Supporting Information

Environmentally Benign and Atom-Economical Protocol for the Regioselective Synthesis of Isoquinolones from *o*-Alkynylaldehydes

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X-Ray Crystallographic Studies



Figure S1. ORTEP diagram for each molecule of the asymmetric unit of compound 3e drawn with 50% ellipsoid probability.

The crystals of **3e** of suitable quality were obtained from $CHCl_2/n$ -hexane. The compound **3e** crystallized in Triclinic crystal system with space group P c. The single-crystal X-ray data were collected on an Oxford XCalibur CCD diffractometer using graphite monochromated Mo K α radiation. The structures was solved using SIR-92 and refined by full matrix least square technique on F² using the SHELXL-97¹⁻⁴ program within the WinGX v 1.80.05 software package. Atomic coordinates, bond lengths, bond angles, and thermal parameters for compounds **3e** has been deposited at the Cambridge Crystallographic Data Centre. CCDC deposit number for **3e** is 2301423.

 Table SI. Crystallographic data and structure refinement for compounds 3e

Identification code	3e
Empirical formula	C ₂₃ H ₂₆ I N O ₂
Formula weight	475.35
Temperature	293 K
Wavelength	0.71073 Å

Crystal system	Monoclinic	
Space group	P c	
Unit cell dimensions	a = 8.95427(16)	$\alpha = 90$
	b = 13.54255(18)	$\beta = 113.787(2)$
	c = 9.03971(16)	$\gamma = 90$
Volume	1003.07 Å ³	
Ζ	2	
Density (calculated)	1.574 g/cm ³	
Absorption coefficient	1.614 mm ⁻¹	
F(000)	480.0	
Index ranges	h=12, k=18, l=12	
Reflections collected	0.0207(5248)	
Completeness to theta = $26.37 \circ$	99.7 %	
Final R indices [I>2 sigma(I)] ^{a,b}	R1 = 0.0207, WR2 = 0.04	449
^a $R = \sum (\ Fo - Fc) / \sum Fo ; bRw = \{\sum$	$\sum [w(Fo^2 - Fc^2)^2] / \sum [w(Fo^2)^2] / \sum [w($	²) ²]} ^{1/2}

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General Experimental

General Method. ¹H NMR (400 MHz) and ¹³C NMR (100 MHz) spectra were recorded in CDCl₃/(CD₃)₂SO. Chemical shifts for protons and carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, br s = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet), coupling constants in Hertz and integration. High-resolution mass spectra were recorded on electrospray mass spectrometer. Crystal structure analysis was accomplished on single needles X-ray diffractometer. TLC analysis was performed on commercially prepared 60 F₂₅₄ silica gel plates. All purchased chemicals were used as received. All melting points are uncorrected. The starting materials were synthesised according to the literature reporting method.¹

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General Procedure for the Synthesis of iodo-substituted isoquinolones(3a-v)



In a 10 ml. oven-dried round bottom flask, o-alkynyl aldehyde **1** (0.25 mmol, 1.0 equiv.), 4-amino-1-butanol **2** (0.75 mmol, 3.0 equiv.) and I₂ (0.40 mmol, 2.0 equiv) was taken and stirred at room temperature for 2 h. The progression of the reaction was monitored by TLC analysis. The reaction mixture was then quenched with satd. aq. Na₂S₂O₃ (5.0 mL) and water (5.0 mL). The resulting solution was extracted using ethyl acetate. The combined organic extracts were dried over anhydrous Na₂SO₄ and concentrated under vacuum. The crude material obtained was purified by column chromatography on silica gel (100–200) (hexane:ethyl acetate; 75/25).

Transformation of 3q via Suzuki coupling reaction :



Representative procedure: An oven-dried vial was charged with the obtained product **3q** (0.10 mmol, 1.0 equiv), phenylboronic acid (0.13 mmol, 1.3 equiv.), $Pd(PPh_3)_2Cl_2(5 \text{ mol }\%)$, K_2CO_3 (0.20 mmol, 2.0 equiv.) in 3:1 DMF/H₂O. The reactants were degassed and filled with N₂ for three times. Then the reaction mixture was stirred at 80 °C for 2 h. When the reaction was completed, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate. Then organic layer was washed with aqueous saturated brine solution and dried over Na₂SO₄ and concentrated under reduced pressure. The crude material obtained was purified by column chromatography on silica gel (100–200) (hexane:ethyl acetate; 70/30) to afford the desired product **11q** in 85% yield.

Conversion of -OH hydroxy group to azide group:



Representative procedure: An oven-dried vial was charged with the obtained product **3q** (0.10 mmol, 1.0 equiv), tosyl chloride (0.15 mmol, 1.5 equiv.),in 3 mL pyridine.. Then the reaction mixture was stirred at room temperature for 10 h. When the reaction was completed, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate. Then organic layer was washed with aqueous saturated brine solution and dried over Na₂SO₄ and concentrated under reduced pressure. The crude material thus obtained was treated with NaN₃ (0.25 mmol, 2.5 equiv.), Cs₂CO₃ (0.25 mmol, 2.5 equiv.) in DMF and the reaction mixture was stirred at 60 °C for 4 h. When the reaction was completed, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate. Then organic layer was washed with aqueous saturated brine solution mixture was diluted with water (10 mL) and extracted with ethyl acetate. Then organic layer was washed with aqueous saturated brine solution and dried over Na₂SO₄ and concentrated with ethyl acetate. Then organic layer was washed with aqueous saturated brine solution and dried over Na₂SO₄ and concentrated under reduced pressure. The crude material obtained was purified by column chromatography on silica gel (100–200) (hexane:ethyl acetate; 70/30) to afford the desired product **5q** in 90% yield.

Transformation of 5q via Click reaction :



Representative procedure: An oven-dried vial was charged with the obtained product **5q** (0.10 mmol, 1.0 equiv), CuI (0.20 mmol), in 2 mL DMF. Then the reaction mixture was stirred at 80 °C for 5 h. When the reaction was completed, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate. Then organic layer was washed with aqueous saturated brine solution and dried over Na_2SO_4 and concentrated under reduced pressure. The crude material obtained was

purified by column chromatography on silica gel (100-200) (hexane:ethyl acetate; 70/30) to afford the desired product 7**q** in 70% yield.



Transformation of 3j via Heck coupling reaction :

Representative procedure: An oven-dried vial was charged with the obtained product 3j (0.10 mmol, 1.0 equiv), 4-methoxystyrene (0.13 mmol, 1.3 equiv.), Pd(PPh₃)₂Cl₂ (10 mol %), K₂CO₃ (0.25 mmol, 2.5 equiv.) in DMF. The reactants were degassed and filled with N₂ for three times. Then the reaction mixture was stirred at 110 °C for 4 h. When the reaction was completed, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate. Then organic layer was washed with aqueous saturated brine solution and dried over Na₂SO₄ and concentrated under reduced pressure. The crude material obtained was purified by column chromatography on silica gel (100–200) (hexane:ethyl acetate; 80/20) to afford the desired product **9***J* in 70% yield.

Mechanistic Control Investigations :

When, we treated the *ortho*-alkynyl aldehyde with amino alcohol in the absence of iodine, the aldimine intermediate **12** was obtained in a 30% yield. The starting material was not completely consumed in the reaction mixture even after 24 h as clear from the crude NMR of the reaction mixture.





Figure S2: ¹H NMR of crude reaction mixture of (Scheme 6, i) showing relative ratio of **12** and **1a** in the reaction mixture.

Characterization data for the products:



2-(4-hydroxybutyl)-4-iodo-3-phenylisoquinolin-1(2H)-one

(**3a**).The product was obtained as a sticky semi-solid (86.1 mg, 82%): ¹H-NMR (400 MHz, CDCl₃) δ 8.40 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.71-7.67 (m, 1H), 7.52-7.48 (m, 1H), 7.36-7.31 (m, 2H), 7.28-7.23 (m, 3H), 3.86 (t, *J* = 7.6 Hz, 2H), 3.50 (t, *J* = 6.4 Hz, 2H), 2.68 (s, 1H), 1.66-1.59 (m, 4H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.7, 142.1, 137.8, 137.2, 134.0, 132.1, 129.4, 128.6, 128.1, 126.1, 80.5, 62.2, 48.1, 29.7, 25.6; HRMS (ESI) [M+H]⁺ Calcd for [C₁₉H₁₉INO₂] 420.0460, found 420.0451.



2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)isoquinolin-1(2H)-one

(3b).The product was obtained as a brown solid (91.5 mg, 85%): mp 136–138 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.36 (dd, J = 8.0, 1.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.67-7.63 (m, 1H), 7.48-7.44 (m, 1H), 7.28 (d, J = 7.8 Hz, 2H), 7.12 (d, J = 8.1 Hz, 2H), 3.81 (t, J = 7.1 Hz, 2H), 3.45 (t, J = 6.5 Hz, 2H), 2.41 (s, 3H), 1.62-1.56 (m, 4H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.1, 145.5, 139.5, 137.3, 136.7, 133.4, 131.6, 129.6, 129.1, 128.1, 127.6, 125.2, 79.8, 61.5, 46.9, 30.7, 29.8, 21.5; HRMS (ESI) [M+H]⁺ Calcd for [C₂₀H₂₁INO₂] 434.0617, found 434.0624.



3-(4-ethylphenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-

1(2*H***)-one (3c).** The product was obtained as a dark brown solid (89.4 mg, 80%): mp 140–142 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 9.1 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.70-7.69 (m, 1H), 7.49 (t, *J* = 8.1 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 4.07 (t, *J* = 5.2 Hz, 2H), 3.64 (t, *J* = 5.3 Hz, 2H), 2.70 (q, *J* = 7.6 Hz, 2H), 1.62-1.56 (m, 4H), 1.25 (t, *J* = 7.6 Hz, 3H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.1, 145.7, 137.3, 136.9, 133.4, 131.6,

129.2, 128.4, 128.2, 127.6, 125.2, 79.8, 63.0, 46.9, 30.7, 29.7, 28.7, 15.4; HRMS (ESI) [M+H]⁺ Calcd for [C₂₁H₂₃INO₂] 448.0773, found 448.0783.



2-(4-hydroxybutyl)-4-iodo-3-(4-methoxyphenyl)isoquinolin-1(2*H***)-one (3d). The product was obtained as a dark brown solid (87.5 mg, 78%): mp 152–156 °C: ¹H-NMR (400 MHz, CDCl₃) 8.36 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.1 Hz, 1H), 7.68-7.64 (m, 1H), 7.49-7.45 (m, 1H), 7.16 (d, J = 11.4 Hz, 2H), 6.99 (d, J = 8.8 Hz, 2H), 3.85-3.81 (m, 6H), 3.47 (t, J = 6.4 Hz, 2H), 1.63-1.55 (m, 4H); ¹³C {1H} NMR (100 MHz, CDCl₃) \delta 160.1, 145.2, 137.3, 133.4, 132.0, 131.7, 130.6, 128.2, 127.6, 125.2, 114.2, 80.5, 61.7, 55.4, 46.9, 30.7, 29.7; HRMS (ESI) [M+H]⁺ Calcd for [C₂₀H₂₁INO₃] 450.0566, found 450.0557.**



3-(4-(tert-butyl)phenyl)-2-(4-hydroxybutyl)-4-

iodoisoquinolin-1(2*H*)-one (3e). The product was obtained as a brown solid (100.7 mg, 90%): mp 160–162 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.35 (d, *J* = 7.7 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.48-7.44 (m, 3H), 7.15 (d, *J* = 8.2 Hz, 2H), 3.81 (t, *J* = 7.8 Hz, 2H), 3.45 (t, *J* = 6.3 Hz, 2H), 2.63 (s, 1H), 1.61-1.54 (m, 2H), 1.33 (s, 9H), 1.30-1.24 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.2, 152.7, 145.6, 137.3, 136.7, 133.4, 131.6, 128.8, 128.1, 127.6, 125.6, 80.0, 61.7, 47.6, 34.9, 31.3, 29.2, 25.0; HRMS (ESI) [M+H]⁺ Calcd for [C₂₃H₂₇INO₂] 476.1086, found 476.1084.



3-(4-fluorophenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-

1(2*H***)-one (3f).** The product was obtained as a dark brown solid (95.0 mg, 87%): mp 142–144 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.36 (dd, J = 8.1, 1.0 Hz, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.68-7.64 (m, 1H), 7.50-7.46 (m, 1H), 7.26-7.22 (m, 2H), 7.21-7.16 (m, 2H + residual CDCl₃),

3.80 (t, J = 7.0 Hz, 2H), 3.49 (t, J = 6.3 Hz, 2H), 1.61-1.56 (m, 4H); ¹³C {1H} NMR (100 MHz, CDCl₃) δ 163.1 (d, $J_{C-F} = 250.6$ Hz), 162.0, 161.8, 144.3, 137.2, 135.6 (d, $J_{C-F} = 3.63$ Hz), 133.6, 131.7, 131.5, 131.4, 128.1 (d, $J_{C-F} = 31.2$ Hz), 125.3, 116.3 (d, $J_{C-F} = 25.4$ Hz), 80.2, 61.8, 47.0, 30.6, 29.8; HRMS (ESI) [M+H]⁺ Calcd for [C₁₉H₁₈FINO₂] 438.0366, found 438.0382.



2-(4-hydroxybutyl)-4-iodo-3-(thiophen-3-yl)isoquinolin-

1(2*H***)-one (3g).** The product was obtained as a dark brown solid (87.1 mg, 82%): mp 120-122 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.35 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.68-7.64 (m, 1H), 7.50-7.46 (m, 2H), 7.33-7.32 (m, 1H), 7.02 (dd, *J* = 4.9, 1.2 Hz, 1H), 3.99-3.91 (m, 1H), 3.77-3.70 (m, 1H), 3.17 (t, *J* = 6.5 Hz, 1H), 1.66-1.57 (m, 4H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.0, 140.9, 139.3, 133.5, 131.7, 128.2, 128.0, 127.9, 126.9, 126.5, 125.3, 80.6, 61.7, 46.9, 30.7, 29.7; HRMS (ESI) [M+H]⁺ Calcd for [C₁₇H₁₇INO₂S] 426.0025, found 426.0013.



2-(4-hydroxybutyl)-4-iodo-3-(4-nitrophenyl)isoquinolin-

1(2*H***)-one (3h).** The product was obtained as a dark brown solid (102.0 mg, 88%): mp 160– 164 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.21 (t, *J* = 8.5 Hz, 2H), 7.78 (dd, *J* = 7.4, 4.4 Hz, 1H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.49-7.45 (m, 1H), 7.31-7.27 (m, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 3.88 (t, *J* = 7.3 Hz, 2H), 3.67 (t, *J* = 6.1 Hz, 2H), 1.84-1.76 (m, 2H), 1.65-1.58 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.2, 149.9, 146.3, 140.2, 136.2, 133.5, 129.8, 128.6, 127.1, 124.9, 124.3, 77.8, 61.8, 48.4, 29.4, 25.2; HRMS (ESI) [M+H]⁺ Calcd for [C₁₉H₁₈IN₂O₄] 465.0311, found 465.0326.



2-(4-hydroxybutyl)-4-iodo-3-(7-methoxynaphthalen-2-

yl)isoquinolin-1(2*H*)-one (3i). The product was obtained as a dark brown solid (118.5 mg, 95%): mp 200-202 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.12 (s, 1H), 7.75 (s, 2H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.17-7.11 (m, 2H), 7.02-6.99 (m, 1H), 6.88-6.84 (m, 1H), 6.72 (d, *J* = 8.7 Hz, 1H), 5.49 (s, 1H), 4.74 (t, *J* = 8.0 Hz, 2H), 3.89 (s, 3H), 3.71 (t, *J* = 6.2 Hz, 2H), 2.04-1.97 (m, 2H), 1.72-1.65 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 184.3, 159.3, 136.6, 135.7, 130.7, 130.6, 130.4, 129.6, 127.9, 127.0, 126.5, 126.0, 125.9, 123.0, 121.6, 120.7, 119.6, 105.7, 82.5, 61.6, 55.4, 51.2, 29.3, 27.4; HRMS (ESI) [M+H]⁺ Calcd for [C₂₄H₂₃INO₃] 500.0723, found 500.0710.



²3-([1,1'-biphenyl]-4-yl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-

1(2H)-one (3j). The product was obtained as a dark brown solid (111.3 mg, 90%): mp 190-192 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.43 (dd, J = 8.0, 1.2 Hz, 1H), 7.92 (d, J = 8.1 Hz, 1H), 7.77 (d, J = 8.1 Hz, 2H), 7.74-7.69 (m, 3H), 7.55-7.53 (m, 1H), 7.51-7.47 (m, 2H), 7.41-7.35 (m, 3H), 3.92 (t, J = 7.8 Hz, 2H), 3.54 (t, J = 6.3 Hz, 2H), 2.97 (s, 1H), 1.71-1.64 (m, 2H), 1.43-1.36 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.1, 145.1, 142.0, 139.7, 138.4, 137.2, 133.5, 131.6, 129.7, 128.9, 128.1, 127.9, 127.7, 127.3, 127.1, 125.1, 79.8, 61.7, 47.7, 29.2, 25.2; HRMS (ESI) [M+Na]⁺ Calcd for [C₂₅H₂₂INaNO₂] 518.0593, found 518.0599.



2-(4-hydroxybutyl)-4-iodo-3-(phenanthren-9-yl)isoquinolin-

1(2H)-one (3k). The product was obtained as a dark brown solid (115.4 mg, 89%): mp 200-204°C: ¹H-NMR (400 MHz, CDCl₃) δ 8.75-8.69 (m, 2H), 8.45 (dt, *J* = 8.0, 1.6 Hz, 1H), 7.98-

7.89 (m, 2H), 7.78-7.62 (m, 5H), 7.52-7.36 (m, 3H), 4.97 (s, 1H), 3.79 (t, J = 6.1 Hz, 2H), 3.38-3.25 (m, 2H), 2.15-2.07 (m, 2H), 1.81-1.74 (m, 2H); ¹³C {1H} NMR (100 MHz, CDCl₃) δ 162.3, 143.3, 142.2, 139.9, 138.6, 137.4, 133.6, 131.8, 130.6, 129.9, 129.1, 128.3, 128.1, 127.9, 127.5, 127.3, 125.3, 80.0, 61.9, 47.9, 29.4, 25.4; HRMS (ESI) [M+Na]⁺ Calcd for [C₂₇H₂₃INNaO₂] 542.0593, found 542.0587.



7-chloro-2-(4-hydroxybutyl)-4-iodo-3-(m-tolyl)isoquinolin-

1(2*H***)-one (5a).** The product was obtained as a dark brown solid (103.9 mg, 89%): mp 150– 152 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.30 (d, J = 2.3 Hz, 1H), 7.77 (d, J = 8.8 Hz, 1H), 7.54 (dd, J = 8.8, 2.3 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.25 (d, J = 7.5 Hz, 1H), 7.01 (d, J = 7.8 Hz, 2H), 3.85-3.70 (m, 2H), 3.44 (t, J = 6.4 Hz, 2H), 2.63 (s, 1H), 2.36 (s, 3H), 1.60-1.52 (m, 2H), 1.33-1.26 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.1, 146.0, 139.3, 138.8, 135.9, 133.8, 133.7, 133.4, 130.3, 129.7, 128.8, 127.3, 126.2, 125.9, 78.3, 61.8, 48.0, 29.3, 25.2, 21.6; HRMS (ESI) [M+H]⁺ Calcd for [C₂₀H₂₀ClINO₂] 468.0227, found 468.0252.



7-chloro-3-cyclopropyl-2-(4-hydroxybutyl)-4-

iodoisoquinolin-1(2*H*)-one(5b). The product was obtained as a creamish white sticky solid (83.4 mg, 80%): ¹H-NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 2.5 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.48 (dd, *J* = 8.8, 2.3 Hz, 1H), 4.46 (t, *J* = 7.6 Hz, 2H), 3.64 (t, *J* = 6.3 Hz, 2H), 2.64 (s, 1H), 1.86-1.79 (m, 1H), 1.78-1.70 (m, 2H), 1.60-1.53 (m, 2H), 1.37-1.32 (m, 2H), 0.89-0.85 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.7, 144.5, 136.1, 133.5, 133.4, 132.9, 127.1, 125.6, 81.4, 62.0, 45.1, 29.8, 25.5, 19.2, 14.4; HRMS (ESI) [M+H]⁺ Calcd for [C₁₆H₁₈CIINO₂] 418.0071, found 418.0085.



7-chloro-3-cyclohexyl-2-(4-hydroxybutyl)-4-

iodoisoquinolin-1(2H)-one (5c). The product was obtained as a creamish white sticky solid

(86.0 mg, 75%): ¹H-NMR (400 MHz, CDCl₃) δ 8.23 (d, J = 2.5 Hz, 1H), 7.81 (d, J = 8.8 Hz, 1H), 7.50 (dd, J = 8.8, 2.3 Hz, 1H), 4.49 (t, J = 7.6 Hz, 2H), 3.67 (t, J = 6.3 Hz, 2H), 2.63 (s, 1H), 2.16-2.07 (m,1H), 1.89-1.18 (m, 14H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.8, 144.6, 136.3, 133.6, 133.5, 133.1, 127.2, 125.7, 81.5, 62.1, 51.5, 46.1, 32.8, 29.9, 26.1, 25.9.; HRMS (ESI) [M+H]⁺ Calcd for [C₁₉H₂₄CIINO₂] 460.0540, found 460.0551.



2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)-7-

(trifluoromethyl)isoquinolin-1(2*H*)-one (5d). The product was obtained as a white solid (112.7 mg, 90%): mp 172–174 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.75 (s, 1H), 8.07 (d, *J* = 8.8 Hz, 1H), 7.91 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 3.95 (t, *J* = 5.6 Hz, 2H), 3.63 (t, *J* = 5.6 Hz, 2H), 2.51 (s, 3H), 2.37 (s, 1H), 1.73-1.62 (m, 4H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.5, 147.9, 139.9, 139.8, 136.3, 132.7, 129.5 (q, *J*_{C-F} = 13.1 Hz), 129.3, 128.3 (q, *J*_{C-F} = 260.1 Hz), 125.9 (q, *J*_{C-F} = 3.6 Hz), 125.0, 78.3, 61.6, 47.2, 30.6, 29.7, 21.6; HRMS (ESI) [M+Na]⁺ Calcd for [C₂₁H₁₉F₃INaNO₂] 524.0310, found 524.0316.





1(2*H***)-one (5e).** The product was obtained as a dark brown solid (117.3 mg, 92%): mp 172– 174 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.45 (d, *J* = 1.5 Hz, 1H), 7.68-7.67 (m, 2H), 7.26 (d, *J* = 7.8 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 3.78 (t, *J* = 7.9 Hz, 2H), 3.44 (t, *J* = 6.4 Hz, 2H), 2.62 (s, 1H), 2.38 (s, 3H), 1.58-1.50 (m, 2H), 1.32-1.25 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.0, 146.1, 139.7, 136.5, 136.4, 136.2, 133.5, 130.5, 129.6, 129.0, 126.2, 121.6, 78.8, 61.7, 48.0, 29.4, 25.2, 21.6; HRMS (ESI) [M+H]⁺ Calcd for [C₂₀H₂₀BrINO₂] 511.9722, found 513.9721.



e 2-(4-hydroxybutyl)-4-iodo-7-nitro-3-(*p*-tolyl)isoquinolin-

1(2*H***)-one (5f).** The product was obtained as a dark brown solid (113.5 mg, 95%): mp 150–152 °C: ¹H-NMR (400 MHz, CDCl₃) δ 9.12 (d, *J* = 2.5 Hz, 1H), 8.33 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.96 (d, *J* = 8.9 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 3.82 (t, *J* = 8.0 Hz, 2H), 3.47 (t, *J* = 6.3 Hz, 2H), 2.67 (s, 1H), 2.41 (s, 3H), 1.62-1.54 (m, 2H), 1.35-1.28 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.1, 149.8, 146.2, 141.7, 140.0, 136.0, 133.3, 129.7, 128.4, 126.9, 124.8, 124.2, 77.6, 61.7, 48.2, 29.2, 25.0, 21.5; HRMS (ESI) [M+H]⁺ Calcd for [C₂₀H₂₀IN₂O₄] 479.0468, found 479.0487.



pentylphenyl)isoquinolin-1(2*H***)-one (5g).** The product was obtained as a dark brown solid (120.1 mg, 90%): mp 130-132 °C: ¹H-NMR (400 MHz, CDCl₃) δ 9.19 (d, J = 2.5 Hz, 1H), 8.41 (dd, J = 9.0, 2.5 Hz, 1H), 8.05 (d, J = 9.0 Hz, 1H), 7.38 (d, J = 8.0 Hz, 2H), 7.21 (d, J = 8.3 Hz, 2H), 3.90 (t, J = 7.9 Hz, 2H), 3.51 (t, J = 6.4 Hz, 2H), 2.74 (t, J = 7.8 Hz, 2H), 1.72-1.62 (m, 6H), 1.45-1.36 (m, 4H), 0.97 (t, J = 7.4 Hz, 3H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.2, 150.0, 146.3, 145.1, 141.8, 136.3, 133.4, 129.0, 128.5, 127.0, 124.9, 124.3, 77.7, 61.7, 48.4, 35.5, 33.3, 29.4, 25.1, 22.4, 14.0; HRMS (ESI) [M+H]⁺ Calcd for [C₂₃H₂₅IN₂O₄] 521.0937, found 521.0972.



2-(4-hydroxybutyl)-4-iodo-3-(3-methoxyphenyl)-7-

nitroisoquinolin-1(*2H*)-one (5h). The product was obtained as a dark brown solid (116.1 mg, 94%): mp 142–144 °C: ¹H-NMR (400 MHz, CDCl₃) δ 9.14 (d, *J* = 2.5 Hz, 1H), 8.35 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.02-6.99 (m, 1H), 6.83-6.81 (m, 1H), 6.77 (t, *J* = 2.0 Hz, 1H), 3.86-3.82 (m, 5H), 3.45 (t, *J* = 6.4 Hz, 2H), 1.67-1.58 (m, 2H), 1.36-1.29 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.0, 159.8, 149.3, 146.2,

141.7, 139.9, 133.3, 130.3, 126.9, 124.8, 124.1, 120.8, 115.3, 114.3, 79.9, 61.5, 55.4, 48.3, 29.2, 25.2; HRMS (ESI) [M+H]⁺ Calcd for [C₂₀H₂₀IN₂O₅] 495.0417, found 495.0425.



2-(4-hydroxybutyl)-4-iodo-6,7-dimethoxy-3-

phenylisoquinolin-1(*2H*)**-one (5i).** The product was obtained as a dark brown solid (83.8 mg, 70%): mp 192–194 °C: ¹H-NMR (400 MHz, CDCl₃) δ 7.79 (s, 1H), 7.51-7.43 (m, 3H), 7.27-7.24 (m, 3H), 3.96 (s, 6H), 3.82-3.79 (m, 2H), 2.96-2.93 (m, 2H), 1.61-1.55 (m, 4H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.0, 159.8, 149.3, 141.7, 139.9, 133.3, 130.3, 126.9, 124.8, 124.1, 120.8, 115.3, 114.3, 107.2, 101.3, 80.5, 61.5, 55.4, 48.3, 29.2, 25.2.; HRMS (ESI) [M+H]⁺ Calcd for [C₂₁H₂₃INO₄] 480.0672, found 480.0706.



Me 7-(4-(*tert*-butyl)phenyl)-6-(4-hydroxybutyl)-8-iodo-

[1,3]dioxolo[4,5-*g*]isoquinolin-5(6*H*)-one (5j). The product was obtained as a dark brown solid (64.9 mg, 50%): mp 200–204 °C: ¹H-NMR (400 MHz, DMSO-*d*₆) δ 7.58 (d, *J* = 8.2 Hz, 2H), 7.45-7.39 (m, 2H), 7.31 (dd, *J* = 8.2, 2.7 Hz, 2H), 6.29 (s, 2H), 4.12 (t, *J* = 6.0 Hz, 2H), 3.63 (s, 1H), 2.94 (t, *J* = 6.2 Hz, 2H), 1.49 (t, *J* = 25.1 Hz, 4H), 1.35 (s, 9H); ¹³C{1H} NMR (100 MHz, DMSO-*d*₆) δ 158.4, 151.6, 147.0, 143.6, 136.6, 131.5, 129.2, 125.4, 124.8, 114.0, 109.7, 102.9, 79.2, 61.3, 45.5, 31.1, 30.4, 29.0; HRMS (ESI) [M+H]⁺ Calcd for [C₂₄H₂₇INO₄] 520.0985, found 520.0988.



2-((7-chloro-2-(4-hydroxybutyl)-4-iodo-1-oxo-1,2-

dihydroisoquinolin-3-yl)methyl)isoindoline-1,3-dione (5k). The product was obtained as a white sticky solid (26.8 mg, 20%): ¹H-NMR (400 MHz, CDCl₃) δ 7.94 (d, J = 1.8 Hz, 1H), 7.90 (d, J = 8.5 Hz, 1H), 7.76-7.73 (m, 1H), 7.60-7.55 (m, 1H), 7.48 (dd, J = 8.4, 1.9 Hz, 2H), 7.40 (dt, J = 7.7, 1.4 Hz, 1H), 3.72 (t, J = 7.8 Hz, 2H), 3.31 (t, J = 7.0 Hz, 2H), 2.76 (s, 2H), 1.84 (t, J = 5.9 Hz, 2H), 1.72 (t, J = 5.3 Hz, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) : The amount of the product 3v was less, so ¹³C NMR could not be recorded; HRMS (ESI) [M+Na]⁺ Calcd for [C₂₂H₁₈ClINaN₂O₄] 558.9897, found 558.9885.



ⁱ ^{Me} **3-(4-ethylphenyl)-2-(2-hydroxyethyl)-4-iodoisoquinolin-1(2***H***)one (6a). The product was obtained as a white sticky solid (83.8 mg, 80%): mp 152–156 °C: ¹H-NMR (400 MHz, CDCl₃) \delta 8.36 (d, J = 9.1 Hz, 1H), 7.88 (d, J = 8.1 Hz, 1H), 7.70-7.69 (m, 1H), 7.49 (t, J = 8.1 Hz, 1H), 7.29 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 8.1 Hz, 2H), 4.07 (t, J = 5.2 Hz, 2H), 3.64 (t, J = 5.3 Hz, 2H), 2.70 (q, J = 7.6 Hz, 2H), 1.25 (t, J = 7.6 Hz, 3H); ¹³C{1H} NMR (100 MHz, CDCl₃) \delta 164.4, 145.9, 145.5, 137.6, 136.8, 133.9, 131.8, 129.2, 128.5, 128.2, 127.9, 124.9, 80.8, 63.0, 51.1, 28.7, 15.2; HRMS (ESI) [M+H]⁺ Calcd for [C₁₉H₁₉INO₂] 420.0460, found 420.0461.**



^{Me} 2-(2-hydroxyethyl)-4-iodo-3-(p-tolyl)-7-

(trifluoromethyl)isoquinolin-1(2H)-one (6b). The product was obtained as a yellow solid (100.7 mg, 85%): mp 182–166 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.64 (s, 1H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.83 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.28 (d, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 8.1 Hz, 2H), 4.06

(t, J = 5.5 Hz, 2H), 3.63 (t, J = 5.5 Hz, 2H), 2.39 (s, 3H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.3, 146.9, 139.0, 135.2, 131.8, 131.3, 128.9, 128.7, 128.3 (q, $J_{C-F} = 260.1$ Hz), 127.9, 124.9, 123.7, 78.1, 61.0, 49.9, 20.5; HRMS (ESI) [M+H]⁺ Calcd for [C₁₉H₁₆F₃INO₂] 474.0718, found 474.0725.



• 7-chloro-2-(2-hydroxyethyl)-4-iodo-3-(m-tolyl)isoquinolin-

1(2*H***)-one (6c).** The product was obtained as a dark brown solid (95.2 mg, 87%): mp 142–146 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.32 (d, *J* = 2.3 Hz, 1H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.55 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.26 (d, *J* = 7.5 Hz, 1H), 7.02 (d, *J* = 7.8 Hz, 2H), 3.86-3.71 (m, 2H), 3.45 (t, *J* = 6.4 Hz, 2H), 2.65 (s, 1H), 2.37 (s, 3H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.1, 146.0, 139.3, 138.8, 135.9, 133.8, 133.7, 133.4, 130.3, 129.7, 128.8, 127.3, 126.2, 125.9, 78.3, 77.4, 77.1, 76.8, 61.8, 48.0, 21.6; HRMS (ESI) [M+H]⁺ Calcd for [C₁₈H₁₆ClINO₂] 439.9914, found 439.9901.



Me 2-(3-hydroxypropyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-

1(2*H***)-one (6d).** The product was obtained as a dark brown solid (105.6 mg, 91%): mp 132–136 °C: ¹H-NMR (400 MHz, CDCl₃) δ 9.12 (d, *J* = 2.5 Hz, 1H), 8.33 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.95 (d, *J* = 8.9 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.06 (t, *J* = 6.3 Hz, 2H), 3.43 (t, *J* = 5.6 Hz, 2H), 2.53 (s, 3H), 1.62-1.56 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.0, 150.7, 147.1, 142.6, 141.0, 137.0, 134.3, 130.6, 129.3, 127.9, 125.7, 125.1, 77.6, 57.0, 43.6, 30.2, 21.4.; HRMS (ESI) [M+H]⁺ Calcd for [C₁₉H₁₇IN₂O₄] 465.0311, found 465.0301.



3-(4-(tert-butyl)phenyl)-2-(5-hydroxypentyl)-4-

iodoisoquinolin-1(2*H*)-one (6e). The product was obtained as a dark brown solid (85.5 mg, 70%): mp 162–164 °C: ¹H-NMR (400 MHz, CDCl₃) δ 8.30 (d, *J* = 7.7 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.43-7.39 (m, 3H), 7.10 (d, *J* = 8.2 Hz, 2H), 3.76 (t, *J* = 7.8 Hz, 2H), 3.40 (t, *J* = 6.3 Hz, 2H), 2.59 (s, 1H), 1.56-1.49 (m, 2H), 1.28-1.22 (m, 11H), 0.83-0.77 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 162.1, 152.6, 145.5, 137.2, 136.6, 133.3, 131.5, 128.7, 128.0, 127.5, 125.5, 79.9, 61.6, 47.5, 34.8, 31.2, 29.1, 25.0, 20.7; HRMS (ESI) [M+H]⁺ Calcd for [C₂₄H₂₉INO₂] 490.1243, found 490.1224.



Ae 2-(4-azidobutyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-

1(2*H***)-one (7f).** The product was obtained as a dark brown solid (113.1 mg, 90%): mp 172–176 °C: ¹H-NMR (400 MHz, CDCl₃) δ 9.21 (d, *J* = 2.3 Hz, 1H), 8.41-8.37 (m, 1H), 8.01 (dd, *J* = 8.9, 3.7 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 2H), 7.12 (d, *J* = 7.8 Hz, 2H), 3.85-3.81 (m, 2H), 3.09-3.05 (m, 2H), 2.43 (s, 3H), 1.62-1.54 (m, 2H), 1.37-1.30 (m, 2H).; ¹³C {1H} NMR (100 MHz, CDCl₃) δ 161.1, 149.7, 146.4, 141.8, 140.2, 136.1, 133.4, 129.8, 128.5, 127.1, 125.0, 124.4, 77.6, 50.6, 48.0, 29.7, 26.0, 21.5; HRMS (ESI) [M+H]⁺ Calcd for [C₂₀H₁₉IN₅O₃] 504.0533, found 504.0547.



2-(4-(4-((8S,9R,13R,14R,17R)-3,17-

dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-

cyclopenta[a]phenanthren-17-yl)-1H-1,2,3-triazol-1-yl)butyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-1(2*H***)-one (9).** The product was obtained as a white solid (139.8 mg, 70%): mp 182-184 °C: ¹H-NMR (400 MHz, CDCl₃) δ 9.32 (d, *J* = 2.5 Hz, 1H), 8.49 (dd, *J* = 9.0, 2.5 Hz, 1H), 8.11 (d, *J* = 9.0 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 3H), 6.68 (dd, *J* = 8.4, 2.6 Hz, 2H), 6.61 (d, *J* = 2.5 Hz, 1H), 3.93 (t, *J* = 7.9 Hz, 2H), 3.15 (t, *J* = 6.8 Hz, 2H), 2.84-2.82 (m, 2H), 2.63 (s, 3H), 2.46 (d, *J* = 8.0 Hz, 1H), 2.26-2.20 (m, 2H), 2.09-2.02 (m, 4H), 1.94-1.87 (m, 2H), 1.78-1.69 (m, 4H), 1.47-1.41 (m, 4H), 0.89 (s, 3H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.3, 153.7, 146.4, 140.2, 138.0, 135.9, 133.4, 132.0, 129.8, 128.4, 127.1, 126.4, 124.4, 115.3, 112.8, 87.4, 79.9, 74.0, 49.3, 47.1, 43.4, 39.3, 38.8, 32.7, 29.6, 29.6, 27.2, 26.3, 22.7, 12.7; HRMS (ESI) [M+H]⁺ Calcd for [C₄₀H₄₃IN₅O₅] 822.2128, found 822.2194.



(E)-3-([1,1'-biphenyl]-4-yl)-2-(4-hydroxybutyl)-4-(4-

methoxystyryl)isoquinolin-1(*2H*)-one (11j). The product was obtained as a dark brown solid (87.7 mg, 70%): mp 192–196 °C: ¹H-NMR (400 MHz, CDCl₃) δ 7.64-7.55 (m, 7H), 7.43-7.28 (m, 8H), 7.07 (d, *J* = 8.7 Hz, 1H), 6.78 (d, *J* = 8.8 Hz, 2H), 6.71 (d, *J* = 8.7 Hz, 1H), 6.40 (t, *J* = 4.7 Hz, 1H), 5.47-5.57 (1H), 3.95 (t, *J* = 7.6 Hz, 2H), 3.73 (s, 3H), 3.51 (t, *J* = 6.3 Hz, 2H), 1.65 (q, *J* = 7.5 Hz, 2H), 1.37 (dd, *J* = 20.0, 6.7 Hz, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃)

*δ*162.0, 150.7, 147.1, 142.6, 141.0, 137.0, 134.3, 130.6, 129.3, 127.9, 125.7, 125.1, 77.6, 57.0, 43.6, 30.2, 21.4.; HRMS (ESI) [M+H]⁺ Calcd for [C₃₄H₃₂NO₃] 502.2382, found 502.2397.



2-(4-hydroxybutyl)-7-nitro-4-phenyl-3-(p-

tolyl)isoquinolin-1(2*H*)-one (13f). The product was obtained as a dark brown solid (90.7 mg, 85%): mp 210–212 °C: ¹H-NMR (400 MHz, CDCl₃) δ 9.28 (d, J = 2.5 Hz, 1H), 8.19 (dd, J = 9.0, 2.5 Hz, 1H), 7.20-7.13 (m, 4H), 7.02-6.97 (m, 6H), 3.84 (t, J = 7.9 Hz, 2H), 3.50 (t, J = 6.3 Hz, 2H), 2.23 (s, 3H), 1.68-1.61 (m, 2H), 1.40-1.33 (m, 2H); ¹³C{1H} NMR (100 MHz, CDCl₃) δ 161.5, 145.7, 145.5, 141.5, 138.7, 135.4, 131.2, 130.8, 129.4, 128.8, 128.5, 128.3, 127.3, 126.9, 125.8, 124.3, 118.8, 61.8, 46.1, 29.3, 25.0, 21.3; HRMS (ESI) [M+H]⁺ Calcd for [C₂₆H₂₄N₂O₄] 428.1736, found 428.1742.

Copies of ¹H, ¹³C and HRMS

Copies of ¹H and ¹³C NMR

¹H NMR (400 MHz, CDCl₃)



2-(4-hydroxybutyl)-4-iodo-3-phenylisoquinolin-1(2H)-one (3a)



HRMS



2-(4-hydroxybutyl)-4-iodo-3-phenylisoquinolin-1(2H)-one (3a)

Qualitative Compound Report



¹H NMR (400 MHz, CDCl₃)



2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)isoquinolin-1(2H)-one (3b)



¹³C {1H} NMR (100 MHz, CDCl₃)



2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)isoquinolin-1(2H)-one (3b)





2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)isoquinolin-1(2H)-one (3b)

Sample Type Instrument Name Acq Method IRM Calibration Status Comment	HSII-408.d Sample Instrument I HS Scanut Success	Sample h Position User Nan Acquired DA Metho	lame MSI-408 p1-44 re Time 19-01-20 ad Default //	123 13:22:07 N			
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Compound Table					Mia	MEG Formula	DB Formula
Compound Label Cpd 1: C28 H20 1 N C	RT Mass 2 0.17 433	Abund 0539 19891 C20	Formula 1H20 I N O2	433.0539	0.13	C20 H20 1 N O2	C20 H20 TN C2
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0.1 0.2 MS Spectrum x1D S Cpel 1: C20 H20 3- 2.5- 2-	0.3 0.4 0.5 Ci	0:6 0.7 0.8 0. wunts vat. Acquisition Terr mum (0.136-0.610 min) I	9 1 1.1 e (min) WSH-4D8.d Subtr	1.2 1.3 rat	14		
0.1 0.2 MS Spectrum x10 s Cpel 1: C20 H20 3 2.5 2. 2. 1.5 1	0.3 0.4 0.5 _{Ci}	0,6 0,7 0,8 0,0 wints vs. Acquisition Ter num (0.136-0.510 min) I	9 1 1.1 e (min)	1.2 1.3 act	14		
0.1 0.2 MS Spectrum x10 5 Gpd 1: C20 H20 3 2.5- 2.5- 1.5- 1.5- 1.5- 0.5-	0.3 0.4 0.5 _{Ci}	0,6 0,7 0,8 0,0 yunis vs. Acquisition Ter rum (0.136-0.510 min) I	a (min) 1	1.2 1.3 ract			
0.1 0.2 MS Spectrum x10.3 Cpe 1: C20 H20 3- 2- 1.5- 1.5- 1.5- 1.5- 435 4	0.3 0.4 0.5 _{Cl} IN C2: + FBF Spec 38 440 442 Cl	0,6 0,7 0,8 0,0 winis vz. Acquisition Ter nym (0,136-0,510 min) 1 esta 44 646 4 punts vz. Mass-to-Chang	a (min) MSH-408.d Subtr MSH-408.d Subtr MSH-408.d Subtr (MSH-408.d Subtr (MSH-408.d Subtr (MSH-408.d Subtr	1.2 1.3 Fact 452 454	1.4		
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6.1 0.2 MS Spectrum x10.9 Gpe 1: C20 H20 3. 2.5 1.5 1.5 4. 0.5 2.5 2.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1	0.3 0.4 0.5 0 IN 02: + FBF Spect 38 440 442 1N 02: + FBF Spect 1N 02: + FBF Spect (N- 422 425 430 -	0.6 0.7 0.8 0. winis vz. Acquisition Ter nym (0.136-0.510 min) 1 ounts vs. Mass-ra-Charg num (0.136-0.510 min) 1 0624 H) -	456 0431 455 0431 455 0431 455 0431 455 0431	1.2 1.3 act 452 454 act	456		
6.1 0.2 MS Spectrum x10.9 Gpd 1: C20 H20 3. 2.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1	0.3 0.4 0.5 0 IN 02: + FBF Spect 38 440 442 10 02: + FBF Spect 10 02: + FBF Spect (N- 425 425 430 0 C	0.6 0.7 0.8 0.7 units vz. Acquisition Ter nym (0.136-0.510 min) 1 units vs. Mass-to-Charg num (0.136-0.510 min) 1 0624 H) - 135 440 445 450 units vs. Mass-to-Charg	455 460 465 e (m/z)	1.2 1.3 act 452 454 act	456		
6.1 0.2 MS Spectrum x10.9 Gpd 1: C20 H20 3. 2.5 1.5 1.5 4.55 4 MS Zoomed Spectrum x10.9 Cpd 1: C20 H20 3. 2.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1	0.3 0.4 0.5 C	0.6 0.7 0.8 0.7 winis vz. Acquisition Ter winis vz. Acquisition Ter winis vz. Acquisition Ter winis vz. Mass-to-Charg rum (0.136-0.510 min) f 0.136-0.510 min) f	455 460 465 455 460 465	1.2 1.3 act 452 454 act 452 454	456		
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0.1 0.2 MS Spectrum x10 3 Gpd 1: C20 H20 3 2.5 2. 1.5 1.5 3.5 2.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1	0.3 0.4 0.5 C	0.6 0.7 0.8 0.0 winis vz. Acquisition Ter- nym (0.136-0.510 min) 1 0.136-0.510 min)	456 0131 MSH-408.4 Subtr 456 0131 M-N3)- 455 460 465 e (m/z)	1.2 1.3 act 452 454 act	456		



3-(4-ethylphenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3c)



¹³C {1H} NMR (100 MHz, CDCl₃)



3-(4-ethylphenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3c)





3-(4-ethylphenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3c)

		100						
Data File Sample Typ Instrument Acq Method IRM Calibra	ne I Name 1 ation Status	MSH- Samp Instru MS Sc	3870.d Ne ment 1 an.m 38	Sample Name Position User Name Acquired Time DA Method	MSH-3878 P1-05 17-05-2022 Default.m	14:55:21		
Comment								
Acquisition Version	5W 62(Q-1	0 series TOF OF B.05.01 (/6500 series (85125)	2010. <u>3</u>				
Compound	Table		-				MEGDIN	
Compo	und Label	RT	Mass	Formula	MFG	Formula	(ppm)	DB Formula
Cpd 14: 4	L21 H22 1 N O.	0.100	447.0693	C21 H22 1 N O2	C21 H	22 1 N OZ	-9.31	C21 H22 TN 02
Compound	Label	m/z	RT	Algorithm	Mass	1		
Cpd 14: C21	HZZ IN OZ	448.0783	0.165	Find by Molecular Featur	447.0695			
		A				-		
MFE MS Snert	THE OTHER	100000000000000000000000000000000000000		No postante de la		10050000000	1000	
x10 6 Cp	d 14: C21 H22	IN 02: +ES	MFE Spec	trum (0.092-0.676 mim) I	rag= 175.0V /	MSH-387B.d	7	
5			· 44	18.0783 +H)+			-	
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3				1				
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	d 14- C21 H22	IN 02: +FS	MEE Snor	num /0.092-0.676 mim) s		1011 2020 4		
.[Co	48.0783	111 02. 123	i mre opec	aram (0.032-0.070 mim) i	rag= 175.0V f	MSH-3878.0		
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x10 6 Cpd								
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×10 6 Cpi	1							
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x10 e Cpi 5 44 4 (M- 3 2							-	
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x10 e Cpi 5 - 44 4 (M- 3 2	500 550	0 600	850	700 750 950	010			
x10 e 5 - 4 4 3 2 1 0	500 550	0 600	650 Counts v	700 750 800 s. Mass-to-Charge (m/z)	850 900	950	1000	
x10 e Cpi 5 - 4 1 2 1 0 5 - 4 1 1 0	500 550 Peak List	0 600	650 Counts v	700 750 800 s. Mass-to-Charge (m/z)	850 900	950	1000	
x10 c Cp 5 44 4 3 2 1 0 15 Spectrum	500 55 Peak List z Abund	0 600 Formula	650 Counts v	700 750 800 s. Mass-to-Charge (m/z)	850 900	950	1000	
x10 e CP/ 5 - 44 10/2 2 1 2 5 Spectrum 1/2 448.0783	500 550 Peak List z Abund 1 446363	0 600 Formula	650 Counts v I N 02	700 750 800 s. Mass-to-Charge (m/z) Ion (M+H)+	850 900	950	1000	
x10 ¢ Cp 5 44 4 3 2 1 0 5 Spectrum V/r 449.0346	500 550 Peak List z Abund 1 446363 1 1017697 1 30904	0 600 Formula 7.5 (21 H23 78 (21 H23 93 (21 H25	650 Counts v I N 02 I N 02 I N 02	700 750 800 s. Mass-to-Charge (m/z) Ion (M+H)+ (M+H)+ (M+H)+	850 900	950	1000	
x10 ¢ CP 5 44 4 3 2 1 0 5 Spectrum (// 448.0783 450.0360 451.0392	500 550 Peak List z Abund 1 446363 1 1017697 1 303964 1 11722	0 600 Formula 7.5 C21 H23 78 C21 H23 93 C21 H23 32 C21 H23	650 Counts v I N 02 I N 02 I N 02 I N 02	700 750 800 s. Mass-to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ (M+H)+	850 900	950	1000	
x10 ¢ Cpc 5 44 4 3 2 1 0 5 5 5 4 4 8 0 3 6 5 5 5 5 4 8 5 5 4 8 5 6 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	500 550 Peak List 2 Abund 1 446363 1 1012697 1 130504 1 31722 1 171836	0 600 Formula 7.5 C21 123 7.9 C21 123 53 C21 123 33 C21 123 52 C21 122	650 Counts v I N 02 I N 02 I N 02 I N 02 I N 02 I N 02	700 750 800 s. Mass-to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	850 900	950	1000	

¹H NMR (400 MHz, CDCl₃)



2-(4-hydroxybutyl)-4-iodo-3-(4-methoxyphenyl)isoquinolin-1(2H)-one (3d)



¹³C {1H} NMR (100 MHz, CDCl₃)



2-(4-hydroxybutyl)-4-iodo-3-(4-methoxyphenyl)isoquinolin-1(2H)-one (3d)





2-(4-hydroxybutyl)-4-iodo-3-(4-methoxyphenyl)isoquinolin-1(2H)-one (3d)

Data Pile Torustance Sample Name Maile N			ANCLE.	5 and				
Instrument Name cq Method reg Method cq Method Instrument 1 Bit Gauge User Name Bit Gauge Instrument 1 Bit Gauge In	Data File Sample Ty	De	Samp	sle	Sample Name	MSH-543B		
Acq Hethod MS Scan.m Acquired Time 18:05-2022 (5:55:21) Default.m Default.m Default.m Default.m Sample Group Info. 3 Acquired Time 18:05-2022 (5:55:21) Default.m Comment Info. 3 Acquired Time 18:05-2022 (5:55:21) Compound Table Info. 3 Compound Label Info. 3 Col 14: CO H20 I N 03 450.0557 0.166 Col 14: CO H20 I N 03 450.0557 0.166 Col 14: CO H20 I N 03: +ESI MFE Spectrum (0.092-0.676 mim) Frag= 175.0V MSH-5438.d 10 Col 14: CO H20 I N 03: +ESI MFE Spectrum (0.092-0.676 mim) Frag= 175.0V MSH-5438.d 100 Col 550 500 500 <td< th=""><th>Instrumen</th><th>t Name</th><th>Instru</th><th>ument 1</th><th>User Name</th><th>1100</th><th></th><th></th></td<>	Instrumen	t Name	Instru	ument 1	User Name	1100		
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Sample Group Acquisition SW Version EXX parties TO//PS/DD series Q-TO'F R.DS.01 (05125) Info. j Compound Table	Comment	ation Status	Presso	AND MICHAEL	Balancian DA Method	Derauktim		
Compound Label RT Mass Formula MFG Formula (JPM) DB Formula Cpd 14: C20 H20 1 N 03 0.166 449.0488 C0 H20 1 N 03 -9.31 C20 H20 1 N 03	Sample Gro Acquisition Version	sw 62 Q-1	0 series TOF OF B.05.01	(/6500 series (85125)	Info. 3			
Compound Label RT Mass Formula MFG Formula (pp) DB Formula Cpd 14: C20 H20 I N 03 0.166 449.0488 C20 H20 I N 03 -9.33 C20 H20 I N 03 +650 S00 S50 S00 S50 S00 S	Compound	Table					HEAD IN	
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Compound Label m/z RT Algorithm Mass Cpd 14: C20 H20 IN 03 450.0557 0.166 Find by Molecular Feature 449.0488	Cpd 14: 1	C20 H20 I N O3	0.166	449.0488	C20 H20 1 N O3	C20 H20 I N O3	-9.3	C20 H20 I N O
Compound Label m/z RT Algorithm Mass Cpd 14: C20 H20 TN 03 450.0557 0.166 Find by Molecular Feature 449.0488 HE MS Spectrum x10 6 Cpd 14: C20 H20 TN 03: +ESI MFE Spectrum (0.092-0.676 mim) Frag= 175.0V MSH-5438.d - 45 - 450.0557 .(M+T) + - 100 150 200 250 300 350 400 450 500 550 500 950 950 FE MS Zhomed Snetham Cpd 14: C20 H20 TN 03: +ESI MFE Spectrum (0.092-0.676 mim) Frag= 175.0V MSH-5438.d - <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th>								
Cpd 14: C20 H20 1 N 03 450.0557 0.166 Find by Molecular Peature 449.0488 ME MS Spectrum x10 6 Cpd 14: C20 H20 I N 03: +ESI MFE Spectrum (0.092-0.676 mim) Frage 175.0V MSH-5438.d 4 450.0557 (M++1) + 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/z) FE MS Zhomed Spectrum Cpd 14: C20 H20 I N 03: +ESI MFE Spectrum (0.092-0.676 mim) Frage 175.0V MSH-5438.d x10 6 4 450.0557 (M++1) + 4 4 4 50.0557 (M++1) + 4 4 4 50.0557 (M++1) + 4 4 4 50.0557 (M++1) + 4 50.0557	Compound	Label	m/z	RT	Algorithm	Mass		
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MEE MS Spectrum x10 6 Cpd 14: C20 H20 I N 03: +ESI MFE Spectrum (0.092-0.676 mim) Frage 175.0V MSH-5438.d 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/2) FE MS Jonned Spectrum Cpd 14: C20 H20 I N 03: +ESI MFE Spectrum (0.092-0.676 mim) Frage 175.0V MSH-5438.d x10 6 - 450.0557 (M+H)+ - 500 550 600 850 700 750 800 950 900 950 1000 Spectrum Peak List 2 2 4 4 4 4 4 4 4 4 5 4 5 5 5 5 5 5 5 5 5 5 5 5 5				and promotion	La contra possibilita en al trabajar en an			
1 500 550 600 850 700 750 800 850 900 950 1000 5 Spectrum Peak List 2 Z Abund Formula Ion 450.0557 1 5463637.5 (20 H20 I N 03 (M+H)+ 452.0367 1 1017697.78 (20 H20 I N 03 (M+H)+ 452.0367 1 1017697	x10 ⁶ Cp 5 4 3- 2	d 14: C20 H20	I N O3: +E5	SI MFE Spec 4! (M4	trum (0.092-0.676 mim) F 50.0557 +1) +	rage 175.0V MSH-5438	3.d	
Spectrum Peak List 2 Z Abund Formula Ion 450.0557 1 5463637.5 C20 H20 I N O3 (M+H)+ 451.0346 1 1017697.78 C20 H20 I N O3 (M+H)+ 452.0367 1 330904.93 C20 H20 I N O3 (M+H)+ 453.0392 1 1372.036 C20 H20 I N O3 (M+H)+ 472.0366 1 117(B36.67) C0 H10 I N H30 C2 (M+H)+ C20 H10 I N H30 C2	MITE MS Spect x10 e Cp 4 3 2 1 5 1 1 5 1 1 5 1 1 5 1 1 0 1 1 1 1 1 5 1 0 1 1 1 1	00 150 200 150 200 150 200 150 200 150 200 151 200 151 200 151 200 151 200 151 200 151 200 151 200 150 200	1 N O3: +E5 250 300 N O3: +ES	SI MFE Spect	ttrum (0.092-0.676 mim) F 50.0557 +1) + +50 500 550 600 650 - vs. Mass-to-Charge (m/2) trum (0.092-0.676 mim) Fi	rag= 175.0V MSH-5438 rób 750 800 850 90 rag= 175.0V MSH-5438	1.d 0 950 1.d	
450.0557 1 5463637.5 C20 H20 I N 03 (M+H)+ 451.0546 1 1017697.78 C20 H20 I N 03 (M+H)+ 452.0367 1 330904.93 C20 H20 I N 03 (M+H)+ 453.0392 1 130904.93 C20 H20 I N 03 (M+H)+ 457.0362 1 117086.72 C20 H20 I N 03 (M+H)+ 457.0362 1 11708.62 D N 03 (M+H)+	MITE MS Spect x10.6 Cp 4 3 2 1 5 1 5 4 3 2 1 0 1 1 0 5 1 1 0	00 150 200 00 50 00 55	1 N O3: +E5 250 300 N O3: +E5	SI MFE Spect 44 (M 350 400 4 Counts I MFE Spect I MFE Spect Counts	trum (0.092-0.676 mim) F 50.0557 +1) + s50 500 550 600 650 - vs. Mass-to-Charge (m/2) trum (0.092-0.676 mim) Fi	rag= 175.0V MSH-5438 róo 750 800 850 90 rag= 175.0V MSH-5438 850 900 950	3.d 0 950 3.d	
451.0346 1 1017697.78 C30 H20 IN 03 (M+H)+ 452.0367 1 130904.93 C20 H20 IN 03 (M+H)+ 453.0392 1 11727.32 (C30 H20 IN 03 (M+H)+ 457.0386 1 117(B36.5C) H10 IN N+72 72.0386 1 117(B36.5C) H10 IN N+72 74.157	MITE MS Spect x10 ° Cp 4 3 2 1 5 5 9 1 1 0 5 5 9 1 0 1 0 5 5 9 1 0 1 5 1 9 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	00 150 200 00 150 200 00 150 200 00 50 514: C20 H20 50.0557 *H)+ 500 55 Peak List	1 N O3: +E5 250 300 N O3: +E5 0 600	SI MFE Spect 44 (M 350 400 4 Counts I MFE Spect 850 Counts	trum (0.092-0.676 mim) F 50.0557 +1) + +1 vs. Mass-to-Charge (m/2) trum (0.092-0.676 mim) Fi 700 750 800 vs. Mass-to-Charge (m/2)	rag= 175.0V MSH-5438 róo 750 800 850 90 rag= 175.0V MSH-5438 850 900 950	l.d 0 950 l.d 1000	
452.0367 1 130904.93 C20 H20 1 N O3 (M+H)+ 453.0392 1 11722.32 C20 H20 1 N O3 (M+H)+ 472.0386 1 17/B36.52 C20 H10 1 N 03 (M+H)+	MTE MS Seed x10 6 Cp 4 3 2 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1	00 150 200 00 150 200 05 Sectum 5 14: C20 H20 50.0557 +0+ 5 500 556 1 Peak List 2 Abuda 1 Galara	250 300 N 03: +ES 0 600	SI MFE Spect 44 (M 350 400 4 Counts I MFE Spect I MFE Spect 850 Counts	trum (0.092-0.676 mim) F 50.0557 ***********************************	rag= 175.0V MSH-5438 róp 750 800 850 90 rag= 175.0V MSH-5438 850 900 950	0 950 3.d	
453.0392 1 11722.32 C20 H20 1 N 03 (M+H)+ 472.0386 1 171836.52 C20 H19 I N No 02 (M+H)+	MTE MS Seed x10 6 Cp 4 3 2 1 0 1 1 5 5 5 6 4 3 2 1 0 1 5 6 6 7 1 1 0 1 5 1 6 7 1 1 1 1 1 1 1 1 1 1 1 1 1	00 150 200 d 14: C20 H20 00 150 200 H Snetnam 514: C20 H20 South Carlor 1: C20 H20 South Carlor 1: C20 H20 South Carlor 1: South Car	250 300 N 03: +ES 0 600 Formul 7.5 C20 H20 7.5 C20 H20	SI MFE Spect 44 (M 350 400 4 Counts 1 MFE Spect 1 MFE Spect 1 MFE Spect	trum (0.092-0.676 mim) F 50.0557 ***********************************	rag= 175.0V MSH-5438 ród 750 800 850 90 rag= 175.0V MSH-5438 850 900 950	1.d 0 950 1.d	
472.0386 1 171836 52 C20 H19 I N Na C2	MITE MS Spectrum *10 6 Cp 4 3 2 1 0 1 *10 6 Cp *10 7 Cp *10 Cp *10 7 Cp *10 Cp *10 Cp *10 Cp *10 Cp	00 150 200 d 14: C20 H20 d 14: C20 H20 d 50ectnum i 14: C20 H20 50.0557 **10+ 50.0 55 Peak List z Abund 1 546363 1 1017697 1 130906	250 300 N O3: +ES 0 600 Formul 7.5 (20 H20 78 (20 H20) 78 (20 H20 78 (20 H20) 78 (20 H20 78 (20 H20) 78 (20	SI MFE Spect 44 (M 350 400 4 Counts I MFE Spect I MFE Spect I M 03 I N 03	trum (0.092-0.676 mim) F 50.0557 ***********************************	rag= 175.0V MSH-5438 roo 750 800 850 90 rag= 175.0V MSH-5438 850 900 950	3.d 0 950 3.d	
473 0463 + 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	MITE MS Spect x10.6 Cp 4 3 2 1 1 0 1 1 FE MS Zhomw x10.6 Cp x10.6	00 150 200 150 200 150 200 154 C20 H20 154 C20 H20 154 C20 H20 150 200 154 C20 H20 150 200 159 200 159 200 159 200 150 200 10	250 300 N O3: +ES 0 600 Formul 7.5 C20 H20 78 C20 H20 93 C20 H20 93 C20 H20 93 C20 H20	850 400 4 0 100 4 0 100 3 0	trum (0.092-0.676 mim) F 50.0557 (*) + (*)	rag= 175.0V MSH-5438 700 750 800 850 90 rag= 175.0V MSH-5438 850 900 950	J.d 0 950 J.d 0 1000	

¹H NMR (400 MHz, CDCl₃)



3-(4-(tert-butyl)phenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3e)



¹³C {1H} NMR (100 MHz, CDCl₃)



3-(4-(tert-butyl)phenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3e)



HRMS



3-(4-(tert-butyl)phenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3e)

Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment	MSI H10.d Sample Instrument 1 MS Scar.m Success in finite		Sample Name Position User Name Acquired Time DA Methnd	HS11-410 P1-C8 18-01-202 Defaultin	9 14:15:15			
Sample Group Acquisition SW 6 Version 6	200 series TOF/6500 seri 2-TOF 0:05:01 (05125)	Info. cs	3					
Compound Table			Formul	.	Tot Mass	(ppm)	MFG Formula	DB Formula C23 H26 EN 02
Compound Label Cpd 1: C23 H26 I N	02 0.195 475.0	973 13621	C23 H26 L7	N 02	475.1008	-7.52	(2) N/61 N 02	
Compound Label Cpd 1: C23 H26 1 N O2 x10 5 Cpd 1: C23 H26 8 1 0.105 6 4	m/z RT 498.0885 0.199	Algorithm Find By Fo 5. 1003, 476.10	n prouta 081, 498,0500) (Mass 475.0973 Scan Frag=	175.0V MSH	-410.d 1		
2- 0-01 02 03 r6 Spectrum x10 5 Cpd 1: C23 H2 1.75- 1.5- 1.5- 1.5- 1.5- 1.5- 1.5- 1.5- 1.	0.4 0.5 0.6 0.7 6 I N O2: + FBF Spects	0.8 0.9 1 unts vs. Acquis um (0.161-0.4)	1.1 1.2 1.3 ation Time (min) 84 min) MSH41	1,4 1,5	1.6 1.7 1.4	8 1.9 2		
2- 0 01 02 03 MS Spectrum x10 5 Cpd 1: C23 H2 1.75 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.	0.4 0.5 0.6 0.7 6 I N O2 + PBF Speck	0.8 0.9 1 Ints vs. Acquis um (0.161-0.4)	1.1 1.2 13 stion Time (min) 84 min) MSH41	1,4 1,5	1.6 5.7 1.4	8 19 2		
2 0 0.1 02 0.3 MS Spectrum x10 5 1.75 1.25 1.25 1.25 1.25 1.25 1.25 1.25 1.25 1.25 1.25 1.75 1.25 1.25 1.25 1.25 1.75 1.25	0.4 0.5 0.6 0.7 6 I N 02: + FBF Spects 460 482 484	28 0.9 1 Inte vs. Acquis um (0.161-0.40 486 4 unts vs. Mass-1	1,1 1,2 1,3 stion Time (min) 84 min) MSH41 86 min) MSH41 10 SH42 10 SCharge (miz)	1,4 1,5 10,d Subra 452 4	1.6 1.7 1.1 et 94 496	8 1.9 2 1 498		
2 0 0.1 0.2 0.3 NS Spectrum x10 5 Cpd 1: C23 H2 1.75 1.25 1	04 0.5 0.6 0.7 Co 6 I N O2: + FBF Spectr 480 482 484 Co	0.8 0.9 1 Inte vs. Acquis um (0.161-0.4) 486 4 Ints vs. Mess-1	1,1 1,2 1,3 Biton Time (mn) 84 min) MSH41 88 400 Iso Charge (m/z) 84 mn) MSH41	1,4 1,5 10.d Subra 492 4	1.6 1.7 1.4 et 34 496 et	8 1.9 2 		
2 0 01 02 03 MS Spectrum x10 5 Cpd 1: C23 H2 1.75 1.5 1.5 1.5 0 478 1028 0 478 1028 0 478 1028 1.75 0.5 0 478 1028 1.75 0.5 0 478 1028 1.75 0.5 0 478 1028 1.75 0.5 0 478 1028 1.75 0.5 0 478 1028 1.75 0.5 0 1.75 0.5 0 1.75 0.5 0 1.75 0.5 0 0 1.75 0.5 0 0 1.75 0.5 0 0 1.75 0.5 0 0 1.75 0.5 0 0 0 0 0 0 0 0 0 0 0 0 0	480 482 484 6 I N O2: + FBF Spectr 480 482 484 6 I N O2: + FBF Spectr 480 (M4	0.6 0.9 1 	1,1 1,2 1,3 Ellon Time (mn) 84 min) M5H41 85 400 Ia-Charge (m/z) 84 min) M5H41	1,4 1,5 10,d Subra 492 4 0,d Subra	1,6 1,7 1,4 et 34 496 et	8 1.9 2		
2 0 0.1 02 0.3 MS Spectrum x10 5 1.75 1.25 1.75 0.25 0 478.1028 (M+H)= 0.23 H2 478.1028 (M+H)= 0.23 H2 478.1028 1.75 0.25 0 478.1028 1.75 0.25 1.75 0.25 1.75 0.25 1.75 0.25 1.75 0.25 1.55 1.	0.4 0.5 0.6 0.7 0.4 0.5 0.6 0.7 6 I N 02: + FBF Spectr 480 482 484 Co 6 I N 02: + FBF Spectr 470 6 I N 02: + FBF Spectr 470 484 484 484 484 484 484 484 48	0.8 0.9 1 	1,1 1,2 1,3 Elion Time (mn) 84 min) M5H41 88 400 Iso-Charge (m/z) 84 min) M5H41	1.4 1.5 10.d Subra 452 4 0.d Subra	1,6 1,7 1,1 et d4 496 ex	468		
2 0 0.1 02 0.3 MS Spectrum x10 5 1.25 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.	0.4 0.5 0.6 0.7 0.4 0.5 0.6 0.7 6 I N 02: + FBF Spectr 480 482 484 Co 6 I N 07: + FBF Spectr 476 G (M-	486 44 um (0.161-0.41 um (0.161-0.41 um (0.161-0.41 um (0.161-0.42 um (0.161-0.42 um (0.161-0.42	1,1 1,2 1,3 Eston Time (mm) 84 min) M5H41 88 490 50 Asrga (m/z) 84 min) M5H41	1.4 1.5 10 d Subra 492 4	1,6 5,7 1,1 et 34 496 et	8 1.9 2		
2 0 0.1 02 0.3 MS Spectrum x10 5 Cpd 1: C23 H2 1.75 1.25 1.25 1.25 1.25 0 478 1028 MHH = 1.75 0.25 0 478 1023 H2 1.75 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.25 1.55 1.	0.4 0.5 0.6 0.7 6 I N 02: + FBF Spectr 480 482 484 CO 6 I N 07: + FBF Spectr 476 G (M-	486 44 um (0.161-0.41 um (0.161-0.41 um (0.161-0.42 um (0.161-0.42 um (0.161-0.42 um (0.161-0.42	1,1 1,2 1,3 Ellon Time (mn) 34 min) M5H41 88 400 89 400 89 (mk) 84 min) M5H41 498 005 (M*H4)	1,4 1,5 10.d Subra 492 4 0.d Subra	1,6 5,7 1,1 et 34 496 et	8 1.9 2		
2 0 0.1 02 0.3 MS Spectrum x10 5 Cpd 1: C23 H2 1.75 1.25 1.25 0.478 1028 (M+H)= KS Jaoned Spectrum x10 5 Cpd 1: C23 H2 1.75 0.5 0.5 1.2	0.4 0.5 0.6 0.7 0.4 0.5 0.6 0.7 6 I N 02: + FBF Spectr 480 482 484 Co 6 I N 02: + FBF Spectr 476 0 (M+	486 44 unis vs. Acquis um (0.161-0.41 unis vs. Mess-1 um (0.161-0.42 0+	11 12 13 Ellon Time (mm) 84 min) MSH41 88 493 82 Charge (mM) 84 min) MSH41 498 085 (M+N4)	1,4 1,5 10.d Subra 452 4 0.d Subra	1.6 1.7 1.1 et 34 496 et	8 1.9 2		
2 0 0.1 0.2 0.3 MS Spottrum x10 5 Cpd 1: C23 H2 1.75 1.25 1.25 0.5 0.5 0.75 0.5 0.5 0.75 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.	480 482 484 6 I N O2: + FBF Spectr 480 482 484 Co 6 I N O2: + FBF Spectr 460 465 470 455 Co	480 485 480	11 12 13 Elion Time (mn) 84 min) MDH41 88 405 82 405 84 min) MDH41 408 055 (M+14) 400 455 50 10-Charge (m8)	1,4 1,5 10.d Subra 452 4 0.d Subra 5 *	1,6 1,7 1,4 et d4 496 et	8 1.9 2 460		
2 0 0.1 0.2 0.3 MS Spectrum x10 5 Cpd 1: C23 H2 1.75 1.25 1.25 0.478 HS Jaomed Spectrum x10 5 Cpd 1: C23 H2 1.75 0.5 0.478 HS Jaomed Spectrum x10 5 Cpd 1: C23 H2 1.75 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.	480 482 484 6 1 N O2: + FBF Spectr 480 482 484 6 1 N O2: + FBF Spectr 460 465 470 476 6 460 465 470 476 6 91 4 1 Formula	480 485 480 485 480 485 480 485 480 485 480 485 480 485 128	11 12 13 Ellon Time (mn) 84 min) MDH41 88 405 85 405 85 405 85 405 85 405 84 min) MDH41 408 055 (M+14) 408 055 (M+14) 408 055 (M+14) 408 055 (M+14)	1,4 1,5 10.d Subra 452 4 0.d Subra 5 *	1,6 1,7 1,4 et 34 496 et	8 1.9 2 460		
2 0 0.1 02 0.3 MS Spectrum x10 5 Cpd 1: C23 H2 1.75 1.25 1.25 1.25 0 478 HS Jaomed Spectrum x10 5 Cpd 1: C23 H2 1.75 0.25 0 478 HS Jaomed Spectrum x10 5 0.25 0 450 455 HS Spectrum Peak L1 m/z a laboration of the laboration	480 482 484 6 I N 02: + FBF Spectr 480 482 484 Co 6 I N 02: + FBF Spectr 460 465 420 455 460 465 420 455 6 Fermula 5 51122 (2310729x02)	486 44 um (0.161-0.44 um (0.161-0.44 um (0.161-0.44 um (0.161-0.44 0.45	1,1 1,2 1,3 Elicon Time (mm) 84 min) M5H41 84 min) M5H41 85 490 80 Charge (m2) 84 min) M5H41 498 0856 (M*H4) 450 455 50 51 Charge (m3) 91 91 91 91 91 91 91 91 91 91	1,4 1,5 10 d Subra 452 4 0.d Subra 15 *	1,6 1,7 1,1 et 34 496 et	8 1.9 2		
2 0 0.1 0.2 0.3 NS Seathum x10 5 Cpd 1: C23 H2 1.75 1.25 1.25 1.25 1.25 4.78 (Vi+I)= 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	450 452 454 450 452 454 450 455 470 475 61N 02: + FBF Spectr 450 475 61N	0,1 0,0 1 1,115 vs, Aoquis 486 4 486 4 486 4 486 4 086 4 094 4 10 10 10 10 10 10 10 10 10 10	11 12 13 13 12 13 13 12 13 14 min) MSH41 84 min) MSH41 88 400 10 Charge (m/s) 84 min) MSH41 498 055 (M*N4) 400 455 10 Charge (m/s) 80 81 410 410 410 410 410 410 410 41	1,4 1,5 10 d Subra 4\$2 4 0.d Subra 15 *	1,6 1,7 1,1 et d4 496 et	8 1.9 2 498		
2 0 0 0 0 0 0 0 0 0 0 0 0 0	480 482 484 480 482 484 6 1 N O2: + FBF Spectr 480 482 484 Co 6 1 N O2: + FBF Spectr 480 485 470 455 6 1 N O2: + FBF Spectr 480 485 470 455 476 Co 6 1 N O2: + FBF Spectr 480 485 470 455 476 Co 81 Co	486 4 486 4 486 4 486 4 486 4 486 4 480 4 48	11 12 13 allon Time (mn) 84 min) M5H41 84 min) M5H41 84 min) M5H41 84 min) M5H41 400 455 45 84 min) M5H41 400 455 45 84 min) M5H41 400 455 45 84 min) M5H41 400 455 45 84 min) M5H41 450 455 45 85 min) M5H41 450 455 45 85 min) M5H41 45 mi	1,4 1,5 10.d Subra 452 4 0.d Subra 15 *	1.6 1.7 1.4 et d4 496 et	8 1.9 2		
2 0 0.1 0.2 0.3 NS Spottrum x10 5 Cpd 1: C23 H2 1.75 1.25 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.	460 465 470 475 6 I N O2: + FBF Spectr 460 465 470 476 6 I N O2: + FBF Spectr 460 465 470 475 6 I N O2: + FBF Spectr 460 465 470 475 6 I N O2: + FBF Spectr 476 Co 6 I N O2: + FBF Spectr 477 Co 7 I N O2: + FBF Sp	480 445 480 445 480 445 480 445 480 465 480 480 465 480 465	11 12 13 2100 Time (min) 24 min) MDH41 24 min) MDH41 25 40 25 40 26 055 26 055	1,4 1,5 10.d Subra 492 4 0.d Subra	1,6 1,7 1,1 et 94 496 et	8 1.9 2 450		
2 0 0.1 0.2 0.3 NS Spectrum x10 5 Cpd 1: C23 H2 1.75 1.25 1.25 0.478 NS Jaomed Spectrum x10 3 Cpd 1: C23 H2 1.75 1.25 0.478 NS Jaomed Spectrum x10 3 Cpd 1: C23 H2 1.75 1.25 0.478 NS Jaomed Spectrum x10 3 Cpd 1: C23 H2 1.75 1.25 1.25 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.	480 482 484 480 482 484 61 N 02: + FBF Spectri 480 482 484 Co 61 N 02: + FBF Spectri 460 465 470 475 61 N 02: + FBF Spectri 475 50 61 N 02: + FBF S	480 445 480 485 480 480 485 480 480 480 480 480 480 480 480 480 480 480 480	1,1,1,2,1,3 2,1,1,2,1,3 2,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1	1,4 1,5 10 d Subres 452 4 0.d Subres 5 *	1,6 1,7 1,1 et 34 496 et	8 1.9 2		
2 0 0.1 0.2 0.3 NS Seathum x10 5 Cpd 1: C23 H2 1.75 1.25 1.25 1.25 1.25 4.78 1.25 1.25 4.78 1.25 1.25 4.78 1.25 1.25 4.78 1.25 1.25 4.78 1.25 1.25 4.78 1.25 1.25 4.78 1.25 1.25 4.78 1.25 1.55 1.55 1.	450 452 454 450 452 454 450 452 454 450 455 470 475 61N 02: + FBF Spectri 450 455 470 475 70 475	0,1 0,0 1 ants vs. Acquis 486 4 486 4 ants vs. Mess-1 um (0,161-0,42 084 094 104 104 104 104 104 104 104 10	11 12 13 13 12 13 14 min) MSH41 84 min) MSH41 85 400 10 Charge (m/z) 84 min) MSH41 498 055 (M*N4) 400 455 10 Charge (m/z) 80 410 400 455 10 Charge (m/z) 81 410 400 455 10 Charge (m/z) 81 410 420 455 10 Charge (m/z) 81 410 420 455 10 Charge (m/z) 81 410 420 455 10 Charge (m/z) 81 410 420 455 10 Charge (m/z) 81 420 455 10 Charge (m/z) 81 81 81 81 81 81 81 81 81 81	1,4 1,5 10 d Subra 4\$2 4 0.d Subra 15 *	1,6 1,7 1,1 et 34 496 et	8 1.9 2		


3-(4-fluorophenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3f)





3-(4-fluorophenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3f)





3-(4-fluorophenyl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3f)

Sample Type Instrument Name Acq Method IRM Calibration Stal Comment	MGH Samp Instru HS Sc Net	434,d rie ment 1 ran m 91	a la finh	Sample Name Position User Name Acquired Time DA Method	MSII-424 P1-85 19-10-202 Default.m	3 13 07 43			
Sample Group Acquisition SW Version	6200 series TDP Q-TDP B.05.01 (/6500 series (85125)	Info.	3					
Compound Labe							D// 1		
Cpd 3: C19 H17 #	IN 02 0.15	437.030	Abund 9 64699	C19 H17 F 1	N 02	Tgt Mass 437.0288	(ppm) 4.78	MFG Formula C19 H17 F 1 N O2	C19 H17 F IN O2
Compound Label Cpd 1: C19 H17 F 1 N	//////////////////////////////////////	RT 0.15	Algorith Find By F	m onmula	Mass 437.0309				
x10 6 Cpd 1: C191	H17 F I N 02: +E	SI EIC(438	0361, 460	0180) Scan Frag	=175.0V M	SH-424 d			
2							: 1		
1.5									
1.									
05									
0.5	-								
01 02	1000 million 1000 million	10 A.A.							
N	0.3 0.4 0								
0.0.2	0.3 0.4 0	Counts	0.7 0. vs. Acquit	8 0.9 1 sition Time (min)	1.1 1.2	2 1.3 1.	4 1.5		
6 Spectrum	0.3 0.4 0	Counts	0.7 0. vs. Acquir	8 019 1 sition Time (min)	1.1 1.2	2 1.3 1.	4 1.5		
5 Spectrum x10 c Cpd 1: C19 H	0.3 0.4 0	BF Spectrur	0.7 0 vs. Acquit	8 0.9 1 sition Time (min) 250 min) MSH-4	1.1 1.2 24.d Subtra	2 1.3 1. ICT	4 1.5		
5 Spectrum x10 6 Cpd 1: C19 H	0.3 0.4 0	BF Spectrur	0.7 0 vs. Acquit	8 09 1 sition Time (mis) 250 min) MSH-43	1.1 1.2 24.d Subtra	2 1.3 1. Het	4 1.5		
5 Spectrum x10 6 Cpd 1: C19 H 12- 1.0.8-	0.3 0.4 0	BF Spectrum	0.7 0 vs. Acquir	8 0.9 1 sition Time (min) 250 min) MSH-4	1.1 1.2 24.d Subtra	2 1.3 1. Ict	4 1.5		
5 Spectrum x10 e Cpd 1: C19 H 1.2 1. 0.8 0.6	03 0.4 0	BF Spectrum	0.7 0 vs. Acquir	8 09 1 pition Time (min) 250 min) MSH-4;	1.1 1.2 24.d Subtra	2 1.3 1. Ici	4 1.5		
5 Spectrum x10 c Cpd 1: C19 H 1.2 1. 0.8- 0.6- 0.4-	03 0.4 0	BF Spectrur	0.7 0 vs. Acquir	8 09 1 bition Time (min) 250 min) MSH-4;	1.1 1.2 24.d Subtra	2 1.3 1.	4 1.5		
S Spectrum x 10 e 12 1 0.8 0.5 0.4 0.2	03 0.4 0	BF Spectrum	0.7 0 vs. Acquir	8 09 1 iilion Time (min) 250 min) MSH-4	1.1 1.2	2 1.3 1.	4 1.5		
CF 0.2 S Spectrum 1.2 0.8 0.6 0.4 0.2 0	0.3 0.4 0	BF Spectrum	ws. Acquit	8 09 1 Jitoo Time (min) 250 min) MSH 4	1.1 1.2	2 1.3 1. HCI 460.019 (M=Naj-	8		
55 Spectrum x10 6 Cpd 1: C19 H 1.2 1 0.8 0.6 0.6 0.4 0.2 0 440	0.3 0.4 0	15 0.5 Courtes BF Spectrum	0.7 0 v3. Acquit = (0.083-0	8 09 1 uition Time (mis) 250 min) MSH-4.	1.1 1.2 24.d Subira 456 4	460.019 (M+Na)+ 58 460	4 1.5		
55 Spectrum x10 6 Cpd 1: C19 H 1.2 1. 0.8 0.5 0.4 0.2 0 440 	0.3 0.4 0	BF Spectrum	9.7 0 vs. Acquit m (0.083-0 vs. Mass-1	8 0.9 1 Jitloo Time (mis) 250 min) MSH-4. 250 min) MSH-4. 452 454 0-Change (miz)	1.1 1.2 24 d Subtra 456 40	2 1.3 1. 460.019 (M*Na)+ 58 460	4 1.5 8 462		
55 Spectrum x10 6 Cpd 1: C19 H 1.2 1. 0.8 0.6- 0.4 0.2 0 440 200med Spectrum x10 6 Cpd 1: C19 H1	0.3 0.4 0	145 445 Counts	0.7 0 vs. Acquit m (0.083-0 vs. Mass-1 vs. Mass-1	452 454 0.9 1 250 min) MSH4 452 454 0-Charpe (m/2) 250 min) MSH4	1.1 1.2 24.d Subtra 456 4	2 1.3 1. HCD 019 (M+Ne)- 55 460	4 1.5 8 462		
55 Spectrum x10 6 Cpd 1: C19 H 1.2 1 0.8 0.6 0.4 0.2 0 440 200med Spectrum x10 6 Cpd 1: C19 H	642 444 4	5 0.5 Courses BF Spectrum 646 448 Counts F Spectrum 438 0382	0.7 0 vs. Acquit m (0.083-0 vs. Mass-1 vs. Mass-1	8 0.9 1 Jition Time (min) 250 min) MSH-4 452 454 b-Change (m/z) 250 min) MSH-42	1.1 1.2 24.d Subtra 456 4:	2 1.3 1. HCD 019 (M+Ne)- 55 460	4 1.5 8 462		
CF 0.2 S Spectrum x10 c Cpd 1: C19 H 1.2 1. 0.8 0.6 0.4 0.2 0 440 200med Spectrum x10 c Cpd 1: C19 H 1.2 1. 0.8 0.6 0.4 0.2 0 440 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2	0.3 0.4 0 117 F I N 02: + F(442 444 4 17 F I N 02: + FB	 5 0.5 Courses 6 Courses 7 Cou	450 vs. Acquir vs. Acquir vs. Mass-1 vs. Mass-1	8 0.9 1 Jition Time (min) 250 min) MSH-4 452 454 e-Change (m/z) 250 min) MSH-42	1.1 1.2 24.d Subtra 456 4: 4.d Subtra	460 019 (M*Na)- 58 460	4 1.5 8 462		
55 Spectrum x10 6 Cpd 1: C19 H 1.2 1. 0.8 0.6 0.4 0.2 0 440 200med Spectrum x10 6 Cpd 1: C19 H 1.2 1.2 0.8 0.6 0.4 0.2 0 440 200med Spectrum	642 646 4	His Courses BF Spectrum Courses F Spectrum 438.0382 (M+H)+	450 450 450 450 450 450 450 450 450 450	8 0.9 1 Jition Time (min) 250 min) MSH-4: 452 454 6-Change (miz) 250 min) MSH-42	1.1 1.2 24 d Subtra 456 4 4.4 Subtra	2 1.3 1. het 460.019 (M*Na)- 58 460 ct	4 1.5 8 462		
55 Spectrum x10 6 Cpd 1: C19 H 1.2 1.2 1.2 0.8 0.6 0.4 0.2 0 440 .2 200med Spectrum x10 6 Cpd 1: C19 H1 1.2 1.2 0.8 0.6 0.4 0.2 0 440 .2 0.8 0.6 0.6 0.6 0.6 0.6 0.6 0.6 0.6	0.3 0.4 0	13 Courtes Courtes BF Spectrum Counts F Spectrum 438.0382 (M+)-()+	9,7,0 9,7,7,0 9,10,083-0 1,450 1,	8 0.9 1 Jition Time (min) 250 min) MSH-4 0-Change (m/2) 250 min) MSH-42	1.1 1.2 24 d Subtra 456 4 4.d Subtrar	2 1.3 1. http://www.com/com/com/com/com/com/com/com/com/com/	4 1.5		
55 Spectrum x10 c Cpd 1: C19 H 1.2 1 0.8 0.6 0.4 0.2 0 440 200med Spectrum x10 c Cpd 1: C19 H 1.2 1 0.8 0.6 0.4 0 0 0 0 0 0 0 0 0 0 0 0 0	0.3 0.4 0	5 O.B. Courses BF Spectrum 438 O.82 (M*)-()*	450 (0.083-0 (0.083-0) (0.083-0)	8 0.9 1 Jition Time (min) 250 min) MSH-4 452 454 0-Change (m2) 250 min) MSH-42	1.1 1.2 24 d Subtra 456 4 4.d Subtrar	2 1.3 1. her (M-Na)- 58 460 ct	4 1.5 8 462		
55 Spectrum x10 c Cpd 1: C19 H 1.2 1. 0.8 0.6 0.4 0.2 0 440 440 200med Spectrum c10 c Cpd 1: C19 H1 1.2 1. 0.8 0.6 0.4 0.2 0 440	0.3 0.4 0 117 F I N 02: + F(442 444 4 7 F I N 02: + FB	5 Outres Courses BF Spectrum F Spectrum 438.0382 (M+H)+	450 450 450 450 10.083-0	452 454 452 454 -Charpe (m/2) 250 min) MSH-42 450 min) MSH-42 460 0158 (M*Na)*	1.1 1.2 24.d Subtra 456 40	2 1.3 1. hct 400 D19 (M+Na)- (M+Na)- 55 460 ct	4 1.5		
55 Spectrum x10 c Cpd 1: C19 H 1.2 1. 0.8 0.6- 0.4 0.2 0 440 200med Spectrum c10 c Cpd 1: C19 H1 1.2 1. 0.8- 0.6- 0.4 0.6- 0.4 0.6- 0.4 0.6- 0.4 0.6- 0.4 0.6- 0.4 0.6- 0.4 0.6- 0.6- 0.4 0.6- 0.6- 0.6- 0.4 0.6- 0.	642 444 4	5 Courtes BF Spectrum Courtes F Spectrum 438 0382 (M+)-()+	450 vs. Mass-1	452 454 452 454 -Change (m/z) 250 min) MSH-42 460 0198 (M+Ha)+	1.1 1.2 24.d Subtra 456 4 4.d Subtrar	2 1.3 1. 6CT 460 019 (M-Na) 55 460 Ct	4 1.5		
55 Spectrum x10 c Cpd 1: C19 H 1.2 1.2 1.2 1.2 0.8 0.6 0.4 0.2 0 440 .2 200med Spectrum c10 c Cpd 1: C19 H1 1.2 1.2 0.4 0.2 0 440 .2 0 440 .2 0 440 .2 0 .2 0 .2 0 .2 0 .2 0 .2 0 .2 .2 .2 .2 .2 .2 .2 .2 .2 .2	642 444 4 17 F I N O2: + F6 17 F I N O2: + F6	Counter Counter Counter Counter Spectrum Gounts FSpectrum Gounts Societ Societ	445 450	452 454 452 454 452 454 6-Change (m/z) 250 min) MSH-42 460 0198 [M+Na)+ -Change (m/z)	1.1 1.2 24.d Subtra 456 4 4.d Subtrar	2 1.3 1. 400 019 (M=N2) 58 460 ct	4 1.5		
55 Spectrum x10 c Cpd 1: C19 H 1.2 1.2 1.2 0.8 0.6 0.4 0.2 0 440 500med Spectrum x10 c Cpd 1: C19 H 1.2 0.8 0.6 0.4 0.2 0 440 500med Spectrum x10 c Cpd 1: C19 H 1.2 1.2 0.8 0.4 0.2 0 440 500med Spectrum x10 c Cpd 1: C19 H 1.2 1.2 0.8 0.6 0.4 0.2 0 440 500med Spectrum x10 c Cpd 1: C19 H 1.2 1.2 0.8 0.6 0.4 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8	0.3 0.4 0 117 F I N 02: + FE 442 444 4 17 F I N 02: + FB 0 425 430 4	BF Spectrum Gounts F Spectrum 438.0382 (M*)()*	9,7,0 9,7,7,0 9,0,083-0 9,0,000 9,0000 9,000 9,000 9,0000 9,0000 9,0000	8 0.9 1 uition Time (min) 250 min) MSH-4: 452 454 0-Charpe (m/2) 250 min) MSH-42 460 0158 (M+Na)+ 0 455 460 4 -Charge (m/2)	1.1 1.2 24 d Subtra 456 4 4.d Subtrar 65 420 -	2 1.3 1. ect (M=Na)- 58 460 et	4 1.5		
S Spectrum x10 c Cpd 1: C19 H 1.2 1.2 0.8 0.6 0.4 0.2 0 440 200med Spectrum x10 c Cpd 1: C19 H 1.2 0.8 0.6 0.4 0.2 0 440 200med Spectrum x10 c (2pd 1: C19 H 1.2 0.8 0.6 0.4 0.5 0.4 0.8 0.6 0.4 0.5 0.4 0.8 0.6 0.4 0.5 0.6 0.4 0.8 0.6 0.4 0.8 0.6 0.4 0.8 0.6 0.4 0.8 0.6 0.4 0.8 0.6 0.4 0.8 0.8 0.6 0.4 0.8 0.8 0.8 0.6 0.4 0.8 0.8 0.8 0.6 0.4 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8	0.3 0.4 0 117 F I N 02: + FE 442 444 4 7 F I N 02: + FB 0 425 430 4 Rt [Formula	5 Guines BF Spectrum F Spectrum F Spectrum 438.0382 (M+H)+ Counts +	0.7 0 vs. Acquir (0.083-0 (0.083-0 (0.083-0; 445 452 445 452 1267	8 0.9 1 Jition Time (min) 250 min) MSH-4: 452 454 0-Charge (m2) 250 min) MSH-42 460 D158 (M+Na)+ -Charge (m/2)	1.1 1.2 24 d Subtra 456 e 4.d Subtras	2 1.3 1. 100 019 (M-Ne)- 58 460 ct	4 1.5 8 462		
5 Spectrum x10 c Cpd 1: C19 H 12 1 0.8 0.6 0.4 0.2 0 440 2 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 0 440 2 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 2 1 1 1 2 1 1 1 2 1 1 1 2 1 1 1 2 1 1 1 2 1 1 1 2 1 1 1 1 2 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1	0.3 0.4 0 117 F I N 02: + F(442 444 4 7 F I N 02: + FB 0 425 430 4 st Formula 668 88 (19H18/2)	County	450 450 465 450 10 083-0 10 083-0	452 454 452 454 0-Crange (m/2) 250 min) MSH-42 460 0198 (M1-Na)* 460 0198 (M1-Na)* 460 0198 (M1-Na)* 460 0198 (M1-2) 455 460 452 454 460 0198 (M2) 455 460 100 - 20	1.1 1.2 24 d Subtra 456 4 4.d Subtran	2 1.3 1. 600 0193 (M=Na)- (M=Na)- 55 460 61 475 460	4 1.5		
S Spectrum x10 c Cpd 1: C19 H 12 1 0.8 0.6 0.4 0.2 0 440 2 200med Spectrum c10 c Cpd 1: C19 H 12 1 0.8 0.6 0.4 0.2 0 440 2 2 0 440 2 2 0 440 2 2 2 2 2 2 2 2 2 2 2 2 2	0.3 0.4 0 117 F I N 02: + F(642 444 4 17 F I N 02: + FB 0 425 430 4 17 F I N 02: + FB 0 425 430 4 18 Formula 64 88 6 (29118)/19 754.39 (19118)/19	Country	0.7 0 vit Acquir (0.083.0 445 450 (0.083.0) 445 450 10.083.0	452 454 452 454 -Change (m/z) 250 min) MSH-42 460 0158 (M+Na)+ -Change (m/z) 460 0158 (M+Na)+ -Change (m/z) 460 455 460 4 -Change (m/z)	1.1 1.2 24.d Subtra 456 4 4.d Subtrar	2 1.3 1. 5CT 460 019 (M*Ra) 55 460 CT 475 480	4 1.5		
S Spectrum x10 c Cpd 1: C19 H 1.2 1.2 1.2 1.2 0.8 0.6 0.4 0.2 0 440 2.2 0 4.5 2.2 0 4.5 2.2 0 4.5 2.2 0 4.5 2.2 0 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.2 4.5 2.5 4.5 4.5 2.5 4.5 4.5 4.5 4.5 4.5 4.5 4.5 4	0.3 0.4 0 117 F I N 02: + Fi 442 444 4 17 F I N 02: + FB 0 425 430 4 at Formula 658.43 (19H18FB 659.432 (19H18FB 659.432 (19H18FB 659.432 (19H18FB	Counts Counts	0.7 0 vit Acquir (0.083.0	8 0.9 1 uition Time (min) 250 min) MSH-4: 452 454 0-Charpe (m/2) 250 min) MSH-42 460 0158 (M+Na)+ 0 455 460 4 -Charge (m/2) 460 0158 (M+Na)+ 0 455 460 4 -Charge (m/2)	1.1 1.2 24 d Subtra 456 4 4.d Subtrar 65 420 4	2 1.3 1. 400.019 (M=N2)- 58 460 et	4 1.5		
S Spectrum x10 c Cpd 1: C19 H 12 1 0.8 0.6 0.4 0.2 0 440 200med Spectrum x10 c Cpd 1: C19 H 12 0.8 0.6 0.4 0.2 0 440 200med Spectrum x10 c Cpd 1: C19 H 12 0.8 0.6 0.4 0.2 0 440 440 440 440 440 440 440	0.3 0.4 0 117 F I N 02: + Fg 442 444 4 7 F I N 02: + FB 0 425 430 4 R Formula 4648 (29418/P) 754.39 (19418/P) 754.39 (19418/P) 755.39 (19418/P) 7	Counts Counts	445 450 445 450 (0.083-0	8 0.9 1 witten Time (min) 250 min) MSH-4: 452 454 0-Charge (m2) 250 min) MSH-42 460 0158 (M+Na)+ -Charge (m/2) 455 460 4 -Charge (m/2) 459	1.1 1.2 24 d Subtra 456 e 4.d Subtran	2 1.3 1. 100 019 (M-Ne)- 58 460 ct	4 1.5 8 462		
S Spectrum x10 c Cpd 1: C19 H 12 1 0.8 0.6 0.4 0.2 0 440 2 2 0 440 45 42 3 5 42 45 45 45 45 45 45 45 45 45 45	0.3 0.4 0 117 F I N 02: + F(442 444 4 7 F I N 02: + FB 0 425 430 4 4 17 F I N 02: + FB 0 425 430 4 17 F I N 02: + FB 0 425 430 4 17 F I N 02: + FB 0 425 430 4 17 F I N 02: + FB 0 425 430 4 17 F I N 02: + FB 0 425 430 4 17 F I N 02: + FB	Countes Countes Countes Countes Spectrum 438.0382 (M+)-()+ (M+)-()+ (M+)-()+ (M+)	445 450 445 450 (0.083-0	452 454 452 454 0-Crange (m/z) 250 min) MSH-4: 460 0198 (M+Na)* 250 min) MSH-42 460 0198 (M+Na)* 460 0198 (M+Na)* 460 0198 (M+Na)* 460 0198 (M-Na)* 460 0198 (M-Na)* (M-N	1.1 1.2 24 d Subtra 456 4 4.d Subtran	2 1.3 1. 501 100 019 (M=Na)- (M=Na)- 58 460 01 01 01 01 01 01 01 01 01 0	4 1.5		
S Spectrum x10 c Cpd 1: C19 H 12 1 0.8 0.6 0.4 0.2 0 440 2 2 2 2 2 2 2 2 2 2 2 4 4 2 2 2 2 2 2 4 4 4 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4	0.3 0.4 0 117 F I N 02: + F(442 444 4 7 F I N 02: + FB 0 425 430 4 17 F I N 02: + FB 0 40 4 17 F I N 02: + FB 0 40 4	Country	445 450 445 450 (0.083-0 445 450 (0.083-0 1 445 450 (0.083-0 1 1 1 1 1 1 1 1 1 1 1 1 1	452 454 452 454 - Charge (m/2) 250 min) MSH-42 460 01585 (M+Na)+ - Charge (m/2) 250 min) MSH-42 460 01585 (M+Na)+ - Charge (m/2) - State (m/2) -	1.1 1.2 24.d Subtra 456 4 4.d Subtrar	2 1.3 1. 400 019 (M+Ra) 55 400 ct	4 1.5		
S Spectrum x10 c Cpd I: C19 H 1.2 1.2 1.2 0.8 0.6 0.4 0.2 0 440 200med Spectrum 10 c Cpd I: C19 H1 1.2 0.8 0.6 0.4 0.2 0 440 200med Spectrum 10 c Cpd I: C19 H1 1.2 1.0 0.8 0.6 0.4 0.2 0 440 200med Spectrum 10 c Cpd I: C19 H1 1.2 1.0 0.8 0.6 0.4 0.2 0 440 200med Spectrum 10 c Cpd I: C19 H1 1.2 1.0 0.8 0.6 0.4 0.2 0 440 200med Spectrum 12 1.0 0.8 0.6 0.4 0.4 0.4 1.2 1.0 0.8 0.6 0.4 0.8 0.6 0.4 0.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 440 2.2 0 4.15 4.2 2.1 1.0 0.8 0.8 0.6 0.4 0.8 0.6 0.4 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8	0.3 0.4 0 117 F I N 02: + Fi 442 444 4 7 F I N 02: + FB 0 425 430 4 8 7 F I N 02: + FB 0 425 430 4 8 7 F I N 02: + FB 0 425 430 4 8 8 7 F I N 02: + FB 0 425 430 4 8 8 7 7 8 8 7 8 8 7 8 8 8 7 8 8 7 8 8 8 7 8 8 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8	Countes C	445 450 445 450 10083-0 100	8 0.9 1 uition Time (min) 250 min) MSH-4: 452 454 0-Charge (m/2) 250 min) MSH-42 460 0158 (M+Na)+ 0-455 460 4 -Charge (m/2) 460 0158 (M+Na)+ 10 10 10 10 10 10 10 10 10 10	1,1 1,2 24 d Subtra 456 e 4,d Subtrae	2 1.3 1. 1400 019 (M*Na)- 58 460 ct	4 1.5		



2-(4-hydroxybutyl)-4-iodo-3-(thiophen-3-yl)isoquinolin-1(2H)-one (3g)





2-(4-hydroxybutyl)-4-iodo-3-(thiophen-3-yl)isoquinolin-1(2H)-one (3g)





2-(4-hydroxybutyl)-4-iodo-3-(4-nitrophenyl)isoquinolin-1(2H)-one (3h)





2-(4-hydroxybutyl)-4-iodo-3-(4-nitrophenyl)isoquinolin-1(2H)-one (3h)





2-(4-hydroxybutyl)-4-iodo-3-(4-nitrophenyl)isoquinolin-1(2H)-one (3h)

Data File Sample Type Instrument Name Acq Nethod IRM Calibration Status Comment	MSH-S78.d Sample Instrument 1 MS Scan m Succest	Sample Name HSI Position P1-1 User Name Acquired Time 24.0	н-528 И ив 2003 13:55:38 ийтт		
Sample Group Acquisition SW 62 Version Q-	Te D0 series TOF/6500 series TOF 8.05.01 (P5125)	fa, 3			
Compound Table			I Diff		
Compound Label Col 1: C19 H17 I N2 O	RT Nass A 0.145 464.0252	2381 C19 H17 I N2 C4	Tgt Mass (ppm) 464.0233 4	C19 II17 1 N2 O4	C19 H17 1 M2 04
x10 3 Cpd 1: C19 H17 4 1 0.145 4 2 1 0 0 1 0 2 0.3 MS Spectrum x10 3 Cpd 1: C19 H17 25 2 1.5 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0	1 N2 C4: +ESI EIC(465.03 0/4 C/5 0/6 0/7 0/8 0/ Counts va 1 N2 C4: + FBF Spectrum (0	06, 482.0571, 487.0125, 502 1, 1, 1, 2, 1, 3, 1, 4 Acculation Time (mm) 205-0.211 min) MSH-578.c 3	9865) Scot Freg=175 5 1.6 1.7 1.8 1.9 2		
0 406 468 MS Zoomed Spectrum	470 472 474 Counts vs.	476 478 480 Mass-to-Charge (m/z)	182 484 488		
x10 2 Cpd 1: C19 H17 2.5 1.5 1. 0.5	1 NZ G4: + FEF Spectrum (0 465 0376 (87+1)-	487,0130 (M+Na)+	usuvCl		
0 440 445	450 455 460 465 470 Courts vs.	425 480 485 400 40 Mass-to-Charge (m/z) Ion (H+10+	5 500 505 510 515		
MS Spectrum Peak List m/z z Abund 465.0376 1 2386.85 466.0351 1 575.03 487.013 1 97.81	C19H18DN2O4 C19H18DN2O4 C19H17DN2O4	(H+H)+ (H+Na)+			
MS Spectrum Peak List m/z s Abund 465.0376 i 7385.85 466.0351 i 575.03 487.013 i 97.83 	C1941803204 20394880309 20394820976804	(H+H)+ (H+Na)+			









2-(4-hydroxybutyl)-4-iodo-3-(7-methoxynaphthalen-2-yl)isoquinolin-1(2H)-one (3i)





3-([1,1'-biphenyl]-4-yl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3j)





3-([1,1'-biphenyl]-4-yl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3j)





3-([1,1'-biphenyl]-4-yl)-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (3j)





2-(4-hydroxybutyl)-4-iodo-3-(phenanthren-9-yl)isoquinolin-1(2H)-one (3k)



¹³C {1H} NMR (100 MHz, CDCl₃)



2-(4-hydroxybutyl)-4-iodo-3-(phenanthren-9-yl)isoquinolin-1(2H)-one (3k)





2-(4-hydroxybutyl)-4-iodo-3-(phenanthren-9-yl)isoquinolin-1(2H)-one (3k)

Qualitative Compound Report

Sample Type Instrument Name Acq Nethod IRM Calibration Status Comment	MSH-562.d Sample Instrument I MS Scan.m Success	Sample Name MSI Position P1-0 User Name Acquired Time 13-0 DA Method Defa	1-562 19 19-2023 15:30:46 mit.m		
Sample Group Acquisition SW 6220 Version Q-TC	1 series TOF/6500 series ₩ 8.05.01 (05125)	info. 3			
Compound Table	RT Mass	Abund Formula	Tut Mass (ppm)	MFG Formula	DB Formul
Cpd 1: C27 H22 I N O2	0.111 519.0732	631592 C27 H22 I N O2	519.0095 7.17	C27 H22 IN 02	C27 H22 1 N
Compound Label Cpd 1: C27 H22 I N O2	m/z RT J 520.0811 0.111 F	Vgorithm Mas find Dy Formula 519.	ss 0732		
x10 6 Cpd 1: C27 H22 1	N 02: +ESI EIC(520.0)	768, 521.0801, 542.0587, 543.0	0620) Scan Frag=175.0V		
1.2					
0.6					
0 01 02 03 0	4 0.5 0.6 0.7 0.8 0	9 1 11 12 13 14			
	Country		15 16 17 18 19 2		
MS Spectrum	County of	s. Acquisition Time (min)	1.5 1.6 1.7 1.8 1.9 2		
MS Spectrum	N O2: + FBF Spectrum (0	 Acquisition Time (min) 0.094-0.211 min) MSH-562.d S 	ubtract		
MS Spectrum *10 5 Cpd 1: C27 H22 I / 7	N C2: + FBF Spectrum (rs. Acquisition Time (min) 0.094-0.211 min) MSH-562.d_S	ubtract		
MS Spectrum x10 5 Cpd 1: C27 H22 H 7 6 5	N O2: + FBF Spectrum (rs. Acquisition Time (min) 3.094-0.211 min) MSH-562.d S	ubtract		
MS Spectrum x10 5 Cpd 1: C27 H22 H 6 5 4	N Q2: + FBF Spectrum (rs. Acquisition Time (min) 2.094-0.211 min) MSH-562.d S	ubfract		
MS Spectrum x10 b Cpd 1: C27 H22 I 7 6 5 4 3 2	N O2: + FBF Spectrum (rs. Acquisition Time (min)	ubfract		
MS Spectrum *10 b Cpd 1: C27 H22 I / 6 5 4 3 2 1	N O2: + FBF Spectrum (rs. Acquisition Time (min)	ubtract 542.0587		
MS Spectrum x10 5 Cpd 1: C27 H22 H 6 5 4 3 2 1 0 522 524	526 528 530	rs. Acquisition Time (min) 3.034-0.211 min) MSH-562.d S 5322 534 536 53	542.0587 (M+Na)+ 8 540 542 544		
MS Spectrum x10 b C Cpd 1: C27 H22 11 7 6 5 4 3 2 5 5 5 4 3 2 5 5 5 4 3 2 5 5 5 5 5 5 5 5 5 5 5 5 5	526 528 530 Counts 4	rs. Acquisition Time (min) 3.094-0.211 min) MSH-562.d S 3.094-0.211 min) MSH-562.d S 532 534 535 53 532 534 535 53	542.0587 (M+Na)- 8 540 542 544		
MS Spectrum x10 5 Cpd 1: C27 H22 H 6 5 4 3 2 1 522 524 MS Zoomed Spectrum x10 5 Cpd 1: C27 H22 H Spectrum	V O2: + FBF Spectrum (0 526 528 530 Counts v 4 O2: + FBF Spectrum (0 520.0811	rs. Acquisition Time (min) 3.094-0.211 min) MSH-562.d S 5.32 534 536 53 rs. Mass-to-Charge (m/z) 3.094-0.211 min) MSH-562.d Si	542.0587 (M+Na)+ 8 540 542 544		
MS Spectrum x10 b 7 6 5 4 3 2 1 5 522 524 MS Zoomed Spectrum x10 6 Cpd 1: C27 H22 II 522 524	V Q2: + FBF Spectrum (0 526 528 630 Counts v 4 Q2: + FBF Spectrum (0 520 0811 (14+1)+	rs. Acquisition Time (min) 3.094-0.211 min) MSH-562.d S 5.532 5.54 536 53 5. Mass-to-Charge (m/z) 3.094-0.211 min) MSH-562.d Si	542.0587 (M+Na)+ 8 540 542 544 ubtract		
MS Spectrum x10 b 7 6 5 4 3 2 1 0 522 524 MS Zoomed Spectrum x10 5 Cpd 1: C27 H22 II 522 524 MS Zoomed Spectrum x10 5 7 6 5 4 3 2 5 6 5 7 6 5 7 7 6 5 7 7 7 7 7 7 7 7 7 7 7 7 7	4 O2: + FBF Spectrum (526 528 630 Counts v 4 O2: + FBF Spectrum (520 0811 (U+H)+	rs. Acquisition Time (min) 3.094-0.211 min) MSH-562.d S 5.52 534 535 53 s. Mass-to-Charge (m/2) 3.094-0.211 min) MSH-562.d Si	15 1.5 1.7 1.8 1.9 2 ubtract 542.0587 (M+Na)+ 8 540 542 544 ubtract		
MS Spectrum x10 b 7 6 5 4 3 2 1 0 522 524 MS Zoomed Spectrum x10 5 Cpd 1: C27 H22 II 522 524 MS Zoomed Spectrum x10 5 Cpd 1: C27 H22 II 522 524 MS Zoomed Spectrum	V G2: + FBF Spectrum (526 528 630 Counts v 4 O2: + FBF Spectrum (520 0811 (U+H)+	rs. Acquisition Time (min) 3.094-0.211 min) MSH-562.d S 5.32 534 536 53 5. Mass-to-Charge (m/2) 3.094-0.211 min) MSH-562.d Si	542.0587 (M+Na)+ 8 540 542 544		
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7-chloro-2-(4-hydroxybutyl)-4-iodo-3-(*m*-tolyl)isoquinolin-1(2*H*)-one (5a)



HRMS



7-chloro-2-(4-hydroxybutyl)-4-iodo-3-(m-tolyl)isoquinolin-1(2H)-one (5a)

Qualitative Compound Report Data File MSH-595.d Sample Tostrument 1 MS Scan.m MSH-596 P1-86 Sample Name Sample Type Instrument Name Acq Method IRM Calibration Status Position P1-06 User Name Acquired Time 19-10-2023 13:11:26 Success DA Hethod Default.m Comment Sample Group Acquisition SW Version 3 Info. 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) Compound Table Diff Compound Label Cpd 1: C20 H19 CI 1 N OZ RT 0.1 Mass Abund 467.018 6943 Tgt Mass (ppm) 467.0149 6.64 MFG Formula C20 H19 CI I N O2 DB Formula C20 H19 CI I N O2 Formula C20 H19 CI I N O2 Compound Label m/z Cpd 1: C20 H19 CI 1 N 02 490.0065 Algorithm Find By Formula RT 0.1 Mass 467.018 Cpd 1: C20 H19 CI I N O2: +ESI EIC(468.0222, 470.0200, 490.0041, 492.0019) Scan Frag=175.0.. 110 € 3.5 2.5 2.5 1.5 0.5 01 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 Counts vs. Acquisition Time (min) 1.2 1.3 1.4 1.5 1.1 MS Spectrum x10 6 Cpd 1: C20 H19 CI I N O2: + FBF Spectrum (0.083-0.233 min) MSH-596.d Subtract 1.75 1.5 1.25 0.75 470.0231 (M+H)+ 0.5 490.0065 (M+Na)+ 0.25 04 472 474 476 478 480 482 484 486 Counts vs. Mass-to-Charge (m/z) 470 488 490 492 MS Zoomed Spectrum x10 6 Cpd 1: C20 H19 C11 N O2: + FBF Spectrum (0.083-0.233 min) MSH-596.d Subtract 1.75 468.0252 468.0252 (M+H)+ 1.5 1.25 0.75 0.5 490.0065 (M+Na)+ 0.25 440 445 450 455 460 485 470 475 480 485 490 495 500 505 510 515 Counts vs. Mass-to-Charge (m/z) MS Spectrum Peak List m/z z Abund Fermula 468.0252 1 1592326.25 C20H20CIINO2 469.0292 1 376870.54 C20H20CIINO2 1270231 1 570254 Ion (M+H)+ (M+H)+ 492.022 1 35204/34 COMPUCINC 470.033 1 532144.48 COMPUCINC 472.025 472.0255 1 199512.77 COMPUCINC 472.027 472.0278 1 12916.94 COMPUCINC 472.01102 473.0314 1 1146.1 COMPUCINC 490.0065 1 69434.58 COMPUCINC (M+H)+ (M+H)+ (M+H)+ (M+Na)+



7-chloro-3-cyclopropyl-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (5b)





7-chloro-3-cyclopropyl-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (5b)



HRMS



7-chloro-3-cyclopropyl-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (5b)

Qualitative Compound Report NSH-995.d Sample flatte MSH-595 Sample Pacifirm PFD Leaturnet 1 User Name NS Schum Acquired Time 16:09-3823 13:09-28 Societ ha Nethed Defailtin Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment Sample Group Info 3 Acquisition SW Version 6709 series T0F/6500 series Q-T0F 8.05 01 (85125) Compound Table DW MEG formula C16 F17 O I NOP C16 H17 CT h OZ Tyl Mars (spm) 416.9952 5.40 Abund 25304 Compound Label RT Opt 1: C16HI2 CIT N 02 0.118 Masi 417.005 CIS #17 O INO2 Mass 417.0014 Compound Label #/2 Cpd 1: C16H:7 CT N C2 439.959 N1 Algorithm 0.118 End By Formula x16 8 [Ced 1: Cf6 H17 Cf | N 02 -ESt EIC/4150065, 420.004 L 438.5845 441.5600) Scan Fragm176.0-1.2 1 0_215 0.8 0.6 0.4 0.2 0 0.0 0.9 02 0.2 04 0.5 00 3.7 Courtaive Acquisition Time (mirr) 0.1 NS Spectrum *10 6 Cpd 1: C16 417 CH N 02: + FBF Spectrum (0015-0235 min) MSH-595.d Subtrad . 3 429.0057 (N+H)+ 2 439.9390 (M*NB)* a 427 412 424 4/6 428 430 435 434 435 Courts /8 Matsho-Charge (m2) 438 440 442 ed Specinum NS 24 x100 Cpd 1: C16 H17 CI I N C2: + F8F Spectrum (0.085-0.235 mir) MSH-595-d Bulances 5 418 0085 2 435 5850 (vf+Na)+ MS Spectrum Pesk Lis. 9/2 X Abund Formula 418 1 475(61.7) Submittive Control 413.0023 1 245(65.4) Submittive Control 420.0057 1 155(12.2) Control Ion (M+H)+ (M+H)+ (N+N)+ (N+N)+ -22.010F 1 439.985 1 +40.9428 1 +42.985 1 442.995 1 442.995 1 2023.91 Clamitolieu 2023.91 Clamitolieu 2023.91 Clamitolieu 2025.91 Clamitolieu 2025.91 Clamitolieu 2024.91 Clamitolieu 2024.91 Clamitolieu 2020.91 Clamitolieu 2020.9 Nefta)e M+Raj+ M+Raj+ M+Raj+ (M+Raj+ 🔅 Aylien Technologies Page 1 of 2 Printed at: 11:51 on: 17-10-2023









7-chloro-3-cyclohexyl-2-(4-hydroxybutyl)-4-iodoisoquinolin-1(2H)-one (5c)





2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)-7-(trifluoromethyl)isoquinolin-1(2H)-one (5d)





2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)-7-(trifluoromethyl)isoquinolin-1(2H)-one (5d)



HRMS



2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)-7-(trifluoromethyl)isoquinolin-1(2H)-one (5d)

MOL 509.0 ml Name binlowed Sample Name Filt POSITER Filt MOL 509.0 ml Name binlowed Sample Name Filt PIL10 User Name Filt Filt MORE STRAM MOL 500.0 MOL 500.0 FOR STRAM Different I Different I Di Di Different I Different I Different I Different I Di Di Di Diffe					and the second		
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24-0310 1 49241-27 C33H19133WH022 (H+Rg)4			545 550	16 94 5 530 535 540 1	524. (M-7 vs.Mss-10 S10 50 vs.Mss-10 Charge (m [M-H])+ [M-H])+ [M-H])+ [M-H])+ [M-H])+	15 490 495 500 1 172155 C11020'31102 172155 C11020'31102 173159 C11020'31102 18110 C11021'3102 1866 52 C11020'3102 1866 52 C11020'3102	1 0.8- 0.6- 0.4- 0.2- 0 475 480 485 MS Spectrum Peak List 500,055 3 111- 500,055 3 1250 500,055 3 1250 500,055 3 1250 500,055 3 1250 500,055 1 250
A SAMPLE IN THE REPORT OF THE			s4s 550	16 9* \$ 530 635 540 1	524 (N+1 is 10 515 520 f is Massic Castor i (N+10) ((N+10) ((N+10) ((N+10) ((N+10) ((N+10) ((N+10) ((N+10) ((N+10) (15 490 495 500 1 Caure 1 Fermula 12155 C11400131002 12155 C11400131002 1310 C11400131002 1366 51 C11400131002 366 52 C11400131002 366 52 C11400131002	1 0.8- 0.6- 0.4- 0.2- 0 475 480 485 MS Spectrum Peak List 550,005 1 250 590,005 1 250 590,0068 1 2225 512,0316 1 2225 512,0316 1 2225
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22:03/5 3 650.11 (21119/304602 [M440] 22:04/5 1 682.6 (21119/304602 [M440]+ 25:05/5 1 164.4 (21119/304602 [M440]+			s4s 550	116 3)+ 5 530 635 540	524 (M+1) rs. Mask to Charge m (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+ (M+1)+	15 450 455 500 1 Fermula 172155 C21420531602 C337.55 C21420531602 1631.65 C21420531602 1631.65 C21420531602 1635.65 C21420531602 1645.25 C34420531602 1635.65 C214155316402 1645.25 C34455316402 1645.45 C214159316402 1645.45 C21415931642 1645.45 C21415954 1645.45 C21415954 1645.45 C21415954.55 C21455556 1645.45 C2145555555555555555555555555	1 0.8- 0.6- 0.4- 0.2- 0 475 400 402 0 475 400 475 40



7-bromo-2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)isoquinolin-1(2H)-one (5e)





7-bromo-2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)isoquinolin-1(2H)-one (5e)







7-bromo-2-(4-hydroxybutyl)-4-iodo-3-(p-tolyl)isoquinolin-1(2H)-one (5e)





2-(4-hydroxybutyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-1(2H)-one (5f)





2-(4-hydroxybutyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-1(2H)-one (5f)



HRMS



2-(4-hydroxybutyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-1(2H)-one (5f)

Qualitative Compound Report



H NMR (400 MHz, CDCl₃)



2-(4-hydroxybutyl)-4-iodo-7-nitro-3-(4-pentylphenyl)isoquinolin-1(2H)-one (5g)











2-(4-hydroxybutyl)-4-iodo-7-nitro-3-(4-pentylphenyl)isoquinolin-1(2H)-one (5g)

Sample Type Instrument Name Acq Method IRM Calibration Status Comment	MSI-580.d Sample Instrument 1 MS Scan m Success	Sample Name Position User Name Acquired Time DA Method	HSH 500 21-15 34 68 2023 Defect m	12:58 22			
Sample Group Acquisition SW 630 Version Q 11	1 series TOI /6500 series OF III 05:01 (II5175)	Info. 3					
Compound Table					6//	MEG Formula	OB Formula
Compound Label Cpd 1: C23 H25 I N2 O4	RT Mass 0.181 520.0896	Aburd Form 11944 (23.0351	NJ 04	520.0859	7.17	C23 H25 T N2 C4	C231H2511M2-04
Compound Label	m/z RT	Algorithm	Mass	1			
Cpd 1: C23 H25 1 N2 O4	543.0765 0.181	Find By Formula	520.0896				
. (o		0022 638 1102 543 07	51 559 0491	1 Scan Fra	0=175		
210 0 181	IN2 04 PESI EIC(52)	10932, 538, 1197, 543, 67	51, 555,0191 -	ing action the			
6							
4							
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1							
01 02 03 0	4 05 06 07 08	09 1 11 12 13	1.4 1.5 1.6	1.7 1.8	1.9 2		
	Counts	i vs. Acquisition Time (min	1				
MER REPAIRING AND							
HS Spectrum	N2 O4: + FBF Spectrum	n (0.081-0.348 min) MSH	580.d Subtrac	1			
x10 5 Cpd 1: C23 H25 I	N2 O4: + FBF Spectrum	n (0.081-0.348 min) MSH	580.d Subtrac	a			
x10 5 Cpd 1: C23 H25 I	N2 O4: + FBF Spectrum	n (0.081-0.348 min) MSH	580.d Subtrac	a			
MS Spectrum x10 5 Cpd 1: C23 H25 I 4- 3-	N2 04: + F0F Spectrum	n (ö.081-0.348 min) MSH	580.d Subtrac	a			
HS Spectrum x10 5 Cpd 1: C23 H25 I 4- 3- 2-	N2 04: + FUF Spectrum	n (ö.081-0.348 min) MSH	580.d Subtrac	1			
HS Spectrum x10 5 4 3 2- 1-	N2 C4: + F0F Spectrum	n (0.081-0.348 min) MSH 8 1274 543.0705 (Mahala	580.¢ Subtrac	a			
HS Spectrum #10 8 Ced 1: C23 H25 I 4 3 2 1 0 522 524 526 52	N2 C4: + FOF Spectrum 53 00. 8 530 532 534 538	n (ö. 081-0. 348 min) MSH 8 1274 543 0705 •Sate]= (M+Na)+ 538 540 542 544 545	580.d Subtrac	ti SÉ4 SÉ6 (sia sio		
HS Spectrum x10 5 Cord 1: C23 H25 I 4 3 - - - - - - - - - - - - - - - - - -	N2 C4: + FDF Spectrum 53 (M) 8 530 532 534 536 Counts	n (ö. 0.81-0.348 min), MSH 8. 1274 543.0 /05 1-04143 (M-143)- 535 450 542 546 546 1-93 450 542 546 546	580.¢ Subtrac 548 550 552	sé4 sé6 (558 SEO		
HS Spectrum x1D % Cpd 1: C23 H26 / 4 3 2 1 522 524 526 52 4 522 524 526 52 522 52 52	N2 D4: + FBF Spectrum 53 (M) 8 530 532 534 535 Counts N2 D4: + FBF Spectrum	n (8.081-0.348 min) MSH 8.1274 543.0.705 1.58149 (M-143)- 535 445 545 546 546 1.48. Massis-Charge (m/2 1.48. Massis-Charge (m/2	580.d Subtrac 548 550 552 580.d Subtrac	séd sée s	ssa seo		
HS Spectrum x10 % Cpd 1: C23 H26 / 4 3 2 1 522 534 536 52 KS Zoond Spectrum x10 % Cpd 1: C23 H26 / 522 C54 52 524 536 52	N2 04: + FDF Spectrum 53 (M) 8 530 532 534 535 Counts N2 04: + FDF Spectrum 521 077 521 077	n (8.081-0.348 min) MSH 8.1274 543.0.105 143443 (M+153)- 1538 540 542 544 545 1538 540 542 544 545 10.081-0.348 min) MSH-	580.d Subtrac 548 550 552 1 580.d Subtrac	t séd sée : x	séa séo		
HS Spectrum x10 b Cpd 1: C23 H26 i 4 3 2 1 522 534 536 52 HS Zooned Spectrum x10 5 Cpd 1: C23 H25 i 4 2	53 00 8 530 532 534 534 02 8 530 532 534 534 531 537 (10)111 531 537	n (8:081-0:348 min) MSH 8:1274 543.0 705 4:5443 4:555 540 542 546 546 1555 540 542 546 546 10:0081-0:348 min) MSH-	580.d Subtrac 548 550 552 580.d Subtrac	t SÉ4 SÉ6 (sta sio		
HS Spectrum x10 & Cod 1: C23 H26 i 4 3 2 1 0 522 524 526 52 HS Zooned Spectrum x10 \$ Cod 1: C23 H26 i 522 524 526 52 HS Zooned Spectrum	533 (M) 8 532 534 538 532 534 538 533 534 538 534 534 534 534 534 534 534 534 534 534	n (8.081-0.348 min) MSH 8.1274 543.0.705 199453 04-7831 1995 542 544 546 533 540 542 544 546 1938 Massis-Charge (min 19.0.081-0.348 min) MSH-	580.d Sabirac 548 550 552 580.d Subred	số4 sốc (sia sio		
HS Spectrum x10 8 Cod 1: C23 H2E i 4 3 2 1 5 522 524 526 52 HS Zooned Spectrum x10 5 Cod 1: C23 H2E i 4 3 - - - - - - - - - - - - -	53 6 8 530 522 534 538 600 8 530 522 534 538 600 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	n (8.081-0.348 min) MSH 8.1274 543.0705 Handy (M-143) 238 540 542 544 546 238 540 542 544 546 1 (8.081-0.348 min) MSH	580.d Sabirac 548 550 552 580.d Subred	số4 sốc :	séa séo		
HS Spectrum x10 8 Ced 1: C23 H2E I 4 3 2 1 5 522 524 526 52 HS Zooned Spectrum x10 5 Ced 1: C23 H2E I 4 3 - 1	53 4 53 53 53 53 53 53 53 53 53 53	n (ö. 081-0.348 min) MSH 8. 1274 543.0 7/15 Harrige (M=Ha)= 538 540 542 544 546 1 vs. Mass-ta-Charge (min 1 (ö. 081-0.348 min) MSH- 543 67/05 1 (51 4 Filig)	580.d Sabrac 548.550 552 580.d Sabrac 580.d Sabrac	số4 sốc :	séa séo		
HS Spectrum x10 8 Ced 1: C23 H25 /	N2 C4: + FUF Spectrum 53 8 530 532 534 535 N2 C4: + FUF Spectrum 52 c073 (M-y1)+ 10 515 530 525 550	n (8.081-0.348 min) MSH 8.1274 543.07/05 http://www.sec.org/ http://www.sec.org/ 553 540 542 544 545 101-101/	580.d Sabirac 548 550 552 580.d Subtrac 590.0 Subtrac	1 564 566 1 1	9 585		
HS Social Section HS Soc	N2 C4: + FBF Spectrum 52 64 8 530 532 534 535 N2 C4: + FBF Spectrum 521 0772 (M7/1)* 10 515 520 525 533 Counts	n (8.081-0.348 min) MSH 8.1274 543.07/05 http:///WH01- 535 540 542 544 546 10.081-0.348 min) MSH- 543.07/05 (M1704) 0.536 540 541 510 55	580. d Sabtrac 548. 550. 552 580. d Sabtrac 580. d Sabtrac (2019)	1 554 556 1 1 1 1 1 1 1 1 1 1 1 1 1	3 585 0 585		
HS Sochum x10 % Cod 1: C23 H26 / 4 3 2 1 0 522 S24 S26 S2 4 522 S24 S26 S2 4 3 2 1 0 522 S24 S26 S2 525 S26 S2 4 3 2 1 4 3 2 1 5 5 5 5 5 5 5 5 5 5 5 5 5	53 (M) 8 520 522 524 528 Control 10 515 520 525 525 (0) 417 (10 515 520 525 525	n (8.081-0.348 min) MSH 8.1274 543.0.705 4.04451 044 7431 533 540 542 544 646 533 540 542 544 646 1.0447434 min) MSH 542 0705 1.0147434 542 0705 1.0147434 543 0705 1.0147434 543 0705 1.0147434 543 0705 1.0147434 543 0705 1.0147434 543 0705 1.0147434 543 0705 1.0147434 543 0705 1.0147434 543 0705 1.0147434 543 0705 1.0147434 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.0147444 1.01474	580. d Sabtrac 548. 550 552 550. d Subtrac 570.000 101.001 10	1 564 566 1 1 1 1 1 1 1 1 1 1 1 1 1	séa séo 0 585		
HS Sochum x10 % Cod 1: C23 H26 / 4 3 2 1 522 534 536 52 HS Zooned Spectrum x10 % Cod 1: C23 H25 / 4 3 - - - - - - - - - - - - -	53 04 53 04 53 04 53 04 51 51 51 51 51 51 51 51 51 51	n (8:081-0:348 min) MSH 8:1274 543.0 7/05 +starteg 6:061-0:348 min) MSH 253 540 542 544 546 (04-140)- (0	580.6 Sabirac 548 550 562 580.6 Submed 580.6 Submed 597 3199 101 101 101 101	1 554 555 5 7	554 560 0 585		
HS Spectrum x10 b Cpd 1: C23 H25 i 4 522 524 526 52 HS Zooned Spectrum x10 b Cpd 1: C23 H25 i 522 524 526 52 HS Zooned Spectrum x10 b Cpd 1: C23 H25 i 4 3 4 5 5 5 5 5 5 5 5 5 5 5 5 5	533 (M) 8 532 534 534 535 531 532 534 535 531 637 (10) 111 10 515 530 535 535 (10) 111 110 515 530 535 535 (10) 110 515 535 535 (10) 110 515 535 535 535 (10) 110 515 535 535 535 535 535 535 535 535 535	n (0.081-0.348 min) MSH 8.1274 543.0.705 1.0015 1.0015 533.540.542.544.546 533.540.542.544.546 1.0081-0.348 min) MSH 0.081-0.348 min) MSH 545.11/75 (M-10) 0.545.540.545 545.11/75 (M-10) 0.545.540.545 500 (M-10) (M-	580.6 Sabirac 548 550 562 580.0 Subirac 580.0 Subirac (20.040) (20.040) (20.040) (20.040) (20.040) (20.040) (20.040) (20.040) (20.040) (20.040)	1 554 556 (7	568 560 0 585		
HS Socrum x10 % Cod 1: C23 H25 i 4 5 522 524 526 52 HS Zooned Spectrum x10 % Cod 1: C23 H25 i 522 524 526 52 HS Zooned Spectrum x10 % Cod 1: C23 H25 i 4 3 - - - - - - - - - - - - -	N2 C4: + FUF Spectrum 53 6 8 530 532 534 535 6 N2 C4: + FUF Spectrum 521 C071 10 515 530 525 534 10 515 530 535 535 10 515 530 535 535 10 515 530 535 535 535 10 515 535 535 535 535 535 10 515 535 535 535 535 535 535 535 535 535	n (8:081-0.348 min) MSH 8:1274 543.07/05 HNH43 (M-Ha)- 538 540 542 544 546 1/31-Flag (0.081-0.348 min) MSH- 543 10/05 (11-Flag) 0:305 540 543 550 55 (14-Flag) 0:305 540 543 550 55 (14-Flag) 0:413 0:413 (M+13)	580.6 Sabirac 548 550 552 580.6 Sebirac 590.0199 (61149) 61.0199 (61149) 61.0199	त इस्टेंग इस्टेंट : त			
HS Sochum x10 % Cpd 1: C23 H26 / 3 2 1 522 S24 S26 S2 HS Zooned Spectrum x10 % Cpd 1: C23 H26 / 522 S24 S26 S2 HS Zooned Spectrum x10 % Cpd 1: C23 H25 / 4 4 5 5 5 5 5 5 5 5 5 5 5 5 5	N2 04: + FBF Spectrum 52 04: 10: 512: 534: 658: 10: 515: 520: 525: 535 10: 515: 520: 525 10: 525: 520: 525 10: 525: 525 10: 525: 525 10: 525	n (0.081-0.348 min) MSH 8.1274 543.0.705 ready (M+5a)+ 553 540 542 544 546 10.081-0.348 min) MSH 543 17/05 n (0.081-0.348 min) MSH 543 17/05 1.12 (M+11)- (580. d Sabtrac 548. 550. 552 580. d Sabtrac 580. d Sabtrac 580. d Sabtrac	1 554 556 1 1 1 1 1 1 1 5 1 5 5 5 5	sta séo 0 885		
HS Sochum x10 % Cpd 1: C23 H26 / 4 3 2 1 522 534 556 52 HS Zooned Spectrum x10 % Cpd 1: C23 H26 / 522 534 556 52 HS Zooned Spectrum x10 % Cpd 1: C23 H25 / 4 3 4 5 5 5 5 5 5 5 5 5 5 5 5 5	53 004 53 004 53 004 53 004 53 007 53 007 53 007 10 515 50 52 53 007 10 515 50 52 53 53 54 54 54 54 54 54 54 54 54 54	n (8:081-0:348 min) MSH 8:1274 543.0 7/05 Harris (M-Ha)- 238 540 542 546 546 148 540 542 546 546 (M-Ha)- (M-HA)-	580.6 Sabirac 548 550 562 580.6 Submed 580.6 Submed 597 3439 101 101 101 101	1 554 556 (8	o sés		
HS Sochum x10 ≥ Cod 1: C23 H26 i 4 3 2 1 552 534 526 52 4 552 534 526 52 4 3 4 552 534 526 52 4 3 4 552 534 526 52 4 3 4 552 534 526 52 4 3 4 552 534 526 52 4 552 534 526 52 4 552 534 526 52 4 552 534 526 52 4 552 534 526 52 552 552 54 552 552 54 552 552 54 552 552 54 552 552 54 552 555 55 552 555 55 555 555 555 555	53 04 53 04 53 04 53 04 53 04 54 54 54 54 54 54 54 54 54 5	n (0.081-0.348 min) MSH 8.1274 543.0.705 harries (M-193)- 533.540.542 544 546 1.0.081-0.348 min) MSH- 543.0705 (A1-Rug) 0.530.540 545 540 547 (A1-Rug) 0.530.540 545 540 547 (M-11)+ (M+11)+	580.6 Sabirac 548 550 552 580.6 Sabirac 580.6 Sabirac 580.6 Sabirac 590.3000 (Minty) 10000 (Minty) 10000 (Minty)	554 556 1 7	-164 500 0 585		
PIS Socrum x10 * Cod 1: C23 H25 i 4 522 524 526 52 PI 522 524 526 52 PI 521 527 12 PI 521 527 12 PI	N2 C4: + FUF Spectrum 53 04 16 520 522 534 538 52 607 52 607 10 515 520 525 535 10 515 520 520 525 535 10 515 520 520 520 520 520 520 520 520 520 52	n (0.081-0.348 min) MSH 8.1274 513.0.7/05 HNHON (M-149) 238 540 542 544 546 (M-149) (M-149) (M-149) (M-11) (M+	580.6 Sabirac 548 550 552 580.d Bubirac 590.0199 (01145) 61.569 565 5	त इस्टेंग इस्टेंस् त	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5		



2-(4-hydroxybutyl)-4-iodo-3-(3-methoxyphenyl)-7-nitroisoquinolin-1(2H)-one (5h)




2-(4-hydroxybutyl)-4-iodo-3-(3-methoxyphenyl)-7-nitroisoquinolin-1(2H)-one (5h)





2-(4-hydroxybutyl)-4-iodo-6,7-dimethoxy-3-phenylisoquinolin-1(2H)-one (5i)





2-(4-hydroxybutyl)-4-iodo-6,7-dimethoxy-3-phenylisoquinolin-1(2H)-one (5i)





2-(4-hydroxybutyl)-4-iodo-6,7-dimethoxy-3-phenylisoquinolin-1(2H)-one (5i)

			4						
Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment	MSII-55 Sample Tristnam MS Scal	S4.d tent 1 outs		Sample Name Position User Name Acquired Time DA Methed	MSII-554 P1-03 10-01-20 Default.m	23 14:30:22			
Sample Group Acquisition SW 6 Version Q	200 series TOF/6 -TOF 8.05.01 (8	5500 series 5125)	Info.	3					
Compound Table							07/		1
Compound Label Cpil 1: C21 II22 TN	RT 0.104	Mass 479.0628	Abund 14701	Formu C21 H22 E	la N 04	Tgt Mass 479.0594	(ppm) 7.19	C21 H22 1 N O4	C1 H22 INC
			·						
Compound Label	m/z	RT	Algorithe	m	Mass				
CD0 1: C21 H22 I N 01	502.0514	0.104	hind By he	ormula	479.0628				
¢- 4- 2-									
6- 4- 2- 0.1 0.2 0.3 M5 Spectrum x10 4 CPel 1: C21 H22 4-	0.4 0.5 0.6 I N O4: + FBF ;	0.7 0/8 Counts Spectrum (0.9 i vs. Acquisi (0.088-0.20	11 12 13 iton Time (min) 24 min) MSH-65	1.4 1.5 1 4.d Subtrac	.6 1.7 1.8 I	1 <u>9</u> 2		
6- 4- 2- 0-1-0-2-0.3 M5 Spectrum x10 4 CPd 1: C21 H22 4- 3-	0.4 0.5 0.6 I N O4: + FBF :	0.7 0.8 Counts Spectrum (0,9 i vs. Acquisi (0.088-0.20	1.1 12 1.3 Bion Time (min) 24 min) MSH-55	1.4 1.5 1 4.d Subtrac	.6 1.7 1.8 I	19 2		
6- 4- 2- 0-1 - 0.2 - 0.3 M5 Spectrum x10 4 CPd 1: C21 H22 4- 3- 2-	0.4 0.5 0.5 IN 04: + FBF :	0.7 0/8 Counts Spectrum (0.9 1 vs. Acquisi (0.088-0.20	1.1 12 1.3 Han Time (min) 24 min) MSH-85 502.0514	1,4 1,5 1 4.d Subtract	.6 1.7 1.8 t	19 2		
6- 4- 2- 0-1 - 0.2 - 0.3 M5 Spectrum x10 4 CPd 1: C21 H22 4- 3- 2- 1-	0.4 0.5 0.6 I N O4: + FBF :	0.7 0/8 Counts Spectrum (0,9 j vs. Acquisi (0.088-0.20	1.1 1.2 1.3 itian Time (min) 24 min) MSH-55 502:0514 (M+Na)+	1/4 1/5 1 4.d Subtract	.6 1.7 1.8 L	19 2		
6 4 2 0.1 0.2 0.3 MS Spectrum xt0 4 Cpd 1: C21 Hd2 4 3 2 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1	0.4 0.5 0.6	0.7 0.8 Counts Spectrum (0,9 i vs. Acquisi (0.088-0.20	1.1 1.2 1.3 Rison Time (min) 94 min) MSH-55 592-0514 (M+Na)+	1/4 1/5 1 4.d Subtract	.6 1.7 1.8 I	19 2		
4 4 5 6 0.1 62 0.3 45 Spectrum x10 4 Cpd 1: C21 H02 4 4 3 2 1 6 6 6 1 1 Cpd 1: C21 H02 1 6 1 1 1 1 1 1 1 1 1 1 1 1 1	0.4 0.5 0.5 IN 04: + PBP 5 488. 490. 455	0.7 0.8 Counts Spectrum (2 494 499 Counts V	0,9 1 vs. Acquisi 0.088-0.20 5 498 500 vs. Mess-to	1.1 1.2 1.3 Itian Time (min) 44 min) MSH-55 592 0514 (M+ha)+ 0 592 304 593 -Gharge (miz)	1.4 1.5 1 4.d Subtrac 5 508 510	.6 1.7 1.8 1 512 514 5	1.9 2		
45 Spectrum x10 4 Cpd 1: C21 H02 455 464 480 465 2 464 480 465 2 464 480 45 2 200med Spectrum x10 4 Cpd 1: C21 H02	0.4 0.5 0.6 1 N O4: + PBF : 488 490 452 N O4: + PBF 5	0.7 0.8 Counts Spectrum (2 494 456 Counts (Spectrum (0.9 1 vs. Acquisi (0.088-0.20 4.408 500 vs. Mass-to 9.088-0.20	1.1 1.2 1.3 1.1 1.2 1.3 1.4 min) MSH-55 592 0514 (M+ha)+ 0 592 304 593 -Ghorge (m2) t min) MSH-554	1/4 1/5 1 4.d Subtract 5 50/6 510	.6 1.7 1.8 t 512 514 5	1.9 Ż		
4 4 5 5 5 5 5 5 5 5 5 5 5 5 5	0.4 0.5 0.5 IN 04: + PBF : 488. 490. 455 N 04: + PBF S 480.0 M 94	0.7 0/s Counts Spectrum (2 454 456 Counts (Spectrum (706	0,9 j vs. Acquisi (0.088-0.20 5 498 500 vs. Mess-to 0.088-0.201	1.1 1.2 1.3 100 Time (min) 34 min) MSH-55 502 0514 (M+ha)+ 0 502 304 503 -Gharge (miz) 4 min) MSH-554	1/4 1/5 1 4.d Subtract 5 50/6 510	.6 1.7 1.8 512 514 5	1.9 Ż		
4 2 0.1 0.2 0.3 45 Spectrum x10 4 Cpd 1: C21 H02 4 4 4 52 484 480 52 500med Spectrum x10 4 Cpd 1: C21 H02 4 6 5 Cpd 1: C21 H02 4 6 7 8 8 8 8 8 8 8 8 8 8 8 8 8	0.4 0.5 0.5 IN 04: + PBP : 488 490 455 N 04: + PBP 5 480 0 IM 94	0.7 0/s Counts Spectrum (2 454 456 Counts (3pectrum (706	0,9 j vs. Acquisi (0.088-0.20 8 498 500 vs. Mass-to 0.088-0.204	1.1 1.2 1.3 Sign Time (min) 44 min) MSH-555 502 0514 (M+Na)+ - - 0 502 354 505 - - - - - - - - - - - - -	1.4 1.5 1 4.d Subtrac 5 508 510 .d Sabtract	.6 1.7 1.8 512 514 5	19 2 is sis		
4 4 5 Spectrum x10 4 Cpd 1: C21 H02 4 4 5 Spectrum x10 4 Cpd 1: C21 H02 4 5 Spectrum x10 4 Cpd 1: C21 H02 5 Spectrum 5 Spe	0.4 0.5 0.5 IN 04: + PBP : 488. 490. 455 N 04: + PBP 5 480.0 (M-94	6.7 0/8 Counts Spectrum (2 494 496 Counts (705 705	0.9 1 9.0088-0.20 0.088-0.20 0.088-0.20 0.088-0.20 0.088-0.20	1.1 1.2 1.3 Itan Time (min) 44 min) MSH-55 502 0514 (MH-ba)+ - - - - - - - - - - - - -	1.4 1.5 1 4.d Subtrac 5 508 510 .d Sabtract	.6 1.7 1.8 512 514 5	1.9 2 is sis		
4 2 0.1 0.2 0.3 45 Spectrum x10 4 Cpd 1: C21 H02 4 3 2 4 5 Zoomed Spectrum x10 4 Cpd 1: C21 H02 4 5 Zoomed Spectrum x10 4 Cpd 1: C21 H02 4 4 3 2 1 4 5 Spectrum x10 4 Cpd 1: C21 H02 4 4 5 Zoomed Spectrum	0.4 0.5 0.5 IN 04: + PBP 3 488 490 455 N 04: + PBP 5 480 0 (M-14	6.7 0.8 Counts Spectrum (Counts (705 705	0.9 1 94. Acquisi 0.088-0.20 0.088-0.20 0.088-0.204 0.088-0.204 502: (M+1	1.1 1.2 1.3 Itian Time (min) 44 min) MSH-55 502 0514 (M+ha)+ 9 502 354 35 - Ghorge (m2) 4 min) MSH-554 0514 Na)+	1,4 1,5 1 4.d Subtrac 5 SÓ8 SÍO .d Subtract	.6 1.7 1.8 512 514 5	19 2 is sis		
4 4 5 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0	0.4 0.5 0.6 IN 04: + FBF 9 488 490 450 N 04: + FBF 9 488 0 (M+4	0.7 0/s Counts Spectrum (Counts v Generals Spectrum (Spectrum (706	0,9 j vs. Acquisi 0.038-0.20 s 408 500 vs. Mess-10 0.088-0.204 0.088-0.204 502- (M+1	1.1 1.2 1.3 Sign Time (min) 44 min) MSH-55 502 0514 (MH-ba)+ 0 552 564 555 - Ghorge (m2) 4 min) MSH-554 0514 NSH- 518 (MH)	1.4 1.5 1 4.d Subtract 5 508 510 .d Subtract .up255 **Q+	.6 1.7 1.8 512 514 5	19 2 is sis		
4 4 4 5 5 5 5 5 5 5 5 5 5 5 5 5	0.4 0.5 0.6 IN 04: + FBF 9 488 490 450 IN 04: + FBF 9 480 0 IM 41 470 475 480	6.7 0/8 Counts Spectrum (2 494 499 Counts (705 705 485 490 Counts (0.9 1 0.088-0.20 0.088-0.20 0.088-0.20 0.088-0.20 0.088-0.20 (M+1 405 500	1.1 1.2 1.3 Bian Time (min) MSH-55 502.0514 (MH-ba)+ 0 502.354 504 0 502.354 505 0 502.354 505 0 502.354 505 0 502.354 505 0 502.354 505 0 502.354 505 0 502.354 505 0 502.354 505 0 502.354 505 0 502.354 505 1 (M 505 1 505 505	1.4 1.5 1 4.d Subtrac 5 508 510 .d Sabtraci 40255 407 520 525 5	512 514 5	1.9 2 i6 5i8		
4 2 0.1 0.2 0.3 MS Spectrum x10 4 Cpd 1: C21 H22 4 4 4 4 5 6 Cpd 1: C21 H22 4 4 4 4 4 4 4 5 6 6 6 5 6 6 6 6 6 6 6 6 6 6 6 6 6	0.4 0.5 0.5 IN 04: + FBF : 488 490 455 480 455 (My) 470 475 480	0.7 0/8 Counts Spectrum (Counts v Counts v Spectrums (19+	0.9 j vs. Acquisi 0.088-0.20 6 408 50 vs. Mass-to 0.088-0.204 502: (M+1 1405 500 5. Mass-to	1,1 1,2 1,3 130 Time (min) 14 min) MSH-55 502 0514 (M+Na)+ 0 502 364 50 - Grange (m2) 4 min) MSH-554 1505 150 615 - Charge (m2)	1.4 1.5 1 4.d Subtract 5 508 510 .d Sabtract .n255 +Q+ 520 525 1	512 514 5	19 2 16 518		
4 2 0.1 0.2 0.3 MS Spectrum x10 4 Cpd 1: C21 H22 4 4 4 4 4 4 5 5 5 5 5 5 5 5 5 5 5 5 5	0.4 0.5 0.5 IN 04: + PBP : 488 490 455 800 455 800 800 455 800 800 800 800 800 800 800 800 800 8	0.7 0/8 Counts Spectrum (2 494 499 Counts v 2 counts v 3pectrums (0 10+	0.9 j vs. Acquisi (0.088-0.20 6 408 50 vs. Mess-to 0.088-0.20 0.088-0.20 0.088-0.20 0.088-0.20 0.088-0.20 0.088-0.20 0.088-0.20 0.088-0.20	1.1 1.2 13 1.60 Time (min) 34 min) MSH-55 502 0514 (M+Na)+ 0 502 504 50 - Gronge (m2) 4 min) MSH-554 (M+Na)+ 505 510 efs - Gronge (m2) 514 - Gronge (m2) - Gro	1.4 1.5 1 4.d Subtract 5 508 510 .d Sabtract .t0255 530 525 1	.6 1.7 1.8 1 512 514 5 510 513 540	19 2 i6 5i8		
4 4 5 5 5 5 5 5 5 5 5 5 5 5 5	0.4 0.5 0.5 IN 04: = PBP : 488 490 455 N 04: = PBP : 488 490 455 N 04: = PBP : 400 455 400 455	0.7 0/8 Counts Spectrum (2 494 49 Counts (2 Counts (1)+ 4 485 490 Counts v	0,9 i vs. Acquisi (0.088-0.20 6 408 50 vs. Mess-to 0.088-0.204 502 (M+1 1 405 500 s. Nass-to- (M+1 1 405 500 s. Nass-to- (M+1)	1.1 1.2 1.3 1.6 Time (min) 14 min) MSH-55 502 0514 (M+Na)* 0 502 504 55 -Charge (m2) 4 min) MSH-554 (M 10) 505 104 55 -Charge (m2) 515 -Charge (m2) 514 (M 10) -Charge (m2) 514 -Charge (m2) -Charge (m2) -Ch	1.4 1.5 1 4.d Subtract 5 508 510 .d Subtract .t0285 .t037 .520 525 1	.6 1.7 1.8 512 514 5	1/9 2 16 518		
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7-(4-(tert-butyl)phenyl)-6-(4-hydroxybutyl)-8-iodo-[1,3]dioxolo[4,5-g]isoquinolin-5(6H)one (5j)





7-(4-(tert-butyl)phenyl)-6-(4-hydroxybutyl)-8-iodo-[1,3]dioxolo[4,5-g]isoquinolin-5(6H)one (5j)





2-((7-chloro-2-(4-hydroxybutyl)-4-iodo-1-oxo-1,2-dihydroisoquinolin-3yl)methyl)isoindoline-1,3-dione (5k)





3-(4-ethylphenyl)-2-(2-hydroxyethyl)-4-iodoisoquinolin-1(2H)-one (6a)





3-(4-ethylphenyl)-2-(2-hydroxyethyl)-4-iodoisoquinolin-1(2H)-one (6a)





3-(4-ethylphenyl)-2-(2-hydroxyethyl)-4-iodoisoquinolin-1(2H)-one (6a)

Sample Trips Here and the second table of the	Data file	MSH-386 d	Sample Name	MSH-386			
And we that we have a state of the	Sample Type	Sample	Position	r1-f2			
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×10 s Cut 1: C*0 + HE IN D2: +ESI E C (423.035, 442.0224) Scen Fmg=175.0V MGH-385.4 *10 s Cut 1: C*0 + HE IN D2: +ESI E C (423.035, 442.0224) Scen Fmg=175.0V MGH-385.4 *10 s Cut 1: C*0 + HE IN D2: +ESI E C (423.035, 442.0224) Scen Fmg=175.0V MGH-385.4 *10 s Cut 1: C*0 + HE IN D2: +ESI E C (423.035, 442.0224) Scen Fmg=175.0V MGH-385.4 *10 s Cut 1: C*0 + HE IN D2: +ESI E C (423.035, 442.0224) Scen Fmg=175.0V MGH-385.4 *10 s Cut 1: C*0 + HE IN D2: +ESI E C (423.035, 442.0224) Inter (1116; (111)) *10 s Cut 1: C*18 + HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s Cut 1: C*18 + HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s Cut 1: C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s Cut 1: C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s Cot 1: C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4 *10 s C*10 HE IN C2: + FGF Spectrum (0.056.0.221 min) MSH-386.4	A CONTRACTOR OF THE OWNER OF THE						
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$x_{10} = \begin{bmatrix} 2 & 2.3 & 0.4 & 0.5 & 0.6 & 0.7 & 2.8 & 0.9 & 1. & 1.1 & 1.2 & 1.3 & 1.4 & 1.5 & 1.6 & 1.7 & 1.8 & 1.9 & 2 \\ \hline \\ MS Spectrum \\ x_{10} = \begin{bmatrix} 2 & 0.4 & 0.5 & 0.6 & 0.7 & 2.8 & 0.9 & 1. & 1.1 & 1.2 & 1.3 & 1.4 & 1.5 & 1.6 & 1.7 & 1.8 & 1.9 & 2 \\ \hline \\ x_{10} = \begin{bmatrix} 2 & 0.4 & 0.5 & 0.6 & 0.7 & 0.8 & 0.221 & mr.] & MS + 386.4 & Subtract \\ \hline \\ x_{10} = \begin{bmatrix} 2 & 0.4 & 0.5 & 0.6 & 0.7 & 0.8 & 0.221 & mr.] & MS + 386.4 & Subtract \\ \hline \\ x_{10} = \begin{bmatrix} 2 & 0.4 & 0.5 & 0.6 & 0.7 & 0.8 & 0.221 & mr.] & MS + 386.4 & Subtract \\ \hline \\ x_{10} = \begin{bmatrix} 2 & 0.7 & $	8-38-7%						
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$\begin{array}{c} \begin{array}{c} 0.35 \\ 0 \\ \end{array} \\ \hline \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 452 \\ 15 \\ 1.5 \\ $	2 0.1 0.2 0.3 0. MS Spectrum x10 3 2 1.75 1.25 1.25 1.25	4 0.5 06 0.7 0.6 Cauri N C2: + F&F Spectrum	0.9 1 1,1 12 13 1 1 1,1 12 13 1 1 1,1 12 13 1 1 (0.055 0.221 min) MSH-386.	4 1.5 16 1.7 1.3 d Subbract	8 1.9 2 2 0273		
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4.20 4.20 4.20 4.25 A22 4.20 4.20 PS 200md Scensum xr10 G_Surgers, Massars-Charge (m/r) 4.00 4.00 yr10 G_God 1: C10 H18 I N G2: + FE# Spectrum (0.058-0.22: min) MSH-S85.c Sulvect 2.00 175 - (M+r)+ 175 - - 175 - <t< td=""><td>2 0 0.1 0.2 0.3 D MS Spectrum x10 5 Cpd 1. C19 H18 1 2- 1.25 1.25 1.25 0.75</td><td>4 0.5 0.6 0.7 D.E. Cauri N C2: + FBF Spectrum</td><td>0 9 1 1 1 12 13 1 1 4 4 4 4 4 4 4 4 1 1 1 1 1 1 1 1 1 1</td><td>4 1.5 1.6 1.7 1.3 d Subbract (M</td><td>8 1.9 2 12 0273 14 Naji</td><td></td><td></td></t<>	2 0 0.1 0.2 0.3 D MS Spectrum x10 5 Cpd 1. C19 H18 1 2- 1.25 1.25 1.25 0.75	4 0.5 0.6 0.7 D.E. Cauri N C2: + FBF Spectrum	0 9 1 1 1 12 13 1 1 4 4 4 4 4 4 4 4 1 1 1 1 1 1 1 1 1 1	4 1.5 1.6 1.7 1.3 d Subbract (M	8 1.9 2 12 0273 14 Naji		
P3 2000md Scatzum x10 € [Cod 1: C13 H18 I N Q2: + FB# Spectrum (2.088-0.22: min) M8H-388.c Subtract 2 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5	2 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0	4 0'S 06 0'7 D.S. Court N C2: + F&F Spectrum	0.9 1 11 12 13 1 s vs. Accutation Time (min) n (0.055 0.221 mr.) MSH386.	4 15 16 17 13 d Subtract (M	8 1.9 2 12 0273 1+Naji		
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0.75 0.25	2 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0	4 05 06 07 0.2 K 02: + FDF Spectrum 426 428 Court N 02: + FBF Spectrum 420 046 (14-11)	1 11 12 13 1 1 14 12 13 1 1 0.055 0.221 min) MSH-386. 452 432 434 455 1 10.056 0.221 min) MSH-588.	4 1.2 1.6 17 1.4 d Subtract 4.6 (M 4.39 440 d Subtract	8 1.9 2 2 0273 9 (24) 442		
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0.25 0 355 400 405 <10 415 420 425 420 435 400 405 470 MS Spectrum Peak List <i>m/r x</i> Abund <i>fermula</i> 41:0x61 <i>i</i> 12272323 (SPISSNO2 41:0x61 <i>j</i> 2010x68 (SPISSNO2 41:11 41:0x61 <i>j</i> 2010x68 (SPISSNO2 41:11 41:0x61 <i>j</i> 2010x68 (SPISSNO2 41:11 42:0x61 <i>j</i> 2010x7 41:11 42:0x61 <i>j</i> 2010x7 41:11 42:0x61 <i>j</i> 2010x7 41:11 41:11 42:0x61 <i>j</i> 2010x7 41:11 4	2 0 0.1 0.2 0.3 D MS Spectrum x10 2 1.25- 1.25- 1.25- 0.35- 0.35- 0.35- 0.35- 0.35- 0.35- 0.42- 1.20- 1.2	4 05 06 07 25 0 02: + FBF Spectrum 426 428 426 428 2041 1 02: + FBF Spectrum 420 046 (14-11)	a <u>69</u> 1 11 12 13 1 a vs. Accusticion Time (mm) n (0.055 0.221 m/r) MSH388. 433 432 434 439 a vs. MatsCharge (m/r) r (0.056-0.221 min) MSH388. r 442.0273 (4414)	4 12 16 17 13 d Subtract 439 440 e Subtract	a 1.9 2 12 0273 11 Maji 442		
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¹H NMR



2-(2-hydroxyethyl)-4-iodo-3-(p-tolyl)-7-(trifluoromethyl)isoquinolin-1(2H)-one (6b)





2-(2-hydroxyethyl)-4-iodo-3-(p-tolyl)-7-(trifluoromethyl)isoquinolin-1(2H)-one (6b)



¹H NMR



7-chloro-2-(2-hydroxyethyl)-4-iodo-3-(m-tolyl)isoquinolin-1(2H)-one (6c)





7-chloro-2-(2-hydroxyethyl)-4-iodo-3-(m-tolyl)isoquinolin-1(2H)-one (6c)





2-(3-hydroxypropyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-1(2H)-one (6d)





2-(3-hydroxypropyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-1(2H)-one (6d)





3-(4-(tert-butyl)phenyl)-2-(5-hydroxypentyl)-4-iodoisoquinolin-1(2H)-one (6e)





3-(4-(tert-butyl)phenyl)-2-(5-hydroxypentyl)-4-iodoisoquinolin-1(2H)-one (6e)





2-(4-azidobutyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-1(2H)-one (7f)





2-(4-azidobutyl)-4-iodo-7-nitro-3-(p-tolyl)isoquinolin-1(2H)-one (7f)





2-(4-(4-((88,9R,13R,14R,17R)-3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17decahydro-6H-cyclopenta[a]phenanthren-17-yl)-1H-1,2,3-triazol-1-yl)butyl)-4-iodo-7nitro-3-(p-tolyl)isoquinolin-1(2H)-one (9)





2-(4-(4-((88,9R,13R,14R,17R)-3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17decahydro-6H-cyclopenta[a]phenanthren-17-yl)-1H-1,2,3-triazol-1-yl)butyl)-4-iodo-7nitro-3-(p-tolyl)isoquinolin-1(2H)-one (9)





(E)-3-([1,1'-biphenyl]-4-yl)-2-(4-hydroxybutyl)-4-(4-methoxystyryl)isoquinolin-1(2H)one (11j)





(E)-3-([1,1'-biphenyl]-4-yl)-2-(4-hydroxybutyl)-4-(4-methoxystyryl)isoquinolin-1(2H)-





2-(4-hydroxybutyl)-7-nitro-4-phenyl-3-(p-tolyl)isoquinolin-1(2H)-one (13f)





2-(4-hydroxybutyl)-7-nitro-4-phenyl-3-(p-tolyl)isoquinolin-1(2H)-one (13f)

