Supporting information for

Radiosynthesis and Biological Evaluation of L and D *S*-(3-[^{18}F]Fluoropropyl)-homocysteine for Tumor Imaging using Positron Emission Tomography

Thomas Bourdier[†]*, *Rachael Shepherd*[†], *Paula Berghofer*[†], *Timothy Jackson*[†], *Christopher J. R. Fookes*[†], *Delphine Denoyer*[‡], *Donna Dorow*[‡], *Ivan Greguric*[†], *Marie-Claude Gregoire*[†], *Rodney J. Hicks*[‡], *Andrew Katsifis*[†]

[†]ANSTO LifeSciences, Australian Nuclear Science and Technology Organisation, Locked Bag 2001, Kirrawee DC NSW 2232, Sydney, Australia.

[‡]Centre for Molecular Imaging, The Peter MacCallum Cancer Centre, 12 St Andrew's Place, East Melbourne, VIC, 3002, Australia.

*To whom correspondence should be addressed. Tel: +61 2 9717 3292, fax: +61 2 9717 9262, E-mail address: bts@ansto.gov.au

Contents

I. Reactivity of precursor 1-3 using potassium carbonate or potassium oxalate for the radiolabeling

Chart 1. Radiolabelling of tosyl, bromo and chloro-precursors **1-3** (5 mg) in acetonitrile (2 mL) with K_{222} (10 mg) and K_2CO_3 (2 mg) as a function of temperature and time.

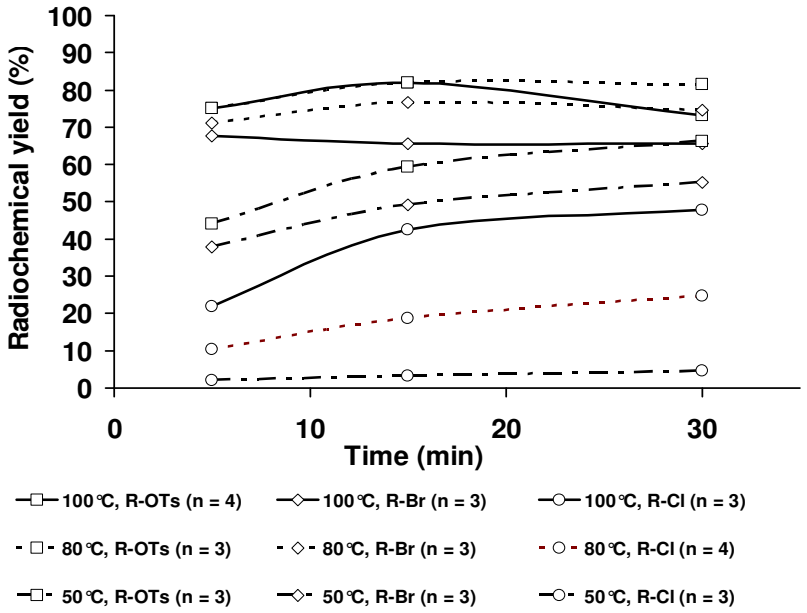
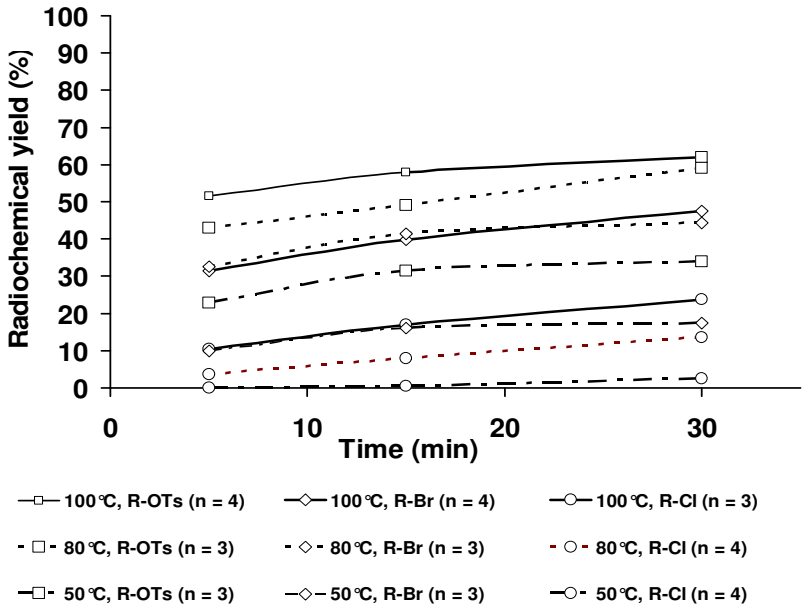


Chart 2. Radiolabelling of tosyl, bromo and chloro-precursors **1-3** (5 mg) in acetonitrile (2 mL) with K_{222} (10 mg), $K_2C_2O_4$ (2.55 mg) and K_2CO_3 (50 μg) as a function of temperature and time.



II. HPLC profile of [^{18}F]FPHCys for the radiosynthesis and QC analysis

Figure 1. HPLC profile of [^{18}F]FPHCys synthesis showing UV and radioactivity traces. [^{18}F]FPHCys has 15 min as retention time.

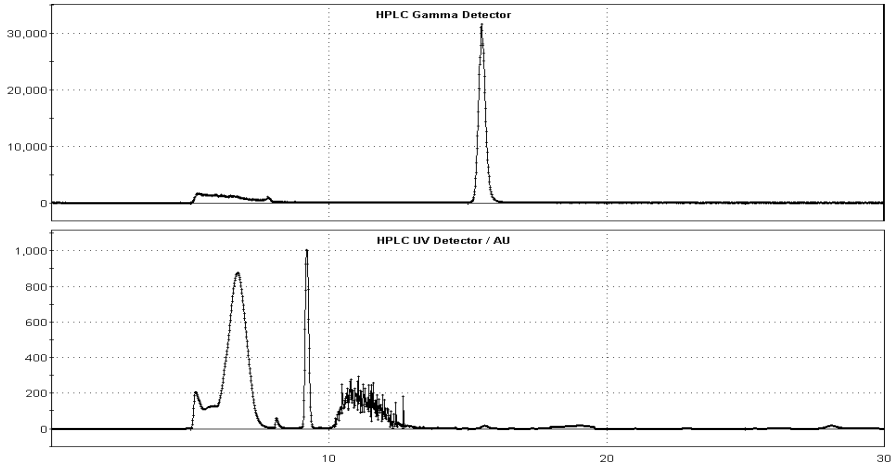
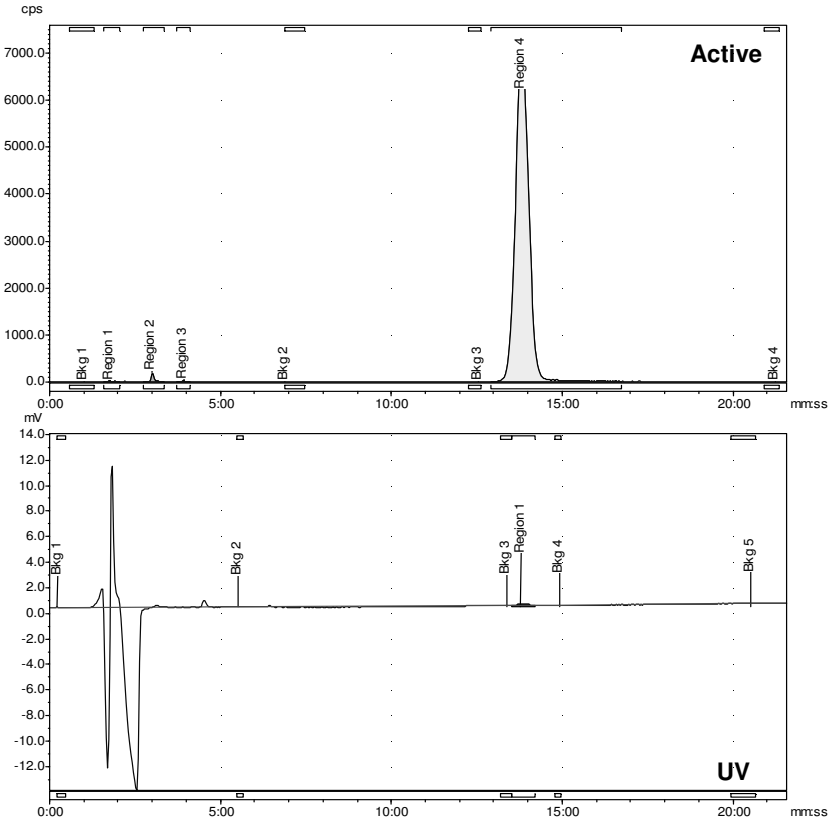


Figure 2. QC analysis of [^{18}F]FPHCys for chemical and radiochemical purity. [^{18}F]FPHCys has 13.5-14.5 min as retention time.



III. Reaction sequence and preparation of reagent for the [^{18}F]FPHCys radiosynthesis

Table 1. Summary of the reaction sequence for [^{18}F]FPHCys radiosynthesis

Fluorination of FPHCys precursor
A. [^{18}F]fluoride trapping on a QMA cartridge
B. [^{18}F]fluoride desorption by eluent
C. Azeotropic evaporation
D. Addition of FPHCys precursor to the reactor vial
E. [^{18}F]fluorination at 100^{o}C for 10 min
Acid hydrolysis
F. Addition of HCl to the reactor vial
G. Hydrolysis at 100^{o}C for 3 min
H. Evaporation of acetonitrile at 100^{o}C for 2 min
I. Addition of NaOH and phosphate buffer
J. Filtration on Alumina cartridge
Purification of [^{18}F]FPHCys
K. Injection on HPLC preparative
L. Collection of [^{18}F]FPHCys
M. Sterile filtration

Table 2. Preparation of reagents for the GE Tracerlab FX_{FN} synthesis module

Entry	Position	Reagents or materials	Quantities
1	V10-V11	Sep-Pak® Light QMA	1
2	V1	$K_2C_2O_4/K_2CO_3$ in H_2O	2.55 mg / 50 μg in 200 μL
3	V1	K_{222} in CH_3CN	10 mg in 800 μL
4	V3	Tosylate precursor **1** in CH_3CN	5 mg in 2 ml
5	V4	6 N HCl	500 μL
6	V5	6 N NaOH	500 μL
7	V6	Phosphate buffer, pH 6, 0.15 M	1 mL
8	V14-V12	Sep-Pak® Light Alumina N	1
9	V16	0.22 μm sterile filter	1