KBr/K$_2$S$_2$O$_8$-Mediated Dibromohydration of

$N$-(2-Alkynylaryl)acetamide

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Supporting Information

1. General experimental methods.
2. General experimental procedure and characterization data.
3. Check CIF report of the Crystal (CCDC: 1498018, Compound 3m)
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 the dibromohydrative reaction of o-alkynylacetaniline and KBr.

\[
\begin{align*}
\text{2-alkynylacetaniline} \; 1 \; (0.2 \; \text{mmol}), \; \text{KBr} \; (3.0 \; \text{equiv}) \; \text{and} \; \text{K}_2\text{S}_2\text{O}_8 \; (3.0 \; \text{equiv}) \; \text{was added to a test tube, and then co-solvent} \; \text{DCE}:\text{H}_2\text{O} \; (2 \; \text{mL}) \; \text{was added. The mixture was stirred at} \; 80 \; ^\circ\text{C}. \; \text{After completion of reaction as indicated by TLC (overnight), the mixture was purified by flash column chromatograph to give the desired product} \; 3. \; \text{The final products} \; 6, \; 8 \; \text{and} \; 9 \; \text{were also synthesized according to the above procedure.}
\end{align*}
\]

$N$-(2-(2,2-dibromo-2-phenylacetyl)phenyl)acetamide (3a)

$^1$H NMR (400 MHz, DMSO) $\delta$ 8.60 (d, $J = 8.4$ Hz, 1H), 8.04 (s, 1H), 7.87 – 7.82 (m, 1H), 7.71 (d, $J = 7.5$ Hz, 1H), 7.43 – 7.30 (m, 6H), 1.90 (s, 3H); $^{13}$C NMR (101 MHz, DMSO) $\delta$ 196.5, 170.2, 153.0, 138.7, 137.5, 129.5, 129.3, 125.5, 125.2, 125.1, 120.3, 117.8, 90.5, 24.8; The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS. HRMS (ESI) calcd for C$_{16}$H$_{13}$NNaO$_3$:$^+$: 290.0788 (M + Na$^+$), found: 290.0784.

$N$-(2-(2,2-dibromo-2-phenylacetyl)-4-methylphenyl)acetamide (3b)

$^1$H NMR (400 MHz, DMSO) $\delta$ 8.48 (d, $J = 8.5$ Hz, 1H), 8.01 (s, 1H), 7.66 (d, $J = 8.5$ Hz, 1H), 7.51 (s, 1H), 7.42 – 7.36 (m, 3H), 7.34 – 7.31 (m, 2H), 2.35 (s, 3H), 1.88 (s, 3H); $^{13}$C NMR (101 MHz, DMSO) $\delta$ 196.5, 167.0, 151.2, 139.5, 137.5, 134.8, 129.5, 129.3, 125.5, 124.7, 120.5, 117.7, 90.7, 24.7, 20.7; The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS. HRMS (ESI) calcd for C$_{17}$H$_{15}$NNaO$_3$:$^+$: 304.0944 (M + Na$^+$), found: 304.0951.
**N-(2-(2,2-dibromo-2-phenylacetyl)-4-fluorophenyl)acetamide (3c)**

\(^1\)H NMR (400 MHz, DMSO) \(\delta\) 8.63 (d, \(J = 9.0\) Hz, 1H), 8.11 (s, 1H), 7.75-7.70 (m, 1H), 7.57-7.55 (m, 1H), 7.43 – 7.34 (m, 5H), 1.89 (s, 3H); \(^{13}\)C NMR (101 MHz, DMSO) \(\delta\) 196.1, 170.1, 159.1 (d, \(J = 244.2\) Hz), 149.7, 137.2, 129.6, 129.5, 125.9, 125.6, 125.6, 121.8 (d, \(J = 7.4\) Hz), 119.8 (d, \(J = 7.5\) Hz), 110.8 (d, \(J = 23.2\) Hz), 91.1, 24.7; The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS. HRMS (ESI) calcd for C\(_{16}\)H\(_{12}\)FNNaO\(_3\)^+: 308.0693 (M + Na^+), found: 308.0690.

**N-(2-(2,2-dibromo-2-phenylacetyl)-4-(trifluoromethyl)phenyl)acetamide (3d)**

\(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 11.19 (s, 1H), 8.87 (d, \(J = 9.2\) Hz, 1H), 7.63 – 7.61 (m, 4H), 7.44 – 7.35 (m, 3H), 2.36 (s, 3H); \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 189.0, 169.5, 145.3, 140.7, 131.4 (q, \(J = 3.2\) Hz), 130.6 (q, \(J = 4.1\) Hz), 130.1, 129.3, 126.2, 124.3, 122.8, 121.7, 121.1 (q, \(J = 272.0\) Hz), 114.9, 25.8; HRMS (ESI) calcd for C\(_{17}\)H\(_{13}\)Br\(_2\)F\(_3\)NO\(_2\): 477.9260 (M + H^+), found: 477.9258.
\(N-(2-(2,2\text{-dibromo}-2-(4\text{-chlorophenyl})\text{acetyl})\text{phenyl})\text{acetamide}\ (3e)\)

\(^1\text{H NMR}\ (400\ \text{MHz, DMSO})\ \delta\ 8.59\ (d, J = 8.4\ \text{Hz}, 1\text{H}),\ 8.16\ (s, 1\text{H}),\ 7.87 - 7.83\ (m, 1\text{H}),\ 7.72\ (d, J = 7.6\ \text{Hz}, 1\text{H}),\ 7.47\ (d, J = 8.8\ \text{Hz}, 2\text{H}),\ 7.37\ (d, J = 8.6\ \text{Hz}, 2\text{H}),\ 7.33-7.31\ (m, 1\text{H}),\ 1.92\ (s, 3\text{H});\ \ ^{13}\text{C NMR}\ (101\ \text{MHz, DMSO})\ \delta\ 196.2,\ 170.2,\ 153.1,\ 138.9,\ 136.7,\ 134.2,\ 129.6,\ 127.6,\ 125.3,\ 120.2,\ 118.0,\ 90.1,\ 24.9;\ \text{The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS.}\ \text{HRMS (ESI) calcd for } C_{16}H_{12}ClNNaO_3^+: 324.0398 (M + Na^+),\ \text{found: 324.0389.}\)

\(N-(2-(2-(4\text{-acetylphenyl})-2,2\text{-dibromoacetetyl})\text{phenyl})\text{acetamide}\ (3f)\)

\(^1\text{H NMR}\ (400\ \text{MHz, CDCl}_3)\ \delta\ 11.07\ (s, 1\text{H}),\ 8.70\ (d, J = 8.4\ \text{Hz}, 1\text{H}),\ 7.96\ (d, J = 8.6\ \text{Hz}, 2\text{H}),\ 7.72\ (d, J = 8.5\ \text{Hz}, 2\text{H}),\ 7.47-7.42\ (m, 1\text{H}),\ 7.35\ (d, J = 8.3\ \text{Hz}, 1\text{H}),\ 6.75-6.71\ (m, 1\text{H}),\ 2.61\ (s, 3\text{H}),\ 2.33\ (s, 3\text{H});\ \ ^{13}\text{C NMR}\ (101\ \text{MHz, CDCl}_3)\ \delta\ 196.7,\ 189.0,\ 169.3,\ 145.7,\ 142.8,\ 137.5,\ 135.5,\ 133.2,\ 128.9,\ 126.6,\ 121.8,\ 121.2,\ 115.2,\ 68.7,\ 26.7,\ 25.7;\ \text{The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS.}\ \text{HRMS (ESI) calcd for } C_{18}H_{15}NNaO_4^+: 332.0893 (M + Na^+),\ \text{found: 332.0893.}\)
N-(2-(2,2-dibromo-2-(4-cyanophenyl)acetyl)phenyl)acetamide (3g)

$^1$H NMR (400 MHz, CDCl$_3$) δ 10.98 (s, 1H), 8.68 (d, $J = 8.6$ Hz, 1H), 7.73 (d, $J = 8.6$ Hz, 2H), 7.68 (d, $J = 8.6$ Hz, 2H), 7.48-7.44 (m, 1H), 7.35 (d, $J = 8.3$ Hz, 1H), 6.78-6.74 (m, 1H), 2.31 (s, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 188.6, 169.3, 145.9, 142.8, 135.7, 133.1, 132.8, 127.2, 121.9, 121.3, 117.5, 115.1, 113.5, 67.6, 25.6; HRMS (ESI) calcd for C$_{17}$H$_{13}$Br$_2$N$_2$O$_2$: 434.9338 (M + H$^+$), found: 434.9333.

N-(2-(2,2-dibromo-2-(4-fluorophenyl)acetyl)phenyl)acetamide (3h)

$^1$H NMR (400 MHz, DMSO) δ 8.59 (d, $J = 8.4$ Hz, 1H), 8.11 (s, 1H), 7.87 – 7.82 (m, 1H), 7.72 (d, $J = 7.6$ Hz, 1H), 7.40 – 7.37 (m, 2H), 7.34-7.30 (m, 1H), 7.25-7.21 (m, 2H), 1.92 (s, 3H); $^{13}$C NMR (101 MHz, DMSO) δ 196.4, 170.2, 162.8 (d, $J = 245.5$ Hz), 153.0, 138.8, 133.8 (d, $J = 2.9$ Hz), 127.9 (d, $J = 8.6$ Hz), 125.3 (d, $J = 4.6$ Hz), 120.2, 118.0, 116.5 (d, $J = 21.8$ Hz), 90.2, 55.4, 24.8; The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS. HRMS (ESI) calcd for C$_{16}$H$_{12}$FNNaO$_3$+: 308.0693 (M + Na$^+$), found: 308.0690.
1H NMR (400 MHz, DMSO) δ 8.63 (d, J = 8.4 Hz, 1H), 8.10 (s, 1H), 7.88 – 7.84 (m, 1H), 7.74 (d, J = 7.2 Hz, 1H), 7.70 (d, J = 8.6 Hz, 2H), 7.64 (d, J = 7.2 Hz, 2H), 7.46 – 7.43 (m, 4H), 7.37-7.31 (m, 2H), 1.97 (s, 3H); 13C NMR (101 MHz, DMSO) δ 196.5, 170.3, 153.1, 141.1, 139.8, 138.8, 136.7, 129.5, 128.3, 127.9, 127.3, 126.2, 125.3, 125.2, 120.4, 117.9, 90.56, 25.0; The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS. HRMS (ESI) calcd for C_{22}H_{17}NNaO_{3}: 366.1101 (M + Na^+), found: 366.1097.

1H NMR (400 MHz, CDCl_3) δ 8.62 (s, 1H), 7.49 (d, J = 8.3 Hz, 1H), 7.42-7.38 (m, 3H), 7.07-7.04 (m, 2H), 3.90 (s, 3H), 1.99 (s, 3H); 13C NMR (101 MHz, CDCl_3) δ 170.7, 160.5, 136.5, 136.4, 131.5, 127.4, 127.3, 123.6, 120.4, 119.9, 119.3, 114.4, 101.7, 55.4, 27.5; HRMS (ESI) calcd for C_{17}H_{14}Br_{2}NO^{-}: 421.9386 (M + H^-), found: 421.9377.
N-(2-(2,2-dibromo-3,3-dimethylbutanoyl)phenyl)acetamide (3k)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.20 (d, $J = 7.8$ Hz, 1H), 7.35 – 7.31 (m, 1H), 7.19 (d, $J = 7.6$ Hz, 1H), 7.08 (t, $J = 7.5$ Hz, 1H), 1.09 (s, 9H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 168.1, 145.1, 134.5, 132.9, 130.1, 129.1, 123.7, 121.5, 118.3, 43.3, 31.5, 24.8; HRMS (ESI) calcd for C$_{14}$H$_{17}$BrNO$: 294.0488$ (M + H$^+$), found: 294.0486.

![Chemical structure of N-(2-(2,2-dibromo-3,3-dimethylbutanoyl)phenyl)acetamide](image1)

N-(2-(2,2-dibromo-2-phenylacetyl)phenyl)cyclohexanecarboxamide (3l)

$^1$H NMR (400 MHz, DMSO) $\delta$ 8.62 (d, $J = 8.4$ Hz, 1H), 8.08 (s, 1H), 7.89 – 7.79 (m, 1H), 7.72 (d, $J = 7.4$ Hz, 1H), 7.42-7.29 (m, 6H), 2.60-2.51 (m, 1H), 1.78 (d, $J = 12.1$ Hz, 1H), 1.64 (d, $J = 4.2$ Hz, 1H), 1.47 (d, $J = 5.0$ Hz, 1H), 1.38 – 1.27 (m, 2H), 1.22 – 1.10 (m, 1H), 1.04 (t, $J = 10.2$ Hz, 2H), 0.73 (d, $J = 12.1$ Hz, 1H), 0.53 – 0.42 (m, 1H); $^{13}$C NMR (101 MHz, DMSO) $\delta$ 196.6, 176.9, 153.3, 138.6, 138.1, 129.2, 129.1, 125.4, 125.2, 125.1, 120.7, 118.1, 90.3, 44.2, 30.1, 28.4, 25.6, 25.2; The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS. HRMS (ESI) calcd for C$_{21}$H$_{21}$NNaO$_3$: 358.1414 (M + Na$^+$), found: 358.1426.

![Chemical structure of N-(2-(2,2-dibromo-2-phenylacetyl)phenyl)cyclohexanecarboxamide](image2)

N-(2-(2,2-dibromo-2-phenylacetyl)phenyl)benzamide (3m)

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 11.96 (s, 1H), 8.91 (d, $J = 8.2$ Hz, 1H), 8.09 (d, $J = 8.0$ Hz, 2H), 7.63 (d, $J = 8.0$ Hz, 2H), 7.60-7.48 (m, 5H), 7.43-7.40 (m, 3H), 6.84-6.79 (m, 4H), 6.76 (s, 2H); $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 168.1, 145.1, 134.5, 132.9, 130.1, 129.1, 123.7, 121.5, 118.3, 43.3, 31.5, 24.8; HRMS (ESI) calcd for C$_{14}$H$_{17}$BrNO$: 294.0488$ (M + H$^+$), found: 294.0486.

![Chemical structure of N-(2-(2,2-dibromo-2-phenylacetyl)phenyl)benzamide](image3)
1H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 190.4, 166.0, 143.1, 140.2, 135.5, 134.6, 133.4, 132.3, 130.0, 129.2, 129.0, 127.5, 125.5, 121.7, 121.5, 116.8; **The dibromo group in the final product was hydrolyzed into carbonyl group when being identified by HRMS.** HRMS (ESI) calcd for C$_{21}$H$_{15}$NNaO$_3$$: 352.0944 (M + Na$^{+}$), found: 352.0951.

![Chemical structure](image1)

N-(2-(2-oxo-2-phenylacetyl)phenyl)benzamide (4)$^1$

$^1$H NMR (400 MHz, CDCl$_3$) δ 12.34 (s, 1H), 9.09 (d, $J = 8.4$ Hz, 1H), 8.13-8.11 (m, 2H), 7.99-7.96 (m, 2H), 7.74-7.63 (m, 3H), 7.61-7.52 (m, 5H), 7.14-7.10 (m, 1H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 199.3, 193.0, 166.1, 142.8, 137.3, 135.1, 134.3, 134.2, 132.7, 132.3, 129.9, 129.2, 128.9, 127.5, 122.8, 120.9, 118.2;

![Chemical structure](image2)

(1Z,3E)-3-(bromo(phenyl)methylene)-N-phenylisobenzofuran-1(3H)-imine 6$^2$

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.64 (d, $J = 8.0$ Hz, 1H), 8.06 (d, $J = 7.7$ Hz, 1H), 7.75-7.52 (m, 5H), 7.40-7.26 (m, 7H), 7.14-7.10 (m, 1H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 152.4, 144.9, 136.8, 135.6, 132.2, 131.7, 130.4, 129.8, 128.8, 128.6, 127.9, 125.1, 124.4, 123.8, 111.4, 104.2;

![Chemical structure](image3)
4-bromo-3-phenyl-1H-isochromen-1-one (8)³

$^1$H NMR (400 MHz, CDCl₃) $\delta$ 8.34 (d, $J = 8.0$ Hz, 1H), 7.97 (d, $J = 7.7$ Hz, 1H), 7.88-7.78 (m, 3H), 7.63-7.61 (m, 1H), 7.49-7.47 (m, 3H); $^{13}$C NMR (101 MHz, CDCl₃) $\delta$ 161.2, 151.8, 136.6, 135.5, 132.8, 130.2, 129.8, 129.7, 129.2, 128.1, 126.7, 120.6, 101.4

Methyl 2-(2-oxo-2-phenylacetyl)benzoate (9a) ⁴

$^1$H NMR (400 MHz, CDCl₃) $\delta$ 8.20 (d, $J = 8.4$ Hz, 2H), 8.01 (d, $J = 8.0$ Hz, 1H), 7.71-7.52 (m, 6H), 3.66 (s, 3H); $^{13}$C NMR (101 MHz, CDCl₃) $\delta$ 193.6, 188.9, 166.8, 138.7, 133.9, 133.0, 132.9, 131.6, 130.8, 130.1, 129.7, 129.5, 128.4, 52.7

Benzyl 2-(2-oxo-2-phenylacetyl)benzoate (9b) ⁴

$^1$H NMR (400 MHz, CDCl₃) $\delta$ 8.20 (d, $J = 8.2$ Hz, 2H), 8.03 (d, $J = 7.7$ Hz, 1H), 7.71-7.70 (m, 2H), 7.65-7.60 (m, 2H), 7.55-7.51 (m, 2H), 7.34-7.27 (m, 5H), 5.15 (s, 2H); $^{13}$C NMR (101 MHz, CDCl₃) $\delta$ 193.7, 189.0, 166.5, 139.0, 135.1, 133.8, 133.1, 131.5, 130.8, 130.1, 129.6, 128.6, 128.4, 128.3, 128.2, 66.9;
Reference:

Crystal data of Compound 3m:

PLATON version of 07/03/2016; check.def file version of 02/03/2016

Datacheck ok0311b - e/p unit cell
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a60311b

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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 C

PLAT911_ALERT_3_C Missing # PFC Refl Between THin & TH/L= 0.600 12 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma > 10 Outliers .... 1 Check

Alert level G

PLAT912_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT912_ALERT_4_G The CIF-Embedded .res File Contains DPIX Records 1 Report
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PLAT922_ALERT_4_G Missing # of PFC Reflections Above 6Th/L= 0.600 5 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 7 Note

0 ALERT level A - Most likely a serious problem - resolve or explain
0 ALERT level B - A potentially serious problem, consider carefully
2 ALERT level C - Check. Ensure it is not caused by an omission or oversight
7 ALERT level G - General information/check it is not something unexpected

2 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
3 ALERT type 3 Indicator that the structure quality may be low
2 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 A, 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.