#### **Supplementary Synthetic Chemistry Information**

#### Synthesis of stereoisomeric probes

The stereoisomeric probes used in this study were prepared by adapting previously reported procedures (**Supplementary Data Fig. 1**)<sup>6, 22</sup> Analytical characterization data is provided for all new compounds.



**Supplementary Data Fig. 1. General scheme for the synthesis of tryptoline acrylamide stereoisomeric probes.** Steps: (i) Pictet-Spengler cyclization followed by chromatographic separation of diastereomers; (ii) ester hydrolysis; (iii) amide coupling; (iv) acrylamide installation.

#### **General considerations**

All NMR spectra were recorded at 298 K unless otherwise noted. <sup>1</sup>H NMR spectra were recorded on Bruker Avance III 400, Avance III HD 400, Avance Neo 400 spectrometers (<sup>1</sup>H, 400 MHz). <sup>13</sup>C NMR spectra were recorded on a Bruker Avance III HD 600 spectrometer (<sup>13</sup>C, 151 MHz). <sup>19</sup>F NMR spectra were recorded on a Bruker AV Neo 399 MHz spectrometer (<sup>19</sup>F, 376 MHz). <sup>1</sup>H NMR data are reported as follows: chemical shift ( $\delta$ ), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet; br = broad), coupling constants, and integration. Chemical shifts are reported in parts per million (ppm) using the appropriate solvent as reference<sup>23</sup>. Analytical supercritical fluid chromatography (SFC) was performed on a Shimadzu LC system (flow rate: 3 mL/min, back pressure: 100 Bar, column temperature: 35 °C) equipped with a polydiode array detector. HRMS was performed on a 6230 TOF LC/MS with a Dual AJS EI source by injecting 5 µM compounds in MeOH with 20% solvent A (0.1% formic acid in water) and 80% solvent B (0.1% formic acid in acetonitrile).



(1S,3S)-2-acryloyl-1-(benzo[d][1,3]dioxol-5-yl)-N-(prop-2-yn-1-yl)-2,3,4,9tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxamide (WX-01-05) WX-01-05 (aka MY-13A) was prepared as reported previously<sup>22</sup>.



(1R,3R)-2-acryloyl-1-(benzo[d][1,3]dioxol-5-yl)-N-(prop-2-yn-1-yl)-2,3,4,9tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxamide (WX-01-07) WX-01-07 (aka MY-13B) was prepared as reported previously<sup>22</sup>.



(1R,3S)-2-acryloyl-1-(benzo[d][1,3]dioxol-5-yl)-N-(prop-2-yn-1-yl)-2,3,4,9tetrahydro-1H-pyrido[3,4-b]indole-3-carboxamide (WX-01-06)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.32 (s, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.11 (dtd, J = 16.1, 7.1, 1.3 Hz, 2H), 6.84 – 6.77 (m, 2H), 6.77 – 6.70 (m, 1H), 6.60 (dd, J = 16.6, 10.4 Hz, 1H), 6.47 – 6.24 (m, 2H), 6.02 (br. s, 1H), 5.95 – 5.89 (m, 2H), 5.70 (d, J = 10.3 Hz, 1H), 4.93 (t, J = 6.0 Hz, 1H),

3.97 – 3.87 (m, 1H), 3.83 (ddd, J = 17.6, 5.2, 2.6 Hz, 1H), 3.48 (dd, J = 15.9, 5.6 Hz, 1H), 3.35 – 3.22 (m, 1H), 2.06 (t, J = 2.5 Hz, 1H).

<sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ 170.74, 169.96, 168.95, 164.81, 148.48, 147.59, 136.65, 135.22, 132.60, 131.49, 131.46, 130.11, 128.29, 126.56, 126.52, 123.32, 122.73, 122.57, 120.42, 120.05, 120.00, 118.69, 118.63, 111.32, 111.22, 108.79, 108.72, 108.68, 107.31, 107.14, 101.74, 101.48, 79.32, 72.05, 71.82, 57.46, 56.56, 51.09, 29.60, 23.21, 22.30.

HRMS ESI-TOF m/z calculated for C<sub>25</sub>H<sub>22</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 428.1605. Found 428.1596.



#### (1S,3R)-2-acryloyl-1-(benzo[d][1,3]dioxol-5-yl)-N-(prop-2-yn-1-yl)-2,3,4,9tetrahydro-1H-pyrido[3,4-b]indole-3-carboxamide (WX-01-08)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.11 (s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.25 (d, *J* = 8.8 Hz, 1H), 7.19 – 7.06 (m, 2H), 6.83 – 6.77 (m, 2H), 6.74 (d, J = 8.1 Hz, 1H), 6.67 – 6.52 (m, 1H), 6.44 – 6.29 (m, 2H), 6.00 – 5.80 (m, 3H), 5.71 (d, J = 10.3 Hz, 1H), 4.90 (t, J = 5.0 Hz, 1H), 4.03 – 3.90 (m, 1H), 3.90 – 3.81 (m, 1H), 3.49 (dd, J = 15.8, 5.9 Hz, 1H), 3.39 – 3.21 (m, 1H), 2.09 (s, 1H).

HRMS ESI-TOF m/z calculated for C<sub>25</sub>H<sub>22</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 428.1605. Found 428.1621.



#### methyl (1S,3S)-2-acryloyl-1-(3-methoxy-4-(prop-2-yn-1-yloxy)phenyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-01-01) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) $\delta$ 7.85 (d, J = 7.7 Hz, 1H), 7.60 (d, J = 7.6 Hz, 1H),

7.30 (dt, J = 8.1, 1.0 Hz, 1H), 7.21 (ddd, J = 8.0, 7.0, 1.5 Hz, 1H), 7.16 (td, J = 7.4, 1.3 Hz, 1H), 7.12 – 6.53 (m, 5H), 6.41 – 6.21 (m, 1H), 5.77 (dd, J = 10.8, 1.7 Hz, 1H), 5.05 (br. s, 1H), 4.71 (d, J = 2.4 Hz, 2H), 3.77 (s, 3H), 3.67 (br. d, J = 15.9 Hz, 1H), 3.25 – 2.99 (m, 4H), 2.46 (t, J = 2.3 Hz, 1H).

<sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ 170.87, 168.02, 149.56, 146.42, 136.55, 133.66, 130.17, 129.27, 128.12, 126.60, 122.59, 121.52, 119.88, 118.74, 113.69, 113.25, 111.16, 107.75, 78.55, 75.95, 56.74, 56.23, 56.19, 56.08, 53.54, 52.30, 51.44, 22.03.

HRMS ESI-TOF m/z calculated for C<sub>26</sub>H<sub>25</sub>N<sub>2</sub>O<sub>5</sub> [M+H]<sup>+</sup> 445.1758. Found 445.1757.



#### methyl (1*R*,3*R*)-2-acryloyl-1-(3-methoxy-4-(prop-2-yn-1-yloxy)phenyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-01-03)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.95 (br. s, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.30 (d, J = 7.9 Hz, 1H), 7.20 (td, J = 7.5, 1.4 Hz, 1H), 7.16 (td, J = 7.4, 1.3 Hz, 1H), 7.11 – 6.54 (m, 5H), 6.29 (br. d, J = 16.3 Hz, 1H), 5.77 (dd, J = 10.8, 1.7 Hz, 1H), 5.04 (br. s, 1H), 4.70 (d, J = 2.4 Hz, 2H), 3.75 (s, 3H), 3.67 (br. d, J = 15.6 Hz, 1H), 3.21 – 3.01 (m, 4H), 2.45 (t, J = 2.4 Hz, 1H).

HRMS ESI-TOF m/z calculated for C<sub>26</sub>H<sub>25</sub>N<sub>2</sub>O<sub>5</sub> [M+H]<sup>+</sup> 445.1758. Found 445.1744.



methyl (1*R*,3*S*)-2-acryloyl-1-(3-methoxy-4-(prop-2-yn-1-yloxy)phenyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-01-02) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.83 (br. s, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.29 – 7.23 (m, 1H), 7.21 – 7.09 (m, 2H), 7.01 – 6.91 (m, 2H), 6.91 – 6.85 (m, 1H), 6.56 (dd, *J* = 16.7, 10.5 Hz, 1H), 6.29 (dd, *J* = 16.7, 1.7 Hz, 1H), 6.16 (s, 1H), 5.64 (d, *J* = 10.5 Hz, 1H), 5.12 – 5.05 (m, 1H), 4.73 – 4.70 (m, 2H), 3.82 (s, 3H), 3.65 (br. s, 3H), 3.61 – 3.54 (m, 1H), 3.37 – 3.16 (m, 1H), 2.48 (t, *J* = 2.1 Hz, 1H).

 $^{13}\text{C}$  NMR (151 MHz, CDCl\_3)  $\delta$  171.46, 169.05, 150.37, 146.73, 136.75, 135.25, 132.54, 129.22, 128.57, 126.54, 122.56, 120.03, 119.04, 118.61, 114.43, 111.26, 111.17, 110.25, 107.83, 78.51, 76.11, 57.56, 56.86, 56.12, 54.27, 52.71, 24.14, 22.86.

HRMS ESI-TOF m/z calculated for  $C_{26}H_{25}N_2O_5$  [M+H]<sup>+</sup> 445.1758. Found 445.1771.



methyl (1*S*,3*R*)-2-acryloyl-1-(3-methoxy-4-(prop-2-yn-1-yloxy)phenyl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-01-04) <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.89 (br. s, 1H), 7.53 (d, J = 7.6 Hz, 1H), 7.25 (d, J = 5.5 Hz, 1H), 7.19 – 7.07 (m, 2H), 7.01 – 6.91 (m, 2H), 6.91 – 6.84 (m, 1H), 6.56 (dd, J = 16.7, 10.5 Hz, 1H), 6.29 (dd, J = 16.7, 1.7 Hz, 1H), 6.16 (br. s, 1H), 5.64 (d, J = 10.5 Hz, 1H), 5.12 – 5.04 (m, 1H), 4.71 (br. s, 2H), 3.81 (s, 3H), 3.65 (br. d, 3H), 3.63 – 3.51 (m, 1H), 3.42 – 3.12 (m, 1H), 2.48 (t, J = 2.5 Hz, 1H).

HRMS ESI-TOF m/z calculated for C<sub>26</sub>H<sub>25</sub>N<sub>2</sub>O<sub>5</sub> [M+H]<sup>+</sup> 445.1758. Found 445.1757.



# methyl (1*S*,3*S*)-2-acryloyl-1-(benzo[*d*][1,3]dioxol-5-yl)-6-(prop-2-yn-1-yloxy)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-01-09)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.81 (br. s, 1H), 7.19 (d, J = 8.7 Hz, 1H), 7.13 (d, J = 2.5 Hz, 1H), 7.02 – 6.82 (m, 3H), 6.79 – 6.53 (m, 3H), 6.41 – 6.22 (m, 1H), 5.90 (s, 2H), 5.77 (dd, J = 10.7, 1.7 Hz, 1H), 5.12 – 4.95 (m, 1H), 4.75

(d, *J* = 2.4 Hz, 2H), 3.61 (br. d, *J* = 16.9 Hz, 1H), 3.21 (br. s, 3H), 3.03 (dd, *J* = 15.6, 6.9 Hz, 1H), 2.53 (t, *J* = 2.4 Hz, 1H).

 $^{13}$ C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  170.84, 167.93, 152.37, 147.79, 147.42, 133.48, 132.20, 132.06, 131.26, 129.13, 128.30, 126.91, 126.87, 122.97, 113.18, 111.86, 111.81, 110.13, 107.83, 103.14, 101.27, 79.39, 75.34, 57.15, 53.56, 52.32, 51.57, 51.03, 22.08.

HRMS ESI-TOF m/z calculated for  $C_{26}H_{23}N_2O_6$  [M+H]<sup>+</sup> 459.1551. Found 459.1571.



methyl (1*R*,3*R*)-2-acryloyl-1-(benzo[*d*][1,3]dioxol-5-yl)-6-(prop-2-yn-1-yloxy)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-01-11)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 (br. s, 1H), 7.19 (d, *J* = 8.7 Hz, 1H), 7.13 (d, *J* = 2.4 Hz, 1H), 7.05 – 6.83 (m, 3H), 6.78 – 6.57 (m, 3H), 6.40 – 6.22 (m, 1H), 5.90 (s, 2H), 5.77 (dd, *J* = 10.7, 1.7 Hz, 1H), 5.04 (s, 1H), 4.75 (d, *J* = 10.7, 1.7 Hz, 1H), 5.04 (s, 1H), 4.75 (d, *J* = 10.7, 1.7 Hz, 1H), 5.04 (s, 1H), 4.75 (d, *J* = 10.7, 1.7 Hz, 1H), 5.04 (s, 1H), 4.75 (d, *J* = 10.7, 1.7 Hz, 1H), 5.04 (s, 1H), 4.75 (d, *J* = 10.7, 1.7 Hz, 1H), 5.04 (s, 1H), 4.75 (d, *J* = 10.7, 1.7 Hz, 1H), 5.04 (s, 1H), 4.75 (d, *J* = 10.7, 1.7 Hz, 1H), 5.04 (s, 1H), 5.04 (s

2.4 Hz, 2H), 3.61 (br. d, J = 15.9 Hz, 1H), 3.21 (br. s, 3H), 3.03 (dd, J = 15.4, 6.7 Hz, 1H), 2.53 (t, J = 2.4 Hz, 1H).

HRMS ESI-TOF m/z calculated for  $C_{26}H_{23}N_2O_6$  [M+H]<sup>+</sup> 459.1551. Found 459.1550.



methyl (1*R*,3*S*)-2-acryloyl-1-(benzo[*d*][1,3]dioxol-5-yl)-6-(prop-2-yn-1-yloxy)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-01-10)

WX-01-10 was prepared as reported previously<sup>6</sup>.



methyl (1*S*,3*R*)-2-acryloyl-1-(benzo[*d*][1,3]dioxol-5-yl)-6-(prop-2-yn-1-yloxy)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-01-12)

WX-01-12 was prepared as reported previously<sup>6</sup>.



(1*S*,3*S*)-2-acryloyl-1-(benzo[*d*][1,3]dioxol-5-yl)-*N*-propyl-2,3,4,9tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxamide (WX-02-16) WX-02-16 was prepared as reported previously<sup>22</sup>.



(1*R*,3*R*)-2-acryloyl-1-(benzo[*d*][1,3]dioxol-5-yl)-*N*-propyl-2,3,4,9tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxamide (WX-02-36) WX-02-36 was prepared as reported previously<sup>22</sup>.



(1*R*,3*S*)-2-acryloyl-1-(benzo[*d*][1,3]dioxol-5-yl)-*N*-propyl-2,3,4,9tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxamide (WX-02-26)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  7.40 (d, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 8.1 Hz, 1H), 7.06 – 7.00 (m, 1H), 6.97 (td, *J* = 7.5, 1.1 Hz, 1H), 6.96 – 6.87 (m, 2H), 6.82 – 6.71 (m, 1H), 6.70 (dd, *J* = 16.7, 10.6 Hz, 1H), 6.32 (s, 1H), 6.17 (d, *J* = 16.8 Hz, 1H), 5.94 – 5.79 (m, 2H), 5.74 – 5.51 (m, 1H), 5.43 – 5.19 (m, 1H), 4.59 (s,

1H), 3.57 - 3.40 (m, 1H), 3.06 - 2.91 (m, 2H), 1.40 - 1.17 (m, 2H), 0.74 - 0.55 (m, 3H), 2 exchangeable protons not observed.

<sup>13</sup>C NMR (151 MHz, CD<sub>3</sub>OD) δ 173.89, 170.85, 149.79, 149.05, 148.60, 147.89, 138.55, 138.21, 138.20, 136.21, 134.78, 130.52, 130.31, 128.75, 127.53, 127.52, 122.52, 120.72, 120.34, 120.11, 118.61, 112.13, 109.42, 109.01, 108.94, 107.99, 107.41, 105.46, 104.25, 102.60, 102.35, 79.47, 59.47, 58.88, 57.98, 57.48, 42.38, 42.26, 25.75, 24.61, 23.49, 11.34.

HRMS ESI-TOF m/z calculated for C<sub>25</sub>H<sub>26</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 432.1918. Found 432.1909.



#### (1S,3R)-2-acryloyl-1-(benzo[d][1,3]dioxol-5-yl)-N-propyl-2,3,4,9tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxamide (WX-02-46)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  7.40 (d, J = 7.8 Hz, 1H), 7.25 (d, J = 8.1 Hz, 1H), 7.04 (t, J = 7.5 Hz, 1H), 7.01 – 6.87 (m, 3H), 6.74 (s, 1H), 6.70 (dd, J = 16.6, 10.6 Hz, 1H), 6.31 (s, 1H), 6.17 (d, J = 16.7 Hz, 1H), 5.95 – 5.83 (m, 2H), 5.75 - 5.57 (m, 1H), 5.43 - 5.21 (m, 1H), 4.69 - 4.50 (m, 1H), 3.57 - 3.39 (m, 1H),

3.00 (t, J = 5.7 Hz, 2H), 1.29 (s, 2H), 0.74 – 0.53 (m, 3H), 2 exchangeable protons not observed. HRMS ESI-TOF m/z calculated for C<sub>25</sub>H<sub>26</sub>N<sub>3</sub>O<sub>4</sub> [M+H]<sup>+</sup> 432.1918. Found 432.1900.



#### methyl (1S,3S)-2-acryloyl-1-(3-fluorophenyl)-2,3,4,9-tetrahydro-1Hpyrido[3,4-b]indole-3-carboxylate (WX-03-57)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) δ 7.54 (d, J = 7.8 Hz, 1H), 7.36 – 7.23 (m, 2H), 7.17 -6.82 (m. 7H). 6.29 (d. J = 16.8 Hz. 1H). 5.84 (d. J = 10.9 Hz. 1H). 5.35 (d. J = 5.5 Hz, 1H), 3.62 (d, J = 16.0 Hz, 1H), 3.14 – 2.92 (m, 4H), 1 exchangeable proton

not observed.

<sup>13</sup>C NMR (151 MHz, CD<sub>3</sub>OD) δ 173.23, 172.12, 170.15, 169.38, 164.86, 163.24, 143.98, 143.93, 138.51, 138.36, 131.35, 130.77, 130.72, 130.22, 130.10, 129.59, 129.15, 127.55, 126.16, 124.74, 123.09, 120.16, 119.11, 117.27, 117.12, 115.86, 115.72, 112.16, 108.18, 108.13, 56.51, 54.63, 52.51. 52.42. 22.59.

<sup>19</sup>F NMR (376 MHz, CD<sub>3</sub>OD) δ -117.11, -118.06.

HRMS ESI-TOF m/z calculated for C<sub>22</sub>H<sub>20</sub>FN<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 379.1452. Found 379.1453.



#### methyl (1R.3R)-2-acryloyl-1-(3-fluorophenyl)-2.3.4.9-tetrahydro-1Hpyrido[3,4-b]indole-3-carboxylate (WX-03-59)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.41 – 7.22 (m, 2H), 7.19 -6.81 (m, 7H), 6.29 (d, J = 16.8 Hz, 1H), 5.83 (d, J = 10.9 Hz, 1H), 5.33 (d, J =6.7 Hz, 1H), 3.61 (d, J = 16.0 Hz, 1H), 3.16 – 2.95 (m, 4H), 1 exchangeable proton

not observed.

HRMS ESI-TOF m/z calculated for C<sub>22</sub>H<sub>20</sub>FN<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 379.1452. Found 379.1447.



#### methyl (1R,3S)-2-acryloyl-1-(3-fluorophenyl)-2,3,4,9-tetrahydro-1Hpyrido[3,4-b]indole-3-carboxylate (WX-03-58)

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.19 – 7.72 (m, 0.4H), 7.53 (d, J = 7.7 Hz, 1H), 7.39 - 7.21 (m, 2.6H), 7.19 (d, J = 7.6 Hz, 1H), 7.16 (t, J = 7.5 Hz, 1H), 7.12 (t, J = 7.4 Hz, 1H), 7.10 – 7.01 (m, 1H), 7.02 – 6.83 (m, 1H), 6.58 – 6.48 (m, 1H), 6.29 (d, J = 16.6 Hz, 1H), 6.20 (s, 1H), 5.65 (s, 1H), 5.18 (s, 1H), 3.63 (s, 4H), 3.52 – 3.11 (m, 1H).

<sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ 171.55, 169.00, 164.07, 162.43, 144.40, 136.84, 136.69, 131.07, 130.42, 129.53, 128.41, 126.38, 122.68, 122.35, 120.10, 118.66, 115.39, 114.61, 113.79, 113.65, 111.32, 111.27, 107.81, 105.11, 57.34, 56.62, 54.33, 52.84, 24.18, 22.84.

<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -113.57, -115.15.

HRMS ESI-TOF m/z calculated for C<sub>22</sub>H<sub>20</sub>FN<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 379.1452. Found 379.1449.



#### (1S,3R)-2-acryloyl-1-(3-fluorophenyl)-2,3,4,9-tetrahydro-1Hmethyl pyrido[3,4-*b*]indole-3-carboxylate (WX-03-60)

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.04 – 7.68 (m, 1H), 7.53 (dd, J = 7.8, 1.2 Hz, 1H), 7.40 – 7.22 (m, 2H), 7.19 (dt, J = 7.7, 1.3 Hz, 1H), 7.16 (t, J = 7.5 Hz, 1H), 7.12 (ddd, J = 8.0, 7.0, 1.1 Hz, 1H), 7.10 – 7.01 (m, 1H), 7.00 – 6.82 (m, 1H), 6.59 – 6.45 (m, 1H), 6.29 (dd, J = 16.5, 1.6 Hz, 1H), 6.19 (s, 1H), 5.76 - 5.56 (m, 1H), 5.19 (d, J = 5.4

Hz, 1H), 3.63 (s, 4H), 3.51 – 3.17 (m, 1H).

HRMS ESI-TOF m/z calculated for C<sub>22</sub>H<sub>20</sub>FN<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> 379.1452. Found 379.1464.



(1S,3S)-2-acryloyl-1-(3-fluorophenyl)-N-(prop-2-yn-1-yl)-2,3,4,9tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxamide (WX-03-338)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  7.54 (d, J = 7.8 Hz, 1H), 7.30 (d, J = 7.9 Hz, 2H), 7.25 - 7.06 (m, 3H), 7.11 (ddd, J = 8.2, 7.1, 1.3 Hz, 1H), 7.04 (ddd, J = 8.0, 1.27.1, 1.1 Hz, 1H), 7.02 – 6.96 (m, 1H), 6.97 – 6.88 (m, 1H), 6.32 (d, J = 16.7 Hz, 1H), 5.85 (dd, J = 10.7, 1.8 Hz, 1H), 5.27 – 5.18 (m, 1H), 3.82 – 3.36 (m, 2H), 3.23 – 2.80 (m,

2H), 2.47 (s, 1H), 2 exchangeable protons not observed.

<sup>13</sup>C NMR (151 MHz, CD<sub>3</sub>OD) δ 170.53, 164.96, 163.33, 144.19, 138.28, 131.01, 130.01, 129.45, 127.46, 125.76, 122.98, 120.15, 119.15, 116.98, 115.86, 115.72, 112.17, 108.23, 80.14, 72.17, 55.93, 52.98, 29.66, 22.60.

<sup>19</sup>F NMR (376 MHz, CD<sub>3</sub>OD) δ -116.90, -117.71. HRMS ESI-TOF m/z calculated for C<sub>24</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>2</sub> [M+H]<sup>+</sup> 402.1612. Found 402.1613.



#### (1R,3R)-2-acryloyl-1-(3-fluorophenyl)-N-(prop-2-yn-1-yl)-2,3,4,9tetrahydro-1H-pyrido[3,4-b]indole-3-carboxamide (WX-03-340)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) δ 7.53 (d, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.27 - 7.04 (m, 3H), 7.11 (ddd, J = 8.2, 7.1, 1.3 Hz, 1H), 7.04 (ddd, J = 7.9, 7.1, 1.1 Hz, 1H), 7.02 - 6.96 (m, 1H), 6.97 - 6.88 (m, 1H), 6.32 (d, J = 16.7 Hz, 1H), 5.84 (dd, J = 10.7, 1.8 Hz, 1H), 5.33 – 5.13 (m, 1H), 3.89 – 3.34 (m, 2H), 3.25 – 2.82 (m,

2H), 2.47 (s, 1H), 2 exchangeable protons not observed.

HRMS ESI-TOF m/z calculated for C<sub>24</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>2</sub> [M+H]<sup>+</sup> 402.1612. Found 402.1625.



#### (1R.3S)-2-acryloyl-1-(3-fluorophenyl)-N-(prop-2-yn-1-yl)-2,3,4,9tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxamide (WX-03-339)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  7.42 (d, J = 7.8 Hz, 1H), 7.38 – 7.11 (m, 4H), 7.04 (t, J = 7.5 Hz, 1H), 6.99 - 6.81 (m, 1H), 6.97 (ddd, J = 8.0, 7.0, 1.1 Hz, 1H), 6.77 – 6.57 (m, 1H), 6.39 (s, 1H), 6.16 (br. d, J = 16.4 Hz, 1H), 5.77 – 5.52

(m, 1H), 5.45 – 5.26 (m, 1H), 3.89 – 3.69 (m, 2H), 3.63 – 3.38 (m, 2H), 2.40 (t, J = 2.5 Hz, 1H), 2 exchangeable protons not observed.

<sup>13</sup>C NMR (151 MHz, CD<sub>3</sub>OD) δ 173.61, 171.15, 171.05, 170.76, 165.15, 163.68, 163.59, 147.59, 147.31, 138.32, 135.35, 133.93, 132.04, 131.12, 130.33, 130.00, 129.30, 128.94, 127.46, 127.42, 122.92, 122.72, 120.19, 118.78, 115.44, 114.59, 114.11, 112.19, 105.73, 104.32, 104.27, 80.36, 72.04, 59.27, 58.67, 57.98, 57.24, 29.72, 25.61, 24.43.

<sup>19</sup>F NMR (376 MHz, CD<sub>3</sub>OD) δ -116.36, -118.07.

HRMS ESI-TOF m/z calculated for C<sub>24</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>2</sub> [M+H]<sup>+</sup> 402.1612. Found 402.1614.



#### (1S,3R)-2-acryloyl-1-(3-fluorophenyl)-N-(prop-2-yn-1-yl)-2,3,4,9tetrahydro-1H-pyrido[3,4-b]indole-3-carboxamide (WX-03-341)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) δ 7.43 (s, 1H), 7.38 – 7.11 (m, 4H), 7.04 (t, J = 7.5 Hz, 1H), 6.99 – 6.81 (m, 1H), 6.97 (ddd, J = 7.9, 7.0, 1.1 Hz, 1H), 6.80 – 6.54 (m, 1H), 6.39 (br. s, 1H), 6.16 (br. d, J = 16.8 Hz, 1H), 5.79 – 5.51 (m, 1H), 5.45

- 5.24 (m, 1H), 3.91 - 3.67 (m, 2H), 3.62 - 3.38 (m, 2H), 2.41 (t, J = 2.5 Hz, 1H), 2 exchangeable protons not observed.

HRMS ESI-TOF m/z calculated for C<sub>24</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>2</sub> [M+H]<sup>+</sup> 402.1612. Found 402.1614.



methvl (1S,3S)-2-acryloyl-1-(3-fluorophenyl)-6-(prop-2-yn-1-yloxy)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-03-346) <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) δ 7.40 – 7.24 (m, 1H), 7.21 (d, J = 8.7 Hz, 1H), 7.15 (d, J = 2.4 Hz, 1H), 7.11 – 6.87 (m, 5H), 6.85 (dd, J = 8.8, 2.5 Hz, 1H), 6.29 (d, J = 16.8 Hz, 1H), 5.84 (d, J = 10.9 Hz, 1H), 5.34 (d, J = 6.8 Hz, 1H),

4.75 (d, J = 2.4 Hz, 2H), 4.59 (s, 1H), 3.66 – 3.47 (m, 1H), 3.19 – 2.95 (m, 3H), 2.91 (t, J = 2.4 Hz, 1H), 1 exchangeable proton not observed.

<sup>13</sup>C NMR (151 MHz, CD<sub>3</sub>OD) δ 172.11, 170.14, 164.84, 163.23, 153.38, 143.97, 143.92, 133.99, 131.24, 130.76, 130.76, 130.08, 129.15, 127.78, 126.13, 124.72, 117.25, 117.10, 115.85, 115.71, 113.80, 112.80, 108.05, 103.63, 80.58, 76.26, 57.84, 56.57, 54.62, 52.96, 52.53, 52.43, 22.61. <sup>19</sup>F NMR (376 MHz, CD<sub>3</sub>OD) δ -117.10, -118.06.

HRMS ESI-TOF m/z calculated for C<sub>25</sub>H<sub>22</sub>FN<sub>2</sub>O<sub>4</sub> [M+H]<sup>+</sup> 433.1558. Found 433.1564.



(1R,3R)-2-acryloyl-1-(3-fluorophenyl)-6-(prop-2-yn-1-vloxy)methvl 2.3.4.9-tetrahydro-1H-pyrido[3.4-b]indole-3-carboxylate (WX-03-348) <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) δ 7.35 – 7.22 (m, 1H), 7.21 (d, *J* = 8.8 Hz, 1H), 7.17 – 7.12 (m, 1H), 7.10 – 6.87 (m, 5H), 6.85 (dd, J = 8.8, 2.5 Hz, 1H), 6.29

(d, J = 16.9 Hz, 1H), 5.84 (d, J = 10.9 Hz, 1H), 5.42 - 5.22 (m, 1H), 4.79 -4.68 (m, 2H), 4.65 – 4.52 (m, 1H), 3.58 (d, J = 16.1 Hz, 1H), 3.14 – 2.95 (m, 3H), 2.91 (t, J = 2.4 Hz, 1H), 1 exchangeable proton not observed.

HRMS ESI-TOF m/z calculated for C<sub>25</sub>H<sub>22</sub>FN<sub>2</sub>O<sub>4</sub> [M+H]<sup>+</sup> 433.1558. Found 433.1557.



methyl (1R,3S)-2-acryloyl-1-(3-fluorophenyl)-6-(prop-2-yn-1-yloxy)-2.3.4.9-tetrahydro-1H-pyrido[3.4-b]indole-3-carboxylate (WX-03-347)

<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  7.47 – 7.09 (m, 4H), 7.05 (d, J = 2.4 Hz, 1H), 7.05 - 6.64 (m, 3H), 6.41 - 6.04 (m, 2H), 5.70 (dd, J = 10.5, 1.8 Hz, 1H), 5.59 – 5.44 (m, 0.5H), 5.06 (s, 0.5H), 4.70 (d, J = 2.4 Hz, 2H), 4.59 (s, 0.5H), 3.72 – 3.50 (m, 3H), 3.50 – 3.38 (m, 1H), 3.26 – 3.12 (m, 0.5H), 2.89 (t, J = 2.4 Hz, 1H), mixture

of rotamers, 1 exchangeable proton not observed.

<sup>13</sup>C NMR (151 MHz, CD<sub>3</sub>OD) δ 173.44, 172.92, 171.57, 170.50, 165.35, 165.02, 163.72, 163.42, 153.46, 147.55, 145.84, 135.98, 134.28, 134.05, 132.89, 131.97, 131.09, 130.43, 129.93, 129.58, 129.42, 128.92, 127.63, 126.12, 123.44, 123.24, 115.84, 115.70, 114.63, 114.48, 113.81, 113.47, 112.91, 111.38, 107.28, 105.18, 103.32, 80.50, 80.06, 76.26, 76.24, 76.01, 75.76, 58.85, 58.60, 57.89, 57.73, 55.82, 53.26, 52.88, 52.43, 24.85, 23.56, 22.61.

<sup>19</sup>F NMR (376 MHz, CD<sub>3</sub>OD) δ -116.51, -118.10.

HRMS ESI-TOF m/z calculated for C<sub>25</sub>H<sub>22</sub>FN<sub>2</sub>O<sub>4</sub> [M+H]<sup>+</sup> 433.1558. Found 433.1571.



methyl (1S,3R)-2-acryloyl-1-(3-fluorophenyl)-6-(prop-2-yn-1-yloxy)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-3-carboxylate (WX-03-349) <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  7.46 – 7.09 (m, 4H), 7.05 (d, J = 2.4 Hz, 1H), 7.03 – 6.61 (m, 3H), 6.41 – 6.03 (m, 2H), 5.70 (d, J = 10.6 Hz, 1H), 5.57 – 5.43 (m, 0.5H), 5.06 (s, 0.5H), 4.70 (d, J = 2.2 Hz, 2H), 4.64 – 4.55 (m, 0.5H),

3.73 – 3.50 (m, 3H), 3.50 – 3.36 (m, 1H), 3.27 – 3.12 (m, 0.5H), 2.89 (t, J = 2.4 Hz, 1H), mixture of rotamers, 1 exchangeable proton not observed.

HRMS ESI-TOF m/z calculated for C<sub>25</sub>H<sub>22</sub>FN<sub>2</sub>O<sub>4</sub> [M+H]<sup>+</sup> 433.1558. Found 433.1570.

# Chiral-phase SFC data





#### WX-01-08



ወ <b>ጋ</b> ል ርኬነ '	220nm		Pe	eak Table		
Peak#	Ret. Time	Height	Height%	USP Width	Area	Area%
1	1.976	952596	100.000	0.099	3428064	100.000

# Co-injection of WX-01-06 and WX-01-08



#### Method details

Column: Cellucoat, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: EtOH (0.05% diethylamine). Gradient elution: 5% to 40% B.





WX-01-03



 PDA Ch1 220nm
 Height
 Height%
 USP Width
 Area
 Area%

 1
 2.869
 133048
 100.000
 0.914
 4588203
 100.000

# Co-injection of WX-01-01 and WX-01-03



#### **Method details**

Column: Chiralcel OJ-3, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: MeOH (0.05% diethylamine). Gradient elution: 40% B.

#### WX-01-02

Chromatogram



Integration Result							
PDA Ch1 2	220nm			Peak Table			
Peak# 1 2	Ret. Time 1.704 2.050	Height 2019982 30139	Height% U 98.530 1.470	USP Width 0.048 0.057	Area 3530459 65356	Area% 98.182 1.818	

#### WX-01-04



# Co-injection of WX-01-02 and WX-01-04



#### **Method details**

Column: Cellucoat, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: EtOH (0.05% diethylamine). Gradient elution: 5% to 40% B.

#### WX-01-09

#### Chromatogram



Integration Result

		Peak Table									
PDA Ch1	220nm										
Peak#	Ret. Time	Height	Height%	USP Width	Area	Area%					
1	2.009	2408696	97.232	0.057	5232029	97.034					
2	2.249	68568	2.768	0.062	159918	2.966					

#### WX-01-11

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#### Integration Result

PDA Ch1 220nm Peak Table									
Peak#	Ret. Time	Height	Height%	USP Width	Area	Area%			
1	2.006	97956	3.580	0.054	192365	2.536			
2	2.238	2638171	96.420	0.071	7394082	97.464			

## Co-injection of WX-01-09 and WX-01-11



#### Method details

Column: Cellucoat, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: EtOH (0.05% diethylamine). Gradient elution: 5% to 40% B.





220nm						
Ret. Time	Height	Height%	Resolution(USP)		Area	Area%
0.510	555996	100.000			1156838	100.000
	220nm Ret. Time 0.510	220nm Ret. Time 0.510 Height 555996	220nm Ret. Time Height Height% 0.510 555996 100.000	220nm Ret. Time Height Height% Resolution(USP) 0.510 555996 100.000	220nm Ret. Time Height Height% Resolution(USP) 0.510 555996 100.000	220nm Ret. Time Height Height% Resolution(USP) Area 0.510 555996 100.000 1156838

#### WX-02-46



			Pea	k ladle		
PDA Ch1	220nm					
Peak#	Ret. Time	Height	Height%	Resolution(USP)	Area	Area%
1	1.088	54104	100.000		 482608	100.000

Co-injection of WX-02-26 and WX-02-46



#### **Method details**

Column: Chiralcel OD-3, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: MeOH (0.05% diethylamine). Gradient elution: 40% B.







Integration Result

			Peal	k Table		
PDA Ch1	220nm					
Peak#	Ret. Time	Height	Height%	Resolution(USP)	Area	Area%
1	1.186	224239	100.000		 871712	100.000

#### WX-03-59



			Peak	Table		
PDA Ch1 2	20nm	Haisht	II. i h + 0/	Perchation (LICP)	<b>A</b>	<b>A</b> ====0/
Peak#	Ret. Time $0.927$	1252115		Resolution(USP)	Area 3829419	Area% 99 906
2	1.185	1138	0.091	3.052	3598	0.094

Co-injection of WX-03-57 and WX-03-59



#### **Method details**

Column: Chiralpak AD-3, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: 2:1 iPrOH/CH<sub>3</sub>CN (0.05% diethylamine). Gradient elution: 40% B.





 Peak Table

 PDA Ch1 220nm
 Peak#
 Ret. Time
 Height
 Height%
 Resolution(USP)
 Area
 Area%

 1
 1.645
 1142936
 100.000
 - 6348111
 100.000

#### Co-injection of WX-03-58 and WX-03-60



#### **Method details**

Column: Chiralcel OD-3, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: MeOH (0.05% diethylamine). Gradient elution: 5% to 40% B.

#### WX-03-338

#### Chromatogram



#### WX-03-340



PDA Ch1	220nm					
Peak#	Ret. Time	Height	Height%	Resolution(USP)	Area	Area%
1	2.612	227335	100.000		 1860721	100.000

#### Co-injection of WX-03-338 and WX-03-340



#### Method details

Column: Chiralcel OD-3, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: MeOH (0.05% diethylamine). Gradient elution: 20% B.

#### WX-03-339





\_\_\_\_\_ \_\_\_\_\_ Integration Result = Peak Table

PDA Ch1 2	20nm		100	k lable		
Peak#	Ret. Time	Height	Height%	Resolution(USP)	Area	Area%
1	1.785	671334	100.000		 3175821	100.000

# Co-injection of WX-03-339 and WX-03-341



#### **Method details**

Column: Chiralcel OD-3, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: MeOH (0.05% diethylamine). Gradient elution: 5% to 40% B.

#### WX-03-346



#### WX-03-348



Signal: DAD1 A, Sig=220,4 Ref=off

RetTime				Area	Area				
[min]	Height	Resolution	Symm.	[mAU*s]	olo				
		-							
1.794	13.644		1.079	32.489	2.808				
2.226	363.449	6.148	0.922	1124.548	97.192				



# Co-injection of WX-03-346 and WX-03-348

#### Method details

Column: Chiralcel OD-3, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: MeOH (0.05% diethylamine). Gradient elution: 5% to 40% B.

#### WX-03-347



#### WX-03-349



Signal: DAD1 A, S	Sig=220,4	Ref=off
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RetTime				Area	Area		
[min]	Height	Resolution	Symm.	[mAU*s]	00		
		-					
1.512	22.907		0.966	49.571	2.772		
1.860	421.790	4.358	0.420	1738.601	97.228		

# Co-injection of WX-03-347 and WX-03-349



#### **Method details**

Column: Chiralcel OD-3, 50 mm length × 4.6 mm internal diameter, 3  $\mu$ m particle size. Mobile phase: A: supercritical CO<sub>2</sub>; B: MeOH (0.05% diethylamine). Gradient elution: 5% to 40% B.

# Spectroscopic data



<sup>1</sup>H NMR spectrum of WX-01-06 (CDCI<sub>3</sub>, 400 MHz)



<sup>13</sup>C NMR spectrum of WX-01-06 (CDCI<sub>3</sub>, 151 MHz)



<sup>1</sup>H NMR spectrum of WX-01-08 (CDCI<sub>3</sub>, 400 MHz)



<sup>1</sup>H NMR spectrum of WX-01-01 (CDCI<sub>3</sub>, 400 MHz)



<sup>13</sup>C NMR spectrum of WX-01-01 (CDCI<sub>3</sub>, 151 MHz)



<sup>1</sup>H NMR spectrum of WX-01-03 (CDCI<sub>3</sub>, 400 MHz)



<sup>1</sup>H NMR spectrum of WX-01-02 (CDCI<sub>3</sub>, 400 MHz)



<sup>13</sup>C NMR spectrum of WX-01-02 (CDCI<sub>3</sub>, 151 MHz)



<sup>1</sup>H NMR spectrum of WX-01-09 (CDCl<sub>3</sub>, 400 MHz)



<sup>1</sup>H NMR spectrum of WX-01-11 (CDCI<sub>3</sub>, 400 MHz)



<sup>1</sup>H NMR spectrum of WX-02-26 (CD<sub>3</sub>OD, 400 MHz)



<sup>13</sup>C NMR spectrum of WX-02-26 (CD<sub>3</sub>OD, 151 MHz)



<sup>1</sup>H NMR spectrum of WX-02-46 (CD<sub>3</sub>OD, 400 MHz)



<sup>1</sup>H NMR spectrum of WX-03-57 (CD<sub>3</sub>OD, 400 MHz)



 $^{13}\text{C}$  NMR spectrum of WX-03-57 (CD<sub>3</sub>OD, 151 MHz)



<sup>19</sup>F NMR spectrum of WX-03-57 (CD<sub>3</sub>OD, 376 MHz)



<sup>1</sup>H NMR spectrum of WX-03-59 (CD<sub>3</sub>OD, 400 MHz)



<sup>1</sup>H NMR spectrum of WX-03-58 (CDCl<sub>3</sub>, 600 MHz)



<sup>13</sup>C NMR spectrum of WX-03-58 (CDCI<sub>3</sub>, 151 MHz)



<sup>19</sup>F NMR spectrum of WX-03-58 (CDCI<sub>3</sub>, 376 MHz)



<sup>1</sup>H NMR spectrum of WX-03-338 (CD<sub>3</sub>OD, 400 MHz)



<sup>19</sup>F NMR spectrum of WX-03-338 (CD<sub>3</sub>OD, 376 MHz)



<sup>1</sup>H NMR spectrum of WX-03-340 (CD<sub>3</sub>OD, 400 MHz)



<sup>1</sup>H NMR spectrum of WX-03-339 (CD<sub>3</sub>OD, 400 MHz)







<sup>1</sup>H NMR spectrum of WX-03-346 (CD<sub>3</sub>OD, 400 MHz)



<sup>19</sup>F NMR spectrum of WX-03-346 (CD<sub>3</sub>OD, 376 MHz)



<sup>1</sup>H NMR spectrum of WX-03-347 (CD<sub>3</sub>OD, 400 MHz)



<sup>19</sup>F NMR spectrum of WX-03-347 (CD<sub>3</sub>OD, 376 MHz)



<sup>1</sup>H NMR spectrum of WX-03-349 (CD<sub>3</sub>OD, 400 MHz)