Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2012

Supplementary information

Single-step radiofluorination of peptides using continuous flow microreactor

Svetlana V. Selivanova,[a] Linjing Mu,[a] Johanna Ungersboeck,[b] Timo Stellfeld,[c] Simon M. Ametamey,*[a] Roger Schibli,[a] and Wolfgang Wadsak*[b]

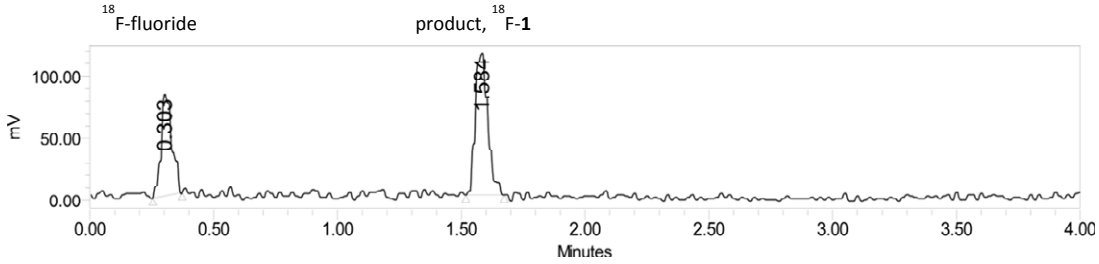
*[*a] Center for Radiopharmaceutical Sciences, ETH Zurich, IPW HCI H427, Wolfgang-Pauli-Strasse 10, 8093 Zurich, Switzerland. Fax: 41 44 633 1367; Tel: 41 44 633 7463; E-mail: simon.ametamey@pharma.ethz.ch*
*[*b] Radiochemistry and Biomarker Development Unit, Department of Nuclear Medicine, Medical University of Vienna, Waehringer Guertel 18-20, A-1090 Vienna, Austria. Fax: 43 1 40400 1557; Tel: 43 1 40400 5255; E-mail: wolfgang.wadsak@meduniwien.ac.at*
[c] Bayer HealthCare, Global Drug Discovery, Berlin, Germany

This journal is © The Royal Society of Chemistry 2012

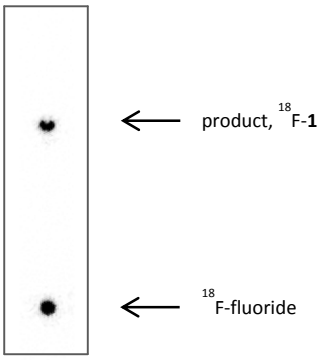
Representative UPLC and TLC analytical chromatograms.

No side products, except unreacted fluoride and radiolabelled peptide, were detected in the reaction mixtures. An example of chromatograms below supports this statement. Reaction was performed at 80°C at 20 µl/min flow rate. Precursor **1** concentration was 0.5 mg/ml.

UPLC radiochromatogram:



TLC radiochromatogram:



Product isolation using Waters Seppak Light C18 cartridge.

The reaction mixture was diluted with 0.1% TFA (12 ml) and loaded on the cartridge. The cartridge was washed with 0.1% TFA (2 ml) to remove remaining unreacted ^{18}F-fluoride. The product was eluted with ethanol (0.5 ml).

Isolated decay corrected RCY was 43%. Radiochemical purity of the isolated product was >99%.

Starting activity	**73.3 MBq**
Cartridge effluent	18.3 MBq
Washing	2.3 MBq
Product eluted	**32.3 MBq**
Residual cartridge activity	6.7 MBq

Comparison of analytical data obtained using UPLC and TLC for peptide 2.

To determine product yield by UPLC, the area under radioactive product peak was divided by the sum of areas of all radioactive peaks present (in this case, only two peaks were observed for each reaction mixture: one was identified as product peak and second was unreacted fluoride).

To determine product yield by TLC, regions of interest were drown on TLC plates using InstantImager software. Percentage was calculated as product counts divided by total counts.

The graph shows that both methods give the same trend, although absolute values are different (being higher for UPLC and lower for TLC).