Supporting Information

Palladium(II)-mediated rapid ^{11}C-cyanation of (hetero)arylborons

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Instrumentals and chemicals

All reactions without using carbon-11 were performed under argon or nitrogen atmosphere unless otherwise indicated. All manipulations of air- and/or moisture-sensitive compounds were performed using standard Schlenk techniques.

Gas chromatography (GC) analysis was carried out on a Shimadzu GC-2014 using an INERT CAP (30 m, 0.25 mm I.D., 0.25 μm df) column and helium as the carrier gas.

Analytical thin-layer chromatography (TLC) was performed on precoated (0.25 mm) silica-gel plates (Merck, Merck Silica Gel 60 F254). Preparative TLC (PTLC) was carried out using precoated (0.5 mm) silica-gel plates (Merck, Merck Silica Gel 60 F254). Flash chromatography was carried out on a YAMAZEN Automated Flash Chromatography System that consists of AI-580 and Parallel Frac FR-360 with silica-gel-packed column (YAMAZEN Universal Column Silica-Gel).

Melting points (mp) were measured with an OptiMelt automated melting point apparatus (Stanford Research Systems, Inc.) and were uncorrected.

^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were obtained from measurements at room temperature on a JEOL 400SS spectrometer. Chloroform-d_1 ($CDCl_3$) containing tetramethylsilane (0.05%, TMS) (99.8%D, Cambridge Isotope Laboratories, Inc.) or dimethylsulfoxide-d_6 (DMSO-d_6, 99.9%D, Cambridge Isotope Laboratories, Inc.) was used as an NMR solvent for NMR measurements. Chemical shifts (δ) are given in parts per million (ppm) downfield from $(CH_3)_4Si$ (δ 0.00 for ^{1}H NMR in $CDCl_3$) or the solvent peak (δ 7.26 for ^{1}H NMR and δ 77.2 for ^{13}C NMR in $CDCl_3$, or δ 2.49 for ^{1}H NMR and δ 39.5 for ^{13}C NMR in DMSO-d_6) as an internal reference with coupling constants (J) in hertz (Hz). The abbreviations s, d, t, and m signify singlet, doublet, triplet, and multiplet, respectively.

IR spectra were measured by diffuse reflectance method on a Shimadzu IRPrestige-21 spectrometer with the absorption band given in cm^{-1}. High-resolution mass spectra (HRMS) were measured on a Thermo Fisher Scientific Exactive™ Plus Orbitrap mass spectrometer under positive electrospray ionization (ESI^+) conditions.

3-Dehydroxy-3-(pinacolylboryl)estrone ((8*R*,9*S*,13*S*,14*S*)-13-methyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-6,7,8,9,1,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthrene-17-one, **1o**),[S1] 4-((4-methylbenzyl)(4*H*-1,2,4-triazole-4-yl)amino)benzonitrile (cetrozole, **2ac**),[S2] 4-((4-bromobenzyl)-(4*H*-1,2,4-triazole-4-yl)amino) benzonitrile (YM511, **2ad**),[S3] and butyl (*R*)-2-(4-(4-(5,5-dimethyl-1,3,2-dioxanborinan-2-yl)-2-fluorophenoxy)phenoxy)propionate (**1ae″**)[S4] were prepared according to the reported methods.

All chemical reagents obtained from commercial suppliers were used without further purification.

N,*N*-Dimethylformamide (DMF), dimethyl sulfoxide (DMSO), and toluene were purchased from Wako Pure Chemical Industries, Ltd.

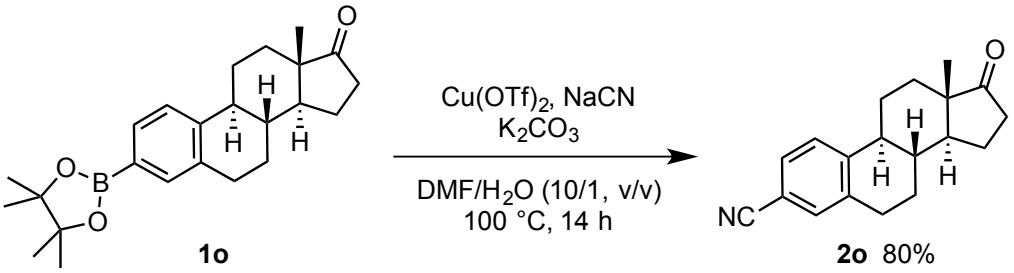
N,*N*-Dimethylacetamide (DMA), *N*,*N*-diethylformamide, *N*-methyl-2-pyrolidinone (NMP), potassium *tert*-butoxide (KO^{t}Bu), 1-fluoro-4-iodobenzene, 4-amino-4*H*-1,2,4-triazole, cyhalofop butyl (**2ae**), bis(pinacolato)diboron ((Bpin)$_2$), 4-methylbenzyl bromide, 4-bromobenzyl bromide, phenylboronic acid pinacol ester (**1a**), phenylboronic acid (**1a′**), 4-methoxyphenylboronic acid pinacol ester (**1e**), 4-formylphenylboronic acid pinacol ester (**1f**), 4-cyanophenylboronic acid pinacol ester (**1h**), 4-cyanophenylboronic acid (**1h′**), 2-cyanophenylboronic acid pinacol ester (**1n**), 4-pyridineboronic acid pinacol ester (**1q**), 4-acetylphenylboronic acid (**1u′**), 4-carbamoylphenylboronic acid (**1v′**), 4-fluorophenylboronic acid (**1w′**), 4-iodophenylboronic acid (**1z′**), 4-phenylbenzonitrile (**2b**), 4-aminobenzonitrile (**2c**), 4-methoxybenzonitrile (**2e**), 4-cyanobenzaldehyde (**2f**), 4-cyanobenzoic acid (**2i**), 2-cyanophenol (**2k**), 2-aminobenzonitrile (**2l**), 2-methoxybenzonitrile (**2m**), phthalonitrile (**2n**), 4-cyanopyridine (**2q**), quinoline-6-carbonitrile (**2r**), quinoline-3-carbonitrile (**2s**), 4-cyanobenzamide (**2v**), 4-chlorobenzonitrile (**2x**), 4-bromobenzonitrile (**2y**), 4-iodobenzonitrile (**2z**), and 2-methylbenzonitrile (**2aa**) were purchased from Tokyo Chemical Industry Co., Ltd.

Phenylboronic acid neopentyl glycol ester (**1a″**), 4-biphenylboronic acid pinacol ester (**1b**), 4-aminophenylboronic acid pinacol ester (**1c**), 4-(hydroxymethyl)phenylboronic acid pinacol ester (**1d**), 4-methoxycarbonylphenylboronic acid pinacol ester (**1g**), 4-methoxycarbonylphenylboronic acid (**1g′**), 4-carboxyphenylboronic acid pinacol ester (**1i**), 2-hydroxyphenylboronic acid pinacol ester (**1k**), 2-aminophenylboronic acid pinacol ester (**1l**), 2-methoxyphenylboronic acid pinacol ester (**1m**), 6-quinolineboronic acid pinacol ester (**1r**), 3-quinolineboronic acid pinacol ester (**1s**), 3-quinolineboronic acid (**1s′**), 4-chlorophenylboronic acid (**1x′**), 4-bromophenylboronic acid (**1y′**), *o*-tolylboronic acid (**1aa′**), 2,4,6-trimethylphenyl boronic acid (**1ab′**), methyl 4-cyanobenzoate (**2g**), 4-(hydroxymethyl)benzonitrile (**2d**), cinnamonitrile (**2p**), 4-cyanoindole (**2t**), 4-acetylbenzonitrile (**2u**), bis(triphenylphosphine)palladium(II) dichloride ($PdCl_2(PPh_3)_2$), bis(tri-*o*-tolylphosphine)-palladium(II) dichloride ($PdCl_2(P(o\text{-}Tol)_3)_2$), (1,1′-bis(diphenylphosphino)ferrocene)palladium(II) dichloride complex with dichloromethane ($PdCl_2(dppf)\cdot CH_2Cl_2$), platinum wire, chloro(1,5-cyclo-octadiene)rhodium(I) dimer ($[RhCl(cod)]_2$), and 4,5-bis(diphenylphosphino)-9,9- dimethylxanthene (xantphos) were purchased from Sigma–Aldrich Japan, Inc.

Sodium cyanide (NaCN), copper(I) iodide (CuI), copper(II) triflate ($Cu(OTf)_2$), *n*-dodecane, benzonitrile (**2a**), terephthalonitrile (**2h**), 4-fluorobenzonitrile (**2w**), triphenylphosphine (PPh_3), potassium carbonate (K_2CO_3), sodium hydroxide (NaOH), 1,4-diazabicyclo[2.2.2]octane (DABCO), and 1,4-dioxane were purchased from Nacalai Tesque, Inc. 2-Cyanobiphenyl (**2j**) was purchased from Trans World Chemicals, Inc. Biphenyl-2-boronic acid pinacol ester (**1j**), indole-4-boronic acid pinacol ester (**1t**), and 2,4,6-trimethylbenzonitrile (**2ab**) were purchased from Alfa Aesar. 4,4,5,5-Tetramethyl-2-styryl-1,3,2-dioxaborolane (**1p**) were purchased from Ark Pharm, Inc. Bis(neopentyl glycolato)diboron was purchased from Frontier Scientific, Inc.

Preparation of non-radiolabeled compounds and labeling precursors

3-Dehydroxy-3-cyanoestrone ((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthrene-3-carbonitrile, 2o)



To a mixture of 3-dehydroxy-3-(pinacolylboryl)estrone (**1o**) (10.2 mg, 26.8 μmol, 1 equiv) and copper(II) trifluoromethanesulfonate (0.72 mg, 2.0 μmol, 0.07 equiv) in DMF (1 mL) equipped with a stir bar was added aqueous NaCN (2.0 mol/L, 100 μL, 0.20 mmol, 7.7 equiv) under air. After sealing the vial with a rubber cap, the reaction mixture was heated at 100 °C for 14 h with stirring. After cooling to room temperature, the reaction mixture was poured into saturated aqueous ammonium chloride (10 mL), and extracted with EtOAc (10 mL × 3). The combined organic extract was washed with brine (10 mL) and dried over Na_2SO_4. After filtration, the volatiles were removed in vacuo. The residue was purified by preparative TLC (hexanes/EtOAc = 6/1) to give **2o** (6.0 mg, 21.5 μmol, 80%) as a white solid;

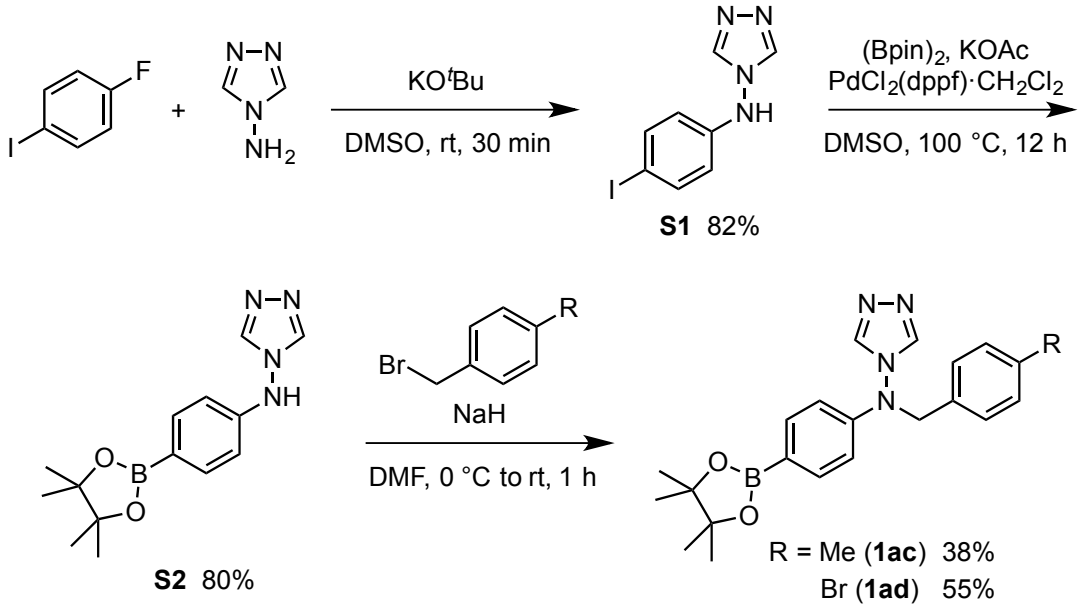
TLC R_f = 0.25 (*n*-hexane/EtOAc = 6/1);

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.92 (s, 3H), 1.45–1.70 (m, 6H), 1.98–2.21 (m, 4H), 2.30–2.45 (m, 2H), 2.53 (dd, *J* = 19.0, 8.8 Hz, 1H), 2.91–2.95 (m, 2H), 7.37–7.44 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 14.0, 21.7, 25.6, 26.2, 29.1, 31.6, 35.9, 37.8, 44.7, 48.0, 50.6, 109.8, 119.3, 126.4, 129.5, 132.7, 138.1, 145.5, 220.5;

The chemical shifts were consistent with those reported in the literature.[S5]

Boronates 1ac and 1ad



N-(4-Iodophenyl)-4*H*-1,2,4-triazole-4-amine (**S1**): 4-Amino-4*H*-1,2,4-triazole (2.32 g, 27.6 mmol, 2 equiv) was added portionwise to a stirred suspension of KO^{t}Bu (3.09 g, 27.5 mmol, 2 equiv) in DMSO (28 mL) at 15 °C. After stirring at room temperature for 30 min, to this mixture was added 1-fluoro-4-iodobenzene (1.59 mL, 13.8 mmol, 1 equiv) dropwise maintaining the temperature below 30 °C. After stirring for 30 min at room temperature, the mixture was poured into water, which resulted in the formation of a precipitate. After neutralization of the mixture with aqueous HCl (1 mol/L), the precipitate was collected by filtration and purified by recrystallization from water to give **S1** (3.26 g, 11.4 mmol, 82%) as a white solid;
mp 199.0–200.0 °C (decomposed);
TLC R_f = 0.20 (EtOAc);
^{1}H NMR (400 MHz, DMSO-d_6) δ 6.32 (dd, J = 8.4, 1.6 Hz, 2H), 7.52 (dd, J = 7.2, 2.4 Hz, 2H), 8.66 (s, 2H), 9.52 (s, 1H);
^{13}C NMR (100 MHz, DMSO-d_6) δ 84.7, 116.2 (2C), 138.8 (2C), 145.1 (2C), 147.7;
IR (ZnSe, cm^{-1}) 806, 842, 937, 964, 999, 1062, 1116, 1180, 1240, 1282, 1305, 1384, 1454, 1485, 1527, 1581, 3122, 3200;
HRMS (ESI$^+$) *m*/*z* 286.9786 (286.9788 calcd for $C_8H_8IN_4^+$, [M+H]$^+$).

N-(4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-4*H*-1,2,4-triazole-4-amine (**S2**): A mixture of PdCl$_2$(dppf)·CH$_2$Cl$_2$ (71.8 mg, 87.9 μmol, 0.05 equiv), **S1** (504 mg, 1.76 mmol, 1 equiv), (Bpin)$_2$ (720 mg, 2.84 mmol, 1.6 equiv), and potassium acetate (517 mg, 5.28 mmol, 3 equiv) in DMSO (10 mL) was stirred at 100 °C for 12 h. After cooling to room temperature, the reaction mixture was poured into saturated aqueous ammonium chloride (100 mL), and extracted with ethyl acetate (100 mL × 3). The combined organic extract was dried over Na_2SO_4. After filtration, the

filtrate was concentrated in vacuo. The residue was purified by flash chromatography ($CHCl_3$/MeOH = 20/1) to give **S2** (400 mg, 1.40 mmol, 80%) as a pale yellow solid;
mp 190.0–191.0 °C (decomposed);
TLC R_f = 0.20 ($CHCl_3$/MeOH = 20/1);
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.33 (s, 12H), 6.57 (d, *J* = 8.6 Hz, 2H), 6.95 (s, 1H), 7.73 (d, *J* = 8.6 Hz, 2H), 8.33 (s, 2H);
^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0 (4C), 84.0 (2C), 112.5 (2C), 136.8 (2C), 144.1 (2C), 148.3 (the signal for the carbon that is attached to the boron atom was not observed);
IR (ZnSe, cm^{-1}) 655, 690, 734, 804, 825, 860, 937, 962, 1014, 1064, 1087, 1139, 1273, 1313, 1357, 1396, 1606, 2976, 3138;
HRMS (ESI^+) *m*/*z* 287.1673 (287.1674 calcd for $C_{14}H_{20}{}^{11}BN_4O_2^+$, $[M+H]^+$).

4-((4-Methylbenzyl)-*N*-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-4*H*-1,2,4-triazol-4-amine (**1ac**): **S2** (555 mg, 1.94 mmol, 1 equiv) and 4-methylbenzyl bromide (555 mg, 3.00 mmol, 1.5 equiv) were dissolved in DMF (10 mL) and cooled with ice-bath. To the solution was added sodium hydride (60% in mineral oil, 100 mg, 2.50 mmol, 1.3 equiv) and after stirring for 30 min at 0 °C, the reaction mixture was warmed to room temperature. After stirring for 1 h at the same temperature, to the mixture was added aqueous $KHSO_4$, and extracted with ethyl acetate (100 mL × 3). The combined organic extract was dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by flash chromatography ($CHCl_3$/MeOH = 20/1) to give **1ac** (290 mg, 0.743 mmol, 38%) as a pale yellow solid;
mp 146.8–147.2 °C;
TLC R_f = 0.30 ($CHCl_3$/MeOH = 20/1);
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.33 (s, 12H), 2.30 (s, 3H), 4.79 (s, 2H), 6.67 (d, *J* = 8.8 Hz, 2H), 7.06–7.12 (m, 4H), 7.74 (d, *J* = 8.8 Hz, 2H), 8.03 (s, 2H);
^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 25.0 (4C), 58.3, 84.0 (2C), 113.3 (2C), 128.6 (2C), 130.0 (2C), 131.4, 136.7 (2C), 138.9, 143.2 (2C), 150.2 (the signal for the carbon that is attached to the boron atom was not observed);
IR (ZnSe, cm^{-1}) 680, 692, 759, 808, 877, 1022, 1041, 1064, 1089, 1112, 1176, 1203, 1269, 1377, 1460, 1494, 1597, 2929, 3101;
HRMS (ESI^+) *m*/*z* 391.2298 (391.2300 calcd for $C_{22}H_{28}{}^{11}BN_4O_2^+$, $[M+H]^+$).

4-((4-Bromobenzyl)-*N*-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-4*H*-1,2,4-triazol-4-amine (**1ad**): This compound was prepared similarly using the procedure for the synthesis of **1ac**. A mixture of compound **S2** (630 mg, 2.20 mmol, 1 equiv) and 4-bromobenzyl bromide (821 mg, 4.44 mmol, 1.5 equiv) in DMF (10 mL) was treated with sodium hydride (60% in mineral oil, 105 mg, 2.63 mmol, 1.2 equiv). The crude mixture was purified by flash chromatography (*n*-hexane/EtOAc = 1/1 to 1/4) to give **1ad** (550 mg, 1.21 mmol, 55%) as a pale yellow solid;

mp 145.5–146.1 °C;
TLC R_f = 0.30 ($CHCl_3$/MeOH = 20/1);
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.33 (s, 12H), 4.79 (s, 2H), 6.65 (d, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 2H), 7.45 (d, *J* = 8.8 Hz, 2H), 7.75 (d, *J* = 8.8 Hz, 2H), 8.11 (s, 2H);
^{13}C NMR (100 MHz, $CDCl_3$) δ 25.0 (4C), 58.2, 84.1 (2C), 113.4 (2C), 123.1, 130.1 (2C), 132.5 (2C), 133.6, 136.8 (2C), 143.0 (2C), 149.9 (the signal for the carbon that is attached to the boron atom was not observed);
IR (ZnSe, cm^{-1}) 738, 810, 827, 858, 962, 999, 1008, 1066, 1093, 1126, 1141, 1228, 1268, 1321, 1363, 1402, 1602, 2970;
HRMS (ESI^+) *m*/*z* 455.1246 (455.1248 calcd for $C_{21}H_{25}{}^{11}B^{79}BrN_4O_2^+$, $[M+H]^+$).

Procedure for the production of [^{11}C]NH_4CN and [^{11}C]HCN

The generation of [^{11}C]cyanides and the ^{11}C-cyanation reactions were conducted on an original automated radiolabeling system in RIKEN CLST/BDR (Figure S1). [^{11}C]CH_4 was initially produced in a CYPRIS HM-12S cyclotron (Sumitomo Heavy Industries, Japan) by irradiating N_2 gas containing 15% H_2 (pressured to 0.8 MPa) with a 12 MeV proton beam (30 μA) via the $^{14}N(p,\alpha)^{11}C$ reaction. The irradiation time was basically fixed for 10 min to give [^{11}C]CH_4 with a radioactivity of approximately 10 GBq. For high-radioactivity syntheses of [*cyano*-^{11}C]cetrozole (**[^{11}C]2ac**) and [*cyano*-^{11}C]YM511 (**[^{11}C]2ad**), the irradiation time was extended to 30 min to afford approximately 25 GBq of [^{11}C]CH_4. The generated [^{11}C]CH_4 was transferred with a stream of N_2 gas (300–400 mL/min) from the target vessel in the cyclotron to a hot cell containing the automated radiolabeling system. The [^{11}C]CH_4 was then trapped by passing through a stainless-steel tube equipped with Porapak Q (80–100 mesh, 400 mg) cooled by liquid nitrogen. After condensation of [^{11}C]CH_4, the stainless-steel tube was warmed by an air heater and purged with helium gas at a flow rate of 150 mL/min. The helium gas containing [^{11}C]CH_4 was mixed with the NH_3 gas (30–40 mL/min), and subsequently passed through a preheated quartz tube (inner diam. 6 mm, 990 °C) containing platinum wire (5.4 g, diam. 0.127 mm) to generate [^{11}C]NH_4CN, which was used for the ^{11}C-cyanation reactions as a gas containing an excess amount of NH_3. This gaseous mixture containing [^{11}C]NH_4CN and NH_3 was passed through a vial containing warm aqueous H_2SO_4 (50%, 1.5 mL, 60–70 °C) to remove NH_3, affording [^{11}C]HCN as a gas. The gases containing either [^{11}C]NH_4CN or [^{11}C]HCN was bubbled into a reaction vessel preloaded with the reagents for the following ^{11}C-cyanation reactions.

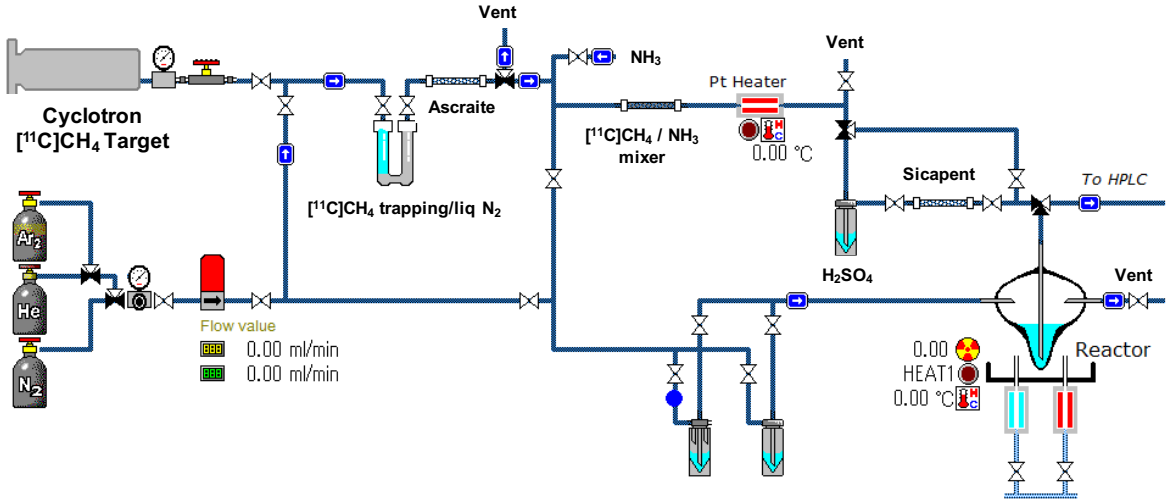
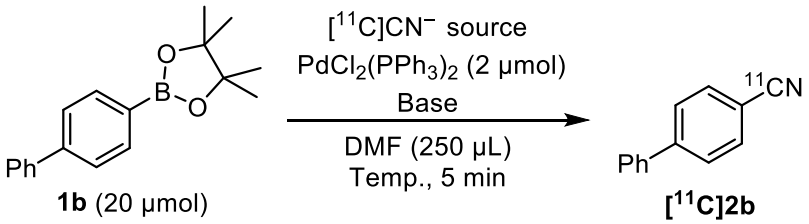


Fig. S1 Experimental setup for palladium-mediated ^{11}C-cyanation.

Palladium(II)-mediated ^{11}C-cyanation of 4-biphenylboronic acid pinacol ester (1b) using various [^{11}C]cyanide sources (Table 2)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 60% **B** (0–15 min), 60–90% **B** (15–20 min), 90% **B** (20–45 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2b**: 4.6 min.

Conditions for the reactions

Entry 1: [^{11}C]NH_4CN used as [^{11}C]cyanide source, NH_3 gas used as base, and reaction conducted at 90 ℃;

Entry 2: [^{11}C]NH_4CN used as [^{11}C]cyanide source, NH_3 gas used as base, and reaction conducted at 100 ℃;

Entry 3: [^{11}C]HCN used as [^{11}C]cyanide source, and aqueous NaOH (2 M, 10 μL, 20 μmol) used as base, and reaction conducted at 100 ℃;

Entry 4: [^{11}C]HCN used as [^{11}C]cyanide source, and K_2CO_3 (2.8 mg, 20 μmol) used as base, and reaction conducted at 100 ℃;

Entry 5: [^{11}C]HCN used as [^{11}C]cyanide source, and aqueous NH_3 (1 M, 20 μL, 20 μmol) used as base, and reaction conducted at 100 ℃.

Entry 6: [^{11}C]HCN used as [^{11}C]cyanide source, without base, and reaction conducted at 100 ℃.

RCYs of each experiment

Run	1	2	3	Average
Entry 1	70%	69%	45%	61 ± 14% (n = 3)
Entry 2	90%	87%	91%	89 ± 2% (n = 3)
Entry 3	64%	58%	55%	59 ± 5% (n = 3)
Entry 4	87%	88%	90%	88 ± 2% (n = 3)
Entry 5	99%	99%	99%	99 ± 0% (n = 3)
Entry 6	trace	trace	trace	trace

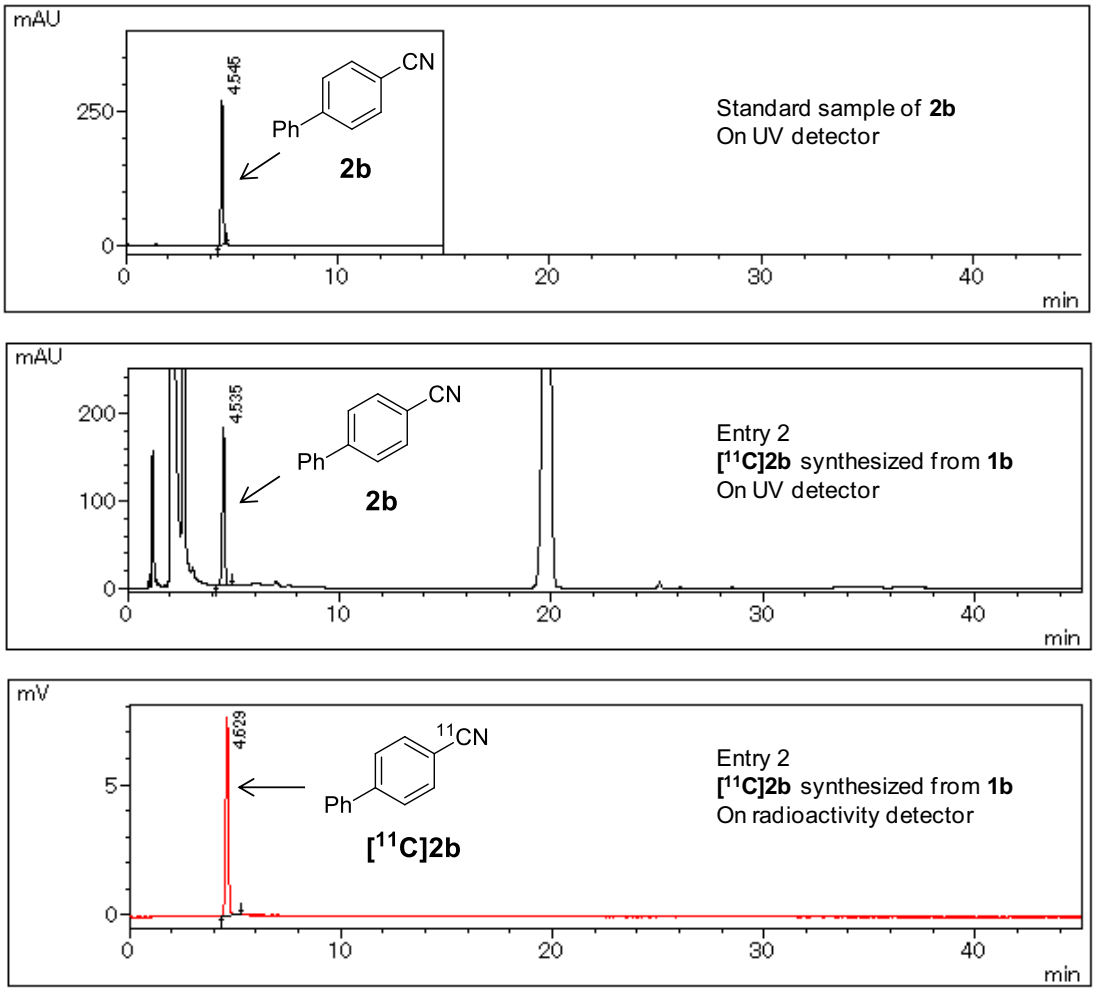


Fig. S2 Representative HPLC chromatograms for the synthesis of **[^{11}C]2b (**Table 2, entry 2).
Top: UV trace of **2b** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2b**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2b**.

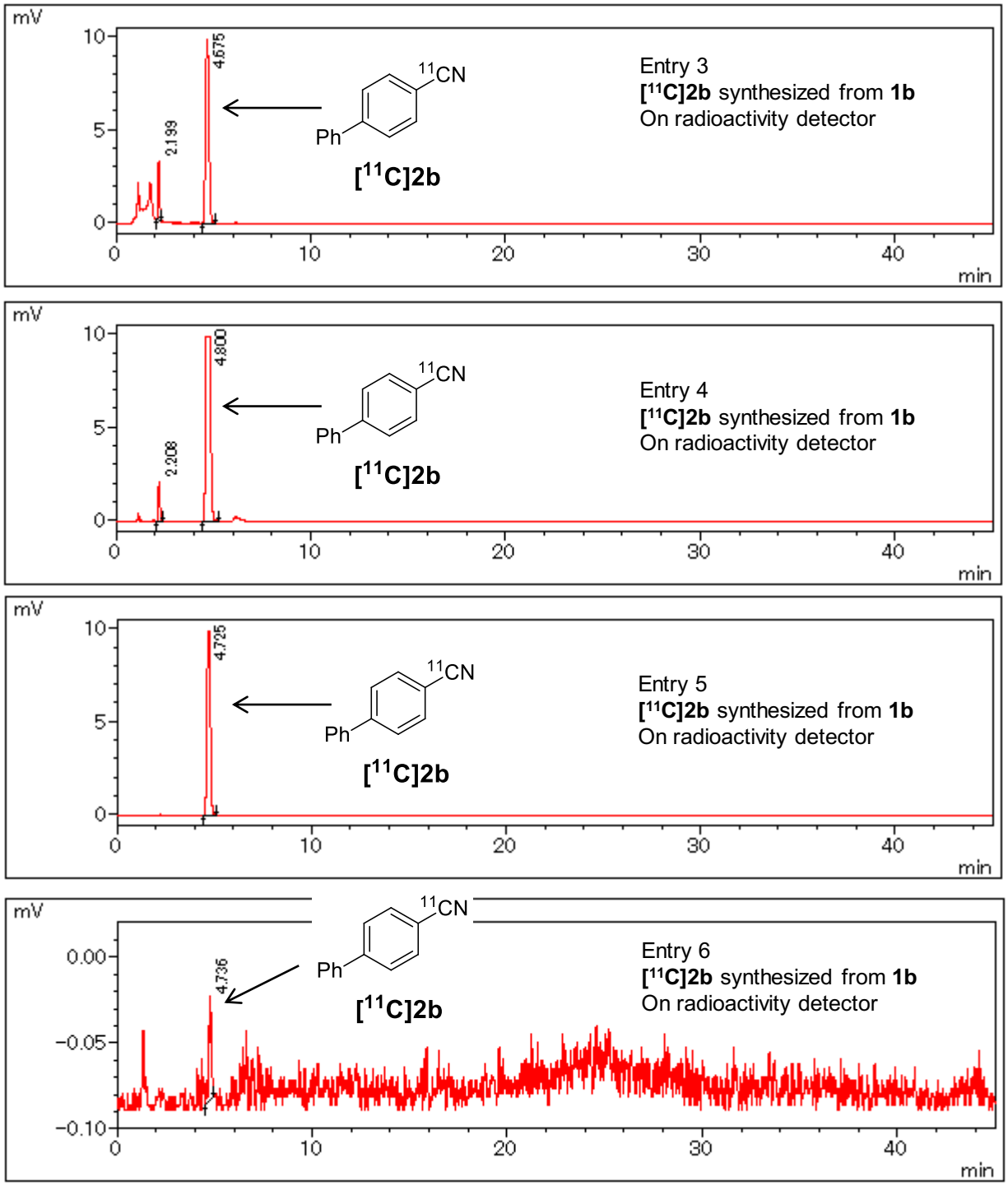
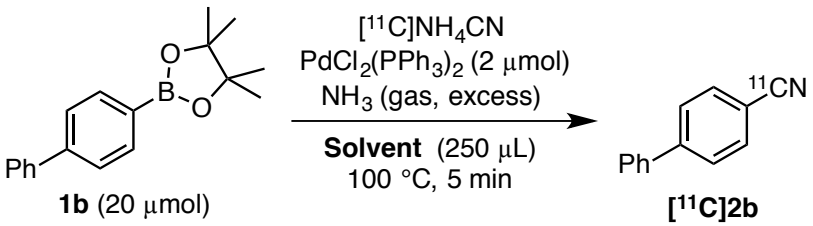


Fig. S3 Representative radio-HPLC chromatograms for the synthesis of **[^{11}C]2b** (Table 2, entries 3–6). RI traces of the reaction mixture of entries 3 (**top**), 4 (**second**), 5 (**third**), and 6 (**bottom**) are shown.

Table S1 Solvent effects on palladium(II)-mediated ^{11}C-cyanation of 1b



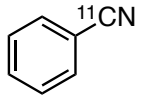
1b (20 μmol) **[^{11}C]2b**

Entry	Solvent	RCY (%)[a]
1	DMF	89 ± 2 (n = 3)[b]
2	DMF (230 μL), H_2O (20 μL)	91 ± 2 (n = 3)[b]
3	DMSO	93 ± 7 (n = 3)[b]
4	DMSO (230 μL), H_2O (20 μL)	87 ± 5 (n = 3)[b]
5	DMA	79 (n = 1)
6	*N*,*N*-Diethylformamide	trace (n = 1)
7	NMP	8 (n = 1)
8	1,4-Dioxane	trace (n = 1)

[a] RCYs based on [^{11}C]NH_4CN were determined by radio-HPLC analysis.
[b] The data were presented as the mean ± SD (n = 3).

Results of palladium(II)-mediated ^{11}C-cyanation of various (hetero)arylborons (Table 3)

[^{11}C]Benzonitrile ([^{11}C]2a)



Entry A: **[^{11}C]2a** was synthesized from phenylboronic acid pinacol ester (**1a**, Table 3A);
Entry B: **[^{11}C]2a** was synthesized from phenylboronic acid neopentyl glycol ester (**1a″**, Table 3A);
Entry C: **[^{11}C]2a** was synthesized from phenylboronic acid (**1a′**, Table 3B).

Conditions for the analytical HPLC
Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 40% **B** (0–15 min), 40–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 220 nm;
Retention time of **[^{11}C]2a**: 4.1 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1a**	98%	96%	91%	95 ± 4% (n = 3)
Entry B: From **1a″**	97%	96%	92%	95 ± 3% (n = 3)
Entry C: From **1a′**	85%	97%	100%	94 ± 8% (n = 3)

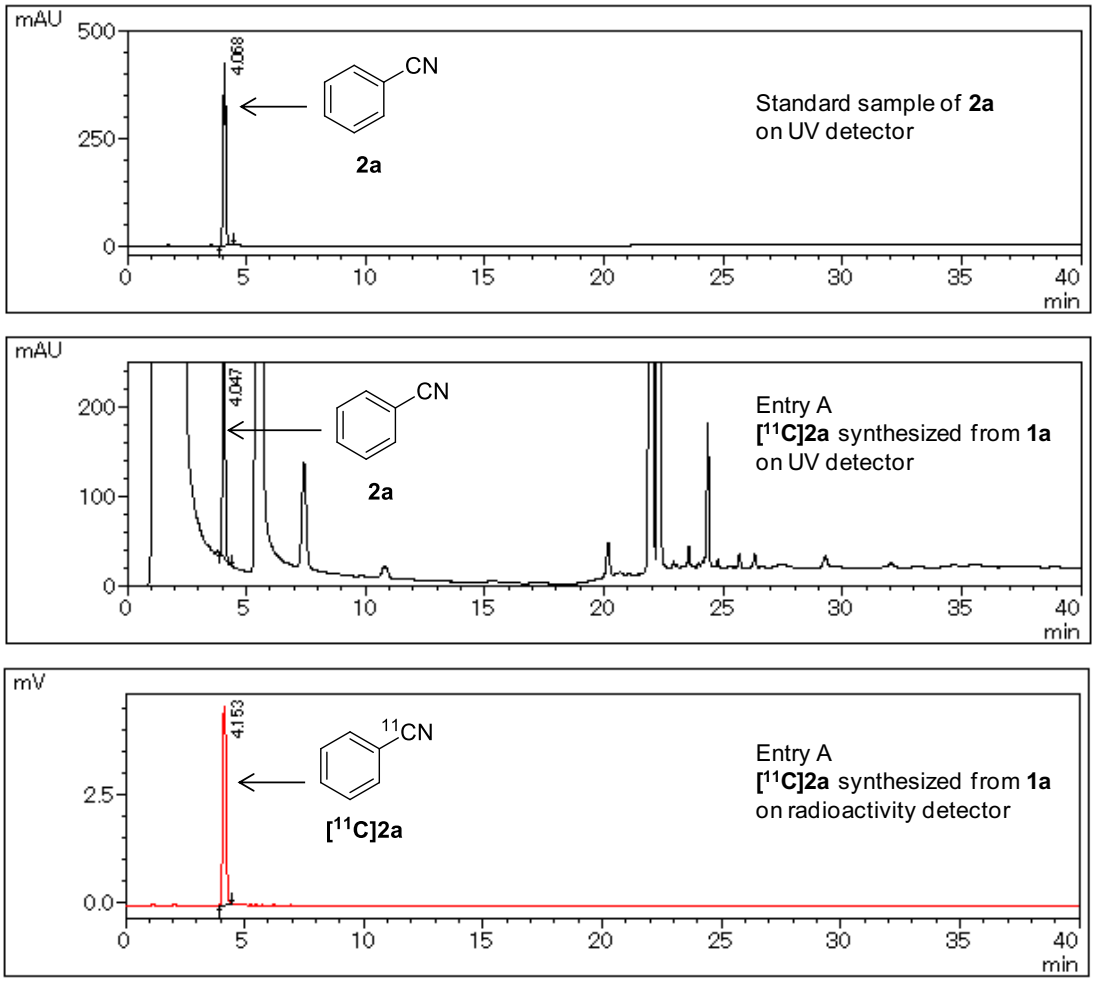


Fig. S4 Representative HPLC chromatograms for the synthesis of **[^{11}C]2a** (Entry A).
Top: UV trace of **2a** as an authentic reference.
Middle: UV trace of the reaction mixture using **1a** as a substrate, containing **[^{11}C]2a**.
Bottom: RI trace of the reaction mixture using **1a** as a substrate, containing **[^{11}C]2a**.

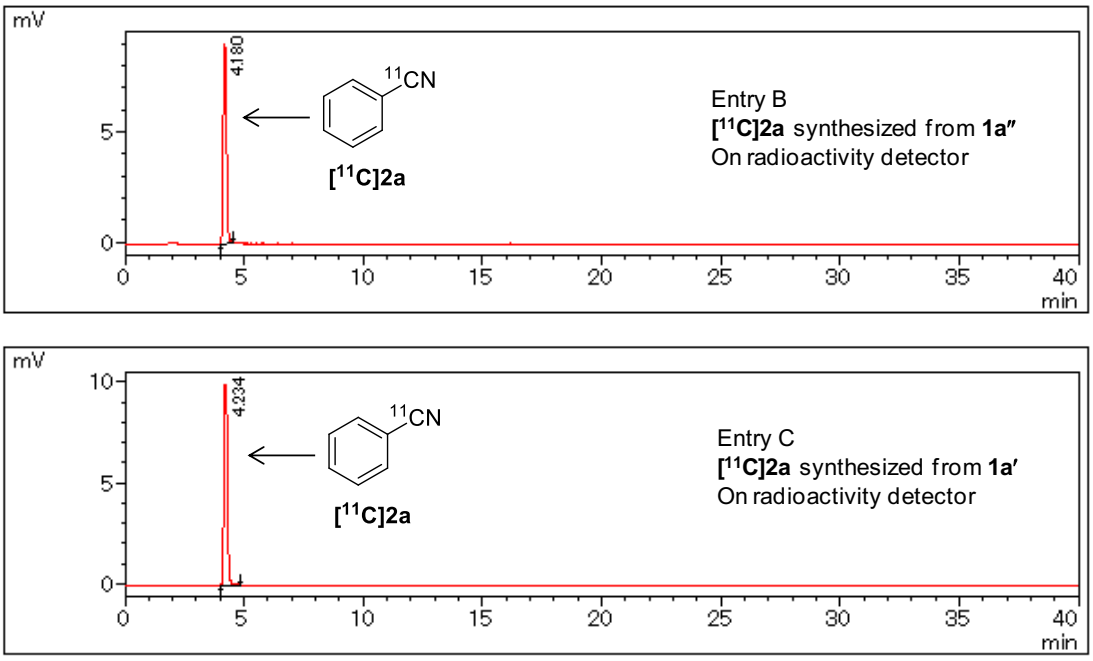
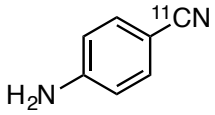


Fig. S5 Representative radio-HPLC chromatograms for the synthesis of **[^{11}C]2a**.
Top: RI trace of the reaction mixture using **1a″** as a substrate, containing **[^{11}C]2a** (Entry B).
Bottom: RI trace of the reaction mixture using **1a′** as a substrate, containing **[^{11}C]2a** (Entry C).

[^{11}C]4-Cyanoaniline ([^{11}C]2c)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 25% **B** (0–15 min), 25–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 230 nm;

Retention time of **[^{11}C]2c**: 4.0 min.

RCYs of each experiment

Run	1	2	3	Average
From **1c**	86%	100%	97%	94 ± 7% (n = 3)

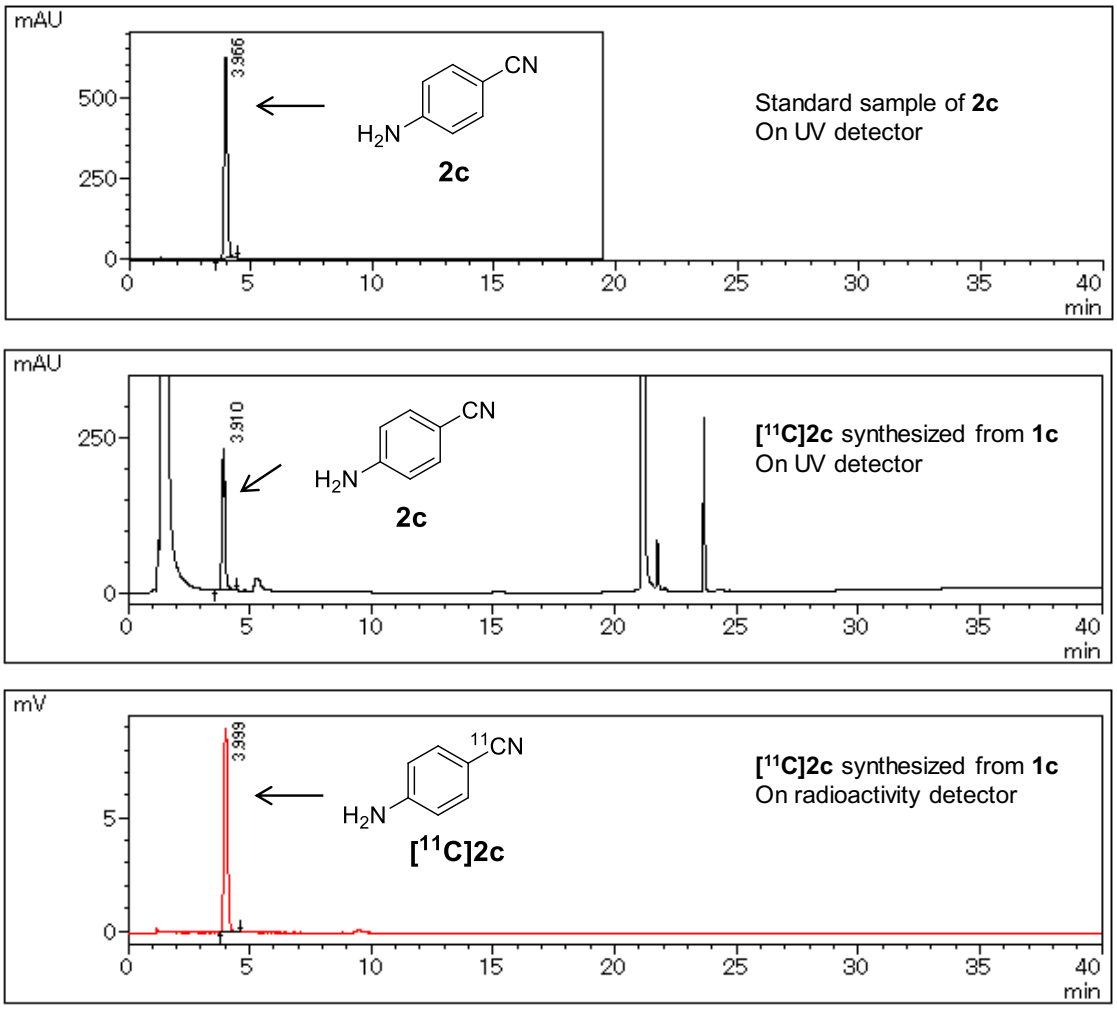
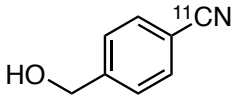


Fig. S6 Representative HPLC chromatograms.
Top: UV trace of **2c** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2c**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2c**.

[^{11}C]4-Hydroxymethylbenzonitrile ([^{11}C]2d)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 20% **B** (0–15 min), 20–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 230 nm;

Retention time of **[^{11}C]2d**: 4.1 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1d**	10%	–	–	10% (n = 1)
Entry B: From **1d**[a]	80%	94%	93%	89 ± 8% (n = 3)

[a] The reaction was conducted in presence of K_2CO_3 (20 μmol).

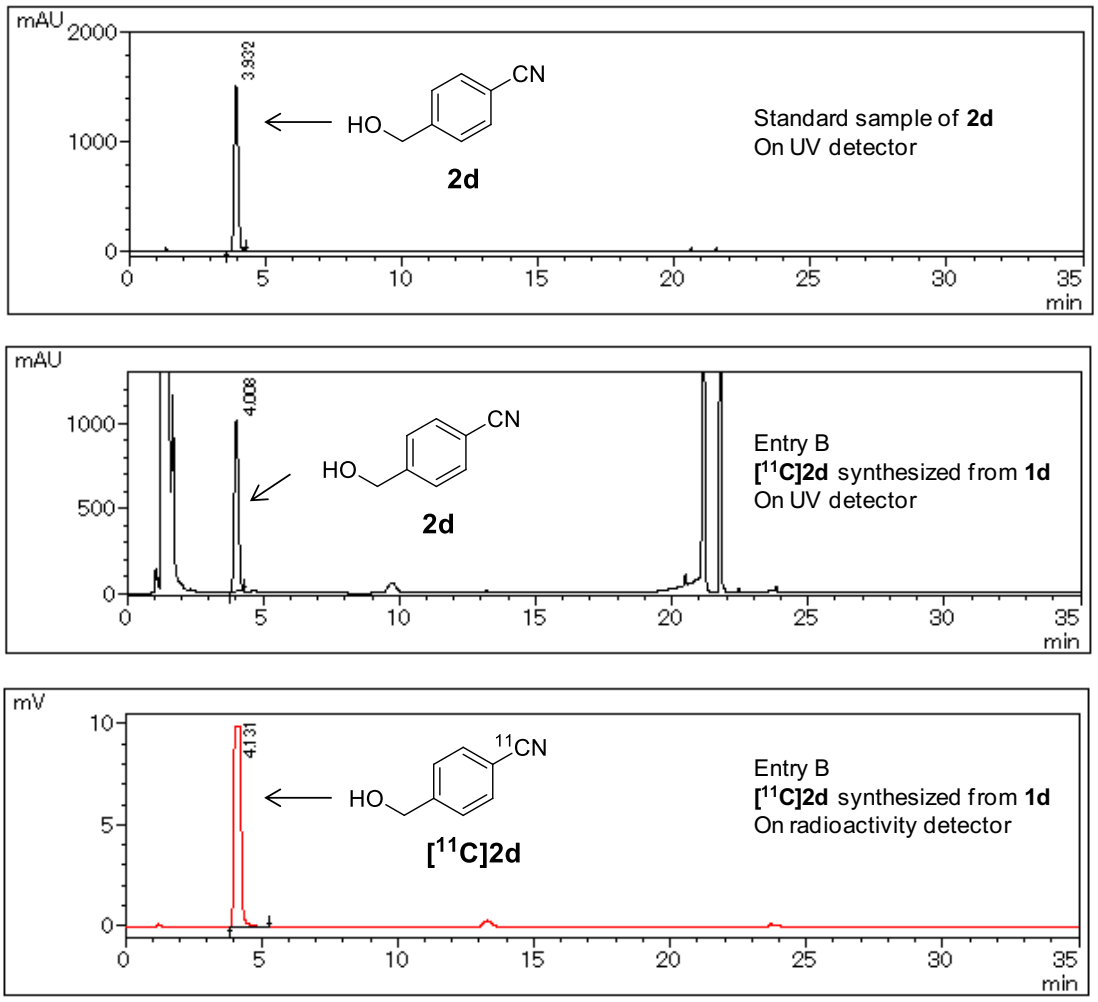
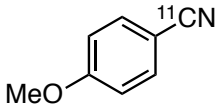


Fig. S7 Representative HPLC chromatograms for the synthesis of **[^{11}C]2d** (Entry B).
Top: UV trace of **2d** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2d**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2d**.

[^{11}C]4-Cyanoanisole ([^{11}C]2e)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 40% **B** (0–15 min), 40–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2e**: 4.7 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1e**	68%	66%	–	67 ± 1% (n = 2)
Entry B: From **1e**[a]	100%	94%	100%	98 ± 4% (n = 3)

[a] The reaction was conducted at 110 °C.

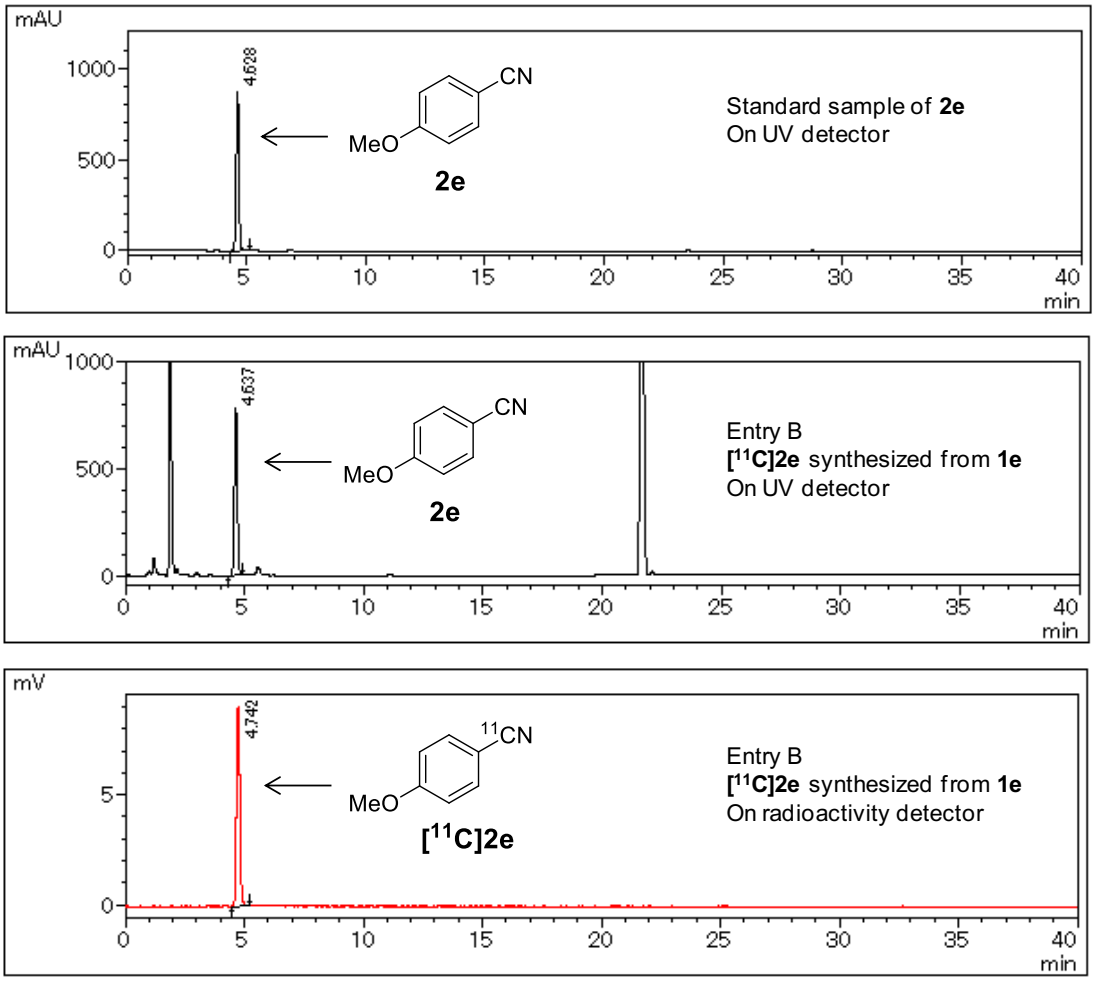
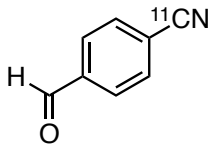


Fig. S8 Representative HPLC chromatograms for the synthesis of **[^{11}C]2e** (Entry B).
Top: UV trace of **2e** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2e**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2e**.

[^{11}C]4-Cyanobenzaldehyde ([^{11}C]2f)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 30% **B** (0–15 min), 30–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 250 nm;

Retention time of **[^{11}C]2f**: 4.6 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1f**	39%	–	–	39% (n =1)
Entry B: From **1f**[a]	69%	53%	64%	62 ± 8% (n = 3)

[a] The reaction was conducted in presence of K_2CO_3 (20 μmol).

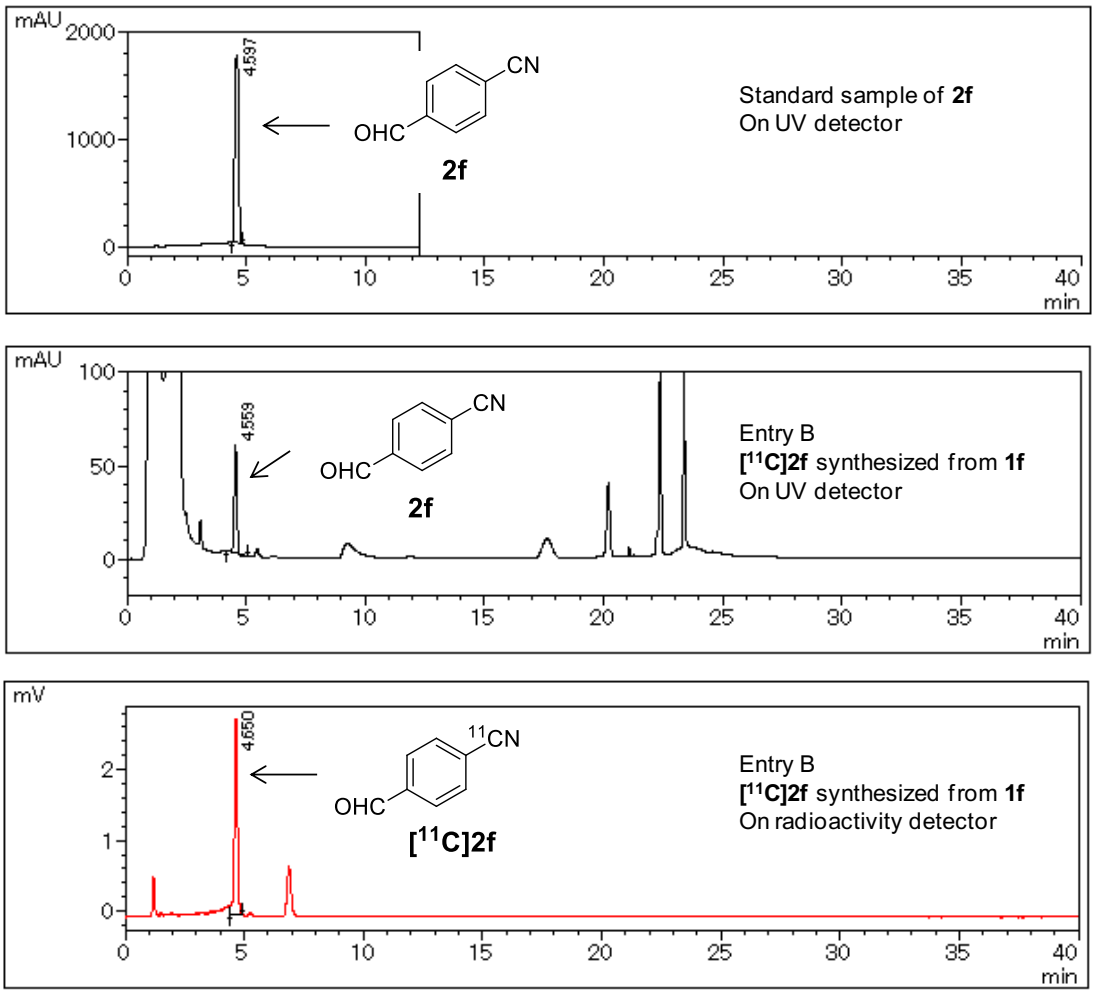
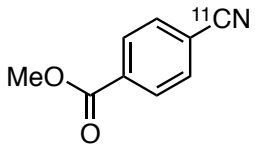


Fig. S9 Representative HPLC chromatograms for the synthesis of **[^{11}C]2f** (Entry B).
Top: UV trace of **2f** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2f**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2f**.

[^{11}C]Methyl 4-cyanobenzoate ([^{11}C]2g)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 35% **B** (0–15 min), 35–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 250 nm;
Retention time of **[^{11}C]2g**: 4.8 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1g**	99%	97%	95%	97 ± 2% (n = 3)
Entry B: From **1g′**	94%	90%	91%	92 ± 2% (n = 3)

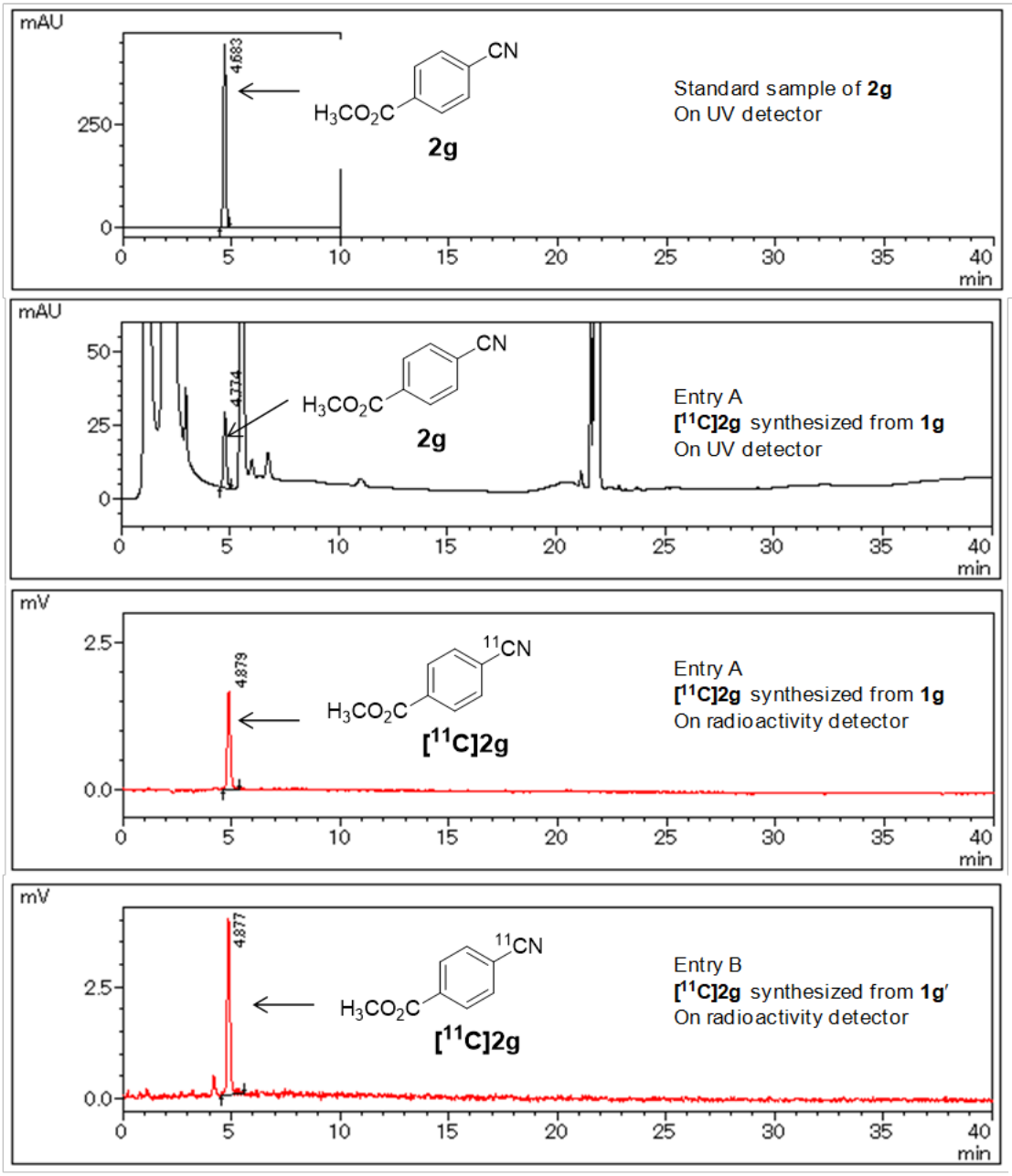
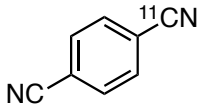


Fig. S10 Representative HPLC chromatograms for the synthesis of **[^{11}C]2g**.
Top: UV trace of **2g** as an authentic reference.
Second: UV trace of the reaction mixture using **1g** as a substrate, containing **[^{11}C]2g** (Entry A).
Third: RI trace of the reaction mixture using **1g** as a substrate, containing **[^{11}C]2g** (Entry A).
Bottom: RI trace of the reaction mixture using **1g′** as a substrate, containing **[^{11}C]2g** (Entry B).

[1-*cyano*-^{11}C]*p*-Dicyanobenzene ([^{11}C]2h)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 35% **B** (0–15 min), 35–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 240 nm;

Retention time of **[^{11}C]2h**: 4.2 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1h**	20%	–	–	20% (n =1)
Entry B: From **1h**[a]	82%	93%	70%	82 ± 12% (n = 3)
Entry C: From **1h′**[a]	80%	97%	87%	88 ± 9% (n = 3)

[a] The reaction was conducted at 110 °C.

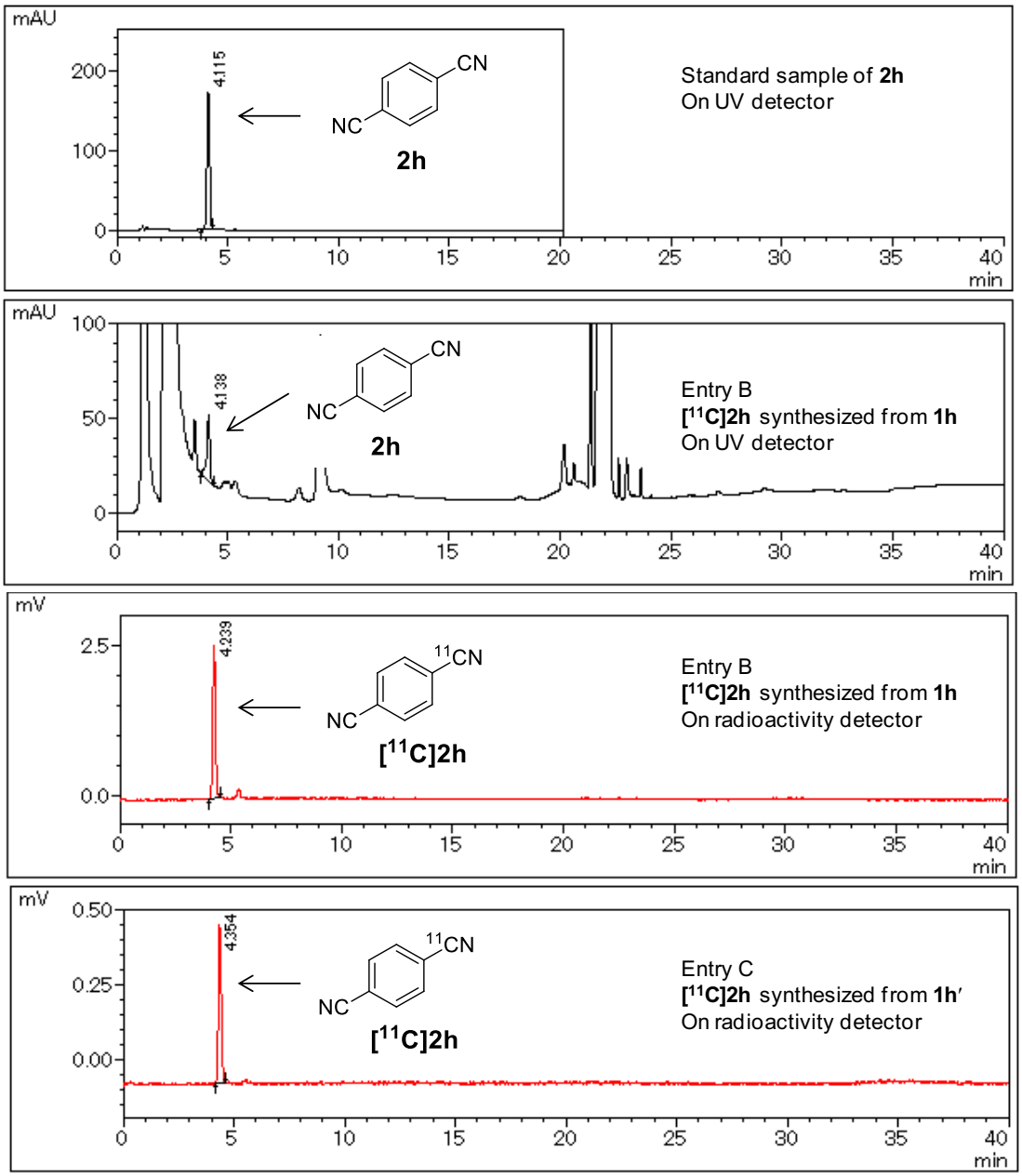
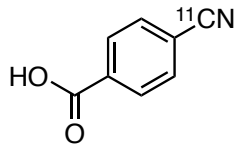


Fig. S11 Representative HPLC chromatograms for the synthesis of **[^{11}C]2h**.
Top: UV trace of **2h** as an authentic reference.
Second: UV trace of the reaction mixture using **1h** as a substrate, containing **[^{11}C]2h** (Entry B).
Third: RI trace of the reaction mixture using **1h** as a substrate, containing **[^{11}C]2h** (Entry B).
Bottom: RI trace of the reaction mixture using **1h′** as a substrate, containing **[^{11}C]2h** (Entry C).

[^{11}C]4-Cyanobenzoic acid ([^{11}C]2i)



Conditions for the analytical HPLC

Mobile phase **A** = phosphate buffer (20 mmol/L (mM), pH 2.5), mobile phase **B** = acetonitrile;
Gradient method: 25% **B** (0–15 min), 25–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 250 nm;
Retention time of **[^{11}C]2i**: 4.3 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1i**	9%	–	–	9% (n = 1)
Entry B: From **1i**[a]	38%	11%	17%	22 ± 14% (n = 3)
Entry C: From **1i**[b]	50%	–	–	50% (n =1)
Entry D: From **1i**[b,c]	81%	60%	65%	69 ± 11% (n = 3)

[a] The reaction was conducted in the presence of K_2CO_3 (20 μmol).
[b] The reaction was conducted at 110 °C, in the presence of **1i** (40 μmol) and K_2CO_3 (70 μmol).
[c] $PdCl_2(P(o\text{-Tol})_3)_2$ (2 μmol) was used instead of $PdCl_2(PPh_3)_2$.

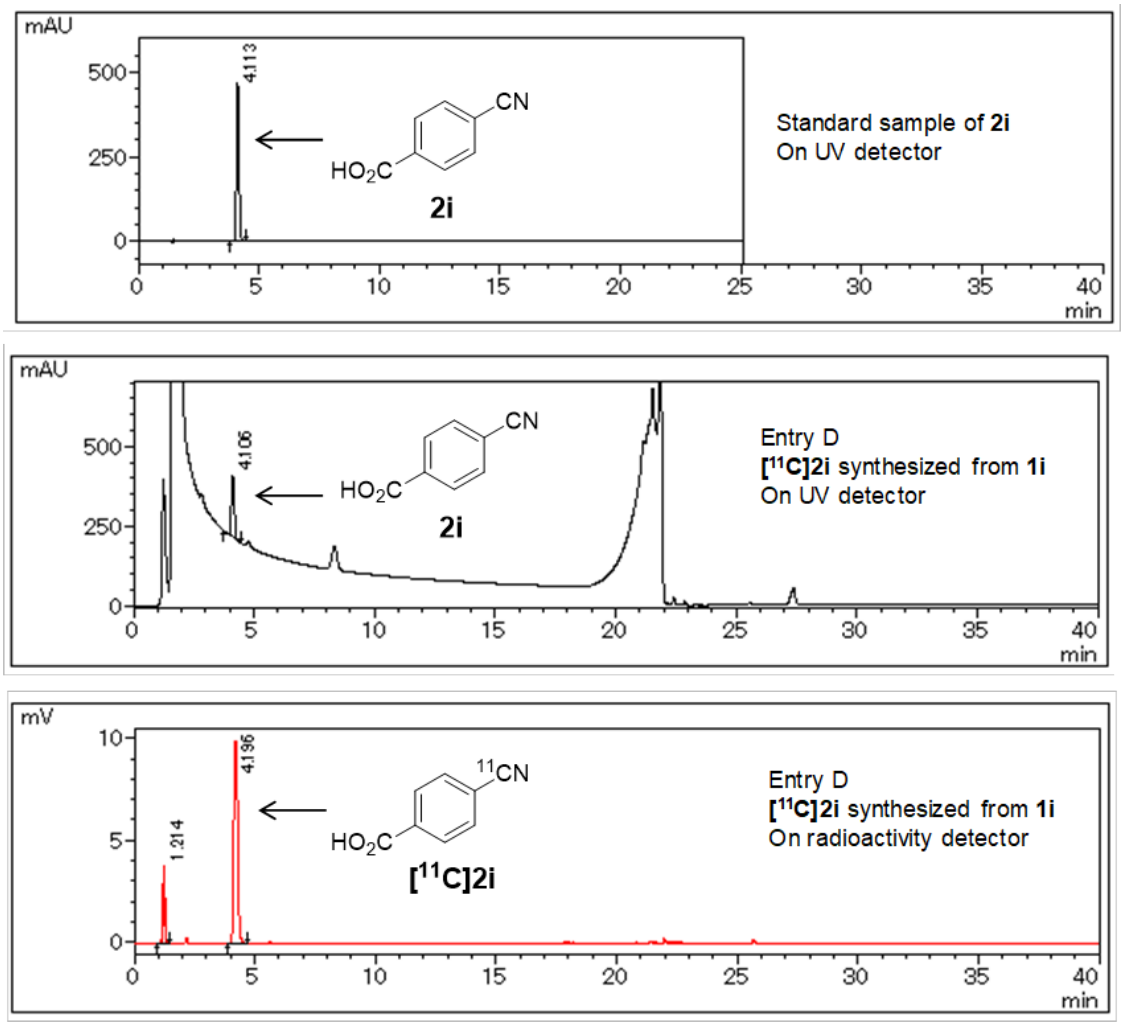
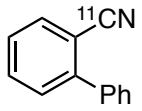


Fig. S12 Representative HPLC chromatograms for the synthesis of **[^{11}C]2i** (Entry D).
Top: UV trace of **2i** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2i**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2i**.

[^{11}C]2-Cyanobiphenyl ([^{11}C]2j)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 60% **B** (0–15 min), 60–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2j**: 3.7 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1j**	8%	–	–	8% (n = 1)
Entry B: From **1j**[a]	68%	84%	85%	79 ± 10% (n = 3)

[a] The reaction was conducted at 110 °C in the presence of K_2CO_3 (20 μmol).

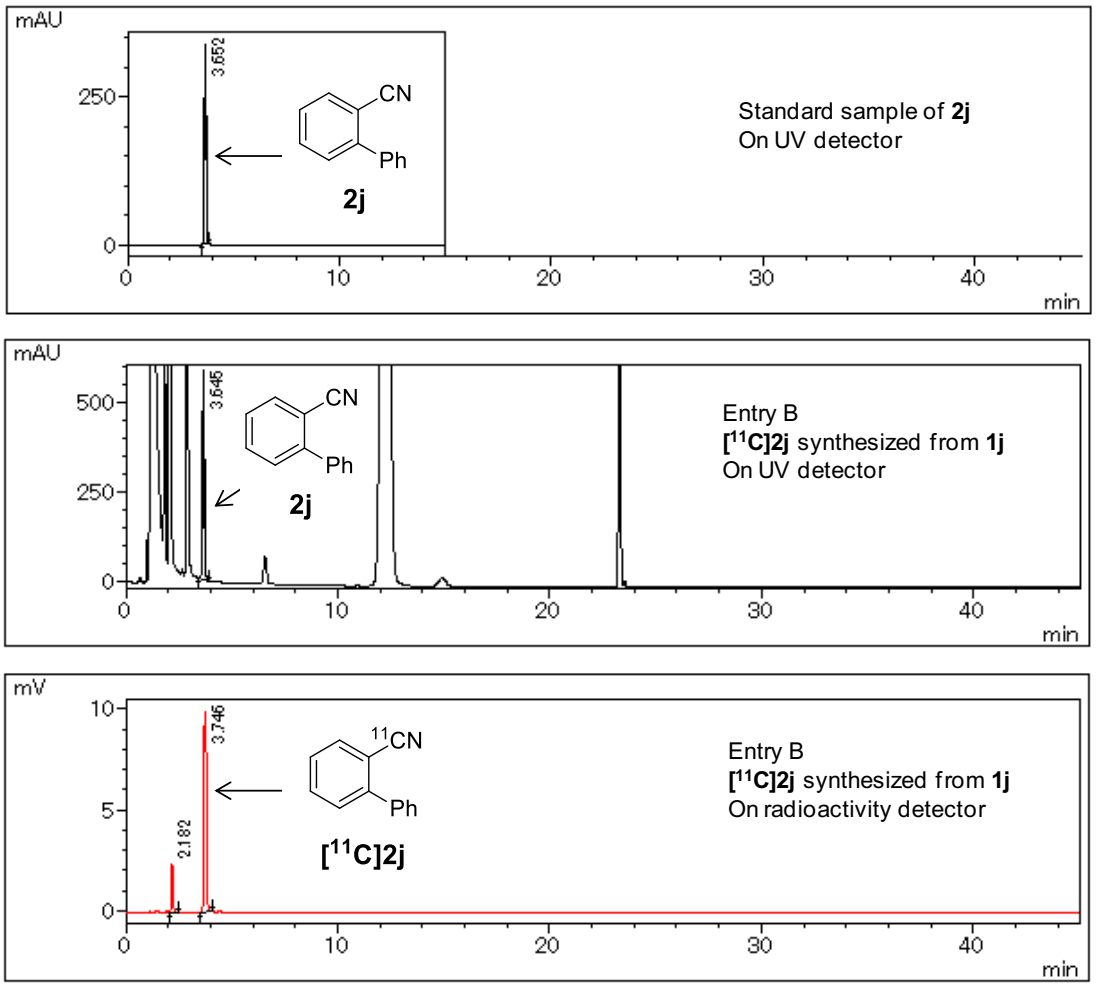
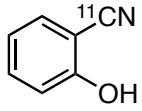


Fig. S13 Representative HPLC chromatograms for the synthesis of **[^{11}C]2j** (Entry B).
Top: UV trace of **2j** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2j**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2j**.

[^{11}C]2-Cyanophenol ([^{11}C]2k)



The reaction was conducted at 110 °C in the presence of K_2CO_3 (20 μmol).

Conditions for the analytical HPLC

Mobile phase **A** = phosphate buffer (20 mM, pH 2.5), mobile phase **B** = acetonitrile;
Gradient method: 28% **B** (0–15 min), 28–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 220 nm;
Retention time of **[^{11}C]2k**: 4.0 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1k**	62%	–	–	62% (n = 1)
Entry B: From **1k**[a]	72%	89%	89%	83 ± 10% (n = 3)

[a] PPh_3 (10 μmol) was added.

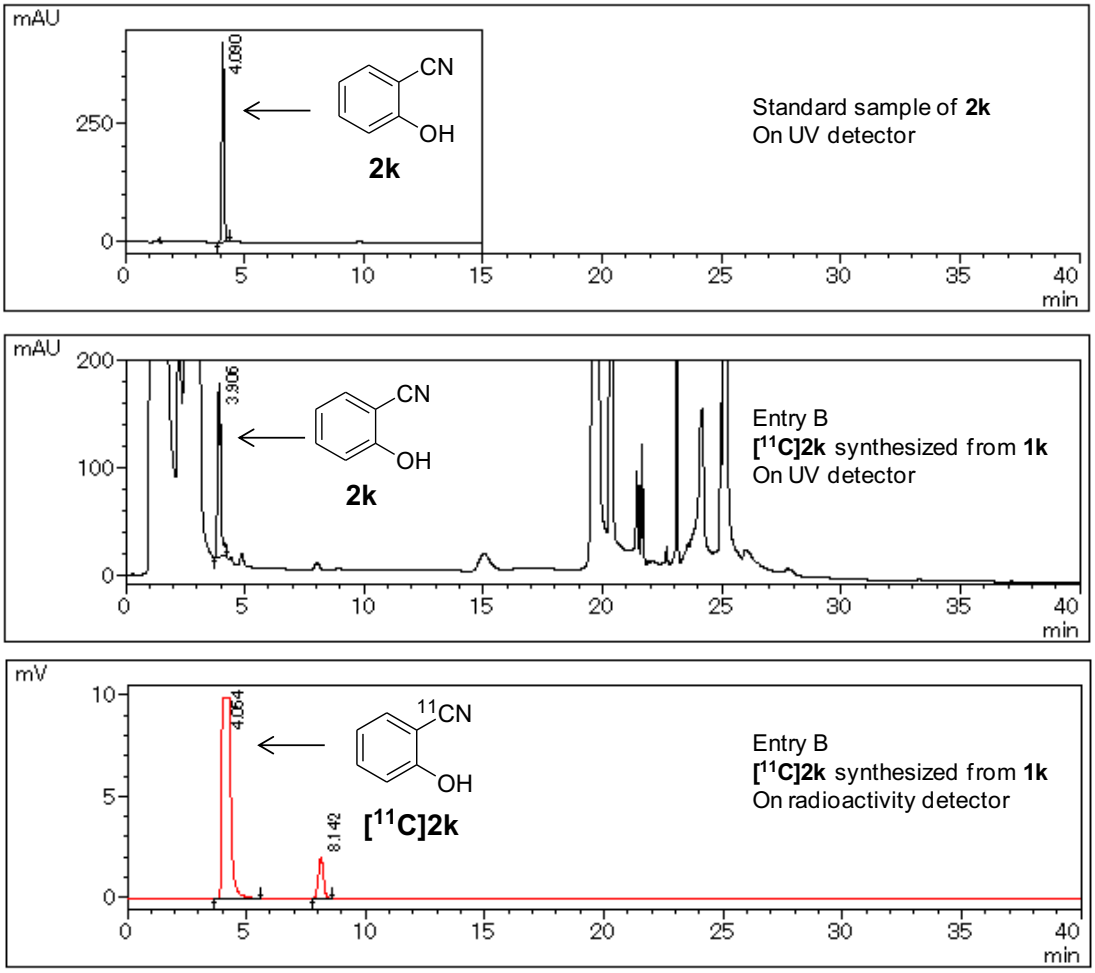
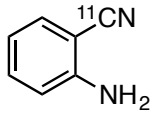


Fig. S14 Representative HPLC chromatograms for the synthesis of **[^{11}C]2k** (Entry B).
Top: UV trace of **2k** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2k**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2k**.

[^{11}C]2-Cyanoaniline ([^{11}C]2l)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 30% **B** (0–15 min), 30–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2l**: 4.5 min.

RCYs of each experiment

Run	1	2	3	Average
From **1l**	100%	99%	97%	99 ± 2% (n = 3)

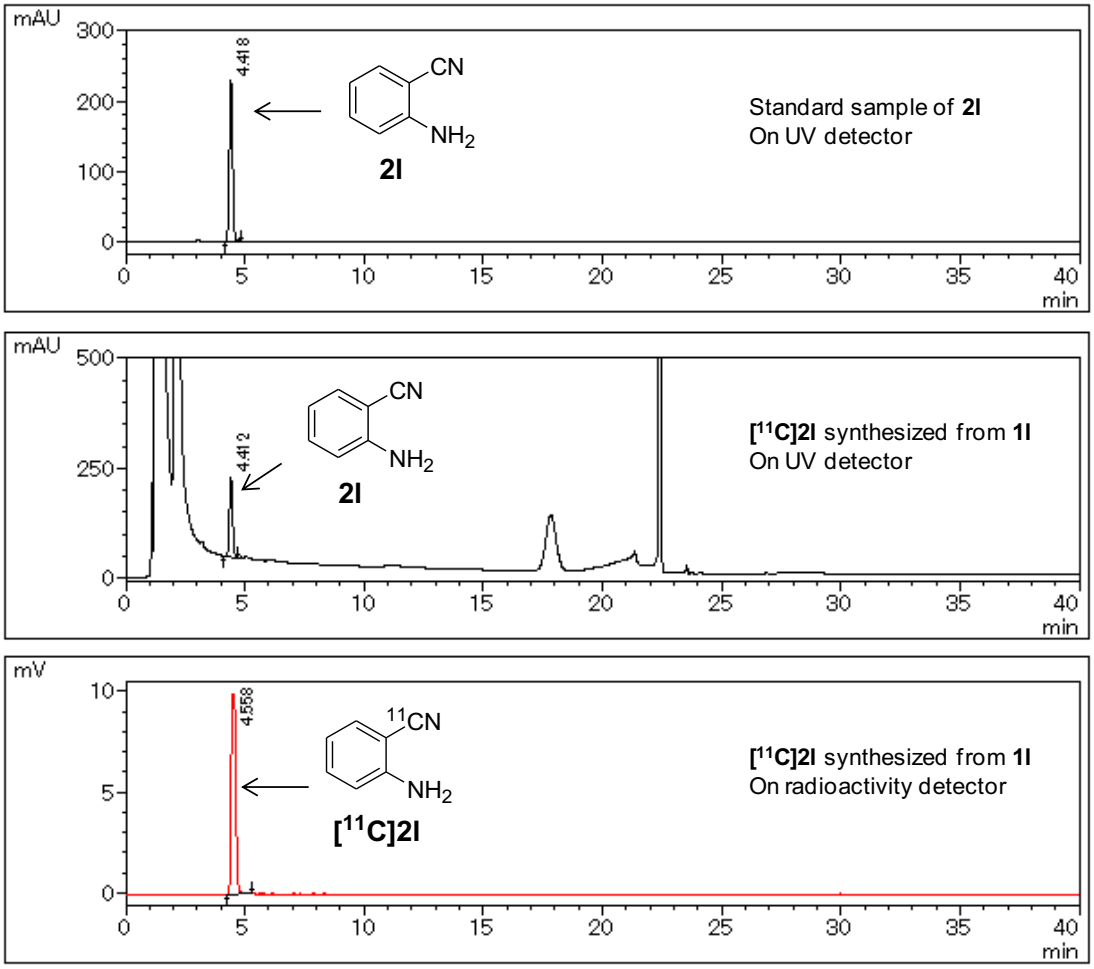
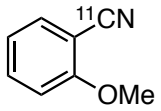


Fig. S15 Representative HPLC chromatograms for the synthesis of **[^{11}C]2l**.
Top: A UV trace of **2l** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2l**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2l**.

[^{11}C]2-Cyanoanisole ([^{11}C]2m)



The reaction was conducted at 110 °C.

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 40% **B** (0–15 min), 40–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 220 nm;
Retention time of **[^{11}C]2m**: 4.3 min.

RCYs of each experiment

Run	1	2	3	Average
From **1m**	87%	91%	93%	90 ± 3% (n = 3)

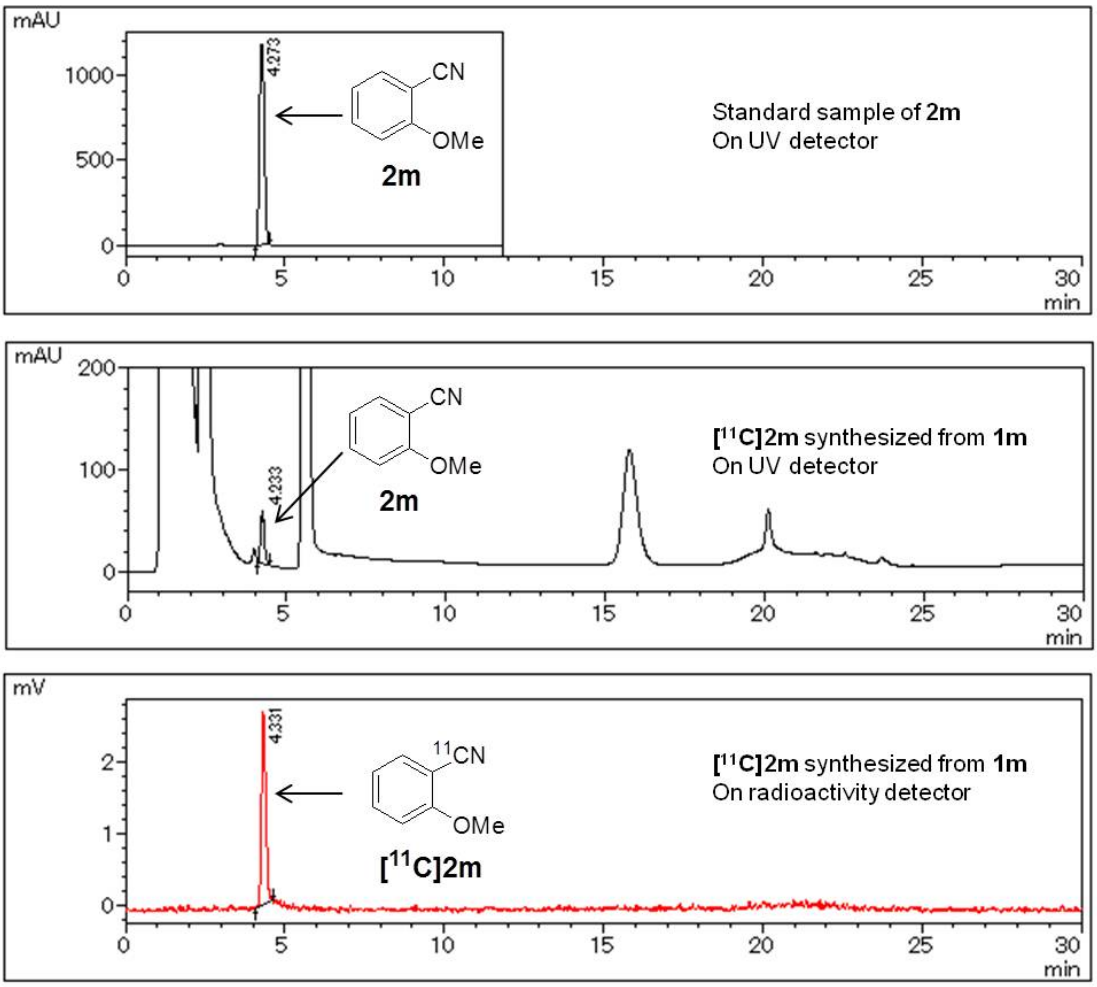
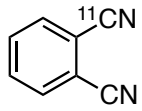


Fig. S16 Representative HPLC chromatograms for the synthesis of **[^{11}C]2m**.
Top: A UV trace of **2m** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2m**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2m**.

[1-*cyano*-^{11}C]*o*-Dicyanobenzene ([^{11}C]2n)



The reaction was conducted at 110 °C.

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 35% **B** (0–15 min), 35–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 220 nm;
Retention time of **[^{11}C]2n**: 4.3 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1n**	46%	45%	48%	46 ± 2% (n = 3)
Entry B: From **1n**[a]	46%	–	–	46% (n = 1)[b]
Entry C: From **1n**[a,c]	70%	73%	71%	71 ± 2% (n = 3)

[a] K_2CO_3 (20 μmol) was added.
[b] [^{11}C]Benzonitrile (**[^{11}C]2a**) was formed as a byproduct (retention time: 5.3 min, RCY: 21%).
[c] PPh_3 (10 μmol) was added.

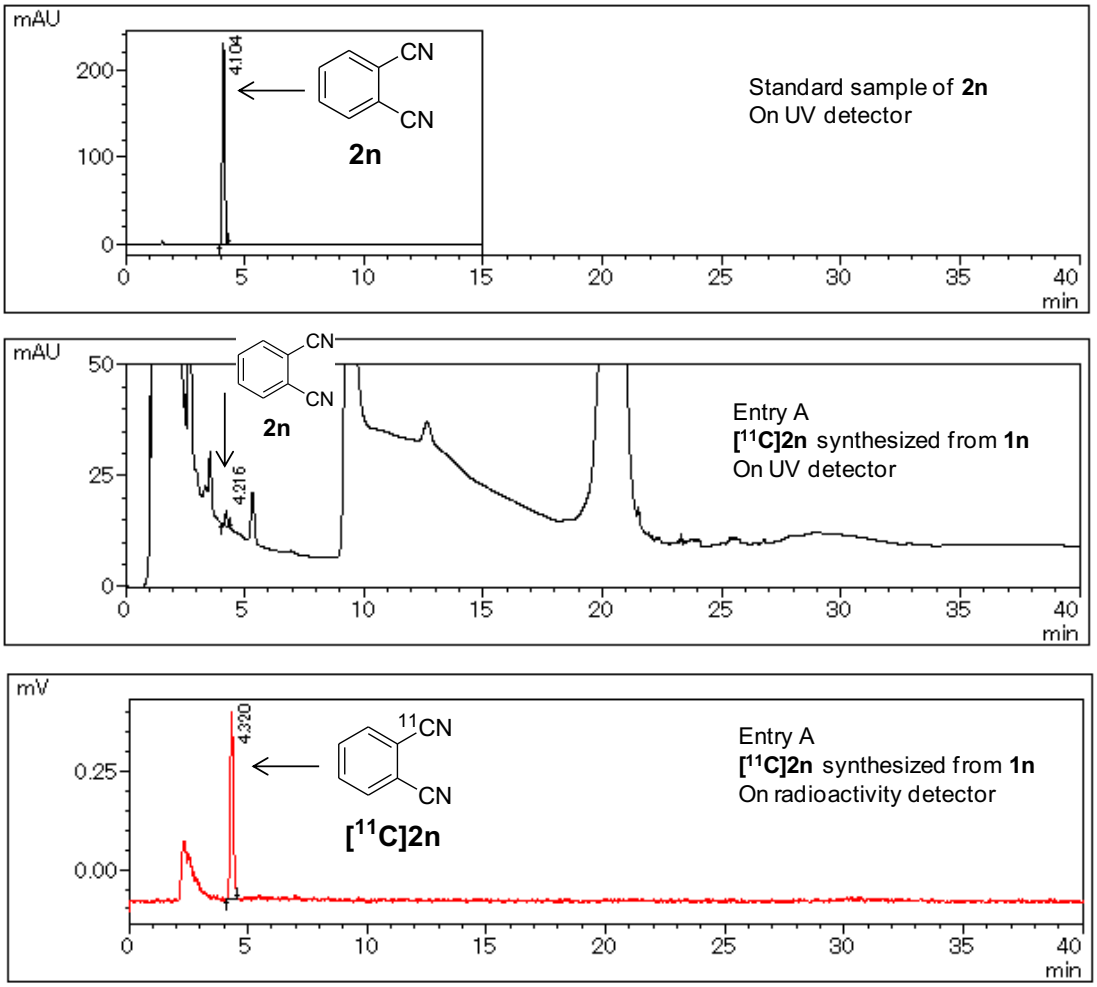


Fig. S17 Representative HPLC chromatograms for the synthesis of **[^{11}C]2n**.
Top: A UV trace of **2n** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2n** (Entry A).
Bottom: RI trace of the reaction mixture containing **[^{11}C]2n** (Entry A).

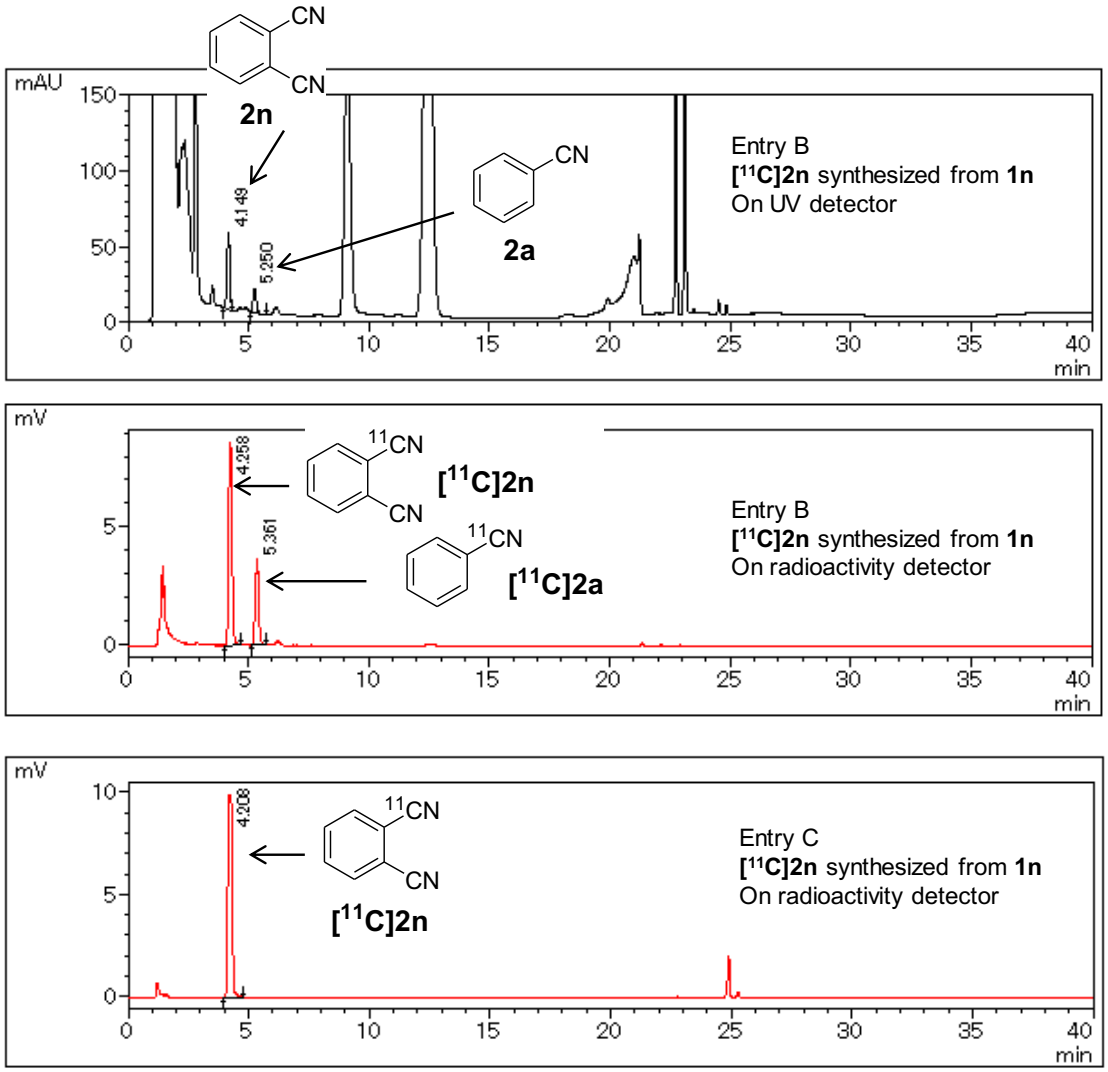
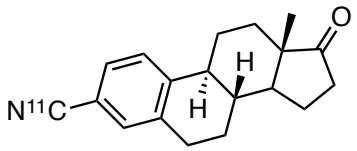


Fig. S18 Representative HPLC chromatograms for the synthesis of **[^{11}C]2n**.
Top: UV trace of the reaction mixture containing **[^{11}C]2n** and **[^{11}C]2a** (Entry B).
Middle: RI trace of the reaction mixture containing **[^{11}C]2n** and **[^{11}C]2a** (Entry B).
Bottom: RI trace of the reaction mixture containing **[^{11}C]2n** (Entry C).

[^{11}C]3-Dehydroxy-3-cyanoestrone ([^{11}C]2o)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 65% **B** (0–15 min), 65–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 250 nm;

Retention time of **[^{11}C]2o**: 4.2 min.

RCYs of each experiment

Run	1	2	3	Average
From **1o**	91%	89%	98%	93 ± 5% (n = 3)

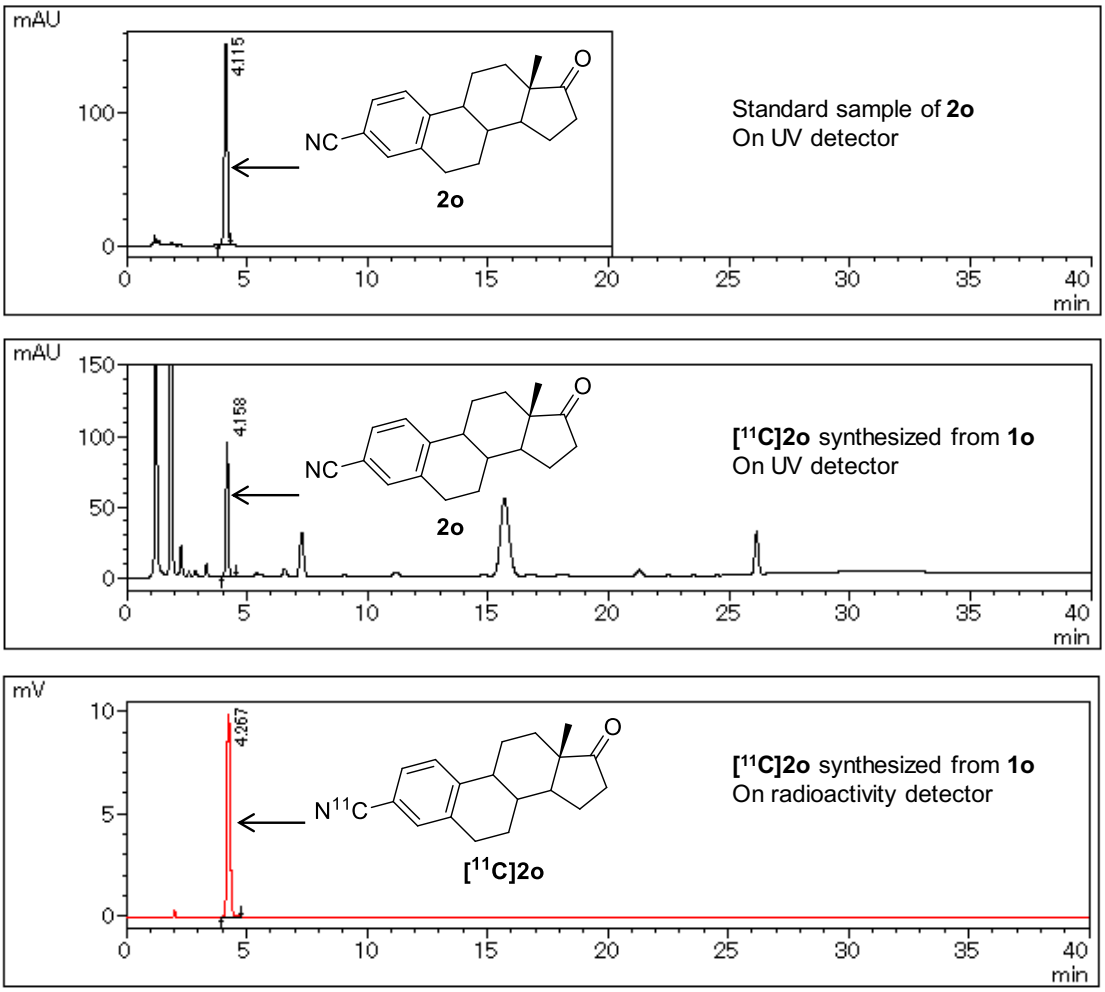
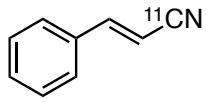


Fig. S19 Representative HPLC chromatograms for the synthesis of **[^{11}C]2o**.
Top: UV trace of **2o** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2o**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2o**.

[^{11}C]Cinnamonitrile ([^{11}C]2p)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 45% **B** (0–15 min), 45–90% **B** (15–20 min), 90% **B** (20–45 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 220 nm;

Retention time of **[^{11}C]2p**: 5.0 min.

RCYs of each experiment

Run	1	2	3	Average
From **1p**	89%	97%	99%	95 ± 5% (n = 3)

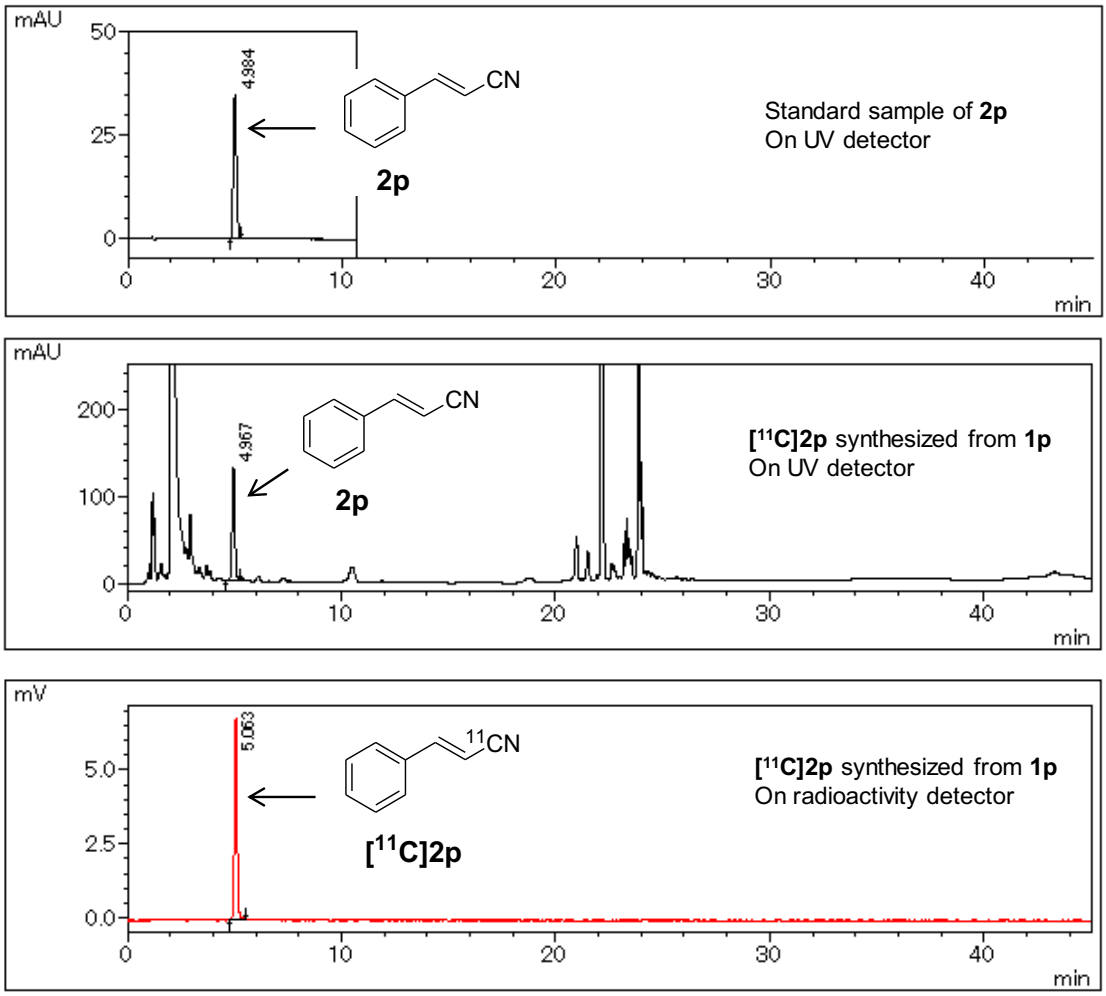
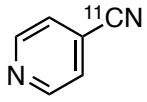


Fig. S20 Representative HPLC chromatograms for the synthesis of **[^{11}C]2p**.
Top: UV trace of **2p** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2p**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2p**.

[^{11}C]4-Cyanopyridine ([^{11}C]2q)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 15% **B** (0–15 min), 15–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2q**: 3.3 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1q**	10%	–	–	10% (n = 1)
Entry B: From **1q**[a]	47%	36%	–	42 ± 8% (n = 2)
Entry C: From **1q**[b]	100%	100%	98%	99 ± 1% (n = 3)

[a] The reaction was conducted in the presence of K_2CO_3 (20 μmol).

[b] The reaction was conducted in the presence of K_2CO_3 (20 μmol) and PPh_3 (10 μmol).

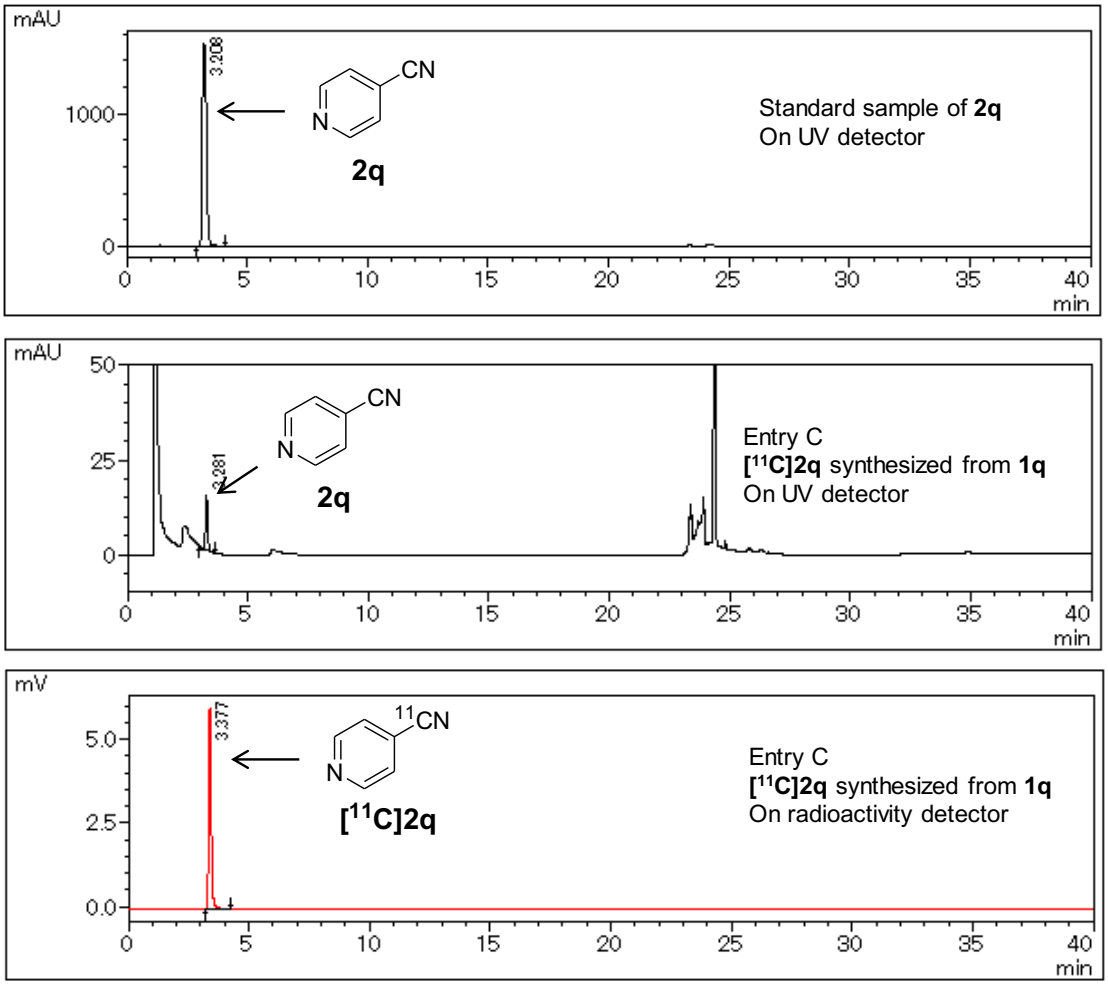
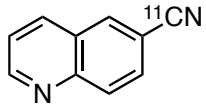


Fig. S21 Representative HPLC chromatograms for the synthesis of **[^{11}C]2q** (Entry C).
Top: UV trace of **2q** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2q**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2q**.

[^{11}C]6-Cyanoquinoline ([^{11}C]2r)



The reaction was conducted in the presence of K_2CO_3 (20 μmol).

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 30% **B** (0–15 min), 30–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;
Retention time of **[^{11}C]2r**: 4.0 min.

RCYs of each experiment

Run	1	2	3	Average
From **1r**	89%	94%	88%	90 ± 3% (n = 3)

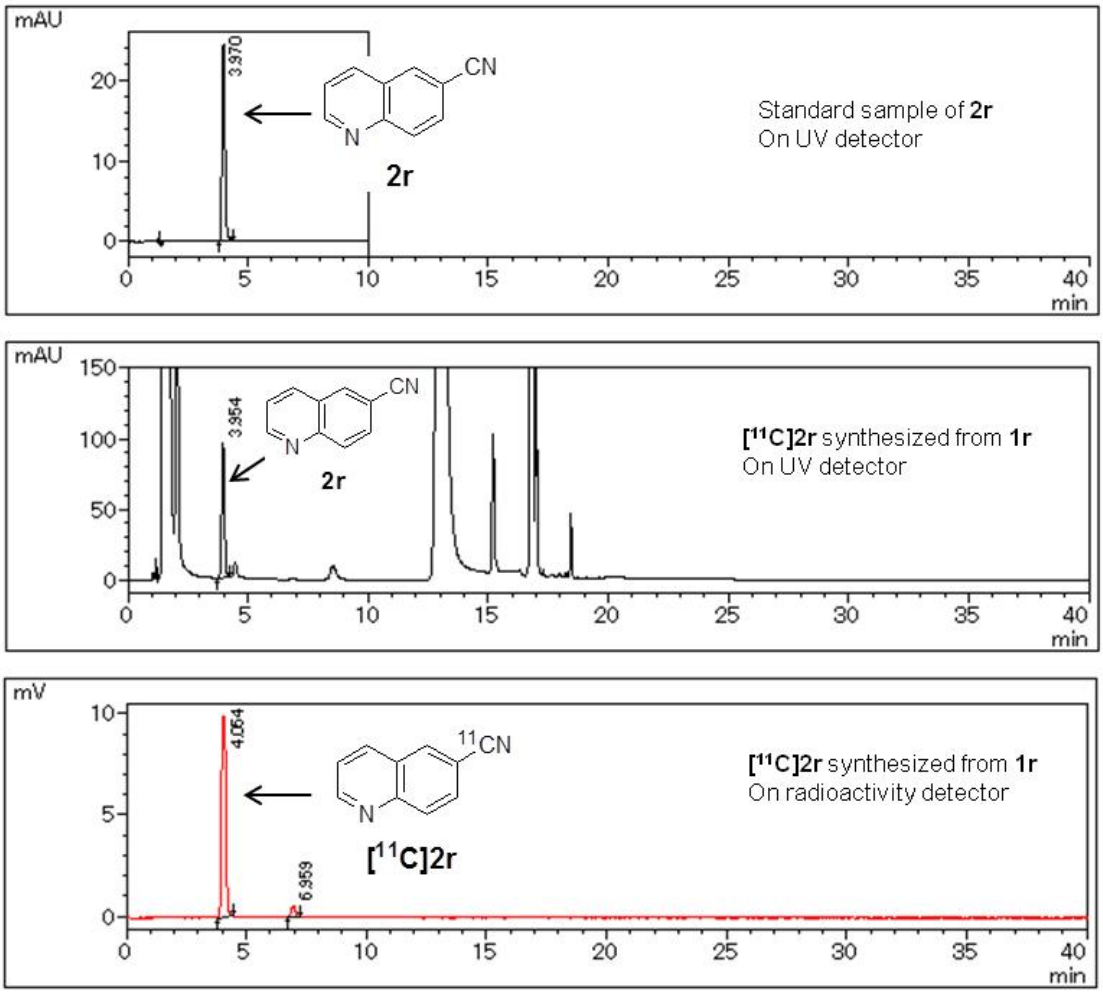
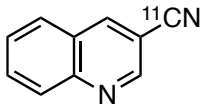


Fig. S22 Representative HPLC chromatograms for the synthesis of **[^{11}C]2r**.
Top: UV trace of **2r** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2r**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2r**.

[^{11}C]3-Cyanoquinoline ([^{11}C]2s)



The reaction was conducted in presence of K_2CO_3 (20 μmol).

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 37% **B** (0–15 min), 37–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 274 nm;

Retention time of **[^{11}C]2s**: 4.0 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A: From **1s**	82%	80%	90%	84 ± 5% (n = 3)
Entry B: From **1s′**	70%	50%	32%	51 ± 19% (n = 3)[a]
Entry C: From **1s′**[b]	98%	70%	70%	79 ± 16% (n = 3)

[a] **[^{11}C]2a** was formed as a byproduct (retention time: 4.8 min, RCY: 32 ± 13% (n = 3)).

[b] PPh_3 (10 μmol) was added.

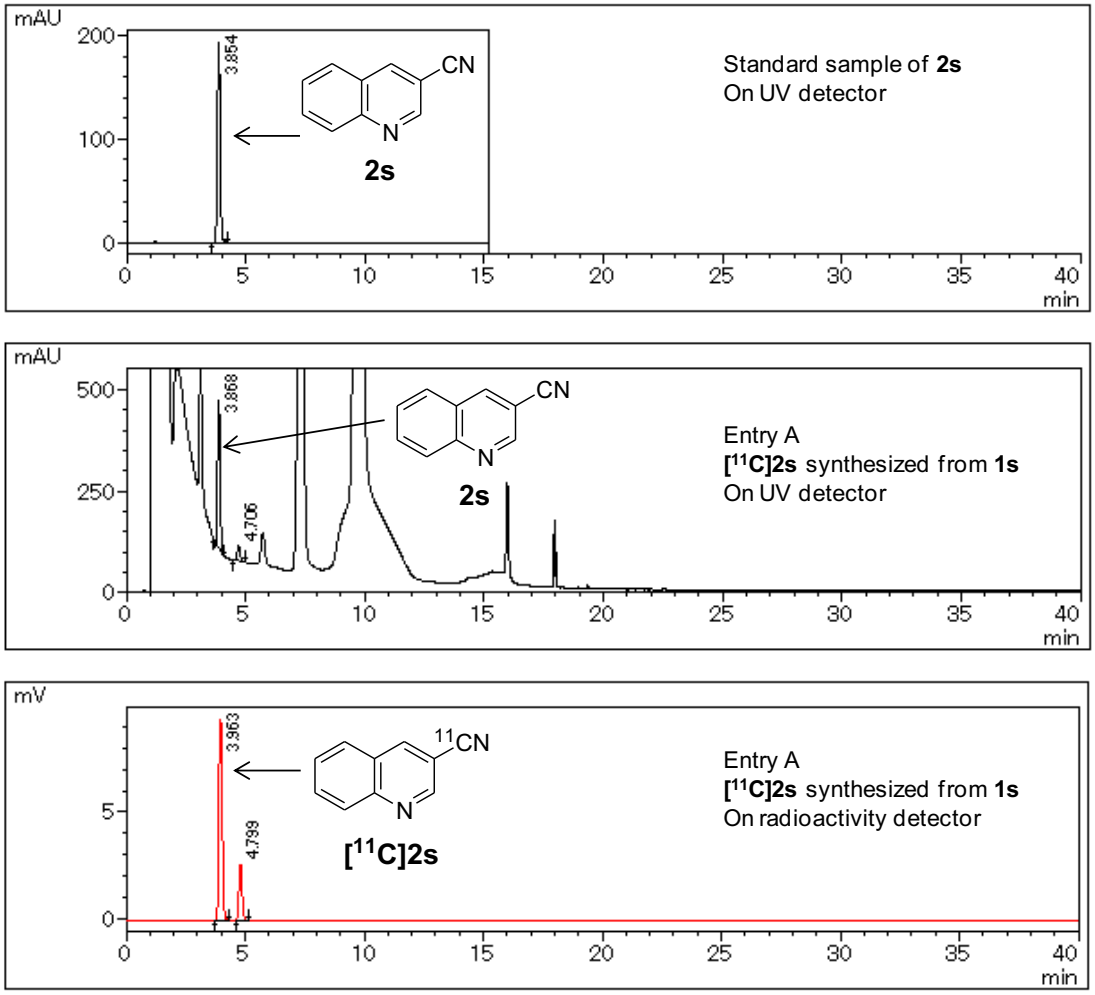


Fig. S23 Representative HPLC chromatograms for the synthesis of **[^{11}C]2s**.
Top: UV trace of **2s** as an authentic reference.
Middle: UV trace of the reaction mixture using **1s** as a substrate, containing **[^{11}C]2s** (Entry A).
Bottom: RI trace of the reaction mixture using **1s** as a substrate, containing **[^{11}C]2s** (Entry A).

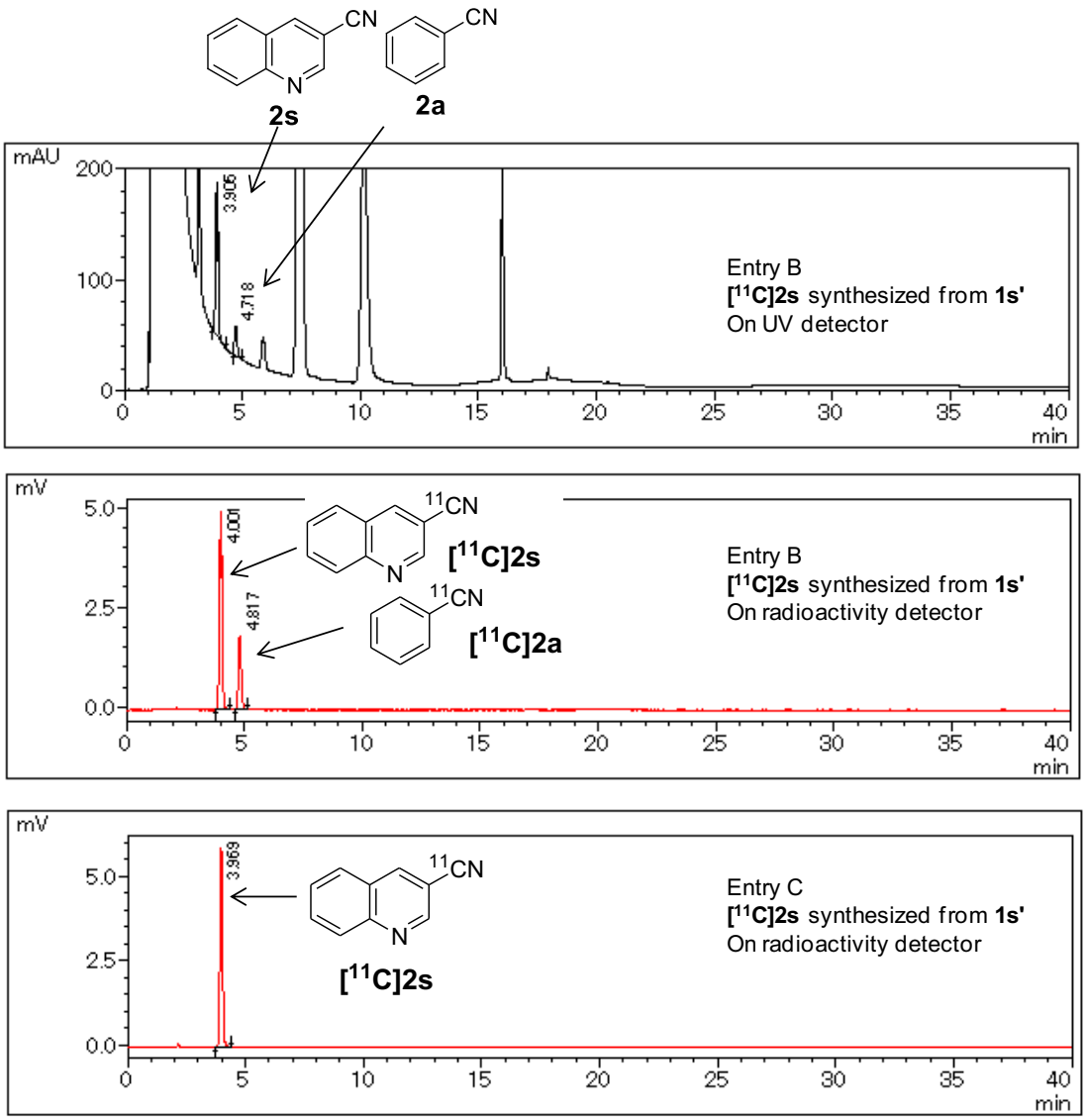


Fig. S24 Representative HPLC chromatograms for the synthesis of **[^{11}C]2s**.

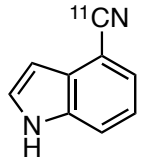
Top: UV trace of the reaction mixture using **1s′** as a substrate, containing **[^{11}C]2s** and **[^{11}C]2a** (Entry B).

Middle: RI trace of the reaction mixture using **1s′** as a substrate, containing **[^{11}C]2s** and **[^{11}C]2a** (Entry B).

Bottom: RI trace of the reaction mixture using **1s′** as a substrate, containing **[^{11}C]2s** (Entry C).

Comparison of the results for entries B and C clearly showed that addition of PPh_3 was effective for reducing the amount of the byproduct **[^{11}C]2a**.

[^{11}C]4-Cyanoindole ([^{11}C]2t)



The reaction was conducted in the presence of K_2CO_3 (20 μmol).

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 37% **B** (0–15 min), 37–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2t**: 4.8 min.

RCYs of each experiment

Run	1	2	3	Average
From **1t**	99%	99%	72%	90 ± 16% (n = 3)

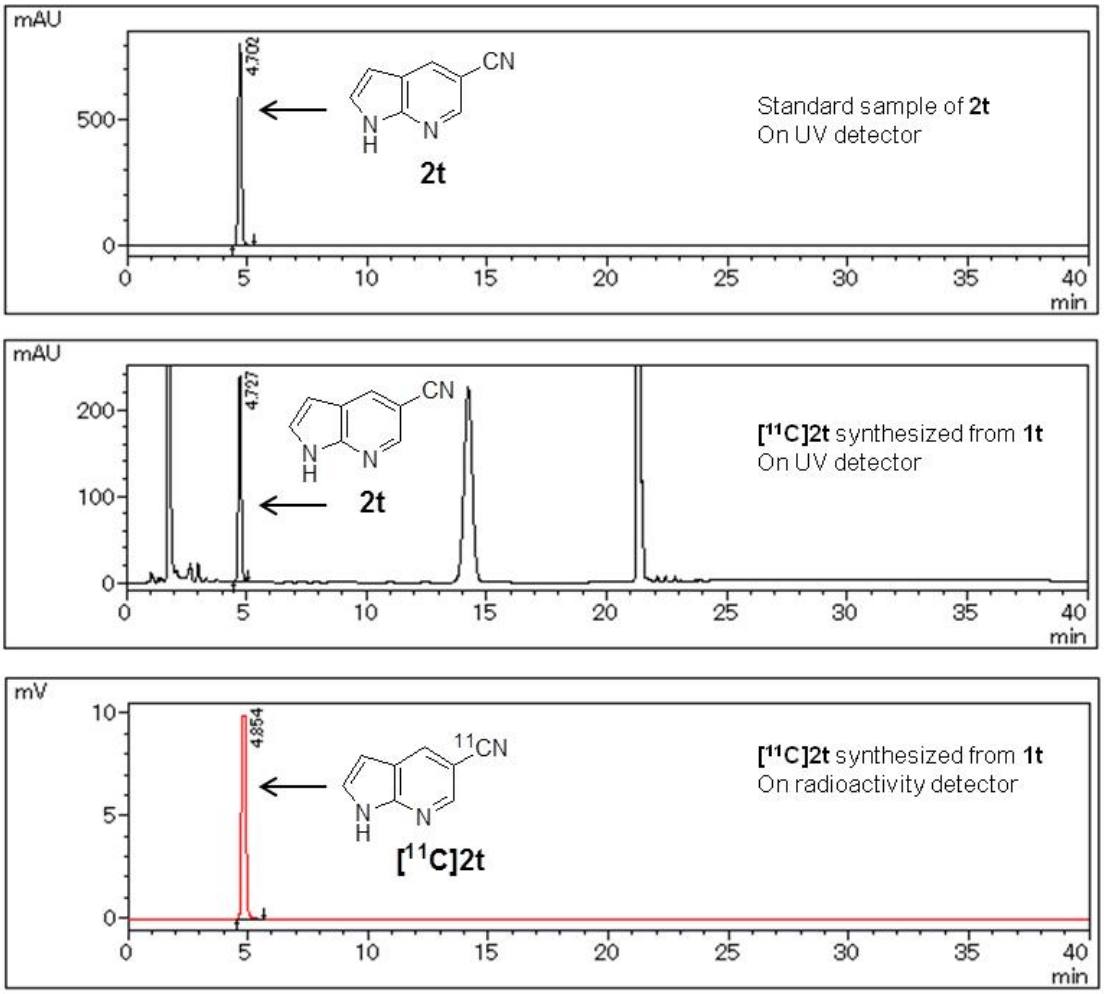
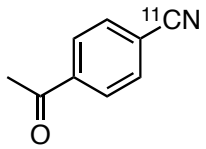


Fig. S25 Representative HPLC chromatograms for the synthesis of **[^{11}C]2t**.
Top: UV trace of **2t** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2t**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2t**.

[^{11}C]4-Cyanoacetophenone ([^{11}C]2u)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 35% **B** (0–15 min), 35–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2u**: 4.2 min.

RCYs of each experiment

Run	1	2	3	Average
From **1u′**	92%	96%	98%	95 ± 3% (n = 3)

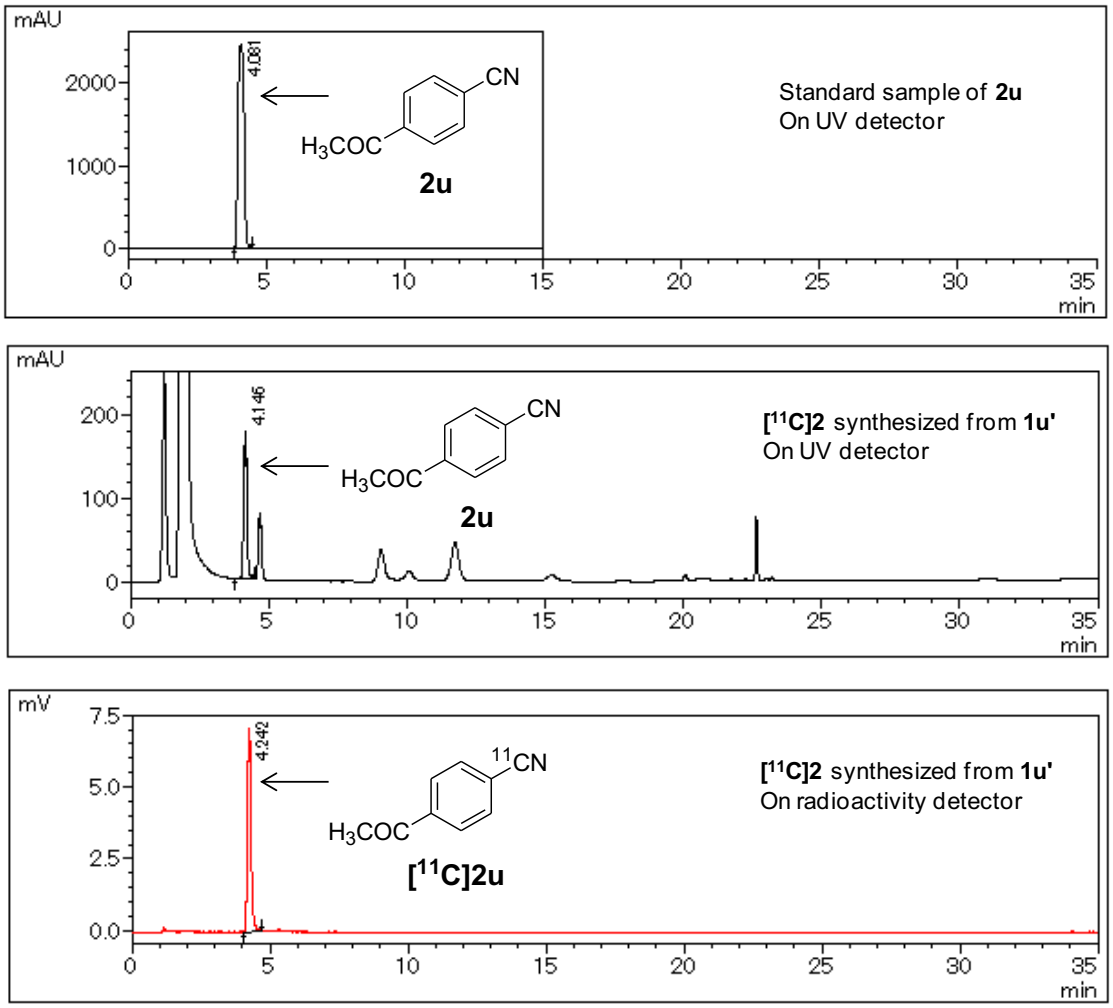
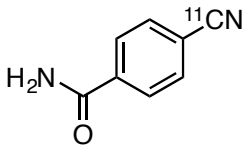


Fig. S26 Representative HPLC chromatograms for the synthesis of **[^{11}C]2u**.
Top: UV trace of **2u** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2u**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2u**.

[^{11}C]4-Cyanobenzamide ([^{11}C]2v)



Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol) and DMF (150 μL) was bubbled a gas containing [^{11}C]NH_4CN until the amount of radioactivity was saturated. To the mixture was added a solution of **1v′** (40 μmol) in DMF (0.1 mL). Then ^{11}C-cyanation was conducted at 110 °C.

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 15% **B** (0–15 min), 15–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 235 nm;
Retention time of **[^{11}C]2v**: 3.5 min.

RCYs of each experiment

Run	1	2	3	Average
From **1v′**	62%	78%	70%	70 ± 8% (n = 3)

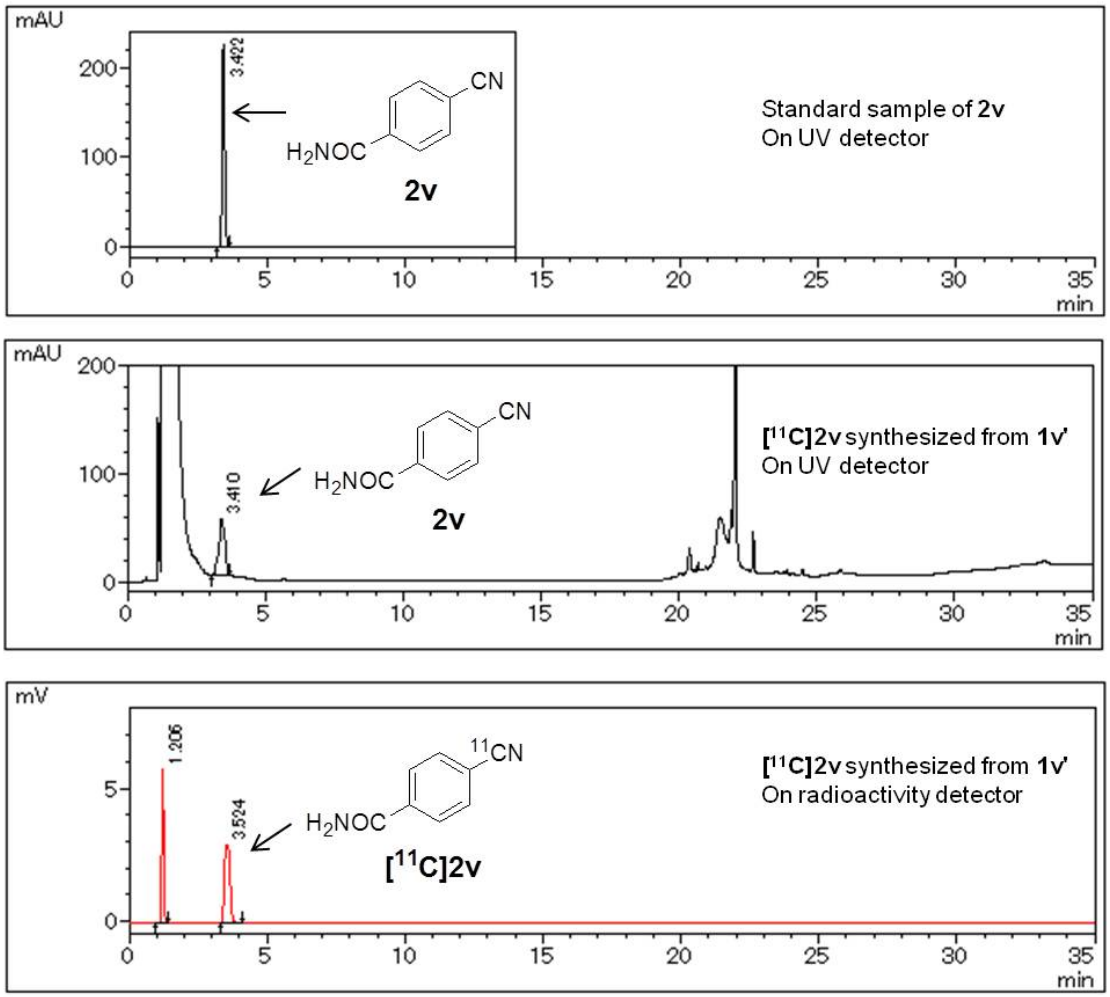
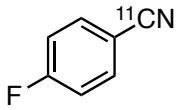


Fig. S27 Representative HPLC chromatograms for the synthesis of **[^{11}C]2v**.
Top: UV trace of **2v** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2v**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2v**.

[^{11}C]4-Fluorobenzonitrile ([^{11}C]2w)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 45% **B** (0–15 min), 45–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 225 nm;

Retention time of **[^{11}C]2w**: 3.6 min.

RCYs of each experiment

Run	1	2	3	Average
Entry A, From **1w′**	60%	51%	54%	55 ± 5% (n = 3)
Entry B, From **1w′**[a]	80%	53%	60%	64 ± 14% (n = 3)

[a] The reaction was conducted at 110 °C, in the presence of K_2CO_3 (20 μmol) and PPh_3 (10 μmol).

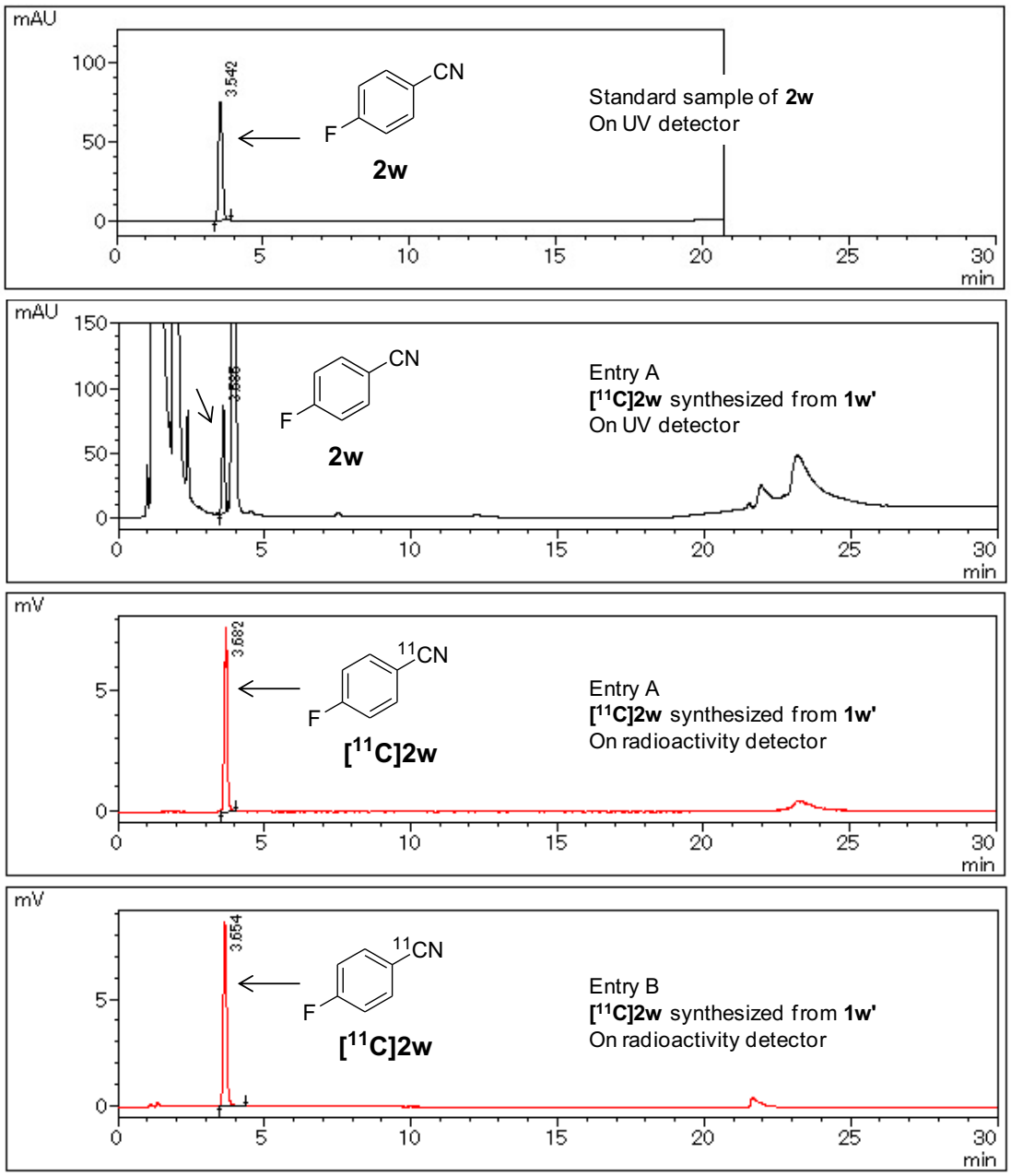
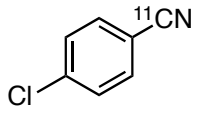


Fig. S28 Representative HPLC chromatograms for the synthesis of **[^{11}C]2w**.
Top: UV trace of **2w** as an authentic reference.
Second: UV trace of the reaction mixture containing **[^{11}C]2w** (Entry A).
Third: RI trace of the reaction mixture containing **[^{11}C]2w** (Entry A).
Bottom: RI trace of the reaction mixture containing **[^{11}C]2w** (Entry B).

[^{11}C]4-Chlorobenzonitrile ([^{11}C]2x)



Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 50% **B** (0–15 min), 50–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 230 nm;

Retention time of **[^{11}C]2x**: 4.2 min.

RCYs of each experiment

Run	1	2	3	Average
From **1x′**	95%	97%	96%	96 ± 1% (n = 3)

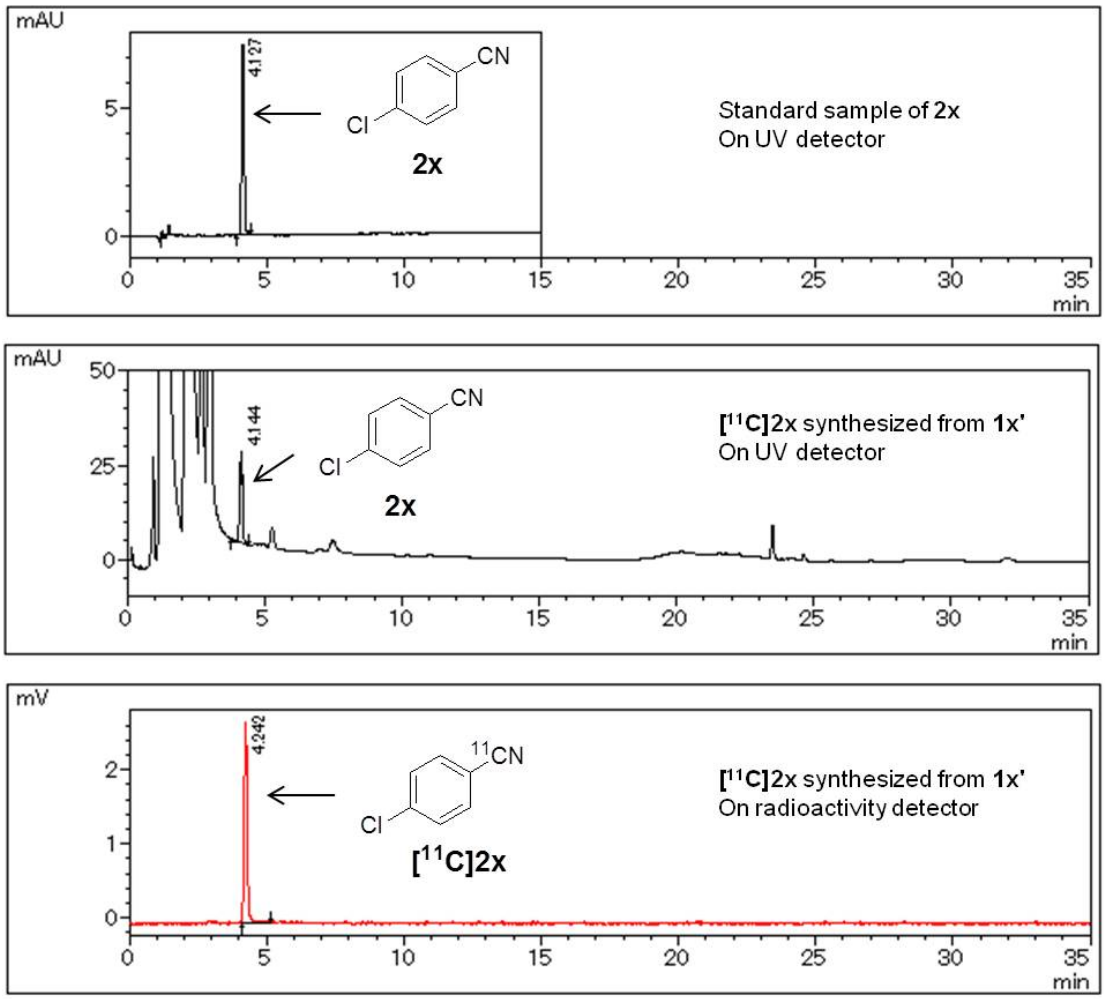
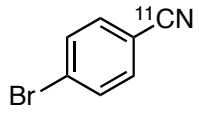


Fig. S29 Representative HPLC chromatograms for the synthesis of **[^{11}C]2x**.
Top: UV trace of **2x** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2x**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2x**.

[^{11}C]4-Bromobenzonitrile ([^{11}C]2y)



Method A (general procedure): Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol), **1y′** (20 μmol), and DMF (250 μL) was bubbled a gas containing [^{11}C]NH_4CN until the amount of radioactivity was saturated. Then the reaction was conducted at 100 °C.

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 25% **B** (0–15 min), 25–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 250 nm;

Retention time of **[^{11}C]2y**: 10.1 min.

RCYs of each experiment

Run	1	2	3	Average
From **1y′**[a]	72%	74%	84%	77 ± 6% (n = 3)

[a] [^{11}C]4-Cyanophenylboronic acid (**[^{11}C]1h**) was formed as a byproduct (retention time: 2.8 min, RCY: 10 ± 3% (n = 3)).

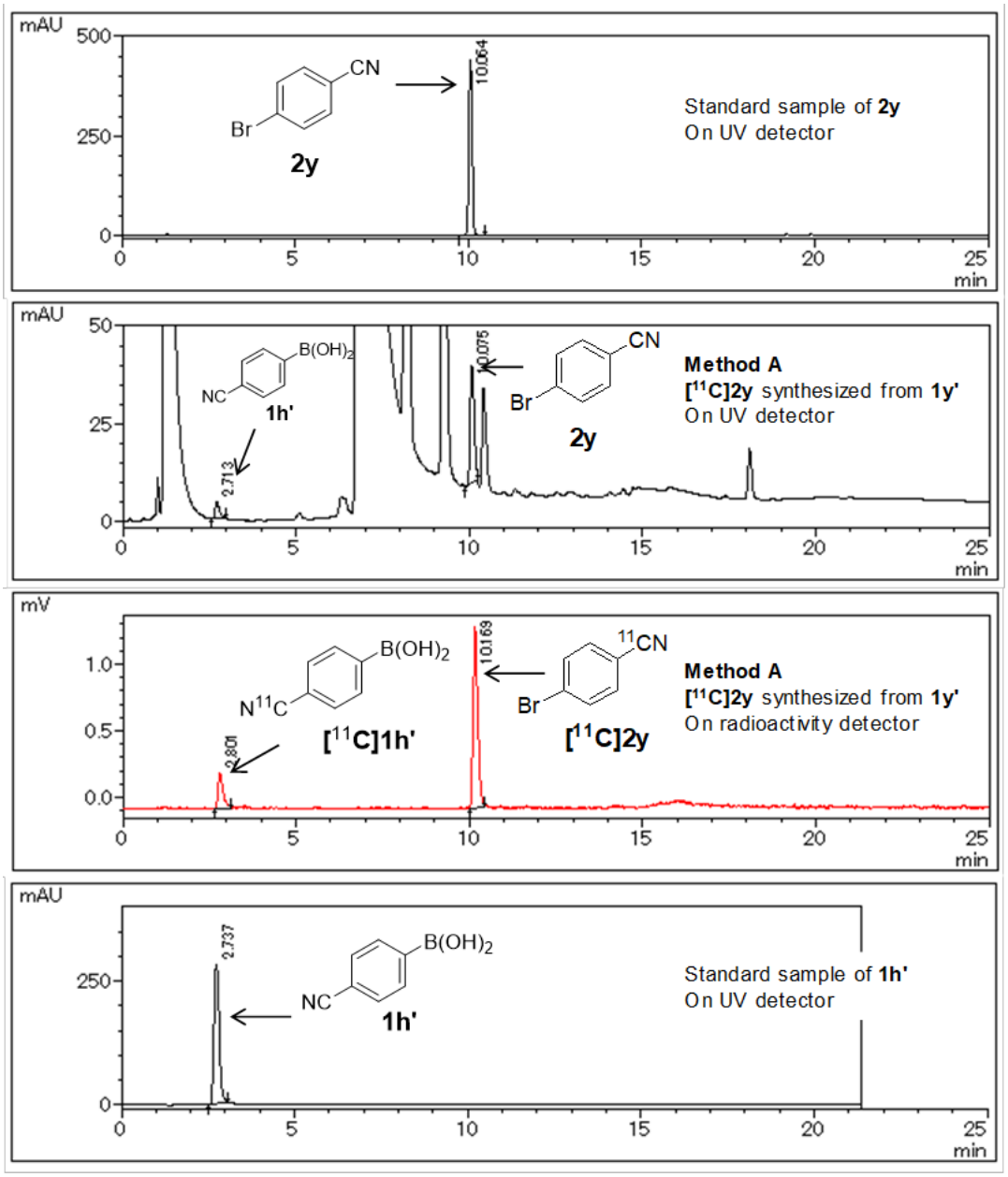


Fig. S30 Representative HPLC chromatograms for the synthesis of **[^{11}C]2y** (**Method A**).
Top: UV trace of **2y** as an authentic reference.
Second: UV trace of the reaction mixture containing **[^{11}C]2y** and **[^{11}C]1h′**.
Third: RI trace of the reaction mixture containing **[^{11}C]2y** and **[^{11}C]1h′**.
Bottom: UV trace of **1h′** as an authentic reference.

Method B: Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol) and DMF (150 μL) was bubbled a gas containing $[^{11}C]NH_4CN$ until the amount of radioactivity was saturated. To the mixture was added a solution of **1y′** (40 μmol) in DMF (100 μL). The reaction was conducted at 100 °C.

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 50% **B** (0–15 min), 50–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 250 nm;
Retention time of **[^{11}C]2y**: 4.5 min.

RCYs of each experiment

Run	1	2	3	Average
From **1y′**	92%	85%	72%	83 ± 10% (n = 3)

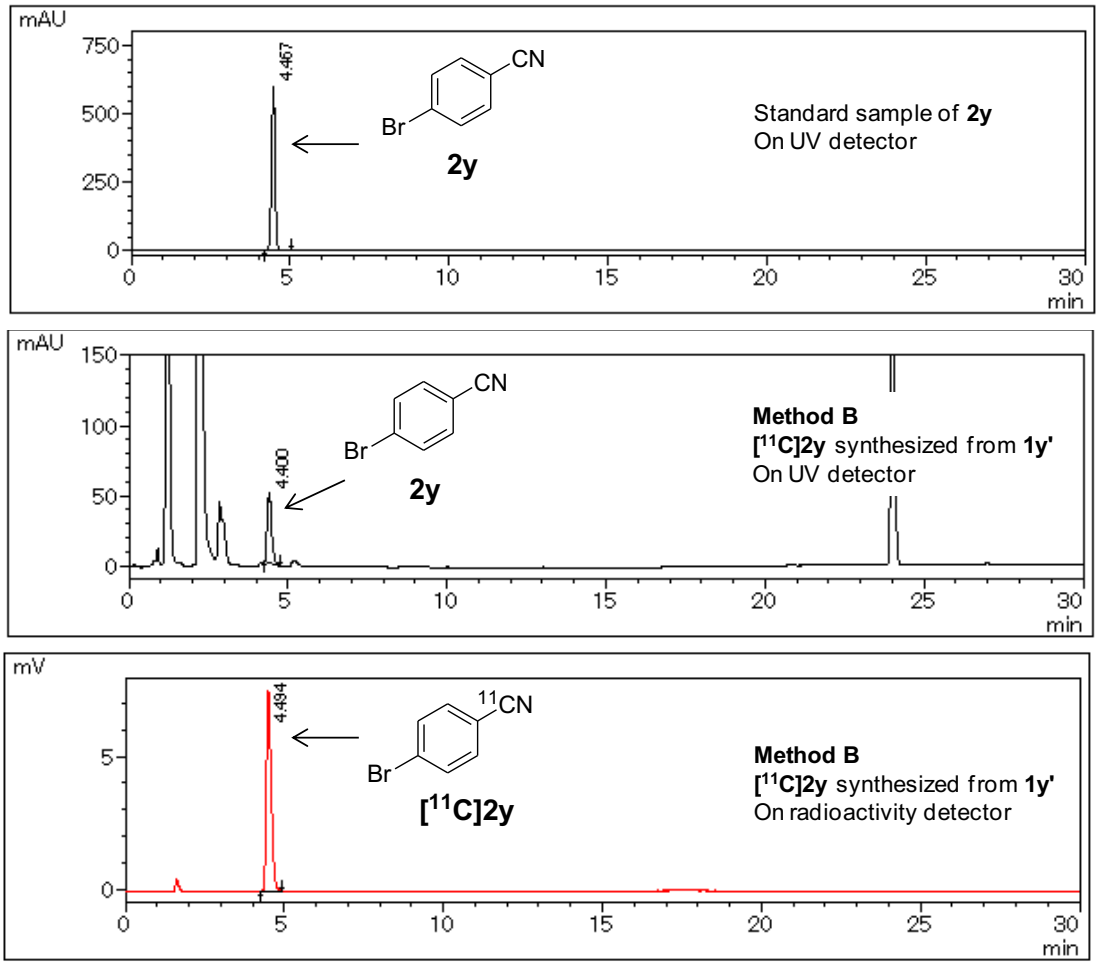
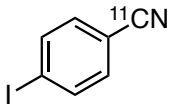


Fig. S31 Representative HPLC chromatograms for the synthesis of **[^{11}C]2y** (**Method B**).
Top: UV trace of **2y** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2y**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2y**.

[^{11}C]4-Iodobenzonitrile ([^{11}C]2z)



Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol) and DMF (150 μL) was bubbled a gas containing [^{11}C]NH_4CN until the amount of radioactivity was saturated. To the mixture was added a solution of **1z′** (40 μmol) in DMF (100 μL). The reaction was conducted at 100 °C.

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 55% **B** (0–15 min), 55–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 250 nm;

Retention time of **[^{11}C]2z**: 4.1 min.

RCYs of each experiment

Run	1	2	3	Average
From **1z′**	86%	68%	84%	79 ± 10% (n = 3)

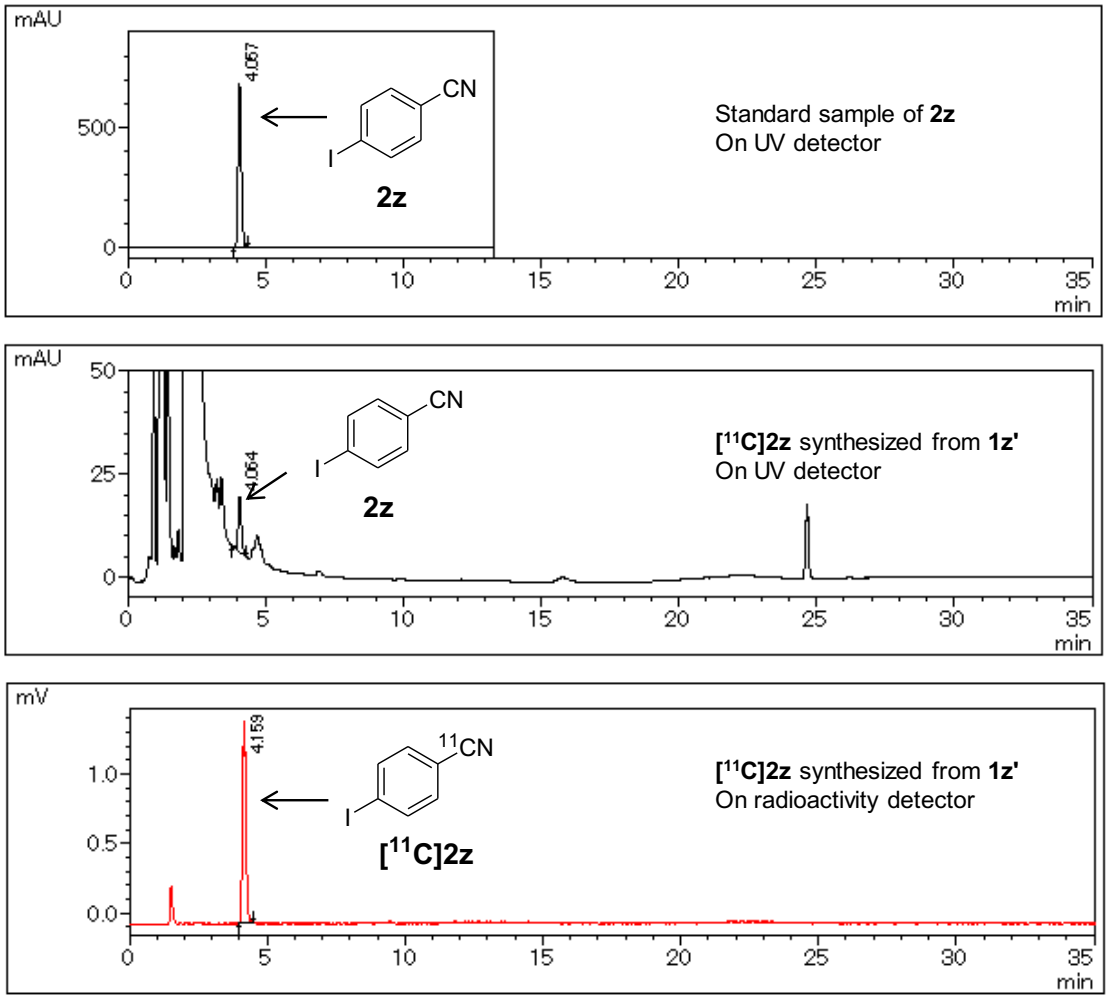
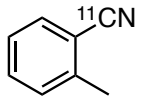


Fig. S32 Representative HPLC chromatograms for the synthesis of **[^{11}C]2z**.
Top: UV trace of **2z** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2z**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2z**.

[^{11}C]2-Methylbenzonitrile ([^{11}C]2aa)



The reaction was conducted in the presence of K_2CO_3 (20 μmol).

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 50% **B** (0–15 min), 50–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 230 nm;
Retention time of **[^{11}C]2aa**: 3.6 min.

RCYs of each experiment

Run	1	2	3	Average
From **1aa′**	79%	80%	74%	78 ± 3% (n = 3)

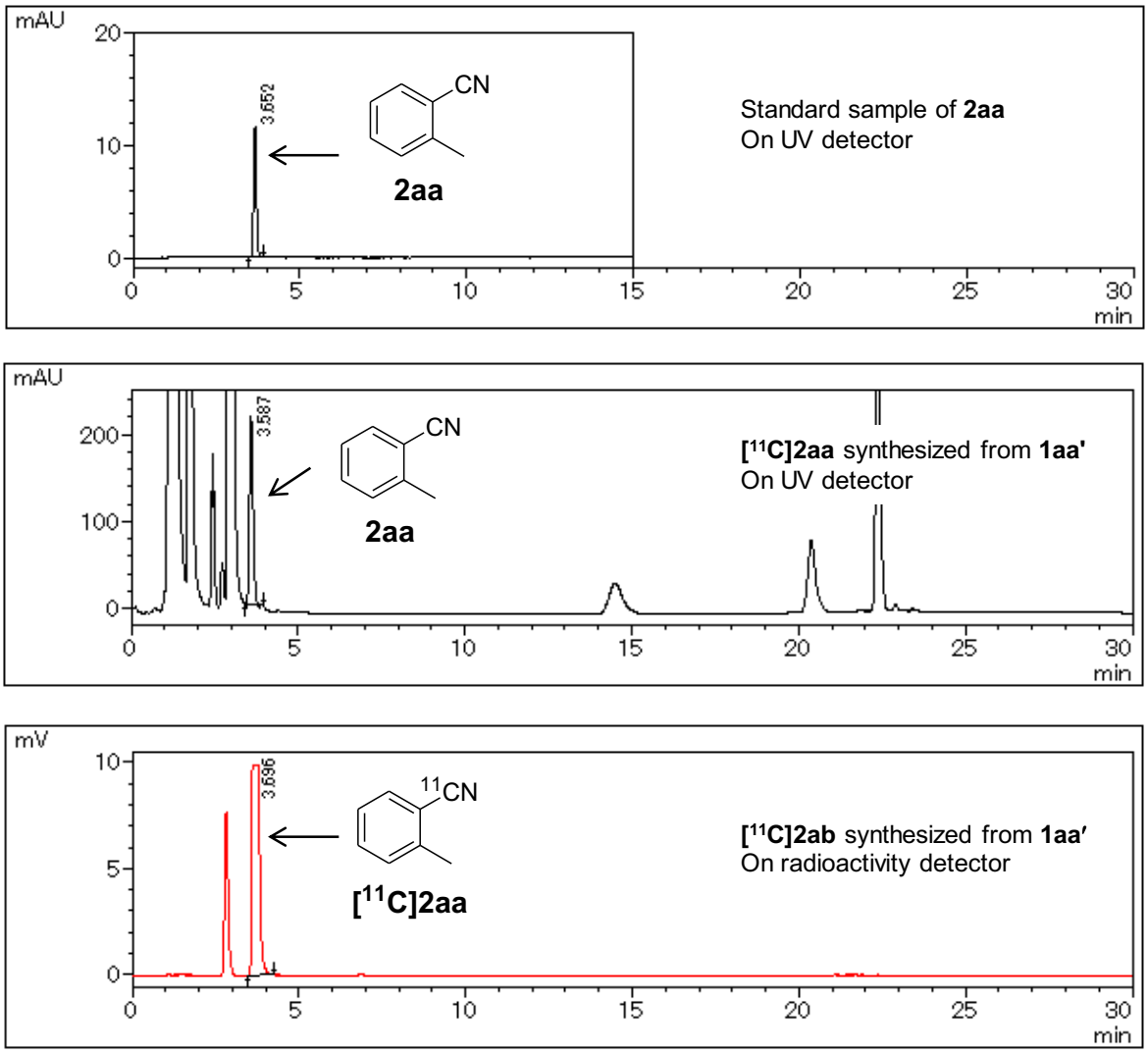
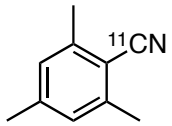


Fig. S33 Representative HPLC chromatograms.
Top: UV trace of **2aa** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2aa**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2aa**.

[^{11}C]2,4,6-Trimethylbenzonitrile ([^{11}C]2ab)



The reaction was conducted using 40 μmol of **1ab′** at 110 °C in the presence of K_2CO_3 (20 μmol).

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 60% **B** (0–15 min), 60–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 230 nm;

Retention time of **[^{11}C]2ab**: 4.5 min.

RCYs of each experiment

Run	1	2	3	Average
From **1ab′**	81%	80%	79%	80 ± 1% (n = 3)

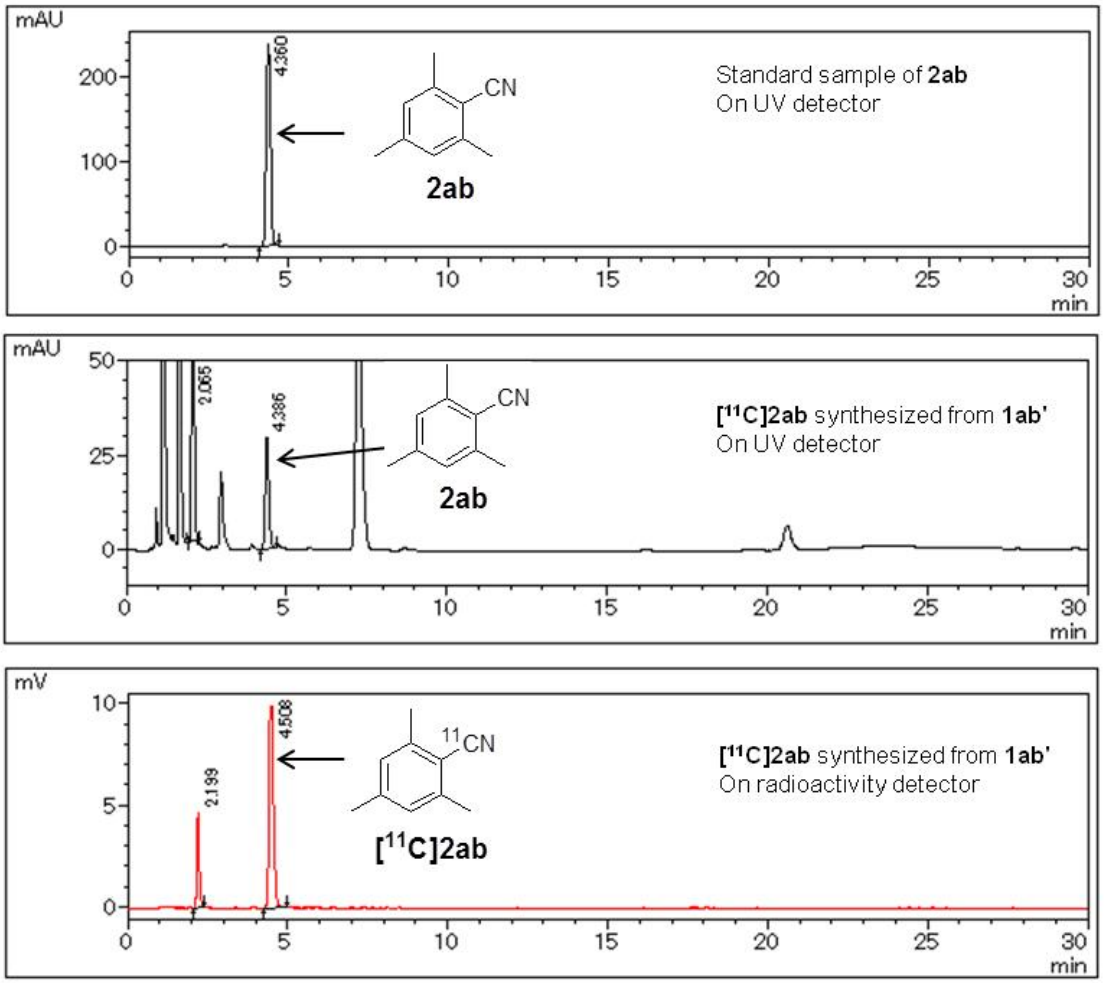
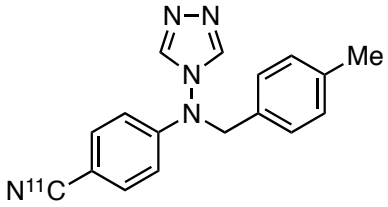


Fig. S34 Representative HPLC chromatograms.
Top: UV trace of **2ab** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2ab**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2ab**.

Radiosynthesis of [*cyano*-^{11}C]cetrozole ([^{11}C]2ac, Fig. 2)



The reaction was conducted in DMSO (250 μL) in the presence of K_2CO_3 (20 μmol).

Conditions for the analytical HPLC

Mobile phase **A** = aqueous NH_4OAc (30 mM, pH 7.0), mobile phase **B** = acetonitrile;
Gradient method: 42% **B** (0–15 min), 42–90% **B** (15–20 min), 90% **B** (20–45 min);
Column: COSMOSIL 5C_{18} AR-II 4.6 mm I.D. × 150 mm
Flow rate: 1.0 mL/min; Wavelength of UV detection: 265 nm;
Retention time of **[^{11}C]2ac**: 5.8 min.

RCYs of each experiment

Run	1	2	3	Average
From **1ac**	80%	90%	85%	85 ± 5% (n = 3)

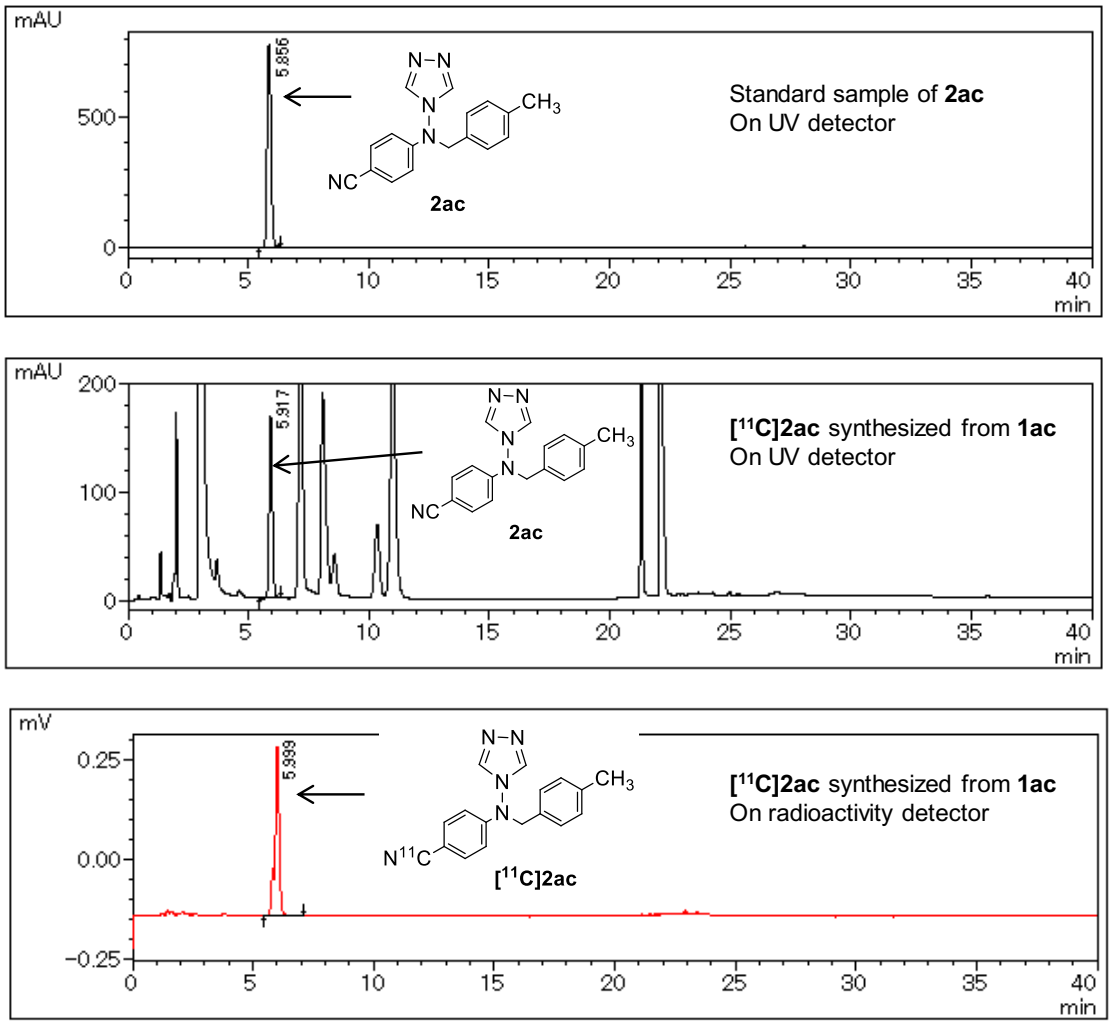
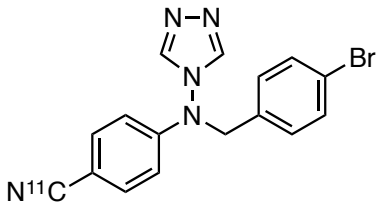


Fig. S35 Representative HPLC chromatograms.
Top: UV trace of **2ac** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2ac**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2ac**.

Radiosynthesis of [*cyano*-^{11}C]YM511 ([^{11}C]2ad, Fig. 2)



The reaction was conducted in DMSO (250 μL) in the presence of K_2CO_3 (20 μmol) and PPh_3 (10 μmol).

Conditions for the analytical HPLC

Mobile phase **A** = aqueous NH_4OAc (30 mM, pH 7.0), mobile phase **B** = acetonitrile;
Gradient method: 45% **B** (0–15 min), 45–90% **B** (15–20 min), 90% **B** (20–40 min);
Column: COSMOSIL 5C_{18} AR-II 4.6 mm I.D. × 150 mm (Nacalai Tesque, Inc.);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;
Retention time of **[^{11}C]2ad**: 5.3 min.

RCYs of each experiment

Run	1	2	3	Average
From **1ad**	89%	69%	65%	74 ± 13% (n = 3)

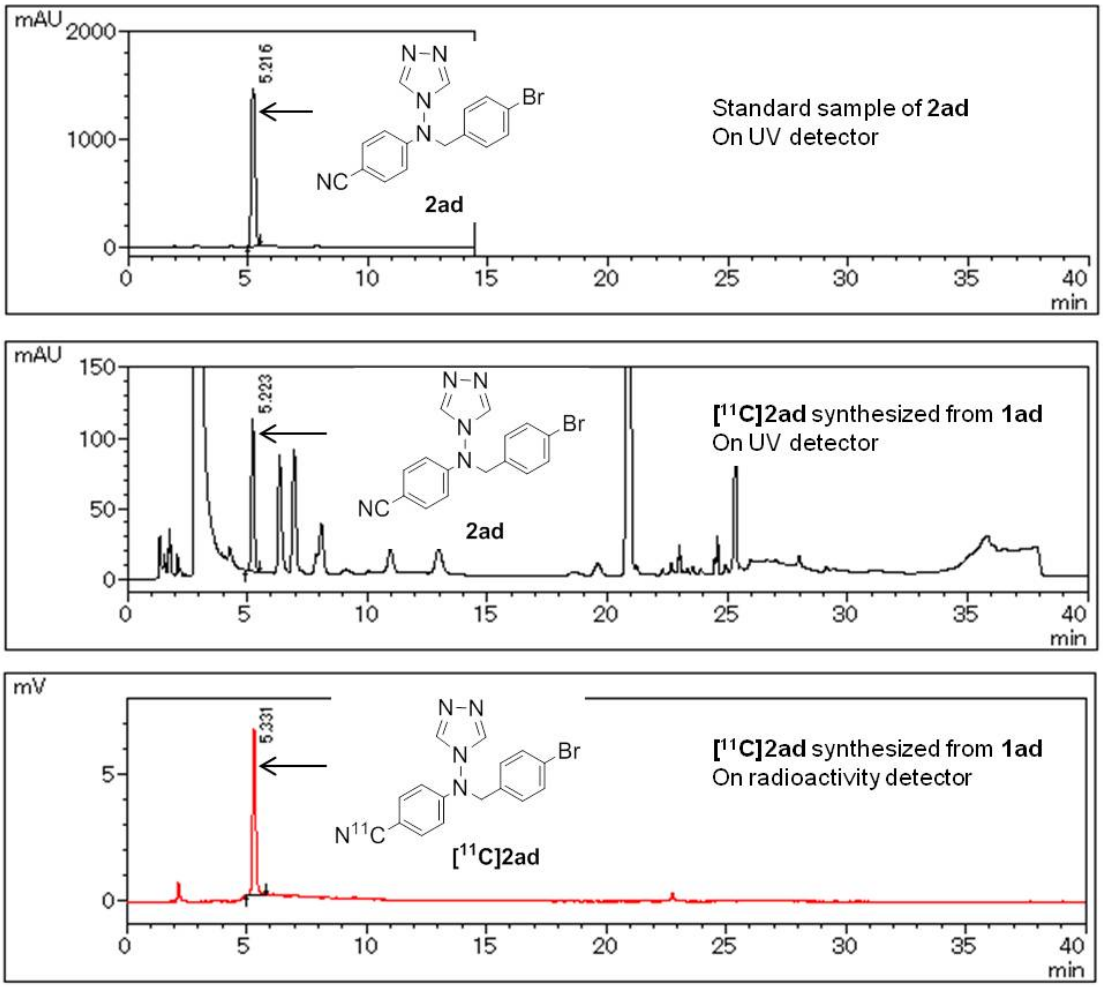
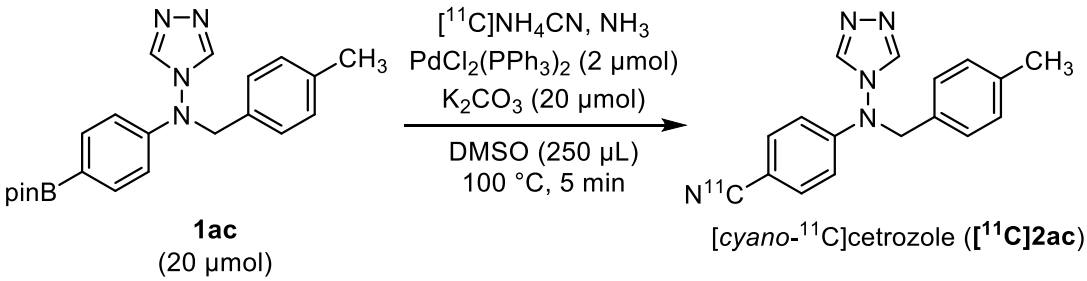


Fig. S36 Representative HPLC chromatograms.
Top: UV trace of **2ad** as an authentic reference.
Middle: UV trace of the reaction mixture containing **[^{11}C]2ad**.
Bottom: RI trace of the reaction mixture containing **[^{11}C]2ad**.

Preparation of [*cyano*-^{11}C]cetrozole ([^{11}C]2ac) with high radioactivity



The gas containing [^{11}C]NH_4CN and NH_3 was prepared by using [^{11}C]CH_4 with a radioactivity of 25 GBq. Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol), **1ac** (20 μmol), K_2CO_3 (20 μmol), and DMSO (250 μL) was bubbled the gas containing [^{11}C]NH_4CN until the amount of radioactivity was saturated. The mixture was heated at 100 °C for 5 min without stirring. After quickly cooling to 25 °C within 1 min, to the reaction mixture was immediately added aqueous acetonitrile (50%, 1.0 mL). The mixture was passed through a short pad of silica wool and syringe filter (filter media, PVDF; pore size, 0.2 mm; Whatman Inc.) sequentially, and injected into a preparative HPLC under the conditions shown below. A fraction containing **[^{11}C]2ac**, which was estimated by using UV and radioactivity detectors, was collected into a flask and concentrated under reduced pressure with heating. The residue was diluted in saline (2 mL) and transferred into a small vial. The desired product **[^{11}C]2ac** was obtained with a radioactivity of 4.4 GBq and a molar radioactivity of 72 GBq/μmol at the end of synthesis. The total time of synthesis was 28 min from the end of bombardment (EOB). The decay-corrected radiochemical yield (DCY) was 45% from [^{11}C]CH_4. The production of **[^{11}C]2ac** was confirmed by HPLC analysis co-injected with non-radioactive standard **2ac**. The chemical and radiochemical purities of **[^{11}C]2ac** were 97% and >99%, respectively.

<u>Conditions for the preparative HPLC</u>

Column: semi-preparative column, COSMOSIL 5C_{18} AR-II 10 mm I.D. × 250 mm (Nacalai Tesque, Inc.);

Mobile phase **A** = phosphate buffer (50 mM, pH 7.0), mobile phase **B** = acetonitrile;

Gradient method: 10% **B** (0–2 min), 41% **B** (2–30 min);

Flow rate: 6.5 mL/min; Wavelength of UV detection: 265 nm;

Retention time of **[^{11}C]2ac**: 13.0 min.

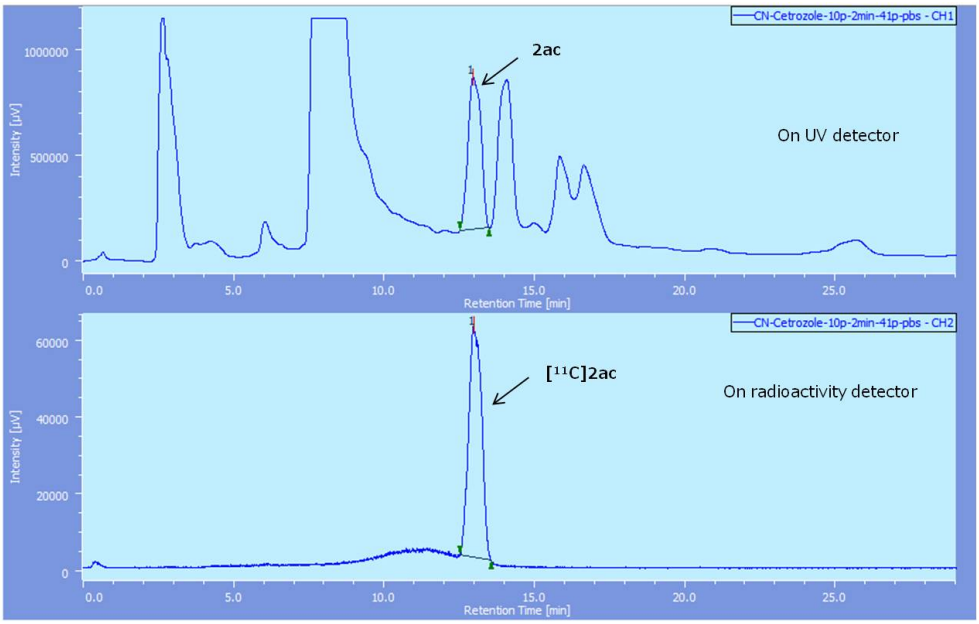


Fig. S37 Preparative HPLC chromatogram for the synthesis of **[^{11}C]2ac**.

Conditions for the analytical HPLC

Column: COSMOSIL 5C_{18} MS-II 4.6 mm I.D. × 150 mm (Nacalai Tesque, Inc.)

Mobile phase: acetonitrile / aqueous NH_4OAc (30 mM, pH 7.0) = 42/58

Flow rate: 1.0 mL/min; Wavelength of UV detection: 265 nm;

Retention time of **[^{11}C]2ac**: 5.8 min.

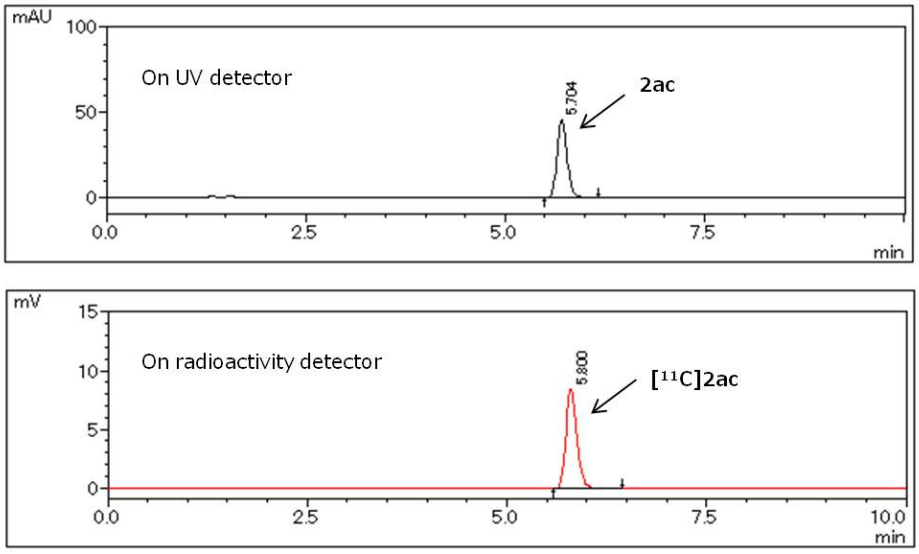


Fig. S38 Analytical HPLC chromatograph of **[^{11}C]2ac** co-injected with non-radioactive standard **2ac**.

Calibration curve for **2ac**

A calibration curve was plotted from five concentrations (1.25, 2.5, 5.0, 10, and 20 nmol/mL) of **2ac** and used for estimating the concentration and molar radioactivity of synthesized **[^{11}C]2ac**.

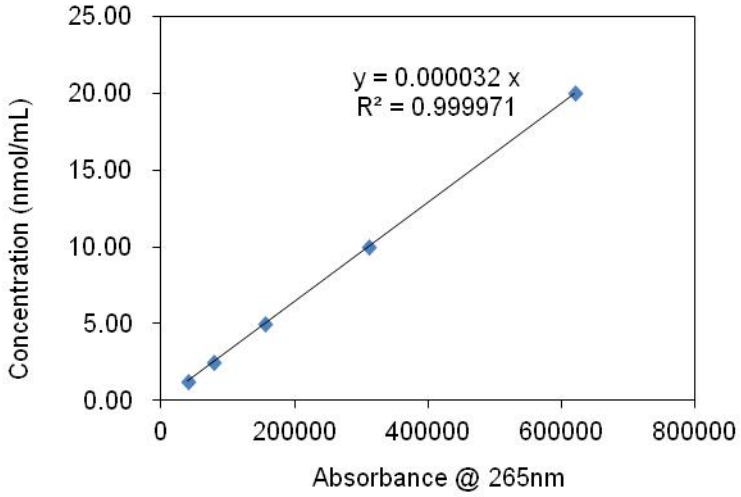
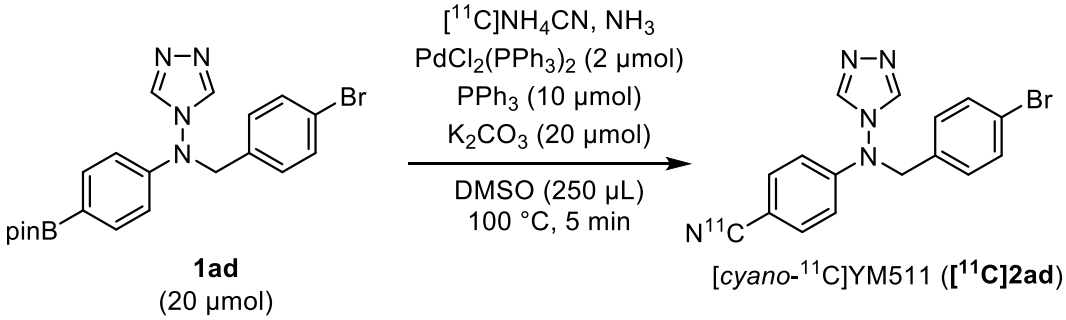


Fig. S39 Calibration curve for **2ac**.

Preparation of [*cyano*-^{11}C]YM511 ([^{11}C]2ad) with high radioactivity



The gas containing [^{11}C]NH_4CN and NH_3 was prepared by using [^{11}C]CH_4 with a radioactivity of 25 GBq. Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol), **1ad** (20 μmol), K_2CO_3 (20 μmol), PPh_3 (2.6 mg, 10 μmol), and DMSO (250 μL) was bubbled the gas containing [^{11}C]NH_4CN until the amount of radioactivity was saturated. The mixture was heated at 100 °C for 5 min without stirring. After quickly cooling to 25 °C within 1 min, to the reaction mixture was immediately added aqueous acetonitrile (50%, 1.0 mL). The mixture was passed through a short pad of silica wool and syringe filter (filter media, PVDF; pore size, 0.2 mm; Whatman Inc.) sequentially, and injected into a preparative HPLC under the conditions shown below. A fraction containing **[^{11}C]2ad**, which was estimated by using UV and radioactivity detectors, was collected into a flask and concentrated under reduced pressure with heating. The residue was diluted in saline (2 mL) and transferred into a small vial. The desired product **[^{11}C]2ad** was obtained with a radioactivity of 3.2 GBq and a molar radioactivity of 93 GBq/μmol at the end of synthesis. The total time of synthesis was 28 min from the end of bombardment (EOB). The decay-corrected radiochemical yield (DCY) was 33% from [^{11}C]CH_4. The production of **[^{11}C]2ad** was confirmed by HPLC analysis co-injected with non-radioactive standard **2ad**. The chemical and radiochemical purities of **[^{11}C]2ad** were 97% and >99%, respectively.

Conditions for the preparative HPLC

Column: semi-preparative column, COSMOSIL 5C_{18} AR-II 10 mm I.D. × 250 mm (Nacalai Tesque, Inc.);

Mobile phase **A** = phosphate buffer (50 mM, pH 7.0), mobile phase **B** = acetonitrile;

Gradient method: 40% **B** (0–30 min);

Flow rate: 3 mL/min (0–2 min), 6.5 mL/min (2–30 min); Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2ad**: 13.6 min.

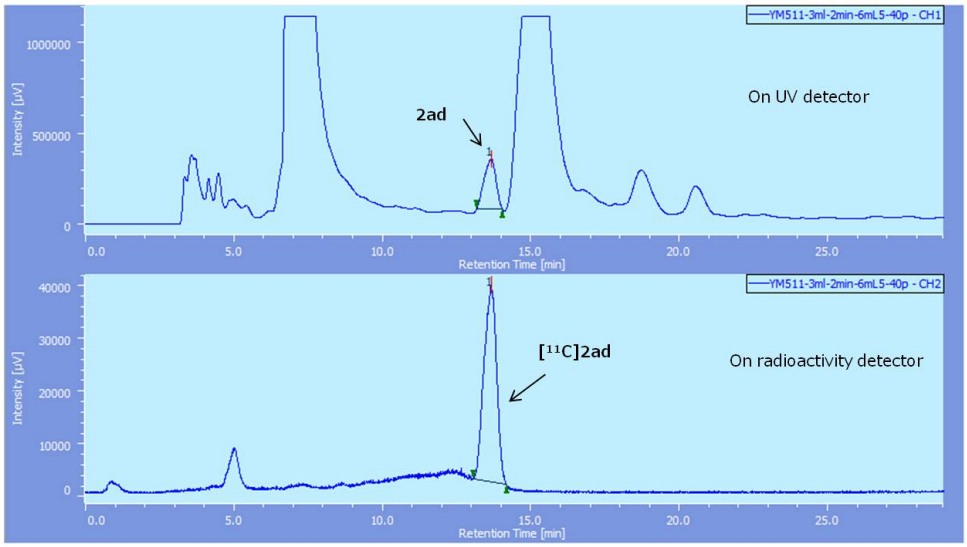


Fig. S40 Preparative HPLC chromatogram for the synthesiss of **[^{11}C]2ad**.

Conditions for the analytical HPLC

Column: COSMOSIL 5C_{18} AR-II 4.6 mm I.D. × 150 mm (Nacalai Tesque, Inc.)

Mobile phase: acetonitrile / aqueous NH_4OAc (30 mM, pH 7.0) = 46/54

Flow rate: 1.0 mL/min; Wavelength of UV detection: 265 nm;

Retention time of **[^{11}C]2ad**: 5.1 min.

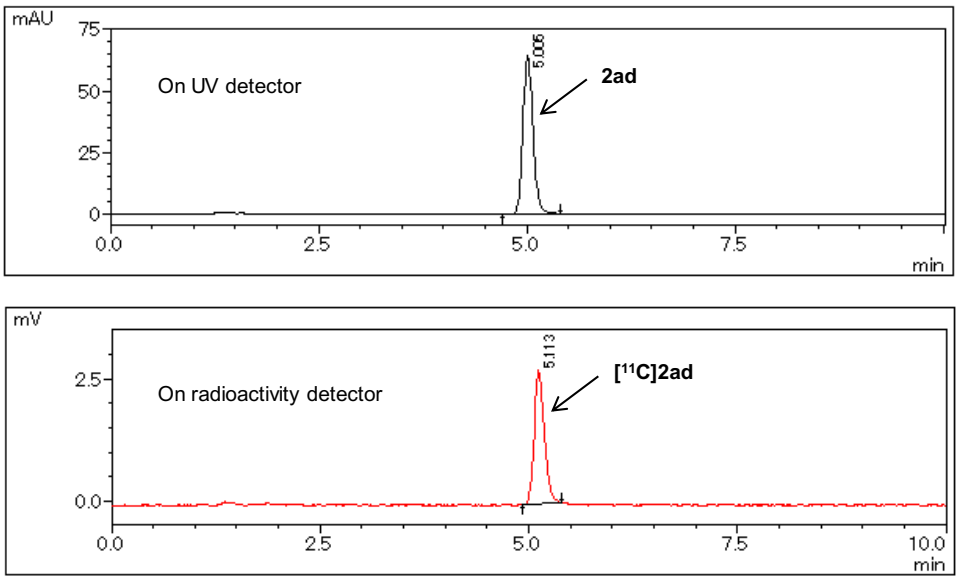


Fig. S41 Analytical HPLC chromatograph of **[^{11}C]2ad** co-injected with non-radioactive standard **2ad**.

Calibration curve for **2ad**

A calibration curve was plotted from five concentrations (1.25, 2.5, 5.0, 10, and 20 nmol/mL) of **2ad** and used for estimating the concentration and molar radioactivity of synthesized **[^{11}C]2ad**.

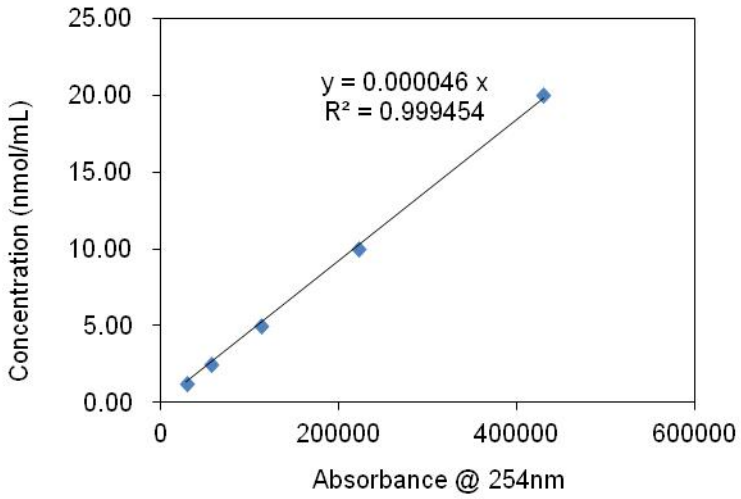
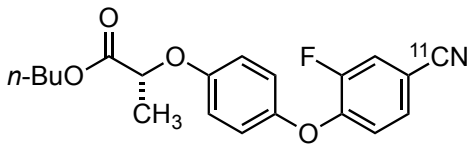


Fig. S42 Calibration curve for **2ad**.

Radiosynthesis of [*cyano*-^{11}C]cyhalofop butyl ([^{11}C]2ae, Fig. 3)



The reaction was conducted in DMSO (250 μL) at 110 °C.

Conditions for the analytical HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;

Gradient method: 70% **B** (0–15 min), 70–90% **B** (15–20 min), 90% **B** (20–40 min);

Flow rate: 1.0 mL/min; Wavelength of UV detection: 254 nm;

Retention time of **[^{11}C]2ae**: 5.2 min.

RCYs of each experiment

Run	1	2	3	Average
From **1ae″**	75%	74%	74%	74 ± 1% (n = 3)

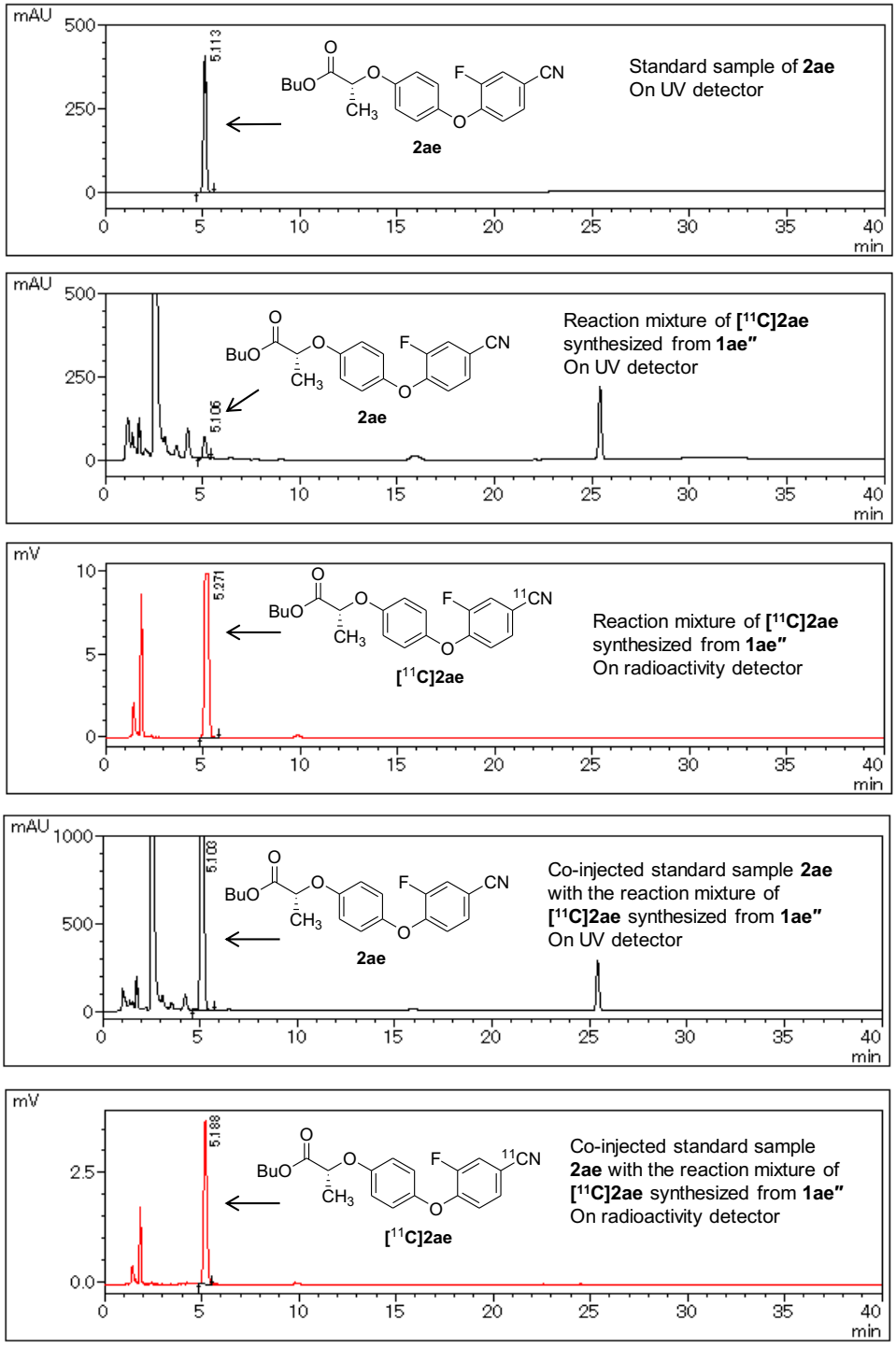


Fig. S43 Representative HPLC chromatograms.

Top: A UV trace of **2ae** as an authentic reference.

Second: UV trace of the reaction mixture containing **[^{11}C]2ae**.

Third: RI trace of the reaction mixture containing **[^{11}C]2ae**.

Fourth: UV trace of co-injected standard **2ae** with the reaction mixture containing **[^{11}C]2ae.**

Bottom: RI trace of co-injected standard **2ae** with the reaction mixture containing **[^{11}C]2ae.**

Molar radioactivity of **[^{11}C]2ae**

Although **[^{11}C]2ae** was not isolated, its molar activity was roughly calculated based on the UV absorbance of **2ae** at 254 nm. A calibration curve was plotted from six concentrations (1.25, 2.5, 5.0, 10, 20, and 100 nmol/mL) of **2ae** and used for estimating the concentration of synthesized **[^{11}C]2ae** in the reaction mixture (Figure S43). The radioactivity of **[^{11}C]2ae** was calculated by counting the total radioactivity of the sample and multiplying by the RCY.

In the experiment shown in Run 1, the total radioactivity of the reaction mixture was 4.21 GBq at the end of synthesis 13 min after the end of bombardment (EOB). Since the RCY for Run 1 was 75%, the radioactivity of **[^{11}C]2ae** was calculated as 3.16 GBq (= 4.21 GBq × 0.75). The amount of **[^{11}C]2ae** was calculated to be 55.3 nmol (integral of the absorbance area: 485,000, concentration: 32.5 nmol/mL, total volume: 1.7 mL) from the calibration curve. Therefore, the molar radioactivity of **[^{11}C]2ae** was calculated to be 57 GBq/μmol. Similarly, the molar radioactivities of **[^{11}C]2ae** for Runs 2 and 3 were calculated to be 64 and 68 GBq/μmol, respectively.

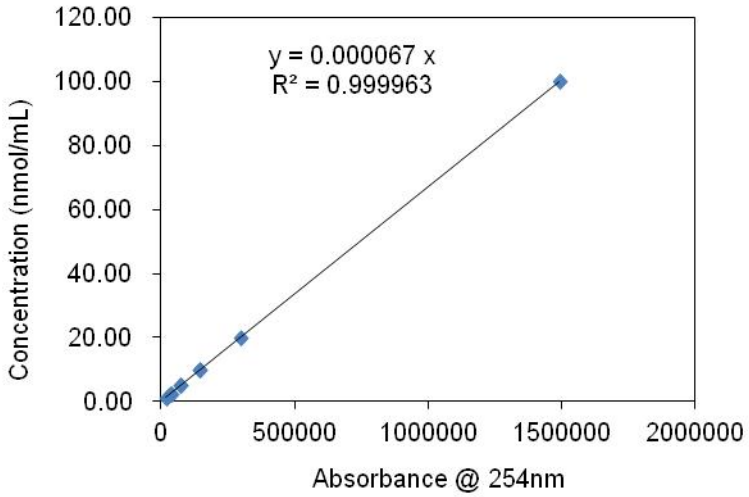


Fig. S44 Calibration curve for **2ae**.

Radio-HPLC analyses of the reaction mixtures of palladium(II)-mediated ^{11}C-cyanation of 1a for mechanistic consideration (Fig. 4)

Preparation of reaction mixtures

Mixture (a): Into a reaction vessel charged with DMF (250 μL) was bubbled the gas containing [^{11}C]NH_4CN at room temperature until the amount of radioactivity was saturated. The mixture was diluted with aqueous acetonitrile (50%, 1.0 mL), and an aliquot of the resulting mixture (20 μL) was injected for radio-HPLC analysis.

Mixture (b): Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol) and DMF (250 μL) was bubbled the gas containing [^{11}C]NH_4CN at room temperature until the amount of radioactivity was saturated. The mixture was diluted with aqueous acetonitrile (50%, 1.0 mL), and an aliquot of the resulting mixture (20 μL) was injected for radio-HPLC analysis.

Mixture (c): Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol), **1a** (4.1 mg, 20 μmol), and DMF (250 μL) was bubbled the gas containing [^{11}C]NH_4CN at room temperature until the amount of radioactivity was saturated. The mixture was diluted with aqueous acetonitrile (50%, 1.0 mL), and an aliquot of the resulting mixture (20 μL) was injected for radio-HPLC analysis.

Mixture (d): Into a reaction vessel charged with $PdCl_2(PPh_3)_2$ (1.4 mg, 2.0 μmol), **1a** (4.1 mg, 20 μmol), and DMF (250 μL) was bubbled the gas containing [^{11}C]NH_4CN at room temperature until the amount of radioactivity was saturated. After heating at 100 °C for 5 min, the mixture was diluted with aqueous acetonitrile (50%, 1.0 mL), and an aliquot of the resulting mixture (20 μL) was injected for radio-HPLC analysis.

Conditions for the analytical radio-HPLC

Mobile phase **A** = water, mobile phase **B** = acetonitrile;
Gradient method: 40% **B** (0–15min), 40–90% **B** (15–20 min), 90% **B** (20–40 min);
Flow rate: 1.0 mL/min; Wavelength of UV detection: 220 nm.

References for Supporting Information

S1 Z. Feng, Q.-Q. Min, Y.-L. Xiao, B. Zhang and X. Zhang, *Angew. Chem., Int. Ed.,* 2014, **53**, 1669.

S2 K. Takahashi, T. Hosoya, K. Onoe, H. Doi, H. Nagata, T. Hiramatsu, X.-L. Li, Y. Watanabe, Y. Wada, T. Takashima, M. Suzuki, H. Onoe and Y. Watanabe, *J. Nucl. Med.,* 2014, **55**, 852.

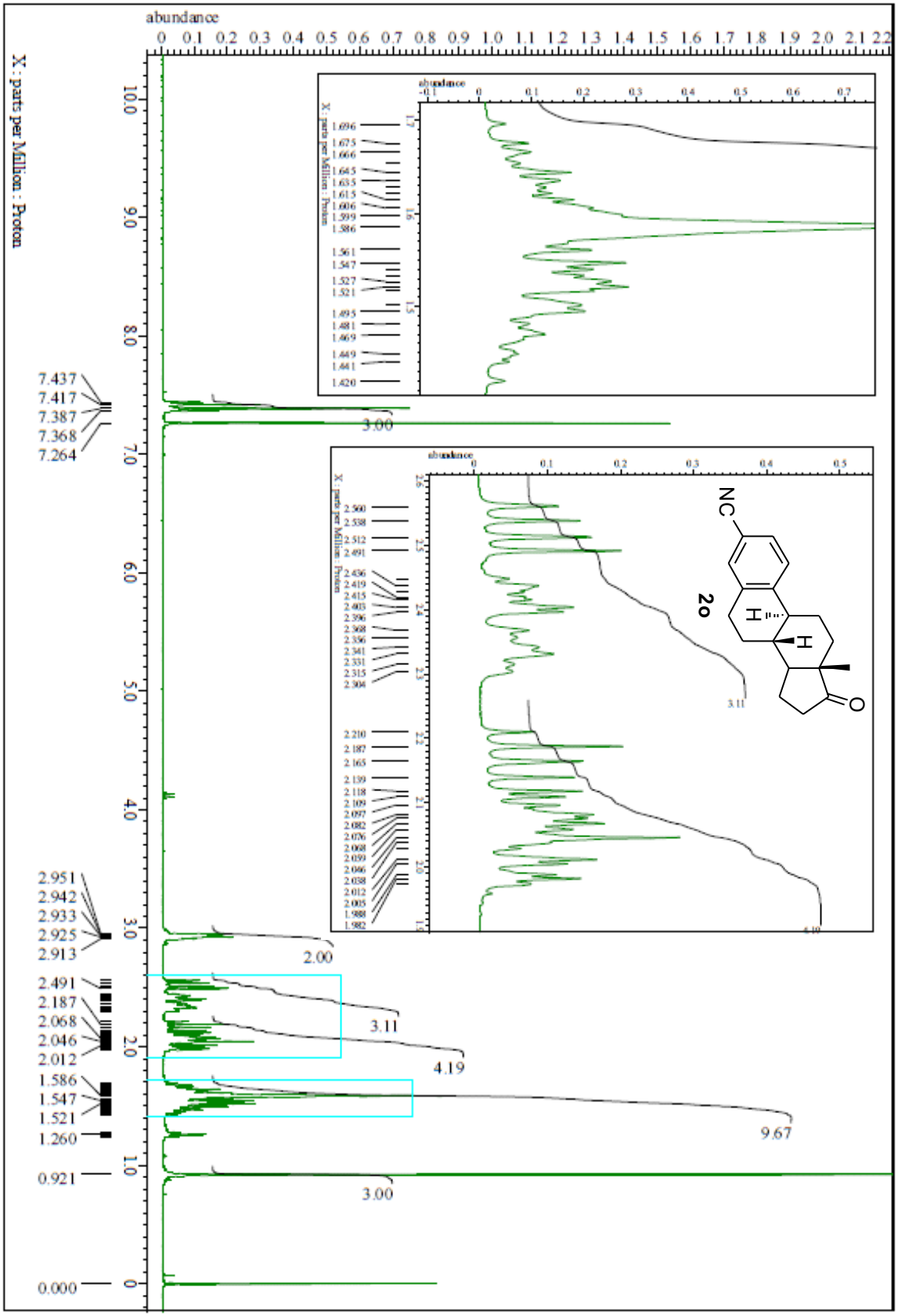
S3 M. Okada, T. Yoden, E. Kawaminami, Y. Shimada, M. Kudoh and Y. Isomura, *Chem. Pharm. Bull.,* 1997, **45**, 333.

S4 M. Tobisu, H. Kinuta, Y. Kita, E. Remond and N. Chatani, *J. Am. Chem. Soc*., 2012, **134**, 115.

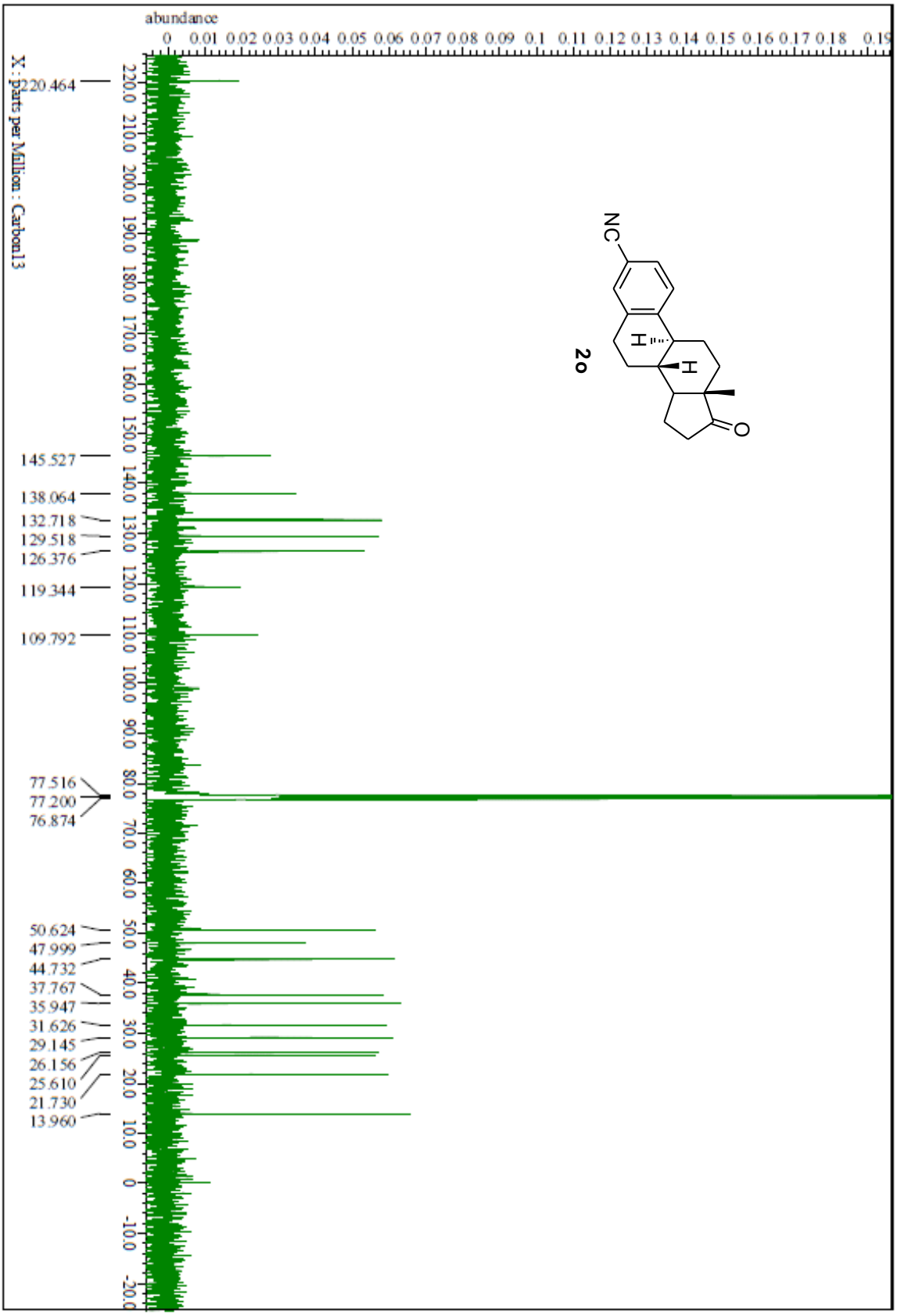
S5 H. G. Lee, P. J. Milner, M. S. Placzek, S. L. Buchwald and J. M. Hooker, *J. Am. Chem. Soc.,* 2015, **137**, 648.

NMR Spectra for compounds

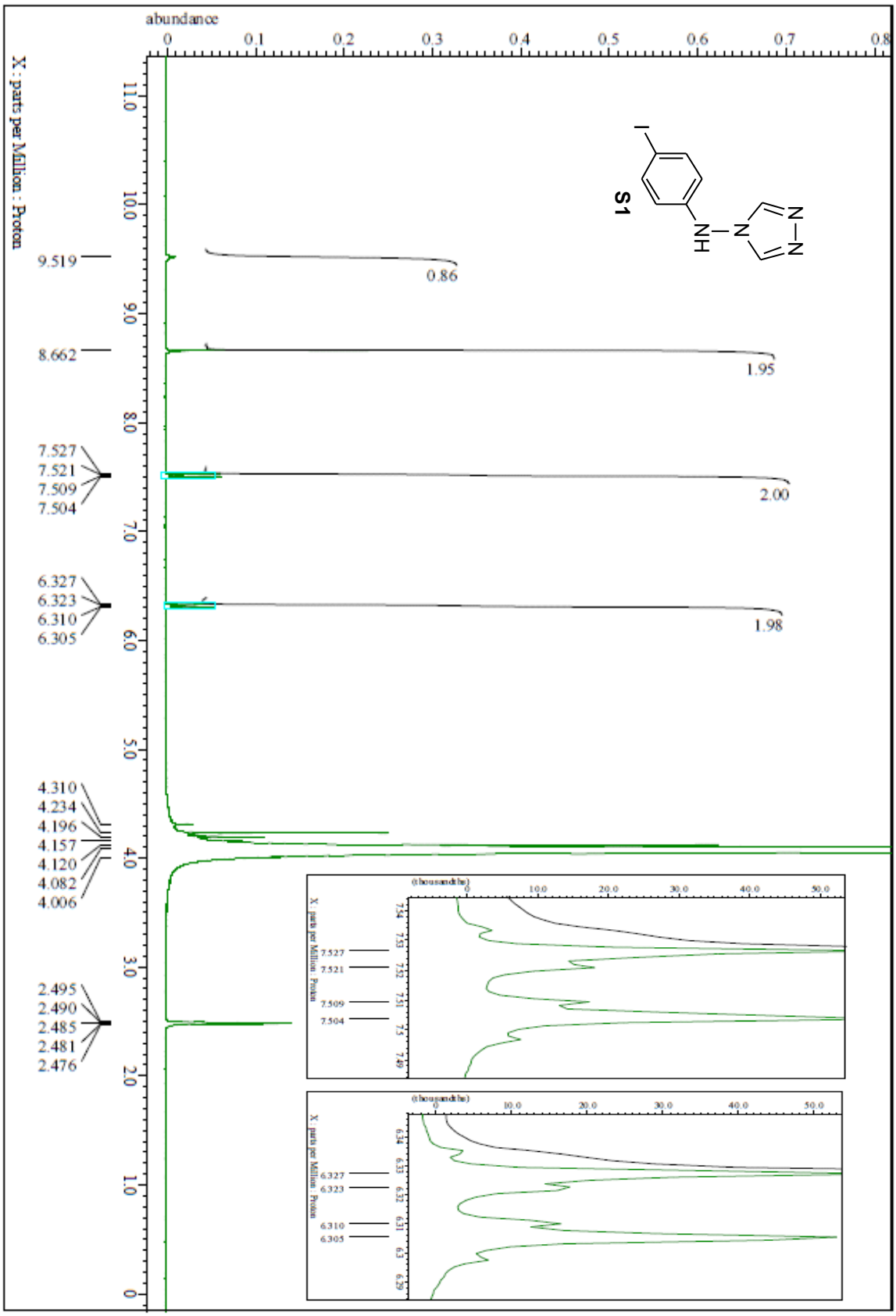
^{1}H NMR (400 MHz) spectrum of **2o** ($CDCl_3$)



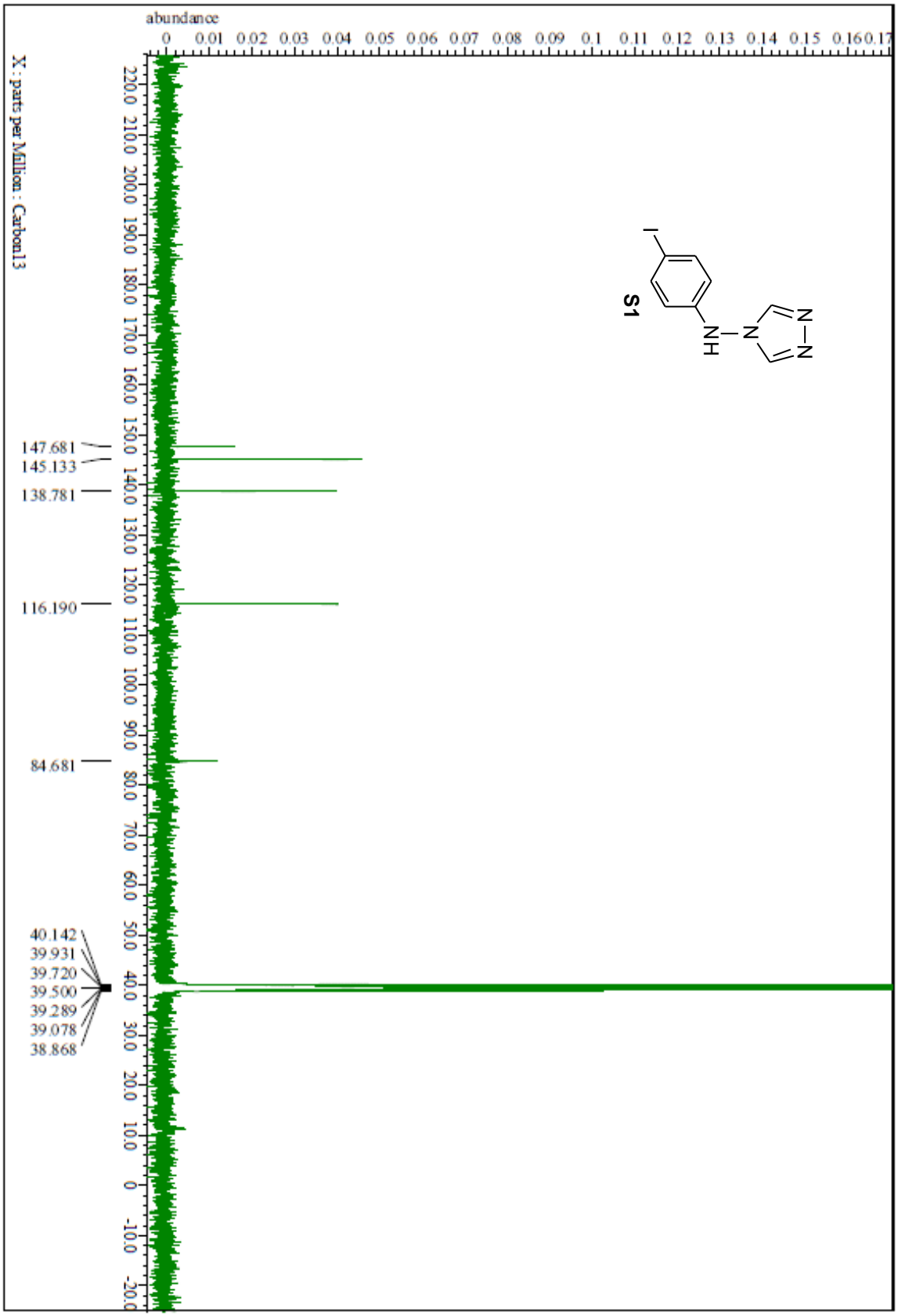
^{13}C NMR (100 MHz) spectrum of **2o** ($CDCl_3$)



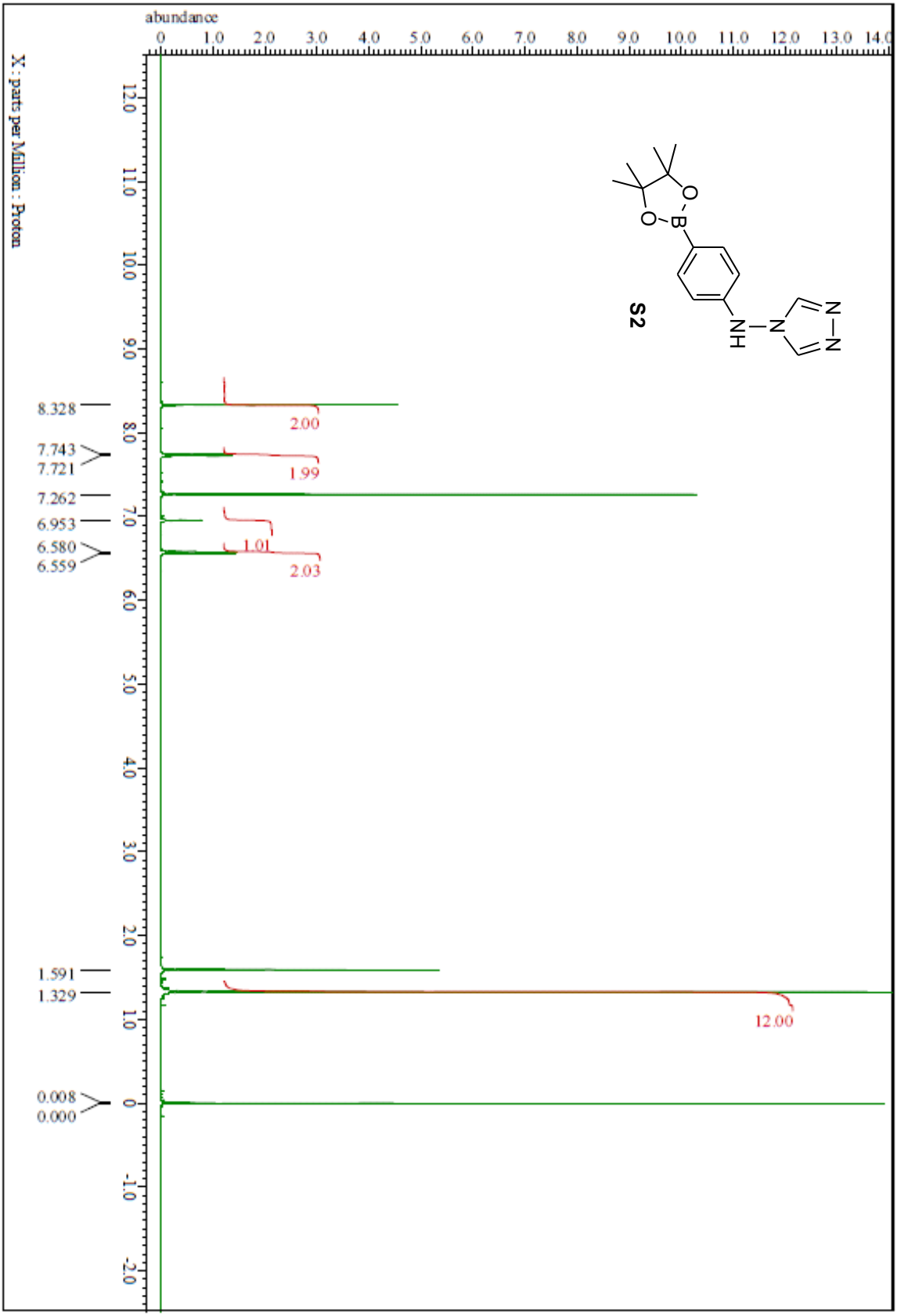
^{1}H NMR (400 MHz) spectrum of **S1** (DMSO-d_6)



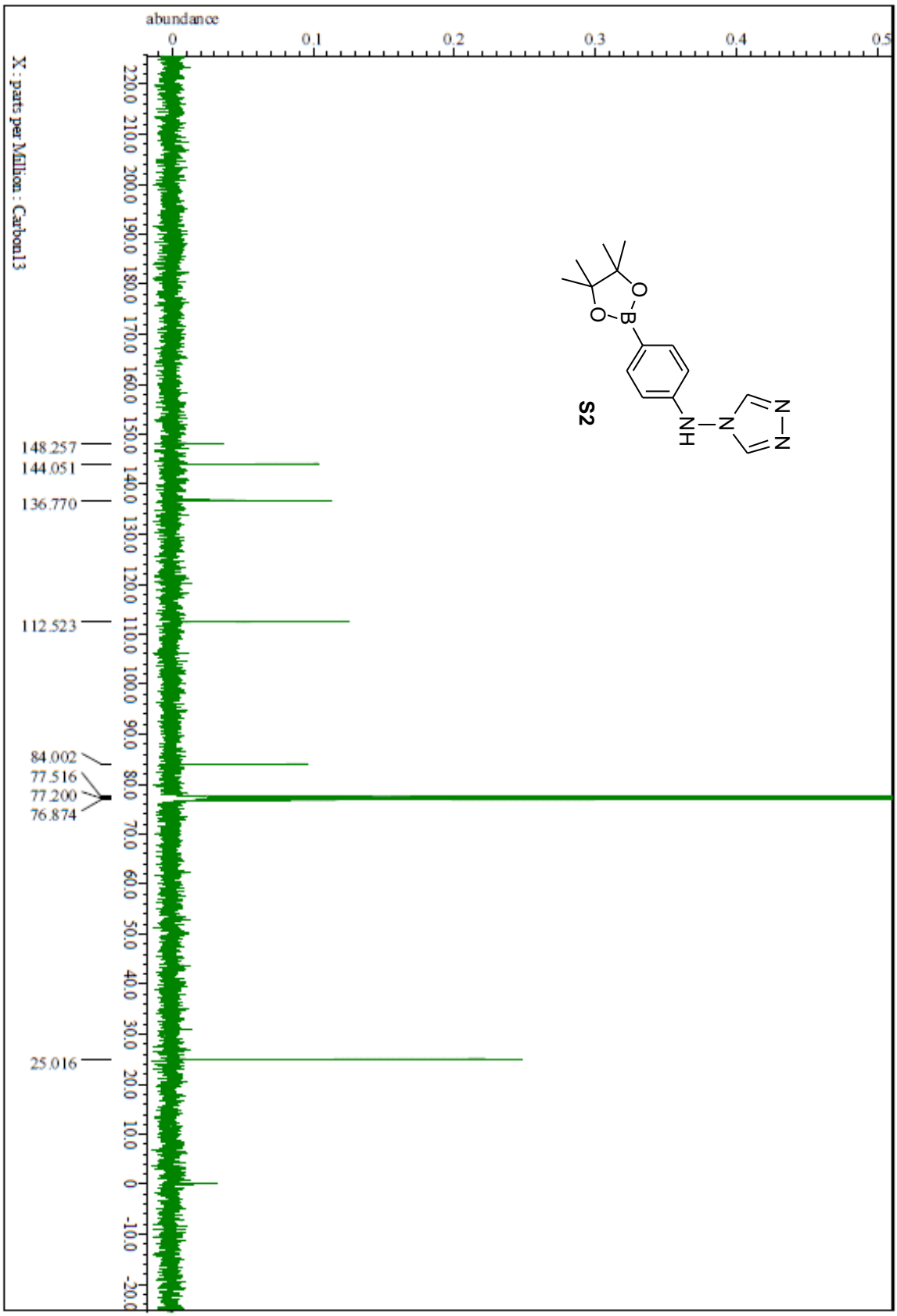
^{13}C NMR (100 MHz) spectrum of **S1** (DMSO-d_6)



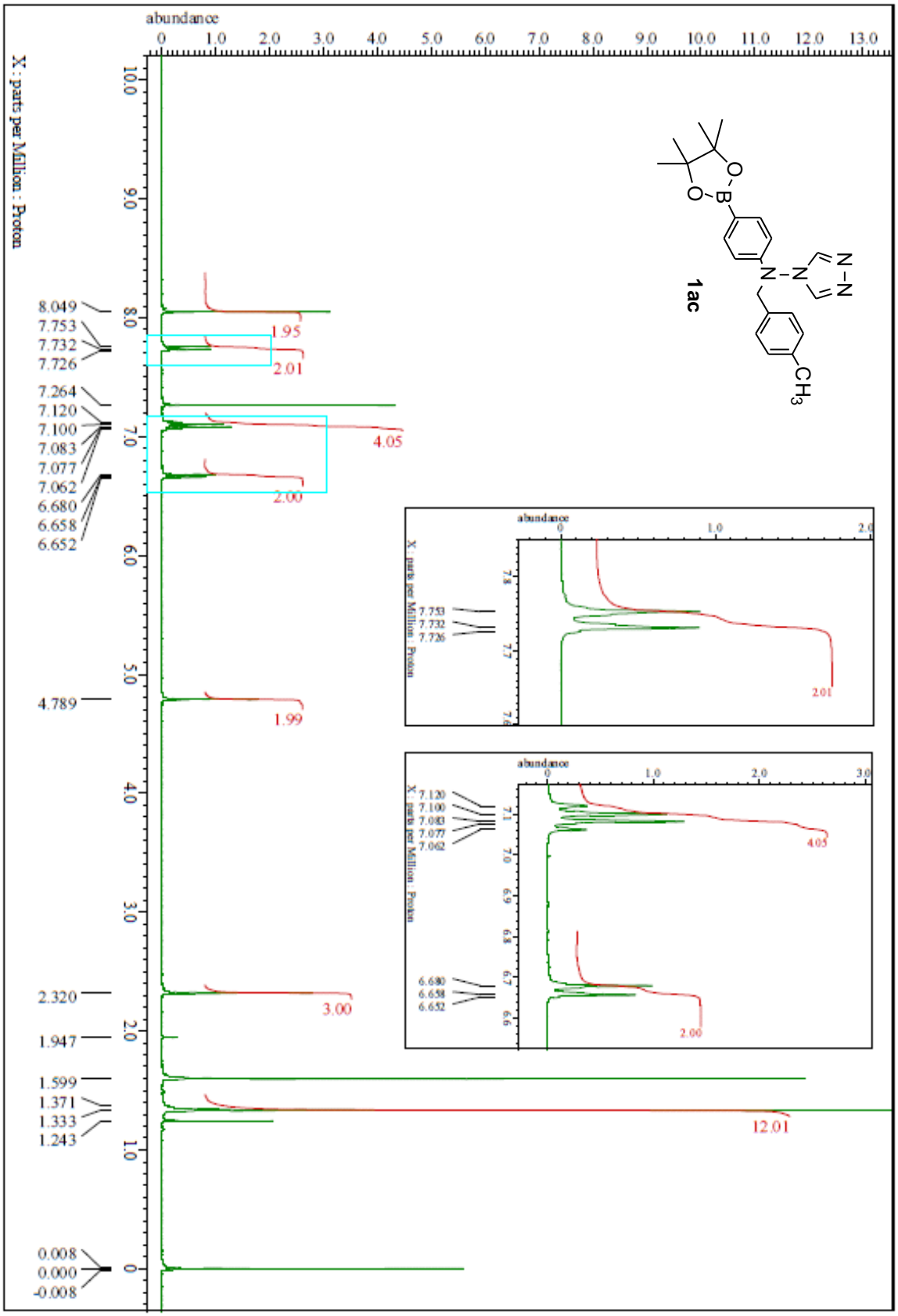
^{1}H NMR (400 MHz) spectrum of **S2** ($CDCl_3$)



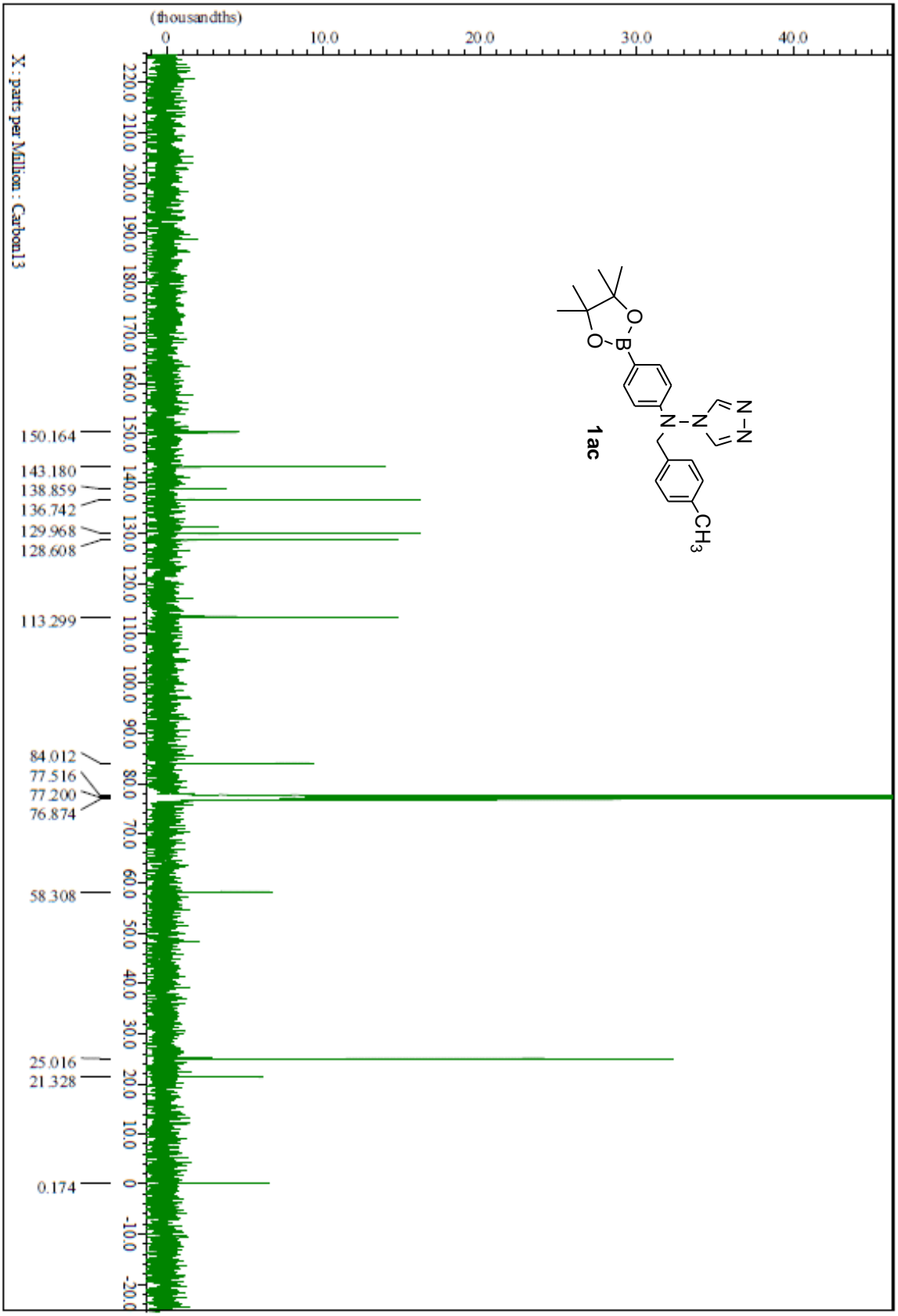
^{13}C NMR (100 MHz) spectrum of **S2** ($CDCl_3$)



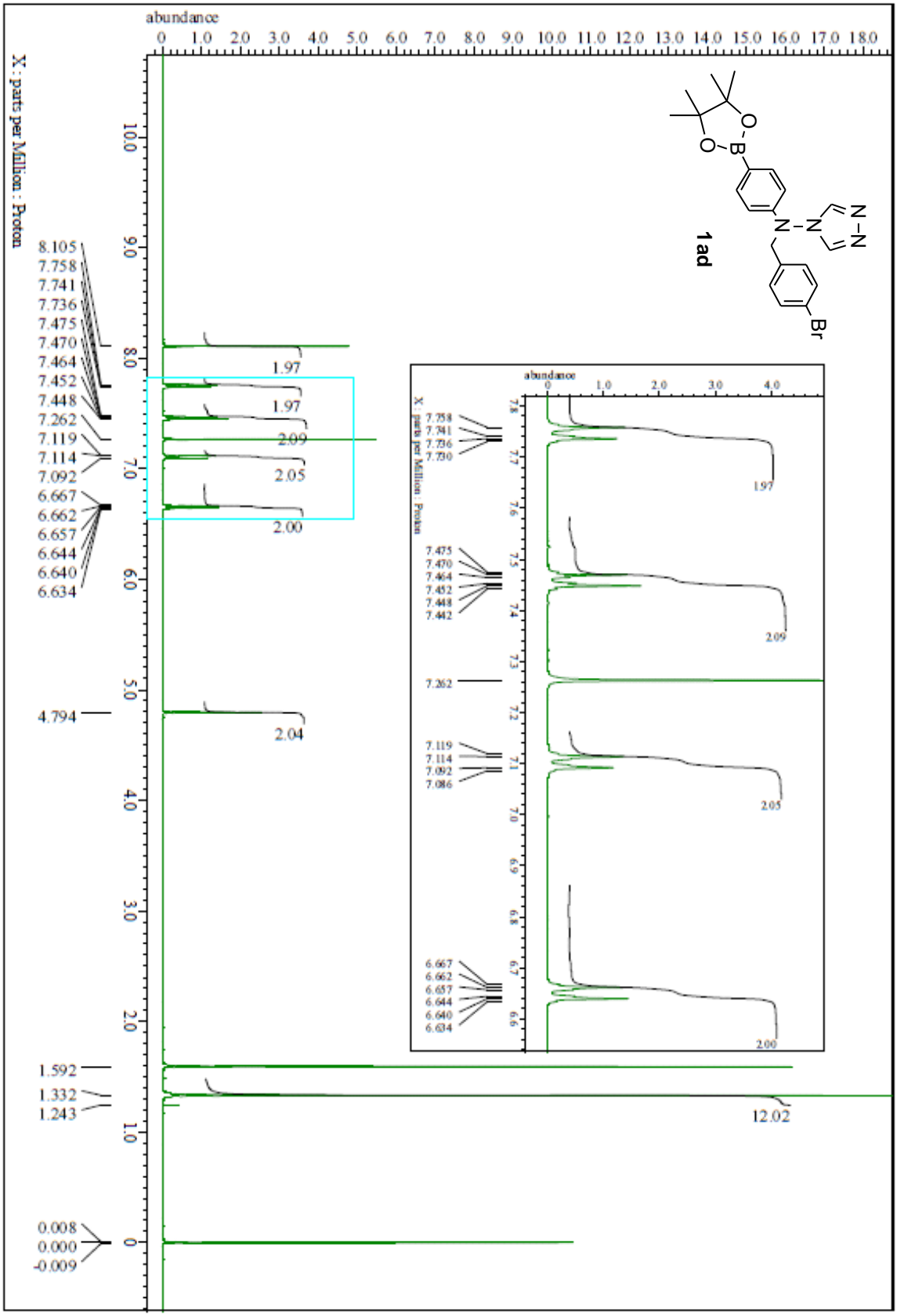
^{1}H NMR (400 MHz) spectrum of **1ac** ($CDCl_3$)



^{13}C NMR (100 MHz) spectrum of **1ac** ($CDCl_3$)



^{1}H NMR (400 MHz) spectrum of **1ad** ($CDCl_3$)



^{13}C NMR (100 MHz) spectrum of **1ad** ($CDCl_3$)