Metal-Free and Open-Air Arylation Reactions of Diaryliodonium Salts for DNA-Encoded Library Synthesis

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Supporting Information

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I. General Information

All commercially available organic compounds were purchased from Sigma-Aldrich, and oligonucleotides were purchased from Shanghai AngewGen Biotech Co., Ltd. in China. Unless otherwise noted, all commercial reagents and solvents were used without additional purification. The substrates 1 were prepared according to literature methods. Water was purified with a Millipore Milli-Q system. NMR spectra were recorded on Bruker AM-500 instruments. Chemical shifts are reported in δ (ppm) referenced to TMS as an internal standard for 1H NMR and CDCl3 (δ 77.0) or DMSO-d6 (δ 39.5) for 13C NMR. High-resolution mass spectra were obtained on High-resolution mass spectra (HRMS-ESI) were obtained on an Agilent Technologies 6230 Accurate Mass TOF LC/MS instrument or an AB Sciex 4600 QTOF MS instrument.

All reagents and DNA headpiece HP-NH2 (5’-/ 5phos / GAGTCA / iSp9 / iUniAmM / iSp9 / TGACTCCC-3’, Figure 1) were obtained from commercial sources unless otherwise noted and used as received. All on-DNA reactions were performed in 1.5 mL or 5 mL Eppendorf tubes. On-DNA reactions in the studies of reaction condition optimization and substrate scope extension were analyzed by UPLC-MS. Typically, samples were dissolved in an appropriate amount of distilled and deionized water (ddH2O) and injected into a reverse-phase chromatography column (Xbridge Oligonucleotide BEH C18 column, 1.7 μm, 2.1×50 mm). The elution was carried out as followings: 5–95% solvent B over 4.5 min, 0.4 mL/min, λ = 260 nm; solvent A: 0.75% v/v hexafluorisopropanol / 0.038% v/v triethylamine in methanol/water = 5/95; solvent B: 0.75% v/v hexafluorisopropanol / 0.038% v/v triethylamine in methanol/water = 90/10. The effluents were analyzed by a Xevo G2-XS Q-TOF with electrospray ionization source was used for detection. On-DNA reaction yield calculation: Ignoring UV coefficient difference for all DNA products and assuming 100% of DNA total recovery, the yield of DNA products were determined from UV absorbance trace (260 nm) peak area.

![Figure S1. The Structure of Headpiece DNA (HP-NH2).](image-url)
II. Abbreviations

BF₃·OEt₂: boron trifluoride ether complex
DAI: diaryliodonium salts
DCM: dichloromethane
DCE: 1,2-dichloroethane
ddH₂O: double distilled water
DIPEA: N,N-diisopropylethylamine
DMA: N,N-dimethylacetamide
DMAP: 4-dimethylaminopyridine
DMF: N,N-dimethylformamide
DMSO: dimethyl sulfoxide
EDC: 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimi
HATU: 2-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate
HOAc: acetic acid
m-CPBA: m-chloroperbenzoic acid
MTBE: methyl tert-butyl ether
THF: tetrahydrofuran
PBS: phosphate buffer saline
PivOH: pivalic acid
sNHS: N-Hydroxysulfosuccinimide sodium salt
TfOH: trifluoromethanesulfonic acid
TMP-H: 1,3,5-trimethoxybenzene
TsOH·H₂O: p-toluenesulfonic acid monohydrate
III. Experimental Procedures and Characterizations

**Figure S2.** Structures of diaryliodonium salts DAI-a–DAI-t

**General procedure (i) for the synthesis of diaryliodonium salts from arenes and iodine:***

$m$-CPBA (85% active oxidant, 15 mmol) and iodine (5 mmol) were dissolved in DCM (50 mL) in a sealed tube, which resulted in a dark purple solution that was cooled to 0 °C. Arene was added followed by dropwise addition of TfOH (10 mmol), resulting in a slight heat increase and change of color to a yellow transparent solution. The solution was stirred at the indicated temperature and time and concentrated in vacuo. MTBE (2–3 mL) was added and the mixture was stirred at rt for 5 min to precipitate out an off-white solid. The flask was stored in the freezer for 30 min, then the solid was filtered off, washed with cold MTBE and dried under vacuum to give diaryliodonium salt.

**General procedure (ii) for the one-pot synthesis of diaryliodonium salts from iodides and arenes:**

$m$-CPBA (85% active oxidant, 5 mmol) and aryl iodide 1 (5 mmol) were dissolved in CH$_2$Cl$_2$ (20 mL) in a sealed tube. Then arene (5 mmol) was added, and the solution was cooled to 0 °C followed by dropwise addition of TfOH (10 mmol), resulting in a slight heat increase. The solution was stirred at the indicated temperature and time and...
concentrated in vacuo. MTBE (2–3mL) was added and the mixture was stirred at rt for 5 min to precipitate out an off-white solid. The flask was stored in the freezer for 30 min, then the solid was filtered off, washed with cold MTBE and dried under vacuum to give diaryliodonium salt.

**General procedure (iii) for the synthesis of diaryliodonium salts from iodides and arylboronic acid:**[2]

\[
\begin{align*}
\text{i) } & \text{m-CPBA, BF}_3\text{OEt}_2 \to \text{R} & \text{BF}_4 \\
\text{CH}_2\text{Cl}_2 & \text{r.t} \to \text{R} & \text{BF}_4 \\
\text{ii) } & \text{AR-B(OH)}_2 \to \text{R} & \text{BF}_4 \\
\text{CH}_2\text{Cl}_2 & \text{r.t} \to \text{R} & \text{BF}_4 \\
\text{ii) } & \text{TfOH} \to \text{R} & \text{OTf} \\
\text{CH}_2\text{Cl}_2 & \text{r.t} \to \text{R} & \text{OTf}
\end{align*}
\]

\( m\)-CPBA (85% active oxidant, 5 mmol) was dissolved in \( \text{CH}_2\text{Cl}_2 \) (20 mL). To the solution was added aryl iodide (5 mmol) followed by \( \text{BF}_3\cdot\text{OEt}_2 \) (10 mmol) at room temperature. The resulting yellow solution was stirred at rt for 1h and then cooled to 0 °C, and aryl boronic acid (5 mmol) was added. After 30 min of stirring at rt, the solution was cooled to 0 °C, followed by dropwise addition of \( \text{TfOH} \) (10 mmol), resulting in a slight heat increase, the solution was stirred at the indicated temperature and time and concentrated in vacuo. Then the crude reaction mixture was applied on a silica plug (10 g) and eluted with \( \text{CH}_2\text{Cl}_2 \) (10 mL) to remove unreacted aryl iodide and \( m\)-CPBA, followed by MeOH/ \( \text{CH}_2\text{Cl}_2 \) (5:95), to elute the product. The latter solution was concentrated in vacuo. MTBE (2–3mL) was added and the mixture was stirred at rt for 5 min to precipitate out an off-white solid. The flask was stored in the freezer for 30 min, then the solid was filtered off, washed with cold MTBE and dried under vacuum to give diaryliodonium salt.

**General procedure (iv) for the synthesis of diaryliodonium salts from iodides and arenes:**[3]

\[
\begin{align*}
\text{i) } & \text{TsOH-H}_2\text{O, m-CPBA} \to \text{R} & \text{I} \\
\text{CH}_3\text{CN} & \text{77 °C} \to \text{R} & \text{I} \\
\text{ii) } & \text{TMP-H} \to \text{R} & \text{I} \\
\text{CH}_3\text{CN} & \text{77 °C} \to \text{R} & \text{I}
\end{align*}
\]

Aryl iodide (1.00 mmol) and acetonitrile (1 ml) were added to a 10 ml round-bottom flask and equipped with a magnetic stir bar. TsOH·H\(_2\)O (1 mmol) was added in one portion at room temperature, followed by \( m\)-CPBA (85% active oxidant, 1 mmol). The flask was lowered into a pre-heated heating block set at 77 °C, and stirred for 30 minutes. 1,3,5-trimethoxynaphthalene (TMP-H) (1 mmol) was then added and the resulting mixture was stirred for 5 minutes at 77 °C. The flask was cooled to ambient temperature before acetonitrile was removed under reduced pressure. Then the resulting crude oil was applied on a silica plug (10 g) and eluted with \( \text{CH}_2\text{Cl}_2 \) (10 mL) to remove unreacted aryl iodide and \( m\)-CPBA, followed by MeOH/\( \text{CH}_2\text{Cl}_2 \) (1:100–1:10) to elute the product.
DAI-a was obtained from the commercial source.

![DAI-a](image)

Synthesized according to **General procedure (ii)**, in 62% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 8.18 – 7.88 (m, 4H), 7.35 – 7.30 (m, 4H), 2.34 (s, 6H). The $^1$H NMR matches that previously reported.$^{[1]}$

![DAI-b](image)

Synthesized according to **General procedure (i)**, in 86% yield. $^1$H NMR (500 MHz, Chloroform-$d$) δ 7.95 – 7.86 (m, 4H), 7.53 – 7.45 (m, 4H), 1.33 (d, $J = 3.5$ Hz, 18H). The $^1$H NMR matches that previously reported.$^{[4]}$

![DAI-c](image)

Synthesized according to **General procedure (ii)**, in 72% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 8.22 – 8.10 (m, 4H), 7.82 – 7.68 (m, 4H). The $^1$H NMR matches that previously reported.$^{[4]}$

![DAI-d](image)

Synthesized according to **General procedure (iii)**, in 72% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 8.26 (d, $J = 8.7$ Hz, 4H), 7.64 (d, $J = 8.8$ Hz, 4H). The $^1$H NMR matches that previously reported.$^{[1]}$

![DAI-e](image)
Synthesized according to *General procedure (iii)*, in 21% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 8.51 (d, $J = 9.0$ Hz, 4H), 8.32 – 8.26 (m, 4H). Exact Mass: 371.9607. Observed mass 371.9636. $^{13}$C NMR (126 MHz, DMSO) δ 150.07, 137.27, 126.92, 123.49. HRMS (ESI) calcd for [M+H]$^+$ [C$_{12}$H$_9$IN$_2$O$_4$]$^+$ 371.9596, observed mass 371.9636.

Synthesized according to *General procedure (iii)*, in 36% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 8.42 – 8.37 (m, 4H), 8.07 – 8.01 (m, 4H), 3.87 (s, 6H). The $^1$H NMR matches that previously reported.$^{[5]}$

Synthesized according to *General procedure (iii)*, in 33% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 8.16 – 8.08 (m, 4H), 7.10 – 7.02 (m, 4H), 3.79 (s, 6H). The $^1$H NMR matches that previously reported.$^{[2]}$

Synthesized according to *General procedure (iii)*, in 42% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 8.44 – 8.37 (m, 4H), 7.62 – 7.55 (m, 4H). The $^1$H NMR matches that previously reported.$^{[6]}$
Synthesized according to *General procedure (iii)*, in 56% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 8.58 – 8.40 (m, 4H), 7.95 (d, $J = 8.4$ Hz, 4H). The $^1$H NMR matches that previously reported.\(^{[2]}\)

![DAI-k](image)

Synthesized according to *General procedure (iii)*, in 37% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 8.82 (d, $J = 1.9$ Hz, 2H), 8.65 – 8.56 (m, 2H), 8.12 – 8.03 (m, 2H), 7.79 (t, $J = 8.0$ Hz, 2H). The $^1$H NMR matches that previously reported.\(^{[2]}\)

![DAI-I](image)

Synthesized according to *General procedure (iii)*, in 74% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 8.50 (t, $J = 1.9$ Hz, 2H), 8.25 (ddd, $J = 8.1$, 1.7, 0.9 Hz, 2H), 7.76 (ddd, $J = 8.1$, 2.1, 0.9 Hz, 2H), 7.58 (t, $J = 8.1$ Hz, 2H). The $^1$H NMR matches that previously reported.\(^{[7]}\)

![DAI-m](image)

Synthesized according to *General procedure (iii)*, in 76% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 8.40 (td, $J = 6.2$, 3.0 Hz, 2H), 7.78 – 7.69 (m, 2H), 7.59 (ddd, $J = 8.5$, 7.2, 1.4 Hz, 2H), 7.38 (ddd, $J = 8.7$, 7.4, 1.4 Hz, 2H). The $^1$H NMR matches that previously reported.\(^{[2]}\)

![DAI-n](image)

Synthesized according to *General procedure (iii)*, in 81% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 8.52 (dd, $J = 8.1$, 1.5 Hz, 2H), 7.84 (dd, $J = 8.1$, 1.5 Hz, 2H), 7.71 (td, $J =
$7.7, 1.5$ Hz, 2H), $7.49$ (td, $J=7.7, 1.5$ Hz, 2H). $^{13}$C NMR (126 MHz, DMSO) $\delta 139.40, 136.44, 135.25, 130.95, 130.68, 120.00$. HRMS (ESI) calcd for [M+H]$^+$ [C$_{12}$H$_6$Cl$_2$I]$^+$ 349.9126. Observed mass 349.9130.

Synthesized according to General procedure (i), in 82% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta 8.14$ (d, $J=8.2$ Hz, 2H), 7.36 (d, $J=2.2$ Hz, 2H), 7.10 (dd, $J=8.3, 2.2$ Hz, 2H), 2.54 (s, 6H), 2.30 (s, 6H). The $^1$H NMR matches that previously reported.$^{[5]}$

Synthesized according to General procedure (i), in 90% yield. $^1$H NMR (500 MHz, Chloroform-$d$) $\delta 7.75$ (s, 2H), 7.36 (s, 4H), 2.59 (s, 6H), 2.37 (s, 6H). The $^1$H NMR matches that previously reported.$^{[4]}$

Synthesized according to General procedure (ii), in 90% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta 7.19$ (s, 4H), 2.46 (s, 12H), 2.29 (s, 6H). The $^1$H NMR matches that previously reported.$^{[4]}$

Synthesized according to General procedure (iii), in 42% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta 8.88$ (dd, $J=7.6, 1.1$ Hz, 2H), 8.49 (d, $J=8.5$ Hz, 2H), 8.21 (d, $J=8.1$ Hz, 2H), 8.07 – 7.98 (m, 2H), 7.81 (ddd, $J=8.4, 6.9, 1.3$ Hz, 2H), 7.68 (ddd, $J=8.1, 6.9, 1.0$ Hz, 2H), 7.57 (t, $J=7.8$ Hz, 2H). The $^1$H NMR matches that previously
Synthesized according to General procedure (iv), in 79% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 8.86 (d, $J = 2.5$ Hz, 1H), 8.36 (dd, $J = 8.5$, 2.4 Hz, 1H), 7.67 – 7.58 (m, 1H), 7.49 – 7.47 (m, 2H), 7.12 (d, $J = 7.9$ Hz, 2H), 6.46 (s, 2H), 4.10 – 3.87 (m, 6H), 3.87 (s, 3H), 2.29 (s, 3H). The $^1$H NMR matches that previously reported.[8]

Synthesized according to General procedure (ii), in 61% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 9.31 – 9.24 (m, 1H), 8.82 (dd, $J = 4.7$, 1.4 Hz, 1H), 8.63 (ddd, $J = 8.2$, 2.3, 1.5 Hz, 1H), 8.24 – 8.18 (m, 2H), 7.58 (ddd, $J = 8.2$, 4.7, 0.7 Hz, 1H), 7.13 – 7.06 (m, 2H), 3.80 (s, 3H). The $^1$H NMR matches that previously reported.[9]
Scheme S1. Synthesis of DNA-conjugated phenols HP1–HP9 and HP11–HP12. i) To a solution of DNA headpiece (HP-NH$_2$) (600 μL, 300 nmol) in borate buffer (250 mM, pH = 9.4) was added a mixture of DMA solution of HATU (60 μL, 200 mM), DIPEA (60 μL, 200 mM) and acids (60 μL, 200 mM). The resultant mixture was vortexed and stood at 25 °C for 8 hours. 5M NaCl (78 μL) and cold ethanol (2.34 mL) were sequentially added, and the resultant mixture was stored at −80 °C for 30 min. The mixture was centrifuged at 4 °C for 30 min at 12000 rpm to remove the supernatant. The resulting pellet was re-dissolved in ddH$_2$O (300 μL), which was used in following reaction without further purification.

Synthesis of DNA-conjugated phenols HP10. Amino acid (5 μL, 200 mM in DMSO) was incubated with EDC (2.5 μL, 400 mM DMSO) and sNHS sodium salt (6.6 μL, 133 mM DMSO/H$_2$O (2:1) for 25 min at 30°C. The solution of HP-NH$_2$ (20 μL, 20 nmol) in borate buffer (250 mM, pH = 9.4) was then added to the mixture and the reaction was let to proceed for 3 hours at 30 °C. The reaction mixture was next added 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet was re-dissolved in ddH$_2$O (20 μL), which was used in following reaction without further purification.
Table S1. Screening of the on-DNA O-arylation reaction parameters

| Entry | DAI-a (equiv) | pH of BBS | Solvent          | Temp. | Time (h) | Yield (%)b |
|-------|---------------|-----------|------------------|-------|----------|------------|
| 1a    | 200           | 9.4       | DMA-BBS (2:3)    | 80    | 2.5      | 87         |
| 2     | 400           |           | DMA-ddH2O (1:9)  | 70    | 2.5      | 37         |
| 3     | 400           |           | DMA-ddH2O (1:9)  | 80    | 2.5      | 65         |
| 4     | 400           |           | DMA-ddH2O (1:9)  | 90    | 2.5      | 46         |
| 5     | 800           | 8         | DMA- BBS (1:9)   | 80    | 2.5      | 14         |
| 6     | 800           | 9         | DMA-BBS (1:9)    | 80    | 2.5      | 48         |
| 7     | 800           | 9.4       | DMA-BBS (1:9)    | 80    | 2.5      | 73         |
| 8     | 800           | 9.4       | DMA-BBS (1:4)    | 80    | 2.5      | 80         |
| 9     | 600           | 9.4       | DMA-BBS (2:3)    | 80    | 2.5      | 76         |
| 10    | 400           | 9.4       | DMA-BBS (2:3)    | 80    | 2.5      | 78         |
| 11    | 200           | 9.4       | DMA-BBS (2:3)    | 70    | 2.5      | 59         |
| 12    | 200           | 9.4       | DMA-BBS (2:3)    | 80    | 2        | 80         |

Reactions were performed at 80°C with HP1 (5 nM, 1 mM in ddH2O) and DAI-a (200 eq, 500 mM in DMA) in total volume of 50 μL aqueous solutions (V_{DMA}/V_{borate buffer (pH 9.4)} = 2 : 3), 2.5h. The conversion yield was determined by LC-MS. BBS: borate buffer solution.

General Procedures (v) for the on-DNA O-arylation reactions

To HP (5 μL, 10 nmol, 1 mM in ddH2O) was added 25 μL of borate buffer (pH 9.4, 250 mM) and 200 equiv. of DAI (20 μL, 50 mM in DMA). The resulting mixture was vortexed and stood at 80 °C for 2.5 h. The reaction mixture was next added 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet (precipitate) was re-dissolved in ddH2O (300 μL) for LC-MS detection.
Scheme S2. Synthesis of P13 and P14

**Step i):** To a solution of HP-NH₂ (10 μL, 10 nmol) in borate buffer (250 mM, pH = 9.4) was added a mixture of DMA solution of HATU (2 μL, 200 mM), DIPEA (2 μL, 200 mM) and acids (2 μL, 200 mM). The resultant mixture was vortexed and stood at 25 °C for 8 hours. The reaction mixture was next added 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4 °C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet was re-dissolved in ddH₂O (10 μL), which was used in following reaction without further purification.

**Step ii):** To a solution of Fmoc protected DNA material (10 μL, 10 nmol) in ddH₂O, was added 5 μL of piperidine. The resultant mixture was vortexed and stood at 25 °C for 2 hours. The reaction mixture was next added 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20 °C) were added, vortexed, and incubated at -80 °C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet was re-dissolved in ddH₂O (10 μL), which was used in following reaction without further purification.

**Step iii):** To a solution of P13s1/P14s1 (5 nmol) in 10 μL borate buffer (250 mM, pH = 9.4) was added HATU (2 μL, 400 mM in DMA), DIPEA (2 μL, 200 mM) and acids (2 μL, 200 mM). The resultant mixture was vortexed and stood at 25 °C for 8 hours. After that 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80 °C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4 °C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet was re-dissolved in ddH₂O (5 μL), which was used in following reaction without further purification.
**Scheme S3.** Synthesis of P15 and P16

**Step i:** To P2c or P12 (5 μL, 5 nmol, 1 mM in ddH2O) was added B2(OH)₄ (5 μL, 750 nmol, 150 mM in ddH2O), NaOH (5 μL, 2500 nmol, 500 mM in ddH2O), 2.5 μL ddH2O and 7.5 μL EtOH (30% by volume). The resulting mixture was vortexed and stood at rt for 2 hours. The reaction mixture was next added 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C), vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet (precipitate) was re-dissolved in ddH2O (300 μL) for LC-MS detection.

**Step ii:** To P15s0 or P16s0 (10 μL, 10 nmol, 1 mM in pH 9.4 borate buffer) was added 1-chloro-4-isocyanato-2-(trifluoromethyl)benzene (1 μL, 500 nmol, 500 mM in MeCN). The resulting mixture was vortexed and stood at 80°C for 16 hours. The reaction mixture was next added 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C), vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet (precipitate) was re-dissolved in ddH2O (10 μL) for LC-MS detection.
Scheme S4. Synthesis of isatin-oximes i1–i20.

**Step i):** To a solution of is1 (2 mmol, 1 equiv.) in 10 mL CH₂Cl₂ was added K₂CO₃ (6 mmol, 3 equiv), followed by dropwise addition of propargyl bromide (6 mmol, 3 equiv). The resulting reaction mixture was stirring at rt for 3 hours. Then the solid was filtered off and the organic was concentrated in vacuo. Then the crude reaction mixture was applied on a silica plug (10 g) and eluted with CH₂Cl₂ (10 mL) followed by MeOH/CH₂Cl₂ (1:100–1:10) to elute the product.

**Step ii):** is2 (1 mmol, 1 equiv.) was dissolved in ethanol (5 ml). To this solution was added hydroxylamine hydrochloride (1.2 mmol, 1.2 equiv.) and KOAc (2 mmol, 2 equiv.) in 3 mL of water. The resulting reaction mixture was stirred at 50°C for 2 hours, then cooled to rt. The yellow precipitate was removed by filtration and dried under high vacuum to produce the isatin oxime (i1–i20).
91% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.73 (td, $J = 7.8$, 1.4 Hz, 1H), 7.60 (dd, $J = 7.5$, 1.3 Hz, 1H), 7.30 – 7.15 (m, 2H), 4.56 (d, $J = 2.5$ Hz, 2H), 3.36 (d, $J = 2.5$ Hz, 1H). The $^1$H NMR matches that previously reported.$^{[14]}$

68% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.77 (td, $J = 8.3$, 5.7 Hz, 1H), 7.08 (d, $J = 7.9$ Hz, 1H), 6.99 (t, $J = 8.8$ Hz, 1H), 4.57 (d, $J = 2.6$ Hz, 2H), 3.37 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO) δ 178.64, 159.10, 157.43, 150.42, 140.93, 111.66, 107.95, 106.19, 77.63, 75.62, 29.95. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_7$FNO$_2$]$^+$ 204.0455, observed mass 204.0496.

40% yield. $^1$H NMR (500 MHz, Chloroform-$d$) δ 7.37 (td, $J = 8.5$, 7.5, 2.4 Hz, 2H), 7.14 – 7.08 (m, 1H), 4.54 (d, $J = 2.6$ Hz, 2H), 2.33 (t, $J = 2.5$ Hz, 1H). The $^1$H NMR matches that previously reported.$^{[15]}$

36% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.71 (dd, $J = 8.3$, 5.7 Hz, 1H), 7.27 – 7.17 (m, 1H), 6.99 (ddd, $J = 10.3$, 8.3, 2.2 Hz, 1H), 4.57 (d, $J = 2.6$ Hz, 2H), 3.37 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 181.00, 169.41, 167.37, 158.14, 152.66, 128.15, 115.05, 110.62, 100.44, 77.60, 75.61, 29.76. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_7$FNO$_2$]$^+$ 204.0455, observed mass 204.0437.
70% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.64 (ddd, $J = 11.6, 8.4, 1.1$ Hz, 1H), 7.48 (dd, $J = 7.3, 1.1$ Hz, 1H), 7.21 (ddd, $J = 8.3, 7.3, 4.0$ Hz, 1H), 4.57 (dd, $J = 2.6, 1.1$ Hz, 2H), 3.34 (d, $J = 2.4$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 181.79, 157.84, 148.83, 146.87, 135.81, 126.36, 125.28, 121.35, 78.42, 75.12, 31.73. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_7$FNO$_2$]$^+$ 204.0455, observed mass 204.0496.

83% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.78 (dd, $J = 8.5, 2.3$ Hz, 1H), 7.66 (d, $J = 2.3$ Hz, 1H), 7.27 (d, $J = 8.4$ Hz, 1H), 4.57 (d, $J = 2.5$ Hz, 2H), 3.37 (s, 1H). The $^1$H NMR matches that previously reported.$^{[14]}$

85% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.62 (d, $J = 8.0$ Hz, 1H), 7.39 (d, $J = 1.8$ Hz, 1H), 7.24 (dd, $J = 8.0, 1.8$ Hz, 1H), 4.58 (d, $J = 2.6$ Hz, 2H), 3.37 (t, $J = 2.6$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO) δ 181.57, 157.92, 151.00, 142.68, 126.51, 123.92, 117.09, 111.99, 77.61, 75.63, 29.68. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_7$ClNO$_2$]$^+$ 220.0160, observed mass 220.0169.

81% yield. $^1$H NMR (500 MHz, Chloroform-$d$) δ 7.59 (d, $J = 7.7$ Hz, 2H), 7.13 (t, $J = 7.8$ Hz, 1H), 4.91 (d, $J = 2.5$ Hz, 2H), 2.31 (t, $J = 2.5$ Hz, 1H). The $^1$H NMR matches that previously reported.$^{[15]}$
85% yield. $^1$H NMR (500 MHz, Chloroform-$d$) $\delta$ 7.76 (d, $J = 10.4$ Hz, 2H), 7.06 (d, $J = 8.3$ Hz, 1H), 4.54 (d, $J = 2.6$ Hz, 2H), 2.34 (d, $J = 2.6$ Hz, 1H). The $^1$H NMR matches that previously reported.$^{[15]}$

89% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 7.52 (dd, $J = 4.8$, 3.1 Hz, 2H), 7.38 (dd, $J = 8.0$, 1.6 Hz, 1H), 4.58 (d, $J = 2.6$ Hz, 2H), 3.37 (d, $J = 2.6$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 181.82, 157.82, 150.77, 132.00, 126.91, 126.46, 117.36, 114.75, 77.60, 75.63, 29.66. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_7$BrNO$_2$]$^+$ 263.9655, observed mass 263.9641.

86% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 7.87 (dd, $J = 8.1$, 1.3 Hz, 1H), 7.62 (dd, $J = 7.3$, 1.3 Hz, 1H), 7.12 (dd, $J = 8.1$, 7.2 Hz, 1H), 4.80 (d, $J = 2.5$ Hz, 2H), 3.37 (t, $J = 2.4$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 181.79, 158.90, 146.68, 143.33, 125.87, 124.56, 121.84, 104.03, 79.29, 75.72, 31.66. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_7$BrNO$_2$]$^+$ 263.9655, observed mass 263.9674.

87% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 8.05 (dd, $J = 8.2$, 1.8 Hz, 1H), 7.85 (d, $J = 1.8$ Hz, 1H), 7.09 (d, $J = 8.3$ Hz, 1H), 4.55 (d, $J = 2.6$ Hz, 2H), 3.36 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 181.63, 157.14, 149.19, 146.02, 132.69, 120.19, 114.05, 87.11, 77.56, 75.65, 29.54. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_7$I NO$_2$]$^+$ 311.9516, observed mass 311.9500.
90% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 7.54 (dd, $J = 8.2$, 1.9 Hz, 1H), 7.43 (d, $J = 1.8$ Hz, 1H), 7.14 (d, $J = 8.0$ Hz, 1H), 4.53 (d, $J = 2.4$ Hz, 2H), 3.34 (t, $J = 2.5$ Hz, 1H), 2.31 (s, 3H). The $^1$H NMR matches that previously reported.\[^{16}\]

89% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 7.50 (d, $J = 7.7$ Hz, 1H), 7.45 (dd, $J = 7.3$, 1.4 Hz, 1H), 7.09 (t, $J = 7.5$ Hz, 1H), 4.68 (d, $J = 2.5$ Hz, 2H), 3.43 (t, $J = 2.5$ Hz, 1H), 2.64 (s, 3H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 183.30, 158.96, 147.75, 142.37, 124.32, 123.14, 122.57, 119.16, 79.82, 75.76, 31.71, 18.04. HRMS (ESI) calcd for [M+H]$^+$ [C$_{12}$H$_{10}$NO$_2$]$^+$ 200.0706, observed mass 200.0707.

88% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 7.32 (d, $J = 1.9$ Hz, 1H), 7.26 (d, $J = 1.9$ Hz, 1H), 4.65 (d, $J = 2.5$ Hz, 2H), 3.42 (t, $J = 2.4$ Hz, 1H), 2.59 (s, 3H), 2.25 (s, 3H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 183.51, 159.02, 145.60, 142.80, 133.68, 123.31, 122.38, 119.17, 79.78, 75.69, 31.66, 20.24, 17.90. HRMS (ESI) calcd for [M+H]$^+$ [C$_{13}$H$_{12}$NO$_2$]$^+$ 214.0863, observed mass 214.0814.

31% yield. $^1$H NMR (500 MHz, Chloroform-$d$) $\delta$ 7.53 (d, $J = 1.9$ Hz, 1H), 7.51 (dd, $J = 8.1$, 2.0 Hz, 1H), 7.05 (d, $J = 8.0$ Hz, 1H), 4.52 (d, $J = 2.6$ Hz, 2H), 2.92 (hept, $J = 6.9$ Hz, 1H), 2.30 (t, $J = 2.5$ Hz, 1H), 1.25 (d, $J = 6.9$ Hz, 6H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 182.91, 157.43, 147.72, 145.31, 136.74, 123.32, 117.79, 110.95, 75.87, 73.22,
33.58, 29.45, 23.81. HRMS (ESI) calcd for [M+H]$^+$ [C$_{14}$H$_{14}$NO$_2$]$^+$ 228.1019, observed mass 228.1024.

![Diagram of is2-17](image)

66% yield. $^1$H NMR (500 MHz, DMSO-$_d_6$) $\delta$ 7.32 (dt, $J$ = 8.6, 2.0 Hz, 1H), 7.18 (dq, $J$ = 5.5, 1.5 Hz, 2H), 4.53 (t, $J$ = 2.0 Hz, 2H), 3.79 (d, $J$ = 1.5 Hz, 3H), 3.34 (q, $J$ = 2.2 Hz, 1H). The $^1$H NMR matches that previously reported.$^{[17]}$

![Diagram of is2-18](image)

72% yield. $^1$H NMR (500 MHz, DMSO-$_d_6$) $\delta$ 7.58 (d, $J$ = 8.4 Hz, 1H), 6.83 (d, $J$ = 2.1 Hz, 1H), 6.70 (dd, $J$ = 8.5, 2.2 Hz, 1H), 4.56 (d, $J$ = 2.5 Hz, 2H), 3.93 (s, 3H), 3.34 (t, $J$ = 2.5 Hz, 1H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 180.37, 168.26, 159.01, 152.68, 127.84, 111.42, 109.18, 98.43, 77.98, 75.35, 56.91, 29.50. HRMS (ESI) calcd for [M+H]$^+$ [C$_{12}$H$_{10}$NO$_3$]$^+$ 216.0655, observed mass 216.0619.

![Diagram of is2-19](image)

80% yield. $^1$H NMR (500 MHz, DMSO-$_d_6$) $\delta$ 7.47 (dd, $J$ = 8.2, 1.2 Hz, 1H), 7.25 – 7.11 (m, 2H), 4.62 (d, $J$ = 2.5 Hz, 2H), 3.91 (s, 3H), 3.24 (t, $J$ = 2.4 Hz, 1H). $^{13}$C NMR (126 MHz, DMSO) $\delta$ 183.22, 158.45, 146.27, 137.70, 125.21, 123.50, 119.59, 117.33, 79.35, 74.40, 57.33, 32.36. HRMS (ESI) calcd for [M+H]$^+$ [C$_{12}$H$_{10}$NO$_3$]$^+$ 216.0655, observed mass 216.0619.

![Diagram of is2-20](image)
75% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 7.77 (dd, $J = 8.7$, 2.6 Hz, 1H), 7.64 (d, $J = 2.5$ Hz, 1H), 7.34 (d, $J = 8.6$ Hz, 1H), 4.58 (d, $J = 2.5$ Hz, 2H), 3.38 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 181.81, 173.27, 157.84, 148.58, 144.55, 139.82, 132.54, 131.01, 123.63, 121.59, 119.25, 118.23, 117.26, 113.00, 111.06, 91.42, 77.52, 75.69, 75.24, 29.62, 29.07. HRMS (ESI) calcd for [M+H]$^+$ [C$_{12}$H$_7$F$_3$NO$_3$]$^+$ 270.0373, observed mass 270.0391.

![Diagram of compound i1](image)

91% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 13.57 (s, 1H), 8.03 (dd, $J = 7.6$, 1.3 Hz, 1H), 7.49 (td, $J = 7.8$, 1.3 Hz, 1H), 7.24 – 7.08 (m, 2H), 4.58 (d, $J = 2.5$ Hz, 2H), 3.29 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 162.76, 143.67, 142.29, 132.51, 127.40, 123.56, 115.76, 110.14, 78.34, 74.94, 29.10. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_9$N$_2$O$_2$]$^+$ 201.0659, observed mass 201.0617.

![Diagram of compound i2](image)

60% yield.$^1$H NMR (500 MHz, DMSO-$d_6$) δ 13.83 – 13.23 (m, 1H), 7.51 (dtd, $J = 40.9$, 8.1, 5.2 Hz, 1H), 7.05 – 6.90 (m, 2H), 4.58 (dd, $J = 15.8$, 2.5 Hz, 2H), 3.30 (dt, $J = 5.3$, 2.5 Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 162.38, 157.83, 157.76, 155.81, 155.70, 155.17, 144.55, 144.49, 143.21, 143.15, 140.52, 140.48, 139.91, 139.85, 135.06, 134.99, 132.98, 132.91, 111.78, 111.59, 110.90, 110.75, 106.66, 106.53, 102.65, 102.47, 78.18, 78.12, 75.11, 75.04, 29.52, 29.25. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_8$FN$_2$O$_2$]$^+$ 219.0564, observed mass 219.0528.

![Diagram of compound i3](image)

63% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 13.85 (s, 1H), 7.79 (dd, $J = 8.2$, 2.8 Hz, 1H), 7.38 (td, $J = 9.1$, 2.8 Hz, 1H), 7.20 (dd, $J = 8.7$, 4.1 Hz, 1H), 4.59 (d, $J = 2.5$ Hz, 2H), 3.30 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO) δ 162.64, 159.60, 157.70, 143.36, 138.61, 118.86, 116.32, 114.53, 111.27, 78.17, 75.09, 29.26. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_8$FN$_2$O$_2$]$^+$ 219.0564, observed mass 219.0528.
75% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.62 (s, 1H), 8.05 (dd, $J = 8.4, 5.8$ Hz, 1H), 7.14 (dd, $J = 9.5, 2.4$ Hz, 1H), 6.94 (dd, $J = 9.9, 8.4, 2.4$ Hz, 1H), 4.59 (d, $J = 2.5$ Hz, 2H), 3.31 (t, $J = 2.4$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 165.55, 163.57, 163.09, 144.62, 144.52, 142.73, 129.45, 112.44, 109.82, 99.08, 78.09, 75.14, 29.38. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_8$FN$_2$O$_2$]$^+$ 219.0564, observed mass 219.0528.

76% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.88 (s, 1H), 7.90 (dd, $J = 7.6, 1.0$ Hz, 1H), 7.40 (ddd, $J = 11.7, 8.6, 1.0$ Hz, 1H), 7.16 (ddd, $J = 8.5, 7.5, 4.5$ Hz, 1H), 4.61 (dd, $J = 2.4, 1.0$ Hz, 2H), 3.30 (t, $J = 2.4$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.63, 148.19, 146.25, 142.91, 128.68, 124.82, 123.72, 120.36, 118.46, 78.92, 74.79, 31.30. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_8$FN$_2$O$_2$]$^+$ 219.0564, observed mass 219.0528.

90% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.90 (s, 1H), 7.99 (d, $J = 2.3$ Hz, 1H), 7.58 (dd, $J = 8.5, 2.2$ Hz, 1H), 7.22 (d, $J = 8.4$ Hz, 1H), 4.59 (d, $J = 2.6$ Hz, 2H), 3.32 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.42, 142.91, 141.03, 131.98, 127.39, 126.68, 116.90, 111.75, 78.05, 75.20, 29.28. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_8$ClN$_2$O$_2$]$^+$ 235.0269, observed mass 235.0208.
87% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.75 (s, 1H), 8.00 (d, $J = 8.1$ Hz, 1H), 7.32 (d, $J = 1.8$ Hz, 1H), 7.20 (dd, $J = 8.1, 1.9$ Hz, 1H), 4.61 (d, $J = 2.6$ Hz, 2H), 3.32 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.79, 143.64, 142.86, 136.73, 128.58, 123.30, 114.53, 110.58, 78.10, 75.18, 29.31. HRMS (ESI) calcd for [M+H]$^+$ [$C_{11}H_8ClN_2O_2]^+$ 235.0269, observed mass 235.0208.

![Image](image.png)

80% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.95 (s, 1H), 8.07 (dd, $J = 7.5, 1.2$ Hz, 1H), 7.49 (dd, $J = 8.3, 1.2$ Hz, 1H), 7.16 (dd, $J = 8.3, 7.5$ Hz, 1H), 4.81 (d, $J = 2.4$ Hz, 2H), 3.31 (t, $J = 2.4$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 163.48, 142.37, 138.08, 134.26, 126.36, 125.11, 118.65, 115.48, 79.69, 75.13, 31.56. HRMS (ESI) calcd for [M+H]$^+$ [$C_{11}H_8ClN_2O_2]^+$ 235.0208.

![Image](image.png)

91% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.97 (s, 1H), 8.12 (d, $J = 2.1$ Hz, 1H), 7.71 (dd, $J = 8.4, 2.2$ Hz, 1H), 7.17 (d, $J = 8.4$ Hz, 1H), 4.59 (d, $J = 2.5$ Hz, 2H), 3.34 – 3.24 (m, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.33, 142.75, 141.35, 134.73, 129.34, 117.34, 115.06, 112.18, 78.02, 75.20, 29.26. HRMS (ESI) calcd for [M+H]$^+$ [$C_{11}H_8BrN_2O_2]^+$ 278.9764, observed mass 278.9718.

![Image](image.png)

78% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.81 (s, 1H), 7.93 (d, $J = 8.0$ Hz, 1H), 7.58 – 7.18 (m, 2H), 4.61 (d, $J = 2.5$ Hz, 2H), 3.33 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 163.53, 162.94, 144.28, 143.22, 129.02, 109.15, 107.79, 97.59, 78.44, 74.90, 56.22, 29.12. HRMS (ESI) calcd for [M+H]$^+$ [$C_{11}H_8BrN_2O_2]^+$ 278.9764, observed mass 278.9718.
81% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.82 (s, 1H), 8.12 (d, $J = 7.3$ Hz, 1H), 7.65 (d, $J = 8.1$ Hz, 1H), 7.13 – 7.06 (m, 1H), 4.85 (d, $J = 2.5$ Hz, 2H), 3.33 – 3.29 (m, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 163.75, 142.25, 139.48, 137.51, 126.73, 125.40, 118.98, 102.85, 79.73, 75.36, 31.45. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_8$BrN$_2$O$_2$]$^+$ 278.9764, observed mass 278.9718.

84% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.87 (s, 1H), 8.29 (d, $J = 1.7$ Hz, 1H), 7.85 (dt, $J = 8.4$, 1.5 Hz, 1H), 7.05 (d, $J = 8.3$ Hz, 1H), 4.57 (d, $J = 2.6$ Hz, 2H), 3.31 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.14, 142.64, 141.84, 140.57, 134.95, 117.72, 112.64, 86.51, 78.04, 75.20, 29.20. HRMS (ESI) calcd for [M+H]$^+$ [C$_{11}$H$_8$N$_2$O$_2$]$^+$ 326.9625, observed mass 326.9617.

83% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.53 (s, 1H), 7.87 (d, $J = 1.8$ Hz, 1H), 7.32 – 7.28 (m, 1H), 7.06 (d, $J = 8.0$ Hz, 1H), 4.55 (d, $J = 2.5$ Hz, 2H), 3.27 (t, $J = 2.5$ Hz, 1H), 2.31 (s, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.80, 143.80, 140.08, 132.68, 132.60, 127.91, 115.80, 109.89, 78.39, 74.86, 29.09, 21.03. HRMS (ESI) calcd for [M+H]$^+$ [C$_{12}$H$_{11}$N$_2$O$_2$]$^+$ 215.0815, observed mass 215.0825.
91% yield. $^1$H NMR (500 MHz, DMSO-$_d^6$) δ 13.58 (s, 1H), 7.95 (dd, $J$ = 7.6, 1.3 Hz, 1H), 7.24 (d, $J$ = 7.8 Hz, 1H), 7.03 (t, $J$ = 7.7 Hz, 1H), 4.71 (d, $J$ = 2.5 Hz, 2H), 3.37 (t, $J$ = 2.5 Hz, 1H), 2.63 (s, 3H). $^{13}$C NMR (126 MHz, DMSO-$_d^6$) δ 163.88, 143.33, 140.27, 136.16, 125.52, 123.65, 120.80, 116.56, 80.33, 75.35, 31.30, 18.33. HRMS (ESI) calcd for [M+H]$^+$ $[C_{12}H_{11}N_2O_2]^+$ 215.0815, observed mass 215.0855.

79% yield. $^1$H NMR (500 MHz, DMSO-$_d^6$) δ 13.52 (s, 1H), 7.78 (d, $J$ = 1.8 Hz, 1H), 7.08 – 7.03 (m, 1H), 4.68 (d, $J$ = 2.5 Hz, 2H), 3.35 (t, $J$ = 2.4 Hz, 1H), 2.58 (s, 3H), 2.25 (s, 3H). $^{13}$C NMR (126 MHz, DMSO-$_d^6$) δ 163.92, 143.49, 138.01, 136.49, 132.61, 125.98, 120.47, 116.67, 80.33, 75.26, 31.24, 20.73, 18.19. HRMS (ESI) calcd for [M+H]$^+$ $[C_{13}H_{13}N_2O_2]^+$ 229.0972, observed mass 229.0924.

65% yield. $^1$H NMR (500 MHz, DMSO-$_d^6$) δ 13.54 (s, 1H), 7.91 (d, $J$ = 1.9 Hz, 1H), 7.38 (dd, $J$ = 8.2, 1.9 Hz, 1H), 7.10 (d, $J$ = 8.1 Hz, 1H), 4.56 (d, $J$ = 2.6 Hz, 2H), 3.28 (t, $J$ = 2.5 Hz, 1H), 2.91 (p, $J$ = 6.9 Hz, 1H), 1.20 (d, $J$ = 6.9 Hz, 6H). $^{13}$C NMR (126 MHz, DMSO-$_d^6$) δ 162.85, 155.91, 143.84, 143.82, 140.42, 130.31, 125.37, 115.85, 110.02, 78.41, 74.90, 33.57, 29.10, 24.47. HRMS (ESI) calcd for [M+H]$^+$ $[C_{14}H_{15}N_2O_2]^+$ 243.1128, observed mass 243.1134.

92% yield. $^1$H NMR (500 MHz, DMSO-$_d^6$) δ 13.61 (s, 1H), 7.61 (dd, $J$ = 2.4, 0.8 Hz, 1H), 7.12 – 7.07 (m, 2H), 4.55 (d, $J$ = 2.6 Hz, 2H), 3.76 (s, 3H), 3.30 – 3.25 (m, 1H). $^{13}$C NMR (126 MHz, DMSO-$_d^6$) δ 162.68, 155.91, 143.93, 135.93, 117.47, 116.33, 113.57, 110.80, 78.42, 74.89, 56.15, 29.14. HRMS (ESI) calcd for [M+H]$^+$ $[C_{12}H_{11}N_2O_3]^+$ 231.0764, observed mass 231.0726.
83% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.18 (s, 1H), 7.94 (d, $J = 8.5$ Hz, 1H), 6.91 – 6.54 (m, 2H), 4.57 (d, $J = 2.6$ Hz, 2H), 3.85 (s, 3H), 3.28 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.68, 143.57, 142.93, 128.72, 126.27, 125.43, 114.84, 113.28, 78.12, 75.19, 29.28. HRMS (ESI) calcd for [M+H]$^+$ [$C_{12}H_{11}N_2O_3$]$^+$ 231.0764, observed mass 231.0726.

83% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.60 (s, 1H), 7.69 (dd, $J = 7.5$, 1.0 Hz, 1H), 7.24 (dd, $J = 8.5$, 1.1 Hz, 1H), 7.11 (dd, $J = 8.5$, 7.6 Hz, 1H), 4.67 (d, $J = 2.5$ Hz, 2H), 3.88 (s, 3H), 3.19 (t, $J = 2.4$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 163.37, 145.29, 143.65, 130.06, 124.56, 120.25, 117.59, 117.08, 79.92, 74.02, 57.12, 31.93. HRMS (ESI) calcd for [M+H]$^+$ [$C_{12}H_{11}N_2O_3$]$^+$ 231.0764, observed mass 231.0726.

80% yield. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 13.97 (s, 1H), 7.93 (d, $J = 2.6$ Hz, 1H), 7.55 (dt, $J = 8.6$, 1.8 Hz, 1H), 7.29 (d, $J = 8.6$ Hz, 1H), 4.61 (d, $J = 2.6$ Hz, 2H), 3.33 (t, $J = 2.5$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.60, 144.07, 144.05, 142.99, 141.25, 125.63, 120.30, 116.35, 111.34, 78.01, 75.25, 29.33. HRMS (ESI) calcd for [M+H]$^+$ [$C_{12}H_8F_3N_2O_3$]$^+$ 285.0482, observed mass 285.0434.
Scheme S5. Synthesis of DNA-conjugated isatin-oxime HO1–HO20.

Step i): To HP-NH$_2$ (50 μL, 50 nmol, 1 mM in ddH$_2$O) was added 250 μL of borate buffer (pH 9.4, 250 mM in ddH$_2$O) and 100 μL of imidazole-1-sulfonyl azide tetrafluoroborate salt (40 mM in ddH$_2$O). The resulting mixture was vortexed and stood at 37°C for 16 hours. After that 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet (precipitate) was re-dissolved in ddH$_2$O (50 μL) for LC-MS detection.
Step ii): To HP-N₃ (10 μL, 10 nmol, 1 mM in pH 9.4 borate buffer) was added isatin oxime (10 μL, 800 nmol, 80 mM in DMSO), isatin oxime (10 μL, 800 nmol, 80 mM in DMSO), THPTA (10 μL, 800 nmol, 80 mM in DMSO), CuSO₄ (10 μL, 800 nmol, 80 mM in ddH₂O), ascorbate (10 μL, 1600 nmol, 160 mM in DMSO). The resulting mixture was vortexed and stood at r.t. for 3 hours. After that 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet (precipitate) was re-dissolved in ddH₂O (10 μL) for LC-MS detection.
**Table S2.** Screening of the reaction parameters of on-DNA N-arylation

| Entry | Base (equiv) | DAI-a (equiv) | Solvent | Temp. | Yield (%)<sup>b</sup> |
|-------|-------------|---------------|---------|-------|-----------------------|
| 1<sup>a</sup> | KOH (2000) | 500 | $ddH_2O/MeOH = 1:4$ | r.t. | 84 |
| 2 | NaOH (2000) | 500 | $ddH_2O/MeOH = 1:1$ | r.t. | 60 |
| 3 | KOH (2000) | 500 | $ddH_2O/DMA = 1:1$ | r.t. | 30 |
| 4 | KOH (2000) | 500 | $ddH_2O/MeOH = 1:1$ | r.t. | 73 |
| 5 | KOH (2000) | 500 | $ddH_2O/MeOH = 4:1$ | r.t. | 50 |
| 6 | KOH (2000) | 500 | $ddH_2O/MeOH = 1:5$ | r.t. | 62 |
| 7 | KOH (2000) | 500 | $ddH_2O/MeOH = 1:9$ | r.t. | 59 |
| 8 | KOH (1500) | 500 | $ddH_2O/MeOH = 1:4$ | r.t. | 68 |
| 9 | KOH (500) | 500 | $ddH_2O/MeOH = 1:4$ | r.t. | 72 |
| 10 | KOH (2000) | 1000 | $ddH_2O/MeOH = 1:4$ | r.t. | 61 |
| 11 | KOH (2000) | 750 | $ddH_2O/MeOH = 1:4$ | r.t. | 71 |
| 12 | KOH (2000) | 250 | $ddH_2O/MeOH = 1:4$ | r.t. | 63 |

<sup>a</sup>Reactions were performed at r.t. with HO1 (2 nmol, 1 mM in $ddH_2O$), DAI-a (500 eq, 500 mM in MeOH), KOH (2000 eq, 500 mM in $ddH_2O$) in total volumes of 50 μL aqueous solutions ($V_{ddH2O}/V_{MeOH} = 1:4$), 2 h. <sup>b</sup>The conversion yield was determined by LC/MS.

**General procedure (vi) for the on-DNA N-arylation of isatin-oxime**

To HO (2 μL, 2 nmol, 1 mM in $ddH_2O$) was added DAI (2 μL, 1000 nmol, 500 mM in MeOH), KOH (8 μL, 4000 nmol, 500 mM in $ddH_2O$) and 38 μL MeOH. The resulting mixture was vortexed and stood at room temperature for 2 hours. After that 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet (precipitate) was re-dissolved in $ddH_2O$ (2 μL) for LC-MS detection.
IV Co-injection Experiment

Co-injection experiment (i) of on-DNA O-arylation of phenols

Scheme S6. Synthesis of P1g from HP1 or HP-NH2 and acid 1gs.

Reaction (i) was performed according to the general procedure (v); Reaction (ii): To a solution of HP-NH2 (10 μL, 10 nmol) in borate buffer (250 mM, pH = 9.4), was added a mixture of DMA solution of DMTMM (2 μL, 200 mM), 1gs (2 μL, 200 mM), 2 μL ddH2O of and 12 μL of borate buffer (250 mM, pH = 9.4). The resultant mixture was vortexed and stood at 25 °C for 8 hours. After that 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet (precipitate) was re-dissolved in ddH2O (10 μL) for LC-MS detection.
Figure S3. LC trace of reaction (i) and reaction (ii).
**Scheme S7.** Synthesis of O1a from HO1 (reaction iii) or i1 (reaction iv).

**Reaction (iii)** was performed according to **general procedure (v).**

**Reaction (iv)** i1 (1 mmol, 1 equiv) was dissolved in 5 mL MeOH, then KOH (1.5 mmol, 1.5 equiv) and DAIa (1.5 mmol, 1.5 equiv) was added to the solution. The reaction mixture was stirred at room temperature for three hours before concentrated in vacuo. Then the crude reaction mixture was extracted with CH₂Cl₂/H₂O, the organic layer was concentrated in vacuo. Then the crude product was applied on a silica plug (10 g) and eluted with CH₂Cl₂ (10 mL) followed by MeOH/CH₂Cl₂ (1:100-1:10) to elute the product. To HP-N₃ (10 μL, 10 nmol, 1 mM in pH 9.4 borate buffer) was added O1as (10 μL, 800 nmol, 80 mM in DMSO), isatin oxime (10 μL, 800 nmol, 80 mM in DMSO), THPTA (10 μL, 800 nmol, 80 mM in DMSO), CuSO₄ (10 μL, 800 nmol, 80 mM in ddH₂O), ascorbate (10 μL, 1600 nmol, 160 mM in DMSO). The resulting mixture was vortexed and stood at r.t. for 3 hours. After that 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C) were added, vortexed, and incubated at -80°C for at least 30 minutes. The sample was centrifuged for 30 minutes at 4°C in a microcentrifuge at 12,000 rpm to remove the supernatant. The resulting pellet (precipitate) was re-dissolved in ddH₂O (10 μL) for LC-MS detection.

**O1as:** 80% yield. ¹H NMR (500 MHz, DMSO-d₆) δ 8.24 (d, J = 7.5 Hz, 1H), 7.62 (td, J = 7.8, 1.4 Hz, 1H), 7.50 – 7.43 (m, 4H), 7.28 – 7.18 (m, 3H), 4.63 (d, J = 2.5 Hz, 2H), 3.34 (s, 1H). ¹³C NMR (126 MHz, DMSO) δ 161.90, 159.02, 146.03, 143.72, 134.54, 130.27, 128.98, 124.66, 124.05, 115.34, 115.17, 110.73, 78.03, 75.26, 29.45. HRMS (ESI) calcd for [M+H]⁺ [C₁₇H₁₅N₂O₂]⁺ 277.0972, observed mass 277.0919.
Figure S4. LC trace of reaction (iii) and reaction (iv).
V. Evaluation of the DNA Tags Degradation

DNA Ligation and sequencing:

The ligation sample was prepared by mixing 5 μL Headpiece (1mM in H₂O) with 5 μL 50 bp oligo DNA (1mM in ddH₂O, prepared by annealing of 2 mM 50 bp-F and 2 mM 50 bp-R). To 0.3 nmol sample in pellet form, 1 μL 10 × T4 DNA reaction buffer (NEB, B0202S), 1 μL T4 DNA ligase (NEB, M0202L), 8 μL ddH₂O were added. The reaction mixtures were kept at room temperature for two hours. Reaction samples were then heated at 65°C for 10 minutes to denature the T4 DNA ligase. Gel electrophoresis is usually executed by using 15% TBE acrylamide gel (5.25 mL 40% acryl (29:1), 7.2 mL MilliQ water,1.4 mL 10 × TBE, 140 μL APS, 6 μL TEMED). The gel box (Bio-Rad, Mini-PROTEAN® Tetra electrophoresis) was filled with 0.5×TAE buffer until the gel was covered. The first lane of the gel was loaded with a DNA ladder, followed by loading 50 ng of DNA sample into each lane. Gel was run at 110 V for 90 min and was stained with 3000 × GelRed from Tanon™ (170-3001) in 15 mL 0.5xTBE buffer for 15 min. DNA fragments were visualized under a UV light device.
Figure S5. DNA ligation reaction analysis for synthesis of diaryl ethers and aryl oximes.
Figure S6. All DNA sample were amplified by two rounds’ PCR steps to reach 184 bp length before sequencing. Following manufacturer’s guidelines, 1 ng of former DNA ligation sample was mix with 1 μL of 10 μM primer PCR1-F and PCR1-R, 25 μL 2 × Primer STAR Max DNA Polymerase (Takara, R045A) to reach a 50 μL system finally. PCR cycles as follows: 98 °C heat activation for 1 min followed by 34 cycles of 98 °C denaturation for 10 seconds, 60 °C annealing for 5 seconds and extension at 72 °C for 10 seconds. DNA sample was evaluation by 2% DNA gel and extracted by NucleoSpin Gel Clean-up Mini kit (MACHEREY-NAGEL, 740609.50). After PCR1, PCR2 was executed as the same step by using PCR1 purified sample. DNA sequencing was sent to Sanger sequencing by using primer Sequencing-F.

PCR1-F: CTCTTTCCCTACACGACGCTCTTCCCGATCTTGGACTCCCAAATC
PCR1-R: G TGACTGGAGTTCAGACGTGTGCTCTTCCGATCAAATAAAGGCCTC
PCR2-F: AATGATACGGCAGACCAGATCTACACTCTTTCCTACACGACGCTC
PCR2-R: CAAGCAGAAGACGGCATACGAGATGTCGTGATGTGACTGAGTTTCAGACG
Sequencing-F: AATGATACGGCAGACC
qPCR Analysis:

qPCR was performed on the Applied Biosystems QuantStudio 7 Real-Time PCR System using 96-well plates. The sample mixtures of 20 µL total volume contained the following: 7 µL ddH₂O, 1 µL primer mix (5 µM each, reverse and forward primer), 2 µL diluted DNA sample and 10 µL Bimake™ 2 × SYBR Green qPCR master mix (Low ROX; B21702). The PCR reaction was carried out with the following thermocycling program: 95 °C, 60 s; 40 cycles of (95 °C, 15 s; 55 °C, 30 s; 72 °C, 30 s). Every assay was repeated at least three times.

Figure S7. qPCR analysis of residual amplifiable material after the reaction condition of synthesis of diaryl ethers (O-Arylation). In a 100 µL polypropylene plate, a solution of a full-length DNA-encoded library (ca. 0.5 mM in water, 10 µL, ca. 5 nmol) was combined with 40 µL ddH₂O (control) or combined with DAI-q (20 µL, 50 mM in DMA) and 25 µL of borate buffer (pH 9.4, 250 mM) (Test 1 and Test 2). The plate was sealed (adhesive aluminum foil), briefly vortexed, and incubated at 80°C for 150 min. All conditions were tested in triplicate (3×3 wells in total). Each sample was then diluted (three times 1:100, 2 µL sample in 198 µL ddH₂O), and desalted by gel filtration (GE healthcare Illustra, G-25 microspin columns) as per the manufacturer’s instruction. Amount of amplifiable material was determined by qPCR analysis in technical sextuplets.
Figure S8. qPCR analysis of residual amplifiable material after the reaction condition of N-arylation aryl oxime. In a 100 µL polypropylene plate, a solution of a full-length DNA-encoded library (ca. 0.5 mM in ddH$_2$O, 4 µL, ca. 5 nmol) was combined with 46 µL water (control) or combined with DAI-a (2 µL, 500 mM in MeOH), KOH (8 µL, 500 mM in ddH$_2$O) and 38 µL of MeOH (pH 9.4, 250 mM) (Test 1 and Test 2). The plate was sealed (adhesive aluminum foil), briefly vortexed, and incubated at room temperature for 120 min. All conditions were tested in triplicate (3 × 3 wells in total). Each sample was then diluted (three times 1:100, 2 µL sample in 198 µL ddH$_2$O), and desalted by gel filtration (GE healthcare Illusta, G-25 microspin columns) as per the manufacturer’s instruction. Amount of amplifiable material was determined by qPCR analysis in technical sextuplets.
VI. References

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VII. Copies of $^1$H, $^{13}$C NMR, HPLC and MS Spectra

$^1$H NMR of DAI-b

$^1$H NMR of DAI-c
$^1$H NMR of DAI-f

$^{13}$C NMR of DAI-f
$^1$H NMR of DAI-g

$^1$H NMR of DAI-h
$^1$H NMR of DAI-k

$^1$H NMR of DAI-l
$^1$H NMR of DAI-m

$^1$H NMR of DAI-n
$^{13}$C NMR of DAI-n

$^1$H NMR of DAI-o
$^1$H NMR of DAI-p

$^1$H NMR of DAI-q
$^1$H NMR of DAI-r

$^1$H NMR of DAI-s
$^1$H NMR of DAI-t

$^1$H NMR of is2-1
$^1$H NMR of is2-2

$^{13}$C NMR of is2-2
$^1$H NMR of $\text{i}s2-3$

$^1$H NMR of $\text{i}s2-4$
\(^{13}\text{C}\) NMR of is2-4

\(^{1}\text{H}\) NMR of is2-5
$^1$H NMR of is2-7

$^{13}$C NMR of is2-7
$^1$H NMR of is2-10

$^{13}$C NMR of is2-10
$^1$H NMR of is2-11

$^{13}$C NMR of is2-11
$^1$H NMR of is2-13

$^1$H NMR of is2-14
$^{13}$C NMR of is2-14

$^1$H NMR of is2-15
$^{13}$C NMR of is2-15

$^1$H NMR of is2-16
$^{13}$C NMR of is2-16

$^1$H NMR of is2-17
$^1$H NMR of is2-18

$^{13}$C NMR of is2-18
$^{1}H$ NMR of is2-19

$^{13}C$ NMR of is2-19
$^1$H NMR of ii

$^{13}$C NMR of ii
$^1$H NMR of i2

$^{13}$C NMR of i2
$^1$H NMR of i3

$^{13}$C NMR of i3
$^1$H NMR of i5

$^{13}$C NMR of i5
$^1$H NMR of i6

$^{13}$C NMR of i6
$^1$H NMR of i7

$^{13}$C NMR of i7
$^1\text{H NMR of i8}$

$^1\text{C NMR of i8}$
$^1$H NMR of i9

$^{13}$C NMR of i9
$^1$H NMR of i10

$^{13}$C NMR of i10
$^{1}H$ NMR of i11

$^{13}C$ NMR of i11
$^1$H NMR of i12

$^{13}$C NMR of i12
$^1$H NMR of i13

$^{13}$C NMR of i13
$^1$H NMR of i14

$^{13}$C NMR of i14
$^1$H NMR of i15

$^{13}$C NMR of i15
$^1$H NMR of i16

$^{13}$C NMR of i16
$^1$H NMR of i7

$^{13}$C NMR of i7
$^1$H NMR of i19

$^{13}$C NMR of i19
$^1$H NMR of i20

$^{13}$C NMR of i20
$^1$H NMR of O1as

$^1$C NMR of O1as
LC Trace and Mass of HP1

Yield: 100%
Exact mass: 5057.33

Triply charged mass \([M/3 - 1.00794\), calculated 1684.7691; observed 1684.3510.\]
LC Trace and Mass of HP2

Yield: 100%
Exact mass: 5057.33
Triply charged mass [M]/3 - 1.00794, calculated 1684.7691; observed 1684.8660.
LC Trace and Mass of HP3

Yield: 96%

Exact mass: 5075.33

Triply charged mass \([M/3 - 1.00794]\), calculated 1690.76906; observed 1690.8722.
LC Trace and Mass of HP4

Yield: 92%
Exact mass: 5102.33
Triply charged mass [M]/3 - 1.00794, calculated 1699.76906; observed 1699.8594.
LC Trace and Mass of HP5

Yield: 100%
Exact mass: 5087.33
Triply charged mass \([M/3 - 1.00794\), calculated 1694.76906; observed 1694.8822.\]
LC Trace and Mass of HP6

Yield: 96%

Exact mass: 5091.83

Triply charged mass [M]/3 - 1.00794, calculated 1696.26906; observed 1696.1976.
LC Trace and Mass of HP7

Yield: 100%

Exact mass: 5075.33

Triply charged mass [M]/3 - 1.00794, calculated 1690.76906; observed 1690.8722.
LC Trace and Mass of HP8

Yield: 96%

Exact mass: 5071.33

Triply charged mass $[{\text{M}}/3 - 1.00794]$, calculated 1689.43573; observed 1689.7273.
LC Trace and Mass of HP9

Yield: 98%
Exact mass: 5107.43
Triply charged mass [M]/3 - 1.00794, calculated 1701.46906; observed 1701.5481.
Yield: 98%

Exact mass: 5142.461

Triply charged mass [M/3 - 1.00794, calculated 1713.1457; observed 1713.0042.
LC Trace and Mass of HP11

Yield: 76%

Exact mass: 5125.471

Triply charged mass [M]/3 - 1.00794, calculated 1707.4824; observed 1707.2305.
LC Trace and Mass of HP12

Yield: 96%
Exact mass: 5058.341
Triply charged mass \([M/3]\) - 1.00794, calculated 1685.1057; observed 1684.9728.
LC Trace and Mass of P1a

Following General Procedure v

Yield: 87%

Exact mass: 5133.45

Triply charged mass \([M/3 - 1.00794\), calculated 1710.14206; observed 1710.1572.\]
LC Trace and Mass of P1b

Following General Procedure v
Yield: 81%
Exact mass: 5147.45
Triply charged mass [M]/3 - 1.00794, calculated 1714.80873; observed 1714.8514.
LC Trace and Mass of P1c

Following General Procedure v

Yield: 90%

Exact mass: 5189.55

Triply charged mass $[M/3 - 1.00794$, calculated 1728.84206; observed 1728.5298.
LC Trace and Mass of P1d

Following General Procedure v

Yield: 68%

Exact mass: 5212.35

Triply charged mass [M/3 - 1.00794, calculated 1736.44206; observed 1736.4899.
LC Trace and Mass of P1e

Following General Procedure

Yield: 76%

Exact mass: 5167.90

Triply charged mass [M/3 - 1.00794, calculated 1721.62539; observed 1721.5054.

![LC Trace and Mass of P1e](image-url)
LC Trace and Mass of P1f

Following General Procedure
Yield: 88%
Exact mass: 5178.45
Triply charged mass [M]/3 - 1.00794, calculated 1725.14206; observed 1725.1943.
LC Trace and Mass of P1g

Following General Procedure

Yield: 86%

Exact mass: 5177.50

Triply charged mass [M]/3 - 1.00794, calculated 1724.82539; observed 1725.0583.
LC Trace and Mass of P1h

Following General Procedure
Yield: 23%
Exact mass: 5163.50
Triply charged mass [M]/3 - 1.00794, calculated 1720.15873; observed 1720.4011.
LC Trace and Mass of P1i

Following General Procedure
Yield: 67%
Exact mass: 5217.45
Triply charged mass [M]/3 - 1.00794, calculated 1738.14206; observed 1738.3845.
LC Trace and Mass of P1j

Following General Procedure

Yield: 78%

Exact mass: 5201.45

Triply charged mass [M]/3 - 1.00794, calculated 1732.80873; observed 1732.8571.
LC Trace and Mass of P1k

Following General Procedure

Yield: 72%

Exact mass: 5201.45

Triply charged mass [M]/3 - 1.00794, calculated 1732.80873; observed 1733.0615.
LC Trace and Mass of P11

Following General Procedure
Yield: 28%
Exact mass: 5167.90
Triply charged mass [M]/3 - 1.00794, calculated 1721.62539; observed 1722.0491.
LC Trace and Mass of P1m

Following General Procedure

Yield: 61%

Exact mass: 5151.45

Triply charged mass [M]/3 - 1.00794, calculated 1716.14206; observed 1716.2083.
LC Trace and Mass of P1n

Following General Procedure
Yield: 85%
Exact mass: 5167.90
Triply charged mass [M]/3 \(- 1.00794\), calculated 1721.62539; observed 1721.5223.
LC Trace and Mass of P1o

Following General Procedure

Yield: 99%

Exact mass: 5161.50

Triply charged mass [M]/3 - 1.00794, calculated 1719.49206; observed 1719.5350.
LC Trace and Mass of P1p

Following General Procedure

Yield: 96%

Exact mass: 5161.50

Triply charged mass [M]/3 - 1.00794, calculated 1719.49206; observed 1719.5181.
LC Trace and Mass of P1q

Following General Procedure
Yield: 92%
Exact mass: 5175.50
Triply charged mass [M]/3 - 1.00794, calculated 1724.15873; observed 1724.1910.
LC Trace and Mass of P1r

Following General Procedure
Yield: 86%
Exact mass: 5183.50
Triply charged mass [M]/3 - 1.00794, calculated 1726.82539; observed 1727.3893.
LC Trace and Mass of P2a

Following General Procedure v

Yield: 92%

Exact mass: 5133.45

Triply charged mass \([M/3] - 1.00794\), calculated 1710.14206; observed 1710.3265.
LC Trace and Mass of P2b

Following General Procedure v

Yield: 93%

Exact mass: 5175.5

Triply charged mass [M]/3 - 1.00794, calculated 1724.15873; observed 1724.3610.
LC Trace and Mass of P2c

Following General Procedure v
Yield: 92%
Exact mass: 5178.45
Triply charged mass [M]/3 - 1.00794, calculated 1725.14206; observed 1725.0059.
LC Trace and Mass of P3a

Following General Procedure v
Yield: 36%
Exact mass: 5151.45
Triply charged mass [M]/3 - 1.00794, calculated 1716.14206; observed 1716.3269.
LC Trace and Mass of P3b

Following General Procedure v
Yield: 95%
Exact mass: 5193.50
Triply charged mass [M]/3 - 1.00794, calculated 1730.15873; observed 1730.3690.
LC Trace and Mass of P3c

Following General Procedure v

Yield: 67%

Exact mass: 5196.45

Triply charged mass [M]/3 - 1.00794, calculated 1731.14206; observed 1731.3743.
LC Trace and Mass of P4a

Following General Procedure v

Yield: 8%

Exact mass: 5178.45

Triply charged mass [M]/3 - 1.00794, calculated 1725.14206; observed 1725.3304.
LC Trace and Mass of P4b

Following General Procedure v
Yield: 80%
Exact mass: 5220.50
Triply charged mass [M]/3 - 1.00794, calculated 1739.15873; observed 1739.3921.
LC Trace and Mass of P4c

Following General Procedure v

Yield: 10%

Exact mass: 5223.45

Triply charged mass [M]/3 - 1.00794, calculated 1740.14206; observed 1740.3828.
LC Trace and Mass of P5a

Following General Procedure

Yield: 95%
Exact mass: 5163.45
Triply charged mass [M]/3 - 1.00794, calculated 1720.14206; observed 1720.3163.
LC Trace and Mass of P5b

Following General Procedure v
Yield: 95%
Exact mass: 5205.50
Triply charged mass [M]/3 - 1.00794, calculated 1734.15873; observed 1734.3916.
LC Trace and Mass of P5c

Following General Procedure v
Yield: 89%
Exact mass: 5208.45
Triply charged mass [M]/3 - 1.00794, calculated 1735.14206; observed 1735.3809.
LC Trace and Mass of P6a

Following General Procedure v

Yield: 86%

Exact mass: 5167.95

Triply charged mass [M]/3 - 1.00794, calculated 1721.64206; observed 1721.6583.
LC Trace and Mass of P6b

Following General Procedure v
Yield: 95%
Exact mass: 5210.00

Triply charged mass [M]/3 - 1.00794, calculated 1735.65873; observed 1735.7220.
LC Trace and Mass of P6c

Following General Procedure v
Yield: 85%
Exact mass: 5212.95
Triply charged mass [M]/3 - 1.00794, calculated 1736.64206; observed 1736.6947.
LC Trace and Mass of P7a

Following General Procedure v
Yield: 95%
Exact mass: 5151.45
Triply charged mass [M]/3 - 1.00794, calculated 1716.14206; observed 1716.3269.
LC Trace and Mass of P7b

Following General Procedure v

Yield: 95%

Exact mass: 5193.50

Triply charged mass [M]/3 - 1.00794, calculated 1730.15873; observed 1730.3860.
LC Trace and Mass of P7c

Following General Procedure v

Yield: 81%

Exact mass: 5196.45

Triply charged mass [M]/3 - 1.00794, calculated 1731.14206; observed 1731.3743.
LC Trace and Mass of P8a

Following General Procedure v
Yield: 95%
Exact mass: 5147.45
Triply charged mass [M]/3 - 1.00794, calculated 1714.80873; observed 1715.0039.
LC Trace and Mass of P8b

Following General Procedure V
Yield: 95%
Exact mass: 5189.50
Triply charged mass [M]/3 - 1.00794, calculated 1728.82539; observed 1729.0746.
LC Trace and Mass of P8c

Following General Procedure v

Yield: 89%

Exact mass: 5192.45

Triply charged mass [M]/3 - 1.00794, calculated 1729.80873; observed 1730.0454.
LC Trace and Mass of P9a

Following General Procedure v
Yield: 15%
Exact mass: 5183.55
Triply charged mass $[M]/3 - 1.00794$, calculated 1726.84206; observed 1727.0149.
LC Trace and Mass of P9b

Following General Procedure v
Yield: 80%

Exact mass: 5225.60

Triply charged mass [M]/3 - 1.00794, calculated 1740.85873; observed 1741.0663.
LC Trace and Mass of P9c

Following General Procedure v
Yield: 41%
Exact mass: 5228.55
Triply charged mass [M]/3 - 1.00794, calculated 1741.84206; observed 1742.0575.
LC Trace and Mass of P10

Following General Procedure v

Yield: 78%

Exact mass: 5218.561

Triply charged mass [M]/3 - 1.00794, calculated 1738.5124; observed 1738.3806.
LC Trace and Mass of P11

Following General Procedure

Yield: 75%

Exact mass: 5201.571

Triply charged mass [M]/3 - 1.00794, calculated 1732.8491; observed 1732.5814.
LC Trace and Mass of P12

Following General Procedure v

Yield: 75%

Exact mass: 5179.441

Triply charged mass [M]/3 - 1.00794, calculated 1725.4724; observed 1725.3290.
LC Trace and Mass of P13

Following General Procedure v

Yield: 66%

Exact mass: 5168.83

Triply charged mass [M]/3 - 1.00794, calculated 1721.9487; observed 1721.6744.
LC Trace and Mass of HP13s0

Following General Procedure
Yield: 98%
Exact mass: 5244.591
Triply charged mass \( [M]/3 - 1.00794 \), calculated 1747.1891; observed 1747.0464.
LC Trace and Mass of P13s1

Yield: 99%

Exact mass: 5022.351

Triply charged mass [M]/3 - 1.00794, calculated 1673.1091; observed 1673.0110.
LC Trace and Mass of P13s2

Yield: 73%

Exact mass: 5285.641

Triply charged mass [M]/3 - 1.00794, calculated 1760.8724; observed 1760.7124.
LC Trace and Mass of P13

Yield: 84%

Exact mass: 5361.741

Triply charged mass $[\text{M}] / 3 - 1.00794$, calculated 1786.2391; observed 1786.0579.
Yield: 100%

Exact mass: 5272.651

Triply charged mass [M]/3 - 1.00794, calculated 1756.5424; observed 1756.3856.
LC Trace and Mass of P14s1

Yield: 98%
Exact mass: 5050.411
Triply charged mass [M]/3 - 1.00794, calculated 1682.4624; observed 1682.3352.
LC Trace and Mass of P14s2

Yield: 78%
Exact mass: 5313.701
Triply charged mass [M]/3 - 1.00794, calculated 1770.2257; observed 1770.0536.
LC Trace and Mass of P14

Yield: 79%
Exact mass: 5389.801
Triply charged mass [M]/3 - 1.00794, calculated 1795.5924; observed 1795.3966.
LC Trace and Mass of P15s0

Yield: 94%

Exact mass: 5148.471

Triply charged mass \([M]/3\) - 1.00794, calculated 1715.1491; observed 1715.0044.
LC Trace and Mass of P15

Yield: 90%
Exact mass: 5370.031
Triply charged mass \([\text{M}] / 3\) - 1.00794, calculated 1789.0024; observed 1788.9833.
LC Trace and Mass of P16s0

Yield: 85%
Exact mass: 5149.451
Triply charged mass [M]/3 - 1.00794, calculated 1715.4757; observed 1715.3265.
LC Trace and Mass of P16

Yield: 90%
Exact mass: 5371.021
Triply charged mass [M]/3 - 1.00794, calculated 1789.3324; observed 1789.3124.
LC Trace and Mass of HP-N₃

Yield: 97%

Exact mass: 4963.231

Triply charged mass [M/3 - 1.00794, calculated 1653.4024; observed 1653.3247.
LC Trace and Mass of HO1

Yield: 90%
Exact mass: 5163.431
Triply charged mass [M]/3 - 1.00794, calculated 1720.1357; observed 1720.0439.
LC Trace and Mass of HO2

Yield: 81%
Exact mass: 5181.421
Triply charged mass [M]/3 - 1.00794, calculated 1726.1324; observed 1726.0093.
LC Trace and Mass of HO3

Yield: 89%

Exact mass: 5181.421

Triply charged mass [M]/3 - 1.00794, calculated 1726.1324; observed 1725.7882.
LC Trace and Mass of HO4

Yield: 84%
Exact mass: 5181.421
Triply charged mass [M]/3 - 1.00794, calculated 1726.1324; observed 1725.7882.
LC Trace and Mass of HO5

Yield: 81%
Exact mass: 5181.421
Triply charged mass \([M/3 - 1.00794]\), calculated 1726.1324; observed 1725.7882.
LC Trace and Mass of HO6

Yield: 94%
Exact mass: 5197.881
Triply charged mass [M]/3 - 1.00794, calculated 1731.6191; observed 1731.4398.
Yield: 80%

Exact mass: 5197.881

Triply charged mass [M]/3 - 1.00794, calculated 1731.6191; observed 1731.4568.
Yield: 80%
Exact mass: 5197.881
Triply charged mass [M]/3 - 1.00794, calculated 1731.6191; observed 1731.0990.
LC Trace and Mass of HO9

Yield: 85%

Exact mass: 5242.331

Triply charged mass [M]/3 - 1.00794, calculated 1746.4357; observed 1746.0881.
LC Trace and Mass of HO10

Yield: 82%
Exact mass: 5242.331
Triply charged mass [M]/3 - 1.00794, calculated 1746.4357; observed 1746.0881.
LC Trace and Mass of HO11

Yield: 81%

Exact mass: 5242.331

Triply charged mass [M]/3 - 1.00794, calculated 1746.4357; observed 1746.0881.
LC Trace and Mass of HO12

Yield: 81%

Exact mass: 5289.331

Triply charged mass [M]/3 - 1.00794, calculated 1762.1024; observed 1761.7434.
Yield: 89%

Exact mass: 5177.461

Triply charged mass $[\text{M}] / 3$ - 1.00794, calculated 1724.8124; observed 1724.4617.
LC Trace and Mass of HO14

Yield: 85%
Exact mass: 5177.461
Triply charged mass [M]/3 - 1.00794, calculated 1724.8124; observed 1724.4617.
LC Trace and Mass of HO15

Yield: 86%

Exact mass: 5191.491

Triply charged mass [M]/3 - 1.00794, calculated 1729.4891; observed 1729.1405.
LC Trace and Mass of HO16

Yield: 87%
Exact mass: 5205.511
Triply charged mass \([M]/3\) - 1.00794, calculated 1734.1624; observed 1733.8087.
LC Trace and Mass of HO17

Yield: 88%

Exact mass: 5193.461

Triply charged mass [M]/3 = 1.00794, calculated 1730.1457; observed 1729.8046.
LC Trace and Mass of HO18

Yield: 82%

Exact mass: 5193.461

Triply charged mass \([M/3]\) - 1.00794, calculated 1730.1457; observed 1729.4641.
Yield: 87%

Exact mass: 5193.461

Triply charged mass [M]/3 - 1.00794, calculated 1730.1457; observed 1729.8046.
Yield: 88%

Exact mass: 5247.421

Triply charged mass \([M]/3\) - 1.00794, calculated 1748.1324; observed 1747.9706.
LC Trace and Mass of O1a

Following General Procedure vi
Yield: 86%
Exact mass: 5239.53
Triply charged mass [M]/3 - 1.00794, calculated 1745.5103; observed 1745.3696.
LC Trace and Mass of O1b

Following General Procedure vi
Yield: 68%
Exact mass: 5253.53
Triply charged mass $[M]/3 - 1.00794$, calculated 1750.1691; observed 1750.1022.
LC Trace and Mass of O1c

Following General Procedure vi
Yield: 85%
Exact mass: 5195.63
Triply charged mass [M]/3 - 1.00794, calculated 1764.2024; observed 1764.1095.
LC Trace and Mass of O1d

Following General Procedure vi
Yield: 83%
Exact mass: 5318.43
Triply charged mass [M]/3 - 1.00794, calculated 1771.8024; observed 1771.7201.
LC Trace and Mass of O1e

Following General Procedure vi

Yield: 84%

Exact mass: 5273.98

Triply charged mass [M]/3 - 1.00794, calculated 1756.9857; observed 1757.0817.
LC Trace and Mass of O1f

Following General Procedure vi
Yield: 95%
Exact mass: 5257.53
Triply charged mass [M]/3 - 1.00794, calculated 1751.5024; observed 1751.4216.
LC Trace and Mass of O1g

Following General Procedure vi
Yield: 77%
Exact mass: 5284.53
Triply charged mass [M]/3 - 1.00794, calculated 1760.5024; observed 1760.4135.
LC Trace and Mass of O1h

Following General Procedure vi
Yield: 93%
Exact mass: 5297.58
Triply charged mass [M]/3 - 1.00794, calculated 1764.8524; observed 1764.7460.
LC Trace and Mass of O1i

Following General Procedure vi
Yield: 32%
Exact mass: 5269.58
Triply charged mass [M]/3 - 1.00794, calculated 1755.5191; observed 1755.4170.
LC Trace and Mass of O1j

Following General Procedure vi

Yield: 70%

Exact mass: 5323.53

Triply charged mass [M]/3 - 1.00794, calculated 1773.5024; observed 1773.3452.
LC Trace and Mass of O1k

Following General Procedure vi
Yield: 80%
Exact mass: 5307.53
Triply charged mass [M]/3 - 1.00794, calculated 1768.1691; observed 1768.0215.
LC Trace and Mass of O11

Following General Procedure vi
Yield: 84%
Exact mass: 5307.53
Triply charged mass [M]/3 - 1.00794, calculated 1768.1691; observed 1768.0215.
LC Trace and Mass of O1m

Following General Procedure vi
Yield: 80%
Exact mass: 5273.88
Triply charged mass [M]/3 - 1.00794, calculated 1756.9524; observed 1757.0034.
LC Trace and Mass of O1n

Following General Procedure vi
Yield: 98%
Exact mass: 5257.53
Triply charged mass \([M/3]\) - 1.00794, calculated 1751.5024; observed 1751.4216.
LC Trace and Mass of O1o

Following General Procedure vi
Yield: 76%
Exact mass: 5273.98
Triply charged mass [M]/3 - 1.00794, calculated 1756.9857; observed 1757.0034.
LC Trace and Mass of O1p

Following General Procedure vi
Yield: $60 + 25\% = 85\%$
Exact mass: 5267.58
Triply charged mass $[M]/3 - 1.00794$, calculated 1754.8524; observed 1754.7650.
LC Trace and Mass of O1q

Following General Procedure vi
Yield: 91%
Exact mass: 5267.58
Triply charged mass $[M]/3 - 1.00794$, calculated 1754.8524; observed 1754.7822.
LC Trace and Mass of O1r

Following General Procedure vi

Yield: 74%

Exact mass: 5281.58

Triply charged mass \([M]/3\) - 1.00794, calculated 1759.5191; observed 1759.4342.
LC Trace and Mass of O1s

Following General Procedure vi
Yield: 92%
Exact mass: 5289.58
Triply charged mass \([M]/3\) - 1.00794, calculated 1762.1857; observed 1762.0977.
LC Trace and Mass of O1t

Following General Procedure vi

Yield: 92%

Exact mass: 5274.95

Triply charged mass [M]/3 - 1.00794, calculated 1757.3091; observed 1757.0206.
LC Trace and Mass of O1u

Following General Procedure vi
Yield: 76%
Exact mass: 5240.51
Triply charged mass [M]/3 - 1.00794, calculated 1745.8291; observed 1745.7118.
LC Trace and Mass of O2a

Following General Procedure vi
Yield: 85%
Exact mass: 5257.52
Triply charged mass [M]/3 - 1.00794, calculated 1751.4991; observed 1751.1560.

![LC Trace and Mass of O2a](image-url)
Following General Procedure vi
Yield: 29 + 53% = 82%
Exact mass: 5285.57
Triply charged mass [M]/3 - 1.00794, calculated 1760.8491; observed 1760.4547.
LC Trace and Mass of O2c

Following General Procedure vi
Yield: 74%
Exact mass: 5315.57
Triply charged mass [M]/3 - 1.00794, calculated 1770.8491; observed 1770.4498.
LC Trace and Mass of O3a

Following General Procedure vi

Yield: 74%

Exact mass: 5257.52

Triply charged mass [M]/3 - 1.00794, calculated 1751.4991; observed 1751.1560.
LC Trace and Mass of O3b

Following General Procedure vi

Yield: 75%

Exact mass: 5285.57

Triply charged mass [M]/3 - 1.00794, calculated 1760.8491; observed 1760.4547.
LC Trace and Mass of O3c

Following General Procedure vi
Yield: 75%
Exact mass: 5315.57
Triply charged mass [M]/3 - 1.00794, calculated 1770.8491; observed 1770.4326.
LC Trace and Mass of O4a

Following General Procedure vi

Yield: 72%

Exact mass: 5257.52

Triply charged mass [M]/3 - 1.00794, calculated 1751.4991; observed 1751.1389.
LC Trace and Mass of O4b

Following General Procedure vi
Yield: 83%
Exact mass: 5285.57
Triply charged mass [M]/3 - 1.00794, calculated 1760.8491; observed 1760.4547.
LC Trace and Mass of O4c

Following General Procedure vi
Yield: 83%
Exact mass: 5315.57
Triply charged mass [M]/3 - 1.00794, calculated 1770.8491; observed 1770.4498.
Following General Procedure vi
Yield: 71%
Exact mass: 5257.52
Triply charged mass \([M]/3\) - 1.00794, calculated 1751.4991; observed 1751.1560.
LC Trace and Mass of O5b

Following General Procedure vi
Yield: 90%
Exact mass: 5285.57
Triply charged mass [M]/3 - 1.00794, calculated 1760.8491; observed 1760.4547.
Following General Procedure vi
Yield: 71%
Exact mass: 5315.57
Triply charged mass [M]/3 - 1.00794, calculated 1770.8491; observed 1770.4498.
LC Trace and Mass of O6a

Following General Procedure vi
Yield: 85%
Exact mass: 5273.98
Triply charged mass [M]/3 - 1.00794, calculated 1756.9857; observed 1756.8147.
LC Trace and Mass of O6b

Following General Procedure vi
Yield: 81%
Exact mass: 5302.03
Triply charged mass [M]/3 - 1.00794, calculated 1766.3357; observed 1765.9906.
LC Trace and Mass of O6c

Following General Procedure vi
Yield: 93%
Exact mass: 5332.03
Triply charged mass [M]/3 - 1.00794, calculated 1776.3357; observed 1776.0878.
LC Trace and Mass of O7a

Following General Procedure vi
Yield: 81%
Exact mass: 5273.98
Triply charged mass [M]/3 - 1.00794, calculated 1756.9857; observed 1756.8147.
LC Trace and Mass of O7b

Following General Procedure vi
Yield: 76%
Exact mass: 5302.03
Triply charged mass \([\text{M}/3 - 1.00794\), calculated 1766.3357; observed 1765.7842.\)
LC Trace and Mass of O7c

Following General Procedure vi

Yield: 77%

Exact mass: 5332.03

Triply charged mass [M]/3 - 1.00794, calculated 1776.3357; observed 1775.7599.
LC Trace and Mass of O8a

Following General Procedure vi

Yield: 89%

Exact mass: 5273.98

Triply charged mass [M]/3 - 1.00794, calculated 1756.9857; observed 1756.4714.
LC Trace and Mass of O8b

Following General Procedure vi
Yield: 80%
Exact mass: 5302.03
Triply charged mass [M]/3 - 1.00794, calculated 1766.3357; observed 1765.7842.
LC Trace and Mass of O8c

Following General Procedure vi
Yield: 82%
Exact mass: 5332.03
Triply charged mass [M]/3 - 1.00794, calculated 1776.3357; observed 1775.7599.
LC Trace and Mass of O9a

Following General Procedure vi
Yield: 76%
Exact mass: 5318.431
Triply charged mass [M]/3 - 1.00794, calculated 1771.8024; observed 1771.4491.
Following General Procedure vi

Yield: 75%

Exact mass: 5346.481

Triply charged mass \([M]/3\) - 1.00794, calculated 1781.1524; observed 1780.7496.
LC Trace and Mass of O9c

Following General Procedure vi
Yield: 80%
Exact mass: 5376.48
Triply charged mass [M]/3 - 1.00794, calculated 1791.1524; observed 1790.9927.
LC Trace and Mass of O10a

Following General Procedure vi
Yield: 65%
Exact mass: 5318.431
Triply charged mass [M]/3 - 1.00794, calculated 1771.8024; observed 1771.4491.
LC Trace and Mass of O10b

Following General Procedure vi
Yield: 82%
Exact mass: 5346.481
Triply charged mass [M]/3 - 1.00794, calculated 1781.1524; observed 1780.7670.
LC Trace and Mass of O10c

Following General Procedure vi
Yield: 65%
Exact mass: 5376.48
Triply charged mass [M]/3 - 1.00794, calculated 1791.1524; observed 1790.7501.
LC Trace and Mass of O11a

Following General Procedure vi

Yield: 73%

Exact mass: 5318.431

Triply charged mass [M]/3 - 1.00794, calculated 1771.8024; observed 1771.4491.
Following General Procedure vi
Yield: 82%
Exact mass: 5346.481
Triply charged mass [M/3 - 1.00794, calculated 1781.1524; observed 1780.7670.
LC Trace and Mass of O11c

Following General Procedure vi

Yield: 83%
Exact mass: 5376.48
Triply charged mass [M]/3 - 1.00794, calculated 1791.1524; observed 1790.9927.
LC Trace and Mass of O12a

Following General Procedure vi

Yield: 66%

Exact mass: 5365.43

Triply charged mass [M]/3 - 1.00794, calculated 1787.4691; observed 1787.2866.
LC Trace and Mass of O12b

Following General Procedure vi

Yield: 70%

Exact mass: 5393.48

Triply charged mass [M]/3 - 1.00794, calculated 1796.8191; observed 1796.4203.
LC Trace and Mass of O12c

Following General Procedure vi
Yield: 73%
Exact mass: 5423.48
Triply charged mass [M]/3 - 1.00794, calculated 1806.8191; observed 1806.6212.
LC Trace and Mass of O13a

Following General Procedure vi

Yield: 87%

Exact mass: 5253.56

Triply charged mass [M]/3 - 1.00794, calculated 1750.1791; observed 1749.4945.
Following General Procedure vi

Yield: 83%

Exact mass: 5281.611

Triply charged mass [M]/3 - 1.00794, calculated 1759.5291; observed 1759.3555.
LC Trace and Mass of O13c

Following General Procedure vi

Yield: 89%

Exact mass: 5311.61

Triply charged mass [M]/3 - 1.00794, calculated 1769.5291; observed 1769.1063.
LC Trace and Mass of O14a

Following General Procedure vi
Yield: 79%
Exact mass: 5253.56
Triply charged mass [M]/3 - 1.00794, calculated 1750.1791; observed 1749.8198.
LC Trace and Mass of O14b

Following General Procedure vi

Yield: 75%

Exact mass: 5281.611

Triply charged mass [M]/3 - 1.00794, calculated 1759.5291; observed 1759.1322.
LC Trace and Mass of O14c

Following General Procedure vi

Yield: 82%

Exact mass: 5311.61

Triply charged mass \([M/3 - 1.00794]\), calculated 1769.5291; observed 1769.3646.
LC Trace and Mass of O15a

Following General Procedure vi
Yield: 82%
Exact mass: 5267.59
Triply charged mass [M]/3 - 1.00794, calculated 1754.8557; observed 1754.4987.
LC Trace and Mass of O15b

Following General Procedure vi
Yield: 87%
Exact mass: 5295.64
Triply charged mass [M]/3 - 1.00794, calculated 1764.2057; observed 1763.8062.
LC Trace and Mass of O15c

Following General Procedure vi

Yield: 89%

Exact mass: 5325.64

Triply charged mass [M]/3 - 1.00794, calculated 1774.2057; observed 1774.0349.
LC Trace and Mass of O16a

Following General Procedure vi
Yield: 86%
Exact mass: 5281.61
Triply charged mass [M]/3 - 1.00794, calculated 1759.5291; observed 1759.3555.
LC Trace and Mass of O16b

Following General Procedure vi
Yield: 83%
Exact mass: 5309.66
Triply charged mass [M]/3 - 1.00794, calculated 1768.8791; observed 1768.6930.
LC Trace and Mass of O16c

Following General Procedure vi
Yield: 80%
Exact mass: 5339.66
Triply charged mass [M]/3 - 1.00794, calculated 1778.8791; observed 1778.6769.
LC Trace and Mass of O17a

Following General Procedure vi

Yield: 87%

Exact mass: 5269.56

Triply charged mass [M]/3 - 1.00794, calculated 1755.5124; observed 1755.3391.
LC Trace and Mass of O17b

Following General Procedure vi
Yield: 90%
Exact mass: 5297.611
Triply charged mass [M]/3 - 1.00794, calculated 1764.8624; observed 1764.4597.
LC Trace and Mass of O17c

Following General Procedure vi
Yield: 76%
Exact mass: 5327.61
Triply charged mass [M]/3 - 1.00794, calculated 1774.8624; observed 1774.4489.
LC Trace and Mass of O18a

Following General Procedure vi
Yield: 80%
Exact mass: 5269.56
Triply charged mass [M]/3 - 1.00794, calculated 1755.5124; observed 1755.1504.
LC Trace and Mass of O18b

Following General Procedure vi
Yield: 80%
Exact mass: 5297.61
Triply charged mass $\frac{[M]}{3} - 1.00794$, calculated 1764.8624; observed 1764.4597.
LC Trace and Mass of O18c

Following General Procedure vi

Yield: 78%

Exact mass: 5327.61

Triply charged mass [M]/3 - 1.00794, calculated 1774.8624; observed 1774.6731.
LC Trace and Mass of O19a

Following General Procedure vi
Yield: 85%
Exact mass: 5269.56
Triply charged mass \([M/3 \cdot 1.00794]\), calculated 1755.5124; observed 1755.1504.
LC Trace and Mass of O19b

Following General Procedure vi
Yield: 80%
Exact mass: 5297.61
Triply charged mass [M]/3 - 1.00794, calculated 1764.8624; observed 1764.4597.
LC Trace and Mass of O19c

Following General Procedure vi
Yield: 77%
Exact mass: 5327.61
Triply charged mass [M]/3 - 1.00794, calculated 1774.8624; observed 1774.4316.
LC Trace and Mass of O20a

Following General Procedure vi
Yield: 70%
Exact mass: 5323.52
Triply charged mass [M]/3 - 1.00794, calculated 1773.4991; observed 1773.3452.
LC Trace and Mass of O20b

Following General Procedure vi
Yield: 70%
Exact mass: 5351.57
Triply charged mass [M]/3 - 1.00794, calculated 1782.8491; observed 1782.7025.
LC Trace and Mass of O20c

Following General Procedure vi
Yield: 92%
Exact mass: 5381.57
Triply charged mass [M]/3 - 1.00794, calculated 1792.8491; observed 1792.6912.