3.5, 1.7 Hz, 1H), 3.64 (s, 2H), 2.12 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 169.2, 164.9, 159.8, 158.2, 151.3, 151.2, 145.5, 137.9, 136.8, 134.5, 131.2, 129.5, 129.4, 129.1, 128.6, 127.5, 127.1, 126.6, 117.2, 113.6, 113.6, 112.7, 109.7, 44.6, 15.9 ppm; HRMS (ESI) calcd for [C₂₃H₁₉N₃O₃+H]+ 386.1426, found 386.1501.



N-(3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)-4-methoxybenzamide: A round bottom flask was charged with 0.26 g 8

3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.16 g of 4-methoxybenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced

pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.37 g of **D3** was obtained in the yield of 92%. HPLC R_t = 16.9 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.43 (d, J = 5.2 Hz, 1H), 8.12 – 7.98 (m, 1H), 7.87 – 7.70 (m, 2H), 7.58 (dd, J = 1.6, 0.6 Hz, 1H), 7.50 (d, J = 2.1 Hz, 1H), 7.46 (dd, J = 8.1, 2.2 Hz, 1H), 7.32 – 7.25 (m, 2H), 7.21 (d, J = 8.2 Hz, 1H), 6.92 – 6.85 (m, 2H), 6.55 (dd, J = 3.5, 1.8 Hz, 1H), 3.82 (s, 3H), 2.15 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.2, 165.0, 162.4, 159.9, 158.2, 151.43, 151.2, 145.4, 137.2, 131.3, 128.9, 127.1, 126.4, 117.5, 113.9, 113.8, 113.5, 112.7, 109.7, 29.7, 16.0 ppm; HRMS (ESI) calcd for [C₂₃H₁₉N₃O₄+H]+ 402.1376, found 402.1451.



N-(3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)-3-methylbenzamide: A round bottom flask was charged with 0.26 g 8

3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.14 g of 3-methylbenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.36 g of **D4** was obtained in the yield of 93%. HPLC R_t = 15.2 min, purity: 96%; ¹H NMR (300 MHz, CDCl₃) δ 8.57 (s, 1H), 8.37 (d, J = 5.2 Hz, 1H), 7.62 – 7.44 (m, 5H), 7.32 – 7.08 (m, 5H), 6.49 (dd, J = 3.5, 1.7 Hz, 1H), 2.25 (s, 3H), 2.08 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 166.3, 164.9, 159.8, 158.2, 151.3, 151.1, 145.5, 138.3, 138.1, 137.3, 134.8, 133.9, 132.4, 131.3, 130.5, 128.4, 128.2, 127.9, 127.2, 126.4, 124.2, 117.7, 114.2, 113.6, 112.7, 109.7, 21.3, 15.9 ppm; HRMS (ESI) calcd for [C₂₃H₁₉N₃O₃+H]+ 386.1426, found 386.1499.



3-chloro-N-(3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)benzamide: A round bottom flask was charged with 0.26 g **8**

3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.14 g of 3-chlorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with

DCM:MeOH = 100:1(v:v) as eluent. 0.38 g of **D5** was obtained in the yield of 94%. HPLC R_t = 14.7 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.62 (s, 1H), 8.38 (d, J = 5.2 Hz, 1H), 7.74 (t, J = 1.7 Hz, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.60 – 7.53 (m, 1H), 7.50 – 7.44 (m, 2H), 7.37 (ddd, J = 7.9, 1.9, 1.0 Hz, 1H), 7.31 – 7.20 (m, 3H), 7.20 – 7.08 (m, 1H), 6.52 (dd, J = 3.5, 1.7 Hz, 1H), 2.08 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 164.9, 164.7, 163.5, 159.7, 158.2, 156.7, 151.3, 151.1, 148.0, 145.5, 140.7, 136.9, 136.7, 134.6, 133.8, 131.6, 131.3, 129.8, 127.5, 126.8, 125.9, 125.3, 123.8, 117.8, 117.2, 114.2, 114.0, 113.6, 112.7, 110.0, 109.8, 101.2, 15.9 ppm; HRMS (ESI) calcd for [C₂₂H₁₆N₃O₃Cl+H]+ 406.0880, found 406.0954.



4-chloro-N-(3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)benzamide: A round bottom flask was charged with 0.26 g **8**

3-((4-(furan-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.14 g of 4-chlorobenzoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.32 g of **D6** was obtained in the yield of 81%. HPLC R_t = 15.3 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.60 (s, 1H), 8.37 (d, J = 5.1 Hz, 1H), 7.70 (d, J = 8.4 Hz, 2H), 7.56 (s, 1H), 7.46 (d, J = 7.1 Hz, 2H), 7.37 - 7.19 (m, 4H), 7.15 (d, J = 8.4 Hz, 1H), 6.53 (d, J = 1.6 Hz, 1H), 2.10 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.0, 164.9, 159.7, 158.2, 151.3, 151.1, 145.5, 137.8, 137.0, 133.2, 131.3, 128.7, 128.7, 126.8, 117.8, 114.3, 113.6, 112.7, 109.8, 15.9 ppm; HRMS (ESI) calcd for [C₂₂H₁₆N₃O₃Cl+H]+ 406.0880, found 406.0951.



N-(3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)acetamide: A round bottom flask was charged with 0.32 g 8

3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.07 g of acetic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were

combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.33 g of **E1** was obtained in the yield of 92%. HPLC R_t = 13.3 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.54 (d, J = 5.1 Hz, 1H), 7.88 (s, 1H), 7.70 – 7.58 (m, 2H), 7.53 (dd, J = 9.5, 6.8 Hz, 2H), 7.46 – 7.23 (m, 5H), 7.19 (d, J = 8.2 Hz, 1H), 2.15 (s, 3H), 2.07 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 168.4, 165.1, 160.3, 158.6, 155.8, 152.3, 151.3, 137.2, 131.3, 128.1, 126.8, 126.2, 123.7, 122.5, 117.2, 113.6, 111.8, 110.8, 109.4, 24.4, 15.9 ppm; HRMS (ESI) calcd for [C₂₁H₁₇N₃O₃+H]+ 360.1270, found 360.1362.



N-(3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)propionamide: A round bottom flask was charged with 0.32 g 8

3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.08 g of propionic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.32 g of **E2** was obtained in the yield of 86%. HPLC R_t = 12.5 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.45 (d, J = 5.1 Hz, 1H), 7.56 (d, J = 8.0 Hz, 2H), 7.52 (s, 1H), 7.46 (d, J = 8.3 Hz, 1H), 7.42 (d, J = 5.1 Hz, 1H), 7.37 – 7.22 (m, 3H), 7.18 (t, J = 7.5 Hz, 1H), 7.10 (d, J = 8.2 Hz, 1H), 2.23 (q, J = 7.5 Hz, 2H), 2.07 (s, 3H), 1.09 (t, J = 7.5 Hz, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.1, 160.3, 158.5, 155.8, 152.4, 151.4, 137.2, 131.3, 128.1, 126.7, 126.07, 123.7, 122.5, 117.1, 115.0, 113.6, 111.8, 110.8, 109.4, 30.6, 15.9, 9.6 ppm; HRMS (ESI) calcd for [C₂₂H₁₉N₃O₃+H]+ 374.1426, found 374.1497.



N-(3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)furan-2-carboxa mide: A round bottom flask was charged with 0.32 g 8 3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.12 g of furan-2-carboxylic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.36 g of **E4** was obtained in the yield of 87%. HPLC R_t = 12.8 min, purity: 96%; ¹H NMR (300 MHz, CDCl₃) δ 8.49 (d, J = 5.1 Hz, 1H), 8.08 (s, 1H), 7.61 – 7.52 (m, 2H), 7.52 – 7.35 (m, 5H), 7.35 – 7.25 (m, 1H), 7.18 (dd, J = 9.0, 5.7 Hz, 2H), 7.11 (d, J = 3.3 Hz, 1H), 6.42 (dd, J = 3.4, 1.7 Hz, 1H), 2.11 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.1, 160.5, 158.5, 156.0, 155.8, 152.5, 151.6, 147.8, 144.2, 136.4, 131.4, 128.2, 126.7, 126.7, 123.6, 122.5, 117.2, 115.2, 113.8, 112.6, 111.8, 110.7, 109.3, 16.0 ppm; HRMS (ESI) calcd for [C₂₄H₁₇N₃O₄+H]+ 412.1219, found 412.1291.



N-(3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)furan-3-carboxa mide: A round bottom flask was charged with 0.32 g 8

3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.12 g of furan-3-carboxylic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 100:1(v:v) as eluent. 0.33 g of **E5** was obtained in the yield of 80%. HPLC R_t = 12.0 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.42 (d, J = 5.1 Hz, 1H), 8.08 (s, 1H), 7.90 (s, 1H), 7.57 – 7.46 (m, 2H), 7.46 – 7.33 (m, 4H), 7.33 – 7.24 (m, 2H), 7.16 (t, J = 7.5 Hz, 1H), 7.09 (d, J = 7.9 Hz, 1H), 6.63 (d, J = 0.9 Hz, 1H), 2.05 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 165.0, 160.9, 160.4, 158.5, 155.8, 152.3, 151.4, 145.2, 143.8, 136.8, 131.4, 128.1, 126.8, 126.6, 123.7, 123.0, 122.5, 117.8, 114.2, 111.8, 110.8, 109.4, 108.5, 15.9 ppm; HRMS (ESI) calcd for [C₂₄H₁₇N₃O₄+H]+ 412.1219, found 412.1289.



N-(3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)-4-((4-methylpipe razin-1-yl)methyl)benzamide: A round bottom flask was charged with 0.32 g 8 3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.50 g of 3-(4-methylpiperazin-1-yl)-2-oxopropanoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 10:1(v:v) as eluent. 0.25 g of G2 was obtained in the yield of 47%. HPLC $R_t = 6.8$ min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.58 (d, J = 5.1 Hz, 1H), 7.87 (s, 1H), 7.79 (d, J = 8.1 Hz, 2H), 7.72 – 7.60 (m, 2H), 7.55 (dd, J = 6.3, 4.6 Hz, 3H), 7.51 – 7.33 (m, 4H), 7.33 – 7.21 (m, 3H), 3.55 (s, 2H), 2.46 (s, 8H), 2.29 (s, 3H), 2.21 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.6, 165.0, 160.5, 158.5, 155.8, 152.4, 151.5, 136.5, 131.4, 128.1, 126.8, 126.7, 125.6, 124.4, 123.7, 122.5, 118.7, 116.9, 113.4, 111.8, 110.8, 110.4, 109.3, 61.5, 54.3, 51.8, 44.7, 16.0 ppm; HRMS (ESI) calcd for [C₃₂H₃₁N₅O₃+H]+ 534.2427, found 534.2520.



N-(3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)-2-(4-methylpiper azin-1-yl)acetamide: A round bottom flask was charged with 0.32 g 8 3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.30 g of 3-(4-methylpiperazin-1-yl)-2-oxopropanoic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 10:1(v:v) as eluent. 0.29 g of G2 was obtained in the yield of 63%. HPLC R_t = 7.9 min, purity: 97%; ¹H NMR (300 MHz, CDCl₃) δ 9.14 (s, 1H), 8.57 (d, J = 5.1 Hz, 1H), 7.66 (d, J = 7.7 Hz, 1H), 7.63 (d, J = 0.8 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.53 (d, J = 5.1 Hz, 1H), 7.48 (d, J = 2.0 Hz, 1H), 7.46 – 7.35 (m, 2H), 7.32 – 7.21 (m, 2H), 3.11 (s, 2H), 2.64 (s, 4H), 2.48 (s, 4H), 2.29 (s, 3H), 2.18 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 164.4, 164.1, 159.5, 157.5, 154.8, 151.5, 150.5, 141.7, 136.0, 132.7, 130.4, 128.3, 127.2, 126.0, 125.7, 122.6, 121.5, 116.4, 112.9, 110.8, 109.7, 108.3, 61.5, 54.1, 52.1, 45.0, 15.0 ppm; HRMS (ESI) calcd for [C₂₆H₂₇N₅O₃+H]+ 458.2114, found 458.1998.



N-(3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)-2-morpholinoace tamide: A round bottom flask was charged with 0.32 g 8

3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.30 g of 2-morpholinoacetic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 10:1(v:v) as eluent. 0.23 g of **G3** was obtained in the yield of 51%. HPLC R_t = 8.1 min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 8.99 (s, 1H), 8.49 (d, J = 5.1 Hz, 1H), 7.62 – 7.52 (m, 2H), 7.52 – 7.38 (m, 3H), 7.32 (dd, J = 7.9, 6.7 Hz, 2H), 7.26 – 7.13 (m, 2H), 3.72 – 3.59 (m, 4H), 3.03 (s, 2H), 2.57 – 2.44 (m, 4H), 2.10 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 167.8, 165.1, 160.5, 158.5, 155.8, 152.4, 151.5, 136.5, 131.4, 128.1, 126.7, 126.6, 123.7, 122.4, 116.8, 113.2, 111.5, 110.7, 109.3, 67.0, 62.4, 53.8, 16.0 ppm; HRMS (ESI) calcd for [C₂₅H₂₄N₄O₄+H]+ 445.1798, found 445.1875.



N-(3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylphenyl)-2-hydroxyaceta mide: A round bottom flask was charged with 0.32 g 8

3-((4-(benzofuran-2-yl)pyrimidin-2-yl)oxy)-4-methylaniline, 0.30 g of 2-hydroxyacetic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 10:1(v:v) as eluent. 0.12 g of G4

was obtained in the yield of 31%. HPLC $R_t = 5.9$ min, purity: 99%; ¹H NMR (300 MHz, CDCl₃) δ 9.73 (s, 1H), 8.72 (d, J = 5.1 Hz, 1H), 7.81 (d, J = 9.1 Hz, 2H), 7.76 – 7.67 (m, 2H), 7.63 (s, 1H), 7.50 (dd, J = 15.7, 8.3 Hz, 2H), 7.35 (t, J = 7.5 Hz, 1H), 7.26 (d, J = 8.3 Hz, 1H), 5.65 (t, J = 5.9 Hz, 1H), 3.98 (d, J = 5.9 Hz, 2H), 3.33 (s, 8H), 2.07 (s, 3H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ 171.3, 165.0, 161.7, 157.9, 155.6, 152.4, 151.4, 138.1, 131.3, 128.1, 127.5, 125.1, 124.3, 123.2, 117.1, 113.5, 112.2, 111.6, 109.9, 62.3, 15.9 ppm; HRMS (ESI) calcd for [C₂₁H₁₇N₃O₄+H]+ 376.1219, found 376.1298.



N-(4-methyl-3-((4-(1-methyl-1H-indol-2-yl)pyrimidin-2-yl)oxy)phenyl)acetamide: A round bottom flask was charged with 0.33 g 8

F1

4-methyl-3-((4-(1-methyl-1H-indol-2-yl)pyrimidin-2-yl)oxy)aniline, 0.07 g of acetic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 50:1(v:v) as eluent. 0.31 g of **F1** was obtained in the yield of 84%. HPLC R_t = 11.7 min, purity: 99%; ¹H NMR (300 MHz, DMSO-*d6*) δ 8.52 (d, J = 5.2 Hz, 1H), 8.40 (s, 1H), 7.86-7.97 (m, 1H), 7.70-7.47 (m, 4H), 7.31 (d, J = 1.8 Hz, 1H), 7.24 (t, J = 7.4 Hz, 1H), 6.99 (t, J = 7.4 Hz, 1H), 3.89 (s, 3H), 2.10 (s, 3H), 2.06 (s, 3H) ppm; ¹³C NMR (75 MHz, DMSO-*d6*) δ 168.7, 165.3, 164.6, 159.1, 151.9, 138.9, 138.0, 134.0, 131.3, 126.0, 125.1, 122.8, 122.7, 121.4, 116.2, 113.4, 112.1, 110.8, 110.7, 33.6, 24.4, 16.0 ppm; HRMS (ESI) calcd for [C₂₂H₂₀N₄O₂+H]+ 373.1586, found 373.1660.



N-(4-methyl-3-((4-(1-methyl-1H-indol-2-yl)pyrimidin-2-yl)oxy)phenyl)propiona mide: A round bottom flask was charged with 0.33 g 8

4-methyl-3-((4-(1-methyl-1H-indol-2-yl)pyrimidin-2-yl)oxy)aniline, 0.08 g of propionic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic

layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 50:1(v:v) as eluent. 0.33 g of **F1** was obtained in the yield of 85%. HPLC R_t = 12.1 min, purity: 99%; ¹H NMR (300 MHz, DMSO-*d6*) δ 9.91 (s, 1H), 8.44 (d, J = 5.4 Hz, 1H), 8.38 (s, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.59 – 7.39 (m, 4H), 7.28 (d, J = 8.3 Hz, 1H), 7.20 (t, J = 7.2 Hz, 1H), 6.96 (t, J = 7.3 Hz, 1H), 3.85 (s, 3H), 3.33 (s, 5H), 2.29 (q, J = 7.5 Hz, 2H), 2.06 (s, 3H), 1.06 (t, J = 7.5 Hz, 3H) ppm; ¹³C NMR (75 MHz, DMSO-*d6*) δ 171.9, 164.8, 164.1, 158.6, 151.5, 138.5, 137.6, 133.5, 130.8, 125.5, 124.5, 122.3, 122.2, 120.9, 115.7, 112.9, 110.4, 110.3, 33.1, 29.5, 15.5, 9.6 ppm; HRMS (ESI) calcd for [C₂₃H₂₂N₄O₂+H]+ 387.1743, found 387.1822.



N-(4-methyl-3-((4-(1-methyl-1H-indol-2-yl)pyrimidin-2-yl)oxy)phenyl)furan-2-ca rboxamide: A round bottom flask was charged with 0.33 g 8 4-methyl-3-((4-(1-methyl-1H-indol-2-yl)pyrimidin-2-yl)oxy)aniline, 0.12 g of furan-2-carboxylic acid and 10 mL DCM. 0.15 g HOBt and 0.21 g of EDCI were added to the solution at room temperature. After stirring for 2 hours, 20 mL distilled water was added and the mixture was extracted with 20 mL DCM for two times. The organic layers were combined and washed with water and brine. The solvent was removed under reduced pressure and the residue was purified through flash chromatography on silica gel with DCM:MeOH = 50:1(v:v) as eluent. 0.37 g of F4 was obtained in the yield of 97%. HPLC $R_t = 11.8$ min, purity: 99%; ¹H NMR (300) MHz, DMSO- $_{d6}$) δ 10.33 (s, 1H), 8.47 (d, J = 5.4 Hz, 1H), 8.38 (s, 1H), 8.00 - 7.91 (m, 2H), 7.88 (d, J = 8.0 Hz, 1H), 7.79 - 7.67 (m, 2H), 7.61 - 7.44 (m, 5H), 7.36 (d, J = 8.2 Hz, 1H), 7.19 (dd, J = 11.3, 4.0 Hz, 1H), 6.99 (t, J = 7.6 Hz, 1H), 3.85 (s, 3H), 2.12 (s, 3H) ppm; ¹³C NMR (75 MHz, DMSO-_{d6}) δ 164.8, 164.1, 158.6, 156.1, 151.4, 147.4, 145.6, 137.7, 137.6, 133.5, 130.8, 125.6, 125.5, 122.3, 122.2, 121.0, 117.0, 114.6, 114.1, 112.1, 111.6, 110.4, 110.3, 33.0, 15.5 ppm; HRMS (ESI) calcd for $[C_{25}H_{20}N_4O_3+H]$ + 425.1535, found 425.1609.

Cell culture

Liver cancer cell lines of Hep3B, MHCC97-L, QGY-7703, SMMC-7721 and SNU368 were obtained from HD Biosciences (China) Co., Ltd. Hep3B cells were cultured in DMEM medium and all the other cell lines in RPMI 1640 medium. All media contained 10% fetal bovine serum (FBS) (Bioind, US origin) and all cells were incubated in a humidified atmosphere of 5 % CO₂ at 37 °C. All the cell lines were

authenticated by using short tandem repeat (STR) matching analysis. No mycoplasma contamination was detected.

CellTiter-Glo luminescent cell viability assay

For experiments hepatocellular carcinoma cells were seeded at 4000 cells per well in 96-well plates. After overnight incubation, solution of compounds in DMSO at various concentrations were added to the cells and further incubated for 120 h. Cell viability was measured with the CellTiter-Glo Luminescent Cell Viability Assay (Promega) according to the manufacturer's instructions. Luminescence was measured using an EnVision Multilabel Plate Reader (Perkin-Elmer). The cytotoxicity of the compounds was expressed as the percentage of luminescence relative to that of untreated cells. The concentration of compound producing 50% of cell proliferation (IC₅₀) was calculated by nonlinear regression analysis of the response-concentration (log) curve, using the Graph-Pad Prism program package (Graph Pad Software; San Diego, CA). Results are expressed as the means of two dependent experiments performed in triplicate.

Compound ID	Inhibition effect (%) ^a		$IC_{50} (\mu M)^b$		Selectivity
	PDGFRα	PDGFRβ	PDGFRa	PDGFRβ	index ^c
A1	39.11	21.40	N.D. ^d	N.D.	N.D.
A2	65.72	40.73	N.D.	N.D.	N.D.
A3	45.45	45.50	N.D.	N.D.	N.D.
A4	66.71	43.74	N.D.	N.D.	N.D.
A5	45.20	33.70	N.D.	N.D.	N.D.
A6	47.73	35.96	N.D.	N.D.	N.D.
A7	62.93	40.23	N.D.	N.D.	N.D.
A8	55.65	43.24	N.D.	N.D.	N.D.
A9	23.63	23.41	N.D.	N.D.	N.D.
A10	40.63	30.94	N.D.	N.D.	N.D.
A11	42.91	6.84	N.D.	N.D.	N.D.
A12	43.17	31.94	N.D.	N.D.	N.D.
B1	2.32	12.87	N.D.	N.D.	N.D.
B2	21.09	17.63	N.D.	N.D.	N.D.
B3	23.12	26.17	N.D.	N.D.	N.D.
B4	35.04	24.42	N.D.	N.D.	N.D.
B5	1.81	19.39	N.D.	N.D.	N.D.
B6	12.21	18.64	N.D.	N.D.	N.D.
B7	31.49	16.63	N.D.	N.D.	N.D.
B8	26.17	37.71	N.D.	N.D.	N.D.
B9	21.34	19.14	N.D.	N.D.	N.D.
B10	19.57	15.63	N.D.	N.D.	N.D.
B11	32.00	5.08	N.D.	N.D.	N.D.
B12	25.66	20.65	N.D.	N.D.	N.D.
C1	33.27	1.32	N.D.	N.D.	N.D.
C2	33.78	2.07	N.D.	N.D.	N.D.
C3	46.46	11.61	N.D.	N.D.	N.D.
C4	13.73	2.83	N.D.	N.D.	N.D.
C5	16.27	5.08	N.D.	N.D.	N.D.
C6	24.14	-0.94	N.D.	N.D.	N.D.
D1	13.74	28.93	N.D.	N.D.	N.D.
D2	36.82	46.75	N.D.	N.D.	N.D.
D3	22.61	37.72	N.D.	N.D.	N.D.
D4	45.70	46.00	N.D.	N.D.	N.D.
D5	51.79	43.49	N.D.	N.D.	N.D.
D6	33.02	37.47	N.D.	N.D.	N.D.
E1	1.56	1.82	N.D.	N.D.	N.D.
E2	19.06	10.10	N.D.	N.D.	N.D.
E3	-2.00	3.83	N.D.	N.D.	N.D.

Supplementary Table S1 PDGFR kinase inhibition of 2-phenyloxypyrimidine derivatives

E4	27.18	7.35	N.D.	N.D.	N.D.
E5	86.12	66.41	0.40	0.93	2.32
E6	-1.24	-0.44	N.D.	N.D.	N.D.
E7	18.56	19.39	N.D.	N.D.	N.D.
E8	26.16	14.62	N.D.	N.D.	N.D.
F1	6.37	2.32	N.D.	N.D.	N.D.
F2	12.21	-4.46	N.D.	N.D.	N.D.
F3	24.14	25.67	N.D.	N.D.	N.D.

^a Inhibition effect (%): kinase inhibition activities of compounds at 1 μ M. ^b IC₅₀: 50% inhibitory concentration (averages of two separate experiments). ^c Selectivity index=IC₅₀ (PDGFR β)/ IC₅₀ (PDGFR α).

^d N.D. = not determined.

Supplementary Table S2 Anti-proliferative activity of 2-phenyloxypyrimidine derivatives on HCC cell lines determined by CellTiter-Glo luminescent cell viability assay (IC₅₀, μ M)

Compound	BEL740	Hep3	MHCC97-	QGY-770	SMMC-772	SNU36
ID	4	В	L	3	1	8
A1	10.8	15.8	15.1	24.5	13.6	85.7
A2	39.3	39.5	>200	59.8	84.3	112.2
A3	32.8	21.2	22.3	47.0	25.1	51.4
A4	12.2	17.5	24.5	39.8	17.5	54.0
A5	15.6	23.3	31.3	40.5	23.5	49.5
A6	9.5	10.7	16.2	21.9	12.3	24.0
A7	32.8	18.9	51.5	57.8	27.2	45.9
A8	20.1	14.3	34.6	24.6	10.1	25.7
A9	23.8	28.4	53.2	48.4	26.8	51.5
A10	28.2	20.1	35.7	43.4	21.1	38.7
A11	74.2	105.4	89.3	252.0	79.7	94.6
A12	133.7	130.3	281.3	170.4	112.6	286.6
B1	10.5	2.7	4.9	5.8	2.7	17.7
B2	14.4	13.0	16.9	20.6	11.7	24.8
B3	3.7	4.6	6.1	7.3	6.0	12.8
B4	9.5	6.4	7.0	10.2	6.2	12.9
B5	7.9	9.2	9.8	14.9	8.4	15.8
B 6	13.4	7.9	10.5	15.4	9.7	15.0
B7	18.3	15.5	>200	25.8	17.0	14.0
B 8	9.9	9.0	14.0	14.4	7.5	12.0
B9	12.9	83.2	>200	19.2	13.8	16.8
B10	8.1	5.8	6.3	10.9	3.9	12.6
B11	21.6	44.2	53.5	81.1	20.2	18.0
B12	13.4	17.7	44.0	27.6	8.8	18.0
C1	36.2	32.0	108.6	91.6	21.0	43.0
C2	48.2	36.3	110.7	119.5	29.5	55.9
C3	39.7	33.5	91.0	70.7	27.2	37.9
C4	8.8	22.9	96.4	14.9	12.0	15.8
C5	20.8	17.0	28.0	35.2	16.8	28.4
C6	6.7	19.7	>200	19.2	14.3	17.2
D1	48.7	11.4	1.6	2.5	1.5	37.3
D2	32.8	28.3	26.4	42.2	21.6	43.8
D3	17.6	9.7	8.5	15.7	7.9	22.2
D4	4.5	6.0	3.4	7.5	3.7	23.2
D5	12.4	11.2	14.7	22.5	12.4	24.0
D6	10.9	7.3	24.6	25.8	8.2	12.7
E1	10.1	86.8	5.7	0.3	0.3	8.5
E2	8.2	74.6	5.5	0.4	0.2	13.2

E3	1.2	125.0	9.6	0.7	0.7	1.3
E4	5.2	15.8	0.0	0.0	0.4	11.4
E5	0.8	2.6	10.0	15.1	1.0	8.9
E6	38.1	11.7	16.7	29.5	27.7	31.6
E7	5.9	9.0	59.1	10.3	4.6	14.7
E8	2.8	3.8	13.6	3.3	2.5	6.3
F1	37.1	31.0	48.4	195.4	34.5	29.3
F2	19.0	33.8	31.8	51.9	27.9	29.1
F3	15.6	41.8	>200	97.7	18.4	26.5



Supplementary Figure S1 Original gel images for Manuscript Fig. 5C

<u>Bel7404</u>

Procaspase-3:



Procaspase-9:



Procapase-7:



PARP:



Bcl-2:



Bax :



GAPDH:



HepG-2

Procaspase-3:



Procaspase-9:



Procapase-7:



PARP:



Bcl-2:



Bax :



GAPDH:



Supplementary Figure S2 Original gel images for Manuscript Fig. 6B B



<u>Bel7404</u>

LC3:



Atg-5:



GAPDH:



HepG-2

LC3:



Atg-5:



GAPDH:



Supplementary Figure S3 Original gel images for Manuscript Fig. 6C C



<u>Bel7404</u>

LC3:



GAPDH:



HepG-2

LC3:



GAPDH:


Supplementary Figure S4 Original gel images for Manuscript Fig. 6D





<u>Bel7404</u>

LC3:



GAPDH:



HepG-2

LC3:



GAPDH:





Supplementary Figure S5 Original gel images for Manuscript Fig. 6E

<u>Bel7404</u>

Atg-5:



GAPDH:



HepG-2

Atg-5:



GAPDH:



Supplementary Figure S6 Original gel images for Manuscript Fig. 7A

<u>Bel7404</u>

Phospho-PDGFRα:



PDGFRa:



PI3K:



Phospho-AKT:

AKT:

Phospho-mTOR:

mTOR:

Phospho-p38 MAPK:



p38 MAPK:



Phospho-MEK:



MEK:



Phospho-ERK:

ERK:

GAPDH:



HepG-2

Phospho-PDGFRα:



PDGFRα:



PI3K:



Phospho-AKT:



AKT:



Phospho-mTOR:



mTOR:



Phospho-p38 MAPK:



p38 MAPK:



Phospho-MEK:



MEK:



Phospho-ERK:



ERK:



GAPDH:





Supplementary Figure S7 Original gel images for Manuscript Fig. 7B B

<u>Bel7404</u>

Phospho-ERK:



ERK:



LC3:



GAPDH:

<u>HepG-2</u>

Phospho-ERK:



ERK:



LC3:



GAPDH:



SP1308303-2-C C13-NMR CDCL3 303K AV-300



15.458

ala na sanana ing kang sa na sana sana ta na mala Mala na sana ng kang sa na sa na sana ta na sa ta na sa ta na

an and the and second and

ppm

and the first from a market second

Constant and







N

-



SP121126 CDCl3 303K C13-NMR AV300

An ing has a set in the last

an the second second

A2

77.533

44.614

5.935

-i

0 ppm





Sample Name						Positio	n		p2d7						Ins	strumen	nt Name		Instrur	nent 1
User Name	QTOF-PC\QTO	F				Inj Vol			0.2						Inj	Positio	n			
Sample Type	Sample					IRM Ca	alibratio	on Status	Succ	ess					Da	ta Filen	ame		A2-p.d	
ACQ Method	20110418-MSc	nly-p.m				Comm	ent								Ac	quired 1	Time		3/12/2	018 2:52:45 PM
	x10 ⁵	+ESI Scan	(rt: 0.5	20-0.5	44 min,	3 scan	s) Frag=	=100.0V	A2-p.d 🖇	Subtra	act									
	5.4 -																			
	5.2																			
	5 -								397.10	665										
	4.8 -								(IVI+F	I) T										
	4.6																			
	4.4 -																			
	4.2																			
	4 -																			
	3.8 -																			
	3.6 -																			
	3.4 -																			
	3.2 -																			
	3 -																			
	2.8 -																			
	2.6																			
	2.4 -																			
	2.2																			
	2 -																			
	1.8 -																			
	1.6 -																			
	1.4 -																			
	1.2 -									ſ										
	1 -																			
	0.8 -																			
	0.6 -																			
	0.4 -																			
	0.2										I									
	0	<u> </u>	······································	····			<u> </u>	<u></u>						<u>.</u>	<u></u>			. <u>.</u>		
		382	384	386	388	390	392	394 Counts	396 s vs. Mas	398 ss-to-	400 Charge	402 (m/z)	404	406	408	410	412	414	416	

SP121128-2 CDCl3 303K C13-NMR AV300



77.486

21.461

of One one

Manallands.

40.000

0 ppm



Sample Name					Position		p2d8				I	instrument	Name	Instrur	nent 1
User Name	QTOF-PC\QTO	F			Inj Vol		0.1				I	njPosition			
Sample Type	Sample				IRM Calib	ration Status	Succes	S			6	Data Filenaı	ne	A3-p.d	
ACQ Method	20110418-MSc	only-p.m			Comment						A	Acquired Tir	ne	3/12/2	018 2:54:56 P
	x10 ⁵	+ESI Scan	(rt: 0.414-	0.450 min	, 4 scans) F	Frag=100.0V A	A3-p.d S	ubtract							
	4.4 -														
	4.2														
	4 -						397.1 (M+⊢	665 \+							
	3.8 -						(101.1	<i>)</i> .							
	3.6 -														
	3.4 -														
	3.2 -														
	3 -														
	2.8 -														
	2.6 -														
	2.4 -														
	2.2 -														
	2 -														
	1.8 -														
	1.6 -														
	14-														
	12-														
	1 -														
	0.8 -														
	0.0														
	0.0														
	0.4														
	0.2														
	0	386	388	390	392	394 Counts	396 vs. Mass	398 -to-Chai	400 ge (m/z)	402	404	406	408	410	





Sample Name						P	osition			р	2d9						I	nstrum	nent Na	ame	1	Instrun	nent 1
User Name	QTOF-PC\QTO	F				Ir	nj Vol			0).1						I	njPosit	ion				
Sample Type	Sample					IF	RM Cal	ibratio	n Statu	is S	Success						D	ata Fil	ename	•		A4-p.d	
ACQ Method	20110418-MSc	only-p.m				C	ommei	nt									A	cquire	d Time	•		3/12/20)18 2:57:46 PN
	x10 5	+ESI Sca	an (rt: (0.594-	0.642	min, 5	scans)	Frag=	=100.0\	/ A4-p	.d Sub	otract											
	62-																						
	6 -																						
	5.8																						
	5.6									3	397.16	64 -											
	5.4 -									,	(101+11)	т											
	5.2																						
	5 -																						
	4.8 -																						
	4.6																						
	4.4 -																						
	4.2																						
	4 -																						
	3.8																						
	3.6 -																						
	3.4 -																						
	3.2 -																						
	3 -																						
	2.8																						
	2.6																						
	2.4 -																						
	2.2 -																						
	2																						
	1.8																						
	1.0																						
	1.4																						
	1.2																						
	0.8 -																						
	0.6 -																						
	0.4 -																						
	0.2												I										
	0			<u></u>	·· · · · · · · · · · · · · · · · · · ·					····· ······	<u></u>					<u></u>		<u></u>	<u></u>		<u> </u>		
		388	389	390	391	392	393	394	395 Coun	396 Its vs	397 Mass-I	398 o-Ch	399 arge (n	400 n/z)	401	402	403	404	405	406	407		

bpm 0 10 E96'SI -20 30 40 303K C13-NMR AV300 20 LID'SS 09 20 or Standove - 76.665 - 77.089 - 77.512 80 60 100 2 SP121119 CDCl3 919.111 -110 113 842 114.038 81.5 · LTT 120 - 123.820 . 126.300 127.023 130 128.981 131.309 ₽LL'IET 140 668'7ET 137.337 148.541 150 005 · TST 668'TST 160 0LS'09T -165.369 164.670 165.369 170 180 190 A5

bpm T980'0--0000.0 -2 - 2.0803 3.12 3 5.95 13.7187 4 5 5.2041 1692.9 -₽862.9 -2708.8 -0811.7 e a v 9 9311 L -2682 L -1262 L -800 L -2.11 7.33152 7.33152 7.33152 22 20.53 3.05 50.5 0135.70 5 00 5.06 1.04 1.03 ດ 00'T 10

SP121105-2 1H-NMR CDCl3 303K AV-300

A5.

Sample Name				Position		p2E1				Inst	rument Name	Instru	ment 1
User Name	QTOF-PC\QTC)F		Inj Vol		0.1				InjP	osition		
Sample Type	Sample			IRM Calibra	ation Status	Succes	\$			Data	Filename	A5-p.d	
ACQ Method	20110418-MS	only-p.m		Comment						Acq	uired Time	3/12/2	018 3:00:14 PM
	x10 ⁵	+ESI Scan (rt: C).416-0.440 m	nin, 3 scans) Fr	ag=100.0V A	5-p.d Su	ıbtract						
	9.5 -												
	9 -												
	8.5 -					413.10 (M+H	514)+						
	8 -												
	7.5												
	7.5												
	7 -												
	6.5 -												
	6 -												
	5.5 -												
	5 -												
	4.5 -												
	4 -												
	3.5 -												
	3 -												
	25-												
	2.0												
	2 -												
	1.5 -												
	1 -												
	0.5							I					
	0 -	· · · · · · · · · · · · · · · · · · ·		, , , , , , , , , , , , , , , , , , , ,		+		<u> .</u>		440 462	404 400 400		
		403 404 40	15 406 407	408 409	410 411 4 Counts v	vs. Mass	414 41 to-Charg∉	15 416 e(m/z)	417 418	419 420	421 422 423	424	

mdd 0 10 186'ST 20 30 40 303K C13-NMR AV300 20 and a contract 09 20 019.91 -260 · LL 915 · LL 80 60 100 **CDCl3** - 111.672 110 222.011 -T\$9.711 -123.836 120 SP121205-1 126.805 128.604 128.833 130 - 131.388 - 131.388 - 133.221 140 - 136.952 -150 ₽ZG.8₽1-688°TST 068°TST 160 995 09T 259 79T E06.491 -170 E0E'991 -180 190 A6. 62

bpm 0000.0-0.5 1.0 1.5 SP121114-3 1HNMR CDCl3 303K AV-300 2.0 3.03 5:1232 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 - 1.1858 - 7.2134 - 7.2837 6.5 ETTE'L 5798.L-9628.L-9907.L-7977.L-7.0 1.08 3.20 1.03 2.07 7.5 17657.7 0723.7 8.0 1911.1 T9TL'L -OFFL'L -LEOE'8 -EOEE'8 -68ES'8 -6555'8 -FT99'8 -85L9'8 -TFFL'8 -6ELT'6 -0.99 1.03 20.1 8.5 9.0 00°T 9.5

				FU	SILIOII			pzlz						msuu	ient na	ille	Insut	
QTOF-PC\QTOF				In	j Vol			0.1						InjPosi	tion			
Sample				IF	M Calib	ration Sta	tus	Success						Data Fi	lename		A6-p.	d
20110418-MSonly-	p.m			Co	omment									Acquire	d Time		3/12/	2018 3:02:19 P
x10 5 +ES	SI Scan	(rt: 0.51	0-0.545	min, 4	scans) F	- rag=100.0	0V A6-	-p.d Su	btract]
6.6																		
6.4																		
6.2																		
6 -								417.1	119									
5.8								(M+I	-l)+									
5.6 -																		
5.4																		
5.2																		
5 -																		
4.8 -																		
4.6																		
4.4																		
4.2																		
4 -																		
3.8																		
3.0																		
3.4																		
3 -																		
2.6																		
2.4																		
2.2																		
2																		
1.8										I								
1.6																		
1.4 -																		
1.2 -																		
1 -																		
0.8																		
0.6																		
0.4																		
0.2																		
0 - ۲		40.4	400	400	440	410		410	410	400	<u></u>	404	400	400	400	400	424	J
	QTOF-PC\QTOF Sample 20110418-MSONI- x10 5 6.6 6.4 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 3 2.8 2.6 2.4 3.2 3 3 2.8 2.6 2.4 3.2 3 3 2.8 2.6 3.4 3.2 3 3 2.8 3 4.2 3 3 4.2 3 3 4.2 3 4 5.2 4 5.2 4 5.2 5 5 4.8 5.2 5 5 4.8 5.2 5 5 4.8 5.2 5 5 4.8 5.2 5 5 4.8 5.2 5 5 4.8 5.2 5 5 4.8 5.2 5 5 4.8 5.2 5 5 5 4.8 5.2 5 5 5 4.8 5.2 5 5 5 4.8 5.2 5 5 5 4.8 5.2 5 5 5 4.8 5.2 5 5 5 5 5 4.8 5.2 5 5 5 5 4.8 5.2 5 5 5 4.8 5.2 5 5 5 5 4.8 5.2 5 5 5 4.8 5.2 5 5 5 5 4.8 5 6 5 4 5 7 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	QTOF-PC\QTOF Sample 20110418-MSonly-p.m x10 5 6.6 6.4 6.4 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 2 1 0 .5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 5 4 .8 5 .8 5	QTOF-PC\QTOF Sample 20110418-MSonly-p.m x10 5 6.6 6.4 6.4 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4.3 8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.4 1.2 1 1 0.8 0.6 0.4 1.4 1.4 1.2 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	QTOF-PC\QTOF Sample 20110418-MSonly-p.m x10 5 6.6 6.4 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0 4 4 2.2 2 1.8 1.6 1.4 1.4 1.2 1.8 1.6 1.4 1.4 1.2 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5	QTOF-PC\QTOF In Sample IR 20110418-MSonUy-p.m Cc x10 5 6.6 6.4 6.4 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4.2 4 4 3.8 3.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 4 3.8 3.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 4 3.8 3.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 4 4 3.8 3.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 4 4 5.2 5 4.8 4.6 5.4 5.2 5 4.8 4.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 4 4.2 4 4 4.2 4 4 5.2 5 5 4.8 5 6 5 4.8 5 6 5 4.8 5 6 5 4.8 5 6 5 4.8 5 6 5 4.8 5 6 5 4.8 5 6 5 4.8 5 6 5 4.8 5 6 5 5 4.8 5 6 5 4.8 5 6 5 5 4.8 5 6 5 5 4.8 5 6 5 5 4.8 5 6 5 5 4.8 5 6 5 5 7 5 7 5 7 5 7 5 7 7 7 7 7 7 7 7	QTOF-PC\QTOF Inj Vol Sample IRM Calib 20110418-MSonly-p.m Comment x10 5 6.6	QTOF-PC\QTOF Inj Vol Sample IRM Calibration State 20110418-MSonly-p.m Comment x10 5 6.6	QTOF-PC\QTOF Inj Vol Sample IRM Calibration Status 20110418-MSonly-p.m Comment x10 * *ESI Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6 6.6 6.4 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4.3 3.6 3.4 3.6 3.4 3.6 3.4 3.6 3.4 3.6 3.4 3.6 3.4 3.2 3 2.6 2.4 2.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6	QTOF-PC\QTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 +ESI Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Sut 6 6.4 6.2 6 6.4 6.2 6 4.4 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 1.1 1.2 1.8 1.6 1.6 1.4 1.2 1 0.8 6 0.4 0.2 0 -	QTOF-PC\QTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 6.6 6.4 6.2 417.1119 6.6 44 6.2 417.1119 6.8 444 6.2 417.1119 6.8 444 6.9 417.1119 7.1 6 7.2 5 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.8 4.6 4.4 <	QTOF-PCQTOF Inj Vol 0.1 Sample IRM Calibration Status Success 2010418-MSonly-p.m Comment x10 5 4ESI Scan (rt: 0.510-0.545 min. 4 scans) Frag=100.0V A6-p.d Subtract 6 417.1119 5.8 417.1119 5.8 (M+H)+ 5.6 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 4.6 3.4 4.2 4 4.2 4 4.8 4.6 4.4 4.2 4 3.8 6.6 3.4 3.2 3.2 3 2.8 4 2.1 4 3.2 4 3.4 4 3.5 4 3.6 4 3.7 4 3.8<	QTOF-PCQUTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonty-p.m Comment *10 5 +ESI Scan (tt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d Subtract 6 44 6 417.1119 5.6 417.1119 5.8 (M+H)+ 5.6 44 4.8 (M+H)+ 5.6 44 4.8 46 4.4 42 4 38 3.6 417.1119 3.8 46 4.4 42 4 42 4 42 4 42 4 42 4 42 4 42 4 42 4 42 4 42 4 42 4 42 4 42 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 1 <td>QTOF-PCQTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 s *ESI Scan (t: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract 66 4 6.6 4 6.6 4 6.6 4 6.6 4 6.7 417.1119 5.8 (M+H)+ 5.6 4 5.4 5.2 5 4 4.8 4.6 4.4 4.2 4.8 4.6 3.8 5.6 3.8 5.6 3.8 5.6 3.4 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.3 4.6 3.4 4.6 3.2 4.7 3.3 4.8 3.6 4.1 3.7 4.1 3.8 4.1 3.6 4.1 3.7 4.1 3.8 4.1 3.9 4.1 4.1 4.1 4.1 4.1 5.2 4.1 4.1</td> <td>QTOF-PC\QTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-Wonly-p.m Comment **ESI Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract 6.6 6.4 6.2 6.4 6.2 6.5 6.4 6.2 6.4 6.2 6.4 6.2 7 7 8 9</td> <td>QTOF-PCQTOF Inj Vol 0.1 InjPosi Sample IRM Calibration State Success Data Fi 20110418-MSonly-p.m Comment Acquire *ESI Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract - - 6.6 - - - - 6.6 - - - - - 7.10 * + - - - - 6.6 - - - - - - 6.6 -</td> <td>QTOF-PC/QTOF Inj Vol 0.1 InjPosition Sample TRM Calibration Status Success Data Filename 20110418 Hesti Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d Subtract Acquired Time * + - - * - - - * - - - * - - - * - - - * - - - * - - - * - - - - * - - - - * - - - - * - - - - * - - - - * - - - - * - - - - * - - - - * -</td> <td>QT0F-PCQTOF Ing Vol 0.1 IngPosition Sample IRM Calibration Status Success Data Filename Z0110418-MSom(rb):-p.m Comment Acquired Time x10 5 +ESI Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract - 66 - - - - 66 - - - - 66 - - - - 66 - - - - 66 - - - - 66 - - - - 7 - - - - 7 - - - - 7 - - - - 6 - - - - - 7 - - - - - - 6 - - - - - - - -</td> <td>QTOF-PCQTOF Inj Vol 0.1 Injestion Sample IRM Calibration Status Success Data Filename A6-p.0 201018-MSonk-p.m Comment Acquired Time 3/12/ x10 s I=SSI Scan (tt 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract - - 66 - - - - - 66 - - - - - - 66 -</td>	QTOF-PCQTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 s *ESI Scan (t: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract 66 4 6.6 4 6.6 4 6.6 4 6.6 4 6.7 417.1119 5.8 (M+H)+ 5.6 4 5.4 5.2 5 4 4.8 4.6 4.4 4.2 4.8 4.6 3.8 5.6 3.8 5.6 3.8 5.6 3.4 4.6 4.4 4.2 4.8 4.6 4.4 4.2 4.3 4.6 3.4 4.6 3.2 4.7 3.3 4.8 3.6 4.1 3.7 4.1 3.8 4.1 3.6 4.1 3.7 4.1 3.8 4.1 3.9 4.1 4.1 4.1 4.1 4.1 5.2 4.1 4.1	QTOF-PC\QTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-Wonly-p.m Comment **ESI Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract 6.6 6.4 6.2 6.4 6.2 6.5 6.4 6.2 6.4 6.2 6.4 6.2 7 7 8 9	QTOF-PCQTOF Inj Vol 0.1 InjPosi Sample IRM Calibration State Success Data Fi 20110418-MSonly-p.m Comment Acquire *ESI Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract - - 6.6 - - - - 6.6 - - - - - 7.10 * + - - - - 6.6 - - - - - - 6.6 -	QTOF-PC/QTOF Inj Vol 0.1 InjPosition Sample TRM Calibration Status Success Data Filename 20110418 Hesti Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d Subtract Acquired Time * + - - * - - - * - - - * - - - * - - - * - - - * - - - * - - - - * - - - - * - - - - * - - - - * - - - - * - - - - * - - - - * - - - - * -	QT0F-PCQTOF Ing Vol 0.1 IngPosition Sample IRM Calibration Status Success Data Filename Z0110418-MSom(rb):-p.m Comment Acquired Time x10 5 +ESI Scan (rt: 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract - 66 - - - - 66 - - - - 66 - - - - 66 - - - - 66 - - - - 66 - - - - 7 - - - - 7 - - - - 7 - - - - 6 - - - - - 7 - - - - - - 6 - - - - - - - -	QTOF-PCQTOF Inj Vol 0.1 Injestion Sample IRM Calibration Status Success Data Filename A6-p.0 201018-MSonk-p.m Comment Acquired Time 3/12/ x10 s I=SSI Scan (tt 0.510-0.545 min, 4 scans) Frag=100.0V A6-p.d. Subtract - - 66 - - - - - 66 - - - - - - 66 -

mdd 0 10 166'ST 20 969.62 -30 40 C13-NMR AV300 20 09 20 989.97 -090'LL -80 £81.77 F 303K 90 100 **CDCl3** 199°TTT -OLT . PIT -110 095'LTT 123.824 - 125.221 120 126.945 SP121202-1 127.422 866.921 -130 131.430 ESL'IET 134.807 140 ₱98.₽€1 -6L9 . 9ET -E61.9E1 -150 T48.571 -- 121.422 721:96S 160 885'09T -LED . 431 -071.491 -170 165.327 180 190 (P) 65









Sample Name					Positi	on		p2E4	4				Ins	trument	t Name	In	strument 1
User Name	QTOF-PC\QTOF				Inj Vo	bl		0.1					Inj	Position			
Sample Type	Sample				IRM C	Calibratio	on Status	Suco	cess				Dat	ta Filena	me	A	3-p.d
ACQ Method	20110418-MSor	ly-p.m			Comn	nent							Acc	uired Ti	ime	3/	12/2018 3:07:26 PM
	x10 5 +	ESI Scan ((rt: 0.295-	0.307 m	nin, 2 scar	ns) Frag	=100.0V A	8-p.d									
	2.6																
	2.5																
	2.4							427.1 (M+⊢	407 1)+								
	2.3								.,								
	2.2																
	2.1																
	2 -																
	1.9																
	1.8																
	1.7 -																
	1.6 -																
	1.5 -																
	1.4 -																
	1.3 -																
	1.2																
	1.1																
	1-																
	0.9																
	0.8																
	0.7																
	0.6									1							
	0.5																
	0.4 -																
	0.3 -																
	0.2																
	0.1 -																
	0 -	424	424 F		425 F	426	426 F	427	407 E	420	100 F	420	420 F	420	420 F	421	<u> </u>
		424	424.5	425	425.5	420	426.5 Counts	427 vs. Ma	427.5 Iss-to-Char	428 ge (m/:	4∠ŏ.5 z)	429	429.5	430	430.5	431	

mdd - martin ملع فتخلفه فتأبير ومقاففه فتعرافك فأحاشان وباعديه علقاتهما إزالك مقدمة فالمجار فالمربق فالمرقا والمتحد والمتلافين والمحاصر فرارا فالمالا فتعاد والمتحد والمتحد والمحاصر فرارا والمحاصر فالمحالية والمحالية فلمحالية والمحالية والم والمركبة والمركبة والمرابع والمرابع والمرابع والمرابع 0 10 696'ST 20 30 40 Indate, 19 Jan Lab 303K C13-NMR AV300 50 60 20 F 80 60 100 工 111.738 114.466 117.887 122.022 123.867 126.176 126.176 127.236 126.176 SP121121-1 CDCl3 110 120 ALL D. & Mr. J. WILL & Mr. 130 201. 131. 133. 134. 134. 140 150 160 والمقطع فالمتعامل فتعارك فيطلعه ومتقا يتستعلما فليكم والترام 170 المعاريق ومعاديها كمان والماسانية فالمعاطي فالتقابة 180 190

8 d


Sample Name				F	Position		p2E5				Ins	strument Na	me	Instrun	nent 1
User Name	QTOF-PC\QTOF			I	inj Vol		0.1				Inj	Position			
Sample Type	Sample			I	RM Calibra	tion Status	Succes	S			Dat	ta Filename		A9-p.d	
ACQ Method	20110418-MSor	ly-p.m		C	Comment						Acc	quired Time		3/12/2	018 3:09:32 PM
	x10 ⁵ +	ESI Scan (r	t: 0.279-0.	.303 min, 3	scans) Fra	ag=100.0V A	9-p.d Sı	ubtract							
	5.6														
	5.4														
	5.2					4	27.1405	5							
	5 -						(IVI+H)+								
	4.8														
	4.6														
	4.4														
	4.2														
	4 -														
	3.8														
	3.6														
	3.4														
	3.2														
	3 -														
	2.8														
	2.6														
	2.4														
	2.2														
	2 -														
	1.8 -														
	1.6 -														
	1.4 -														
	1.2														
	1 -														
	0.8														
	0.6														
	0.4														
	0.2								1						
	0			·····	· · · · · · · · · ·		<u> </u>		<u> </u>		······	· ·· ·			
		422	423	424	425	426 Counts v	427 /s. Mass	428 -to-Charg	429 ge (m/z)	430	431	432	433		





Sample Name					Po	sition			p2E6				I	nstrume	ent Nam	e	Instrur	nent 1
User Name	QTOF-PC\QTC)F			Inj	j Vol			0.1				I	njPositi	on			
Sample Type	Sample				IR	M Calibi	ation St	atus	Success				0	oata File	name		А10-р.	d
ACQ Method	20110418-MS	only-p.m			Co	mment							A	cquired	Time		3/12/2	018 3:16:43 P
	x10 ⁵	+ESI Scan (rt: 0.351	1-0.422	min, 7 s	cans) F	rag=100).0V A1	0-p.d Su	btract								
	6 75 -																	
	6.5 -																	
	6 25 -								401.	1414								
	6-								(M+	H)+ ∣								
	5.75 -																	
	5.5																	
	5.25																	
	5 -																	
	4.75 -																	
	4.5 -																	
	4.25 -																	
	4 -																	
	3.75 -																	
	3.5																	
	3.25 -																	
	3 -																	
	2.75 -																	
	2.5																	
	2.25 -																	
	2 -																	
	1.75 -																	
	1.5 -																	
	1.25 -																	
	1 -																	
	0.75 -																	
	0.5																	
	0.25										I							
	0 -	<u>,</u>						<u></u>				 			<u></u>			

mdd -----0 10 -510.91 20 30 E 40 E C13-NMR AV300 20 60 20 989.97 090'LL 80 \$85.TT 303K 90 100 CDCl3 57 110 971.726 -P76.911 -STL'LTI . 120 151:020 SP121205-2 928.521. - 127.423 130 131.512 169.151 EE8.9E1 -140 L9₽.9EI 142.092 SLS . 80T . 150 815'0ST -SEP'ISI . ₱96'IST 160 LT9.09.1 968'E9T -- 164.714 170 180 190 An 77

mdd 0000.0 -0.5 1.0 1.5 2.0 SP121205-2 1H-NMR CDCl3 303K AV-300 3.12 - 2.1823 2.5 3.0 3.5 4.0 4.5 3 5.0 6) 5.5 6.0 6.5 - 7.2450 7.0 - 7.4042 9917 L -1127 L -2137 L -01.1 80.8 7.5 5.99 - 7.4685 - 7.6623 8.0 6918.8 -1.02 PEPE.8 -8.5 - 8.5831 10°S 9689 8 -9891 8 -9161 6 -0.6 00'T 9.5 AH

				Posit	tion			p2E7						I	instrun	nent Na	ame	Ir	nstrument 1
QTOF-PC\QTOF				Inj V	'ol			0.1						I	njPosi	tion			
Sample				IRM	Calibra	tion St	atus	Succe	SS					0	Data Fi	lename	•	A	11-p.d
20110418-MSon	ly-p.m			Com	ment									A	Acquire	d Time	1	3,	/12/2018 3:19:42 PM
x10 ⁵ +	ESI Scan (rt	: 0.265-0	.277 mi	n, 2 sca	ans) Fra	ag=100	0.0V A1	l-p.d	Subtr	act									
9 -																			
8.5 -							38 (1	34.146 M+H)+	63 +										
8 -							(
7.5																			
7 -																			
6.5 -																			
6 -																			
5.5 -																			
5																			
4.5																			
4.5																			
4																			
3.5 -																			
3 -																			
2.5																			
2 -									I										
1.5 -																			
1 -																			
0.5																			
0 -	· · · · · · ·	· · · · · ·			· · · · · · · · · · · · · · · · · · ·	<u></u>	<u> </u>					· · · · · ·							
	376 37	7 378	379	380	381	382 Co	383 ounts vs	384 . Mas	385 s-to-C	386 harge	387 (m/z)	388	389	390	391	392	393	394	
	QTOF-PC\QTOF Sample 20110418-MSon x10 5 + 9 8.5 8 7.5 7 6.5 6 5 4.5 5 4.5 5 4.5 5 4.5 3 2.5 2 1.5 1 0.5 0	QTOF-PC\QTOF Sample 20110418-MSonly-p.m x10 5 +ESI Scan (rt 9 8.5 8 7.5 7 6.5 6 5 4.5 5 4.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 1 0 376 37	QTOF-PC\QTOF Sample 20110418-MSonly-p.m x10 5 +ESI Scan (rt: 0.265-0 9 8.5 8 7 6.5 7 6.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 376 377 378	QTOF-PC\QTOF Sample 20110418-MSonly-p.m *10 5 +ESI Scan (rt: 0.265-0.277 mi 9 8.5 8 7.5 7 6.5 6 5.5 6 5 5 4.5 5 4.5 5 4.5 5 4.5 5 4.5 5 4.5 5 4.5 5 4.5 5 4.5 5 4.5 5 6 5 5 5 6 6 5 5 5 6 6 5 5 7 6 7 6 5 5 7 6 7 6	Positi QTOF-PC\QTOF Sample IRM 20110418-MSonly-p.m Com x10 5 +ESI Scan (rt: 0.265-0.277 min, 2 sca 9 8.5 8 7.5 7 6.5 5 4.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 	Position Inj Vol Sample 20110418-MSonly-p.m x10 5 +ESI Scan (rt: 0.265-0.277 min, 2 scans) Fra 9 8.5 8 7 6.5 6 5.5 5 4 3.5 3 2.5 4 3.5 3 2.5 4 5 4 3.5 3 2.5 4 5 4 3.5 5 4 5 4 3 5 4 5 5 4 5 5 4 5 5 4 5 5 4 5 5 4 5 5 4 5 5 4 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 5 5 6 6 5 5 6 6 5 5 6 6 5 5 6 6 5 5 6 6 5 5 6 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 7 8 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 8 7 7 7 8 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 8 7 7 7 7 7 7 7 7 7 7 7 7 7	Position QTOF-PC\QTOF Sample 20110418-MSonly-p.m Comment	Position QTOF-PC\QTOF Inj Vol Sample IRM Calibration Status 20110418-MSonly-p.m Comment x10 5 +ESI Scan (rt: 0.265-0.277 min, 2 scans) Frag=100.0V A1 9 8.5 7 6.5 6 5.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 	Position p2E7 QTOF-PC\QTOF Inj Vol 0.1 Sample IRM Calibration Status Succe 20110418-MSonly-p.m Comment x10 5 +ESI Scan (t: 0.265-0.277 min, 2 scans) Frag=100.0V A11-p.d 9 8.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 37 37 37 37 37 37 37 37 37 37	Position p2E7 QTOF-PCQQTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment	Position p2E7 QTOF-PC\QTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 +ESI Scan (rt: 0.265-0.277 min, 2 scans) Frag=100.0V A11-p.d Subtract 9 8.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 2.5 5 4.5 4 3.5 3 4.5 4 3.5 5 4.5 4 3.5 5 5 4.5 4 5 5 5 5 5 5 5 5 5 5 5 5 5	Position p2E7 QTOF-PCQTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 +ESI Scan (rt: 0.265-0.277 min, 2 scans) Frag=100.0V A11-p.d. Subtract 9 8.5 384.1463 (M+H)+ 8 7.5 7 6.5 6 5.5 5 4.5 4.5 4 3.5 3 2.5 2 1.5 4.5 4 3.5 3 2.5 2 1.5 4.5 4.5 4.5 4.5 4.5 5 4.5 4.5	Position p2E7 QTOF-PCQTOF INV Calibration Status Success 20110418-MSonly-p.m Comment x10 s +ESI Scan (rt: 0.265-0.277 min, 2 scans) Frag=100.0V A11-p.d Subtract 9 8.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 4.5 4 3.5 3 2.5 2 1.5 4.5 4 3.5 3 2.5 2 1.5 4.5 4 3.5 3.5 4.5 4.5 4.5 4.5 4.5 4.5 4.5 4	Position p2E7 QTOF-PCQUTOF Int Vol Ulbration Status Success 20110418-MSonly-p.m Comment x10 <s< td=""> +ESI Scan (rt: 0.265-0.277 min. 2 scans) Frag=100.0V A11-p.d. Subtract 9 </s<>	Position p2E7 1 QTOF-PCQTOF IRM Calibration Status Success I 20110418-MSonly-p.m Comment ////////////////////////////////////	Position p2F7 instrum QTOF-PCQTOF inj Vol 0.1 instrum Sample IRM Calibration Status Success Data H 20110418-MSon/y-p.m Comment Acquire +ESI Scan (rt: 0.265-0.277 min, 2 scans) Frag=100.0V A11-p.d Subtract +ESI Scan (rt: 0.265-0.277 min, 2 scans) Frag=100.0V A11-p.d Subtract 	Pesition p2E7 Instrument Na QTOF-PCQTOF Inj Vol 0.1 InjPosition Sample IRM Calibration Status Success Data Filename 20110118-MSonly-p.m Comment Acquired Time x10 f fSI Scan (rt: 0.265-0.277 min, 2 scans) Frag=100.0V A11-p.d. Subtract Success 384.1463 9 8.5 384.1463 (M+H)+ Success Success 7 6.5 6 5.5 5 Success Success 3 3 344.1463 (M+H)+ Success Success Success 8.5 3 Success Success Success Success Success 7 6.5 6 5.5 Success Success Success Success 3 3 3 3 3 Success Success Success 3 3 3 3 3 Success Success Success 3 5 5 Success Su	Position p2Z7 Instrument Name QTOF-PCQTOF Inj Voi 0.1 InjPosition Sample IRM Calibration Status Success Data Filename 20110118-MSonty-p.m Comment Acquired Time x10 f fESI Scan (rt. 0.265-0.277 min.2 scans) Frag=100.0V A11-p.d. Subtract Acquired Time 9 8.5	Position p227 Instrument Name In y for Sample IRM Calibration Status Success Data Filename A 20110H18/HSontly-p.m Comment Acquired Time 3 x10 #ESI Scan (t: 0.265-0.277 min, 2 scans) Frag=100.0V A11-p.d. Subtract Subtract Subtract 9 8.5

mdd 10 006'ST----20 30 40 50 303K AV-300 60 20 973.576 77.526 973.526 うちゃく たいていたい ちょうちょう ちょうちょう 80 SP130830-3-C C13-NMR CDCL3 80 100 869'TTT SDD DII 110 698'LTT 123.5821 120 186.92T 130.884 131.379 131.379 130 Contraction of the local division of the loc /.06.121 509.321 7136.921 140 840.841-844.841-856.181-150 The second والمستقبل والموافقة ومحمومة فالزاج مستقبسين فليتوقف ومحملت المستقبل والمستقبل والمستقبل ومغلم لمنافر فللمرافع 262 191 262 191 010 291 875 091 965 791 265 791 160 170 180 190 200 210 A12 80



A12

Sample Name					Position			p2E8					Instr	ument Na	ame	Instru	ment 1
User Name	QTOF-PC\QTO	F			Inj Vol			0.1					InjPo	sition			
Sample Type	Sample				IRM Cali	bration S	tatus	Success					Data	Filename		А12-р	.d
ACQ Method	20110418-MSc	only-p.m			Commen	nt							Acqui	ired Time		3/12/2	2018 3:24:41
	×10.6	+ESI Scan	(rt: 0.478-0	.514 min,	4 scans)	Frag=10	0.0V A12	2-p.d Su	btract]
	x10 °		(,	,	- J											
	1 -																
	0.95 -																
	0.0						(384.1459 (M+H)+									
	0.9																
	0.85 -																
	0.8 -																
	0.75 -																
	0.70																
	0.7 -																
	0.65																
	0.6 -																
	0.55																
	0.55 -																
	0.5 -																
	0.45																
	04-																
	0.1																
	0.35 -																
	0.3 -																
	0.25 -																
	0.0																
	0.2																
	0.15 -																
	0.1 -																
	0.05																
	0.05																
	0 –	370 37	۸ דد <u>(</u>	376	270	200	202		296	200	200	202	204	306	<u></u>	400	Ì

bpm 0 10 - 16.002 20 30 40 C13-NMR AV300 50 60 20 886:91 -⊅98:11 -80 681.TT . 303K 90 100 CDCl3 OFL'TTT -110 114.321 818 LTT --126.500 120 - 127.257 SP121205-4 · 127.359 128.466 130 · 128.925 191.291 199.151 -140 609'TET -734.847 -T18'SET -150 617 LET -655°TST 160 \$28.631 · ₽81.284 -80E . 308 -170 EST . 753 -180 190 0

mdd 0000.0 -0.5 1.0 1.5 SP121205-4 1H-NMR CDCl3 303K AV-300 2.0 9560.2 3.00 2.5 3.0 3.5 4.0 4.5 5 65 5.0 5.5 ₽6TT'L 0*L*₽T'L 6.0 7.2349 7.2389 6.5 7.2643 1.04 5.05 1.01 2.05 1.01 5.05 5.02 7.0 7.5 -= 8.0 ELZL'L 00'T LISL L --LISL L --LSS6 L --Z9L6 L --76SE 8 --L9LE 8 --7758 8 -8.5 00°T 0.6 9.5 ā 1

ampie mame					Positic	on		p2E9				In	strument	Name	Instru	ument 1
Jser Name	QTOF-PC\QTOF				Inj Vo	I		0.1				In	jPosition			
ample Type	Sample				IRM Ca	alibratio	n Status	Success				Da	ata Filenar	ne	B1-p.	d
CQ Method	20110418-MSor	nly-p.m			Comm	ent						Ac	quired Tir	ne	3/12/	2018 3:27:08
	x10 5 +	ESI Scan (rt: 0.460-0.	495 min	, 4 scan	s) Frag=	100.0V B	1-p.d Sul	otract							
	5.8 -															
	5.6															
	5.4 -							382 155	4							
	5.2							(M+H)+								
	5 -															
	4.8 -															
	4.6															
	4.4															
	4.2															
	4 -															
	3.8 -															
	3.6 -															
	3.4 -															
	3.2 -															
	3 -															
	2.8 -															
	2.6															
	2.4															
	2.2															
	2 1 8 -															
	1.6															
	1.0															
	1.2								1							
	1															
	0.8 -															
	0.6															
	0.4 -															
	0.2 -															
	0			·····						h	 			<u></u>	·····]

		udd
		10
	ES6'SI	20
		30
	000.00	40
300	009 //	20
AV-2		09
)3K	959.97	20
3 30	\$05.17 670.77	80
DCL		8
0	7.88°TIT	100
NMF	129.121	110
C13-	127.345	120
-4-C	121.221 121.228 121.228	130
0830	₽/E ' 1E1 /GV ' DE1	140
SP13	146 981 082.981 764.181	150
	200°01 192°591 281°291	160
	\$20.024	0 177
		190
		200
		210



Sample Name						Posi	tion			p2F1						Ir	strum	ent Nar	ne	Instr	ument 1
User Name	QTOF-PC\QTOF					Inj ۱	/ol			0.1						Ir	jPositi	on			
Sample Type	Sample					IRM	Calibra	tion St	atus	Succes	s					D	ata File	name		В2-р	.d
ACQ Method	20110418-MSonl	ly-p.m				Com	ment									A	quired	Time		3/12	/2018 3:29:48
	x10 ⁵ +E	ESI Sca	an (rt: 0	.367-0.	403 mi	n, 4 sc	ans) Fra	ag=100).0V B2	-p.d Sı	ubtrac	ct									
	6.2																				
	6 -																				
	5.8 -								2	00 171	-										
	5.6								3	96.171 (M+H)+	і										
	5.4 -																				
	5.2																				
	5 -																				
	4.8 -																				
	4.6																				
	4.4 -																				
	4.2																				
	4 -																				
	3.8 -																				
	3.6 -																				
	3.4 -																				
	3.2 -																				
	3 -																				
	2.8 -																				
	2.6																				
	2.4 -																				
	2.2 -																				
	2 -																				
	1.8																				
	1.0																				
	1.4																				
	1.2																				
	0.0																				
	0.0																				
	0.4											I									
	0.2																				
	0	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	_

bpm 0 B3 10 566'SI -20 - 21.334 30 40 303K C13-NMR AV300 50 60 20 76.700 77.547 80 51 90 889.111. 100 EE0.PII. CDC13 E95.711 124.064 110 126.614 128.929 128.520 128.520 128.520 SP121128-3 120 130 730°265 131.348 568'TET 140 - 132.463 - 134 012 - 134 808 - 135 821 - 915 821 - 915 21 150 160 - 120.929 - 120.929 - 165.269 - 165.289 - 167.189 170 180 190

mdd 6000.0 -0.5 1.0 1.5 SP121128-3 1HNMR CDCl3 303K AV-300 2.0 - 2.3277 2.94 2.92 2.5 3.0 3.5 4.0 22 4.5 5 5.0 5 5.5 6.0 - 7.2020 6.5 7.2535
\$2532 L

\$2000 L -7.0 2.99 86°₽ 80°£ 7.5 8.0 20.5 PL99 L -EST9 L -TE00 8 -P800 8 -9820 8 -S820 8 -P2L4 8 -9685 8 -8.5 00°T 9.0 2 3 20 4 41 .

Sample Name					Pos	ition		p2F2						Instr	ument N	lame	Inst	rument 1
User Name	QTOF-PC\QTOF				Inj	Vol		0.1						InjPo	osition			
Sample Type	Sample				IRM	1 Calibra	tion Status	Success						Data	Filenam	e	B3-p	o.d
ACQ Method	20110418-MSonly	y-p.m			Cor	nment								Acqu	ired Tim	e	3/12	2/2018 3:32:10 PM
	x10 5 +E	SI Scan	(rt: 0.49	9-0.558	min, 6 s	cans) Fra	ag=100.0V E	3-p.d Su	btract	t								
	7.75 -																	
	7.5 -																	
	7.25 -																	
	7 -							396.1	714									
	6.75 -							(IVI+F)+									
	6.5 -																	
	6.25 -																	
	6 -																	
	5.75 -																	
	5.5 -																	
	5.25 -																	
	5 -																	
	4.75 -																	
	4.5 -																	
	4.25																	
	4 -																	
	3.75 -																	
	3.5 -																	
	3.25 -																	
	3 -																	
	2.75																	
	2.5																	
	2.25																	
	2 -																	
	1.75 -								1									
	1.5 -																	
	1.25 -																	
	1 -																	
	0.75																	
	0.5																	
	0.25									1								
	0 -		<u>. </u>			· · · · · · · · · · · · · · · · · · ·		, l	.1				·····					
		382	384	386	388	390	392 39 Counts	94 396 vs. Mass-	to-Ch	398 Narge	400 (m/z)	402	404	406	408	410	412	

mdd 0 10 STO'9T 20 - 21.483 30 40 303K C13-NMR AV300 50 60 20 29.653 910:11 TOS:11 80 in st E 06 100 **CDCl3** 120 110 089.111 173.941 125.711 SP121202-2 127.054 130 128.936 ₽75.151 ₽86.251 140 137.135 150 585'IST . 160 LL6.651 165.316 261.792 170 180 190 B4 AND AND A



Sample Type Sample Type CQ Method Sources Lipitation Data Fileane X quired Time H p.d. CQ Method Sources Acquired Time 9/12/2018 3:31:31 X100 \$\$ 7.5 7.5 7.5 7.5 7.5 7.5 7.5 7.5 7.5 7.5	Sample Name					Positi	on		p2F3						I	nstrum	ent Nam	e	Instr	ument 1
ample Type Simple TMC Calibration Status Success Data Filename 64-p.d. CQ Method 20110418-45000+p.m. Comment Acquired Time 3/12/2018/3:43:11 V 1 Simple FEISI Scen (rt. 0.603-0.639 min. 4 scene) Frage=100.0V 84-p.d. Subtract	User Name	QTOF-PC\QTC	F			Inj Vo	bl		0.1						I	njPositi	on			
CQ Method 2011/01/18/#Somty-pum Comment Acquired Time 3/12/2018 33:43:11 r 1 FESI Scan (tf: 0:603-0:639 min, 4 scans) Frag=100.0V B4-p.d Subtract -	Sample Type	Sample				IRM C	Calibratio	on Status	Succe	SS					0	Data File	ename		В4-р	.d
*ESI Scan (rt. 0.603-0.639 min, 4 scans) Frag=100.0V B4-p.d Subtract 7.5 7.6 7.7 8.70 6.75 6.75 6.75 6.75 6.75 7 306.1713 (M+H)+ 6.25 6.75 7 3.5 3.25 3.25 3.25 3.25 3.25 3.25 3.26 3.275 2.26 2.27 3.26 3.27 3.25 3.26 3.275 3.26 3.275 3.26 3.275 3.26 3.275 3.26 3.275 3.26 3.275 3.26 3.275 3.26 3.275 3.26 3.275 3.26 3.27	ACQ Method	20110418-MS	only-p.m			Comn	nent								A	cquired	l Time		3/12	/2018 3:34:31 PI
7,25 7,26 7,26 7,26 7,26 6,25 6,25 6,25 5,22 5,55 5,22 5,55 5,22 5,55 5,22 5,55 5,22 5,55 5,22 5,55 5,22 5,55 5,22 5,55 5,22 5,55 5,22 5,55 5,25		x10 ⁵	+ESI Scan	(rt: 0.603-0	.639 mi	n, 4 scai	ns) Frag	=100.0V B	4-p.d S	ubtra	ct									
725 7 6.75 6.25 6 6.5 7.75 5.55 7 7 7 7 7 7 7 7 7 7 7 7 7 7		7.5 -																		
7 396.1713 6.5 (M+H)+ 6.5 6 5.5 5 7.5 5 2.5 5 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 1.5 1 <t< td=""><td></td><td>7.25</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>		7.25																		
6.75		7 -																		
65 625 6 575 55 526 5 525 5 525 5 525 5 525 5 5 5 5 5 5 5 5 5 5 5 5 5		6.75							396.1	713										
6 25 6 5.75 5.25 5 4.75 4.5 4.25 4 3.75 3.5 3.25 3 2.25 2 2 1.75 1.5 1.25 2.5 2.5 3.5 3.25 3 3.5 3.25 3 3.5 3.25 3.5 3.5 3.25 3.5 3.5 3.5 3.5 3.5 3.5 3.5 3.		6.5 -							(111)	U+										
6 5.75 5.25 5.25 5.5 5.25 5.5 5.25 5.5 5.25 5.5 5.		6.25																		
5.75 5.6 5.26 5.75 4.75 4.75 4.75 4.75 4.75 4.75 3.75 3.75 3.75 3.225 3.225 2.25 2.25 2.25 2.25 1.75 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.		6 -																		
5.5 5.25 5 4.75 4.5 4.5 4.5 4.5 4.5 4.5 3.5 3.5 3.5 3.5 3.5 3.25 3.25 2.5 2.5 2.5 2.5 2.5 2.5 2.5 2.5 2.5		5.75 -																		
525 5 475 4.5 4.25 4 3.75 3.5 3.26 2.5 2.5 2.5 2.5 2.5 2.5 2.5 2.5		5.5 -																		
5 4.75 4.5 4.25 4 3.75 3.5 3.25 3 2.75 2.5 2.25 2 1.75 1.5 1.25 1 0.75 0.5 0.25 0.		5.25																		
4.75 4.5 4.25 4 3.75 3.5 3.25 3 2.75 2.5 2.25 2 1.75 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.		5 -																		
4.5 4.25 4 3.75 3.5 3.25 3 2.75 2.5 2.25 2.5 2.5 2.5 2.5 2.5 2		4.75 -																		
4 25 4 3.75 3.5 3.25 3.5 3.25 3.75 2.5 2.25 2.25 2 1.75 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1.5 1.25 1		4.5 -																		
4 3.75 3.5 3.25 3 2.75 2.5 2.25 2 1.75 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.		4.25 -																		
3.75 3.5 3.25 3.25 2.5 2.5 2.5 2.5 2.5 2.5 2.5		4 -																		
3.5 3.25 3.25 2.5 2.5 2.25 2.75 1.5 1.5 1.25 1.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0		3.75 -																		
3.25 3 2.75 2.5 2.25 2 1.75 1.5 1.25 1 0.75 0.5 0.25 0 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charge (m/z)		3.5 -																		
3 2.75 2.5 2.25 2 1.75 1.5 1.25 1 0.75 0.5 0.25 0 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charge (m/z)		3.25 -																		
2.75 2.5 2.25 2 1.75 1.5 1.25 1 0.75 0.5 0.25 0 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charce (m/z)		3 -																		
2.5 2.25 2 1.75 1.5 1.25 1 0.75 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.		2.75																		
2.25 2 1.75 1.5 1.25 1 0.75 0.5 0.5 0.5 0.25 0 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charge (m/z)		2.5 -																		
2 1.75 1.5 1.25 1.25 1.25 0 		2.25 -																		
1.75 1.5 1.25 1.25 1.25 1.25 0.75 0.5 0.25 0.25 0.25 0.25 0.387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charce (m/z)		2 -																		
1.5 1.25 1 0.75 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.		1.75 -																		
1.25 1 0.75 0.5 0.25 0 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charge (m/z)		1.5 -																		
1 0.75 0.5 0.25 0 		1.25 -																		
0.75 0.5 0.25 0 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charge (m/z)		1 -																		
0.5 0.25 0 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charge (m/z)		0.75 -																		
0.25 0 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charge (m/z)		0.5 -																		
0		0.25 -																		
387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 Counts vs. Mass-to-Charge (m/z)		0 -		· _ · · · · · ·	· ··· · · · · · · · · ·	·										· · · · ·	· · · · · · · · · · · · · · · · · · ·	<u></u>	<u> </u>	Ļ
			387	388 389	390	391 39	92 393	394 39 Counts v	5 396 /s Mas	397 s-to-0	7 398 Charge	399 (m/z)	400	401	402 40)3 404	405	406	407	

mdd Line. 0 10 816.SI 20 30 40 15- vore 303K C13-NMR AV300 50 ₹LE'SS. 60 20 32 20 991.97 -081.77 -80 909 · LL 51 90 100 CDC13 SS9'TTT -110 091'ETT -811.911 16.5 . LTT 120 SP121212-2 - 126.324 .127.042 127.347 130 ₽16.921 · 950.051 -ST2.151 -140 131'38¢ 568'SET 137.418 150 005'TST -160 759.892 -- 165.262 895 S91 -170 141.74T 180 190 B5



Sample Name		Position	p2F4	Instrument Name	Instrument I
User Name	QTOF-PC\QTOF	Inj Vol	0.1	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	B5-p.d
ACQ Method	20110418-MSonly-p.m	Comment		Acquired Time	3/12/2018 3:36:31 PI
	x10 5 +ESI Scan (rt: 0.8	350-0.957 min, 10 scans) Frag=100.0V E	35-p.d Subtract		
	3.3 -				
	3.2				
	3.1		412 1662		
	3 -		(M+H)+		
	2.9 -				
	2.8 -				
	2.7				
	2.6				
	2.5 -				
	2.4 -				
	2.3				
	2.2				
	2.1				
	2 19-				
	18				
	1.7				
	1.6 -				
	1.5				
	1.4 -				
	1.3 -				
	1.2 -				
	1.1 -				
	1 -				
	0.9 -				
	0.8 -				
	0.7				
	0.6				
	0.5				
	0.2				
	0.2				
	0.1				

bpm 10 E Z00.91 -----20 30 40 SP140506-1-C C13-NMR CDCL3 303K AV-300 50 60 20 -76.612 -77.037 -77.460 80 6 100 717.672 110 LOT . PII 914.TI 120 000.727.040 -127.349 130 173.271 -133.271 -133.930 140 606 · SET --136.755 150 151.602 160 976.921-119.991 -165.250 -167.240 170 180 190 200 0 20 210



Sample Name						Positi	on			p2F5							Instr	ument	Name		Instrun	nent 1
User Name	QTOF-PC\QTO	=				Inj Vo	bl			0.1							InjPo	osition				
Sample Type	Sample					IRM C	Calibrat	tion Stat	tus	Succes	S						Data	Filenar	ne		B6-p.d	
ACQ Method	20110418-MSo	nly-p.m				Comn	nent										Acqu	ired Tin	ne		3/12/2	018 3:39:16 PM
	x10 5	ESI Sca	n (rt: 0.	541-0.	576 min	n, 4 scar	ns) Fra	g=100.0)V B6-	p.d Sı	ubtra	ct										
	2.7 -																					
	2.6																					
	2.5								4	416.11	65											
	2.4 -									(M+H))+											
	2.3 -																					
	2.2																					
	2.1 -																					
	2 -																					
	1.9 -																					
	1.8 -																					
	1.7 -																					
	1.6 -																					
	1.5 -																					
	1.4 -																					
	1.3																					
	1.2																					
	1.1 -																					
	1-																					
	0.9																					
	0.8 -																					
	0.7																					
	0.6																					
	0.5																					
	0.4 -																					
	0.3																					
	0.2												1									
	0.1 -																					
	0	<u>Ib</u>	·····	··· ·		·			. .	<u> </u>		<u> </u>	<u> </u>	. <u></u> I		····· · · · ·	····	h.	<u> </u>		<u> </u>	
		400	402	404	406	408	410	412 Cou	414 Ints vs	416 Mass.	4 s-to-C	18 Char	420 ge (m/z	422 z)	424	426	428	430	432	434		

bpm 0 10 - 12.982 20 30 40 303K C13-NMR AV300 50 60 20 858.97 -77.282 77.707 80 60 100 CDC13 082.111-\$LE . \$TI -110 198 LTT -- 125.380 126.849 SP121205-3 120 127.331 127.540 - 128.922 130 129.784 ₱22°721 -095'TET -140 · 131 .525 213.912 -- J32 .762 150 ES9'9ET -- 131.052 -₽I₽.IZI 160 LI8.651 668 . P91 . 601 S91 . 170 161.761 -180 190 2

0.0 ppm - 0.0002 0.5 1.0 1.5 SP121205-3 1H-NMR CDCI3 303K AV-300 2.0 3.00 2.0858 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 2.08 3.14 2.14 7.5 7.4265 7.4266 7.5096 7.5045 7.5057 7. 8.0 5.10 E0.1 8.5 9.0 00°T 1 9.5 F

Sample Name					Positio	n		p2F6					Instrum	ent Name	e	Instrum	ent 1
User Name	QTOF-PC\QTO	:			Inj Vol			0.1					InjPosit	ion			
Sample Type	Sample				IRM Ca	libration S	Status	Success					Data Fil	ename		B7-p.d	
ACQ Method	20110418-MSo	nly-p.m			Comme	ent							Acquire	d Time		3/12/20	18 3:41:26 PM
	x10 ⁵	·ESI Scan (ı	t: 0.436-0	0.496 mir	n, 6 scans	s) Frag=10	0.0V B7-	-p.d Sub	otract								
	4.2 -																
	4 -																
	38-						4	416.116 (M+H)+	5								
	0.0																
	3.6																
	3.4 -																
	3.2																
	3 -																
	2.8 -																
	2.6																
	24																
	2.4																
	2.2 -																
	2 -																
	1.8 -																
	1.6 -																
	1.4 -																
	1.2								I								
	1 -																
	0.8 -																
	0.0																
	0.6																
	0.4									1							
	0.2																
	0				<u> </u>				<u> </u>	<u></u>						·····	
		404	406	408	410	412	414 Counts vs	416 Mass-I	418 o-Charge	420 e (m/z)	422	424	426	428	430	·	

mdd 0 10 TE0.01 -20 30 40 303K C13-NMR AV300 50 S 60 3:0 20 689.97 -22 290.77 -284.77 -80 90 100 SP121202-3 CDCl3 110 918.111 -545.411 -994.LTT -120 - 123.802 +22.721 -- 128.382 130 128.965 685'TET 135.722 140 196.441 PIP.0PI L\$5.6\$1 . 150 975.151 -160 828.6S1 -598'E9T -LOT' 59T 170 EIE . 751 180 88 190



Sample Name					Posit	ion		p2F7				I	Instrumen	t Name	Ins	trument 1	
User Name	QTOF-PC\QTC	F			Inj Ve	ol		0.1				I	InjPositio	ı			
Sample Type	ple Type Sample			IRM (on Status	Success			Data Filenar			ame	B8-	B8-p.d	
ACQ Method	20110418-MSonly-p.m			Comr	Comment						4	Acquired Time			3/12/2018 3:43:49 PM		
	x10 ⁵	+ESI Sca	ın (rt: 0.25	0-0.261 n	nin, 2 sca	ns) Frag-	=100.0V B8	3-p.d S	ubtract								
	5.8 -																
	5.6 -																
	5.4 -							427.14	103								
	5.2 -							(M+H)+								
	5 -																
	4.8 -																
	4.6																
	4.4 -																
	4.2 -																
	4 -																
	3.8 -																
	3.6 -																
	3.4 -																
	3.2 -																
	3-																
	2.0																
	2.0																
	2. 1 2.2 -																
	2 -																
	1.6 -																
	1.4 -																
	1.2 -																
	1 -																
	0.8 -																
	0.6																
	0.4																
	0.2 -																
	0 -			400						<u></u>		46.4		462			
		421	422	423	424	425	426 Counts v	427 s. Mass	428 s-to-Charg	429 ge (m/z)	430	431	432	433	434		

mdd 096 . SI ----303K AV-300 019.97 120.77 120.77 SP130828-C C13-NMR CDCL3 111'.42 114'32.4 114'32.4 151'342 152'342 152'326 152'326 153'48 153'4 Short 日日にたたいのないである


Sample Name						Position			p2F8					Instrun	nent Nan	ne	Instrur	nent 1
User Name	QTOF-PC\QT0	DF			:	Inj Vol			0.1					InjPosi	tion			
Sample Type	Sample				:	IRM Calil	bration St	tatus	Success	;				Data Fi	lename		B9-p.d	
ACQ Method	20110418-MS	only-p.m				Commen	t							Acquire	ed Time		3/12/2	018 3:45:31 PM
	x10 ⁵	+ESI Sca	an (rt: 0	.421-0.4	80 min, 6	6 scans)	Frag=100	0.0V B9-	p.d Su	btract								
	-																	
	4.2																	
	4 -								427.14	407								
	3.8 -								(IVI+H)+								
	3.6																	
	3.4 -																	
	3.2 -																	
	3 -																	
	2.8 -																	
	2.6 -																	
	2.4 -																	
	2.2																	
	2 -																	
	1.8 -																	
	1.6 -																	
	1.4 -																	
	1.2 -																	
	1 -																	
	0.8 -																	
	0.6																	
	0.4																	
	0.2 -																	
	0 -							· · · · · · · · · · · · · · · · · · ·			<u> </u>			· · · · · · · · ·			<u>_</u>	
	-	420	421	422	423	424	425 C	426 ounts vs	427 Mass-	428 to-Charg	429 e (m/z)	430	431	432	433	434	435	

			invited before the	bpm
				10
	£00.91			20
			Land dealers	30
				40
300				20
-VA				60
03K	565.94		The state of the s	20
3	244.77			80
DCL				90
R C	849.111 200.01			100
MN-	576.SII 688.TII			110
C13	128.931	· · · · · · · · · · · · · · · · · · ·		0 12(
-3-C	175.621 659.621 123.456			0 13
1108	ZET.IEI 056.2EI 98/.921			0 14
2013	649'IGI			0 15
SF	166.937 266.537			10 16
				80 1
				90 1
				000
				10 2
BIO				
		110		



Sample Name				P	osition		p2F9				Ir	nstrument Na	me I	nstrument 1
User Name	QTOF-PC\QTO	F		Ir	nj Vol		0.1				Ir	jPosition		
Sample Type	Sample			IF	RM Calib	ration Status	Success				D	ata Filename	E	310-p.d
ACQ Method	20110418-MSc	only-p.m		C	omment						A	cquired Time	3	/12/2018 3:53:13 PM
	x10 ⁵	+ESI Scan (rt: 0	538 min)	Frag=10	0.0V B1	0-p.d								
	5.8 -													
	5.6													
	5.4 -						400.1463							
	5.2						(M+H)+							
	5 -													
	4.8													
	4.6													
	4.4 -													
	4.2													
	4 -													
	3.8													
	3.6													
	3.4													
	3.2													
	3 -													
	2.8													
	2.6													
	2.4													
	2.2 -													
	2 -													
	1.8 -													
	1.6 -													
	1.4 -													
	1.2 -													
	1 -													
	0.8													
	0.6													
	0.4 -													
	0.2								1					
	0 -	<u></u>	1	i	<u> 1</u> .	······	 	_,I,		······	-*	·····	· · · · · · · · · · · · · · · · · · ·	
		392 393	394 3	95 39	6 397	398 399 Counts	400 4 vs. Mass-t	401 402 o-Charge	2 403 e (m/z)	404 40	5 406	407 408	409 410	

mdd 0 10 ₽T0'9T -20 30 40 303K C13-NMR AV300 20 60 20 - 76.789 - 76.789 -----80 689.LL 90 100 CDC13 110 208.111 -284.432 -T18.711 -120 SP121210-1 - 121.296 - 151.308 -- 128.937 -130 PPP.IEI . 881 TEL -971.921 · 140 - 136.712 T42.247 150 961'091 -845 TST -160 288.6SI -941.191 -011.201 -170 - 167.202 180 119 190





bpm 0 10 166'SI -20 30 40 303K C13-NMR AV300 50 F 60 E. 20 - 16.681 - 77.106 - 77.530 -80 90 100 SP121210-2 CDCl3 110 ₽91"TTT -L62.PII -951 . TIT 120 - 153 · 275 - 127.336 826.921 -130 078'0ET 131.451 -091 SET -140 408'SET -L08'981 -140.841 ---150 067 TST -- T25' 103 160 478.6SI -- J.ed: 055 ELT . 391 -170 - J67.258 180 190 812



SP121210-2 1H-NMR CDCI3 303K AV-300

Sample Name					Pos	ition		p1A2						Inst	rument Nar	ne	Instru	ment 1
User Name	QTOF-PC\QTO	F			Inj	Vol		0.1						InjF	osition			
Sample Type	Sample				IRM	I Calibrat	tion Status	Succe	SS					Data	a Filename		B12-p.	d
ACQ Method	20110418-MSc	only-p.m			Con	nment								Acq	uired Time		3/12/2	2018 3:55:07 PM
	x10 ⁵	+ESI Scan (r	t: 0.611-0	0.670 r	min, 6 sc	ans) Fra	ag=100.0V B	12-p.d	Subtra	ct								
	5.8 -																	
	5.6 -																	
	5.4							383.1	507									
	5.2 -							(M+H	ł)+									
	5 -																	
	4.8 -																	
	4.6																	
	4.4 -																	
	4.2																	
	4 -																	
	3.8 -																	
	3.6 -																	
	3.4 -																	
	3.2 -																	
	3 -																	
	2.8																	
	2.0																	
	2.4																	
	2.2																	
	1.8 -																	
	1.6																	
	1.4																	
	1.2 -								1									
	1 -																	
	0.8																	
	0.6																	
	0.4 -																	
	0.2									1								
	0	<u> </u>								, [.			·····		i			ļ
		374 375	376	377	378 3	79 380) 381 38 Counts	32 383 vs. Mas	s-to-Cl	 385 arge (386 m/z)	387	388	389 39	90 391 3	392 39	93	





Sample Name					Position		p1A	3			Instr	ument Name	e Ir	nstrument 1
User Name	QTOF-PC\QTO	DF			Inj Vol		0.1				InjPo	osition		
Sample Type	Sample				IRM Calib	oration Status	Suc	cess			Data	Filename	C	1-p.d
ACQ Method	20110418-MS	only-p.m			Comment	:					Acqu	ired Time	3,	/12/2018 3:57:44 PM
	x10 ⁵	+ESI Scan (r	t: 0.838 ı	min) Frag	=100.0V C1	1-p.d Subtract								
	1.55 -													
	1.5 -													
	1.45 -						70 15	56						
	1.4 -					c c	(M+H)	+						
	1.35 -						Ì							
	1.3 -													
	1.25 -													
	1.2 -													
	1.15 -													
	1.1 -													
	1.05 -													
	1 -													
	0.95 -													
	0.9 -													
	0.85 -													
	0.8 -													
	0.75 -													
	0.7 -													
	0.65 -													
	0.6 -													
	0.55 -													
	0.5 -													
	0.45 -													
	0.4 -													
	0.35 -													
	0.3 -													
	0.25 -													
	0.2 -													
	0.15 -													
	0.1 -													
	0.05 -													
	0 =	365	366	367	368	369	370	371	372	373	374	375	376	
				007	000	Counts	vs. Ma	ass-to-Cha	rge (m/z)	570	U / T	0,0	0,0	



303K AV-300 SP130325-3-C C13-NMR CDCL3



User Name QrOF-PACUPT Ind Vol 0.1 Implementation Sample Type Sample Type RRM Calibration Status Scosss Dab Filename Q:2 od ALQ Method 20110418-55 Machane C2 od 312/2018.355 ALS Method Sample Type Comment Subjects Acquired Time 312/2018.355 ALS Method Sample Type Sample Type Sample Type Sample Type Sample Type Sample Type ALS Method Sample Type Sample Type Sample Type Sample Type Sample Type Sample Type ALS Method Sample Type Sample Type Sample Type Sample Type Sample Type Sample Type ALS Method Sample Type Sample Type Sample Type Sample Type Sample Type Sample Type ALS Method Sample Type Sample Type Sample Type Sample Type Sample Type Sample Type ALS Method Sample Type Sample Type Sample Type Sample Type Sample Type Sample Type ALS Method Sample Type Sample Type Sample Type Sample Type Sample Type Sample Type ALS Method Sample Type Sample Type Sample Type Sample Type	Sample Name						Posit	tion			p1A4						Instru	ment N	ame	In	strument 1
Sample Type Sample TeM Calibation Status Success Data Filename Co.p.d ACQ Method 20110415 Comment Comment Acquired Time 3/12/2018 353 ALS ************************************	User Name	QTOF-PC\QTC	DF				Inj V	/ol			0.1						InjPos	ition			
ACQ Method 20110418-HSSUm/p.m. Comment Acquired Time 3/12/2018 3/85 No 4	Sample Type	Sample					IRM	Calibra	tion Sta	tus	Succes	S					Data F	ilename	e	C	2-p.d
x10 s 483 463 464 464 464 464 464 464 464 474 48 48 49 41 42 43 44 44 45 46 47 48 49 49 41 41 42 43 44 45 46 47 48 49 41 42 42 42 42 42 42 41 42 42 43 44 44 45 46 47 48 49 41	ACQ Method	20110418-MS	only-p.m				Com	ment									Acquir	ed Time	e	3/	12/2018 3:59:34
4.8 4.6 4.4 4.2 4 3.8 3.9 3.9 3.9 3.9 3.9		x10 ⁵	+ESI Sc	an (rt: (0.496-0	.508 mi	n, 2 sca	ans) Fra	ag=100.0	0V C2-j	o.d Su	ubtract									
4.6 334.1712 4.2 (M+H)+ 4.2 (M+H)+ 3.8 3.6 3.4 3.2 3 3.4 3.2 3 2.8 4 2.8 4 2.8 4 2.4 4 3.2 4 3.3 4 3.4 4 3.2 4 3.4 4 3.2 4 3.4 4 3.2 4 3.4 4 3.2 4 3.4 4 3.2 4 3.4 4 3.2 4 3.4 4 3.5 4 3.6 4 1.6 4 1.8 4 1.8 4 1.9 4 1.9 4 1.9 4 1.9 4 1.9 4 1.9		4.8 -																			
44 384.1712 (M+H)+ 42 (M+H)+ 38 36 34 32 35 3 26 24 22 2 18 16 1.4 12 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.4 1.2 1.5 1.4 1.6 1.4 1.7 1.4 1.8 1.4 1.4 1.2 1.5 1.4 1.5 1.4 1.5 1.4 1.6 1.4		4.6																			
42 4 38 36 34 32 3 28 26 24 22 2 18 16 14 12 1 08 06 04 02 0 0 0 0 0 0 0 0 0 0 0 0 0		4.4 -									384.1 (M+H	712)+									
		4.2 -																			
		4 -																			
		3.8 -																			
		3.6																			
32 3 28 26 24 22 2 18 16 14 12 1 08 06 04 02 0		3.4 -																			
		3.2 -																			
		3 -																			
		2.8 -																			
		2.6 -																			
		2.4 -																			
		2.2																			
		2 -																			
		1.8 -																			
		1.6 -																			
		1.4 -																			
		1.2 -																			
		1-																			
		0.8 -																			
		0.6																			
		0.4																			
		0.2 -																			
376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393		0 -	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	



SP131216-3 CDCL3 1HNMR AV300



Sample Name				I	Position		p	1A5				1	instrume	nt Name	In	strument 1
User Name	QTOF-PC\QTO	F		1	Inj Vol		0.	.1				1	njPositio	n		
Sample Type	Sample			1	IRM Calib	oration Stat	tus Si	uccess				I	Data Filer	name	CE	-p.d
ACQ Method	20110418-MSc	nly-p.m		(Comment	t						1	Acquired	Time	3/	12/2018 4:01:18 PM
	x10 ⁵	+ESI Scan (rt:	0.528-0.5	552 min, 3	3 scans)	Frag=100.()V C3-p.	d Subtr	act							
	4.8 -															
	4.6															
	4.4 -						4	l22.1504 (M+H)+	1							
	4.2 -															
	4 -															
	3.8 -															
	3.6															
	3.4 -															
	3.2															
	3 -															
	2.8															
	2.6															
	2.4 -															
	2.2															
	2 -															
	1.8 -															
	1.6 -															
	1.4 -															
	1.2 -															
	1 -															
	0.8 -															
	0.6 -															
	0.4 -															
	0.2															
	0-				<u> </u>				₁						···· ·· ·· ···	
	0	410	412	414	416	418 Соц	420 Ints vs. M	422 Mass-to-	424 Charge	426 (m/z)	428	430	432	434	436	



C4

SP131216-4 CDCL3 1HNMR AV300



c4







SP131216-5 CDCL3 1HNMR AV300







SP140310-1 CDCL3 1HNMR AV300

User Name ODF-PCQUTOF Inj Vol 0.1 Englestion Sample Type Sample Type Comment Saccass Data Filename C5 p.d. KQ Method 20110181 MSGoty.p.m. Comment Acquired Time 3/12/2018 4:11:01 I x10 s 4 3.6 -	Sample Name					Position			p1A8					Instrum	ent Name	e 1	Instrument 1
Sample Single Dide Deta Object Convext Acquired Time 3/1/2/0014 1:13:11 XQ Method 20110H1450mjc,m Convext Acquired Time 3/1/2/0014 1:13:11	User Name	QTOF-PC\QTO	:			Inj Vol			0.1					InjPositi	on		
XQQ Method 20110418+South-p.m. Comment Acquired Time 3/1/2/2018-411.03 IF x10 4 5 5 Can (rt. 0.983-1.054 min, 7 scans) Frag=100.0V C6-p.d. Subtract - - 4 3.8 466.1313 - - - - 3.4 3.2 - - - - - 3.2 3 2.8 - - - - 2.4 2.2 2.2 - - - - - 3.8 2.6 - - - - - - 3.2 2.6 - - - - - - 3.4 - - - - - - - 3.2 - - - - - - - 3.2 - - - - - - - 3.4 - - - - - - - 3.4 - - - - - - - 3.4 - - - - - - - - 3.5 - - - -	Sample Type	Sample				IRM Cali	bration Sta	atus	Success					Data File	ename	(C6-p.d
x10 FESI Scen (rt. 0.983-1.054 min, 7 scens) Freg=100.0V C8-pd Subtract 4 3.8 3.6 (M+T)+ 3.7 (M+T)+ 3.8 (M+T)+ 3.9 (M+T)+ 3.1 (M+T)+ 3.2 (M+T)+ 3.3 (M+T)+ 3.4 (M+T)+ 3.5 (M+T)+ 3.6 (M+T)+ 3.7 (M+T)+ 3.8 (M+T)+ 3.9 (M+T)+ 3.1 (M+T)+ 3.2 (M+T)+ 3.3 (M+T)+ 3.4 (M+T)+ 3.5 (M+T)+ 3.6 (M+T)+ 3.7 (M+T)+ 3.8 (M+T)+ 3.9 (M+T)+ 3.9 (M+T)+ <th>ACQ Method</th> <th>20110418-MSo</th> <th>nly-p.m</th> <th></th> <th></th> <th>Commen</th> <th>nt</th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th>Acquired</th> <th>l Time</th> <th>:</th> <th>3/12/2018 4:11:03 F</th>	ACQ Method	20110418-MSo	nly-p.m			Commen	nt							Acquired	l Time	:	3/12/2018 4:11:03 F
4 38 466.1313 36 (M+I)+ 32 3 34 32 35 34 36 10 37 10 38 10 39 10 30 10 31 10 32 10 33 10 34 10 35 10 36 10 37 10 38 10 39 10 39 10 30 10 31 10 32 10 33 10 34 10 36 10 37 10 38 10 39 10 39 10 30 10 31 10 32 10 33 10 34 10 35 10 36		10.5	ESI Scan (rt:	0.983-1.	054 min.	7 scans)	Frag=100	0V C6-	p.d Subt	ract							
466.1313 (M++1)+ 476.476.478.480 476.476.478.480 476.476.478.480 476.476.478.480 476.476.478.480 476.478.476.478.476.478.480 476.478.476.478.476.478.480 476.478.476.478.476.478.480 476.478.476.476.478.476.478.476.476.478.476.476.		x10 3	(,	,	g										
3.8 466.1313 3.6 (M+H)+ 3.2 (M+H)+ 3.3 (M+H)+ 3.4 (M+H)+ 3.5 (M+H)+ 3.6 (M+H)+ 3.7 (M+H)+ 3.8 (M+H)+ 3.9 (M+H)+		4 -															
33 466.1313 36 (M+H)+ 34 32 3 36 28 3 26 3 28 4 29 4 10 4 10 4 10 4 11 4 12 4 14 4 12 4 14 4 12 4 14 4 15 4 16 4 16 4 17 4 18 4 19 4 10 4 13 4 14 4 15 4 16 4 17 4 18 4 19 4 10 4 10 4 10 4 10 4 10 4 10 4 10 4 10 4 10 4 10 4 10 4 10 4		3.8 -															
36 34 32 3 38 28 26 24 22 2 18 16 14 12 1 08 06 04 02 0 		5.6							466.1313 (M+H)+								
34 32 38 26 24 22 2 18 16 14 12 1 08 06 04 02 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Massto-Charge (mz)		3.6 -															
$\begin{array}{c} 32\\ 3\\ 3\\ 28\\ 26\\ 24\\ 22\\ 2\\ 18\\ 16\\ 14\\ 12\\ 1\\ 1\\ 08\\ 06\\ 04\\ 02\\ 0\\$		3.4 -															
3 3 28 26 24 22 2 18 16 14 12 1 0.8 0.6 0.4 0.4 0.4 0.4 0.4 0.4 0.4 0.4		3.2 -															
$ \begin{array}{c} 3\\ 28\\ 26\\ 24\\ 22\\ 2\\ 18\\ 16\\ 14\\ 12\\ 1\\ 08\\ 06\\ 04\\ 02\\ 0\\ 454\\ 456\\ 458\\ 400\\ 452\\ 454\\ 456\\ 458\\ 400\\ 452\\ 454\\ 466\\ 468\\ 470\\ 472\\ 474\\ 476\\ 478\\ 480\\ 488\\ 400\\ 472\\ 474\\ 476\\ 478\\ 480\\ 488\\ 488\\ 488\\ 488\\ 488\\ 488\\ 48$		0.2															
$ \begin{array}{c} 28\\ 26\\ 24\\ 22\\ 2\\ 18\\ 16\\ 14\\ 12\\ 1\\ 18\\ 16\\ 14\\ 12\\ 1\\ 18\\ 16\\ 14\\ 12\\ 1\\ 12\\ 1\\ 18\\ 16\\ 14\\ 12\\ 1\\ 12\\ 1\\ 14\\ 12\\ 1\\ 12\\ 1\\ 14\\ 12\\ 1\\ 12\\ 1\\ 14\\ 12\\ 1\\ 14\\ 12\\ 1\\ 12\\ 1\\ 14\\ 12\\ 1\\ 14\\ 12\\ 1\\ 14\\ 12\\ 1\\ 14\\ 12\\ 1\\ 14\\ 12\\ 14\\ 12\\ 14\\ 14\\ 12\\ 14\\ 14\\ 12\\ 14\\ 14\\ 12\\ 14\\ 14\\ 14\\ 12\\ 14\\ 14\\ 14\\ 14\\ 14\\ 14\\ 14\\ 14\\ 14\\ 14$		3 -															
2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 		2.8															
$ \begin{array}{c} 24\\ 22\\ 2\\ 18\\ 16\\ 14\\ 12\\ 1\\ 08\\ 06\\ 04\\ 02\\ - 454 456 458 460 462 464 466 468 470 472 474 476 478 480 \end{array} $		2.6															
2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		24															
$ \begin{array}{c} 22\\ 2\\ 18\\ 16\\ 14\\ 12\\ 1\\ 0\\ 0\\ 0\\ 0\\ 0\\ 454 456 458 460 462 464 466 468 470 472 474 476 478 480 \end{array} $		2.4															
2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		2.2															
1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		2 -															
$\begin{array}{c} 1.6 \\ 1.4 \\ 1.2 \\ 1 \\ 0.8 \\ 0.6 \\ 0.4 \\ 0.2 \\ 0 \\ 454 \\ 456 \\ 458 \\ 460 \\ 462 \\ 464 \\ 466 \\ 466 \\ 468 \\ 470 \\ 472 \\ 474 \\ 476 \\ 478 \\ 480 \\ \end{array}$		18-															
1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		1.0															
1.4 1.2 1 0.8 0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		1.6 -															
1.2 1 1 1 1 1 1 1 1 1 1 1 1 1		1.4 -															
1 0.8 0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		1.2															
0.8 0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		1 -															
0.8 0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		I I															
0.6 0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		0.8 -															
0.4 0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		0.6															
0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		0.4 -															
0.2 0 454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		0.4															
0		0.2															
454 456 458 460 462 464 466 468 470 472 474 476 478 480 Counts vs. Mass-to-Charge (m/z)		0	· · · · · · · · ·								<u> </u>				······································		<u> </u>
			454	456	458	460	462 Co	464 unts vs.	466 . Mass-to	468 -Charge	470 (m/z)	472	474	476	478	480	











-3500

-3000

-0







Sample Name				Posit	ion	p1	LA9				Instrumen	t Name	Instru	ment 1
User Name	QTOF-PC\QTC	DF		Inj V	ol	0.	1				InjPosition	l		
Sample Type	Sample			IRM	Calibration Sta	tus Su	uccess				Data Filena	ame	D1-p.0	ł
ACQ Method	20110418-MS	only-p.m		Com	ment						Acquired T	ime	3/12/2	2018 4:13:43 PN
	x10 ⁵	+ESI Scan (rt	: 0.648-0.695	ō min, 5 sca	ins) Frag=100.	0V D1-p.	d Subtract							
	4.8 -													
	4.6						070 1014							
	4.4 -						372.1344 (M+H)+							
	4.2 -													
	4 -													
	3.8 -													
	3.6 -													
	3.4 -													
	3.2 -													
	3 -													
	2.8 -													
	2.6 -													
	2.4 -													
	2.2 -													
	2 -													
	1.8 -													
	1.6 -													
	1.4 -													
	1.2 -													
	1 -							1						
	0.8 -													
	0.6 -													
	0.4													
	0.2 -													
	0 -												·····	J
	Ū	362	364	366	368 Coi	370 untsivs M	372 Aass-to-Ch	374 arge (m/z)	376	378	380	382	384	





SP130116-2 CDCL3 1HNMR AV300

Sample Name				Posi	tion		p1B1				Inst	rument Na	ame	Instrum	ent 1
User Name	QTOF-PC\QTOF			Inj V	/ol		0.1				InjF	osition			
Sample Type	Sample			IRM	Calibratio	n Status	Success				Data	a Filename	•	D2-p.d	
ACQ Method	20110418-MSon	ly-p.m		Com	ment						Acq	uired Time	1	3/12/20	18 4:16:05 F
	x10 ⁵ +	ESI Scan (rt: 0.	642-0.701	min, 6 sca	ans) Frag=	=100.0V D2	-p.d Subt	ract							
	4.4 -														
	4.2														
	4 -						(M+H)+								
	3.8 -														
	3.6														
	3.4														
	3.2 -														
	3 -														
	2.8 -														
	2.6														
	2.4 -														
	2.2														
	2 -														
	1.8 -														
	1.6 -														
	1.4 -														
	1.2 -														
	1 -							1							
	0.8 -														
	0.6														
	0.4 -														
	0.2														
	0 -	376	378	380	382	384	386	388	390	392	394	396	398	400	





SP130116-4 CDCL3 1HNMR AV300
Sample Name					P	osition	1		p1	.B2						Ins	trume	nt Nan	ne	Ins	trument 1
User Name	QTOF-PC\QTC	F			I	nj Vol			0.1	1						Inj	Positic	on			
Sample Type	Sample				I	RM Cal	ibratio	on Statu	is Su	iccess						Dat	ta File	name		D3	-p.d
ACQ Method	20110418-MS	only-p.m			C	omme	nt									Acc	quired	Time		3/1	2/2018 4:18:57 PM
	x10 ⁵	+ESI Scan (r	t: 0.551·	-0.563	min, 2	scans)) Frag=	=100.0\	/ D3-p.c	d Subtr	act										
	8 25 -																				
	8-																				
	7.75																				
	7.5 -								4(02.1451	1										
	7.25 -								(1	M+H)+											
	7 -																				
	6.75																				
	6.5																				
	6.25																				
	6 -																				
	5.75 -																				
	5.5																				
	5.25																				
	5 -																				
	4.75 -																				
	4.5 -																				
	4.25 -																				
	4 -																				
	3.75 -																				
	3.5 -																				
	3.25 -																				
	3 -																				
	2.75																				
	2.5																				
	2.23																				
	2 1 75 -																				
	1.5																				
	1.25 -																				
	1 -																				
	0.75																				
	0.5																				
	0.25											I									
	0 -	<u>_</u>		'	<u> </u>			. In.		<u> </u>										<u> </u>]
		393 394	395	396	397	398	399	400 Coun	401 ts vs. N	402 Aass-to-	403 Char	404 ge (m/	405 z)	406	407	408	409	410	411	412	

mdd 0 10 L06 . SI -20 -21.255 30 40 303K AV-300 50 60 70 -77.219 -77.219 CDCL3 80 589.11-60 SP130116-3-C C13-NMR 100 901.601 V -112.721 009.511~ 651.411~ 110 171.720 120 124.169 126.417 006.721. 130 128.375 -131.252 975.376 140 018.461-137.287 078.340 150 145.521 -121.090 160 -128.182 -128.182 -164.917 -166.258 170 180 190

pd



SP130116-3 CDCL3 1HNMR AV300

User Name OFO-PCQ(OPF Inj Vol 0.1 Lipbestion Sample Ype Sample Ype Comment Acquired Time 9 + p.4 KCQ Method 20110418-MScnity-p.m Comment Acquired Time 3/12/2018 + 22:07 P x10 s +ESI Scan (t 0. 722-0.746 min.3 scans) Frag=100.0V D+p.0 Subtract -	Sample Name						Ро	sition			I	p1B3							Instr	umen	t Nam	е	In	strument	1
Sample Strok Date Date Date Det Det <th< th=""><th>User Name</th><th>QTOF-PC\QTC</th><th>F</th><th></th><th></th><th></th><th>Inj</th><th>Vol</th><th></th><th></th><th>(</th><th>0.1</th><th></th><th></th><th></th><th></th><th></th><th></th><th>InjPo</th><th>ositior</th><th>ı</th><th></th><th></th><th></th><th></th></th<>	User Name	QTOF-PC\QTC	F				Inj	Vol			(0.1							InjPo	ositior	ı				
XQ Method 20110418 + MSonly p.m. Comment Acquired Tme 3/12/2008 + 421:07 P X10 FESI Scan (tt 0.722-0.746 min, 3 scans) Frag=100.0V D4-p.d. Subtract	Sample Type	Sample					IR	M Cali	bratio	n Stat	us :	Succes	S						Data	Filen	ame		D	4-p.d	
x10 5 FSI Scan (it. 0.722-0.746 min, 3 scans) Frag=100.0V D4-p.d Subtract 4 385 1409 44 (M+H)+ 43 (M+H)+ 44 (M+H)+ 45 36 36 34 36 34 36 34 36 34 36 34 36 34 36 34 36 34 36 34 36 34 36 34 36 34 37 370 30 36 36 37 370 30 31 32 33 34 35 36 37 38 38 36 37 38 38 36 37 39 </th <th>ACQ Method</th> <th>20110418-MS</th> <th>only-p.m</th> <th></th> <th></th> <th></th> <th>Co</th> <th>mmen</th> <th>t</th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th>Acqu</th> <th>ired T</th> <th>ime</th> <th></th> <th>3/</th> <th>/12/2018</th> <th>4:21:07 F</th>	ACQ Method	20110418-MS	only-p.m				Co	mmen	t										Acqu	ired T	ime		3/	/12/2018	4:21:07 F
48 385.1493 44 (M+H)+ 42 1 43 1 44 1 36 1 36 1 37 378 381 38 1 42 1 43 1 44 1 45 1 46 1 47 378 379 360 381 382 385 386 387 386 398		x10 ⁵	+ESI Scar	n (rt: 0.	722-0.	746 mi	n, 3 s	cans)	Frag=	=100.0	V D4-p	o.d Su	ubtra	ct											
46 386,1439 44 (M+H)+ 42 (M+H)+ 43 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 36 37 37 37 37 37 39 38 38 39 </td <td></td> <td>4.8 -</td> <td></td>		4.8 -																							
380.1499 ((M+H))+ 42 4 38 36 36 34 32 3 3 3 3 4 28 26 24 22 2 1.8 1.6 1.4 1.2 1 1.8 1.6 1.4 1.2 1 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.8 1.6 1.4 1.2 1.8 1.8 1.6 1.4 1.2 1.8 1.8 1.6 1.4 1.2 1.8 1.8 1.6 1.4 1.2 1.8 1.8 1.6 1.4 1.2 1.8 1.8 1.6 1.4 1.2 1.8 1.8 1.6 1.4 1.2 1.8 1.8 1.6 1.4 1.7 1.8 1.8 1.8 1.8 1.8 1.8 1.8 1.8 1.8 1.8		4.6											~~												
42 4 38 36 34 32 3 28 26 24 22 2 18 16 14 12 1 08 06 04 02 		4.4 -									3	386.14 (M+H)	.99)+												
4 38 36 34 32 3 28 26 24 22 2 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 1 18 16 14 12 10 19 19 19 19 19 19 19 19 19 19		4.2 -										Ì													
38 36 34 32 3 28 26 24 22 18 16 14 12 18 16 14 12 18 16 14 12 18 19 10 10 10 11 12 13 14 12 13 14 12 13 14 15 16 17 37<38<379<380 361 382 383 364 385 366 387 386 389 390 391 392 393 394 395 396 397		4 -																							
36 34 32 3 3 28 26 24 22 2 18 16 14 12 1 0.8 0.6 0.4 0.2 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		3.8 -																							
34 32 3 38 38 38 38 38 38 38 38 39 30 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		3.6 -																							
32 3 3 3 3 3 3 3 3 3 3 3 3 3		3.4 -																							
3 28 26 24 22 2 18 16 14 12 1 08 06 04 02 - 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		3.2 -																							
28 26 24 22 18 16 14 12 1 0 377 378 379 380 381 382 383 394 385 386 387 388 389 390 391 392 393 394 395 396 397		3 -																							
26 24 22 2 18 16 14 12 1 08 06 0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		2.8 -																							
2.4 2.2 2 1.8 1.6 1.4 1.2 1 0 		2.6 -																							
2.2 2 1.8 1.6 1.4 1.2 1 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		2.4 -																							
2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		2.2 -																							
1.8 1.6 1.4 1.2 1 0 377 378 379 380 381 382 385 386 387 388 389 390 391 392 393 394 395 396 397		2 -																							
1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		1.8 -																							
1.4 1.2 1 0.8 0.6 0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		1.6 -																							
1.2 1 0.8 0.6 0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		1.4 -																							
1 0.8 0.6 0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		1.2 -																							
0.8 0.6 0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		1 -											1												
0.6 0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		0.8 -																							
0.4 0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		0.6 -																							
0.2 0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		0.4																							
0 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		0.2 -																							
377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397		0.2							<u></u>			<u> </u>					<u> </u>	<u> </u>					l.		
		0	377	378	379	380	381	382	383	384	385	386	387	7 388	389	390	391	392	393	394	395	396	397		





SP130116-5 CDCL3 1HNMR AV300

DJ







Sample Name			Positi	on	p1B5					Instrument Name	Instru	ment 1
User Name	QTOF-PC\QTOF		Inj Vo	I	0.1					InjPosition		
Sample Type	Sample		IRM C	alibration Status	Success	5				Data Filename	D6-p.c	
ACQ Method	20110418-MSon	ly-p.m	Comm	ient						Acquired Time	3/12/2	018 4:25:23 PM
	x10 5 +	ESI Scan (rt: 0.405-0.	.441 min, 4 scar	ns) Frag=100.0V D	6-p.d Su	btract						
	7 -											
	6.75 -											
	6.5				406.095	51						
	6.25				(M+H)- │	ł						
	6 -											
	5.75 -											
	5.5											
	5.25											
	5 -											
	4.75 -											
	4.5											
	4.25											
	4 -											
	3.75											
	3.5											
	3.25 -											
	3 -											
	2.75											
	2.5											
	2.25											
	2						I					
	1.75											
	1.5					I						
	1.25											
	0.75											
	0.75											
	0.5											
	0.25		<u></u>							<u></u>	.	
	0	396 397 398 39	9 400 401 4	102 403 404 40	5 406	407 40	08 409	9 410 4	11 412 4	13 414 415 416	417 418	

Alleh Mildle	all plants	
alud buis		
delivered in		986.91
di tolioni		904.42
a and a start is		
All-aparta		
herbillapt		
Humpha		
Rinderhis		
adduble in		₽₽9·9L 890·LL
hat the St		061.77
al a la la la		
partition of		924.001
and when		542.TTT \$09.ETT
AND AND		122.493
and a sub-		681.921 681.921
of the type lit		260.821
Philar Phase		522·LET -
May May are		122.332
Mantala ta		542.051 572.051 660.251
at which the		SPP.891
Hadilly		
And and		
and plant		
and the		- C)
di Malia		



Sample Name			Position	p1B6		Instrument Name	Instrument 1
User Name	QTOF-PC\QTOF		Inj Vol	0.1		InjPosition	
Sample Type	Sample		IRM Calibration Status	Success		Data Filename	E1-p.d
ACQ Method	20110418-MSonly	-p.m	Comment			Acquired Time	3/12/2018 4:27:24 PM
	x10 5 +E	SI Scan (rt: 0.648-0.695 r	min, 5 scans) Frag=100.0V E	1-p.d Subtrac	ct		
	6.6						
	6.4						
	6.2						
	6 -			360.1342			
	5.8 -			(M+H)+			
	5.6 -						
	5.4						
	5.2						
	5						
	4.8						
	4.6						
	4.4 -						
	4.2						
	4 -						
	3.8						
	3.6						
	3.4 -						
	3.2 -						
	3 -						
	2.8 -						
	2.6						
	2.4						
	2.2						
	1 0						
	1.0						
	1.0						
	1.4						
	1.2						
	0.8 -						
	0.0						
	0.4						
	0.2 -						
	0						

	C
	2
	0
	2
-	
	0
. 1	0
	2
	-
-	š
. 1	0
	4
	-
-	20
	~
	0
	9
	-
- 1	0
	-
	0
-	š
	0
	S
	0
-	0
	Z
	-
	0
	5
	0
-	N
	-
	-
	0
	6.3
	0
-	4
	-
	-
	0
	47
	-
2	0
-	0
	-
	-
8	0
	2
	-
	0
1	80
	-
	-
	0
-	0
	1-
	0
_	õ
	3
2	-
	-
1	0
-	5
	11

annia thabhadhadhadhadhadhadh આવા અને કાર્યની જેવાન્સ અને સાથી પુસ્ત કાર્યકાર કે પણ આવે છે. તે અવસ્થી અનુસાય બંધુ કાર્ય સંઘર્ત છે કે પ્રિક્રે પ્રક્રિયની છે પિત્ર કાર્યકાર કે શાસ્ય કે શાસ્ય કે છે. والمتحدث والمتحالة والإنصافات والمتعام المتحمية متحالهما المارية متعرجها والمرابع independent Mill A Marine Marine Milling photo a solution of the later of the solution hundred a brind of which the al das bi Heater by Supervision and Supervised States Liphuill Anaryking bolo and hy lipher

LLS.6-006'ST-845.05-569.97-77.057 77.483 -100'305 -110'123 -111'125 -113'25 -113'25 -155'461 -155'461 -155'461 -155'461 -155'461 -155'461 -155'461 -155'53 -156'135'133 -156'135'13 -156'13 -156'13 -156'13 -156'13 -156'13 -156'135'13 -SLE'ISI 66E'ZSI 6E8'SSI 0ES'8SI 6EE'09I \$60'S9I

158

SP130619-1-C C13-NMR CDCL3 303K AV-300



SP20130619-1 CDCL3 1HNMR AV300

EZ

Sample Name				Po	sition		p1B7					Instr	ument Nam	e Ir	nstrument 1
User Name	QTOF-PC\QTC)F		Inj	j Vol		0.1					InjPo	osition		
Sample Type	Sample			IR	M Calibra	ation Status	Succe	SS				Data	Filename	E	2-p.d
ACQ Method	20110418-MS	only-p.m		Co	mment							Acqu	ired Time	3,	/12/2018 4:29:34 PM
	x10 ⁵	+ESI Scan (ri	t: 0.533-0.557	7 min, 3 s	cans) Fr	ag=100.0V E	2-p.d S	ubtract							
	7.25 -														
	7 -														
	6.75 -						374.1	497							
	6.5 -						(M+ł	H)+							
	6.25														
	6 -														
	5.75														
	5.5														
	5.25														
	5 -														
	4.75 -														
	4.5 -														
	4.25														
	4 -														
	3.75 -														
	3.5 -														
	3.25 -														
	3 -														
	2.75														
	2.5														
	2.25 -														
	2 -														
	1.75 -														
	1.5 -							1							
	1.25 -														
	1 -														
	0.75														
	0.5														
	0.25								I						
	0 -	··· ·						<u>,</u>						···· · · · · · · · · · · · · · · · · ·	J
		367	368 369	370	371	372 373 Counts	374 vs. Mas	l 375 s-to-Cha	376 rge (m/z	377 :)	378	379	380 381	382	

SP130621-2-C C13-NMR CDCL3 303K AV-300

15.972

Webbards for over the second till all and a second product of stars a fellow a branchistic and be better and be better and be and for and

alme, to reache the structure of the office second diversity limit infertee, the set of state, a second size in the infertee state and size of the second size of

ppm



aber miest, ber iftelitate men mine unter ten band verbenst anfen infer aber utilient der stel este alle method ficher mit er

is a second and the second on the second we have a second with the second second with the

190 180 170 160



Sample Name				Pos	sition		p1B9					Instru	ment Name	Ins	trument 1
User Name	QTOF-PC\QTO	F		Inj	Vol		0.1					InjPos	ition		
Sample Type	Sample			IRM	4 Calibration S	Status	Success					Data F	ilename	E3-	p.d
ACQ Method	20110418-MSc	only-p.m		Con	nment							Acquir	ed Time	3/1	2/2018 4:33:55 PM
	x10 ⁵	+ESI Scan (rt	:: 0.517-0.552	2 min, 4 so	cans) Frag=10	0.0V E4-	p.d Subtra	ct							
	6.4														
	6.2														
	6 -						412.1291								
	5.8 -						(M+H)+								
	5.6														
	5.4 -														
	5.2 -														
	5 -														
	4.8														
	4.6														
	4.4 -														
	4.2														
	4														
	3.0														
	3.4														
	3.4														
	3 -														
	2.8 -														
	2.6														
	2.4														
	2.2 -														
	2 -														
	1.8 -														
	1.6 -														
	1.4 -							I							
	1.2 -														
	1 -														
	0.8 -														
	0.6 -														
	0.4 -														
	0.2 -														
	0 -	402 402	404 405	406 40	7 409 400	410 47	11 410 4	10 4			417 44	0 410	420 421	400 400	
		402 403	404 405	406 407	408 409 / (410 41 Counts vs	11 412 4 Mass-to-C	13 4 harge	14 41 (m/z)	o 416	417 41	8 419	420 421	422 423	

SP130624-C C13-NMR cdcl3 303K AV-300



15.902

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



E4

User Name													
		=	Inj	Vol	0.1					Inj	Position		
Sample Type	Sample		IRI	M Calibration Status	Success					Dat	a Filename	ł	E4-p.d
ACQ Method	20110418-MSo	nly-p.m	Co	mment						Acq	uired Time	3	3/12/2018 4:36:07 PI
	x10 5 4.2	ESI Scan (rt: 0.599-	0.623 min, 3 s	cans) Frag=100.0V E	5-p.d Sub	otract							
	4 -												
	3.8 -				412.12 (M+H)	289							
	3.6 -				(ועודרו))+							
	3.4 -												
	3.2 -												
	3 -												
	2.8												
	2.6 -												
	2.4 -												
	2.2 -												
	2 -												
	1.8 -												
	1.6 -												
	1.4 -												
	1.2 -												
						I							
	0.0												
	0.4												
	0.2	<u></u>		<u></u>									
	0 –	403 404 40	5 406 407	408 409 410 4	411 412	413	414	415	416 41	7 418 4	19 420 42	21 422	423





ppm



ample Name						Pos	sition			P2	a5						Instru	Iment	Name		Instrur	nent 1
ser Name	QTOF-PC\QTOF	=				Inj	Vol			0.1	L						InjPo	sition				
ample Type	Sample					IRM	M Calib	ration	Status	Su	ccess						Data	Filenan	ne		E5-p.d	
CQ Method	20110418-MSo	nly-p.m				Cor	mment										Acqui	red Tin	ne		3/13/2	018 1:50:42
	×10 5 +	-ESI Sca	an (rt: 0	.599-0	.658 m	iin, 6 se	cans) F	- rag=1	00.0V G	а́1-р.с	d Subt	ract										
	4																					
	3.8 -																					
	3.6								Ę	534.2	502											
	3.4 -									(101+F	1)+											
	3.2 -																					
	3 -																					
	2.8 -																					
	2.6 -																					
	2.4 -																					
	2.2																					
	2 -																					
	1.8 -																					
	1.6 -																					
	1.4 -																					
	1.2 -																					
	1 -																					
	0.8 -																					
	0.6																					
	0.4																					
	0.4											1										
	0.2 -																					
	0 -	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	 545	

	SP20131	220-2 - C	C13-NMR	CDCL3	303K	AV-300)
124 71 71	204 203 204 203 204 204 204 204 204 204 204 204 204 204	91 91 42 72 72 72 72 72	65 65 69 69 69 73 73	222 0	റയറ	ть м	m
0.04	0000440 0000440	1000004	000000	- 9. 9 - 9. 9	65	31 31 76	73
990 101	13112	112212	111	1 10	77	54	44
11	1111-		11/1/		\bigvee	$ \rangle /$	

-15.979

E6

i i i a a batarat ana tarrah an aritherina han da a ya da ita and bia casha hara da taran a sa mananginya kana gapar pasaraan manana ya sa sa mananginya	hallo al diglas Tayaqattaash	da basanan Mananan	electronic in the second s	al la colorada Tili boorda a	and the	unnudaa. Munudaa.e	der bieligen der program	nlandulu Nisaran	na na hagalan Alir na gula	.day, bredd, metraffarw	al al parata	ertanette raufseen	ibbadallana. Marappirana	alla line din	lavu ababdu avu ababdu	aldest allet to



E6



SP-20131011 CDCL3 1HNMR AV300

3.6763 3.6616 3.6463

0314 .

3

5317 5166 5017 1034

NNNN

.

• . . -0.0853

9871 4935 55865 55865 55865 49621 4601 4601 4602 33191 33181 33181 22904 2214 1032 11871 1693 1602 1602 ~ ~ L. T. 1 ε. 1

E7

. .





Sample Name				F	Position		P2a6						Instr	ument N	ame	Instr	ument 1
User Name	QTOF-PC\QTOF			I	nj Vol		0.1						InjPo	sition			
Sample Type	Sample			I	RM Calibra	ation Status	s Succe	SS					Data	Filenam	e	Е7-р	.d
ACQ Method	20110418-MSonl	Comment									Acquired Time				3/13/2018 1:53:04 PM		
	×10 5 +E	SI Scan (rt:	0.330-0.40)1 min, 7	scans) Fr	ag=100.0V	G3-p.d S	Subtra	ct								
	x10 -	·				-											
	9 -																
	8.5 -						445.18 (M+H)	75									
	8 -																
	7.5 -																
	7 -																
	6.5 -																
	6 -																
	5.5 -																
	5 -																
	4.5 -																
	4 -																
	3.5 -																
	3 -																
	2.5 -																
	2 -																
	1.5 -																
	1 -																
	0.5 -								1								
	0	····									10 1		450				
		436 43	7 438 4	39 440	441 44	2 443 4 Count	44 445 s vs. Mas	446 s-to-C	447 Charge (448 4 m/z)	49 450	451	452 45	3 454	455 4	56 457	







				Posit	ion		P	2a7						Instrum	ent Nar	ne	Instru	ument 1
QTOF-PC\QTO	=			Inj V	ol		0	.1						InjPosit	ion			
Sample	IRM Calibration Status					S S	Success							ename	E8-p.d			
20110418-MSo		Comment									Acquire	d Time		3/13/2018 1:56:22 PM				
x10 ⁵ 3.8	ESI Scan	(rt: 0.251-	-0.286 mi	in, 4 sca	ns) Fra	g=100.0V	G4-p	.d Sub	otract									
3.6 -																		
3.4 -							3	376.129	98									
3.2 -								(ואדיוא)	F									
3_																		
28-																		
2.0																		
2.0																		
2.4																		
2.2 -																		
2 -																		
1.8 -																		
1.6 -																		
1.4 -																		
1.2																		
1 -																		
0.8 -																		
0.6 -																		
0.4 -								1										
0.2																		
0 -						<u> </u>	<u></u>							<u></u>			<u> </u>	
	368 3	69 370	371	372	373	374 : Count	375 s vs. l	376 Mass-t	377 o-Char	378 ge (m/z)	379	380	381	382	383	384	385	
	QTOF-PC\QTOF Sample 20110418-MSo x10 5 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0	QTOF-PC\QTOF Sample 20110418-MSonly-p.m x10 5 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 368 3	QTOF-PC\QTOF Sample 20110418-MSonly-p.m x10 5 3.8 3.6 3.4 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 1 0.8 0.6 0.4 0.2 368 369 370	QTOF-PC\QTOF Sample 20110418-MSonly-p.m x10 5 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 368 369 370 371	Positi QTOF-PC\QTOF Sample IRM 20110418-MSonly-p.m Comm x10 5 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 368 369 370 371 372	Position Inj Vol Sample 20110418-MSonly-p.m x10 5 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 3 3 2.8 2.6 2.4 2.2 3 3 2.8 3.6 3.4 3.6 3.4 3.2 3 3 2.8 3.6 3.4 3.2 3 3 3 3 3 3 3 3 3 3 3 3 3	Position QTOF-PC\QTOF Sample 20110418-MSonly-p.m Comment +ESI Scan (rt: 0.251-0.286 min, 4 scans) Frag=100.0V +ESI Scan (rt: 0.251-0.286 min, 4 scans) Frag=100.0V * * * * * * * *	Position P QTOF-PC\QTOF In Vol 0 Sample IRM Calibration Status S 20110418-MSonly-p.m Comment x10 5 +ESI Scan (rt: 0.251-0.286 min, 4 scans) Frag=100.0V G4-p 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 	Position P2a7 QTOF-PC\QTOF Inty Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 3.8 3.6 3.4 3.6 3.4 3.6 3.4 3.6 3.4 3.6 3.4 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 3.8 3.6 3.4 3.76.124 (M+H) 3.2 3.8 2.6 2.4 2.2 3.8 2.6 2.4 2.2 3.8 2.6 3.4 3.76.124 (M+H) 3.2 3.8 3.6 3.4 3.76.124 (M+H) 3.2 3.8 3.6 3.7 3.7 3.7 3.7 3.7 3.7 3.7 3.7	Position P2a7 QTOF-PCQQTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment *ESI Scan (rt: 0.251-0.286 min, 4 scans) Frag=100.0V G4-p.d Subtract 3.8 3.6 3.4 3.6 3.4 3.6 3.4 3.76.1298 (M+H)+ 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 3.8 3.6 3.4 3.76.1298 (M+H)+ 3.2 3 3.76.1298 (M+H)+ 3.77 3.76.1298 (M+H)+ 3.77 3.76.375 3.76.376 3.77 Counts vs. Mass-to-Charles 3.76.1298 (M+H)+ 3.77 3.77 3.77 3.77 3.76.375 3.76 3.77 3.77 3.77 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.76 3.77 3.76 3.76 3.77 3.76 3.77 3.76 3.76 3.77 3.76 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.76 3.77 3.77 3.76 3.77 3.7	Position P2a7 QTOF-PC\QTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 4 4 5 38 36 34 36 34 36 34 376.1298 (M+H)+ 32 3 28 26 24 22 2 1.8 1.6 1.4 2.2 2 3 3 2.8 2.6 2.4 2.2 2 3 3 2.8 3 2.8 3 2.8 3 2.8 3 2.8 3 2.8 3 2.8 3 2.8 3 2.8 3 2.6 2.4 3 3 2.8 3 2.6 2.4 3 3 3 3 3 3 3 4 3 3 5 3 7 5 3 7 5 3 7 3 3 7 3	Position P2a7 QTOF-PCQTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment *ESI Scan (rt: 0.251-0.286 min, 4 scans) Frag=100.0V G4-p.d Subtract 3.6 3.4 3.6 3.6 3.4 3.6 3.4 3.6 3.6 3.6 3.4 3.6 3.6 3.6 3.6 3.6 3.6 3.6 3.6	Position P237 QTOF-PCQTOF IPM Calibration Status Success 20110418-MSonly-p.m Comment x10 s +ESI Scan (rt: 0.251-0.286 min, 4 scans) Frag=100.0V G4-p.d. Subtract 3.8 376.1298 3.4	Position P2a7 QTOF-PCQTOF Inj Vol 0.1 Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment	Position P2a7 Instrum QT0F-PCQTOF Int Calibration Status Success Data Fill 20110418-MSon/y-p.m Comment Acquire x10 5 +ESI Scan (rt: 0.251-0.286 min, 4 scans) Frag=100.0V G4-p.d Subtract - 38 - - - - - 38 - - - - - - 38 - <t< td=""><td>Position P2a7 Instrument Nar QTOF-PCQQTOF Inj Vol 0.1 LipPosition Sample 20110118/MSontly-p.m Comment Success Data Filename 20110118/MSontly-p.m Comment Success Acquired Time x10 #ESI Scan (rt. 0.251-0.286 min, 4 scans) Frag=100.0V G4-p.d. Subtract Success Success 3.8 3.6 </td><td>Position P2a7 Instrument Name GTGF-PCQTDF Inj Vol 0.1 InjPosition Sample IRM Calibration Status Succes Data Filename 20110418-MSonly-p.m Comment Acquired Time x10 4 Calibration Status Succes Acquired Time 3.8 </td><td>Position P2a7 Instrument Name Instrument Name</td></t<>	Position P2a7 Instrument Nar QTOF-PCQQTOF Inj Vol 0.1 LipPosition Sample 20110118/MSontly-p.m Comment Success Data Filename 20110118/MSontly-p.m Comment Success Acquired Time x10 #ESI Scan (rt. 0.251-0.286 min, 4 scans) Frag=100.0V G4-p.d. Subtract Success Success 3.8 3.6	Position P2a7 Instrument Name GTGF-PCQTDF Inj Vol 0.1 InjPosition Sample IRM Calibration Status Succes Data Filename 20110418-MSonly-p.m Comment Acquired Time x10 4 Calibration Status Succes Acquired Time 3.8	Position P2a7 Instrument Name Instrument Name

SP1300701-C C13-NMR cdcl3 303K AV-300

40.575 40.295 39.738 39.738 33.462 33.560 -24.435 15.979

 $\begin{array}{c} 168.663\\ 165.306\\ 165.306\\ 164.588\\ 159.096\\ 151.965\\ 138.988\\ 138.945\\ 138.945\\ 138.045\\ 138.045\\ 138.045\\ 138.045\\ 138.045\\ 138.045\\ 138.045\\ 138.045\\ 1122.011\\ 122.017\\ 1122.077\\ 1122.077\\ 1122.077\\ 112.077\\ 1$

FI





Sample Name					Po	osition			P1C2						Instru	ment Na	ame	Inst	rument 1		
User Name	QTOF-PC\QTOF				In	ij Vol			0.1						InjPos	sition					
Sample Type	Sample				IR	RM Calib	oration S	Status	Succe	SS					Data F	ilename	2	F1-p	o.d		
ACQ Method	20110418-MSor	only-p.m Comment													Acquired Time			3/12	3/12/2018 4:38:05 PM		
	40.5 +	FSI Scan	(rt [.] 0 46	5-0 500	min 4	scans)	Frag=10	0 0V F1	-nd S	ubtract											
	x10 5		(,				p.a. 0												
	9 -																				
	8.5 -																				
								3	373.16	60											
	8 -								(111-11)	т											
	7.5																				
	7 -																				
	6.5 -																				
	6 -																				
	5.5 -																				
	5 -																				
	4.5																				
	4 -																				
	35-																				
	0.0																				
	3 -																				
	25																				
	2.0																				
	2 -																				
	15-																				
	1.5																				
	1 -																				
	0.5																				
	0.5										I										
	0 -								<u> </u>									<u> </u>			
		366	367	368	369	370	371 C	372 Counts ve	373 s. Mas	374 s-to-Ch	375 arge (m	376 /z)	377	378	379	380	381	382			
SP130703-3-C C13-NMR DMSO 303K AV-300

F2



9.573

ha di Katan	uh di bind	happing	(Underped	Wheeh		manh	man	ubbla p	lu lunop		al la land	yklloph.dy	Hisaluh	u Weinklau	Hubber H	phanter	har ha	hille		rality	aulticklala
ALL ARE AND HAVEN	114 khunht	ahaindh	Hole has	Lakapatinil	ir fritt de lit	en hur h	ay and only at	did Arthur	nilmed	hall have	mblied	lie dial	i, hën dib	en de la composición d	alm)Heb	norik.Weal	usin Ha	amaldal	annid	alborballo	hhaddlin in to
210	200	190	180	170	160	150	140	130	120	110	100	90	80	70	60	50	40	30	20	10	ppm



Sample Name					Positi	on		P2a1					In	strumen	t Name	In	strument 1	
User Name	QTOF-PC\QTO	F			Inj Vo	bl		0.1					In	jPositior	ı			
Sample Type	Sample				IRM C	alibratio	on Status	Success					Data Filename			F2	F2-p.d	
ACQ Method	20110418-MSc	only-p.m			Comm	nent							Ac	Acquired Time			3/13/2018 1:42:53 PM	
	x10 5	+ESI Scan (r	t: 0.470-	0.482 mi	n, 2 scar	ns) Frag=	=100.0V F	2-p.d Sı	ubtract									
	9.5 -																	
	9 -																	
	9 F							387.1 (M+H	822 1)+									
	6.0																	
	8 -																	
	7.5 -																	
	7 -																	
	6.5 -																	
	6 -																	
	5.5 -																	
	5 -																	
	4.5 -																	
	1 -																	
	3.5 -																	
	3 -																	
	2.5 -																	
	2 -																	
	1.5 -																	
	1 -																	
	0.5																	
	0 -	·····					<u> </u>							· · · · ·		<u></u>		
		374	376	378	380	382	384 Counts	386 vs. Mass	388 -to-Ch	390 arge (m/z	392 2)	394	396	398	400	402		

SP130705-2-C C13-NMR DMSO 303K AV-300

073 515 240 964 051 40.(339.(33.(33.(33.()

50

40

ppm

534

. ഹ

-

L64.823 164.112 156.112 156.103 151.435 145.640 145.640 145.640 133.535 133.535 133.535 133.535 125.467 125.329 122.204 124.134 124.134 124.134 124.134 124.134 125.14 ----

the site of a standard strend with the sense of the standard strends to the standard strends to the standard st n ministration de la calencia de la ba hatti a ti a heat da hudi ti ini taki ti 110 210 200 180 130 120 100 90 80 70 60 30 20 10

190

170

160

150

140



£J

OTOF-PC\OTOF																
			Inj	Vol		0.1					InjPosi	tion				
Sample				IRM Calibration Status							Data Fi	F3-p.	F3-p.d			
20110418-MSonl	/-p.m		Con	nment							Acquired Time			3/13/2018 1:46:49 PM		
x10 5 +E	SI Scan (rt: 0).343-0.355	min, 2 sc	ans) Frag	=100.0V F	4-p.d Sub	tract									
6.2 -																
6 -																
5.8																
5.6						425.16	09									
5.4 -						(IVI+L)	Ŧ									
5.2																
5																
4.8																
4.6																
4.4 -																
4.2																
4 -																
3.8 -																
3.6 -																
3.4 -																
3.2 -																
3 -																
2.8 -																
2.6 -																
2.4 -																
2.2 -																
2 -																
1.8 -																
1.6																
1.4							1									
1.2																
1 -																
0.8																
0.6																
0.4																
0.2																
0			<u></u>	<u> </u>		<u> </u>		<u> </u>				· · · · · · · · · · · · · · · · · · ·	. <u></u>			
	Sample 20110418-MSonly x10 5 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 1.4 1.2 1 0.8 0.6 0.4 0.2 1.4 0.6 0.4 0.2 1.4 0.2 1.4 0.6 0.4 0.2 1.4 0.6 0.4 0.2 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.6 0.4 0.2 0.4 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	Sample 20110418-MSonly-p.m x10 5 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 4.2 4 4 3.8 3.6 3.4 4.4 4.2 4 4 4 3.8 3.6 3.4 4.4 4.2 4 4 4 4 4 4 4 4 4 4 4 4 4	Sample 20110418-MSonly-p.m x10 5 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8 0.6 0.4 4.2 4 4.2 4 4.3 4.5 5.4 4.5 4.8 4.6 4.4 4.2 4 4.5 4.8 4.6 4.4 4.2 4 4.5 4.8 4.6 4.4 4.2 4 4.5 4.8 4.6 4.4 4.2 4.5 4.8 4.6 4.4 4.2 4.5 4.8 4.6 4.4 4.2 4.5 4.8 4.6 4.4 4.2 4.5 4.8 4.6 4.4 4.2 4.5 4.8 4.6 4.4 4.2 4.5 4.8 4.6 4.4 4.2 4.5 4.8 4.6 4.4 4.5 4.5 4.8 4.6 4.4 4.2 4.5 4.5 4.8 4.6 4.6 4.4 4.5 4.6 4.7 4.5 4.8 4.6 4.7 4.5 4.8 4.6 4.7 4.7 4.7 4.7 4.7 4.7 4.7 4.7	Sample IRM 20110418-MSonly-p.m Con x10 5 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 4 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 2.2 2 1.8 1.6 1.4 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.2 1.8 1.6 1.4 1.4 1.2 1.8 1.6 1.4 1.4 1.2 1.8 1.6 1.4 1.4 1.2 1.8 1.6 1.4 1.4 1.2 1.8 1.6 1.4 1.4 1.2 1.8 1.6 1.4 1.8 1.6 1.4 1.4 1.2 1.8 1.6 1.4 1.4 1.2 1.8 1.6 1.4 1.4 1.4 1.4 1.4 1.4 1.4 1.4	Sample IRM Calibration 20110418-MSonly-p.m Comment x10 5 6.2 6 5.8 5.6 5.4 5.2 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4 3.2 3 2.8 2.6 2.4 4 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4 4 3.2 3 2.8 2.6 2.4 4 3.2 3 2.8 2.6 2.4 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4 3.8 3.6 3.8 3.8 3.8 3.8 3.8 3.8 3.8 3.8	Sample IRM Calibration Status 20110418-MSonly-p.m Comment x10 +ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F 6 6 5.6 5.4 5.6 5.4 5.6 5.4 5.6 5.4 5.7 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.8 3.6 3.4 3.2 3.6 3.4 3.6 3.4 3.6 3.4 3.7 3.8 3.8 3.6 3.9 3.8 3.6 3.4 <td>Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 6 6 6 6 5.8 5.6 425.16 5.4 425.16 6.2 6 5.8 425.16 5.4 6 4.8 4.6 4.4 4.2 4.3 3.6 3.4 3.2 3 2.8 2.6 2.4 1.8 1.6 1.4 1.2 1.8 6.6 0.4 0.2 1.8 0.6 0.4 0.2 1.2 414 412 416</td> <td>Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 6.2 6 5.8 5.6 5.4 5.4 5.4 5.4 4.52 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4.3 3.6 3.4 3.6 3.4 3.2 3 2.8 2.6 2.4 4.3 3.6 3.4 3.2 3 2.8 2.6 2.4 4.3 3.6 3.4 3.6 3.4 3.6 3.4 3.2 3 2.8 2.6 2.4 4.3 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.4 3.6 3.6 3.4 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.6 3.4 3.6 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.6 3.4 3.6 3.6 3.6 3.6 3.6 3.6 3.6 3.6</td> <td>Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 Fest Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract 6 425.1609 6 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 55 4.8 4.6 4.4 4.2 4 32 3 34 32 35 426 46 44 47 426 48 426 49 426 41</td> <td>Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 62 6 5.8 5.6 5.4 5.2 5 6 425.1609 (M+H)+ 425.160 (M+H)+ 425</td> <td>Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment ×10 \$ +ESI Scan (tt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract 6 6 6 7 4 5 6 6 7 4 5 6 7 8 6 7 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8</td> <td>Sample IRM Calibration Status Success Deta Fi 20110418-MSonly-p.m Comment Acquire *10 5 +ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract 6 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 4 4 4 4 4 4 4 4 4 4 4 4</td> <td>Sample IM Calibration Status Success Data Filename 20110418-MSon/u-p.m Comment Acquired Time *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d S</td> <td>Sample ItM Calibration Status Success Data Filename F3p. 201104184MSon/p.p.m Comment Acquired Time 3/13/ x10 s +ESI Scan (rt. 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract 4 - 6 4 - - - - 5.6 425.1609 (M+H)+ - - - 5.4 - - - - - - 425.1609 (M+H)+ -</td>	Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 6 6 6 6 5.8 5.6 425.16 5.4 425.16 6.2 6 5.8 425.16 5.4 6 4.8 4.6 4.4 4.2 4.3 3.6 3.4 3.2 3 2.8 2.6 2.4 1.8 1.6 1.4 1.2 1.8 6.6 0.4 0.2 1.8 0.6 0.4 0.2 1.2 414 412 416	Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 6.2 6 5.8 5.6 5.4 5.4 5.4 5.4 4.52 5 4.8 4.6 4.4 4.2 4 3.8 3.6 3.4 3.2 3 2.8 2.6 2.4 4.3 3.6 3.4 3.6 3.4 3.2 3 2.8 2.6 2.4 4.3 3.6 3.4 3.2 3 2.8 2.6 2.4 4.3 3.6 3.4 3.6 3.4 3.6 3.4 3.2 3 2.8 2.6 2.4 4.3 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.4 3.6 3.6 3.4 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.6 3.4 3.6 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.4 3.6 3.6 3.6 3.4 3.6 3.6 3.6 3.6 3.6 3.6 3.6 3.6	Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 Fest Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract 6 425.1609 6 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 54 425.1609 55 4.8 4.6 4.4 4.2 4 32 3 34 32 35 426 46 44 47 426 48 426 49 426 41	Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment x10 5 62 6 5.8 5.6 5.4 5.2 5 6 425.1609 (M+H)+ 425.160 (M+H)+ 425	Sample IRM Calibration Status Success 20110418-MSonly-p.m Comment ×10 \$ +ESI Scan (tt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract 6 6 6 7 4 5 6 6 7 4 5 6 7 8 6 7 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8	Sample IRM Calibration Status Success Deta Fi 20110418-MSonly-p.m Comment Acquire *10 5 +ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract 6 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 5 4 4 4 4 4 4 4 4 4 4 4 4 4	Sample IM Calibration Status Success Data Filename 20110418-MSon/u-p.m Comment Acquired Time *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract *ESI Scan (rt: 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d S	Sample ItM Calibration Status Success Data Filename F3p. 201104184MSon/p.p.m Comment Acquired Time 3/13/ x10 s +ESI Scan (rt. 0.343-0.355 min, 2 scans) Frag=100.0V F4-p.d Subtract 4 - 6 4 - - - - 5.6 425.1609 (M+H)+ - - - 5.4 - - - - - - 425.1609 (M+H)+ -		