Supporting Information

Copper(II)-Mediated [^{11}C]Cyanation of Arylboronic Acids and Arylstannanes

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1. General Procedures, Materials and Methods

Instrumental Information. NMR spectra were obtained on a Varian vnmrs700 (699.76 MHz for ^{1}H; 175.95 MHz for ^{13}C), a Varian vnmr500 (500.09 MHz for ^{1}H; 470.56 MHz for ^{19}F; 125.75 MHz for ^{13}C), or a Varian MR400 (400.53 MHz for ^{1}H; 376.87 MHz for ^{19}F) spectrometer. All ^{13}C NMR data presented are proton-decoupled ^{13}C NMR spectra, unless noted otherwise. ^{1}H and ^{13}C NMR chemical shifts (δ) are reported in parts per million (ppm) relative to TMS with the residual solvent peak used as an internal reference. ^{19}F NMR spectra are referenced based on the internal standard 1,2-difluorobenzene, which appears at –140.53 ppm. ^{1}H and ^{19}F NMR multiplicities are reported as follows: singlet (s), doublet (d), triplet (t), quartet (q), and multiplet (m). Melting point data (mp) were collected on an OptiMelt Automated Melting Point System and are uncorrected. High performance liquid chromatography (HPLC) was performed using a Shimadzu LC-2010A HT system equipped with a Bioscan B-FC-1000 radiation detector. Radio-TLC analyses were performed using a Bioscan AR 2000 Radio-TLC scanner with EMD Millipore TLC silica gel 60 plates (3.0 cm wide x 6.5 cm long).

Materials and Methods. All commercial products were used as received unless otherwise stated. Arylstannane and arylboronic acid precursors were purchased from Frontier Scientific, Oakwood Products, Acros Organics, Synthonix, and Sigma Aldrich. Arylnitrile reference standards were sourced commercially. 3-Bromo-1-phenyl-5-(pyridine-2-yl)-1,2-dihydropyridin-2-one (CAS 381248-06-2) was purchased from Key Organics and used as received. Perampanel (CAS 380917-97-5) was purchased from AChemBlock.

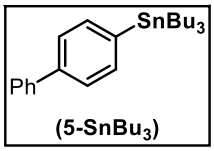
2. Synthesis and Characterization of Substrates

General Procedure A: Preparation of Trialkylarylstannane Substrates

General procedure A was adapted from the literature.[1,2,3] In a nitrogen atmosphere glovebox, a 20 mL vial was charged with aryl iodide or aryl bromide (1 mmol), $Pd(PPh_3)_4$ (0.1-0.25 mmol), and lithium chloride (4.8 mmol). The combined solids were dissolved in toluene (12.5 mL, 0.08 M) at room temperature. Hexabutylditin (2.6 mL, 5.2 mmol) or hexamethylditin (1.1 mL, 5.2 mmol) was added via syringe, and the vial was sealed and removed from the glovebox. The sealed vial was heated at 100 ºC. Once the reaction mixture turned black (generally 2-4 h), it was cooled to room temperature. Aqueous potassium fluoride (5.0 mL, 2 M solution) was added, and the mixture was stirred vigorously. After 30 min, the mixture was filtered through a plug of Celite (eluting with hexanes or toluene). The filtrate was washed with brine (25 mL), dried over magnesium sulfate, filtered, and concentrated under vacuum. The crude product was purified via flash column chromatography.

General Procedure B: Preparation of Arylboronic Acid Substrates

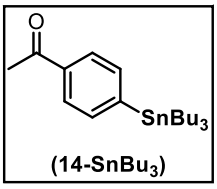
General procedure B was adapted from the literature.[4] *n*-BuLi (1.2 equiv) was added dropwise to a solution of the aryl bromide (1 equiv) in anhydrous THF at –78 ºC under a nitrogen atmosphere in an oven-dried vial. The reaction was then stirred at –78 ºC for ~1 h. An excess of $B(OMe)_3$ (10 equiv) was added slowly under a nitrogen atmosphere. The resulting solution was allowed to warm slowly to room temperature and stirred overnight. The reaction was quenched with distilled water and acidified with HCl (1M solution), and the product was extracted into EtOAc. The combined organic extracts were washed with brine, dried over $MgSO_4$, and concentrated under vacuum.



(5-SnBu$_3$)

4-Tributylstannyl-1,1'-biphenyl (5-SnBu$_3$)

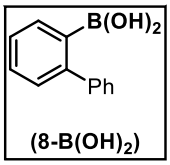
General procedure A was followed using 4-iodo-1,1'-biphenyl (279.5 mg, 1.0 mmol) and heating for 3 h. Purification by flash column chromatography eluting with hexanes afforded **5-SnBu$_3$** as a colorless oil (191.0 mg, 43% yield, R_f = 0.6 in 100% hexanes). The ^{1}H and ^{13}C NMR spectra matched those reported in the literature.[5] HRMS (EI) [M – $C_4H_9^+$] Calculated for $C_{20}H_{27}Sn$: 387.1135; Found 387.1135.



(14-SnBu$_3$)

4-Tributylstannylacetophenone (14-SnBu$_3$)

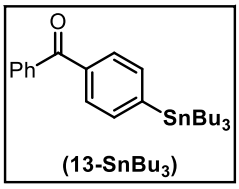
General procedure A was followed using 4-iodoacetophenone (246.3 mg, 1.0 mmol) and heating for 4 h. Purification by flash column chromatography eluting with hexanes afforded **14-SnBu$_3$** as a colorless oil (284.3 mg, 69% yield, R_f = 0.56 in 5% ethyl acetate in hexanes). The ^{1}H and ^{13}C NMR spectra matched those reported in the literature.5 HRMS (ESI$^+$) [M + K$^+$] Calculated for $C_{20}H_{34}KOSn$: 449.1263; Found 449.1263.



(8-B(OH)$_2$)

[1,1'-Biphenyl]-2-ylboronic Acid (8-B(OH)$_2$)

2-Bromobiphenyl (0.25 mL, 1.45 mmol) was dissolved in 15 mL of anhydrous THF, and *n*-BuLi (0.7 mL, 1.75 mmol, 1.2 equiv, 2.48 M in hexane) and then $B(OMe)_3$ (1.6 mL, 14.4 mmol, 10 equiv) were added sequentially according to general procedure B. Triturating the resulting mixture with pentanes and a small amount of EtOAc yielded the desired boronic acid (**8-B(OH)$_2$**) as an off-white solid (220.3 mg, 77% yield, mp = 184-185 ºC). The ^{1}H and ^{13}C NMR spectra matched those reported in the literature.4 HRMS (EI) [M$^+$] Calculated for $C_{12}H_{11}BO_2$: 198.0852; Found 198.0858.



(13-SnBu$_3$)

4-Tributylstannylbenzophenone (13-SnBu$_3$)

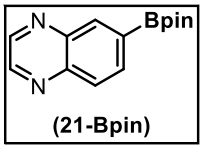
In a nitrogen atmosphere glovebox, a 20 mL vial was charged with 4-iodobenzopheone (308.6 mg, 1.0 mmol), $Pd(PPh_3)_2Cl_2$ (175.3 mg, 0.25 mmol, 0.25 equiv) and dioxane (12.5 mL, 0.08 M) at room temperature. Hexabutylditin (1.3 mL, 2.6 mmol) was added via syringe and the vial was sealed and removed from the glovebox. The sealed vial was heated at 100 ºC for 4 h. After cooling to room temperature, the reaction mixture was filtered through a silica plug that was washed with EtOAc. The solvent was removed under vacuum, and the crude product was

purified via preparative TLC (5% ethyl acetate in hexanes) affording the product (**13-SnBu$_3$**) as a yellow oil (231.5 mg, 59% yield, R_f = 0.5 in 5% ethyl acetate in hexanes).

^{1}H NMR ($CDCl_3$): δ 7.82 (m, 2H), 7.73 (m, 2H), 7.57-7.63 (multiple peaks, 3H), 7.48 (m, 2H), 1.56 (m, 6H), 1.35 (m, 6H), 1.11 (m, 6H), 0.90 (m, 9H)

^{13}C NMR ($CDCl_3$): δ 197.05, 149.22, 137.70, 136.92, 136.26, 132.24, 130.04, 128.94, 128.18, 29.04, 27.34, 13.66, 9.66

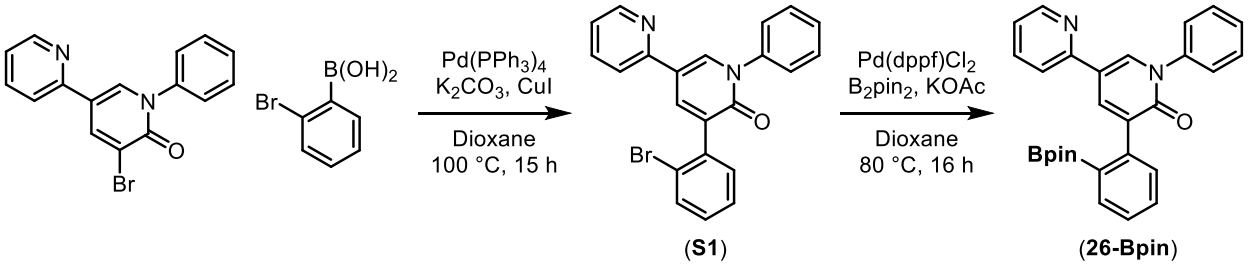
HRMS (ESI+) [M + K^+] Calculated for $C_{25}H_{36}KOSn$: 511.1420; Found 511.1418.



(21-Bpin)

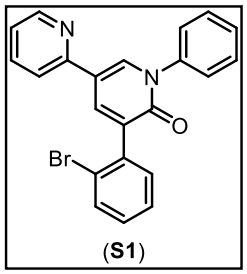
6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)quinoxaline (21-Bpin)

The following procedure was adapted from the literature.[6] In a nitrogen atmosphere glovebox, a 20 mL vial was charged with 6-bromoquinoxaline (419 mg, 2.0 mmol, 1 equiv), Pd(dppf)Cl_2 dichloromethane complex (186.0 mg, 0.23 mmol, 0.11 equiv), KOAc, (394.2 mg, 4.0 mmol, 2.0 equiv), bis(pinacoloato)diboron (612.5 mg, 2.4 mmol, 1.2 equiv) and dioxane (10 mL, 0.2 M). The resulting solution was heated at 90 ºC for 1.5 h. The reaction mixture was allowed to cool to room temperature and then concentrated *in vacuo*. The resulting residue was dissolved in CH_2Cl_2 and filtered through a plug of celite. After removing the CH_2Cl_2 under vacuum, the product was purified by column chromatography (20% ethyl acetate in hexane), affording **21-Bpin** as a yellow oil (103.2 mg, 15% yield, R_f = 0.3 in 20% ethyl acetate in hexanes). The ^{1}H and ^{13}C NMR spectra matched those reported in the literature.6 HRMS (ESI+) [M + H]$^+$ Calculated for $C_{14}H_{18}BN_2O_2$: 257.1456; Found 257.1463.



(**S1**) (**26-Bpin**)

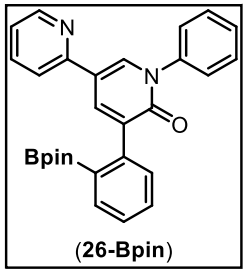
Perampanel-Bpin (26-Bpin) was prepared via the following 2 step procedure that was adopted from the literature.[7,8]



(**S1**)

Step 1:

Aryl bromide **S1** was prepared via a literature procedure. In a nitrogen-filled glovebox, the pyridne bromide (319.2 mg, 0.98 mmol, 1 equiv), 2-bromophenylboronic acid (1651.6 mg, 8.2 mmol, 8.4 equiv), tetrakis(triphenylphosphine)palladium(0) (180.5 mg, 0.16 mmol, 0.16 equiv), copper(I) iodide (48.9 mg, 0.26 mmol, 0.26 equiv), and potassium carbonate (1653.6 mg, 12.0 mmol, 12.3 equiv) were dissolved in dioxane (6 mL, 0.16 M) at room temperature. This solution was heated at 100 ºC for 15 h with vigorous stirring. The reaction was cooled to room temperature and quenched with water (5 mL). The aqueous phase was extracted with EtOAc (2 x 25 mL) and the combined organic extracts were dried over $MgSO_4$ and concentrated. The crude residue was purified by column chromatography (silica gel, 35% ethyl acetate in hexanes) to afford **S1** as a yellow oil (210.0 mg, 53% yield, R_f = 0.4 in 50% ethyl acetate in hexanes). The ^1H and ^{13}C NMR spectra matched those reported in the literature.7 HRMS (ESI^+) $[M + H]^+$ Calculated for $C_{22}H_{16}BrN_2O$: 403.0441; Found 403.0444.



(**26-Bpin**)

Step 2:

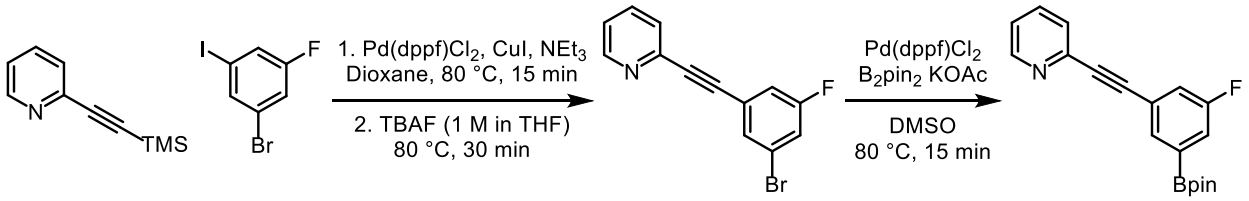
In a nitrogen-atmosphere glovebox, a suspension of aryl bromide (**S1**, 60.8 mg, 0.15 mmol), $Pd(dppf)Cl_2$ dichloromethane complex ((20.3 mg, 0.02 mmol, 0.16 equiv), KOAc, (372.9 mg, 1.5 mmol, 9.7 equiv), and bis(pinacoloato)diboron (214.8 mg, 2.2 mmol, 14.5 equiv) in dioxane (3.8 mL, 40 mM) was heated at 80 ºC for 16 h. The reaction mixture was allowed to cool to room temperature, quenched with water, and washed with EtOAc (3 x 25 mL). The combined organic extracts were washed with brine, dried over $MgSO_4$, and concentrated under vacuum. The crude residue was purified by column chromatography (20% ethyl acetate in hexane with 1-5%

NEt_3) to afford **26-Bpin** as a white solid (31.7 mg, 47% yield, R_f = 0.2 in 70% ethyl acetate in hexanes with 15% NEt_3, melting point: decomposes above 138 ºC).

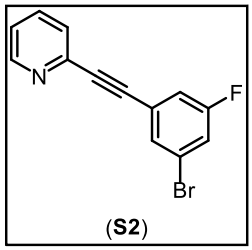
^{1}H NMR ($CDCl_3$): δ 8.84 (d, *J* = 1.3 Hz, 1H), 8.66 (dt, *J* = 0.8, 2.5, 1H), 8.35 (d, *J* = 1.3 Hz, 1H), 7.80-7.83 (multiple peaks, 3H), 7.72 (d, *J* = 4.6 Hz, 1H), 7.52-7.57 (multiple peaks, 5H), 7.37 (dtd, *J* = 18.0, 7.4, 0.8 Hz, 2H), 7.30 (dd, *J* = 2.5, 9.8 Hz, 1H), 1.11 (s, 12H).

^{13}C NMR ($CDCl_3$): δ 161.1, 152.3, 150.0, 140.4, 137.3, 134.6, 133.7, 133.5, 133.2, 129.6, 129.4, 129.0, 127.9, 127.5, 126.8, 123.4, 123.0, 122.9, 122.8, 119.3, 80.49, 25.89

HRMS (ESI+) [M + H^+] Calculated for $C_{28}H_{28}BN_2O_3$: 451.2187; Found 451.2175.



PEB-Bpin,F (27-Bpin) was prepared by the following 2 step procedure adapted from the literature.[9,10,11]



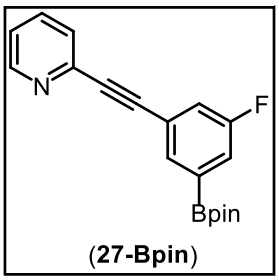
Step 1:
In a nitrogen filled glovebox, 2-((trimethylsilyl)ethynyl)pyridine (177.0 mg, 1.01 mmol, 1 equiv), 1-bromo-3-fluoro-5-iodobenzene (316.9 mg, 1.05 mmol, 1 equiv), $Pd(PPh_3)Cl_2$ (87.1 mg, 0.12 mmol, 0.1 equiv), CuI (43.0 mg, 0.23 mmol, 0.2 equiv), and NEt_3 (0.3 mL, 2.2 mmol, 2.1 equiv) were dissolved in dioxane at room temperature. The reaction mixture was heated to 80 ºC under nitrogen for 15 min. TBAF (1 M solution in THF, 1.1 mL, 1.2 mmol, 1.1 equiv) was added dropwise over 10 min. The resulting solution was allowed to stir for an additional 30 min at 80 ºC under nitrogen before being cooled to room temperature. The reaction was filtered through a celite plug, concentrated under vacuum, and dissolved in DCM. The organic later was washed with H_2O (2 x 25 mL) and brine, dried over $MgSO_4$, and concentrated under vacuum. The crude residue was purified by column chromatography (5% ethyl acetate in hexanes) to afford **S2** as a yellow oil (182.2 mg, 65% yield, R_f = 0.43 in 20% ethyl acetate in hexanes).

^{1}H NMR ($CDCl_3$): δ 8.63 (m, 1H), 7.70 (m, 1H), 7.52-7.54 (multiple peaks, 2H), 7.26-7.29 (multiple peaks, 2H), 7.23 (m, 1H)

^{13}C NMR ($CDCl_3$): δ 162.11, 150.24, 142.57, 136.28, 130.84, 127.38, 125.41, 123.35, 122.44, 119.99, 117.76, 90.45, 86.07

^{19}F NMR ($CDCl_3$): δ –110.46

HRMS (ESI+) [M + H^+] Calculated for $C_{13}H_8BrFN$: 275.9819; Found 275.9821.



(**27-Bpin**)

Step 2:
In a nitrogen atmosphere glovebox, aryl bromide (**S2**, 430.8 mg, 1.6 mmol), Pd(dppf)Cl_2 dichloromethane complex (179.4 mg, 0.02 mmol, 0.14 equiv), KOAc (459.7 mg, 4.7 mmol, 3.0 equiv), and bis(pinacoloato)diboron (436.3 mg, 1.7 mmol, 1.1 equiv) were suspended in DMSO (8.8 mL, 0.18 M). The reaction mixture was heated at 80 ºC for 15 h. The reaction was allowed to cool to room temperature and quenched with water, and the product was extracted into EtOAc (3 x 50 mL). The combined organic extracts were washed with brine, dried over $MgSO_4$, and concentrated under vacuum. Triturating the resulting mixture with pentanes and a few drops of EtOAc yielded **27-Bpin** as a yellow solid (386.1 mg, 76% yield, R_f = 0.32 in 20% ethyl acetate in hexanes, mp = 77-78 °C).

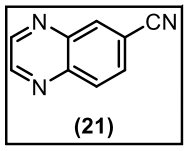
^{1}H NMR ($CDCl_3$): δ 8.62 (dq, *J* = 4.9, 1.0 Hz, 1H), 7.84 (s, 1H), 7.68 (td, *J* = 7.7, 2.0 Hz, 1H), 7.50 (dt, *J* = 7.7, 1.0 Hz, 1H), 7.47 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.35 (dq, *J* = 8.9, 1.3 Hz, 1H), 7.24 (dd, *J* = 4.9 1.3 Hz, 1H), 1.34 (s, 12H)

^{13}C NMR ($CDCl_3$): δ 161.98, 150.11, 143.10, 136.16, 134.38, 127.18, 123.71, 122.93, 121.66, 121.00, 89.27, 87.74, 84.32, 29.68, 24.83

^{19}F NMR ($CDCl_3$): δ –113.84

HRMS (ESI+) [M + H^+] Calculated for $C_{19}H_{20}BFNO_2$: 324.1566; Found 324.1575.

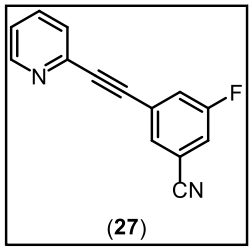
3. Synthesis and Characterization of Arylnitrile Standards



(21)

Quinoxaline-6-carbonitrile (21)

Quinoxaline-6-carbonitrile (**21**) was prepared via an adapted literature procedure.[12] In a nitrogen atmosphere glovebox, $Pd(PPh_3)_4$ (110.7 mg, 0.10 mmol, 0.1 equiv) was added to a vial and removed from the glovebox. The same vial was charged with 6-bromoquinoxaline (210.6 mg, 1.0 mmol, 1 equiv) and $K_4[Fe(CN)_6]\bullet 3H_2O$ (174.5 mg, 0.41 mmol, 0.4 equiv). The vial was placed under N_2. A solution of *t*-BuOH/H_2O (1:1, 3 mL, 0.33 M) and DBU (0.05 mL, 0.33 mmol, 0.33 equiv) was added via syringe, and the resulting mixture was stirred at room temperature for 10 min and then at 85 ºC for 15 h. The reaction mixture was allowed to cool to room temperature and filtered through a celite plug that was washed with methanol and DCM. The organic solution was washed with H_2O and brine, was dried over $MgSO_4$, and was then concentrated under vacuum. The crude residue was purified by flash chromatography on silica gel (25% ethyl acetate in hexanes), which afforded **21** as a white solid (55.0 mg, 21% yield R_f = 0.4 in 50% ethyl acetate in hexanes, mp = 173-174 ºC). The ^1H and ^{13}C NMR spectra matched those reported in the literature.[13] HRMS (ESI+) $[M + H]^+$ Calculated for $C_9H_6N_3$: 156.0562; Found 156.0553.



(**27**)

F-PEB (27)

Aryl fluoride **27** was prepared via a literature procedure.[3,10] The product was purified by flash chromatography on silica gel (15% ethyl acetate in hexanes), to afford **27** as a brown solid (142.9 mg, 63% yield R_f = 0.15 in 20% ethyl acetate in hexanes, mp = 75-77 °C). The ^1H and ^{13}C NMR spectra matched those reported in the literature.[10,14]

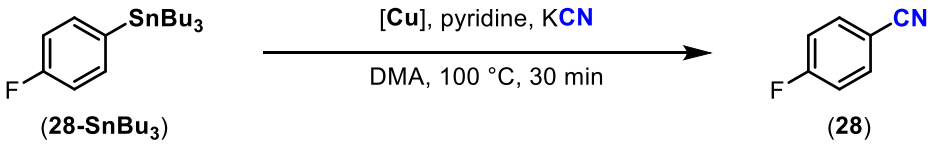
^{19}F NMR ($CDCl_3$): δ –108.9

HRMS (ESI+) $[M + H^+]$ Calculated for $C_{14}H_8FN_2$: 223.0666; Found 223.0664.

4. Experimental Details (Optimization)

General procedure: Stock solutions of the aryl organometallic substrate (0.1 mL, 0.1 M solution, 10 µmol, 1 equiv), $Cu(OTf)_2$ (20 µmol, 2 equiv), pyridine (0.15 mL, 1.0 M solution,150 µmol, 15 equiv), and KCN (1.5 mg, 20 µmol, 2 equiv) were added to a 4 mL vial and diluted with DMA (to 1.0 mL total volume). The vial was sealed with a Teflon-lined cap, and the reaction mixture was stirred at 100 ºC for 30 min. The resulting solution was cooled to room temperature, 1,2-difluorobenzene was added as an internal standard, and the crude reaction was analyzed by ^{19}F NMR spectroscopy.

Copper Screen



(**28-SnBu$_3$**) (**28**)

Table S4-1. Copper Salt Screen

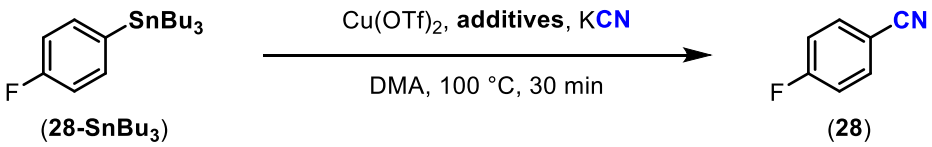
entry	[Cu]	28 (%)
1	$Cu(OTf)_2$	35
2	$Cu(TFA)_2$ hydrate	19
3	$Cu(NO_3)_2$ $3H_2O$	27
4	$Cu(BF4)_2$ $6H_2O$	39
5	$Cu(SO_4)$	30
6	$(MeCN)_4Cu(PF_6)$	12
7	$(MeCN)_4Cu(BF_4)$	18

Reaction conditions: **28-SnBu$_3$** (10 µmol), copper salt (2 equiv), pyridine (15 equiv), and KCN (2 equiv) in DMA at 100 ºC for 30 min. Yield was determined by ^{19}F NMR spectroscopy with 1,2-difluorobenzene as an internal standard.

• Copper sources that did not form product: $Cu(acac)_2$, Cu(OAc), $Cu(OAc)_2$, CuF_2, CuI, CuO

• Copper sources that formed a trace (<5%) amount of product: $(MeCN)_4Cu(OTf)$, $CuCl_2$, CuCl, Cu(TFA) benzene

Additive Screen



(**28-SnBu$_3$**) (**28**)

Table S4-2. Additive Screen

entry	additive	28 (%)
1	none	17
2[a]	pyridine	39
3[a]	2-picoline	14
4[a]	2,4-lutidine	18
5[a]	2,6-lutidine	21
6[a]	piperidine	8
7[a]	morpholine	17
8[b]	18-crown-6 (w/o pyr)	23
9[a]	18-crown-6 (w/ pyr)	42
10[b]	DIPEA	18
11[b]	K_2CO_3	12
12[b]	K_3PO_4	14
13[b]	NaTFA	13
14[b]	NEt_3	18

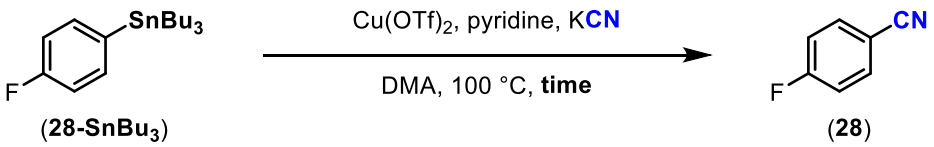
Reaction conditions: **28-SnBu$_3$** (10 µmol), $Cu(OTf)_2$ (2 equiv), additive, and KCN (2 equiv) in DMA, set to 100 ºC for 30 min. Yield was determined by ^{19}F NMR spectroscopy with 1,2-difluorobenzene as an internal standard.

[a]15 equiv of additive used. [b]3 equiv of additive used

• Additives that provided no product: 1,10-phenanthroline, quinaldic acid, DBU

• Additives that provided <5% product: 2,2'-bipyridine, DMAP

Time Study

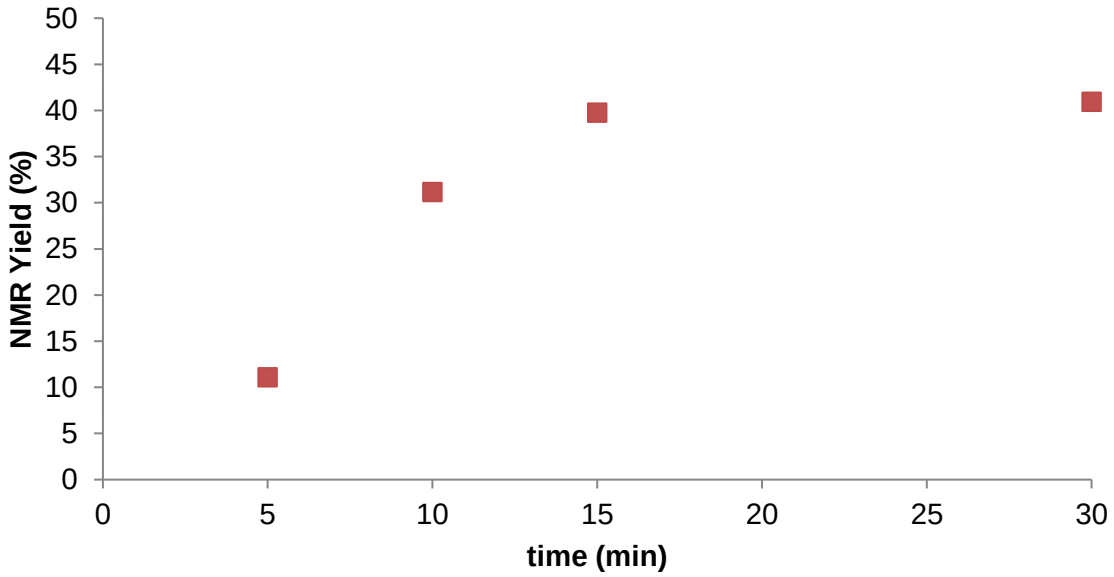


(**28-SnBu$_3$**) (**28**)

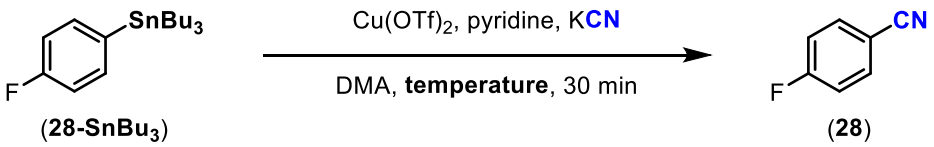
Table S4-3. Time Study

entry	time (min)	28 (%)
1	5	11
2	10	31
3	15	40
4	30	41

Reaction conditions: **28-SnBu$_3$** (10 µmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), and KCN (2 equiv) in DMA at 100 ºC for a selected amount of time. Yield was determined by ^{19}F NMR spectroscopy with 1,2-difluorobenzene as an internal standard.



Temperature Study



(**28-SnBu$_3$**) (**28**)

Table S4-4. Temperature Study

entry	temperature (°C)	28 (%)
1	50	--
2	80	16
3	100	40
4	120	47
5	140	37

Reaction conditions: **28-SnBu$_3$** (10 µmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), and KCN (2 equiv) in DMA at a selected temperature for 30 min. Yield was determined by ^{19}F NMR spectroscopy with 1,2-difluorobenzene as an internal standard.

Comparison of Substrates in DMF and DMA

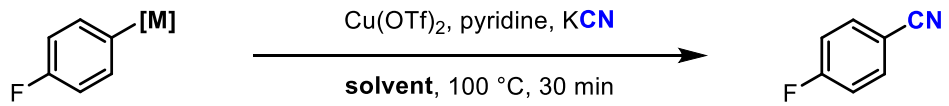
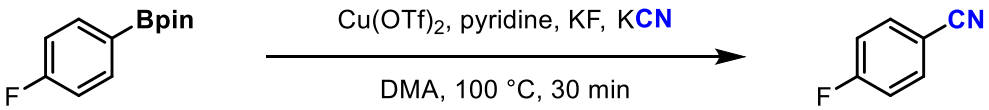


Table S4-5. Small Scope in DMF and DMA

entry	[M] (substrate #)	% yield (in DMA)	% yield (in DMF)
1	$SnBu_3$ (**28-$SnBu_3$**)	44	52
2	$B(OH)_2$ (**28-$B(OH)_2$**)	65	62
3	BF_3K (**28-BF_3K**)	61	59
4	Bpin (**28-Bpin**)	15	12

Reaction conditions: substrate (10 µmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), and KCN (2 equiv) in DMA or DMF at 100 ºC for 30 min. Yield was determined by ^{19}F NMR spectroscopy with 1,2-difluorobenzene as an internal standard.

Activator for Arylboronate Ester Substrates



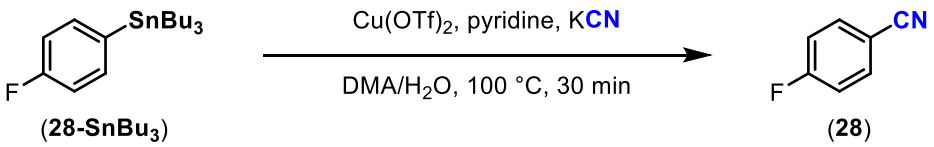
(**28-Bpin**) (**28**)

Table S4-6. Activator for Arylboronate Ester Substrates

entry	KF (equiv)	28 (%)
1	--	14
2	1	41
3	2	40

Reaction conditions: **28-Bpin** (10 µmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), KF, and KCN (2 equiv) in DMA at 100 ºC for 30 min. Yield was determined by ^{19}F NMR spectroscopy with 1,2-difluorobenzene as an internal standard.

Effect of Water



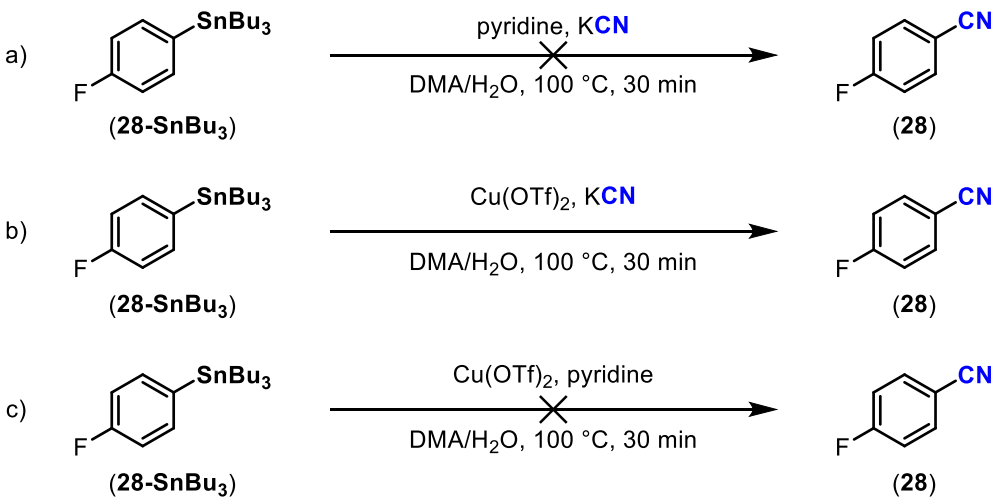
(**28-SnBu$_3$**) (**28**)

Table S4-7. Effect of Water

entry	DMA (mL)	H_2O (mL)	28 (%)
1	1.0	--	40
2	1.0	0.1	45
3	1.0	0.2	37

Reaction conditions: **28-SnBu$_3$** (10 µmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), H_2O, and KCN (2 equiv), DMA (1 mL total, 10 mM) at 100 ºC for 30 min. Yield was determined by ^{19}F NMR spectroscopy with 1,2-difluorobenzene as an internal standard.

Control Reactions



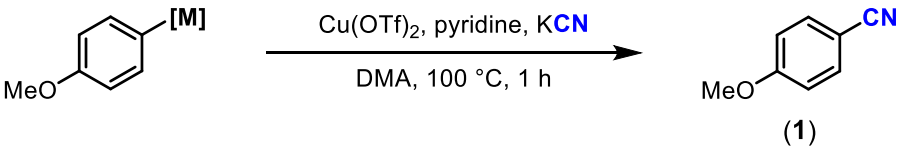
(**28-SnBu$_3$**) (**28**)

(**28-SnBu$_3$**) (**28**)

(**28-SnBu$_3$**) (**28**)

Control reactions for the cyanation of substrate **28-SnBu$_3$** were conducted (a) without $Cu(OTf)_2$, (b) without pyridine, (c) and without KCN. In (a) and (c), the cyanation product **28** was not detected. In (b), the cyanation product **28**, was observed in 12%.

Cu-Mediated Cyanation of Anisole Substrates



(**1**)

Table S4-8. Cu-Mediated Cyanation of Anisole Substrates

entry	[M]	1 (%)
1	**1-SnBu$_3$**	28
2	**1-B(OH)$_2$**	32
3	**1-BF$_3$K**	26
4	**1-Bpin**	6
5[a]	**1-Bpin**	22

Reaction conditions: substrate (10 µmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), and KCN (2 equiv), DMA (1 mL total, 10 mM) at 100 ºC for 1 h. Work up: cooled to room temperature, washed with brine (2 mL) and ethyl acetate (3 x 1 mL), dried, filtered through silica gel, and concentrated. Yield was determined by ^{1}H NMR spectroscopy with 1,3,5-trifluorobenzene as an internal standard. [a]KF (1.2 equiv)

5. Radiochemistry

5.1 Materials and Methods

Unless otherwise stated, reagents and solvents were commercially available and used without further purification. HPLC-grade acetonitrile, anhydrous *N*,*N*-dimethylformamide, anhydrous *N,N*-dimethylacetamide, potassium trifluoromethanesulfonate, and potassium carbonate were purchased from Fisher Scientific. Sterile product vials were purchased from Hollister-Stier. QMA-light Sep-Paks were purchased from Waters Corporation. QMA-light Sep-Paks were flushed with 10 mL of ethanol, followed by 10 mL of 90 mg/mL potassium trifluoromethanesulfonate solution, and finally 10 mL of sterile water prior to use.

5.2 Synthesis of [^{11}C]KCN[15]

A GE PETtrace cyclotron (40 µA for 30 min) was used to produce [^{11}C]CO_2 by the ^{14}N(p,α)^{11}C reaction. The resulting [^{11}C]CO_2 was converted to [^{11}C]HCN using a GE PETtrace Carbon-11 Process Panel. Briefly, [^{11}C]CO_2 (3,000 mCi) from the target was trapped on molecular sieves at room temperature. The [^{11}C]CO_2 was released and mixed with hydrogen gas at 350 ºC then passed through a preheated nickel oven at 420 ºC for conversion to [^{11}C]CH_4. The [^{11}C]CH_4 gas was purified by passing it through Ascarite and Sicapent columns to remove water and unreacted [^{11}C]CO_2. The [^{11}C]CH_4 was mixed with anhydrous ammonia and passed through a high temperature (950 ºC) platinum oven, resulting in the formation of [^{11}C]HCN (non-decay corrected radiochemical yields of 700-1000 mCi).

Modifications were made to a commercial GE TRACERLab FX_M. Two electronic valves were installed in the front of the chemistry module to direct [^{11}C]HCN from the GE process panel to the FX_M. V30 and V31 were removed from the HPLC pump and connected to a system to capture the [^{11}C]HCN from the process panel. The system consists of a helically shaped platinum wire in a Teflon tube inserted between V30 and V31. To capture and purify [^{11}C]HCN (removal of excess NH_3), the helical platinum wire was treated with 0.2 mL of a 1 M solution of KOH followed by 2 mL of dry air. The [^{11}C]HCN was trapped on the platinum wire, and then the flow was switched from the process panel to N_2, which removed the ammonia. This purification was carried out because we hypothesized that residual NH_3 could have a negative effect on the reaction conditions. The [^{11}C]CN was then eluted as [^{11}C]KCN by directing the three way valve from waste to the reactor and eluting with H_2O.

5.3 Synthesis of ^{11}CN-Labeled Molecules (Manual Synthesis)

Unless otherwise noted, this procedure was used for all [^{11}C]cyanation reactions. Stock solutions of precursor (0.1 M), $Cu(OTf)_2$ (0.2 M) and pyridine (1.0 M) in DMA were prepared immediately prior to the start of the reaction. Aliquots of these solutions were used to carry out subsequent [^{11}C]cyanation reactions. Reactions were typically set up in the following order: $Cu(OTf)_2$ (0.1 mL, 20 µmol, 2 equiv) and pyridine (0.15 mL, 0.15 mmol, 15 equiv) were mixed in a 4 mL vial at room temperature. The resulting solution was diluted with DMA (0.55 mL, 1.0 mL total volume) and then charged with substrate (0.1 mL, 0.01 mmol, 1 equiv). The reaction vial was sealed under an atmosphere of ambient air with a PTFE/Silicone septum cap, and a 0.1 mL aliquot of [^{11}C]KCN (150-3000 µCi, depending on the time required for HPLC analysis) was added to the reaction vial through the septum via a syringe. The vial was heated in an aluminum block without stirring at 100 ºC for 5 min and then immediately cooled to room temperature. Radio-TLC analysis was conducted to determine the radiochemical conversion (% RCC). The crude reaction mixture was spotted onto a standard silica-coated glass plate and the TLC was coducted using 1:1 hexane/EtOAc or 100% EtOAc as the eluant. The RCC was then determined by dividing the integrated area under the cyanated product spot by the total integrated area of the carbon-11 on the TLC plate. To prepare samples for HPLC analysis: 0.1

mL of the reaction mixture (or for the co-injection analysis 0.1 mL of the reaction mixture spiked with 0.1 mL of 1 mg/mL cyanation authentic standard solution) were transferred to an HPLC autosampler vial. Eluent systems and columns used for HPLC analysis are described below.

RCC = integration of ^{11}C product peak / sum of integration of all ^{11}C peaks

5.4 General HPLC Conditions

Four general HPLC conditions were used: two different gradient methods (Conditions A or B) and two different isocratic methods (Conditions C or D).

HPLC Conditions A

Condition: 5-95% gradient of (CH_3CN + 0.05% TFA) in (H_2O + 0.05% TFA)
Flow rate: 2 mL/min
Column: Luna C-18 Column 150 x 4.6 mm; 5 µm

0-3 min	5% MeCN	isocratic
3-20 min	5% to 95% MeCN	linear increase
20-30 min	5% MeCN	isocratic

HPLC Conditions B

Condition: 0-50% gradient of (CH_3CN + 0.05% TFA) in (H_2O + 0.05% TFA)
Flow rate: 2 mL/min
Column: Omega Polar RP Column 150 x 4.6 mm; 5 µm

0-1 min	0% MeCN	isocratic
1-10 min	0% to 50% MeCN	linear increase
10-12 min	50% MeCN	isocratic
12-15 min	0% MeCN	isocratic

HPLC Conditions C

Condition: 20% (MeCN + 0.05% TFA) in (H_2O + 0.05% TFA)
Flow Rate: 2 mL/min
Column: Luna C-18 Column 150 x 4.6 mm; 5 µm

HPLC Condition D

Condition: 40% (MeCN + 0.05% TFA) in (H_2O + 0.05% TFA)
Flow Rate: 1.5 mL/min
Column: Luna C-18 Column 150 x 4.6 mm; 5 µm

5.5 Additional Optimization Results of radiocyanation (manual synthesis conditions)

Water Effects

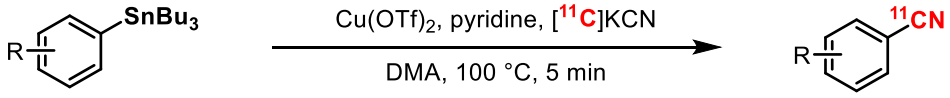
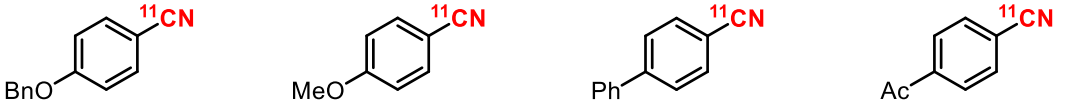


Figure S5-1. Water Effects



([^{11}C]**2**)
with H_2O: 44 ± 4%
anhydrous: 50 ± 4%

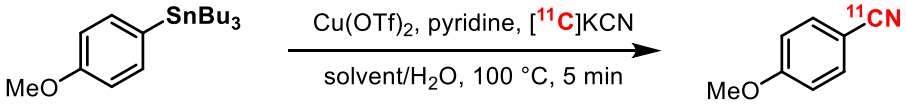
([^{11}C]**1**)
with H_2O: 41 ± 1%
anhydrous: 42 ± 1%

([^{11}C]**5**)
with H_2O: 48 ± 3%
anhydrous: 58 ± 1%

([^{11}C]**14**)
with H_2O: 42 ± 1%
anhydrous: 43 ± 1%

Reaction conditions: substrate (10 µmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), [^{11}C]KCN in DMA (0.1 mL) diluted to 1 mL in DMA/H_2O (4:1) at 100 ºC for 5 min. RCCs were determined via radio-TLC (n = 2).

Solvent Effects



(**1-SnBu$_3$**)

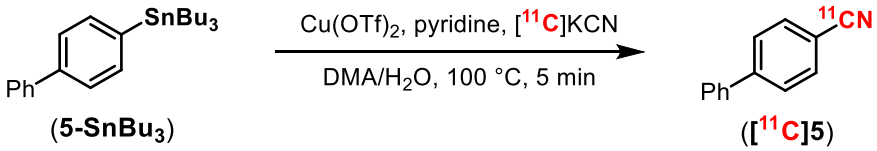
([^{11}C]**1**)

Table S5-1. Solvent Effects on Cu-Mediated [^{11}C]Cyanation

entry	Solvent	% RCC
1	DMA	68
2	DMF	48

Reaction conditions: substrate (0.01 mmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), and [^{11}C]KCN in H_2O (0.1 mL) diluted to 1 mL in DMA at 100 ºC for 5 min. RCCs were determined via radio-TLC.

Temperature Study



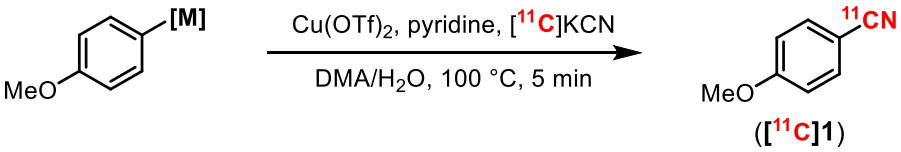
(**5-SnBu$_3$**) (**[^{11}C]5**)

Table S5-2. Temperature Study

entry	Temperature (°C)	% RCC
1	100	74
2	80	53
3	50	6

Reaction conditions: substrate (0.01 mmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), and [^{11}C]KCN in H_2O (0.1 mL) diluted to 1 mL total volume of a DMA/H_2O mixture at the selected temperature for 5 min. RCCs were determined via radio-TLC.

Optimal DMA:H_2O Ratio



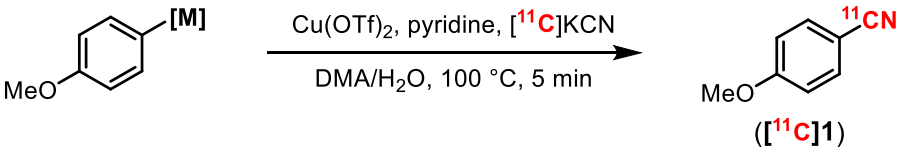
([^{11}C]**1**)

Table S5-3. Optimal DMA:H_2O Ratio

entry	[M]	DMA:H_2O	1 (% RCC)
1	**1-SnBu$_3$**	9:1	64
2	**1-SnBu$_3$**	5:1	43
3	**1-SnBu$_3$**	3:1	30
4	**1-B(OH)$_2$**	9:1	76
5	**1-B(OH)$_2$**	5:1	59
6	**1-B(OH)$_2$**	3:1	45
7	**1-B(OH)$_2$**	1:1	25

Reaction conditions: substrate (0.01 mmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), H_2O and [^{11}C]KCN in H_2O (0.1 mL) diluted to 1 mL total volume of a DMA/H_2O mixture at 100 ºC for 5 min. RCCs were determined via radio-TLC.

TLC Control Reactions



([^{11}C]**1**)

Table S5-4. TLC Control Reactions

entry	[M]	TLC Condition	1 (% RCC)
1	**1-SnBu$_3$**	A	57
2	**1-SnBu$_3$**	B	52
3	**1-SnBu$_3$**	D	51
4	**1-B(OH)$_2$**	A	71
5	**1-B(OH)$_2$**	B	71
6	**1-B(OH)$_2$**	C	76

Reaction conditions: substrate (0.01 mmol), $Cu(OTf)_2$ (2 equiv), pyridine (15 equiv), and [^{11}C]KCN in H_2O (0.1 mL) diluted to 1 mL total volume of a DMA/H_2O mixture at the selected temperature for 5 min. RCCs were determined via radio-TLC.

TLC Conditions
A: traditional acidic silica plates
B: Silica plates pre-treated with NEt_3
C: Neutral alumina plates
D: Basic alumina plates

5.6 General Procedure/Methods for Automated Syntheses

All loading operations were conducted under an ambient atmosphere. Nitrogen was used as a pressurizing gas during automated sample transfers. [^{11}C]Cyanide was produced via the ^{14}N(p,α)^{11}C nuclear reaction using a GE PETTrace cyclotron and process panel. [^{11}C]KCN was produced as indicated above. A solution containing precursor (0.1 mL, 0.1 M stock, 10 µmol, 1 equiv) in 0.4 mL of anhydrous DMA was prepared in vial 2. $Cu(OTf)_2$ (0.1 mL, 0.2 M stock, 20 µmol, 2 equiv) and pyridine (0.15 mL, 1.0 M stock, 150 µmol, 15 equiv) in 0.25 mL of DMA was mixed in the reaction vessel. H_2O (0.2 mL in vial 1) was used to wash the [^{11}C]KCN into the reaction vessel containing the catalyst solution. After vial 2 was added, the mixture was heated at 100 ºC for 4 min (it took approximately 1 min to heat to 100 ºC). After 4 min, the reaction was cooled to 40 ºC and vial 4 containing 0.5 mL of buffer was added. The mixture was then transferred to an HPLC loop for injection and purification by semi-preparative chromatography (Phenomenex Luna C18, 250 x 10 mm, 10µ, 4 mL/min). The product peak (retention time ~12 min) was collected and transferred out of the hot cell. Time from EOB ~30-32 min.

5.6.1 Specific Activity Calculation

An aliquot of the purified sample was injected onto an analytical HPLC. The UV peak corresponding to the [^{11}C]radionitrile product was determined by overlaying the UV and RAD traces (with a 0.2 min offset as described in the HPLC section). The UV area was then used to calculate the concentration of the product based on linear regression analysis of appropriate arylnitrile standards. A standard curve was generated from the standard solutions, each performed in duplicate (0.0001 mg/mL to 1.0 mg/mL). This provided the concentration of the product in mmol/mL. Dividing the activity concentration (Ci/mL) by the HPLC-derived concentration of product (mmol/mL) provided the specific activity in Ci/mmol. This reflects an end of synthesis (EoS) specific activity.

5.6.2 Automated Synthesis of [^{11}C]4-methoxybenzonitrile ([^{11}C]1)

The general procedure from Section 5.6 was followed with no deviations.
Starting material: **1-SnBu$_3$**
Activity Isolated, non-decay corrected: 16 mCi/220 mCi
RCY, non-decay corrected: 7%
RCY, decay corrected: 22%
Specific Activity: 1800 Ci/mmol

5.6.3 Automated Synthesis of [^{11}C]4-methoxybenzonitrile ([^{11}C]1)

The general procedure from Section 5.6 was followed with no deviations.
Starting material: **1-B(OH)$_2$**
Activity Isolated, non-decay corrected: 71 mCi/400 mCi
RCY, non-decay corrected: 18%
RCY, decay corrected: 53%
Specific Activity: 4400 Ci/mmol

5.6.3 Automated Synthesis of [^{11}C]Perampanel ([^{11}C]26)

The general procedure from Section 5.6 was followed with no deviations.
Starting material: **26-Bpin**
Activity Isolated, non-decay corrected: 46 mCi/450 mCi
RCY, non-decay corrected: 10 ± 1% (n = 2)
RCY, decay corrected: 29 ± 1% (n = 2)
Specific Activity: 1900 Ci/mmol

6. References

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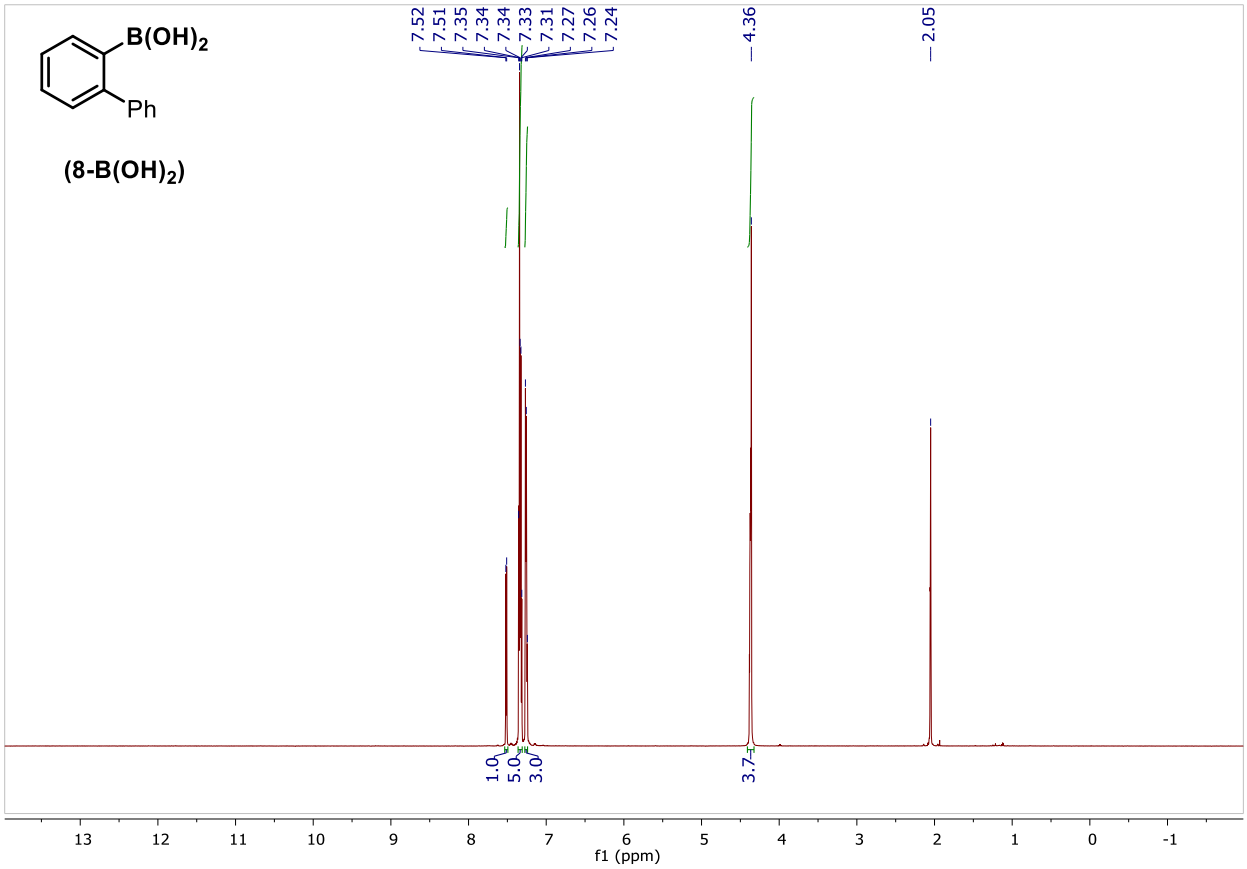
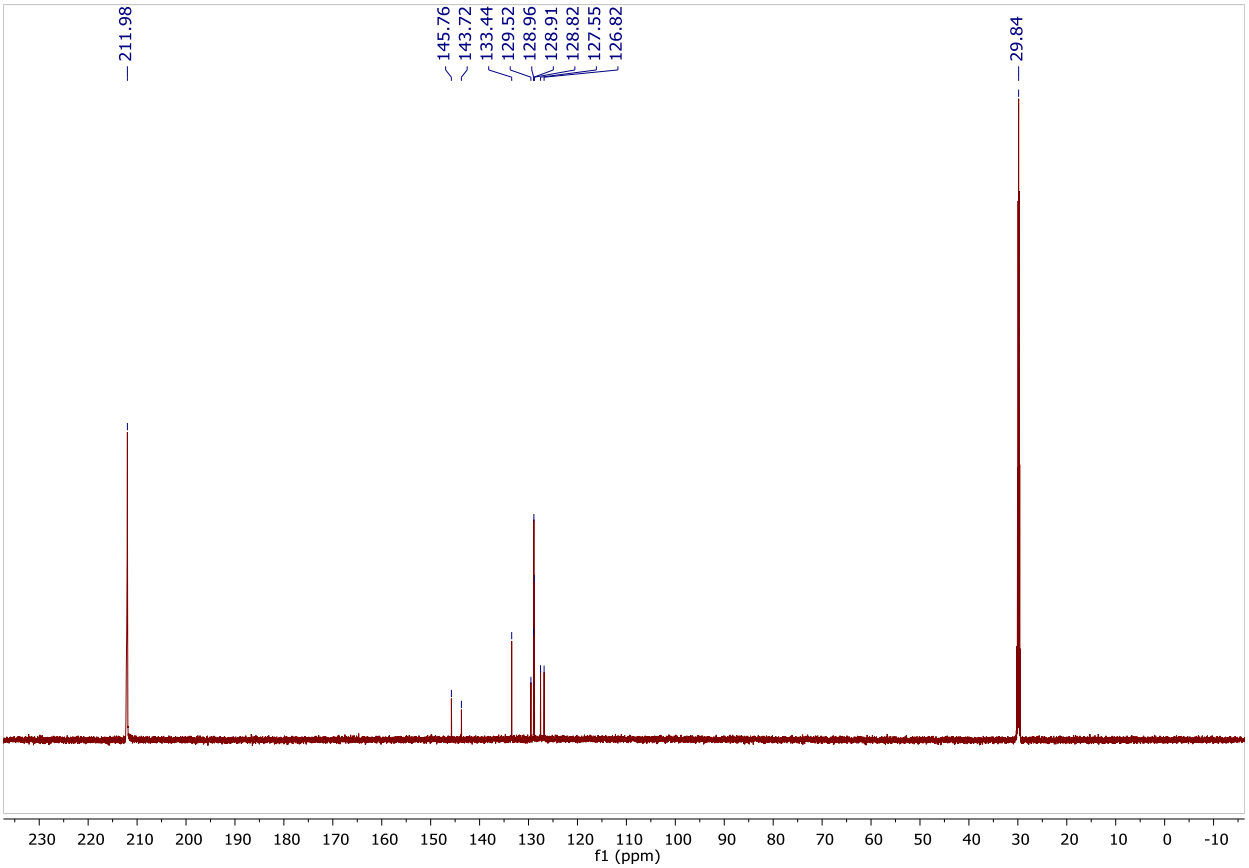
7 Spectral Data
7.1 ^{1}H, ^{13}C, ^{19}F NMR Spectra

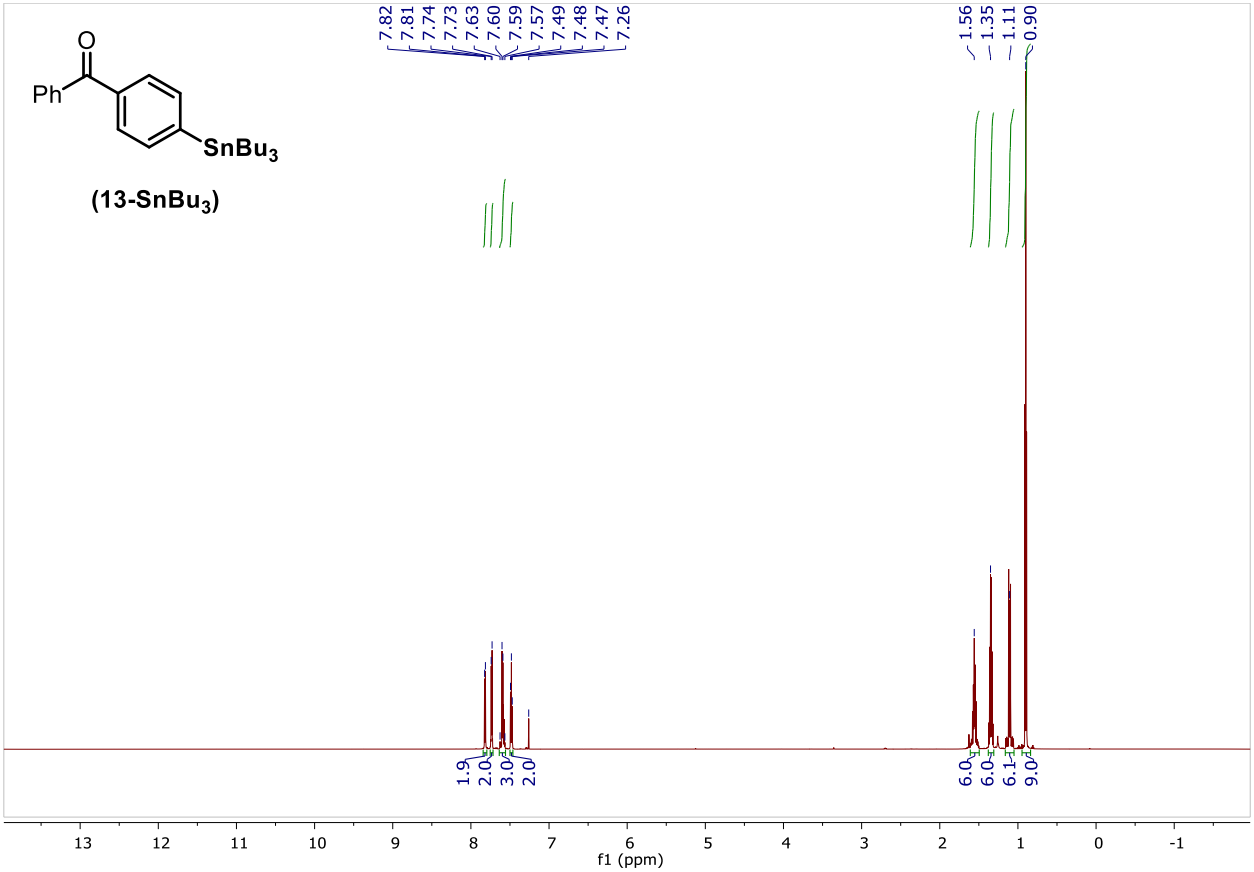
^{1}H NMR



^{13}C NMR



^{1}H NMR

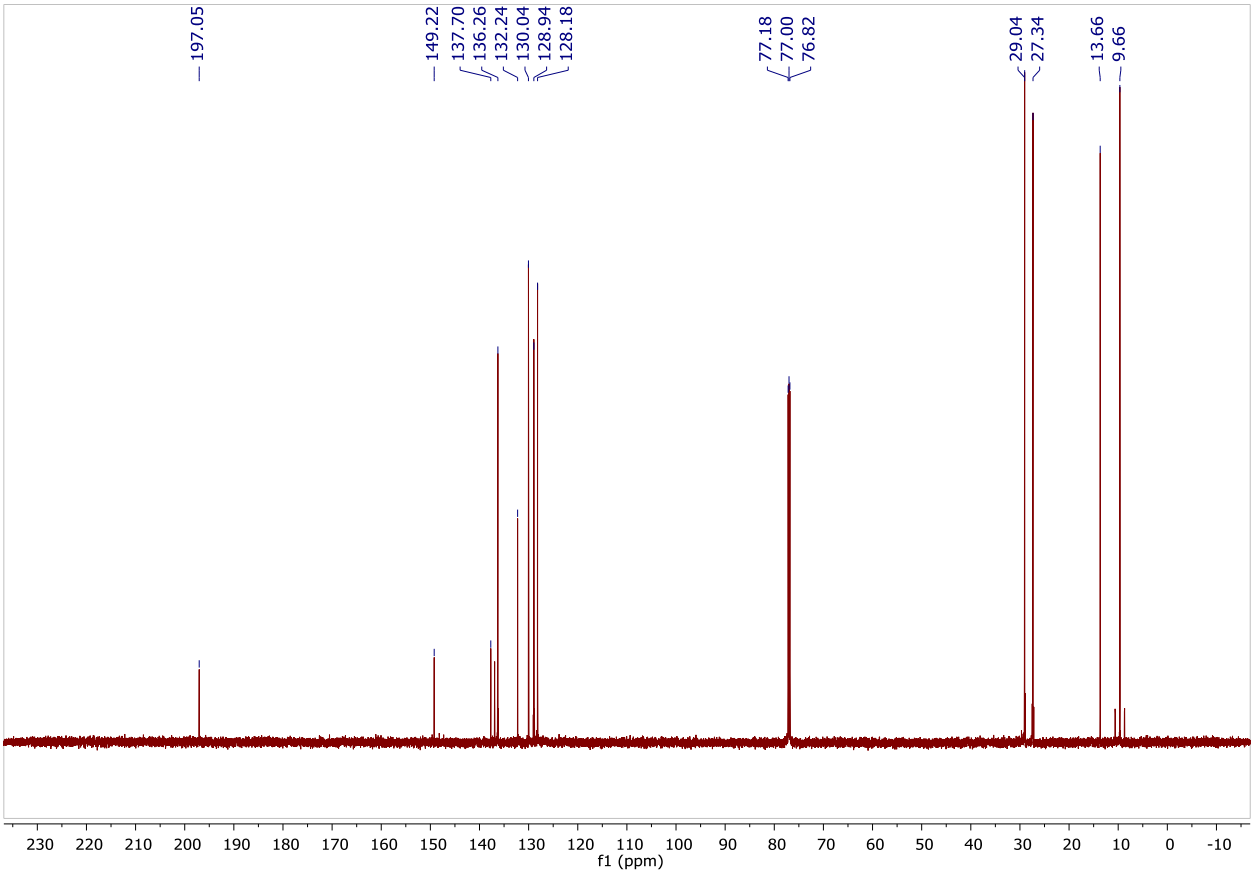


Ph

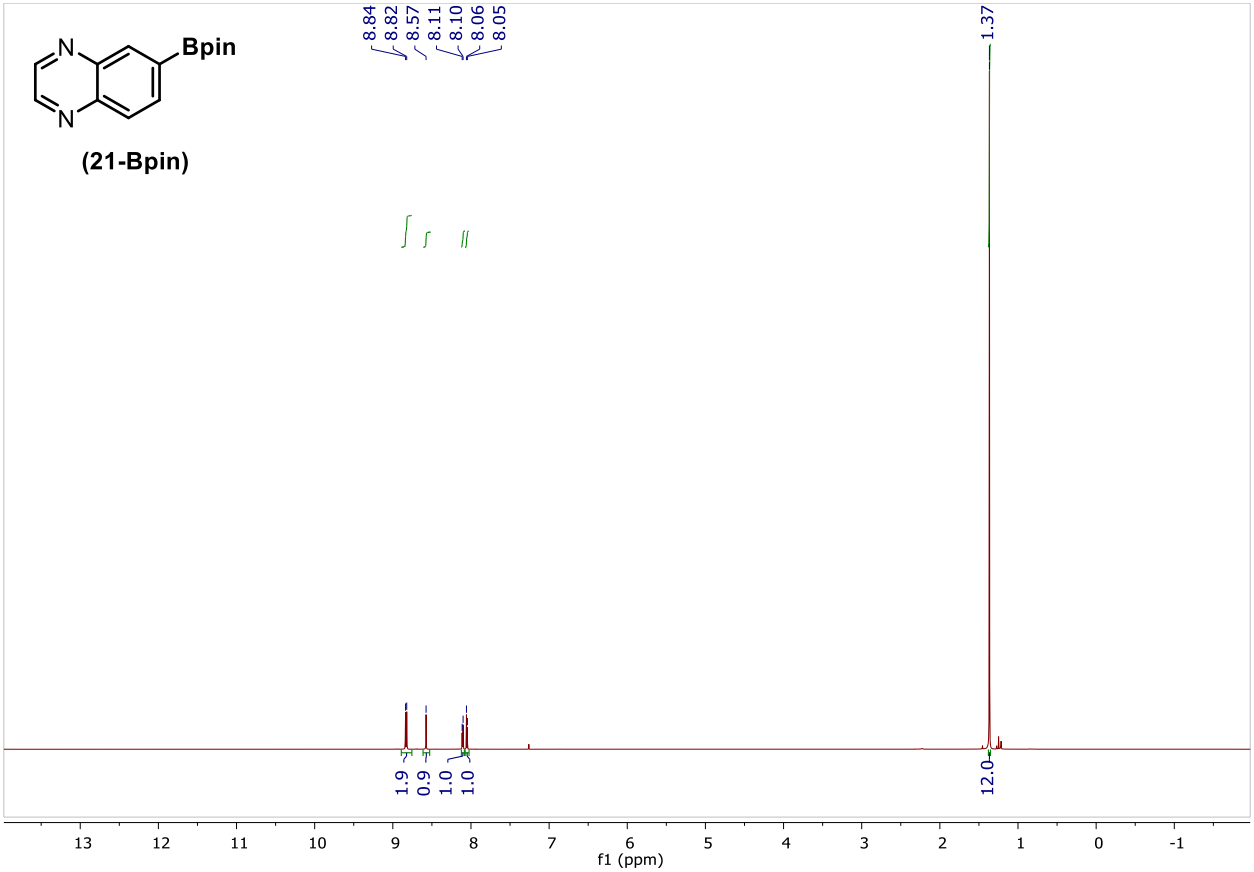
$SnBu_3$

(13-$SnBu_3$)

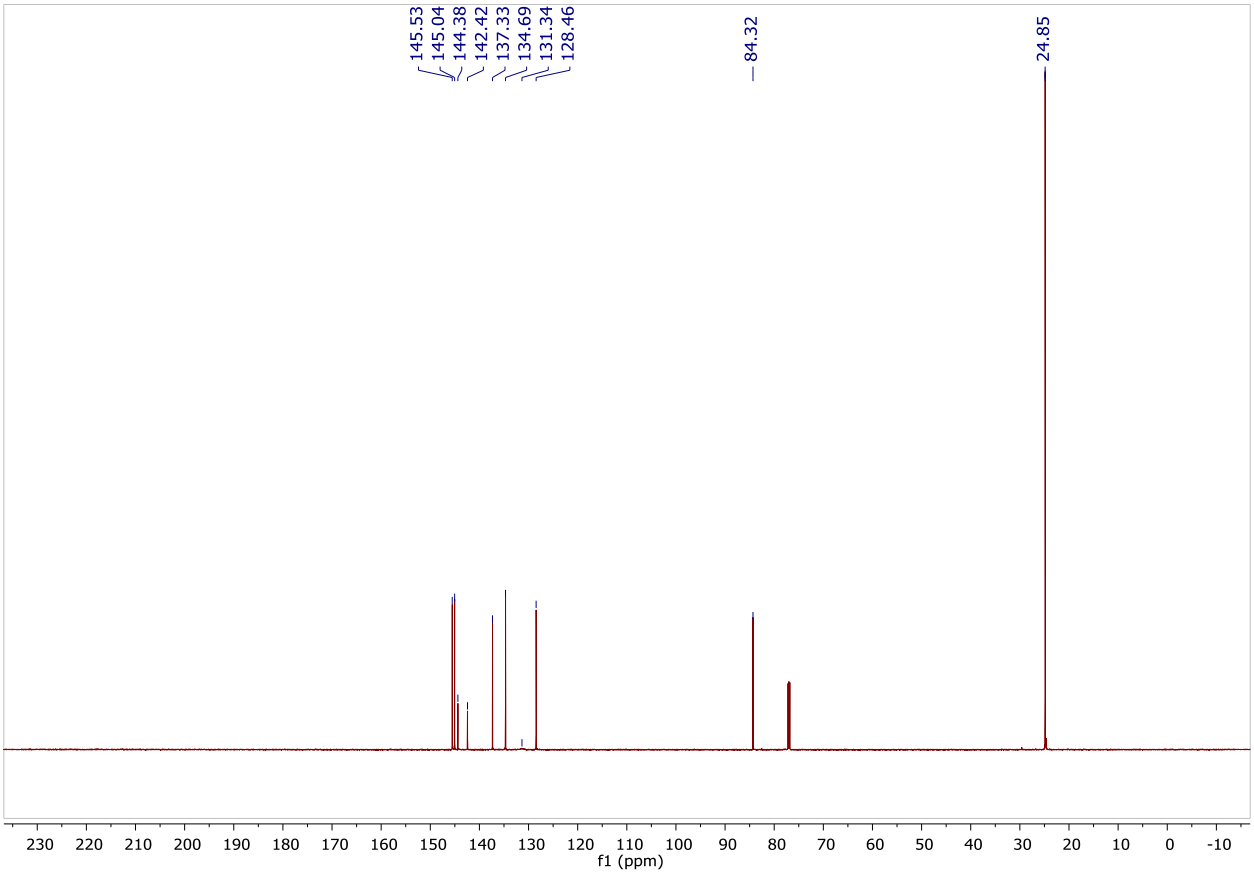
^{13}C NMR



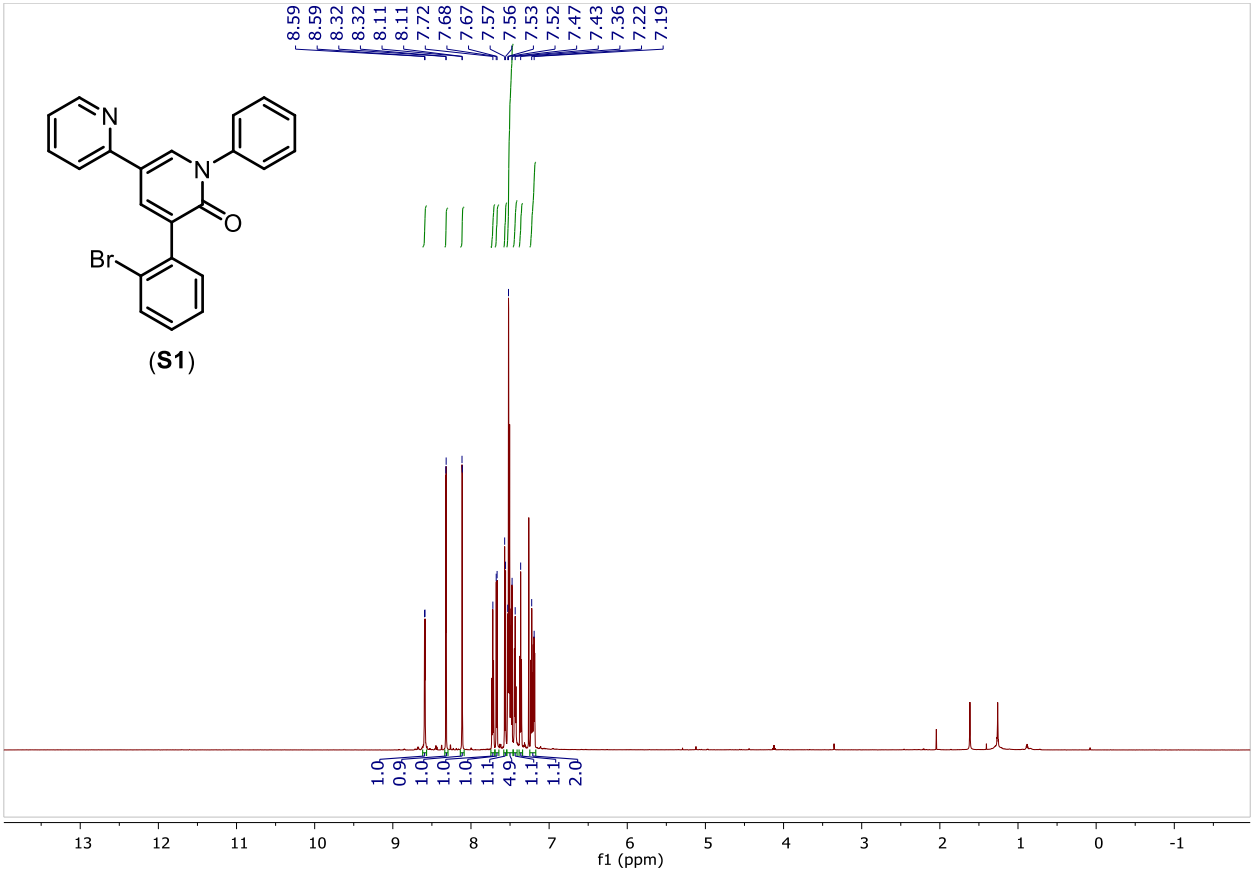
^{1}H NMR



^{13}C NMR

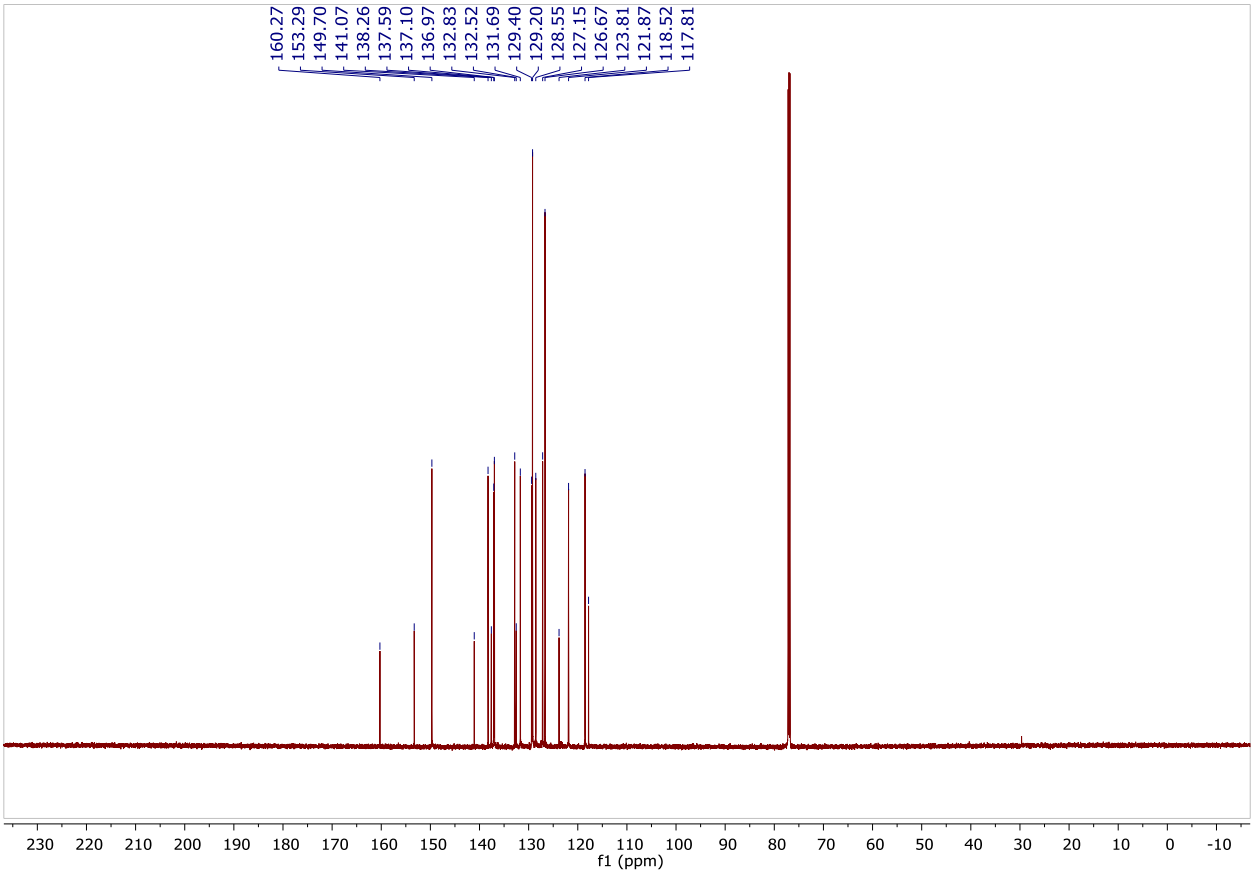


^{1}H NMR

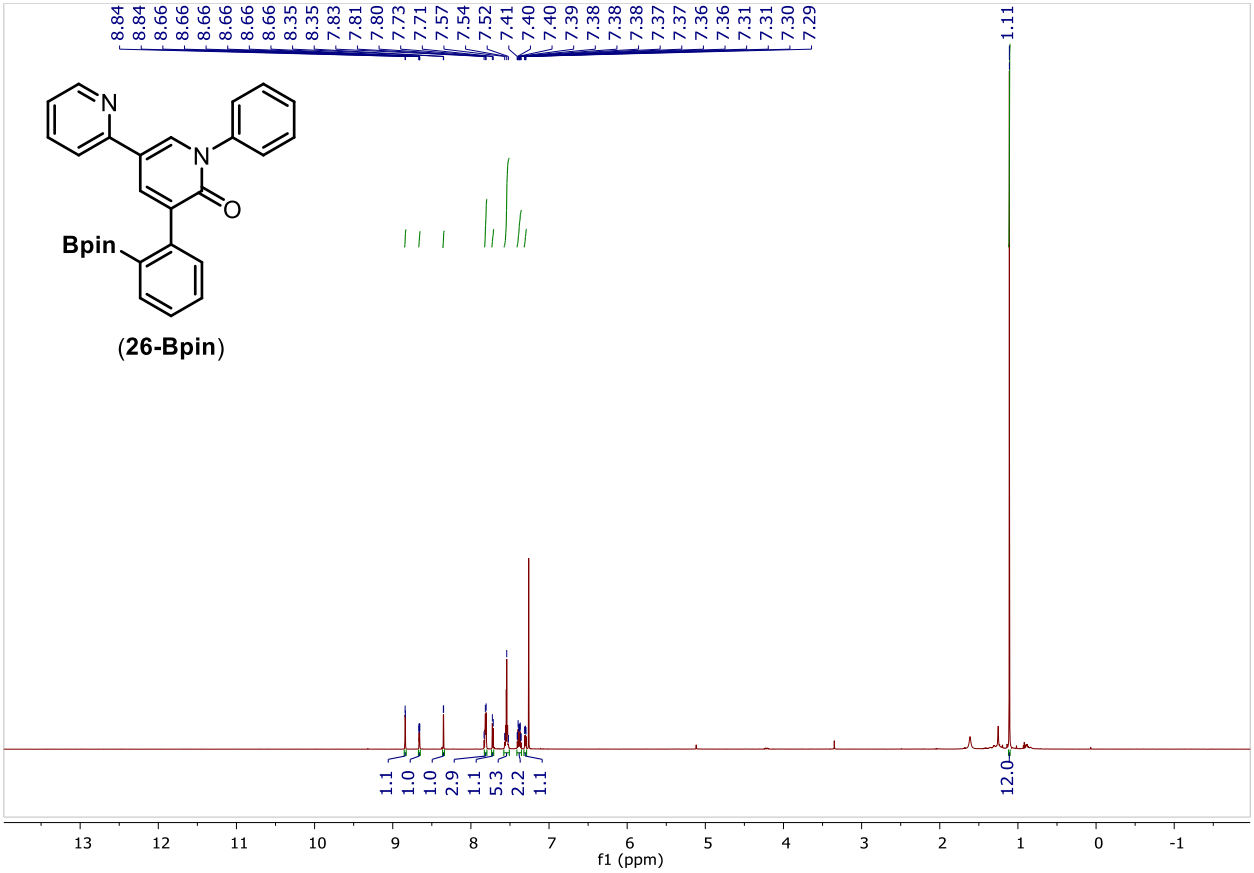


(**S1**)

^{13}C NMR

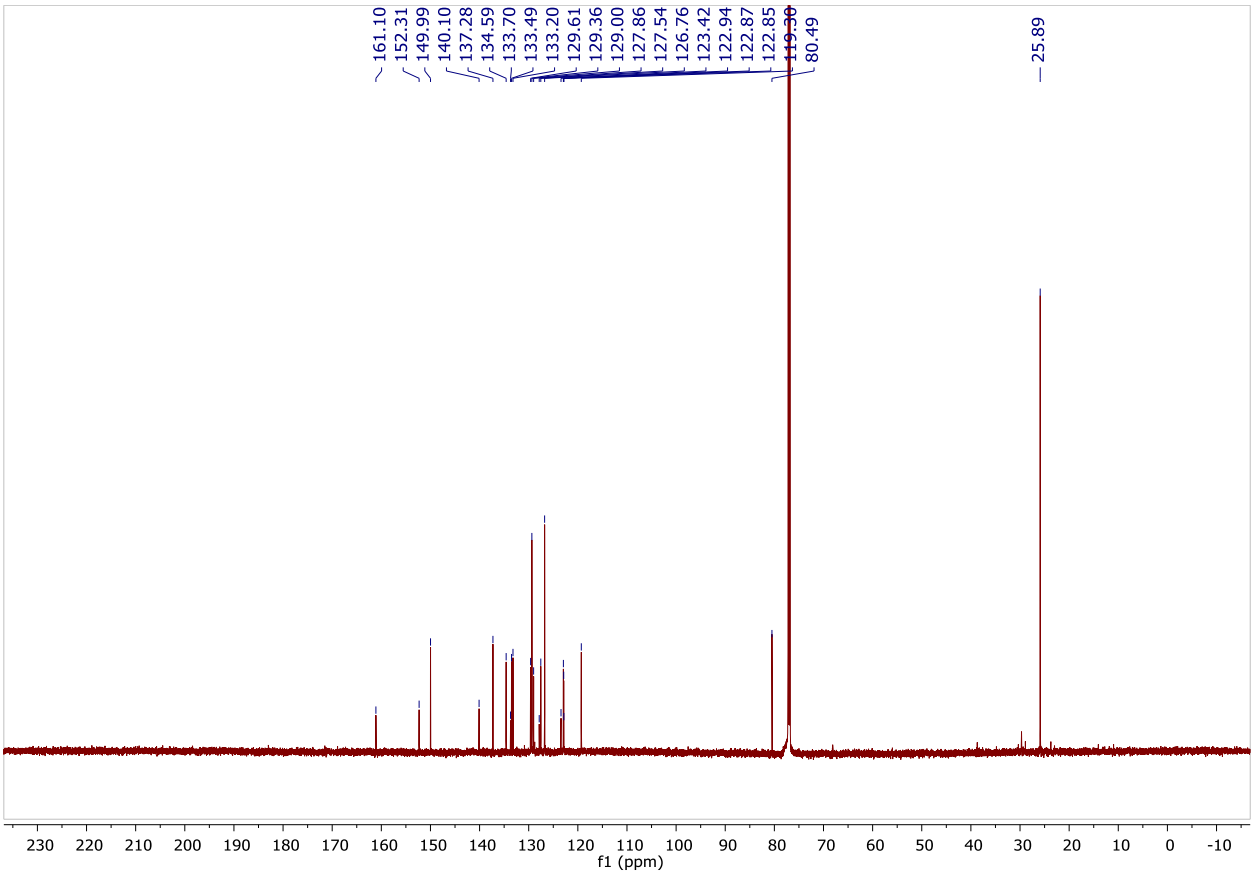


^{1}H NMR

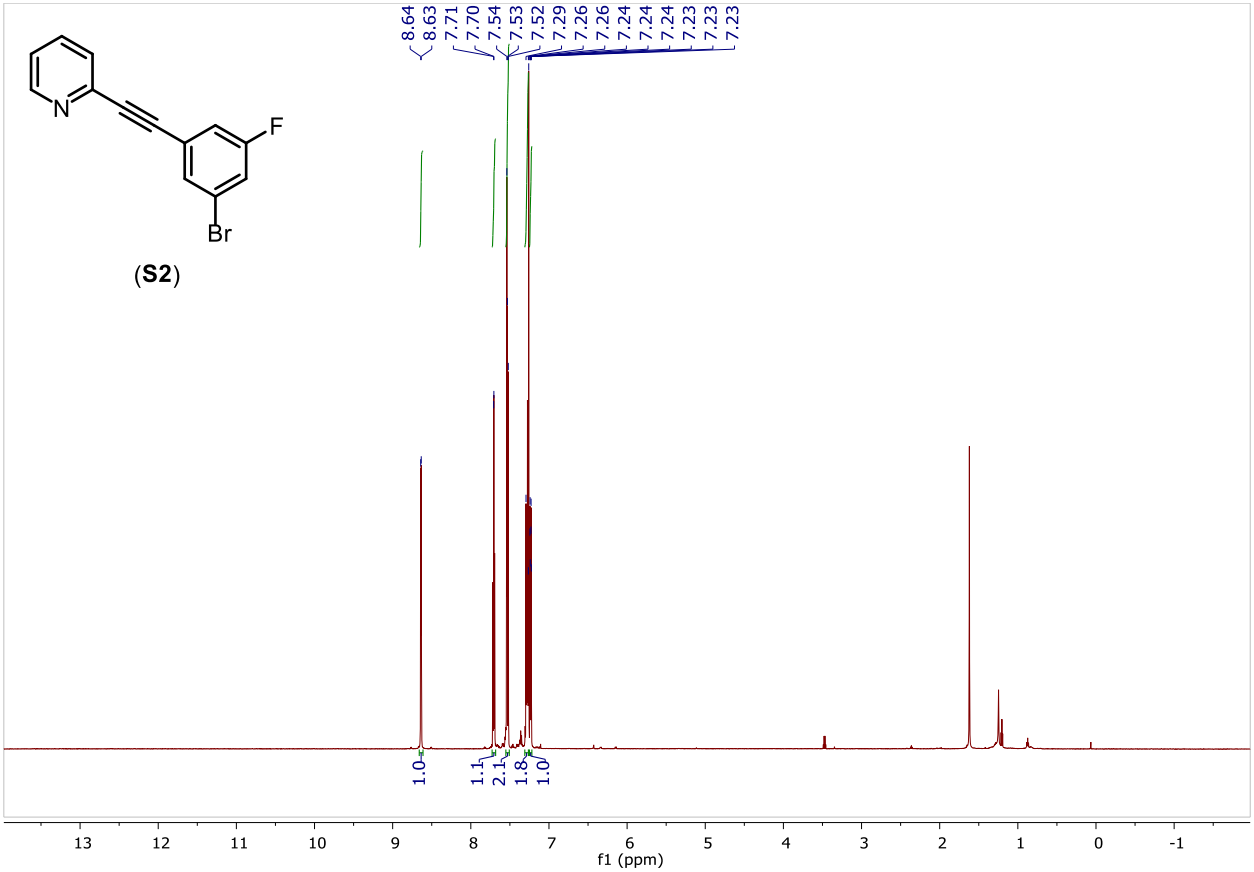


(**26-Bpin**)

^{13}C NMR

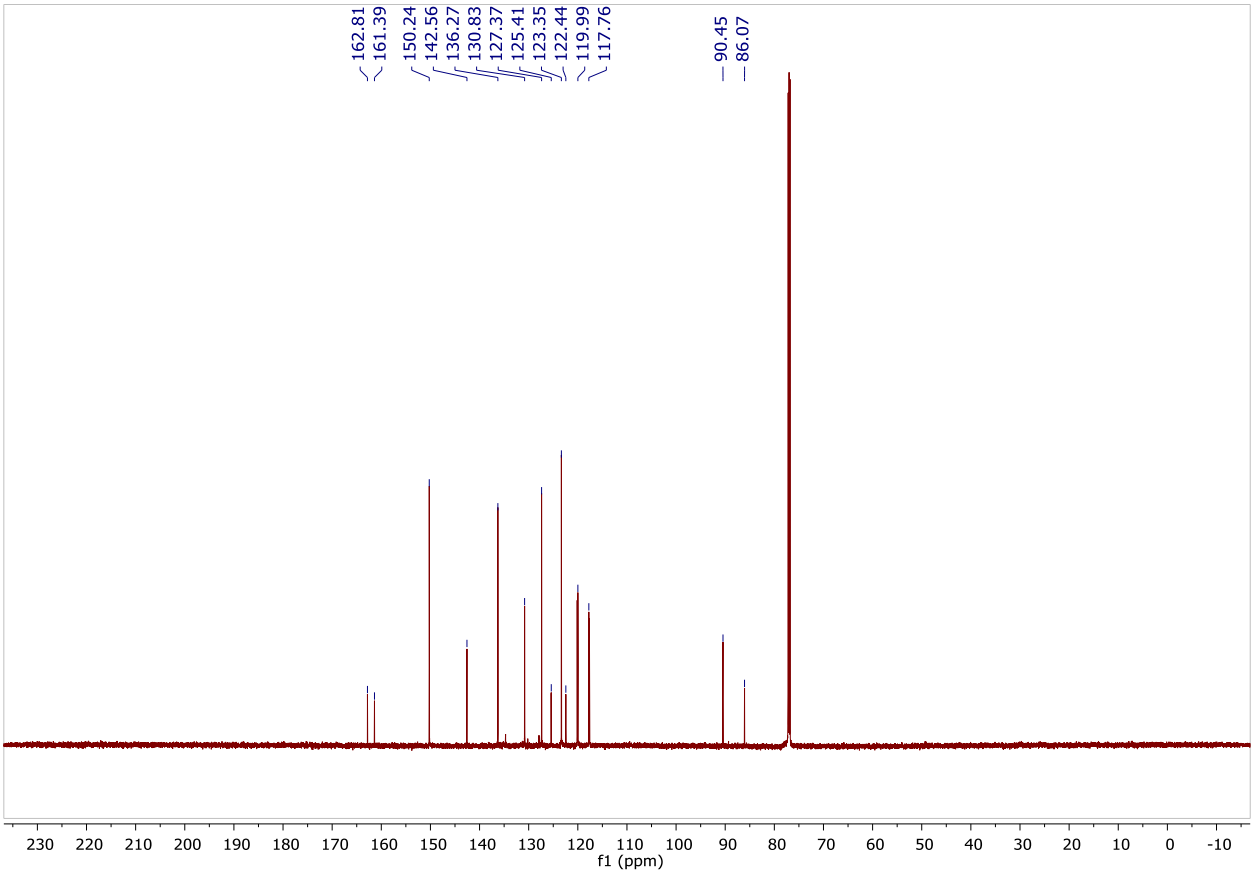


^{1}H NMR

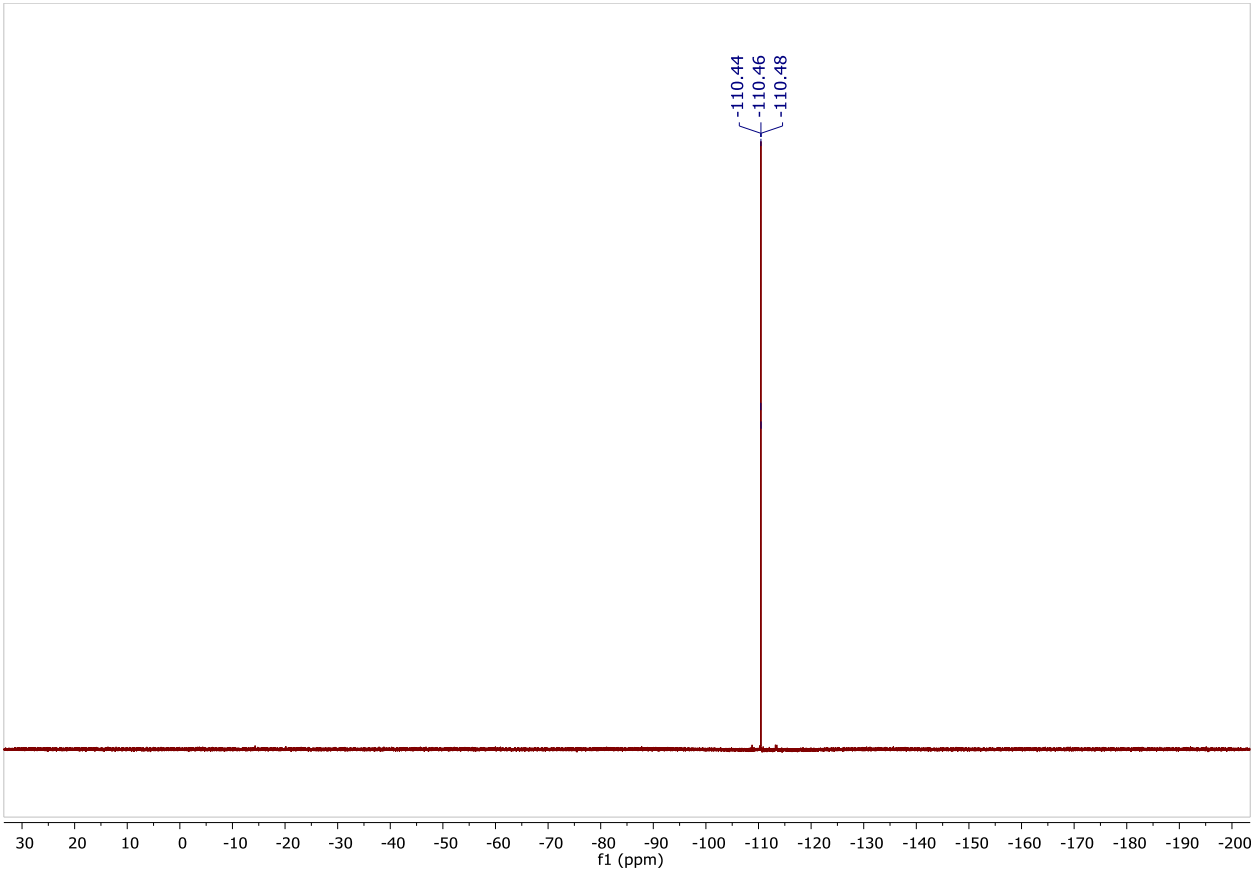


(**S2**)

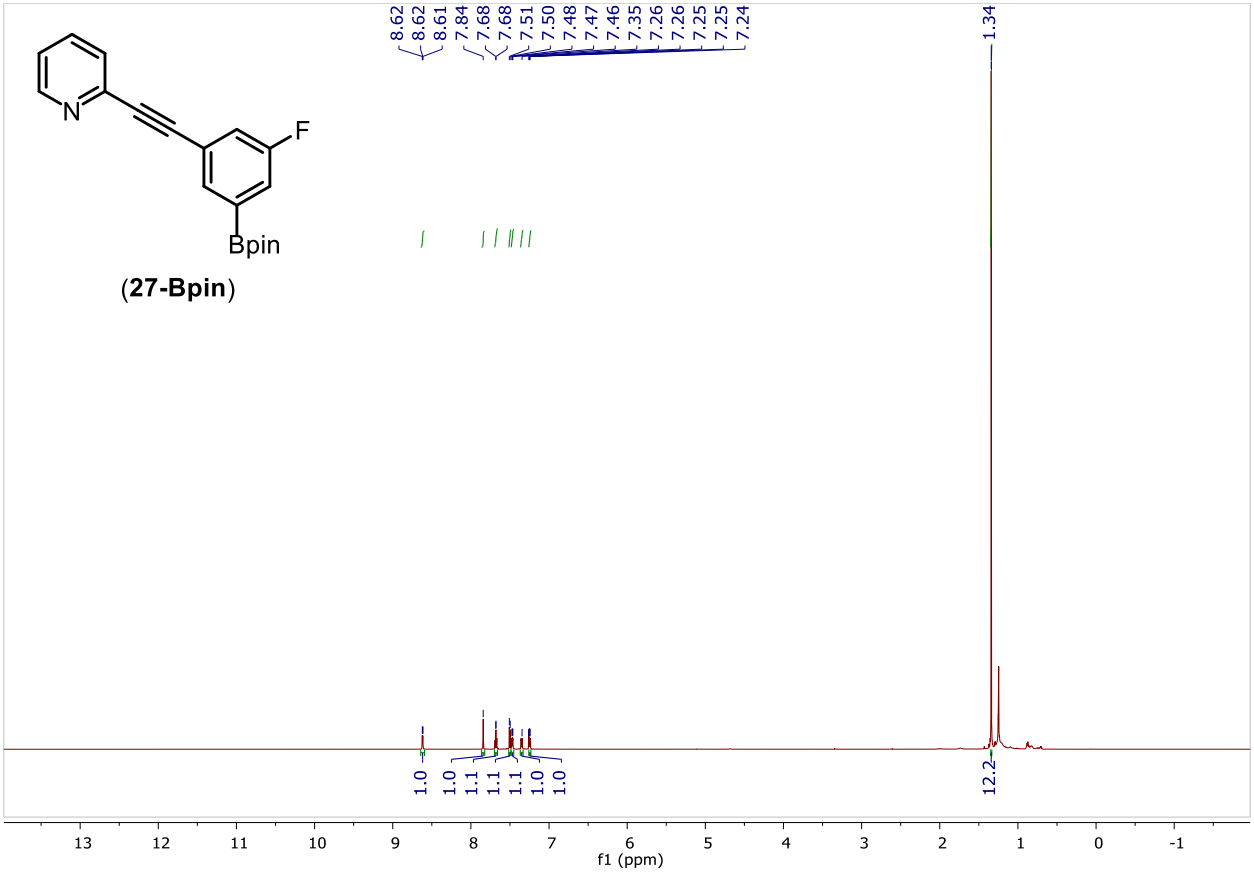
^{13}C NMR



^{19}F NMR

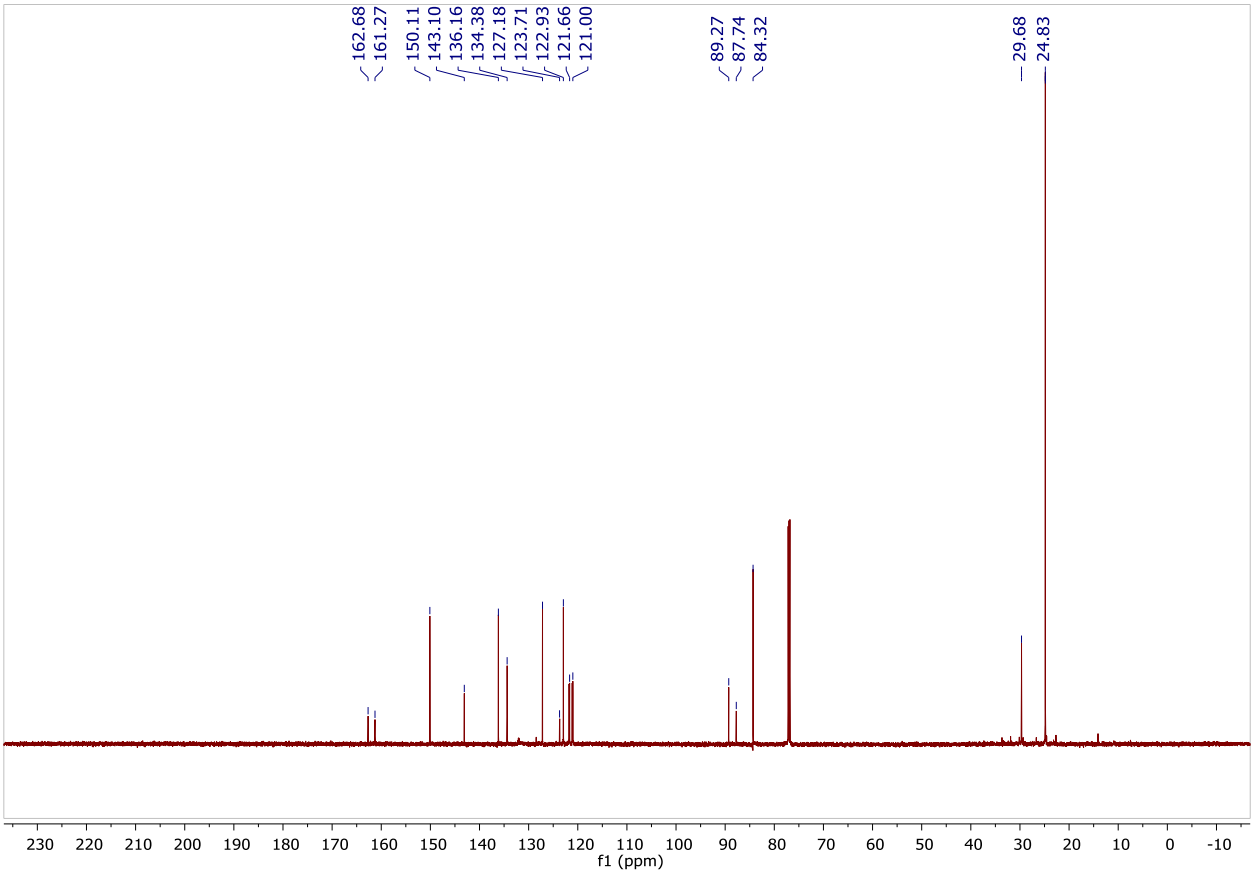

-110.44
-110.46
-110.48
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

^{1}H NMR

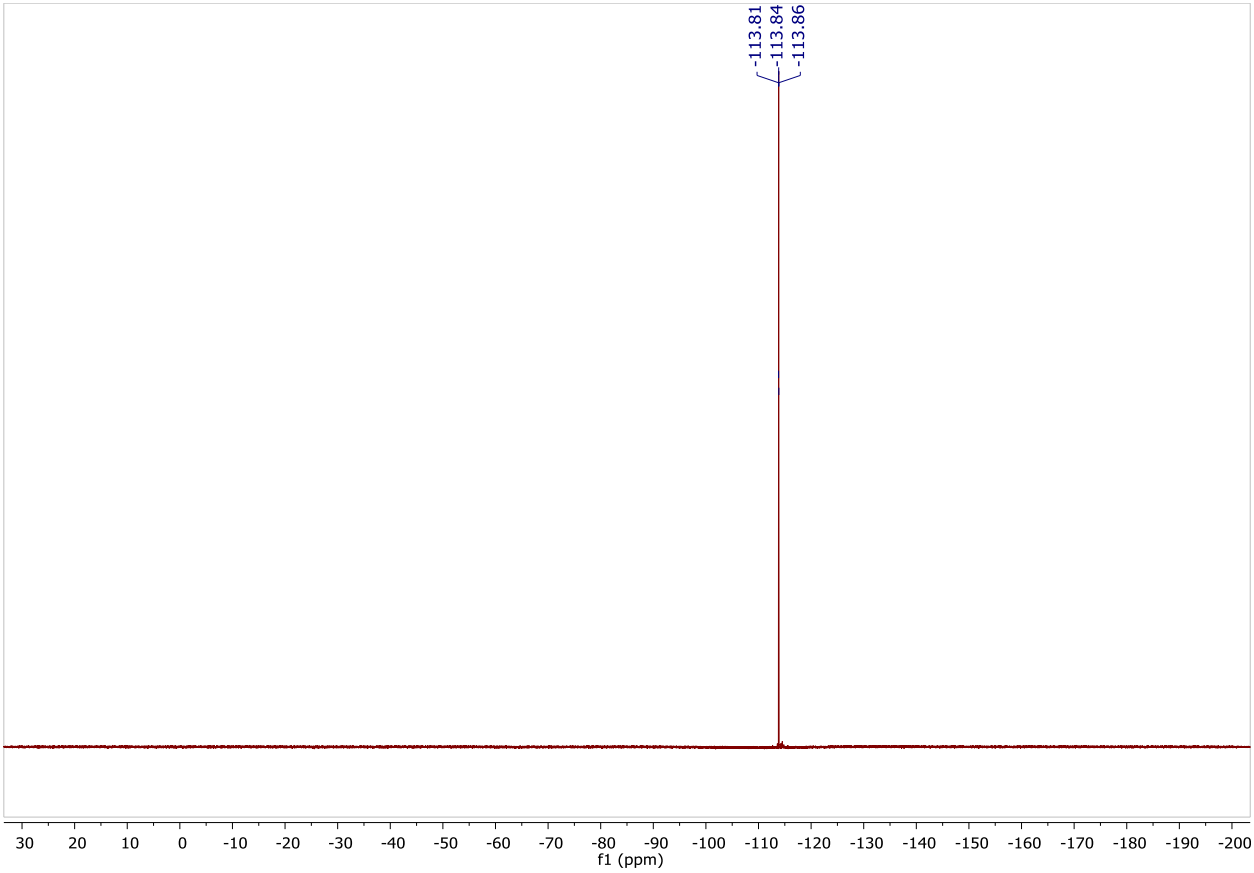


(**27-Bpin**)

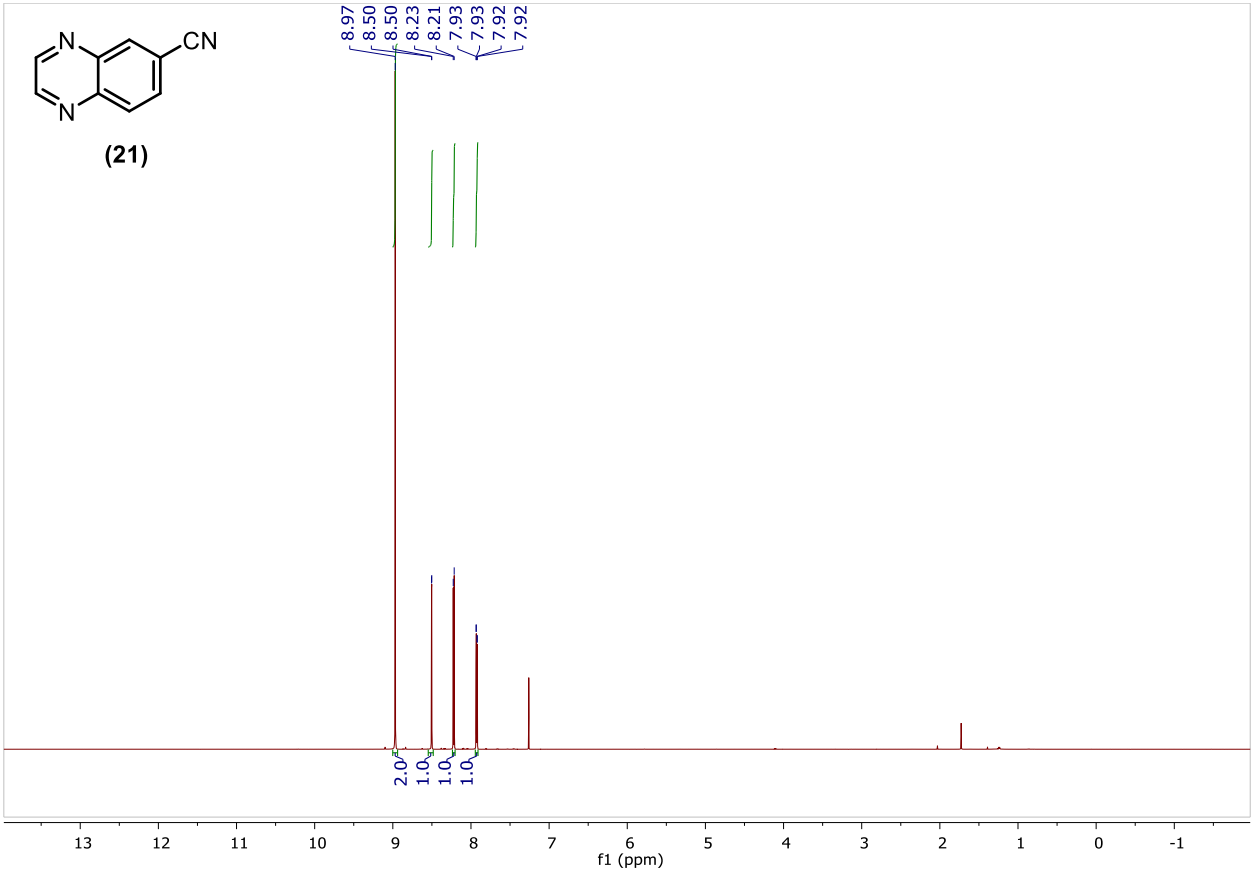
^{13}C NMR



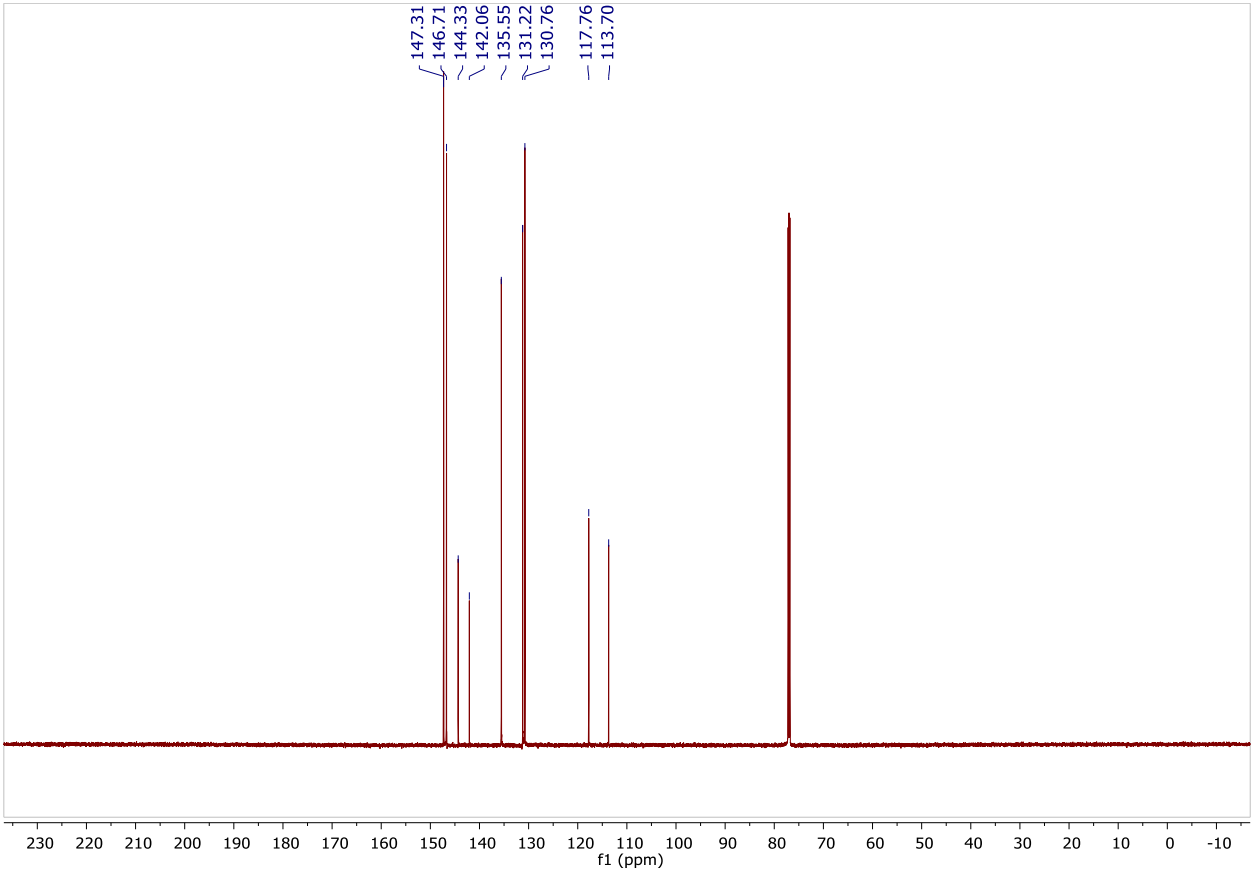
^{19}F NMR


-113.81
-113.84
-113.86
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

^{1}H NMR

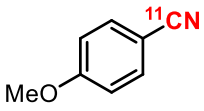


^{13}C NMR



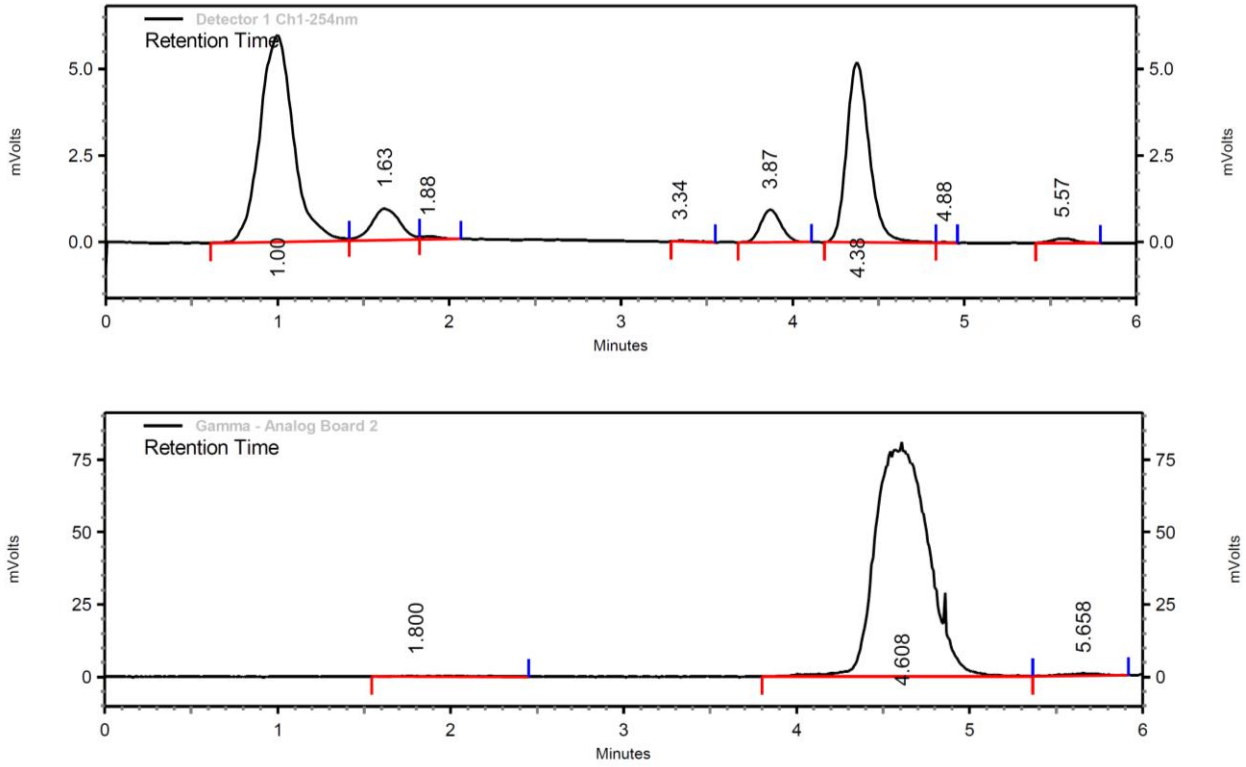
7.2 Radio-HPLC/Radio-TLC Analysis for ^{18}F-Labeled Compounds

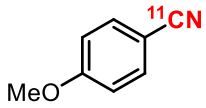
As a way to confirm the identity of the radiolabeled substrate, a HPLC co-injection of the crude reaction mixture with an aliquot of the authentic product was performed. The two HPLC traces presented, show the RAD and UV trace (254 nm or 280 nm) from the crude reaction mixture spiked with an authentic standard of the product. The wavelength shown is the wavelength where the analyte compound exhibited greatest absorptivity. Because of the physical separation of the two detectors, the two traces are offset by 0.2 min. HPLC conditions are from Section 5.4.



([^{11}C]1)

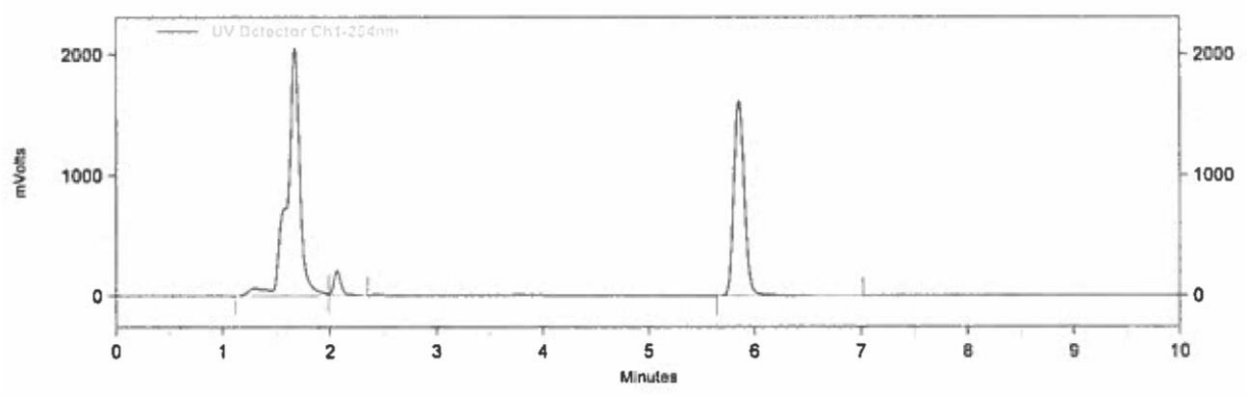
HPLC Conditions: A
Starting material: **1-SnBu$_3$**

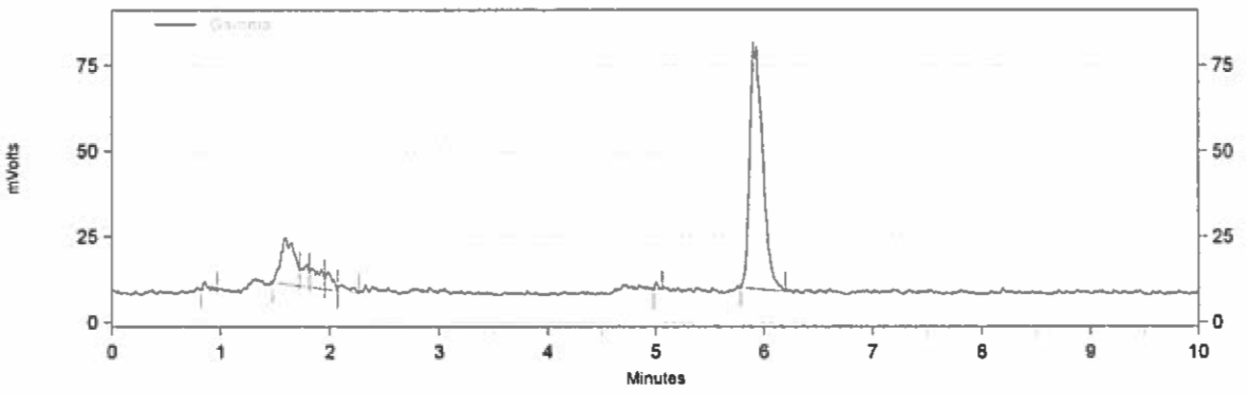


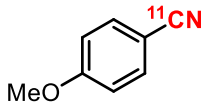


([^{11}C]1)

HPLC Conditions: A
Starting material: **1-B(OH)$_2$**

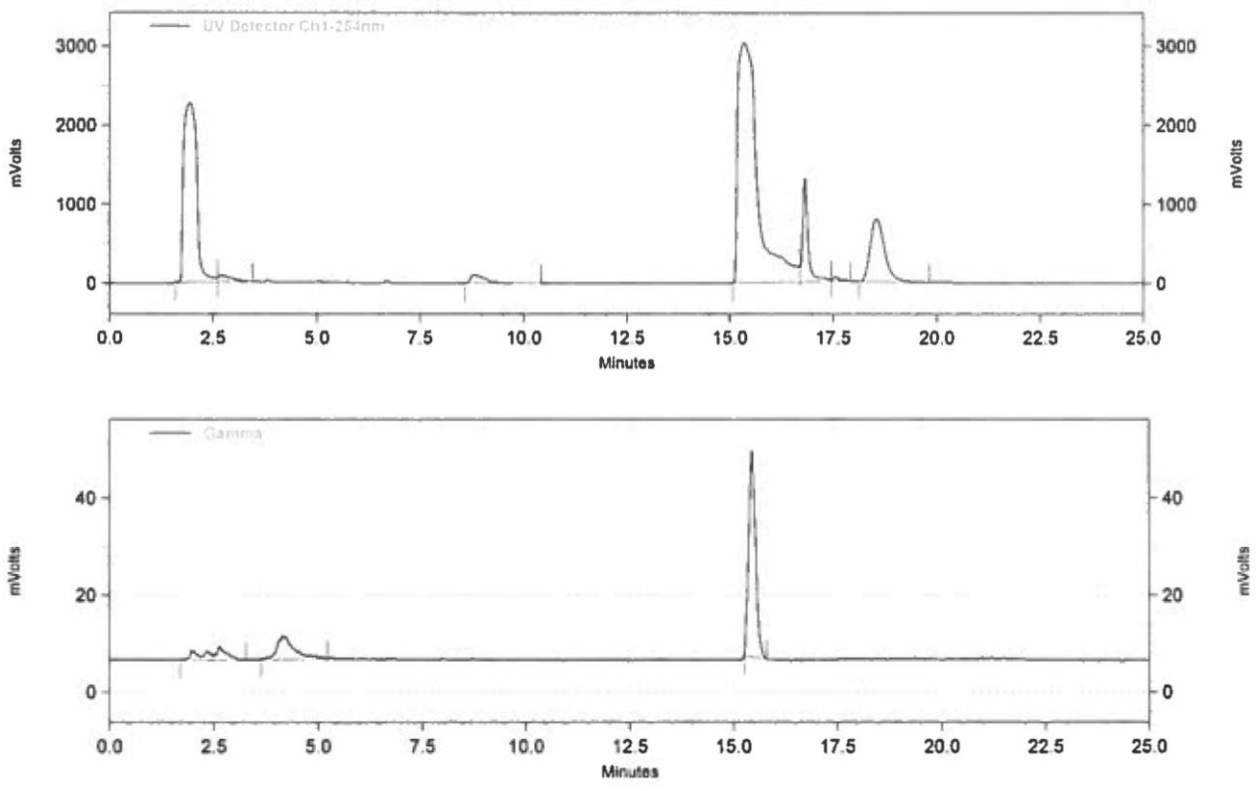


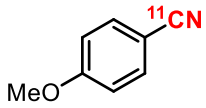




([^{11}C]1)

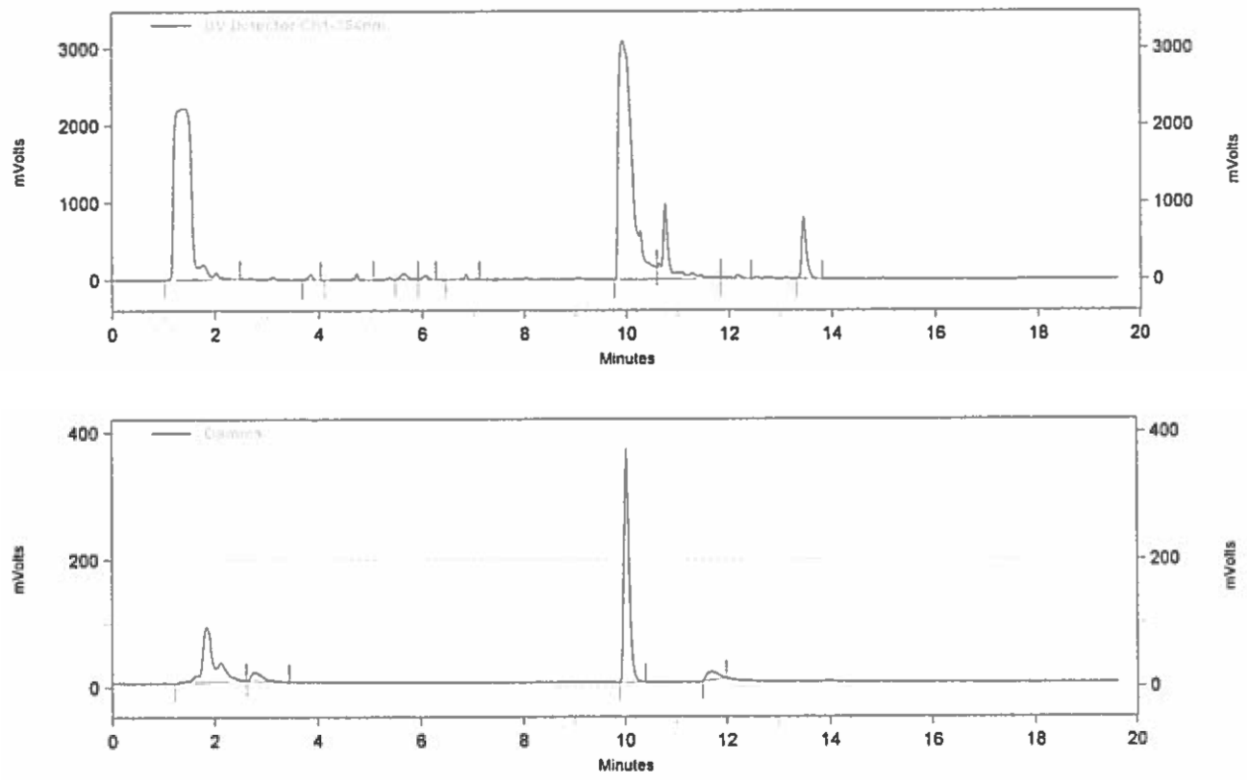
HPLC Conditions: A
Starting material: **1-BF_3K**

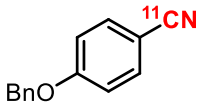




([^{11}C]1)

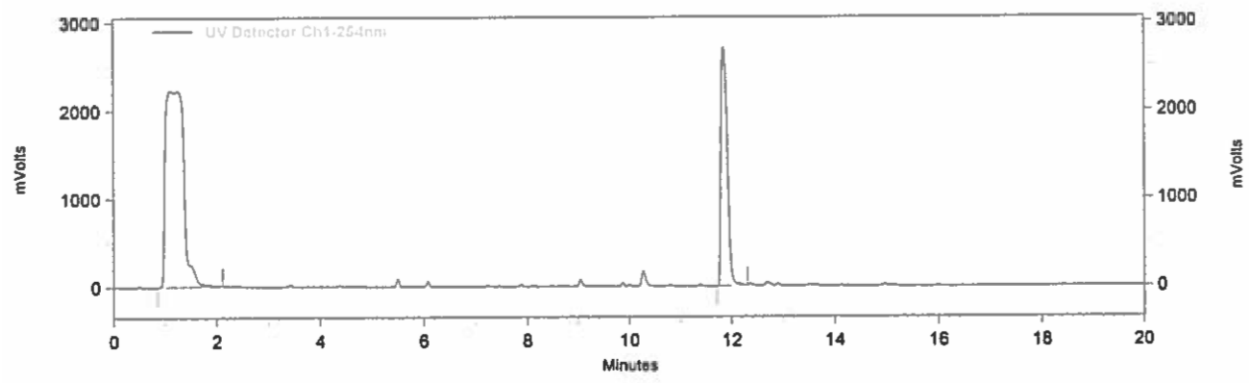
HPLC Conditions: A
Starting material: **1-Bpin**

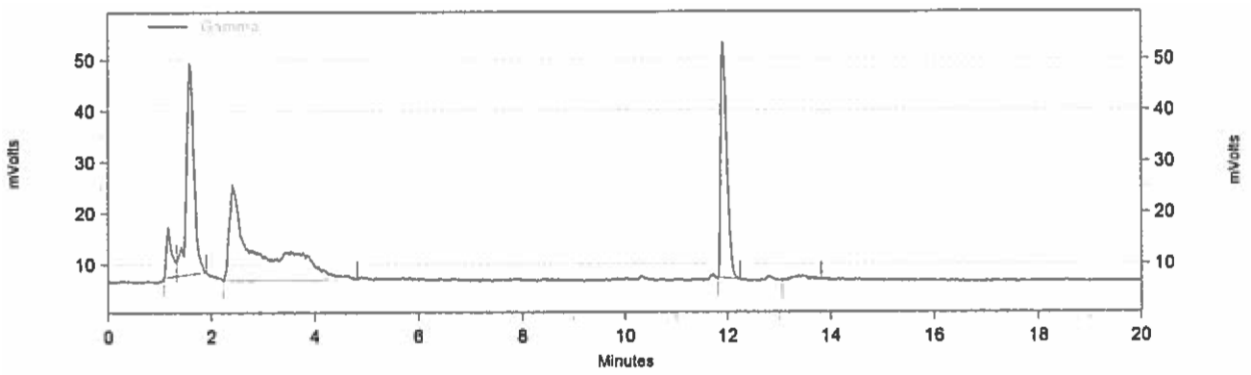


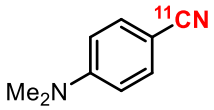


([^{11}C]2)

HPLC Conditions: A
Starting material: **2-SnBu$_3$**

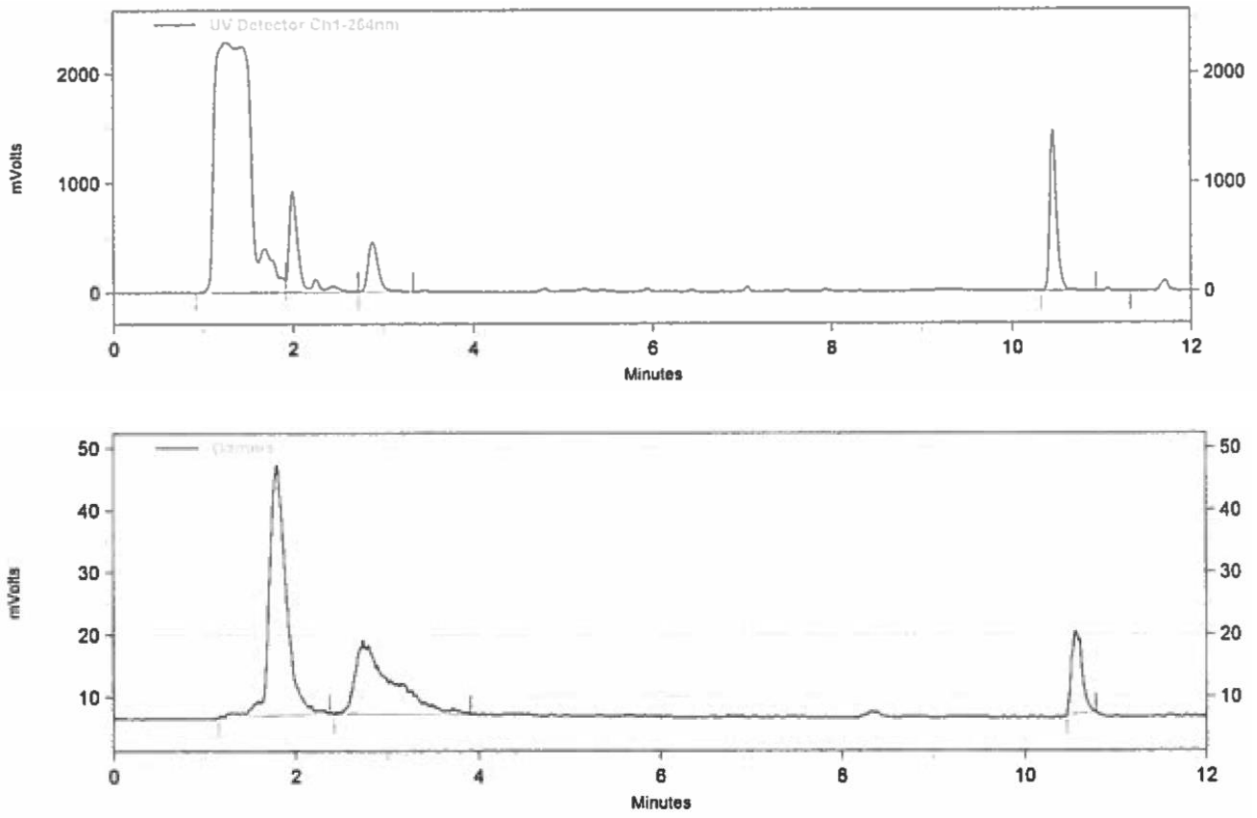


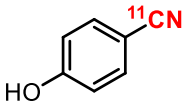




([^{11}C]3)

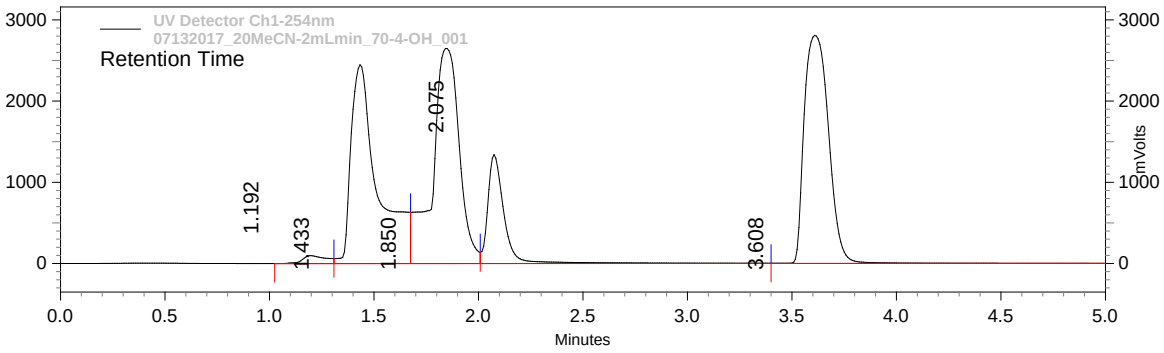
HPLC Conditions: A
Starting material: **3-SnBu$_3$**

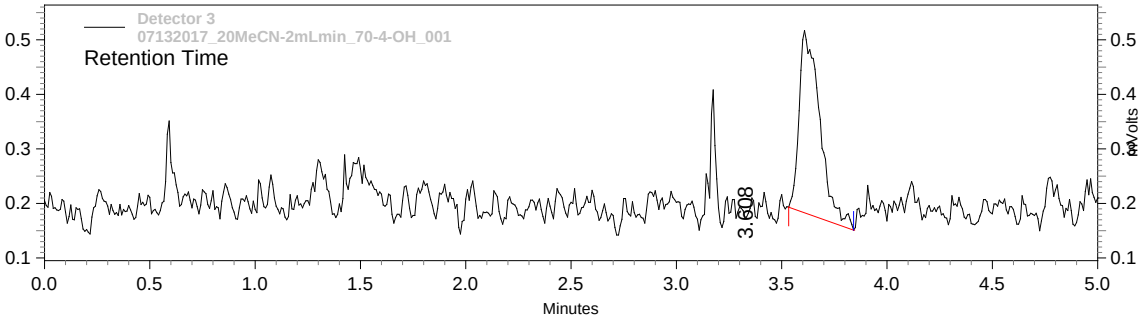


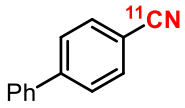


([^{11}C]4)

HPLC Conditions: A
Starting material: **4-B(OH)$_2$**

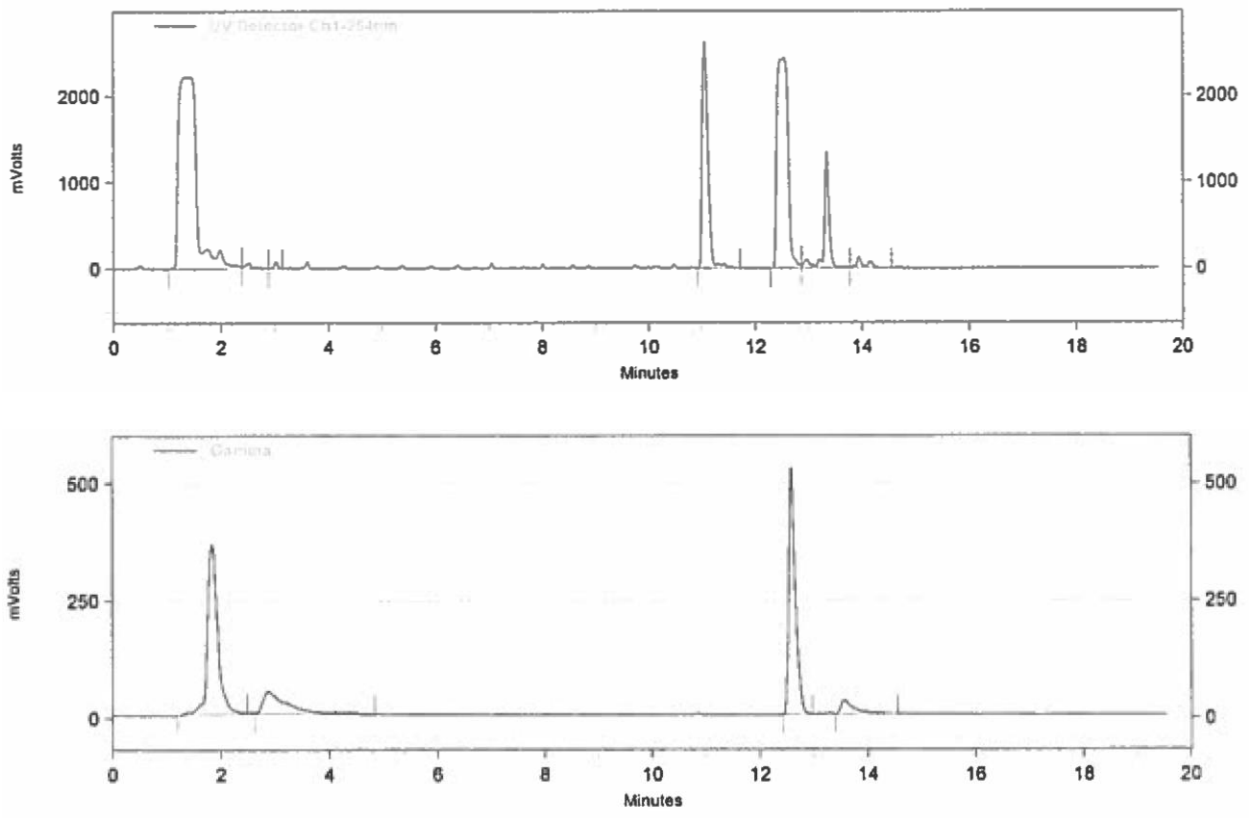


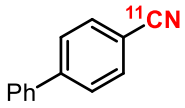




([^{11}C]5)

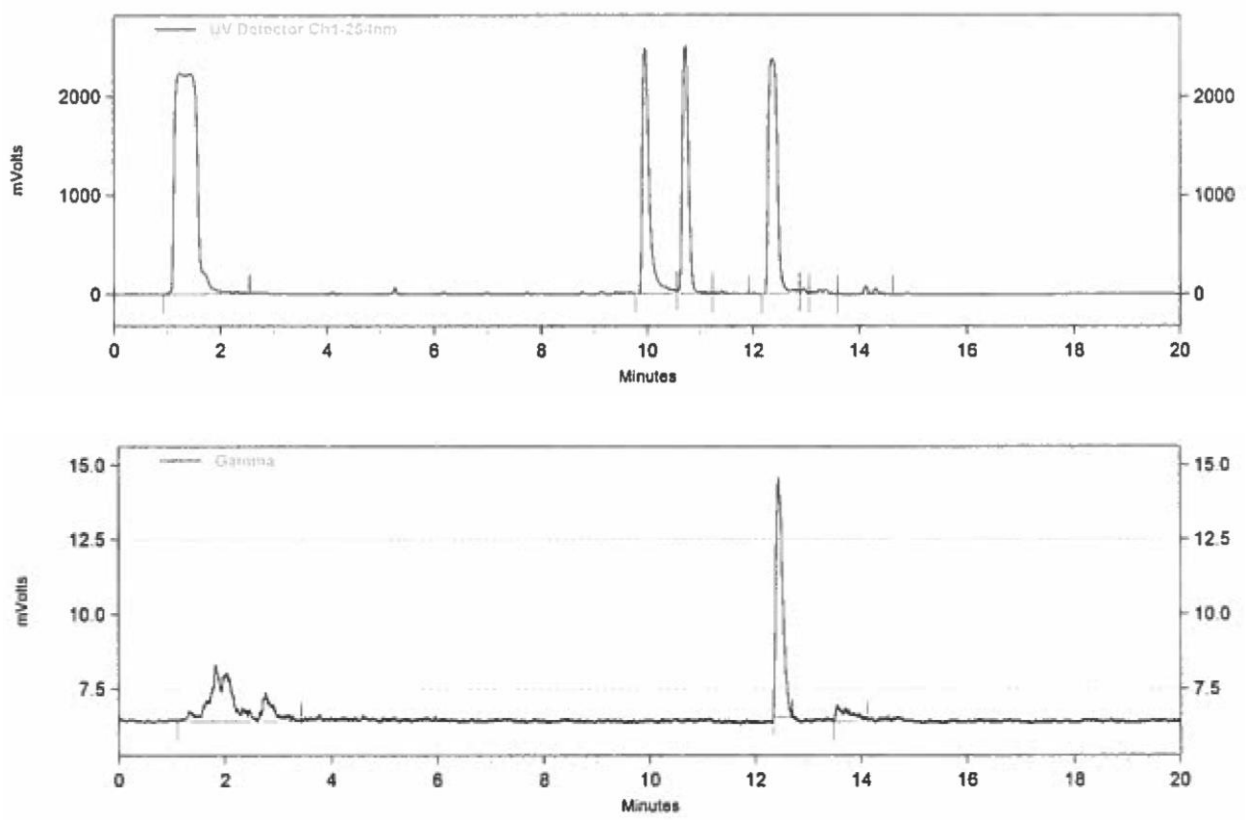
HPLC Conditions: A
Starting material: **5-SnBu$_3$**

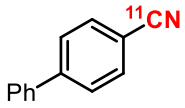




([^{11}C]5)

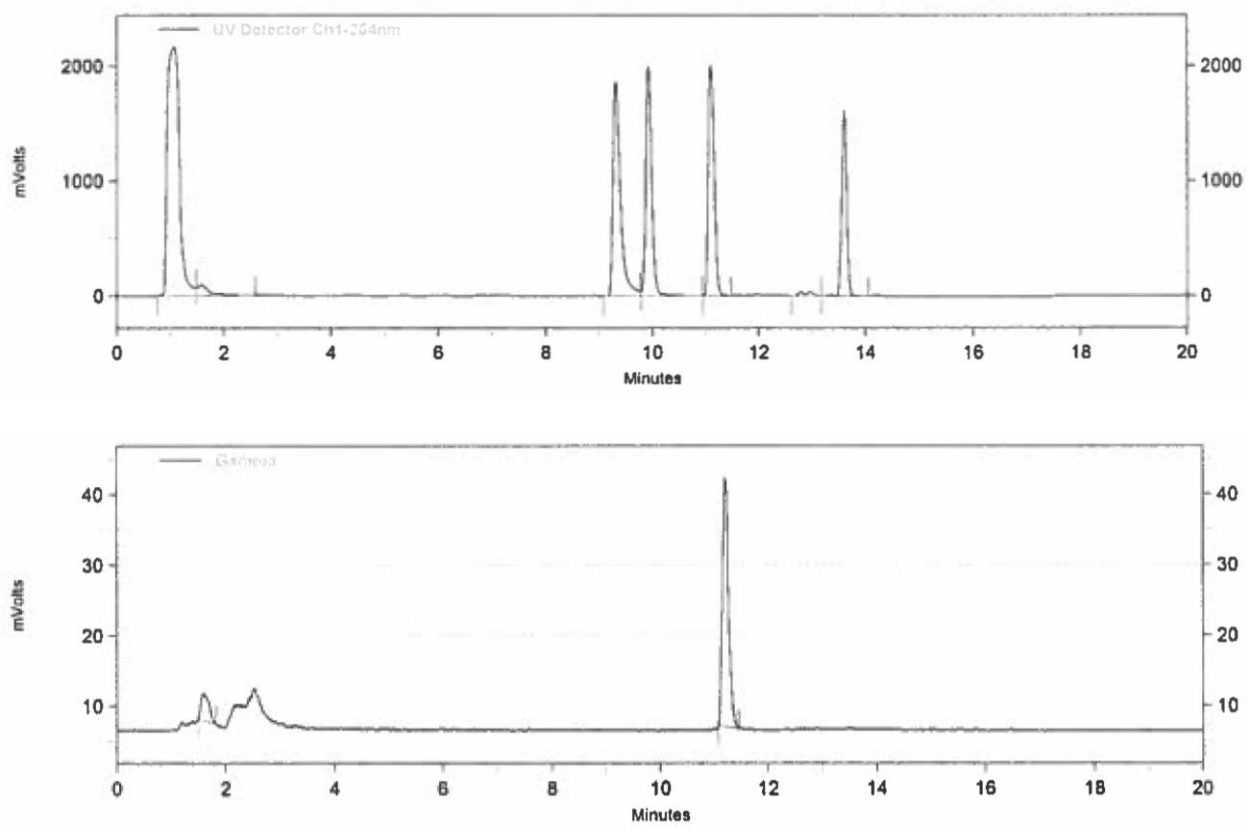
HPLC Conditions: A
Starting material: **5-B(OH)$_2$**

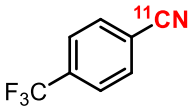




([^{11}C]5)

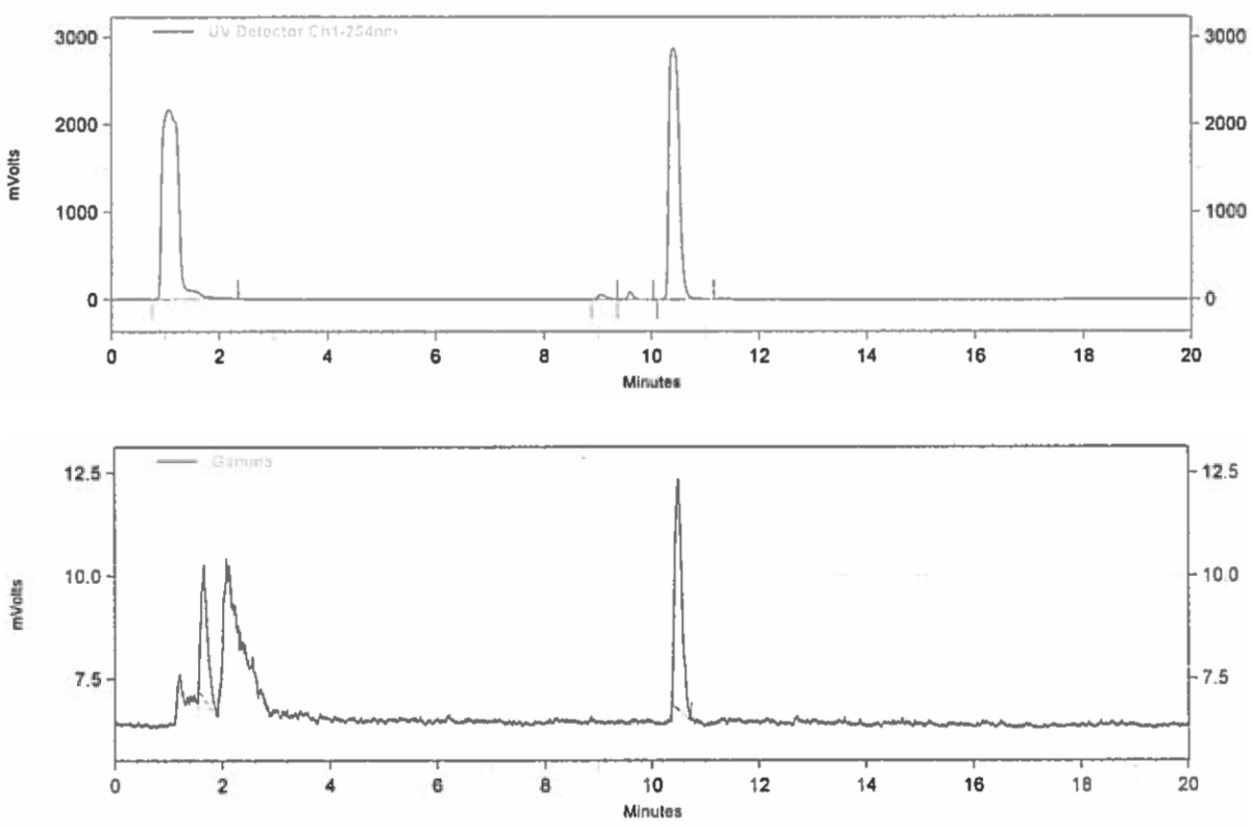
HPLC Conditions: A
Starting material: **5-Bpin**

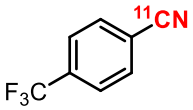




([^{11}C]6

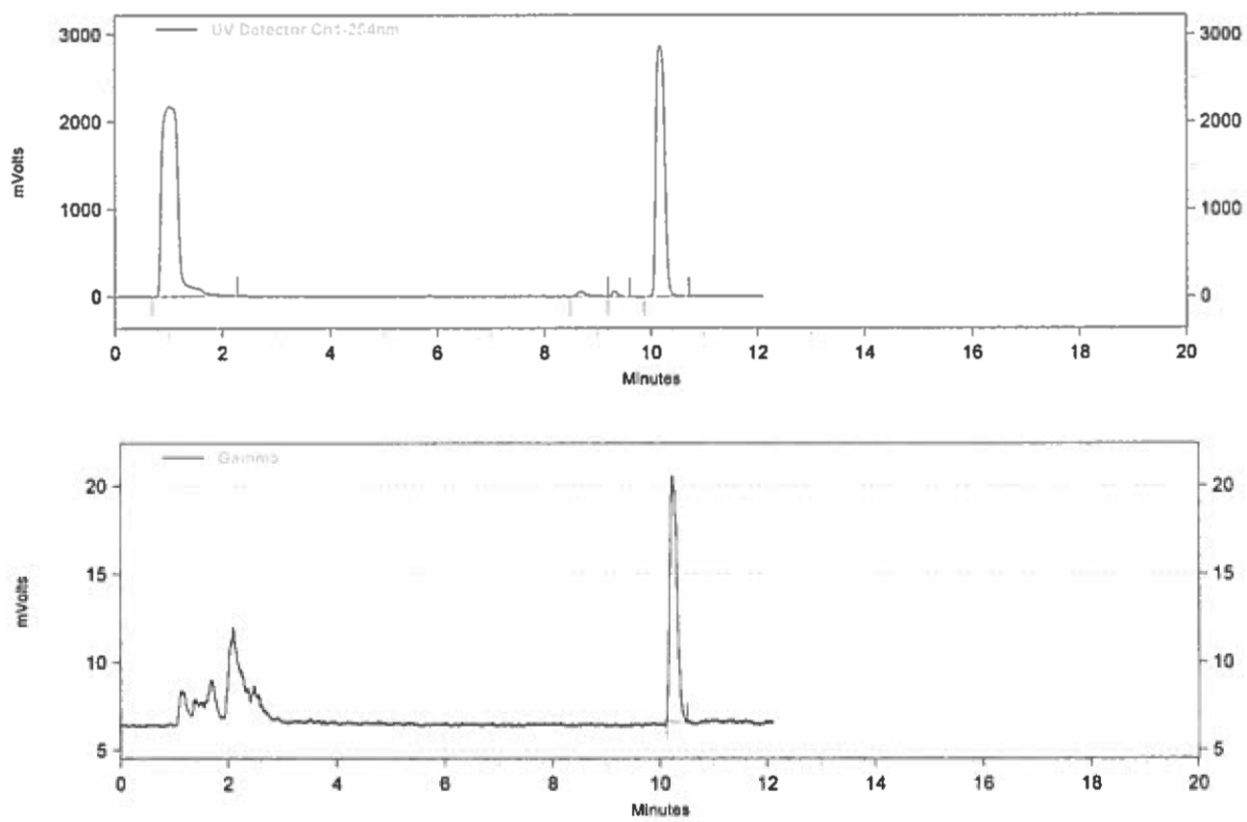
HPLC Conditions: A
Starting material: **6-B(OH)$_2$**

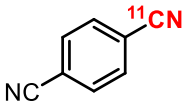




([^{11}C]6

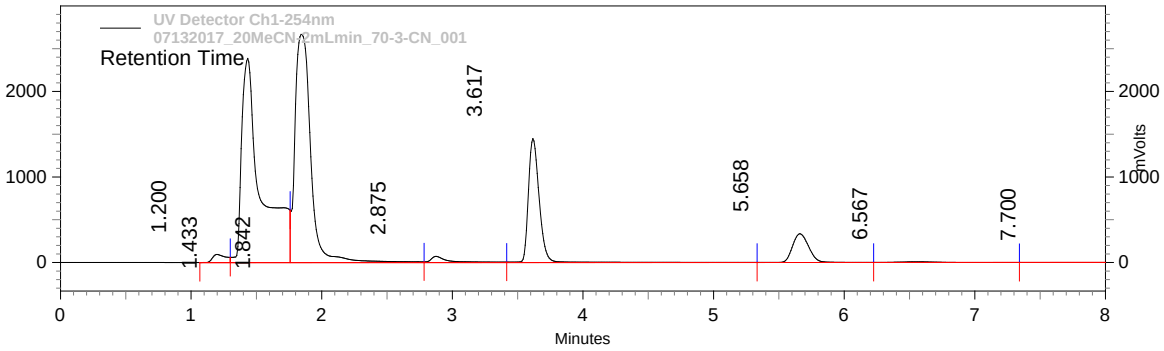
HPLC Conditions: A
Starting material: **6-BF_3K**

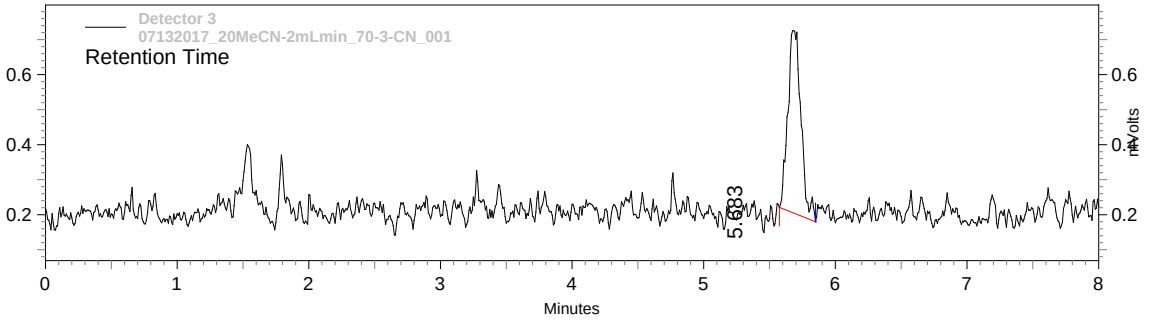


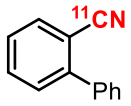


([^{11}C]7)

HPLC Conditions: A
Starting material: **7-B(OH)$_2$**

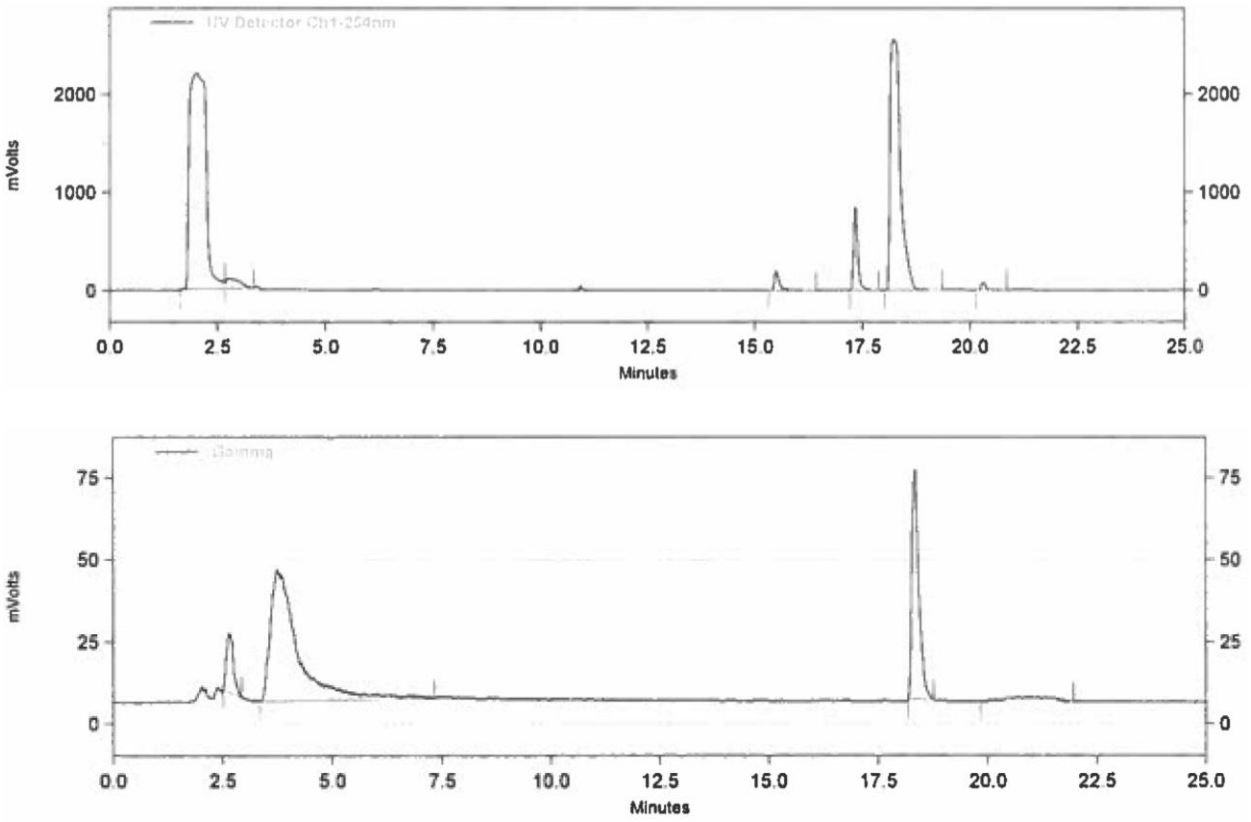


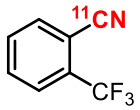




([^{11}C]8)

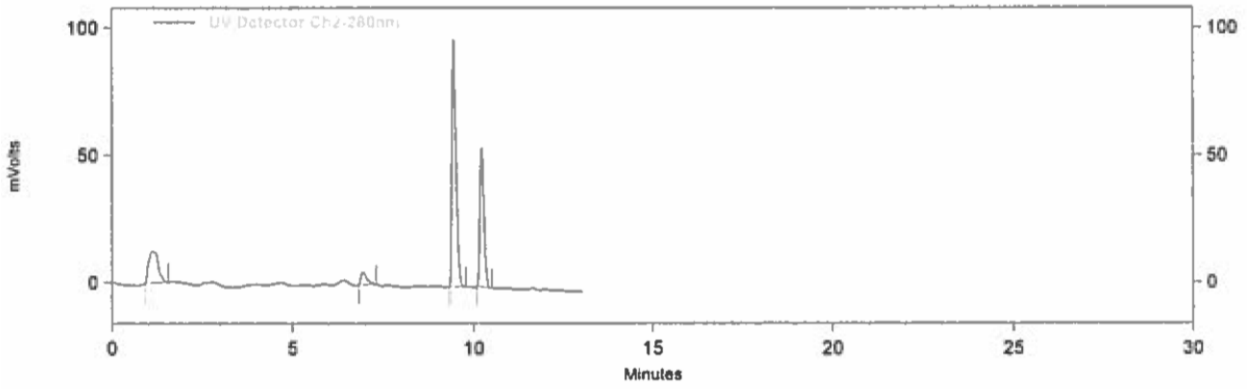
HPLC Conditions: A
Starting material: **8-Bpin**

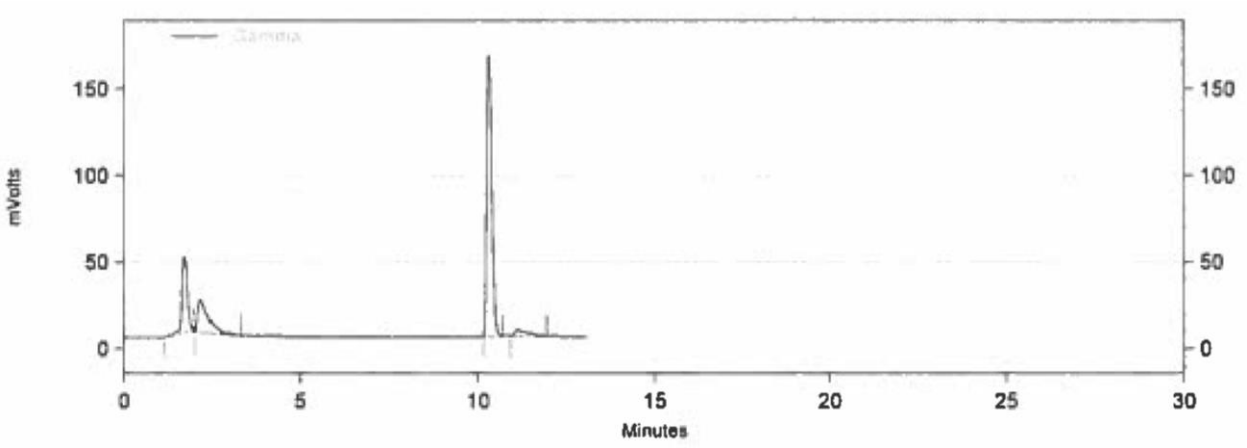


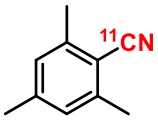


([^{11}C]9)

HPLC Conditions: A
Starting material: **9-B(OH)$_2$**

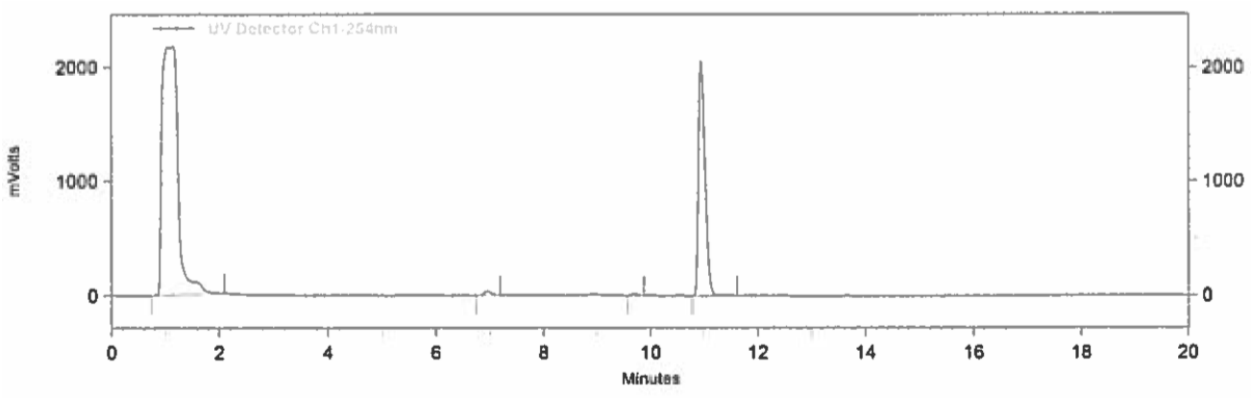


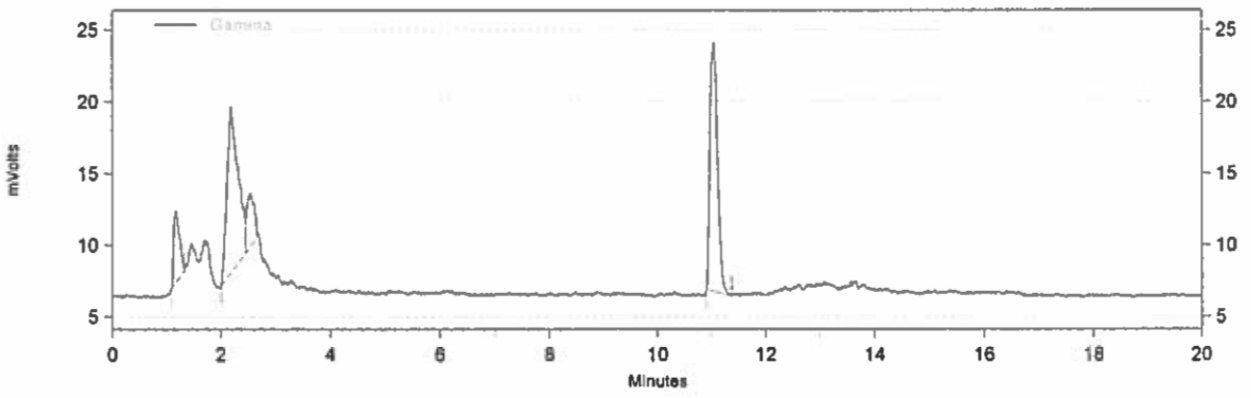


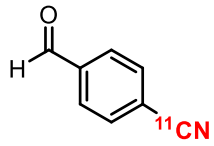


([^{11}C]10)

HPLC Conditions: A
Starting material: **10-B(OH)$_2$**

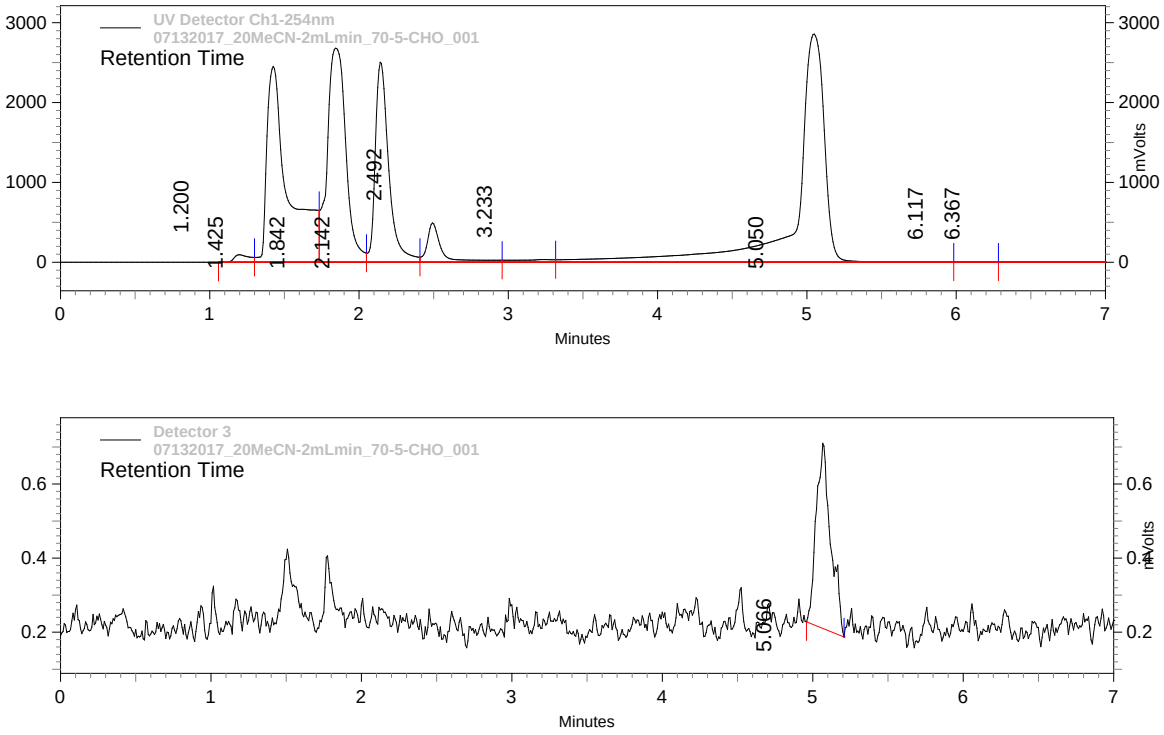


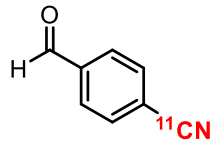




([^{11}C]**11**)

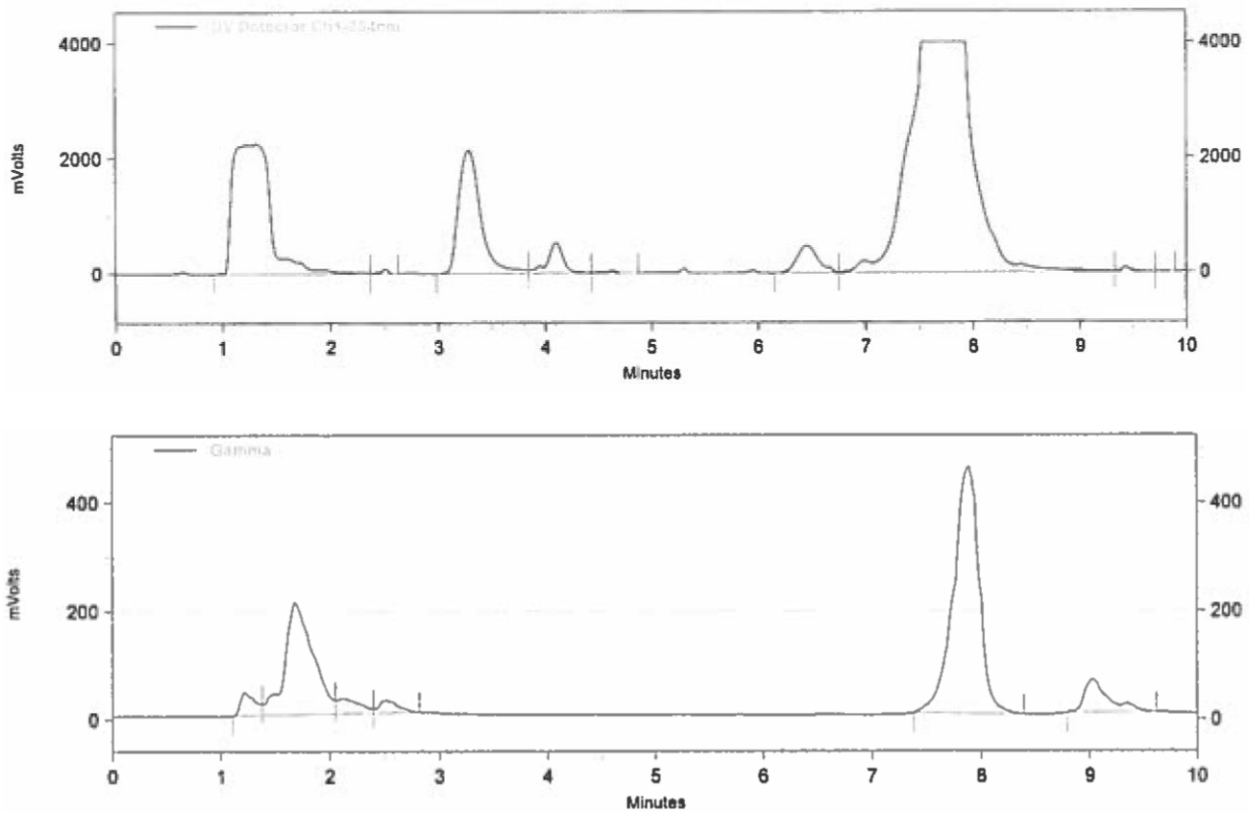
HPLC Conditions: A
Starting material: **11-B(OH)$_2$**

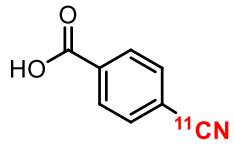




([^{11}C]11)

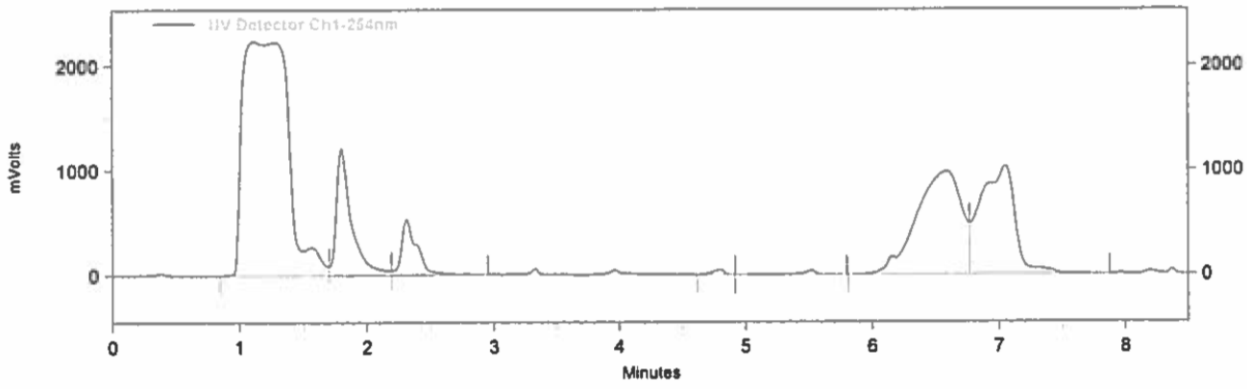
HPLC Conditions: A
Starting material: **11-BF_3K**

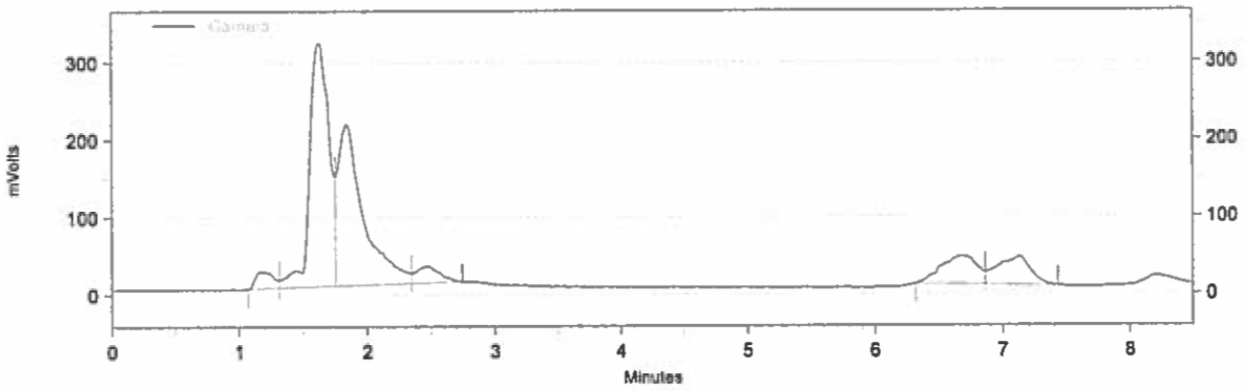


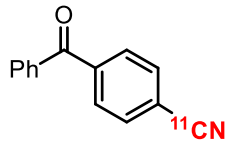


([^{11}C]12)

HPLC Conditions: A
Starting material: **12-B(OH)$_2$**

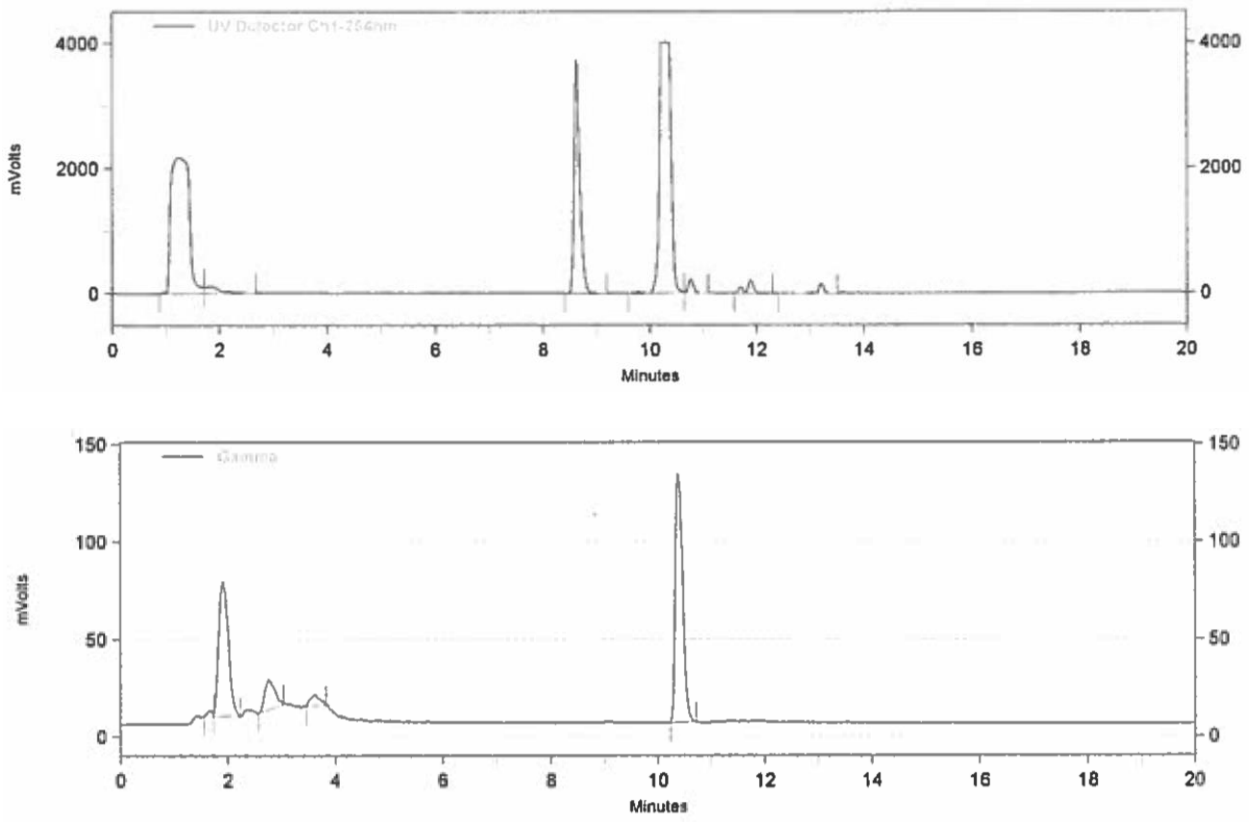


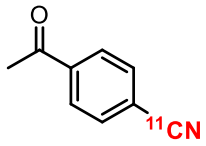




([^{11}C]13)

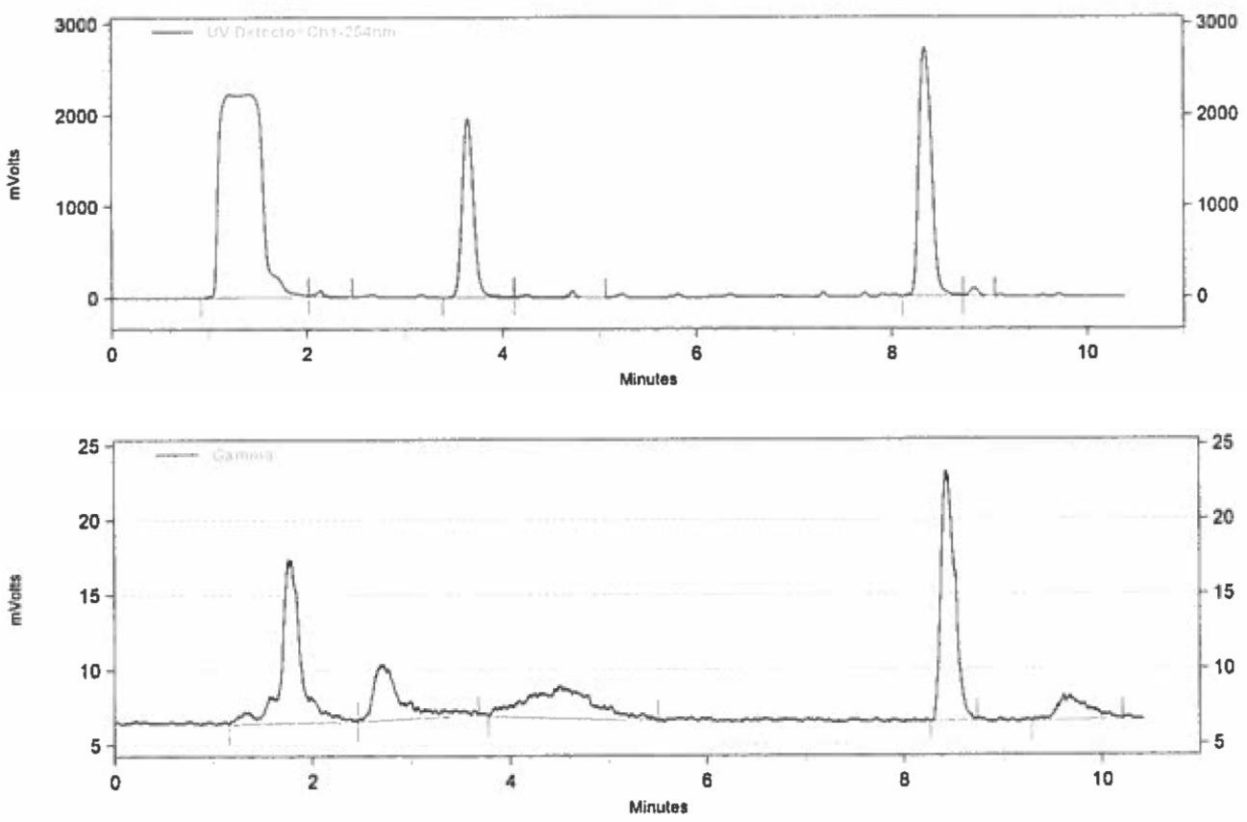
HPLC Conditions: A
Starting material: **13-SnBu$_3$**

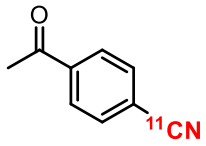




([^{11}C]14)

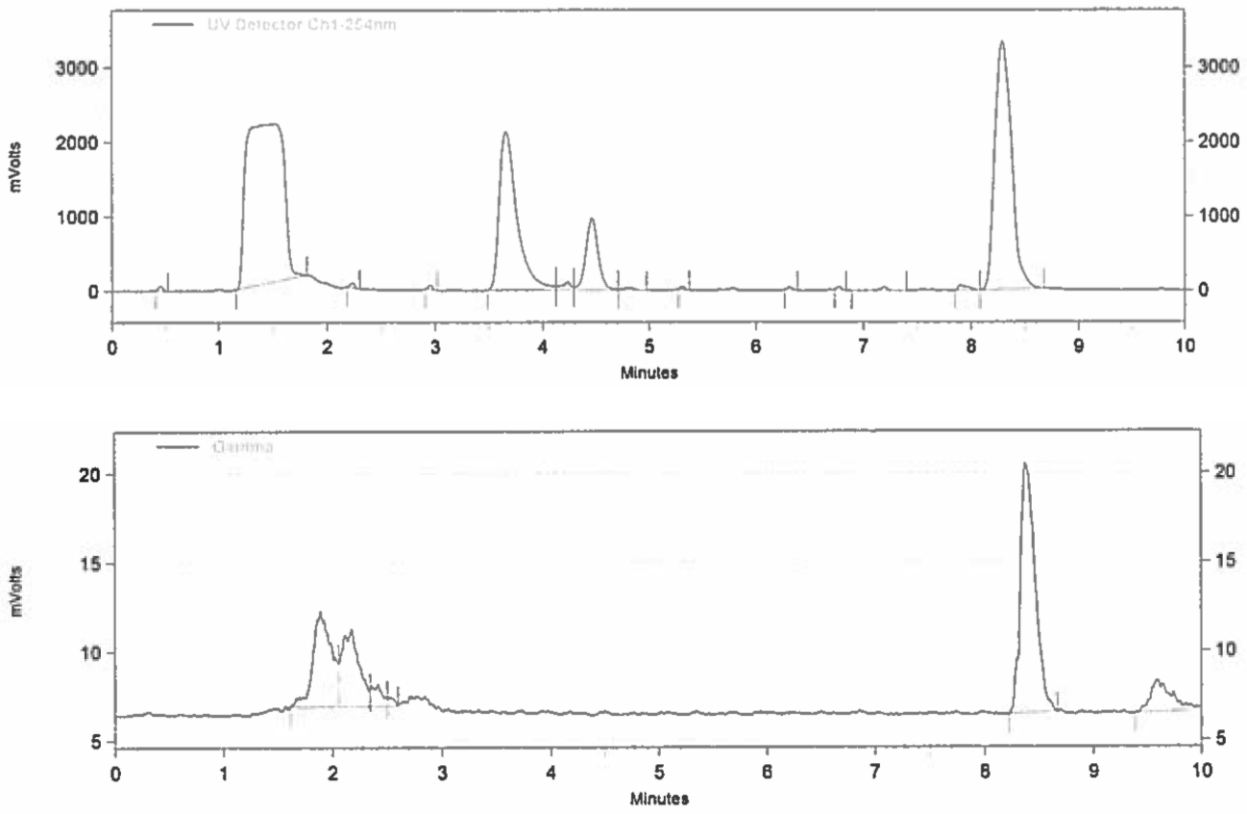
HPLC Conditions: A
Starting material: **14-SnBu$_3$**

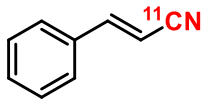




([^{11}C]14)

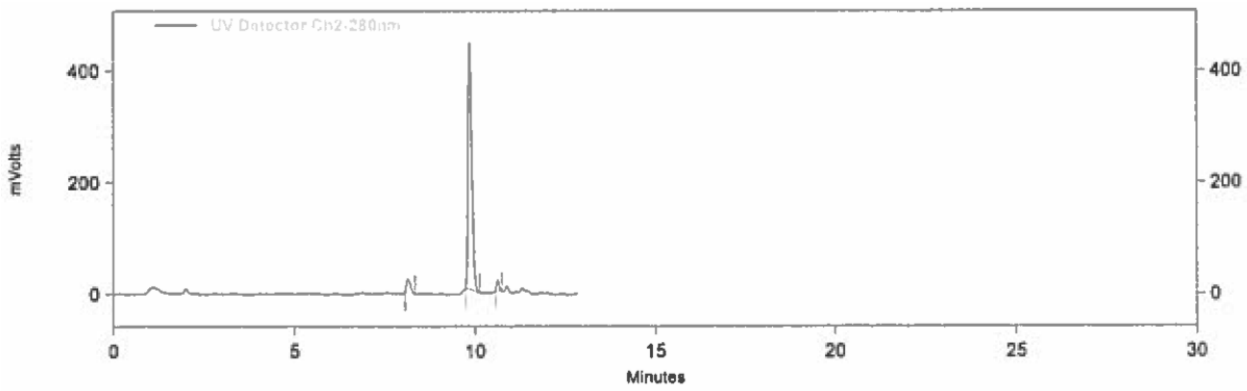
HPLC Conditions: A
Starting material: **14-B(OH)$_2$**

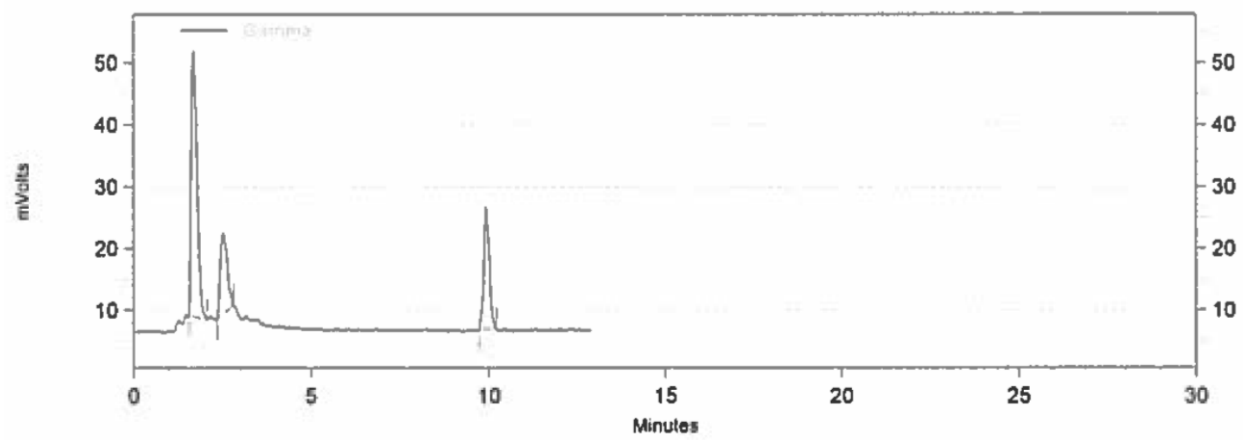


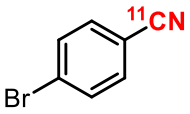


([^{11}C]15)

HPLC Conditions: A
Starting material: **15-SnBu$_3$**

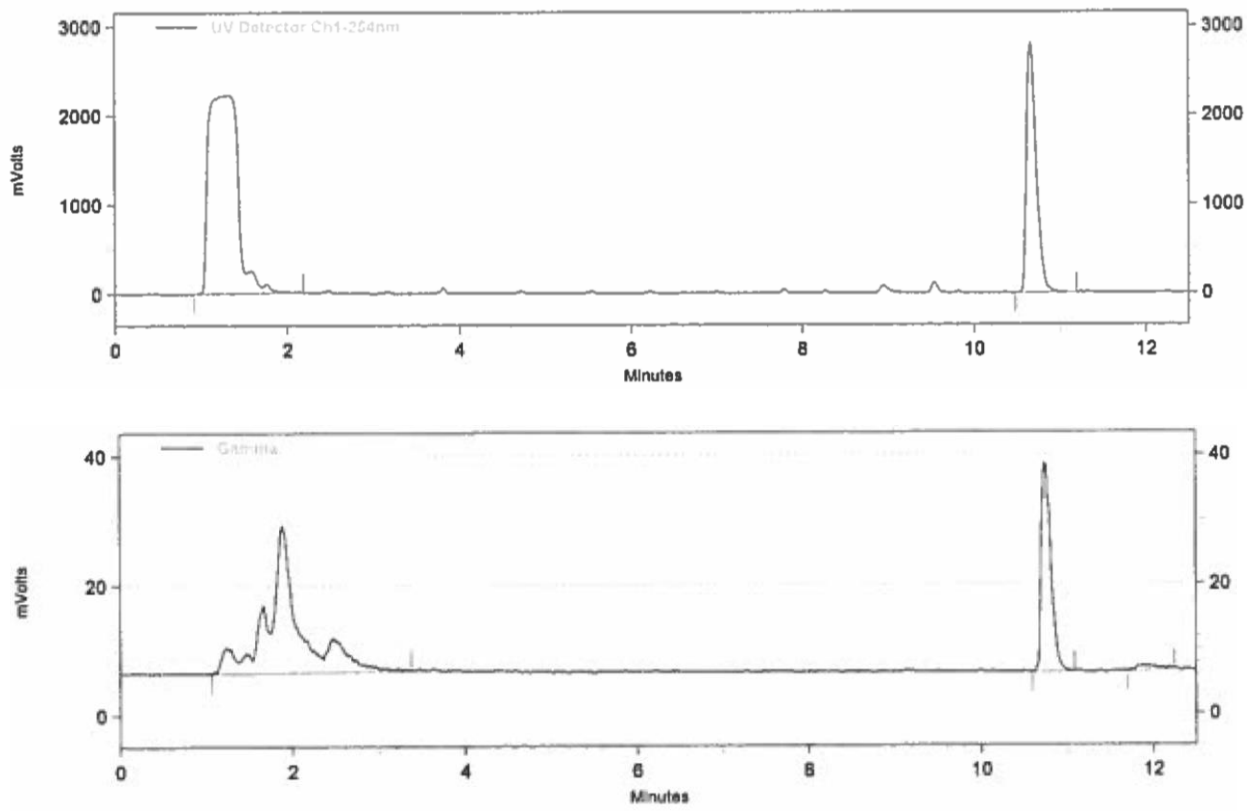


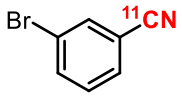




([^{11}C]16)

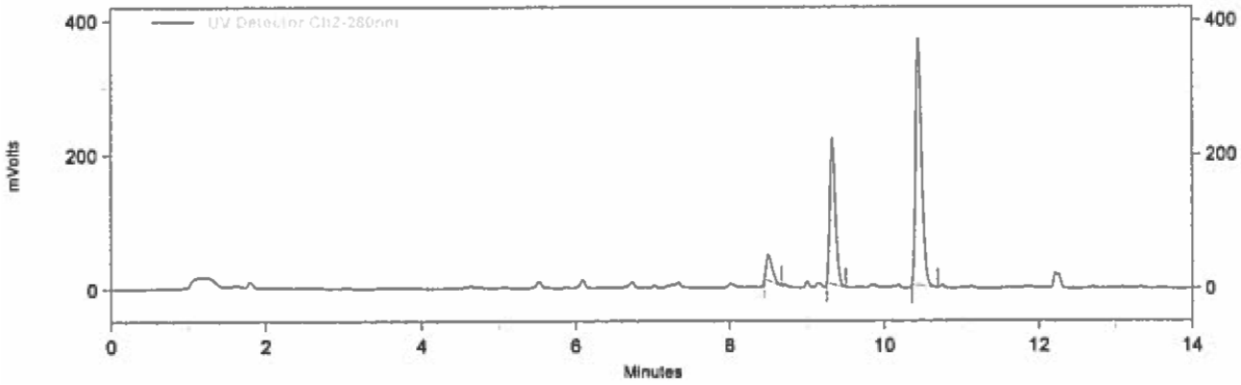
HPLC Conditions: A
Starting material: **16-B(OH)$_2$**

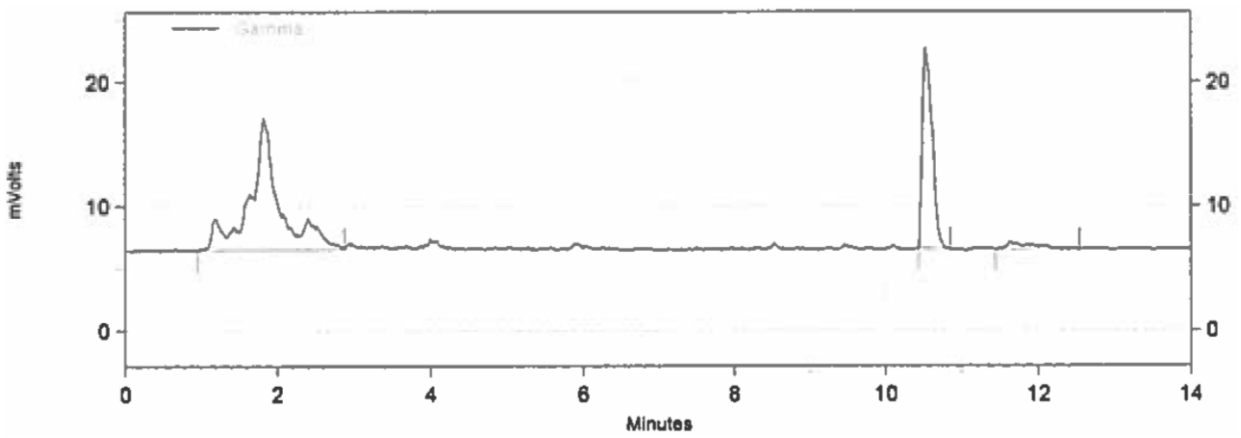


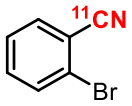


([^{11}C]17)

HPLC Conditions: A
Starting material: **17-B(OH)$_2$**

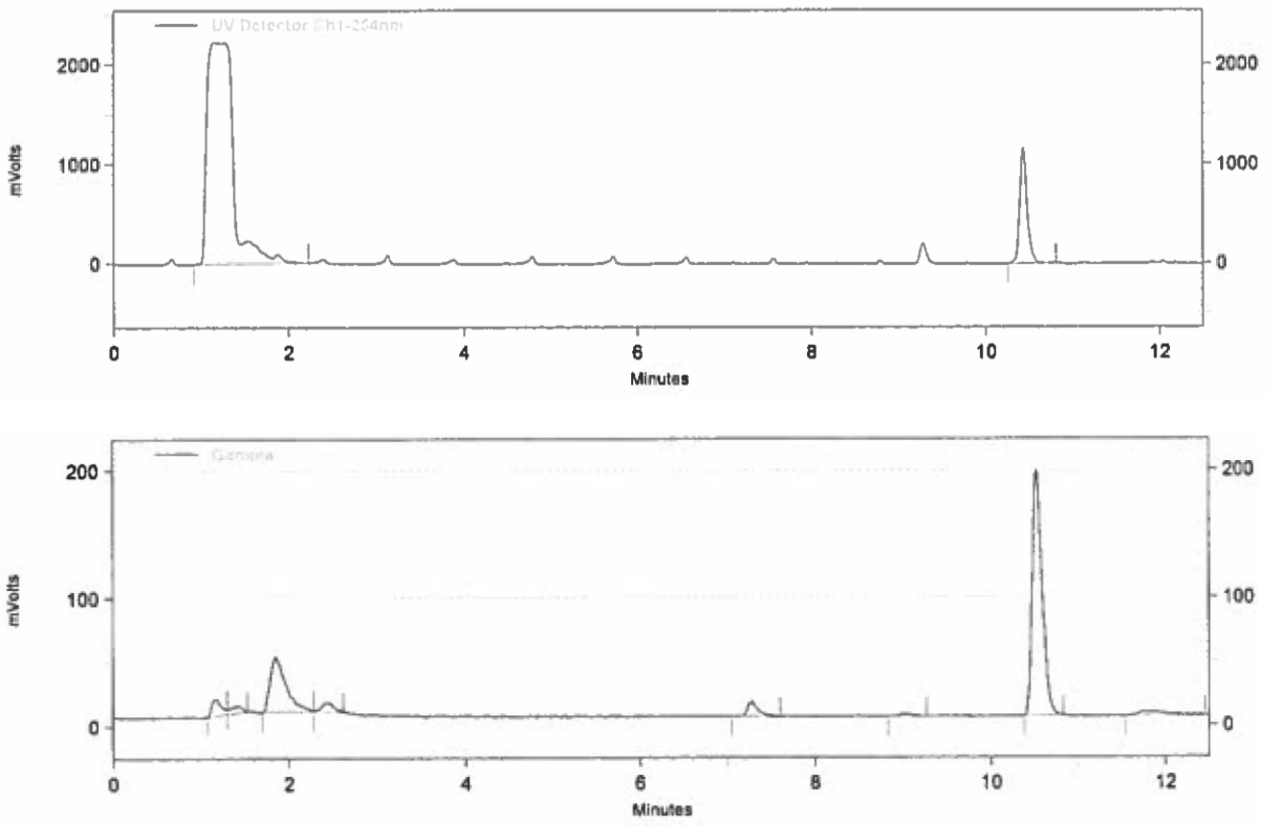


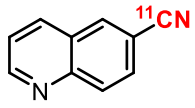




([11C]18)

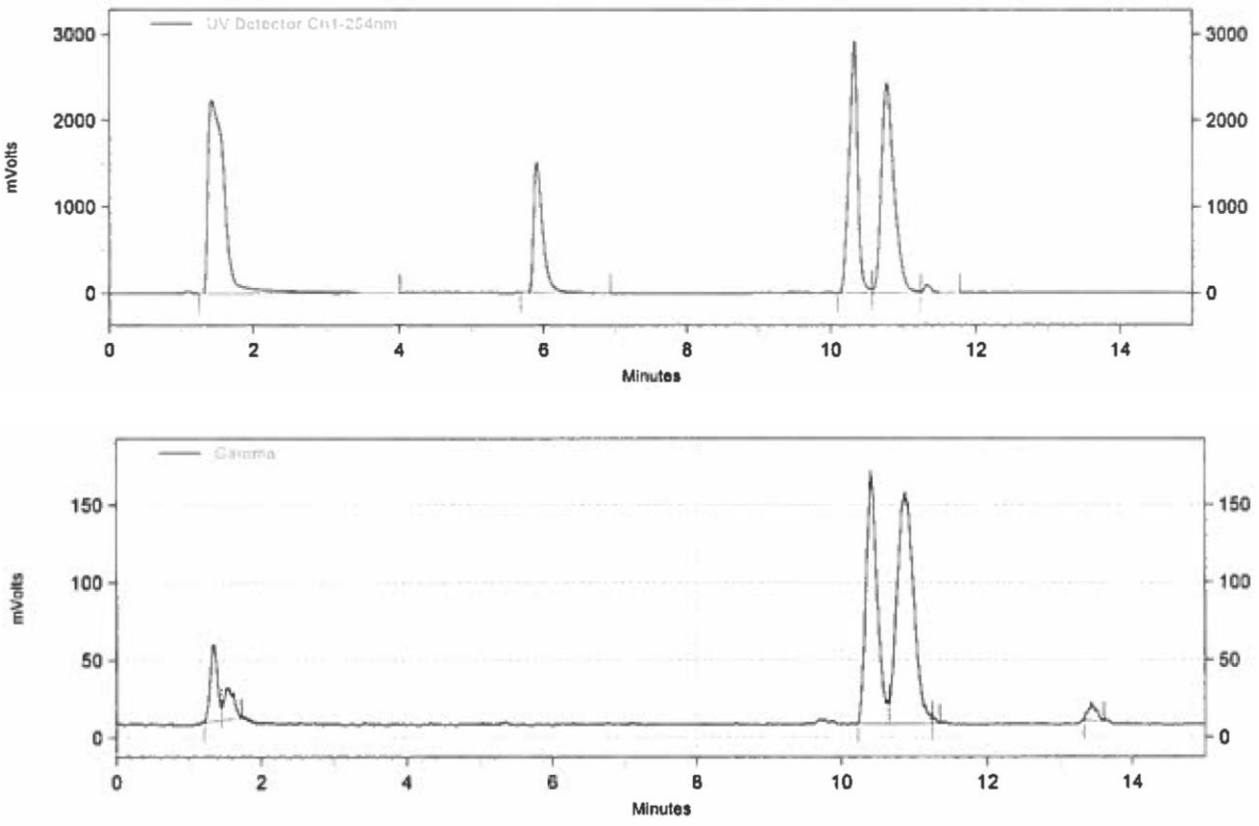
HPLC Conditions: A
Starting material: **18-B(OH)$_2$**

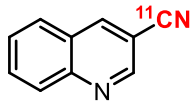




([^{11}C]**19**)

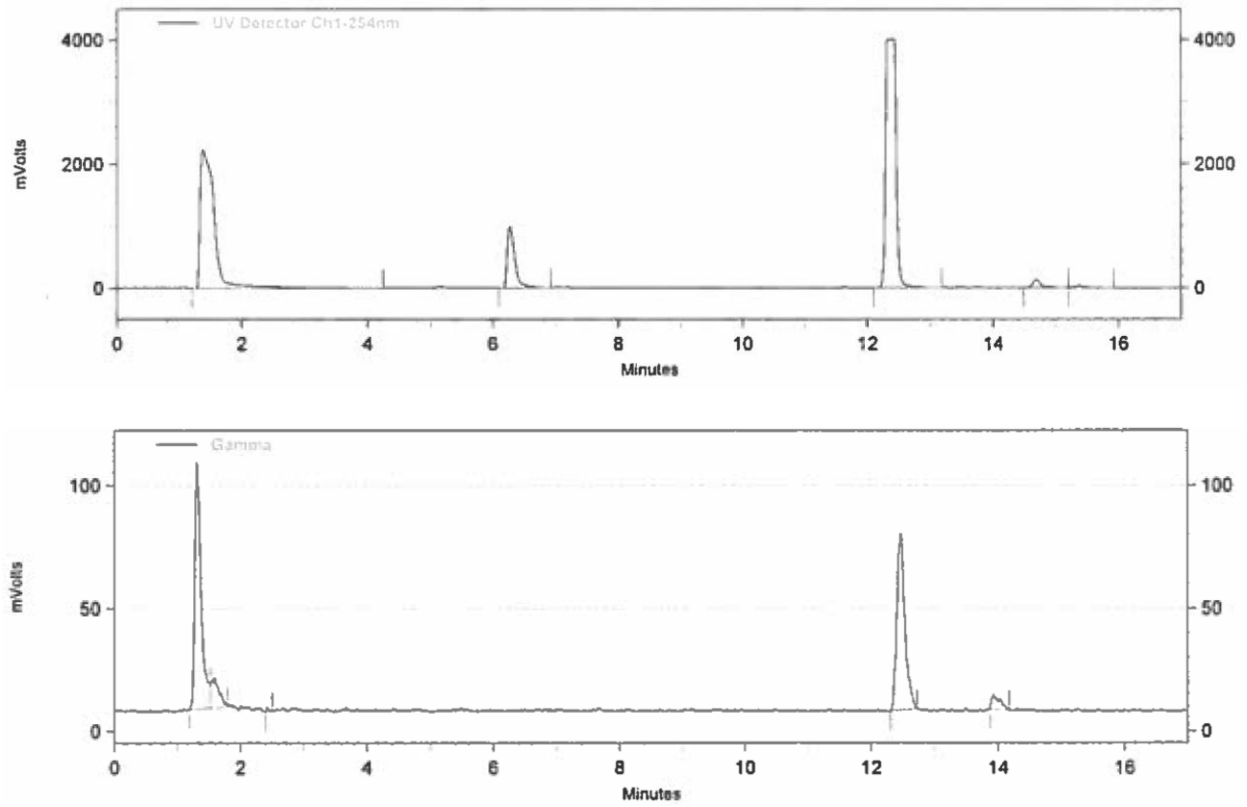
HPLC Conditions: B
Starting material: **19-B(OH)$_2$**

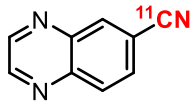




([11C]20)

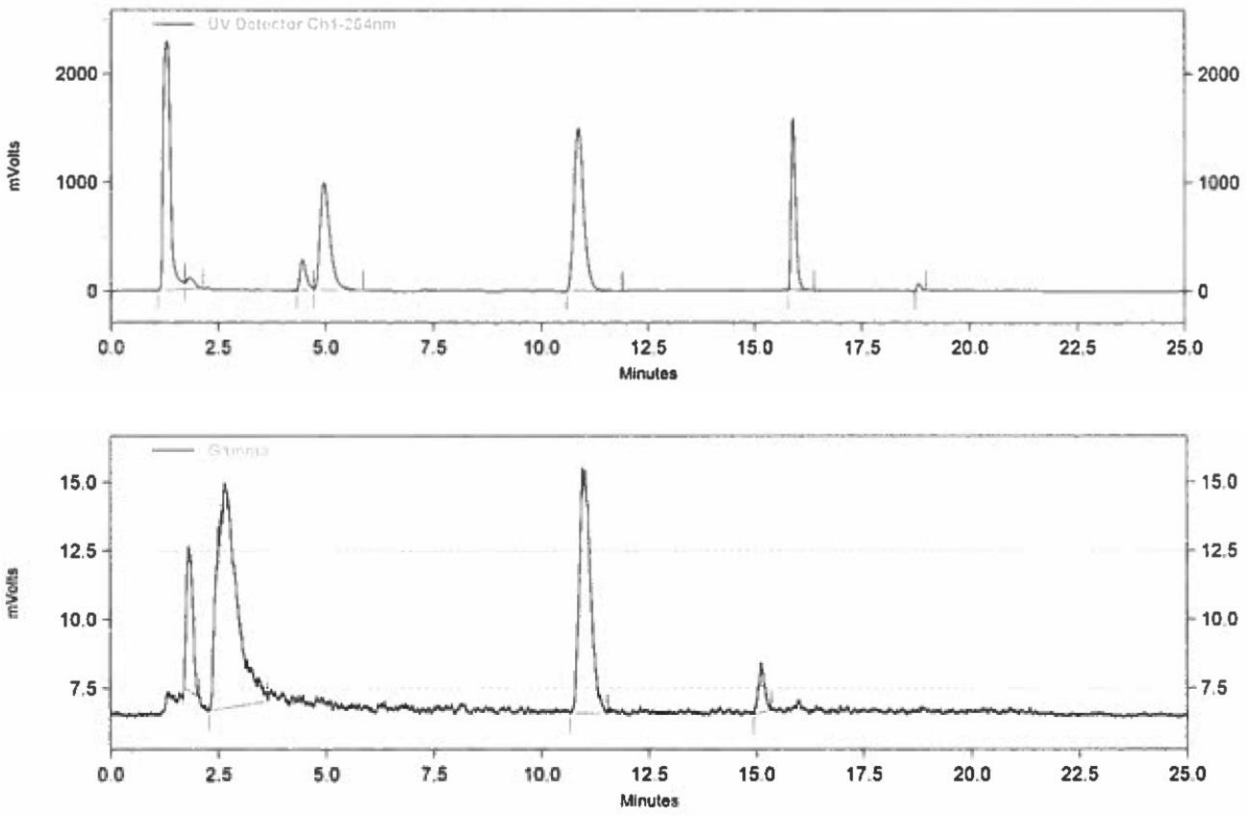
HPLC Conditions: B
Starting material: **20-B(OH)$_2$**





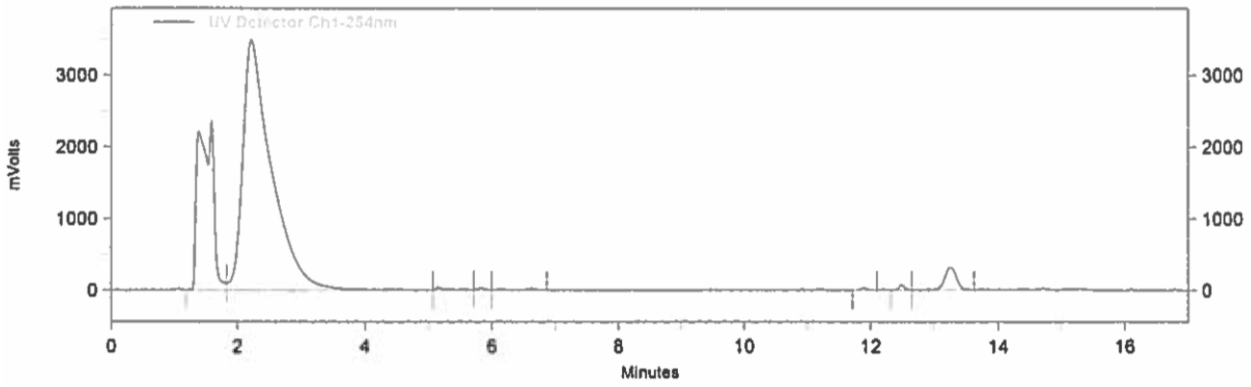
([^{11}C]21)

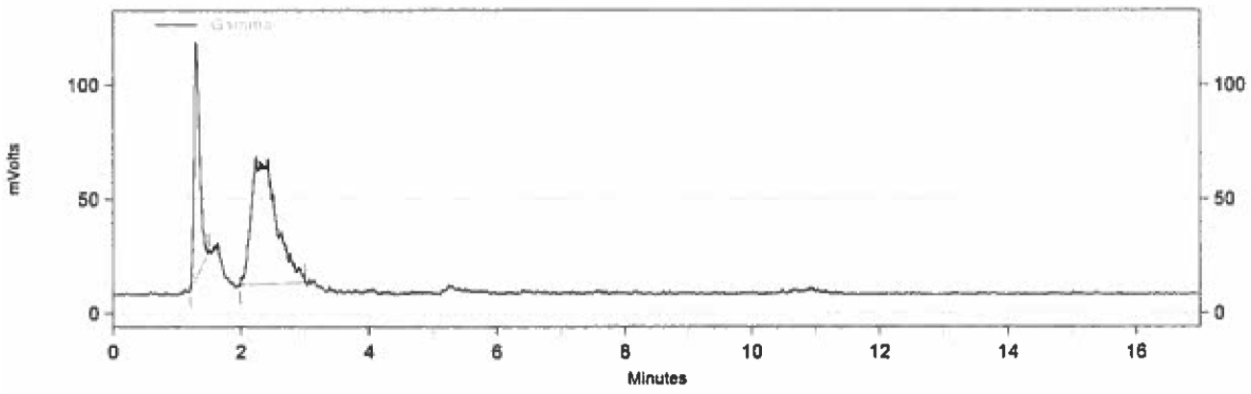
HPLC Conditions: A
Starting material: **[^{11}C]21-Bpin**

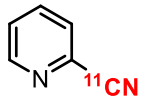


([^{11}C]22)

HPLC Conditions: B
Starting material: **22-B(OH)$_2$**

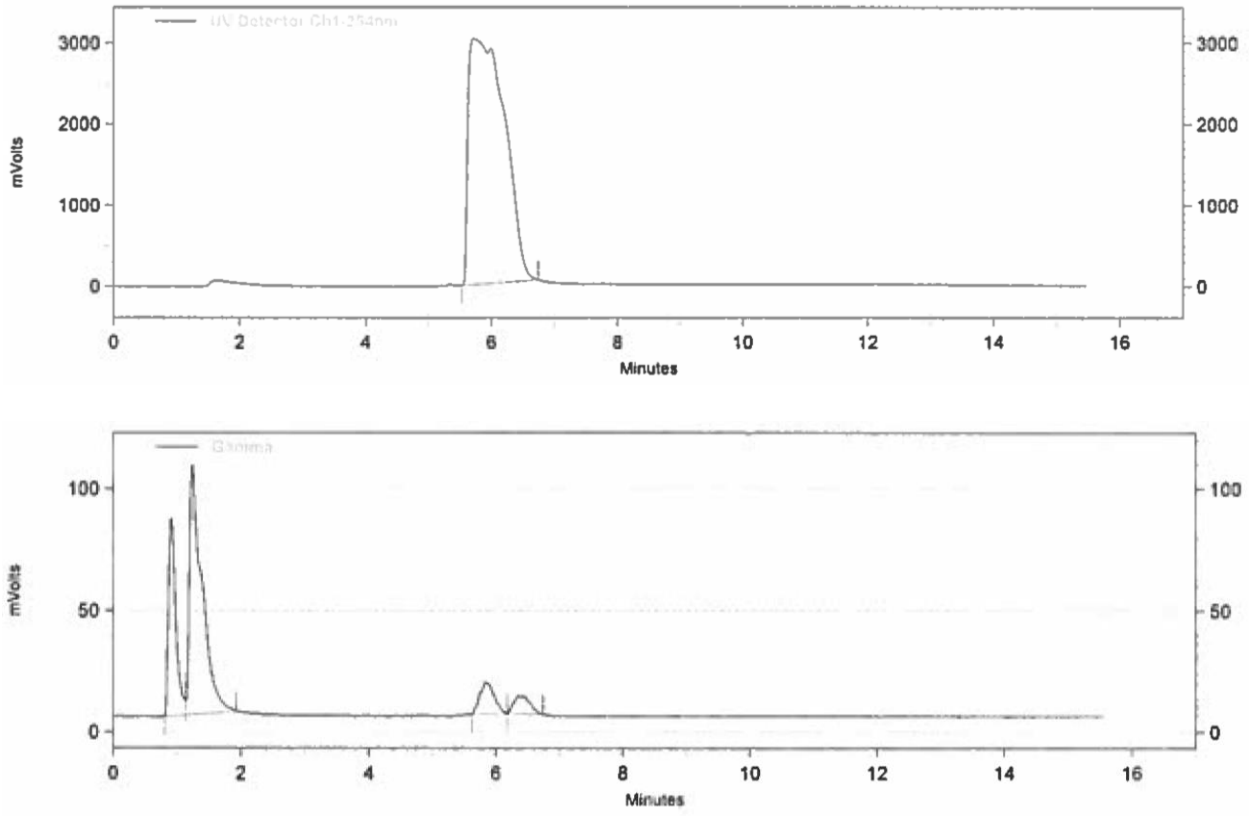






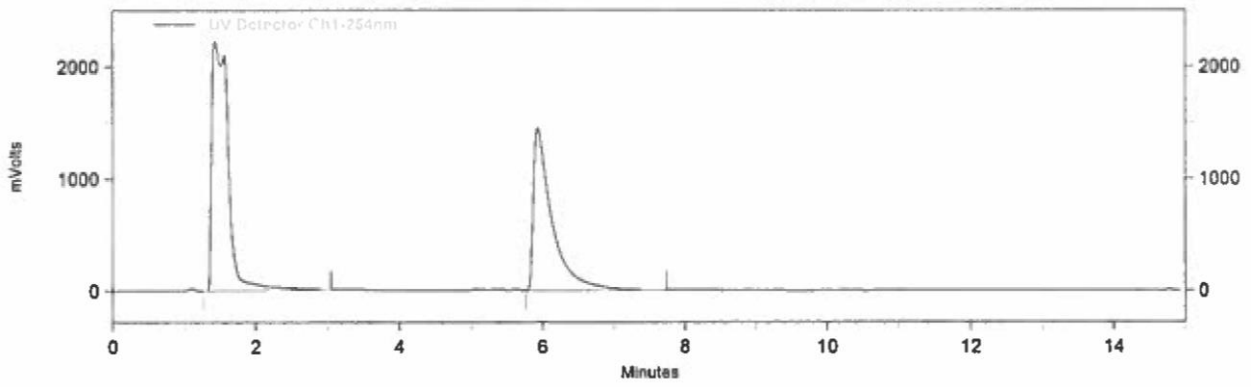
([^{11}C]23)

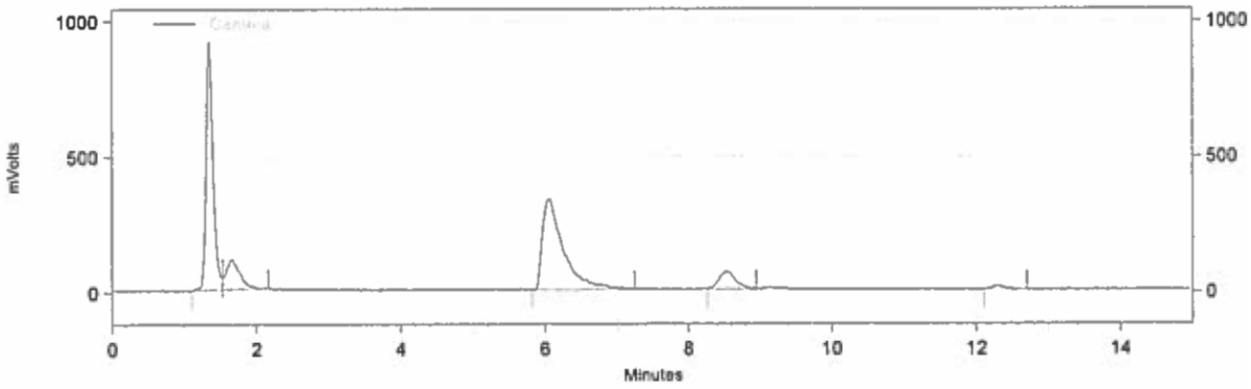
HPLC Conditions: B
Starting material: **23-SnBu$_3$**

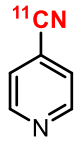


([^{11}C]24)

HPLC Conditions: B
Starting material: **24-SnBu$_3$**

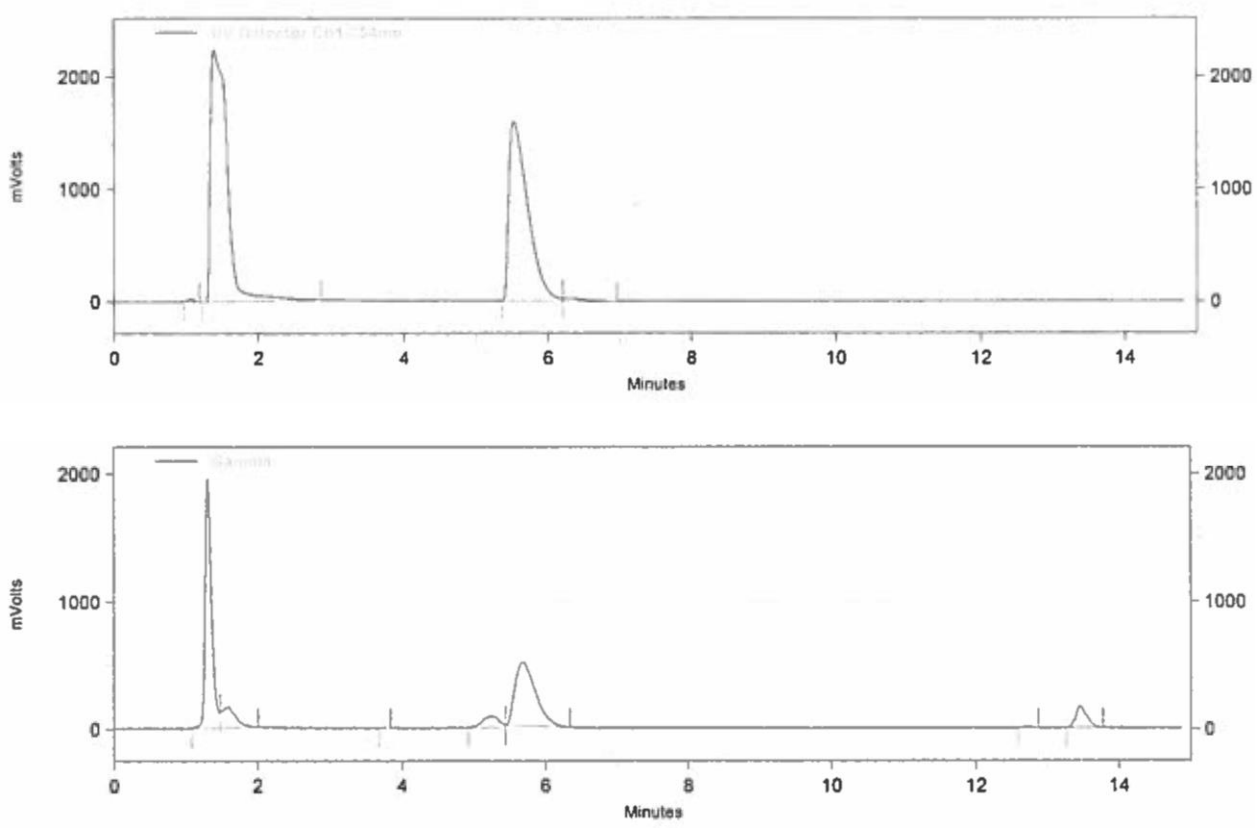


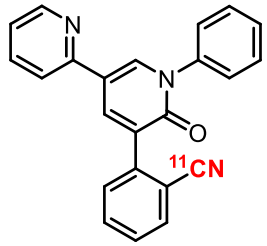




([^{11}C]25)

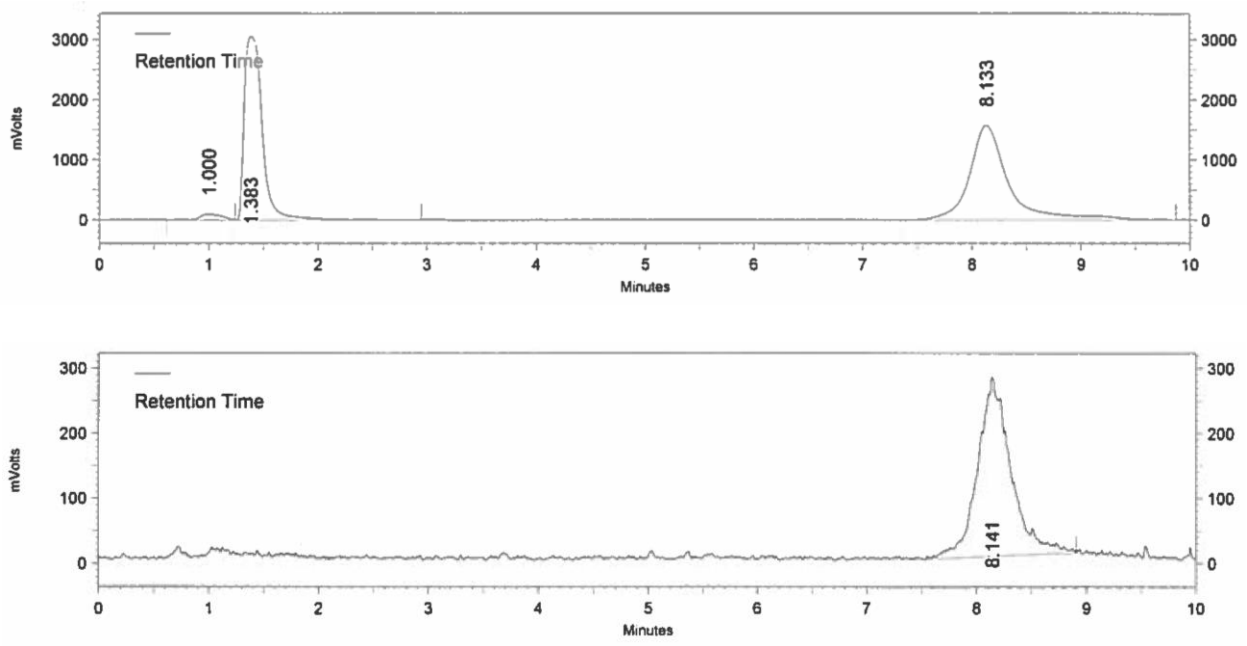
HPLC Conditions: B
Starting material: **25-SnBu$_3$**

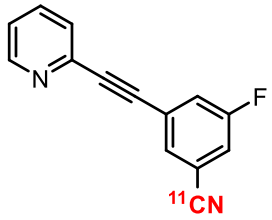




([^{11}C]26)

HPLC Condition D
Starting material: **26-Bpin**





([^{11}C]27)

HPLC Condition D
Starting material: **27-Bpin**