ZnBr$_2$-Mediated Oxidative Spiro-Bromocyclization of Propiolamide for the Synthesis of 3-Bromo-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione

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Supporting Information

1. General experimental methods.
2. General experimental procedure and characterization data.
3. Check CIF report of the Crystal (Compound 3a)
4. $^1$H and $^{13}$C NMR spectra of compound 3.
General experimental methods:

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale.

General experimental procedure for ZnBr₂-Mediated Oxidative Spiro-Bromocyclization of Propiolamide.

\[ \begin{align*}
R^1 & \quad N-arylpropolamide 1 (0.2 \text{ mmol}), \quad ZnBr_2 (1.0 \text{ equiv}) \quad \text{and} \quad \text{Oxone (2.0 equiv)} \\
\text{MeCN:H₂O (4:1, v/v)} & \quad \text{at} \quad \text{rt} \\
& \quad \text{provided} \quad \text{the} \quad \text{desired} \quad \text{product} \quad 3.
\end{align*} \]

The final products 6 and 8 were also synthesized according to the above procedure.
3-bromo-1-methyl-4-phenyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3a)\textsuperscript{1}

\textbf{\textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3})} $\delta$ 7.40-7.35 (m, 5H), 6.52 (d, $J$ = 10.1 Hz, 2H), 6.47 (d, $J$ = 10.1 Hz, 2H), 2.91 (s, 3H); \textbf{\textsuperscript{13}C NMR (101 MHz, CDCl\textsubscript{3})} $\delta$ 183.7, 165.7, 151.3, 144.1, 133.4, 130.2, 130.1, 128.7, 127.7, 119.8, 68.3, 26.6; HRMS (ESI) calcd for C\textsubscript{16}H\textsubscript{13}BrNO\textsubscript{2}: 330.0124 (M + H\textsuperscript{+}), found: 330.0124.

3-bromo-1-methyl-4-(p-tolyl)-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3b)\textsuperscript{1}

\textbf{\textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3})} $\delta$ 7.29 (d, $J$ = 8.0 Hz, 2H), 7.14 (d, $J$ = 8.0 Hz, 2H), 6.50 (d, $J$ = 10.5 Hz, 2H), 6.46 (d, $J$ = 10.4 Hz, 2H), 2.91 (s, 3H), 2.32 (s, 3H); \textbf{\textsuperscript{13}C NMR (101 MHz, CDCl\textsubscript{3})} $\delta$ 183.7, 165.9, 151.2, 144.3, 140.6, 133.3, 129.4, 127.6, 127.2, 119.2, 68.3, 26.6, 21.4; HRMS (ESI) calcd for C\textsubscript{17}H\textsubscript{13}BrNO\textsubscript{2}+: 344.0281 (M + H\textsuperscript{+}), found: 344.0271.

3-bromo-4-(4-methoxyphenyl)-1-methyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3c)\textsuperscript{1}

\textbf{\textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3})} $\delta$ 7.45 (d, $J$ = 8.9 Hz, 2H), 6.88 (d, $J$ = 8.8 Hz, 2H), 6.52-6.51 (m, 4H), 3.81 (s, 3H), 2.91 (s, 3H); \textbf{\textsuperscript{13}C NMR (101 MHz, CDCl\textsubscript{3})} $\delta$ 183.8,
166.0, 161.0, 150.5, 144.6, 133.2, 129.2, 122.3, 118.2, 114.1, 68.1, 55.3, 26.5; HRMS (ESI) calcd for C_{17}H_{15}BrNO_{3}^{+}: 360.0230 (M + H^{+}), found: 360.0229.

3-bromo-4-(4-chlorophenyl)-1-methyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3d)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.40-7.35 (m, 4H), 6.51-6.50 (m, 4H), 2.93 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.4, 165.5, 150.0, 143.9, 136.5, 133.6, 129.1, 129.0, 128.5, 68.1, 26.6; HRMS (ESI) calcd for C$_{16}$H$_{12}$BrClNO$_2^{+}$: 363.9734 (M + H$^{+}$), found: 363.9730.

3-bromo-1-methyl-4-(o-tolyl)-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3e)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.28-7.20 (m, 2H), 7.13-7.09 (m, 1H), 6.87 (d, $J = 7.6$ Hz, 1H), 6.60 (d, $J = 10.0$ Hz, 1H), 6.52-6.46 (m, 2H), 6.29 (d, $J = 10.0$ Hz, 1H), 2.93 (d, $J = 1.2$ Hz, 3H), 2.20 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.4, 165.5, 152.5, 143.5, 143.3, 136.0, 133.8, 133.2, 130.7, 129.8, 128.7, 125.4, 122.0, 69.8, 27.2, 19.9; HRMS (ESI) calcd for C$_{17}$H$_{15}$BrNO$_2^{+}$: 344.0281 (M + H$^{+}$), found: 344.0285.
3-bromo-4-(2,6-dimethylphenyl)-1-methyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3f)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.15 (t, $J = 7.7$ Hz, 1H), 7.01 (d, $J = 8.8$ Hz, 2H), 6.64 (d, $J = 9.6$ Hz, 2H), 6.35 (d, $J = 9.6$ Hz, 2H), 2.99 (s, 3H), 2.13 (s, 6H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.5, 165.5, 153.6, 144.4, 136.0, 132.7, 129.4, 128.3, 128.1, 122.7, 71.2, 27.3, 21.0; HRMS (ESI) calcd for C$_{18}$H$_{17}$BrNO$_2$: 358.0437 (M + H$^+$), found: 358.0438.

\[
\begin{align*}
\text{O} & \quad \text{Ph} \\
\text{O} & \quad \text{Br} \\
\text{N} & \quad \text{Br}
\end{align*}
\]

4-([1,1'-biphenyl]-2-yl)-3-bromo-1-methyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3g)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.44-7.40 (m, 1H), 7.36-7.33 (m, 5H), 7.23-7.21 (m, 2H), 6.99-6.96 (m, 1H), 6.32 (d, $J = 10.0$ Hz, 1H), 6.22 (d, $J = 10.0$ Hz, 1H), 5.83 (dd, $J = 10.0$, 1.7 Hz, 1H), 4.99 (dd, $J = 10.0$, 2.8 Hz, 1H), 2.76 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.6, 165.4, 154.8, 144.1, 143.1, 141.0, 140.5, 132.9, 130.4, 130.1, 129.6, 128.7, 128.3, 128.0, 127.3, 123.8, 69.1, 26.8; HRMS (ESI) calcd for C$_{22}$H$_{17}$BrNO$_2$: 406.0437 (M + H$^+$), found: 406.0440.

\[
\begin{align*}
\text{O} & \quad \text{CN} \\
\text{O} & \quad \text{Br} \\
\text{N} & \quad \text{Br}
\end{align*}
\]

2-(3-bromo-1-methyl-2,8-dioxo-1-azaspiro[4.5]deca-3,6,9-trien-4-yl)benzonitrile (3h)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.74-7.72 (m, 1H), 7.59-7.51 (m, 2H), 7.15 (d, $J = 8.8$ Hz, 1H), 6.67-6.61 (m, 2H), 6.49-6.37 (m, 2H), 2.97 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.2, 164.7, 148.5, 143.3, 142.5, 133.5, 133.4, 132.7, 130.3, 129.2, 124.5,
3-bromo-1-methyl-4-(3-nitrophenyl)-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3i)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.27-8.25 (m, 2H), 7.71-7.68 (m, 1H), 7.60-7.58 (m, 1H), 6.51-6.55 (m, 4H), 2.96 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.0, 164.9, 148.6, 148.1, 143.3, 134.0, 133.6, 131.7, 130.1, 124.9, 123.1, 122.2, 68.2, 26.8; HRMS (ESI) calcd for C$_{17}$H$_{12}$BrN$_2$O$_2$: 355.0077 (M + H$^+$), found: 355.0010.

3-bromo-1,4-dimethyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3j)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 6.47 (d, $J$ = 9.7 Hz, 2H), 6.32 (d, $J$ = 9.7 Hz, 2H), 2.81 (s, 3H), 1.77 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.7, 165.8, 149.8, 144.6, 133.4, 118.9, 68.4, 26.9, 12.4; HRMS (ESI) calcd for C$_{16}$H$_{12}$BrN$_2$O$_4$: 374.9975 (M + H$^+$), found: 374.9985.

3-bromo-1-methyl-4-(trimethylsilyl)-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3k)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 6.52 (d, $J$ = 9.6 Hz, 2H), 6.31 (d, $J$ = 9.6 Hz, 2H), 2.83 (s, 3H), 0.25 (s, 9H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.9, 165.7, 152.4, 144.5, 133.2, 132.9, 69.4, 26.4, -1.2; HRMS (ESI) calcd for C$_{13}$H$_{13}$BrNO$_2$Si: 326.0206 (M + H$^+$), found: 326.0208.
3-iodo-1-methyl-4-phenyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3l)$^1$

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.41-7.34 (m, 3H), 7.29-7.27 (m, 2H), 6.51 (d, $J = 10.0$ Hz, 2H), 6.46 (d, $J = 10.6$ Hz, 2H), 2.96 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.7, 167.4, 157.9, 144.0, 133.3, 131.8, 130.1, 128.7, 127.7, 98.2, 70.3, 27.0

1-benzyl-3-bromo-4-phenyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3n)$^1$

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.33-7.21 (m, 10H), 6.33 (d, $J = 10.2$ Hz, 2H), 6.22 (d, $J = 10.7$ Hz, 2H), 4.54 (s, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.9, 165.9, 151.8, 144.2, 137.0, 132.6, 130.1, 128.9, 128.6, 128.5, 128.0, 127.8, 119.8, 68.8, 45.4; HRMS (ESI) calcd for C$_{22}$H$_{17}$BrNO$_2$$: 406.0437 (M + H$^+$), found: 406.0439.

3-bromo-1-(2-bromobenzyl)-4-phenyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3o)$^1$

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.43-7.10 (m, 9H), 6.29-6.26 (m, 4H), 4.76 (s, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.8, 165.9, 152.2, 143.3, 136.2, 132.8, 130.7, 130.2, 129.9, 129.7, 128.6, 127.8, 124.0, 119.5, 68.6, 44.7; HRMS (ESI) calcd for C$_{22}$H$_{16}$Br$_2$NO$_2$$: 483.9542 (M + H$^+$), found: 483.9541
1-acetyl-3-bromo-4-phenyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione (3p)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.48-7.35 (m, 3H), 7.23-7.17 (m, 2H), 6.56 (d, $J = 10.1$ Hz, 2H), 6.40 (d, $J = 10.6$ Hz, 2H), 2.64 (s, 2H); $^1$C NMR (100 MHz, CDCl$_3$) $\delta$ 183.69, 168.50, 164.41, 156.22, 142.81, 132.49, 130.53, 128.57, 128.11, 119.15, 68.49, 25.59; HRMS (ESI): $m/z$ [M + Na]$^+$ calcd for C$_{17}$H$_{13}$BrNO$_3$: 358.0079; found: 358.0072.

methyl 2-(3-bromo-2,8-dioxo-4-phenyl-1-azaspiro[4.5]deca-3,6,9-trien-1-yl)acetate (3q)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.40-7.36 (m, 5H), 6.65 (d, $J = 9.7$ Hz, 2H), 6.42 (d, $J = 9.7$ Hz, 2H), 4.03 (s, 2H), 3.74 (s, 3H); $^1$C NMR (101 MHz, CDCl$_3$) $\delta$ 183.7, 168.5, 165.8, 152.6, 143.4, 133.1, 130.4, 128.8, 127.7, 119.3, 105.0, 68.3, 52.6, 41.7; HRMS (ESI) calcd for C$_{18}$H$_{15}$BrNO$_4$: 388.0179 (M + H$^+$), found: 388.0161

2-(3-bromo-2,8-dioxo-4-phenyl-1-azaspiro[4.5]deca-3,6,9-trien-1-yl)-N-(tert-butyl)-2'-phenylacetamide (3r)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.42-7.22 (m, 10H), 6.72 (dd, $J = 10.0$, 2.8 Hz, 1H), 6.49 (dd, $J = 10.0$, 2.9 1H), 6.25 (d, $J = 10.0$ Hz, 1H), 6.21 (d, $J = 10.0$ Hz, 1H), 5.49
(s, 1H), 4.79 (s, 1H), 1.28 (s, 9H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 184.0, 166.6, 165.7, 152.4, 144.3, 144.1, 135.2, 132.5, 132.3, 130.1, 129.4, 129.3, 129.1, 128.6, 127.8, 120.0, 69.6, 62.8, 52.0, 28.5; HRMS (ESI) calcd for C$_{27}$H$_{26}$BrN$_2$O$_3$: 505.1121 (M + H$^+$), found: 505.1116

3-bromo-1,6-dimethyl-4-phenyl-1-azaspiro[4.5]deca-3,6,9,triene-2,8-dione (3s)$^1$

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.43-7.36 (m, 5H), 6.49-6.45 (m, 2H), 6.36 (s, 1H), 2.84 (s, 3H), 1.74 (d, $J = 1.1$ Hz, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 184.4, 166.2, 152.6, 151.2, 144.4, 132.9, 132.2, 130.4, 129.9, 128.9, 127.5, 119.7, 70.4, 26.2, 17.7; HRMS (ESI) calcd for C$_{17}$H$_{15}$BrNO$_2$: 344.0281 (M + H$^+$), found: 344.0289

3-bromo-1,7-dimethyl-4-phenyl-1-azaspiro[4.5]deca-3,6,9,triene-2,8-dione (3t)$^1$

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.37-7.34 (m, 5H), 6.46-6.45 (m, 2H), 6.28 (s, 1H), 2.91 (s, 3H), 1.92 (d, $J = 1.3$ Hz, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 184.5, 165.8, 151.7, 143.9, 140.7, 138.8, 133.2, 130.3, 128.7, 127.7, 119.4, 68.8, 26.5, 15.9; HRMS (ESI) calcd for C$_{17}$H$_{15}$BrNO$_2$: 344.0281 (M + H$^+$), found: 344.0280

3-bromo-4-phenyl-1-oxaspiro[4.5]deca-3,6,9,triene-2,8-dione (6)$^1$

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.48-7.41 (m, 5H), 6.67 (d, $J = 10.1$ Hz, 2H), 6.42 (d, $J = 10.2$ Hz, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 183.5, 166.9, 159.8, 141.7, 132.2, 131.4, 129.0, 128.6, 127.4, 112.3, 83.0; HRMS (ESI) calcd for C$_{15}$H$_{10}$BrO$_3$: 316.9808 (M + H$^+$), found: 316.9818
4-(4-acetylphenyl)-3-bromo-6-iodo-1-tosyl-1-azaspiro[4.5]deca-3,6,9-trien-8-one (8)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.85 (d, $J = 8.4$ Hz, 2H), 7.76 (d, $J = 8.0$ Hz, 2H), 7.34 (d, $J = 8.1$ Hz, 2H), 7.23 (d, $J = 8.2$ Hz, 2H), 6.95-6.89 (m, 2H), 6.30 (dd, $J = 9.9$, 1.8 Hz, 1H), 4.60-4.51 (m, 2H), 2.55 (s, 3H), 2.45 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 197.2, 181.0, 144.9, 144.7, 141.6, 137.6, 137.0, 136.0, 134.1, 129.9, 129.1, 128.3, 127.8, 119.4, 59.3, 26.6, 21.6; HRMS (ESI) calcd for C$_{24}$H$_{20}$BrINO$_4$S$^+$: 623.9336 (M + H$^+$), found: 623.9348

Reference:

Crystal data of Compound 3a:
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_60406b

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found  CIF dictionary  Interpreting this report

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The following ALERTs were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.
Alert level B
PLAT94_ALERT_3_B Number of (Jobs-Input)/SigmA > 10 Outliers .... 4 Check

Alert level C
PLAT94_ALERT_3_C Short Inters HL-HL Contact Brl ... Brl ... 3.34 Ang.
PLAT911_ALERT_3_C Missing # PFC Refl Between Tmin & 3T/L= 0.600 13 Report

Alert level G
PLAT912_ALERT_4_G Missing # of PFC Reflections Above STH/L= 0.600 4 Note
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0 ALERT level A = Most likely a serious problem - resolve or explain
1 ALERT level B = A potentially serious problem, consider carefully
2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
2 ALERT level G = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit to Acta Crystallographica Section C or E or IUCrData, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 30/03/2016; check.def file version of 30/03/2016