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Supplementary Material

[^{18}F]Fluorination Optimisation and the Full Automated Production of [^{18}F]MEL050 using a Microfluidic System

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Table of Contents

General Experimental

All reagents and solvents were purchased from ABX (Radeberg, Germany) or Sigma-Aldrich. The chlorinated precursor **2** was synthesised in-house.[1] Aqueous [^{18}F]fluoride was produced on an IBA Cyclone 18 Twin cyclotron (ANSTO, Camperdown, Australia) by the ^{18}O(p, n)^{18}F nuclear reaction and delivered to the NanoTek Microfluidic Synthesis System (Advion, Ithaca, NY, USA). Up to 150 GBq of [^{18}F]fluoride was trapped on a MP-1 resin (ORTG, Oakdale, TN, USA), eluted with 15-20 mg of $K_{2.2.2}$ in 1 mL of CH_3CN and 80 µL of 10% w/v aqueous K_2CO_3 and azeotropically dried with CH_3CN under vacuum and N_2 flow. The dried [^{18}F]complex was reconstituted with 700 µL of CH_3CN and 200 µL of DMSO before being loaded into the storage loop of P3. The precursor **2** (3 mg) was dissolved in 600 µL DMSO and loaded into the storage loop of P1. [^{18}F]Fluorination optimisation was performed as described previously.[2] The automated radiosynthesis of **[^{18}F]1** was performed with the aid of a custom-made electrical connection board to facilitate HPLC/SPE purification and formulation.[3] The dummy reactions (generally 30 µL of radioactive complex) were used in the estimation of the RCY of the product, whereby the amount of radioactivity could be extrapolated from the amount present in the dummy reaction. Specific activity values for **[^{18}F]1** were calculated by measuring the radioactivity injected into an analytical HPLC system and assessing the UV absorbance associated with the radioactive peak.

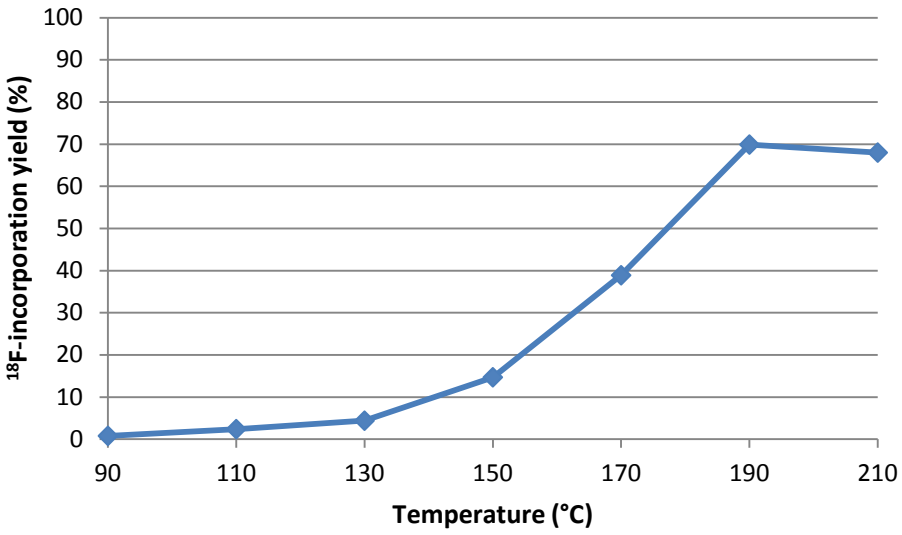

Figure S1. [^{18}F]Fluorination incorporation yield of **[^{18}F]1** at varying temperatures, using a 20 µL/min flow rate for each reagent.

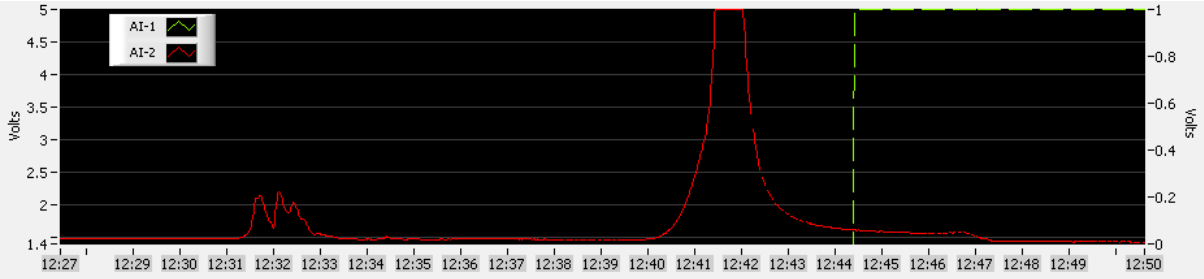

Figure S2. Crude radio-HPLC chromatogram of **[^{18}F]1**.

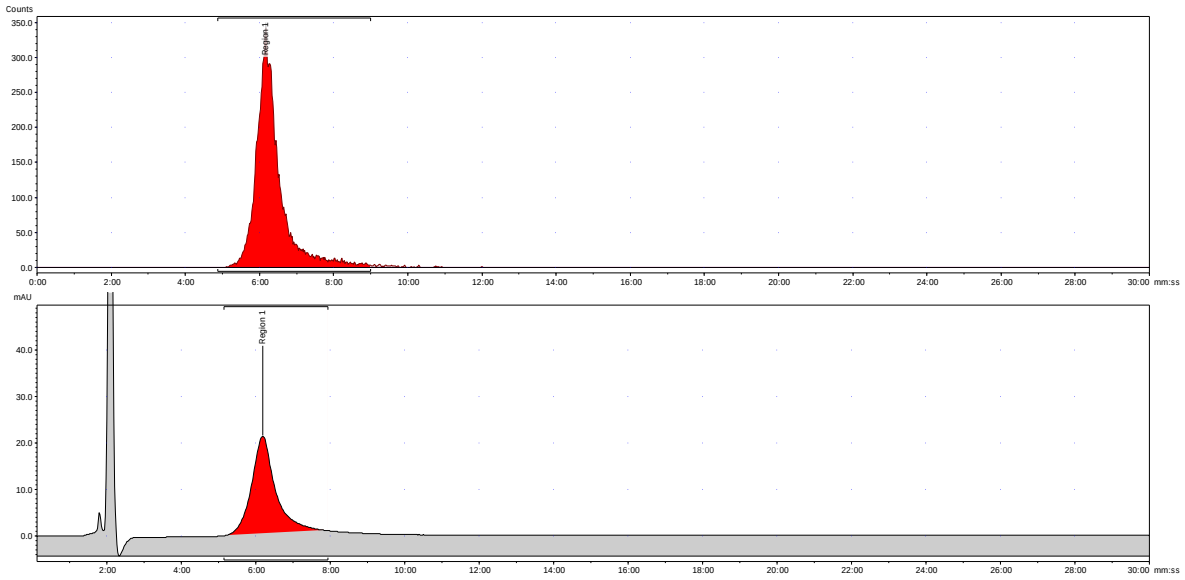

Figure S3. Radio-HPLC of purified **[^{18}F]1** and the corresponding non-radioactive reference standard.

[1] I. Greguric, S. R. Taylor, D. Denoyer, P. Ballantyne, P. Berghofer, P. Roselt, T. Q. Pham, F. Mattner, T. Bourdier, O. C. Neels, D. S. Dorow, C. Loc'h, R. J. Hicks, A. Katsifis, *J. Med. Chem.* **2009**, *52*, 5299. doi: 10.1021/jm9008423

[2] G. Pascali, G. Mazzone, G. Saccomanni, C. Manera, P. A. Salvadori, *Nucl. Med. Biol.* **2010**, *37*, 547. doi: 10.1016/j.nucmedbio.2010.03.006

[3] G. Pascali, A. Berton, M. DeSimone, N. Wyatt, L. Matesic, I. Greguric, P. A. Salvadori, *Appl. Rad. Isot.* **2014**, *84*, 40. doi: 10.1016/j.apradiso.2013.10.020