Supporting Information

Copper Mediated Radiobromination of (Hetero)Aryl Boronic Pinacol Esters

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Experimental Section

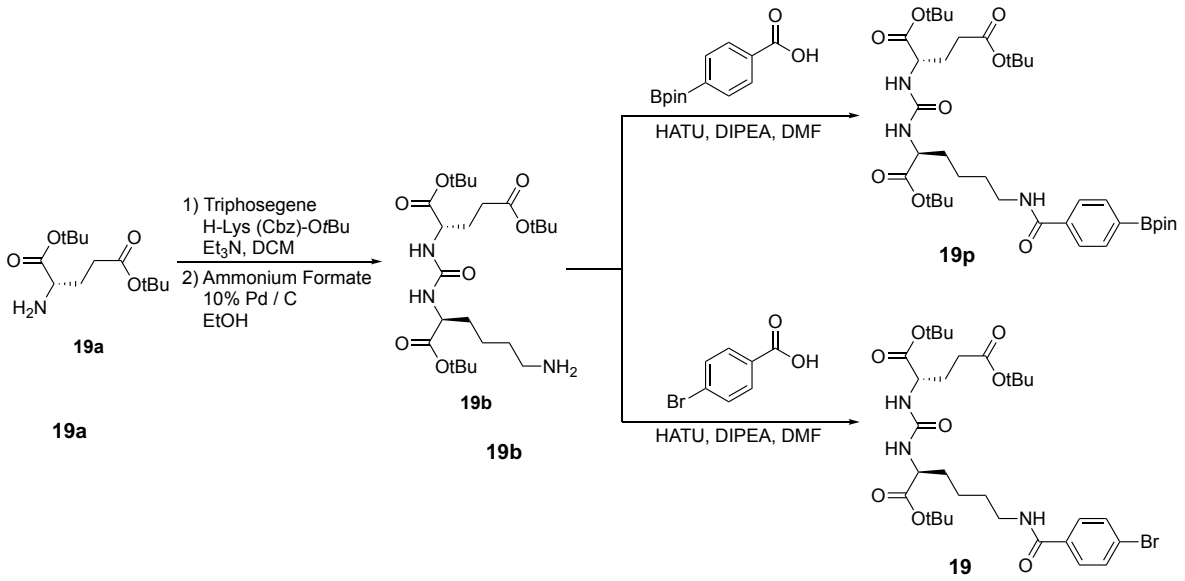
Methods and Reagents.

All aryl-bromide standards and aryl-boronic pinacol ester precursors unless otherwise mentioned were purchased through either: Ambeed, Combi-blocks, Sigma-Aldrich, Alfa-Aesar, TCI Chemicals, or Fisher Scientific. Anhydrous solvents were purchased from Sigma-Aldrich and used as received. Flash chromatography was performed on a Teledyne Isco CombiFlash R_f system utilizing normal phase pre-column cartridges and gold high performance columns. Purifications were performed using ethyl acetate/*n*-hexane eluting with a gradient method starting at 0:100 ethyl acetate: *n*-hexane and ending at 100:0 ethyl acetate: *n*-hexane. Organic solutions were concentrated by rotary evaporation below 40 °C at 25 torr. Identification of products was determined via high-performance liquid chromatography (HPLC) using a Kinetix XB-C18 column (5 µm, 100 Å, 10 x 250 mm) with rates and mobile phases as indicated. All aryl-bromide standards and aryl-boronic pinacol esters were concentrated into 20 mL scintillation vials and stored under argon in a freezer (0 °C) until further use or characterization. Quaternary methylammonium- (QMA-)functionalized solid phase extraction (SPE) cartridges (Sep-Pak Accell Plus QMA Plus Light Cartridge, 130 mg/cart, 37 – 55 µm, Waters Corp.) were pre-conditioned before use as described in the manuscript. Octadecyl- (C18-)functionalized SPE cartridges (Sep-Pak C18 Plus Light Cartridge, 130 mg/cart, 55 – 105 µm, Waters Corp.) were preconditioned with 5 mL EtOH and 10 mL water before use.

Analytical Data

All proton (^{1}H) nuclear magnetic resonance (NMR) spectra were recorded on a 400 MHz spectrometer (Bruker Avance-400) at the University of Wisconsin Paul Bender Chemistry Instrumentation Center NMR facility. Chemical shifts are expressed in parts per million (δ scale) and are referenced to residual $CHCl_3$ (^{1}H: δ 7.26 ppm) and $(CD_3)_2SO$ (^{1}H: δ 2.50 ppm). Data are presented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and bs = broad singlet), integration, and coupling constant in hertz (Hz).

Figure S1: **Standard and precursor for glutamate-urea-lysine derivative:**



Step 1: **19a** (10 g, 34 mmol) was dissolved in DCM (300 mL) and Et_3N (15.4 mL) and cooled to -78 °C. Triphosgene (3.4 g, 11.5 mmol) was dissolved in DCM (100 mL) and added dropwise via cannula. Upon completion the solution was allowed to warm to room temperature over 30 minutes. H-Lys (Cbz)-O*t*Bu (7.6 g, 20.2 mmol) and Et_3N (2.8 mL) were added sequentially and the solution was stirred under static argon for 3 days.

After 3 days the solution was diluted with DCM and washed with water (3x). The solution was dried over Na_2SO_4 and concentrated in vacuo. Flash chromatography was performed to yield 11.6 g (92%) of the intermediate which was used in Step 2 without any further manipulation.

Step 2: The product of Step 1 was dissolved in EtOH (370 mL) and ammonium formate (11.8 g, 187 mmol) and 10% Pd / C (1.2 g, 1.9 mmol) were added the solution and stirred at room temperature overnight under static argon.

The crude solution was passed through a pad of Celite and concentrated in vacuo before flash chromatography was performed yielding 8.5g (93%) of **19b** as an amorphous solid.

Step 3:

Precursor: **19b** (600 mg, 1.2 mmol), HATU (1.6 mmol), and 4-Bpin-benzoic acid (320 mg, 1.3 mmol) were dissolved in DCM (40 mL) in a flame dried Schlenk flask under argon. DIPEA (0.48 mL, 2.7 mmol) was added to the stirred solution in one portion and allowed to react for 2 days at room temperature.

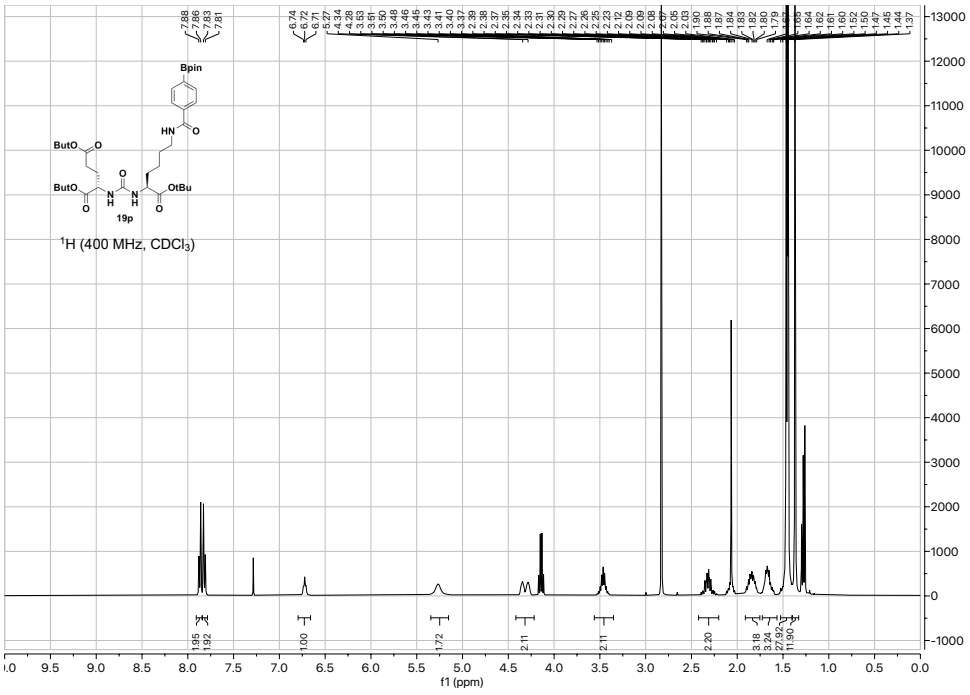
The crude solution was concentrated in vacuo and directly purified via flash-chromatography to yield **19p**, 375 mg (42%) as an amorphous solid.

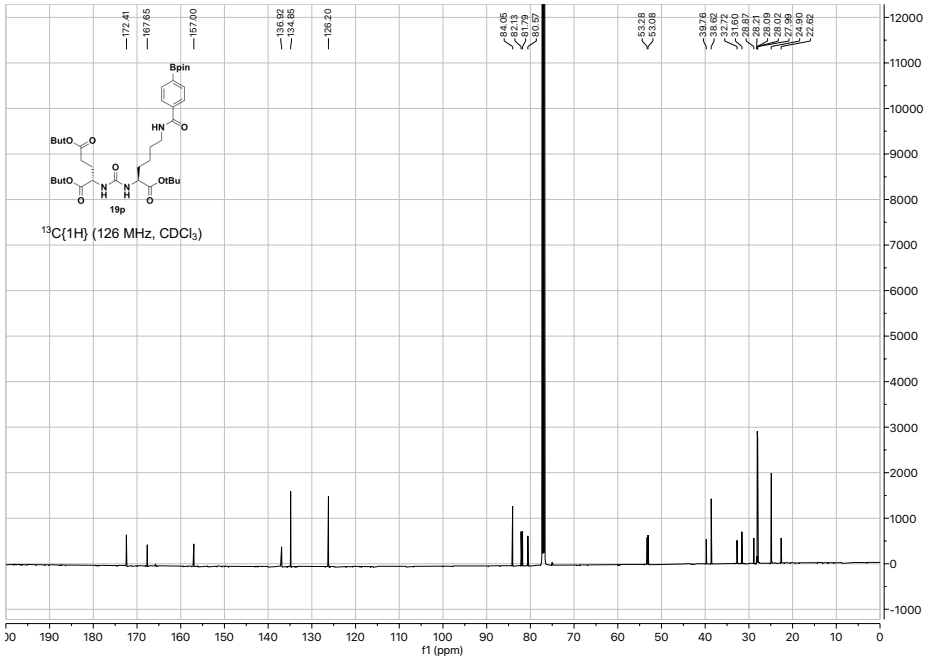
^{1}H NMR spectra literature data.[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 (d, *J* = 8.3 Hz, 2H), 7.82 (d, *J* = 8.3 Hz, 2H), 6.72 (t, *J* = 5.4 Hz, 1H), 5.27 (s, 2H), 4.31 (d, *J* = 23.6 Hz, 2H), 3.58 – 3.36 (m, 2H), 2.45 – 2.20 (m, 2H), 2.07 (s, 1H), 1.93 – 1.76 (m, 3H), 1.66 (dd, *J* = 14.2, 5.7 Hz, 3H), 1.47 (s, 9H), 1.45 (s, 9H), 1.44 (s, 9H), 1.37 (s, 12H).

^{13}C{1H} NMR (126 MHz, $CDCl_3$) δ = 172.4, 167.7, 157.0, 136.9, 134.9, 126.2, 84.1, 82.1, 81.8, 80.6, 53.3, 53.1, 39.8, 38.6, 32.7, 31.6, 28.9, 28.2, 28.1, 28.0, 28.0, 24.9, 22.6.

HRMS (TOF ESI) m/z: [M + H]+ Calcd for $C_{37}H_{61}BN_3O_{10}$: 718.4445; found 718.4453.





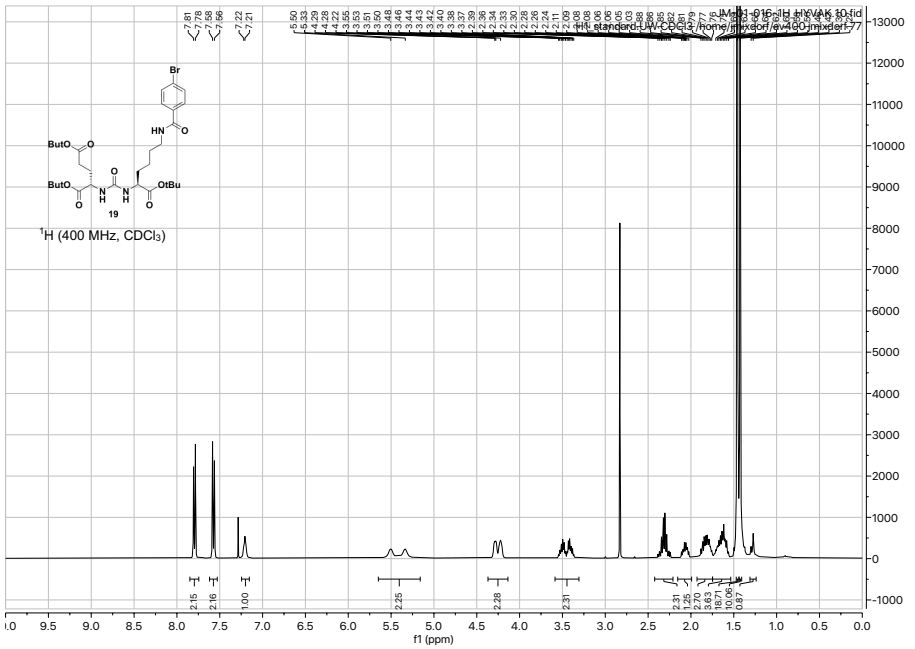
Standard: **19b** (300 mg, 0.6 mmol), HATU (310 mg, 0.8 mmol), and 4-Br-benzoic acid (130 mg, 0.65 mmol) were dissolved in DCM (20 mL) in a flame dried Schlenk flask under argon. DIPEA (0.24 mL, 1.4 mmol) was added to the stirred solution in one portion and allowed to react for 2 days at room temperature.

The crude solution was concentrated in vacuo and directly purified via flash-chromatography to yield **19**, 230 mg (56%) as an amorphous solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.79 (d, *J* = 8.5 Hz, 2H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.21 (t, *J* = 5.6 Hz, 1H), 5.42 (d, *J* = 68.1 Hz, 2H), 4.39 – 4.20 (m, 2H), 3.60 – 3.34 (m, 2H), 2.40 – 2.22 (m, 2H), 2.16 – 1.99 (m, 1H), 1.93 – 1.75 (m, 3H), 1.65 (qd, *J* = 14.2, 8.6 Hz, 3H), 1.46 (s, 18H), 1.43 (s, 9H), 1.29 – 1.27 (m, 1H).

^{13}C{1H} NMR (126 MHz, $CDCl_3$) δ = 173.4, 172.4, 172.2, 166.8, 157.3, 133.6, 131.5, 129.1, 125.8, 82.5, 81.7, 80.7, 53.5, 53.0, 39.9, 38.6, 32.6, 31.5, 28.8, 28.1, 28.0, 27.9, 23.2.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{31}H_{49}BrN_3O_8$ 670.2698; Found 670.2699.



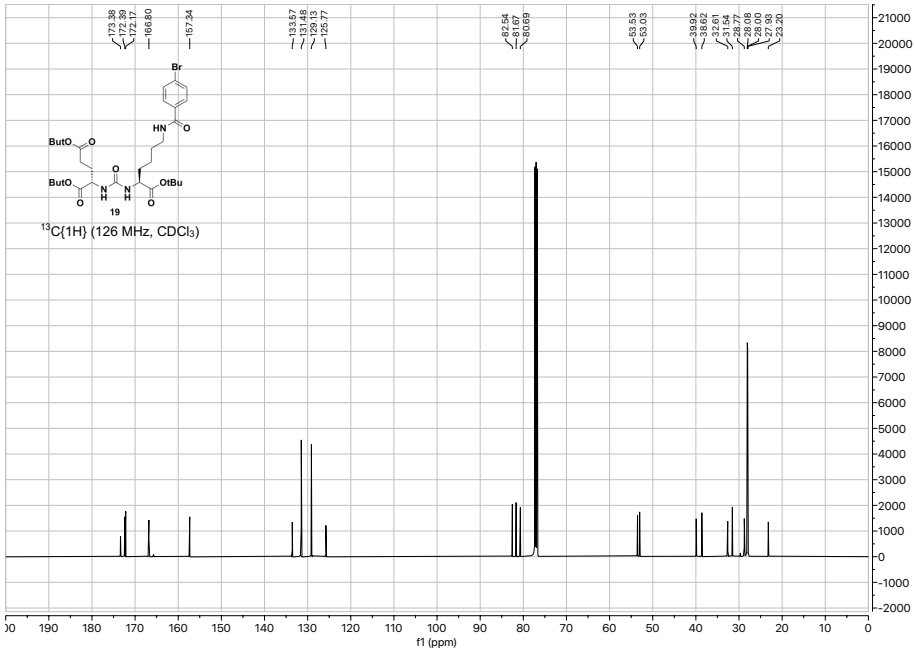
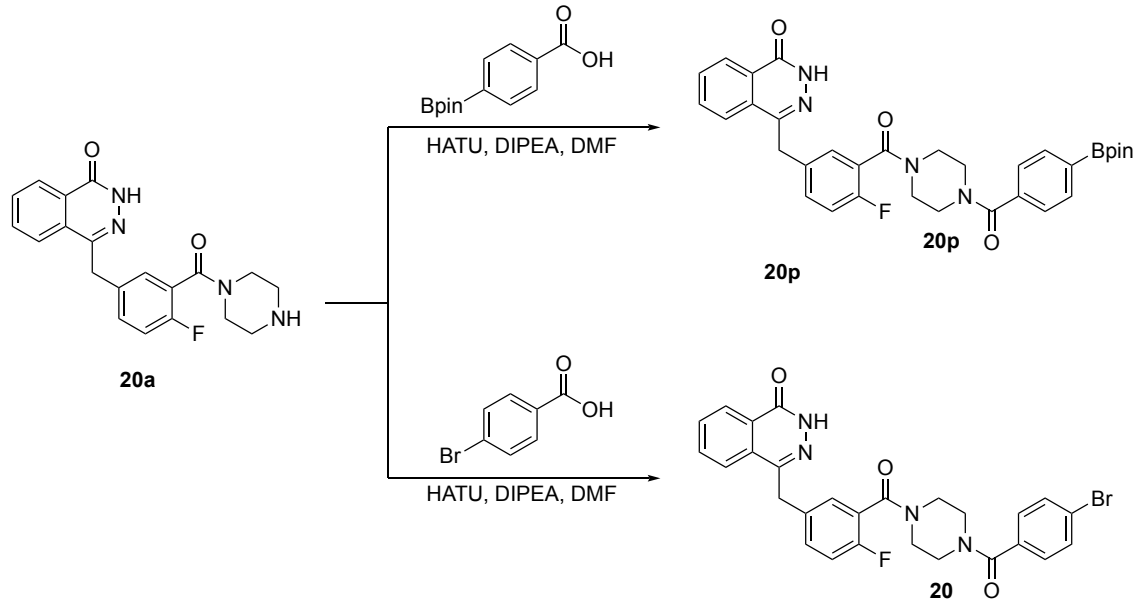


Figure S2: Standard and precursor for olaparib derivative:



Precursor: **20a** (100 mg, 0.28 mmol), HATU (120 mg, 0.32 mmol), and 4-Bpin-benzoic acid (75 mg, 0.31 mmol) were dissolved in DCM (2 mL) in a flame dried Schlenk flask under argon. DIPEA (0.1 mL, 0.29 mmol) was added to the stirred solution in one portion and allowed to react for 2 days at room temperature.

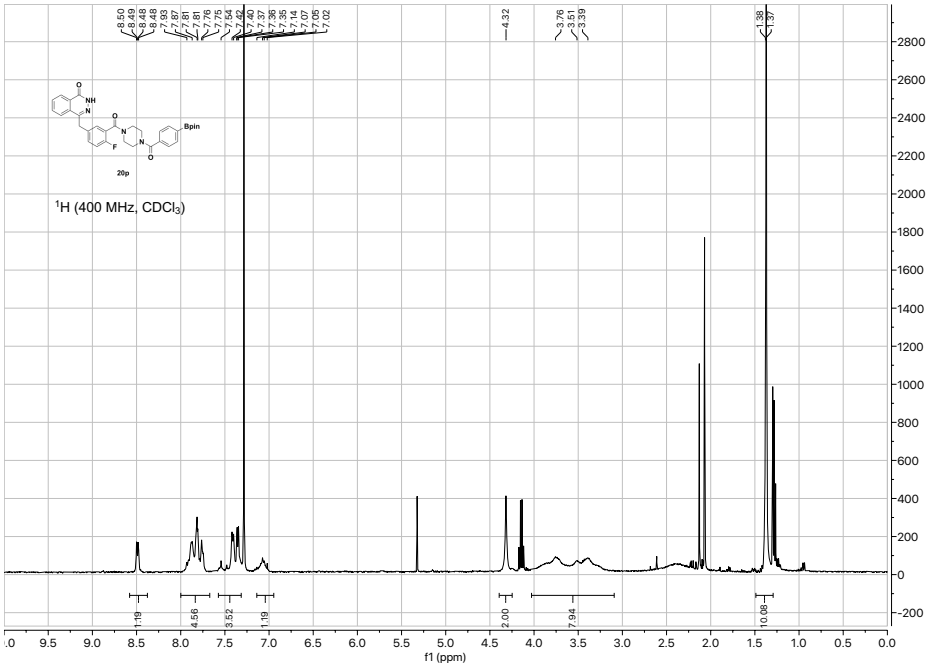
The crude solution was concentrated in vacuo and directly purified via flash-chromatography to yield **20p**, 101 mg (57%) as an amorphous solid.

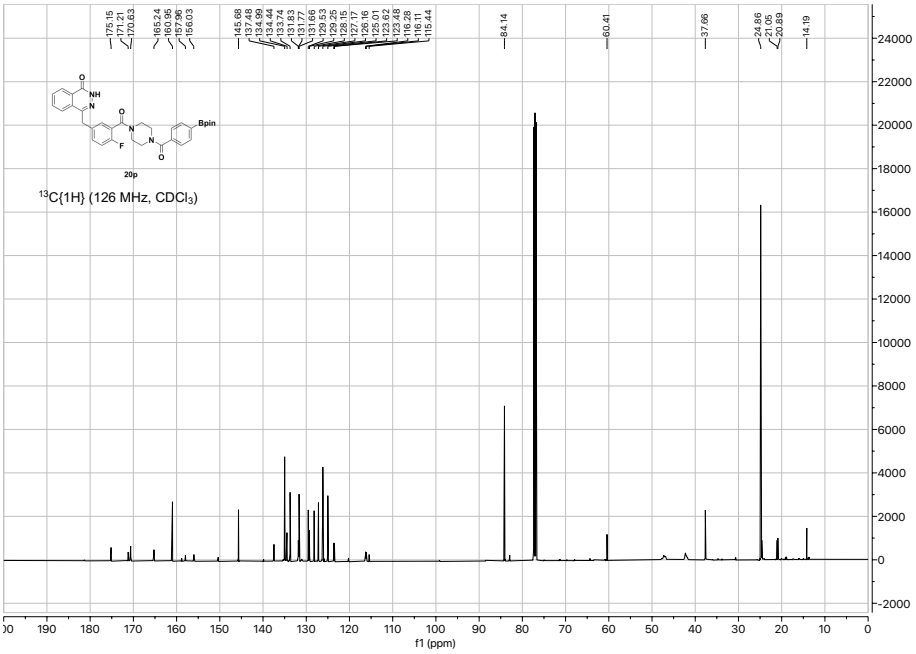
^{1}H NMR spectra literature data.[2]

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.49 – 8.46 (m, 1H), 7.96 – 7.73 (m, 5H), 7.49 – 7.32 (m, 4H), 7.16 – 7.00 (m, 1H), 4.32 (s, 2H), 3.76 (bs, 4H), 3.39 (bs, 4H), 1.37 (s, 12H).

^{13}C{1H} NMR (126 MHz, $CDCl_3$) δ = 175.2, 171.2, 170.6, 165.2, 161.0, 157.0 (d, J = 242.0 Hz), 145.7, 137.5, 135.0, 134.4, 133.7, 131.8 (d, J = 8.2 Hz), 129.5, 129.3, 127.2, 126.2, 125.0, 123.6 (d, J = 18.0 Hz), 116.2 (d, J = 21.8 Hz), 115.4, 84.1, 60.4, 37.7, 24.9, 21.0 (d, J = 19.9 Hz), 14.2.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{33}H_{35}BFN_4O_5$ 597.2679; Found 597.2680.





Standard: **20a** (125 mg, 0.34 mmol), HATU (140 mg, 0.37 mmol), and 4-Bpin-benzoic acid (72 mg, 0.36 mmol) were dissolved in DCM (3.5 mL) in a flame dried Schlenk flask under argon. DIPEA (0.12 mL, 0.34 mmol) was added to the stirred solution in one portion and allowed to react for 2 days at room temperature.

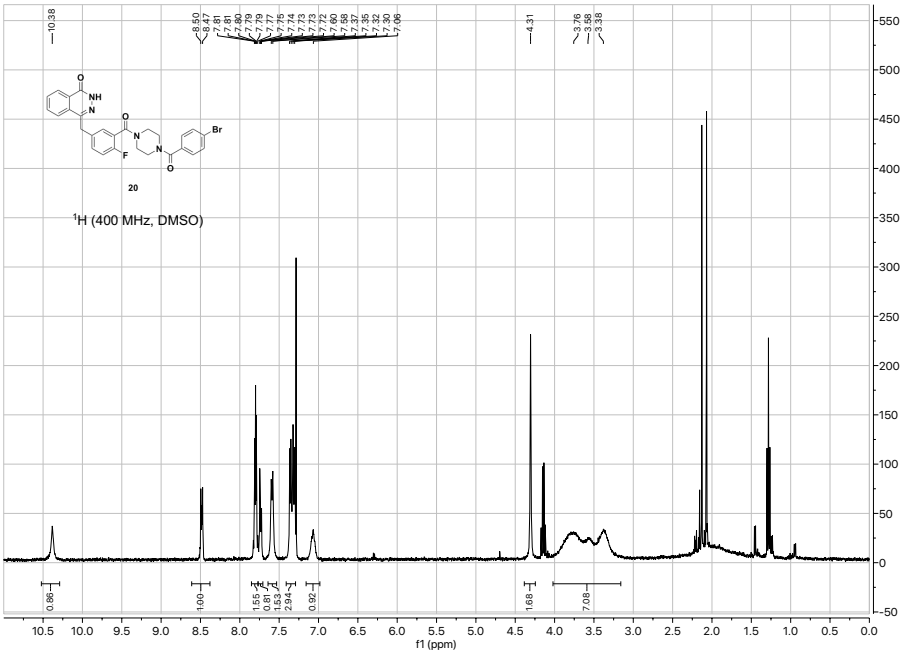
The crude solution was concentrated in vacuo and directly purified via flash-chromatography to yield **20**, 149 mg (80%) as an amorphous solid.

^{1}H NMR spectra literature data.[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.43 (s, 1H), 8.52 – 8.46 (m, 1H), 7.84 – 7.77 (m, 2H), 7.76 – 7.71 (m, 1H), 7.59 (d, *J* = 7.9 Hz, 2H), 7.38 – 7.30 (m, 4H), 7.06 (s, 1H), 4.31 (s, 2H), 3.76 (bs, 4H), 3.37 (bs, 4H).

^{13}C{1H} NMR (126 MHz, $CDCl_3$) δ = 175.0, 171.2, 169.7, 165.2, 160.7, 158.0, 156.0, 145.6, 133.8, 131.9, 131.7, 129.5, 129.3, 128.8, 128.2, 127.2, 125.0, 124.6, 123.6 (d, J = 18.0 Hz), 116.2 (d, J = 22.1 Hz), 60.4, 37.7, 20.7, 14.2.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{27}H_{23}BrFN_4O_3$ 549.0932; Found 549.0932.



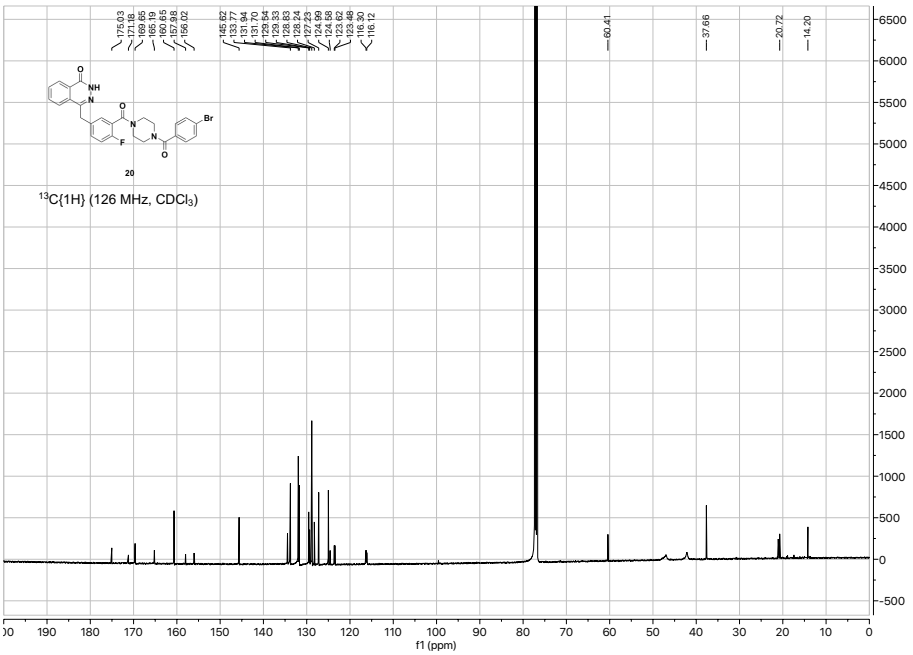
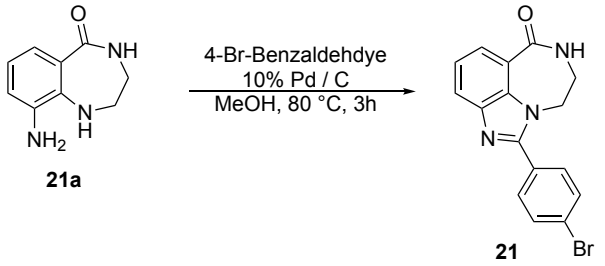


Figure S3: Standard and precursor for rucaparib derivative:

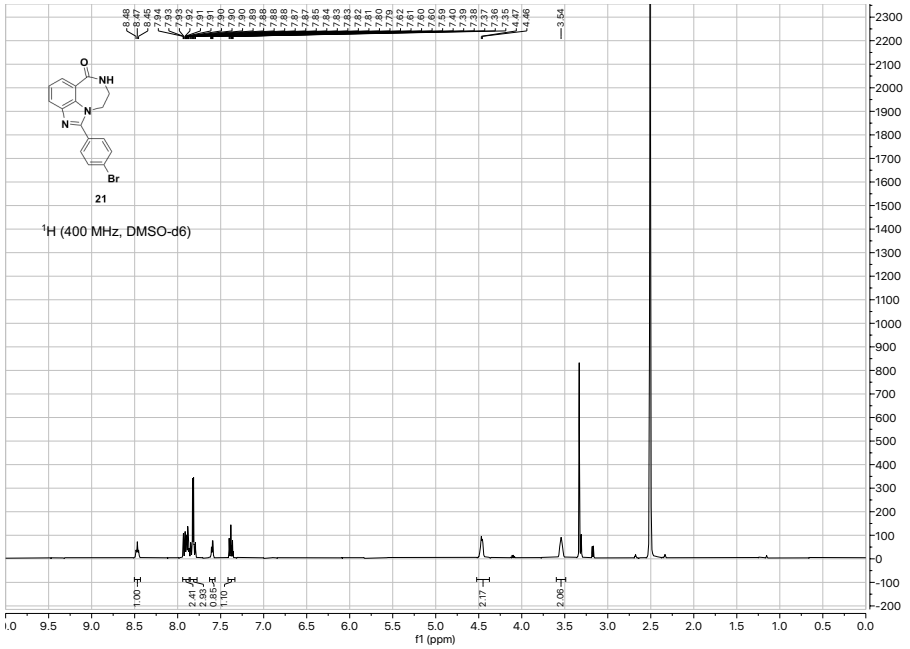


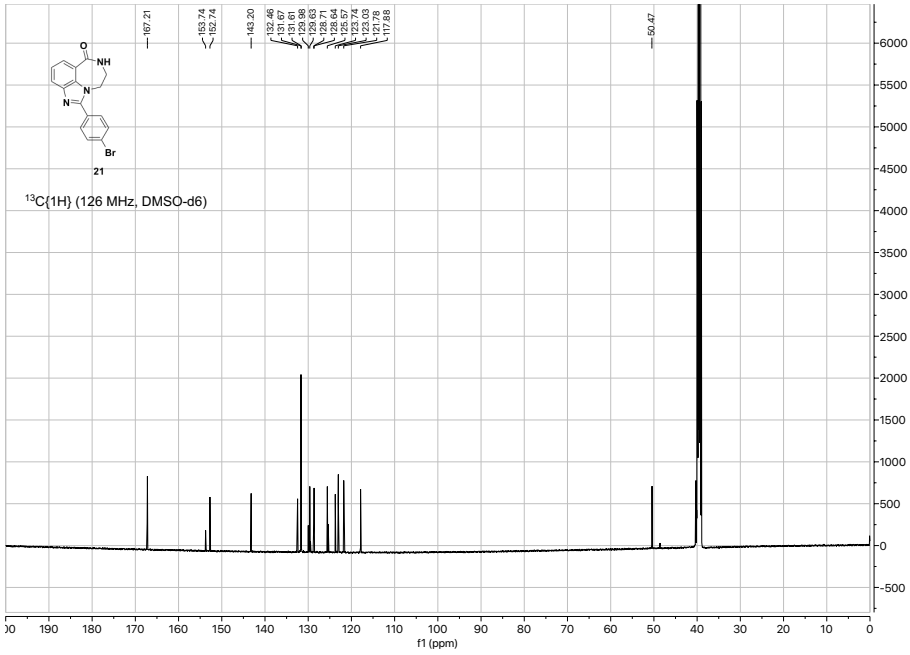
Aryl-boronic pinacol ester precursor for the rucaparib derivative was synthesized as previously published[4] and graciously provided by Professor Mehran Makvandi of the University of Pennsylvania.

In a flame dried glass vial, 10% Pd / C (6 mg, 0.06 mmol) and **21a** (100 mg, 0.56 mmol) were dissolved in MeOH (2 mL) under argon. 4-Br-Benzaldehyde (104 mg, 0.56 mmol) was added dropwise to the vial and heated in an oil bath to 80 °C for 3 h.

The crude solution was passed through a pad of celite 515 and washed with MeOH (25 mL) and concentrated in vacuo and purified via flash-chromatography to yield **21**, 60 mg (35%) as an amorphous solid.

^{1}H NMR (400 MHz, d_6-DMSO) δ = 8.50 (t, *J* = 5.7 Hz, 1H), 7.99 – 7.89 (m, 2H), 7.88 – 7.80 (m, 3H), 7.65 – 7.59 (m, 1H), 7.43 – 7.38 (m, 1H), 4.48 (bs, 2H), 3.57 (bs, 2H).
^{13}C{1H} NMR (126 MHz, DMSO) δ = 167.2, 153.7, 152.7, 143.2, 132.5, 131.6 (d, J = 7.1 Hz), 129.6, 128.7 (d, J = 8.7 Hz), 125.6, 123.7, 123.0, 121.8, 117.9, 50.4.
HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{13}BrN_3O$ 342.0237; Found 342.0232.



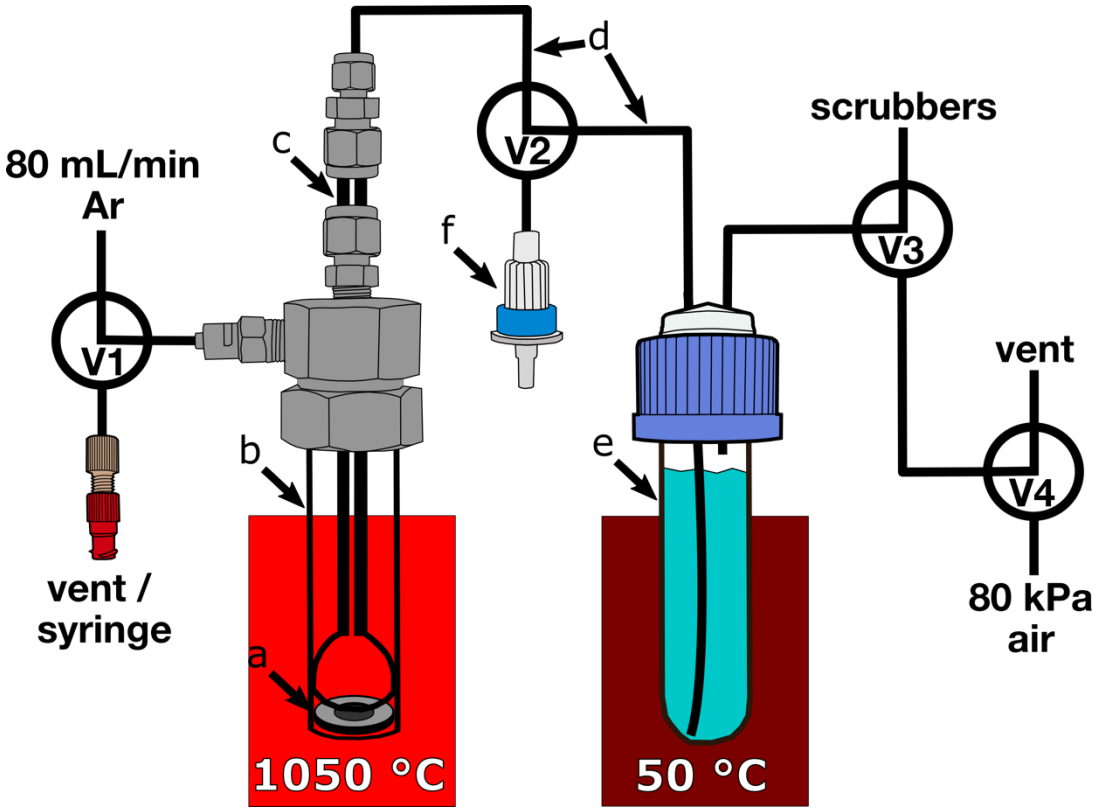


General Procedure for Production & Distillation of Radiobromide

Bromine-76 and bromine-77 were produced as previously described through the proton irradiation of isotopically enriched $Co^{76}Se$ and $Co^{77}Se$, respectively.[5] Briefly, water-jet cooled $Co^{76}Se$ or $Co^{77}Se$ on Nb coins were irradiated with 35 μA protons (12.5 MeV, 500 μm aluminum degrader) for one hour with the University of Wisconsin's cyclotron (PETtrace, GE Healthcare) using an

solid target transport system (QIS, ARTMS), producing 14 ± 2 mCi ^{77}Br (n = 10) and 54 ± 1 mCi ^{76}Br (n = 2) at end of bombardment.

Figure S4: **Radiobromine distillation and reclamation apparatus.**



Radiobromine was isolated from irradiated CoSe targets by dry distillation using a vertical tube furnace assembly (see above). Following irradiation, the CoSe target (a) was removed from the QIS transfer capsule, dried, placed in the flat-bottomed quartz tube (b), and sealed inside the assembly. Argon was flowed constantly at 80 mL/min over the CoSe target, through quartz (c) and PTFE tubing (d) and bubbled through a water trap (e). The quartz tube was subsequently lowered into a preheated tube furnace (TF1 11/32/150, Carbolite Gero) at 1050 °C. After 5 minutes of heating, the quartz tube was lifted from the furnace and immediately immersed in room temperature water, rapidly cooling the CoSe target. Argon flow continued while the assembly thermally cooled for up to 10 minutes. The assembly was vented to atmospheric pressure (actuating V1 and V3) and the quartz tube inverted. Using a 60 mL syringe attached to the furnace assembly inlet vent, the warm water (50 °C) from the water trap was drawn up to fill the quartz and PTFE tubing with water five times to rinse radiobromide into the water trap. After rinsing, the contents of the water trap were passed through a pre-conditioned QMA light cartridge using air pressure (80 kPa) by actuating V2 and V4. After trapping the radiobromide, the QMA cartridge was eluted

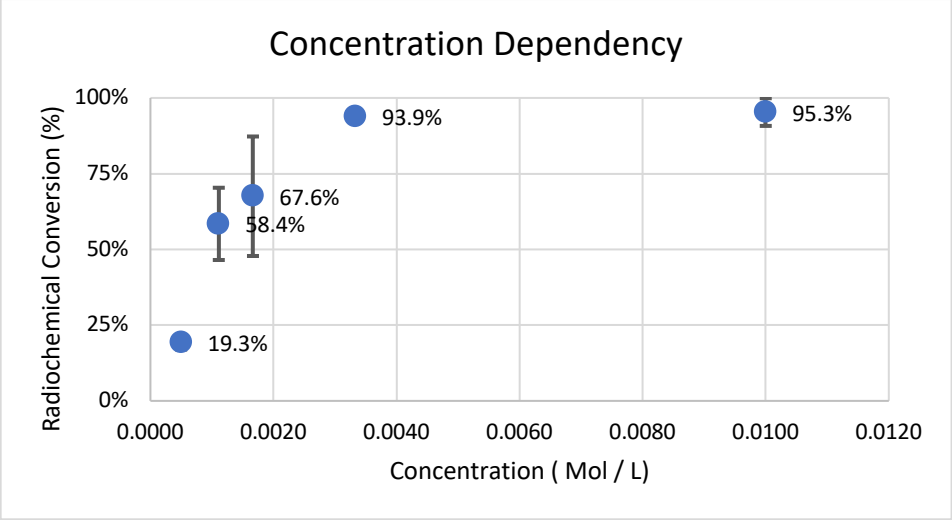
with 600 - 1200 µL of corresponding QMA equilibration and elution solutions (See Manuscript – Table 1). The total $^{76/77}$Br radiochemical yield for the distillation and QMA trap/release process was (72 ± 12)%, n = 12. This radiobromide solution was either evaporated until dryness under a constant stream of argon while heated in an aluminum hot-block at 110 °C or was portioned into smaller quantities before evaporation in the same manner.

General Procedure for Radiobromide Labeling

Dry [$^{76/77}$Br]bromide was dissolved in a mixture of [$Cu(py)_4OTf_2$] / 3,4,7,8-tetramethyl-1,10-phenanthroline (50 mol%, prepared fresh as 50 mM stock in MeOH) and an aryl Bpin precursor (1 µmol, prepared fresh as 12.5 mM stock in MeOH) in 9:1 MeOH/H_2O (100 µL). The solution was stirred for 30 min at room temperature. Upon completion the solution was diluted in water (10 mL) and passed through a preconditioned C18 Sep-Pak to trap the radiolabeled compound. The cartridge was rinsed with water (10 mL) and the radio labeled compound was eluted from the C18 Sep-Pak with subsequent additions of pure ethanol (0.5 mL) and water (0.5 mL). The combined load/rinse solution (~20 mL), elution solution (~1 mL), and eluted C18 cartridge were assayed with a radioactive dose calibrator (CRC-15R setting #120 for ^{77}Br, #690÷2 for ^{76}Br, Capintec). A crude radiochemical conversion (RCC) was calculated by dividing the activity of the elution solution by the total summed activity. The elution solution was then injected onto a preparative HPLC (Kinetix XB-C18, 5 µm, 100 Å, 10 x 250 mm) using the corresponding elution conditions mentioned below. Purified RCC was calculated by multiplying the crude RCC by the radiochemical purity of the product peak determined by integration of radioactivity peak areas of the HPLC chromatogram. Non-decay corrected radiochemical yield (RCY) was determined by the quantity of radiolabeled product isolated from the preparative HPLC divided by the starting activity in the reaction.

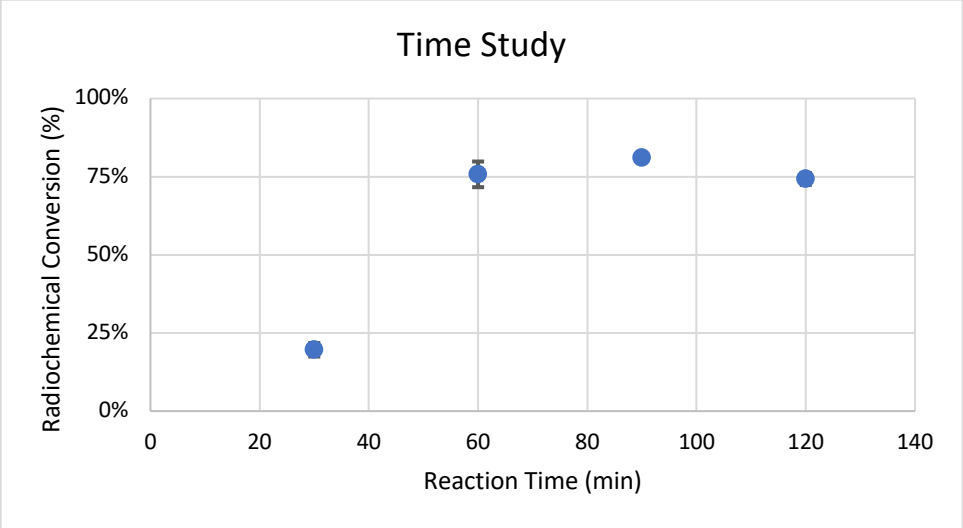
Preliminary data investigating the dependence of reactant concentration, time and temperature on [$^{76/77}$Br]**21** optimized reaction conditions are shown below.

Figure S5. Concentration dependency of Cu-mediated radiobromodeborylation



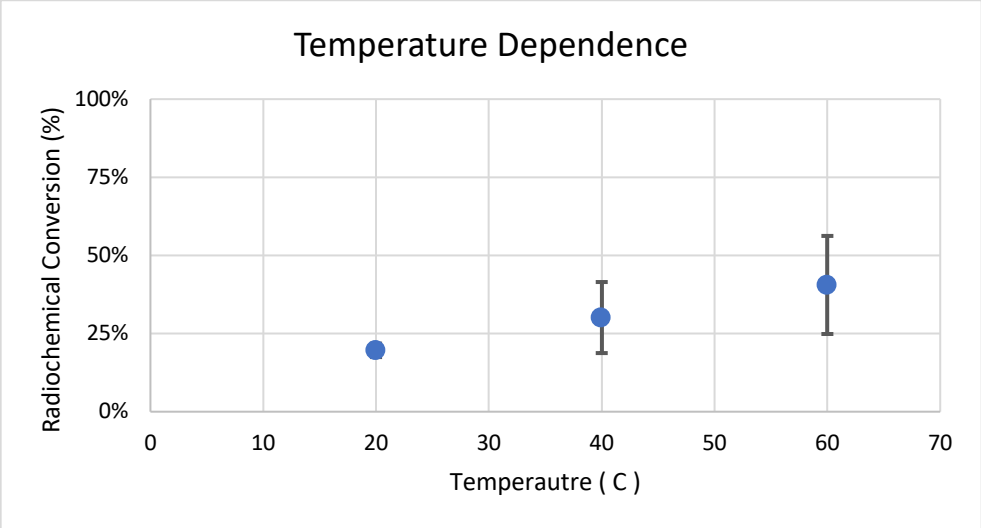
Concentration studies were undertaken with the same reaction conditions as seen in **Scheme 2**, with the following modifications. 1) reactions were performed in v-vial (4 mL) instead of pulled point vials (1 mL), except for the lowest concentration reaction. 2) Stirring was not conducted for these reactions. 3) In order to account for varying concentration different overall solvents amounts were varied (0.1, 0.3, 0.6, 0.9, and 2 mL) while holding precursor (1 µmol), catalyst (0.5 µmol), and ^{77}Br constant.

Figure S6. Time dependency of Cu-mediated radiobromodeborylation



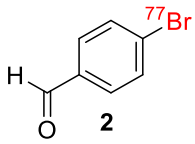
Time studies were undertaken with the same reaction conditions as seen in **Scheme 2**, with the following modification. 1) Stirring was not conducted for these reactions.

Figure S7. Temperature dependency of Cu-mediated radiobromodeborylation



Temperature studies were undertaken with the same reaction conditions as seen in **Scheme 2**, with the following modifications. 1) Stirring was not conducted for these reactions. 2) Reactions were completed in an aluminum hot block that had equilibrated to the set temperature for 20 minutes. 3) The 20 °C reaction was done at room temperature and not in a hot block.

HPLC Traces of Standards and Radiolabeled Products



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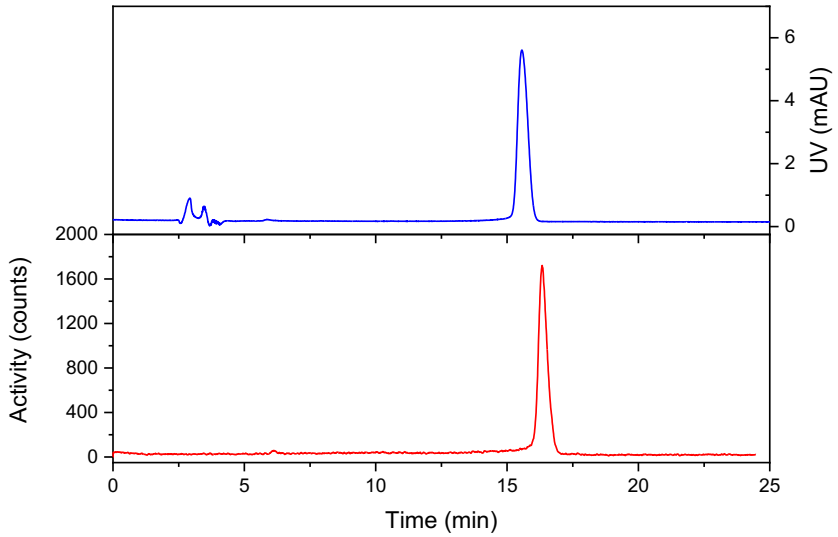
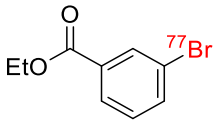


Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 95 ± 5% (n = 2)
Injected onto Prep-HPLC: 15.8 MBq
Collected off Prep-HPLC: 12.6 MBq (80% Recovery, n = 1)



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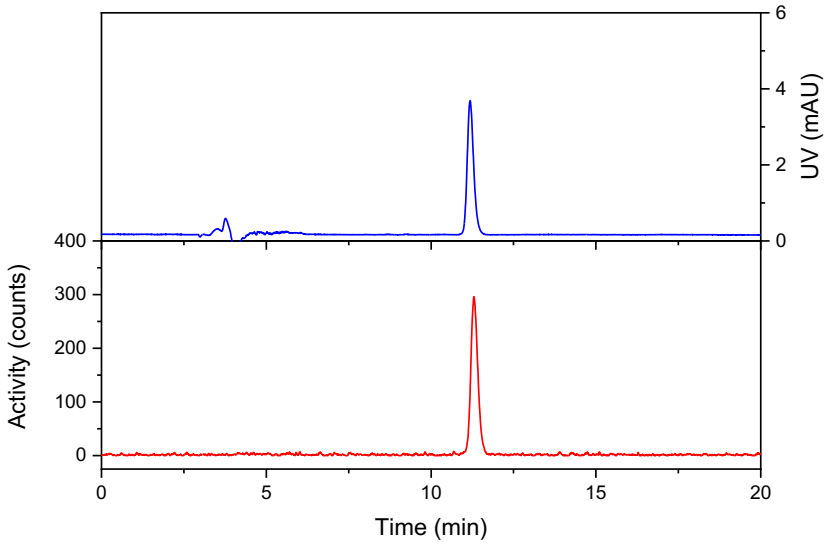
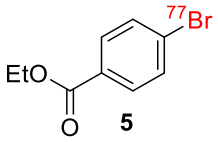


Eluent: 70:30 MeCN / 0.1 M NH_4HCO_2 (aq) – 3 mL / min
RCC: 87 ± 0% (n = 2)
Injected onto Prep-HPLC: 5.3 MBq
Collected off Prep-HPLC: 4.7 MBq (89% Recovery, n = 1)



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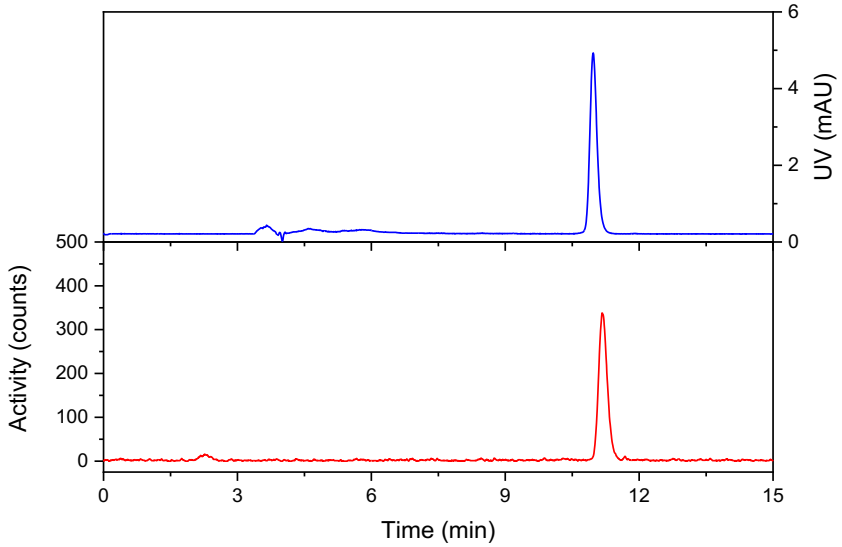
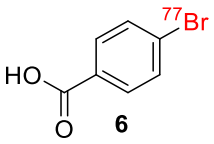
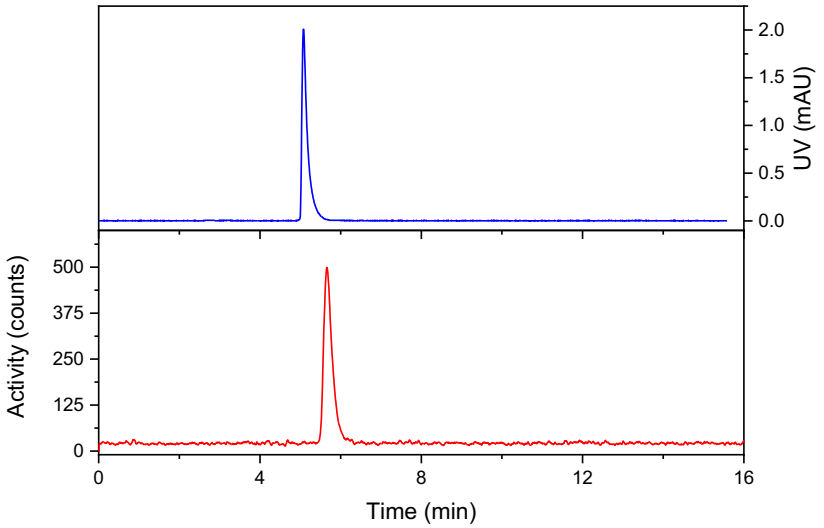


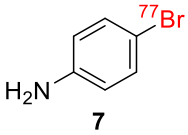
Eluent: 70:30 MeCN / 0.1 M NH_4HCO_2 (aq) – 3 mL / min
RCC: 87 ± 0% (n = 2)
Injected onto Prep-HPLC: 5.4 MBq
Collected off Prep-HPLC: 4.9 MBq (91% Recovery, n = 1)



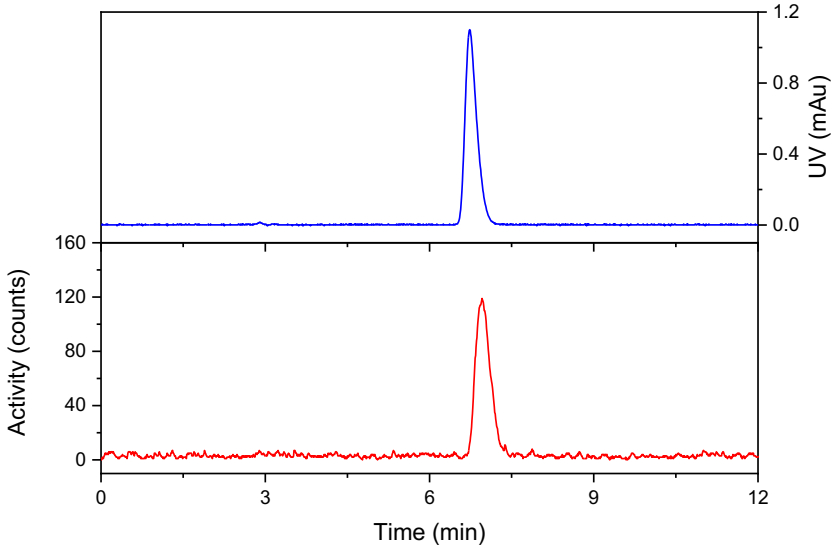
6



Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 97 ± 1% (n = 2)
Injected onto Prep-HPLC: 6.3 MBq
Collected off Prep-HPLC: 5.6 MBq (89% Recovery, n = 1)

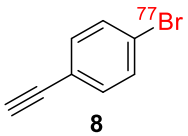


7



Eluent: 50:50 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 54 ± 1% (n = 2)
Injected onto Prep-HPLC: 3.3 MBq

Collected off Prep-HPLC: 3.0 MBq (91% Recovery, n = 1)



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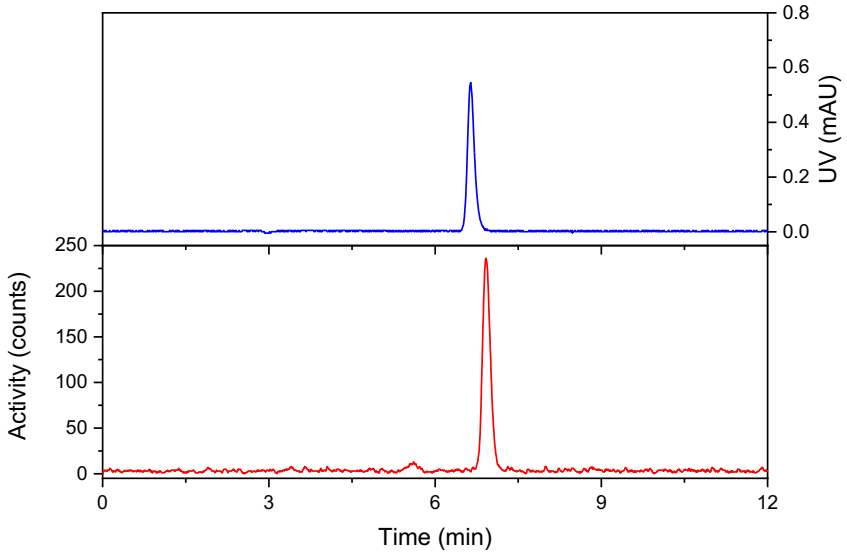
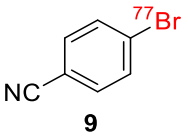


Eluent: 70:30 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 67.5 ± 0.5% (n = 2)
Injected onto Prep-HPLC: 4.4 MBq
Collected off Prep-HPLC: 3.5 MBq (80% Recovery, n = 1)



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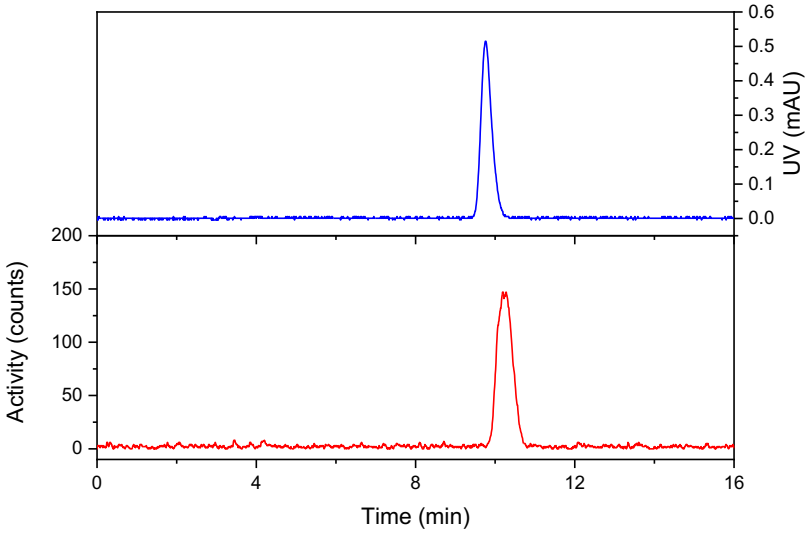
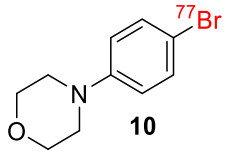


Eluent: 50:50 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min

RCC: 85.5 ± 0.5% (n = 2)
Injected onto Prep-HPLC: 6.5 MBq
Collected off Prep-HPLC: 5.4 MBq (83% Recovery, n = 1)



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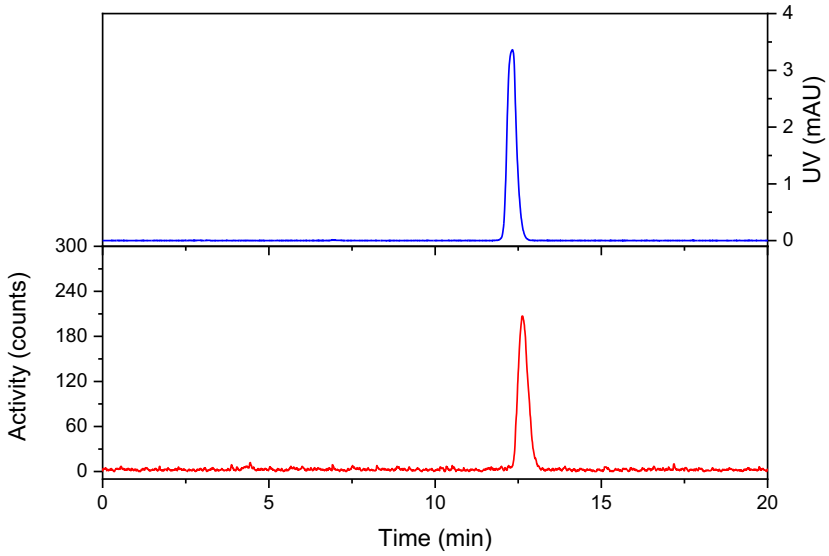
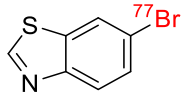


Eluent: 50:50 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 92 ± 1% (n = 2)
Injected onto Prep-HPLC: 6.7 MBq
Collected off Prep-HPLC: 6.1 MBq (91% Recovery, n = 1)



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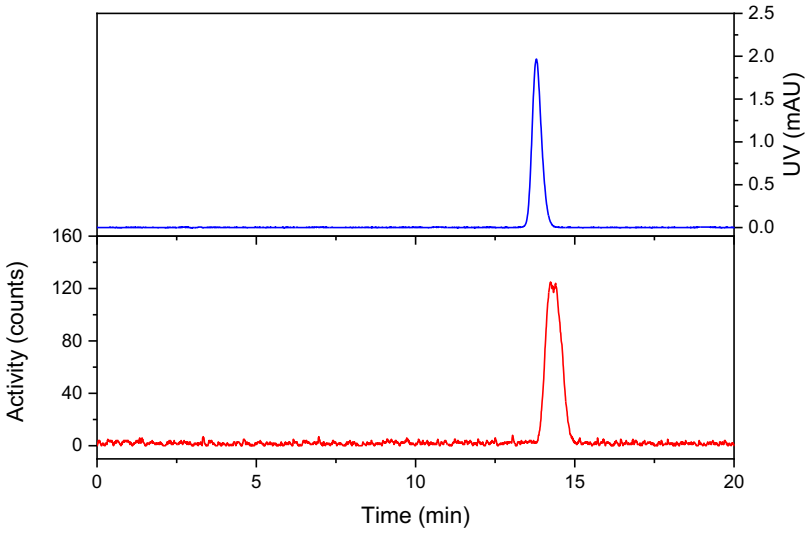
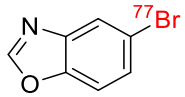


Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 90.5 ± 0.5% (n = 2)
Injected onto Prep-HPLC: 6.8 MBq
Collected off Prep-HPLC: 5.6 MBq (82% Recovery, n = 1)



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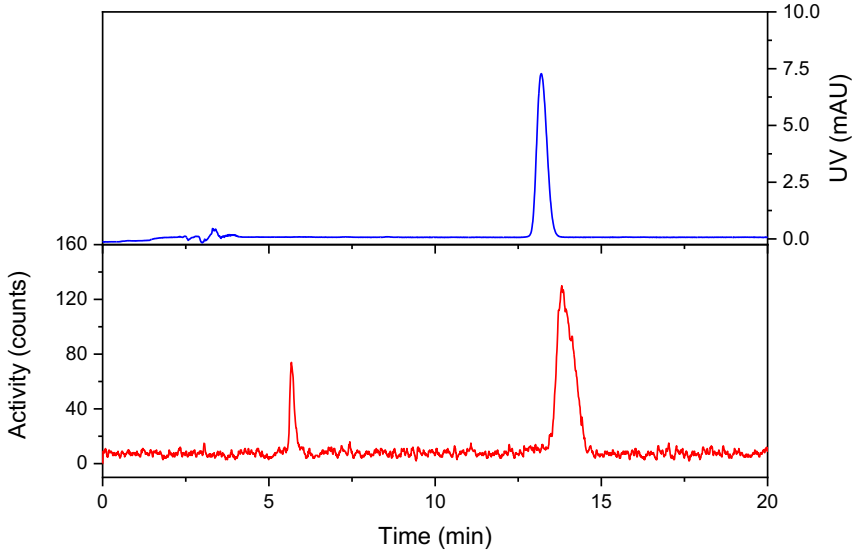
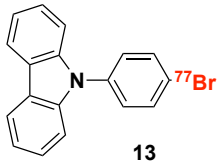
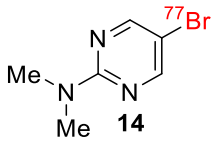


Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 75 ± 15% (n = 2)
Injected onto Prep-HPLC: 5.4 MBq
Collected off Prep-HPLC: 4.9 MBq (91% Recovery, n = 1)

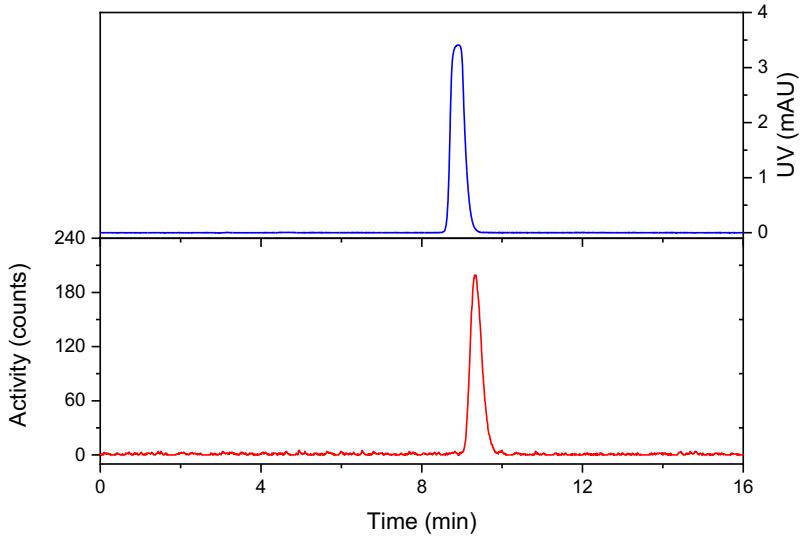


13

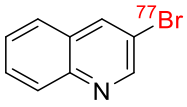
Eluent: After numerous trials we were unable to obtain preparative HPLCs for either the standard or radiolabeled product. We believe this is due to its poor solubility in our system. Due to this challenge, RCC for compound **13** is representative of crude radiochemical conversion.
RCC: 17 ± 8% (n = 2)



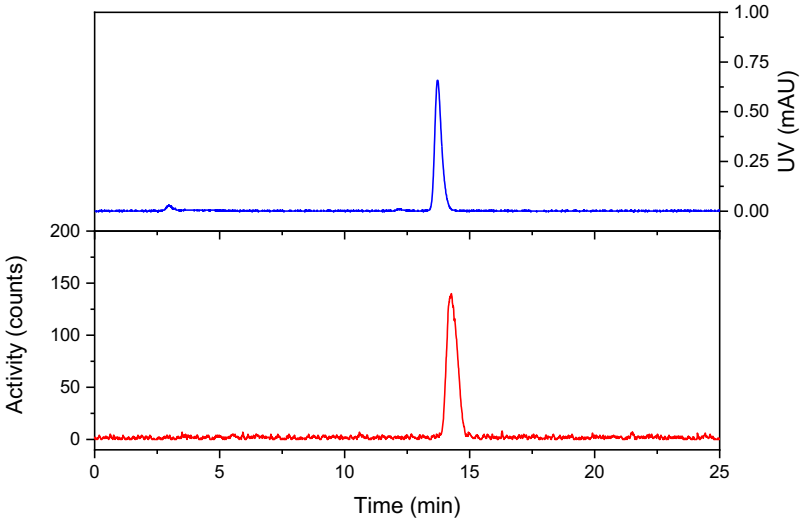
14



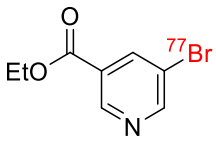
Eluent: 50:50 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 89 ± 1% (n = 2)
Injected onto Prep-HPLC: 5.4 MBq
Collected off Prep-HPLC: 5.2 MBq (96% Recovery, n = 1)



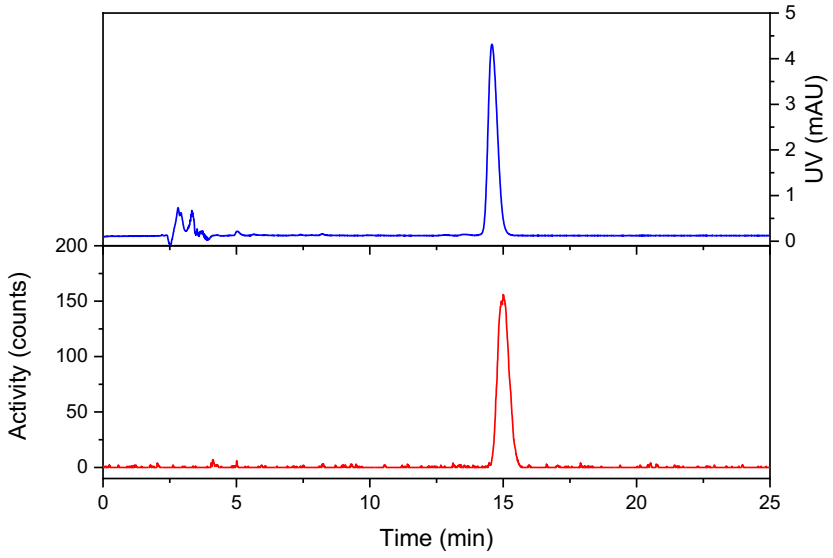
15



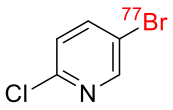
Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 89.5 ± 0.5% (n = 2)
Injected onto Prep-HPLC: 6.6 MBq
Collected off Prep-HPLC: 5.5 MBq (83% Recovery, n = 1)



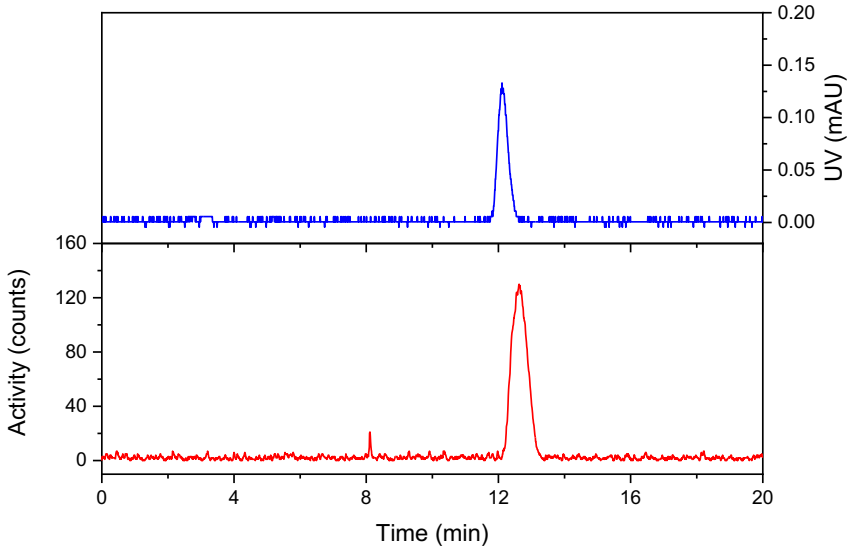
16



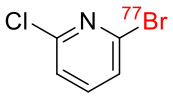
Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 91 ± 0% (n = 2)
Injected onto Prep-HPLC: 5.3 MBq
Collected off Prep-HPLC: 4.6 MBq (87% Recovery, n = 1)



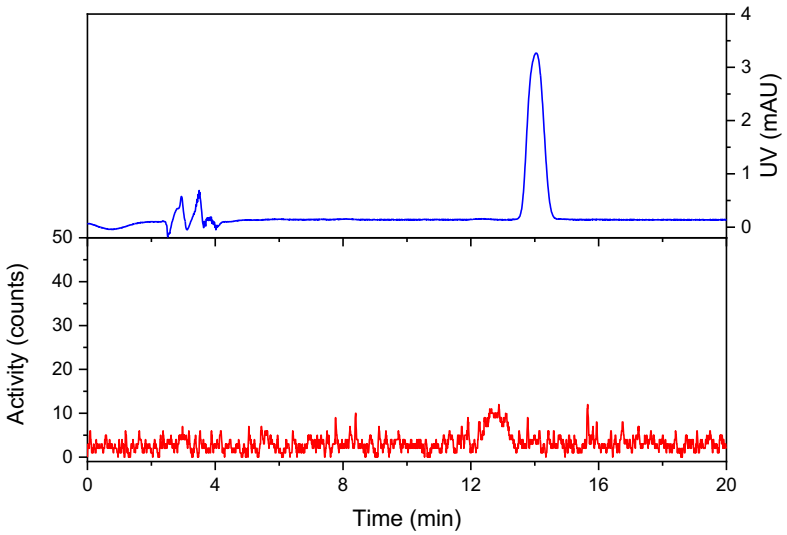
17



Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 85 ± 2% (n = 2)
Injected onto Prep-HPLC: 6.1 MBq
Collected off Prep-HPLC: 5.6 MBq (92% Recovery, n = 1)

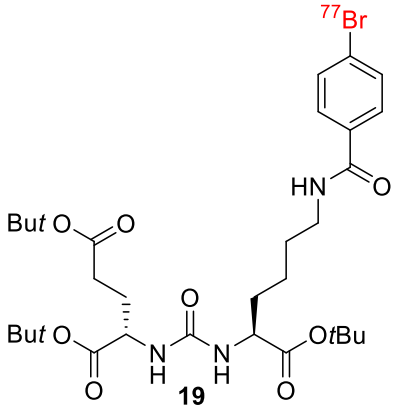


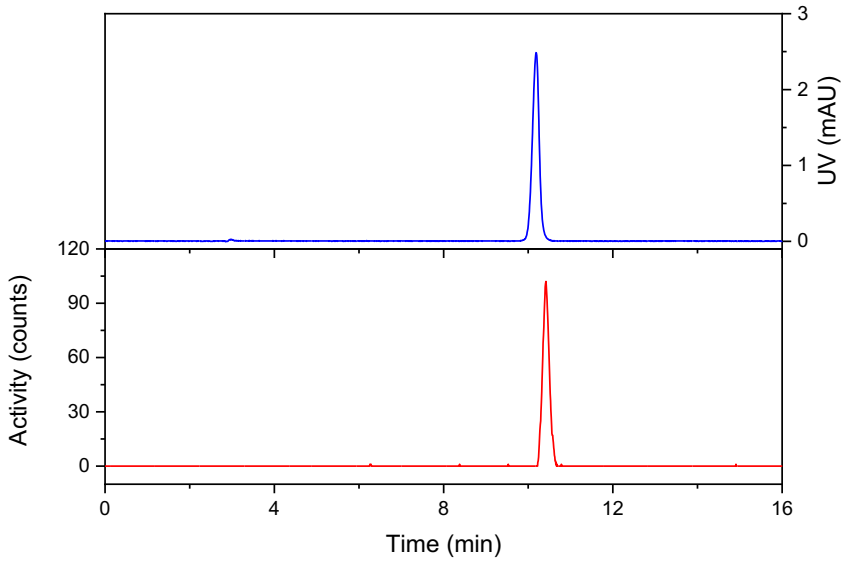
18



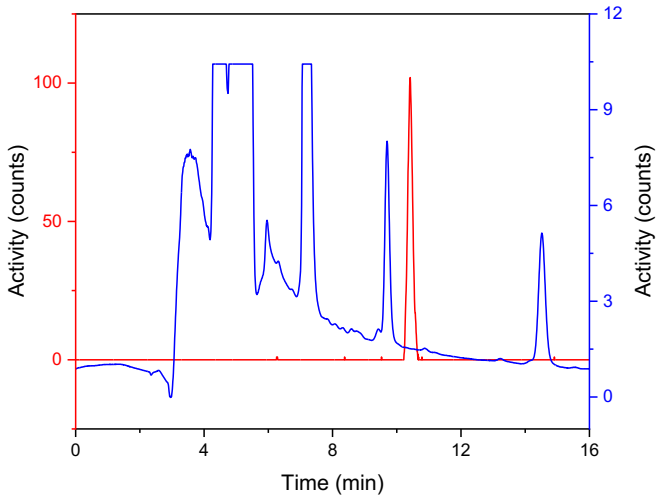
Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) –4 mL / min

RCC: 9 ± 2% (n = 2) Only small amounts of activity were isolated, so preparative HPLC analysis was challenging. Due to this challenge, RCC for compound **18** is representative of crude radiochemical conversion.
Injected onto Prep-HPLC: 0.44 MBq
Collected off Prep-HPLC: NA MBq (NA Recovery, n = 1)

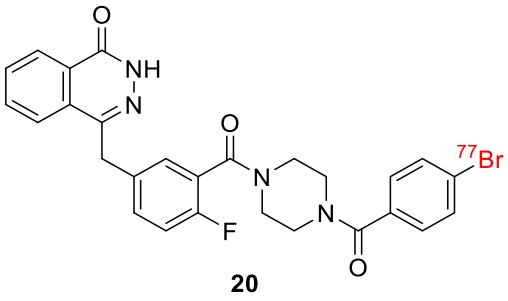




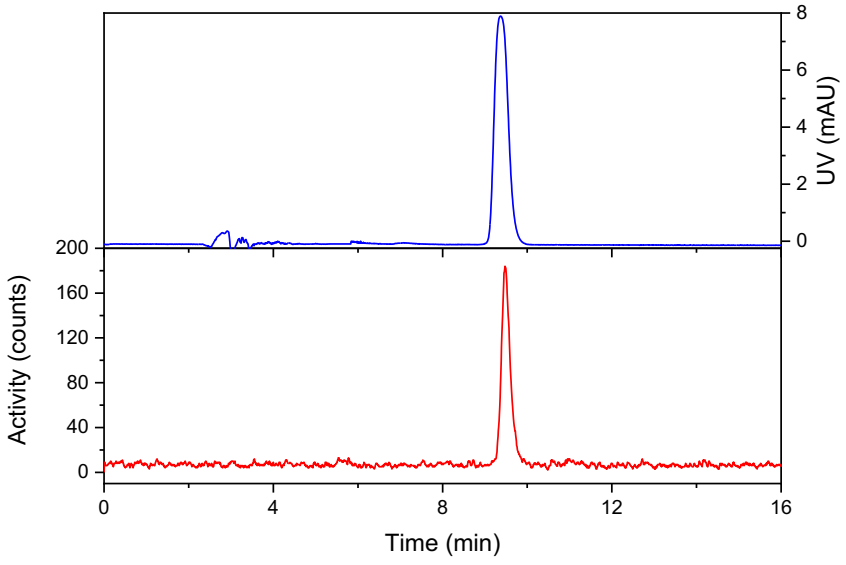
Crude preparatory HPLC chromatogram of compound **19**:



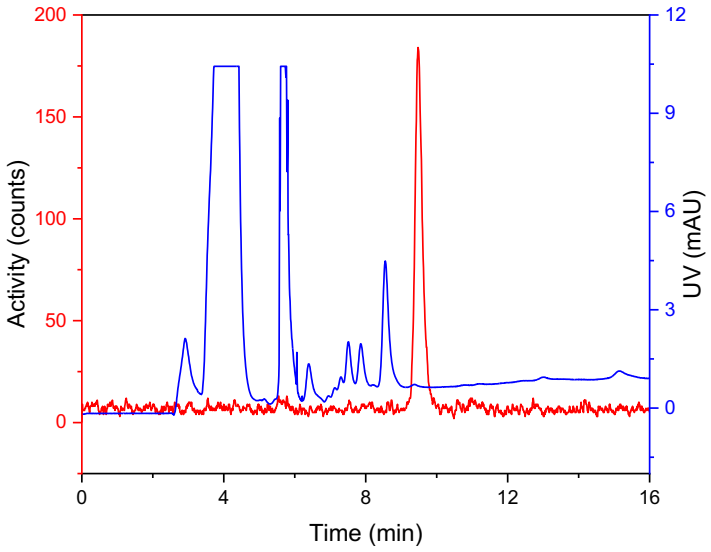
Eluent: 70:30 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 31 ± 4% (n = 2)
RCY: 23 ± 2% (n = 2)



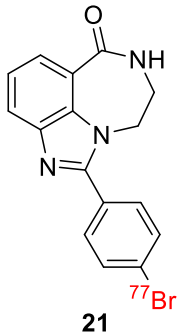
20



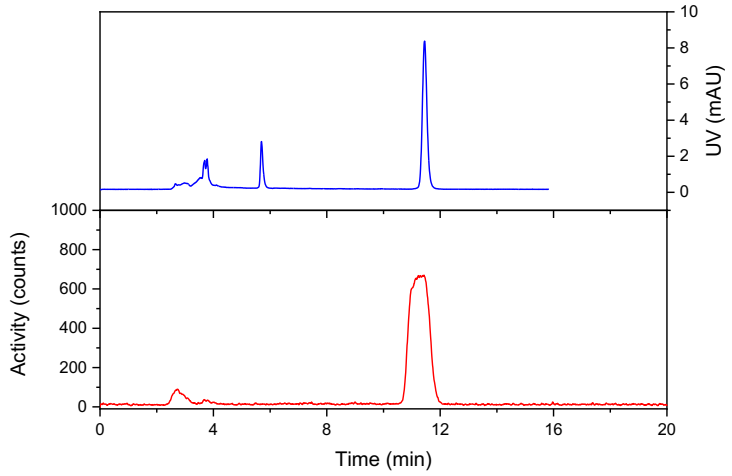
Crude preparatory HPLC chromatogram of compound **20**:



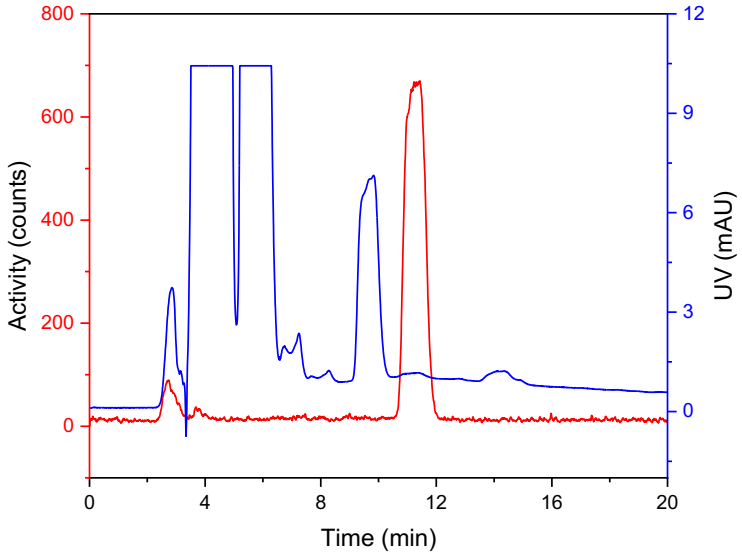
Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 90 ± 3% (n = 2)
RCY: 76 ± 1% (n = 2)



21



Crude preparatory HPLC chromatogram of compound **21**:



Eluent: 40:60 MeCN / 0.1 M NH_4HCO_2 (aq) – 4 mL / min
RCC: 89 ± 4% (n = 7)
RCY : 74 ± 7% (n = 7)

References

(1) Wang, S.; Blaha, C.; Santos, R.; Huynh, T.; Hayes, T. R.; Beckford-Vera, D. R.; Blecha, J. E.; Hong, A. S.; Fogarty, M.; Hope, T. A.; Raleigh, D. R.; Wilson, D. M.; Evans, M. J.; VanBrocklin, H. F.; Ozawa, T.; Flavell, R. R. Synthesis and Initial Biological Evaluation of Boron-Containing Prostate-Specific Membrane Antigen Ligands for Treatment of Prostate Cancer Using Boron Neutron Capture Therapy. *Mol. Pharm.* **2019**, *16* (9), 3831–3841. https://doi.org/10.1021/acs.molpharmaceut.9b00464.

(2) Zhou, D.; Chu, W.; Voller, T.; Katzenellenbogen, J. A. Copper-Mediated Nucleophilic Radiobromination of Aryl Boron Precursors: Convenient Preparation of a Radiobrominated PARP-1 Inhibitor. *Tetrahedron Lett.* **2018**, *59* (20), 1963–1967. https://doi.org/10.1016/j.tetlet.2018.04.024.

(3) Zmuda, F.; Malviya, G.; Blair, A.; Boyd, M.; Chalmers, A. J.; Sutherland, A.; Pimlott, S. L. Synthesis and Evaluation of a Radioiodinated Tracer with Specificity for Poly(ADP-Ribose) Polymerase-1 (PARP-1) in Vivo. *J. Med. Chem.* **2015**, *58* (21), 8683–8693. https://doi.org/10.1021/acs.jmedchem.5b01324.

(4) Reilly, S. W.; Makvandi, M.; Xu, K.; Mach, R. H. Rapid Cu-Catalyzed [^{211}At]Astatination and [^{125}I]Iodination of Boronic Esters at Room Temperature. *Org. Lett.* **2018**, *20* (7), 1752–1755. https://doi.org/10.1021/acs.orglett.8b00232.

(5) Ellison, P. A.; Olson, A. P.; Barnhart, T. E.; Hoffman, S. L. V; Reilly, S. W.; Makvandi, M.; Bartels, J. L.; Murali, D.; DeJesus, O. T.; Lapi, S. E.; Bednarz, B.; Nickles, R. J.; Mach, R. H.; Engle, J. W. Improved Production of ^{76}Br, ^{77}Br and ^{80m}Br via CoSe Cyclotron Targets and Vertical Dry Distillation. *Nucl. Med. Biol.* **2020**, *80–81*, 32–36. https://doi.org/10.1016/j.nucmedbio.2019.09.001.