

Supporting Information

Synthesis and evaluation of new ^{18}F -labelled acetamidobenzoxazolone-based radioligands for imaging of translocator protein (18 kDa, TSPO) in brain

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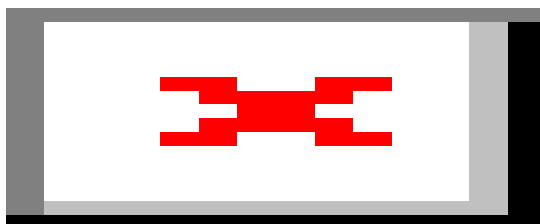
Supplemental Table 1. G_{score} of **1–3** for TSPO ligand interaction

Ligand	G_{score}
1	-10.455
2	-12.319
3	-11.839

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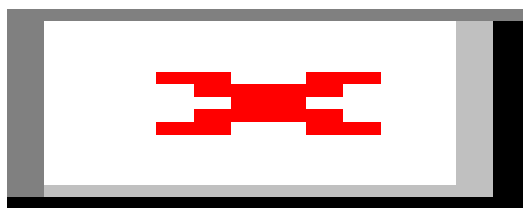
Analysis chart of **2**

HPLC (Capcell Pack UG80 C₁₈ column (4.6 mm i.d. × 250 mm). MeCN/H₂O/ Et₃N, 6.0/4.0/0.01 (v/v/v), flow rate = 1.0 mL/min, λ_{uv} = 254 nm)



Analysis chart of **3**

HPLC (Capcell Pack UG80 C₁₈ column (4.6 mm i.d. × 250 mm). MeCN/H₂O/ Et₃N, 65/35/0.01 (v/v/v), flow rate = 1.0 mL/min, λ_{uv} = 254 nm)



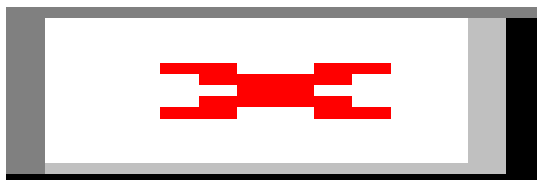
Supplemental Figure 1. HPLC analytic charts for **2** and **3**

[¹⁸F]**2** HPLC analytical chart

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HPLC (Capcell Pack UG80 C₁₈ column (10.0 mm i.d. × 250 mm). MeCN/H₂O/ Et₃N, 6.0/4.0/0.01 (v/v/v), flow rate = 5.0 mL/min, λ_{uv} = 254 nm)

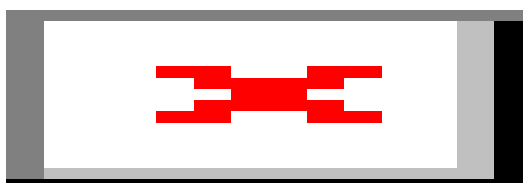
Detector: UV-254 nm (blue) and RI (red)



[¹⁸F]3 HPLC analytical chart

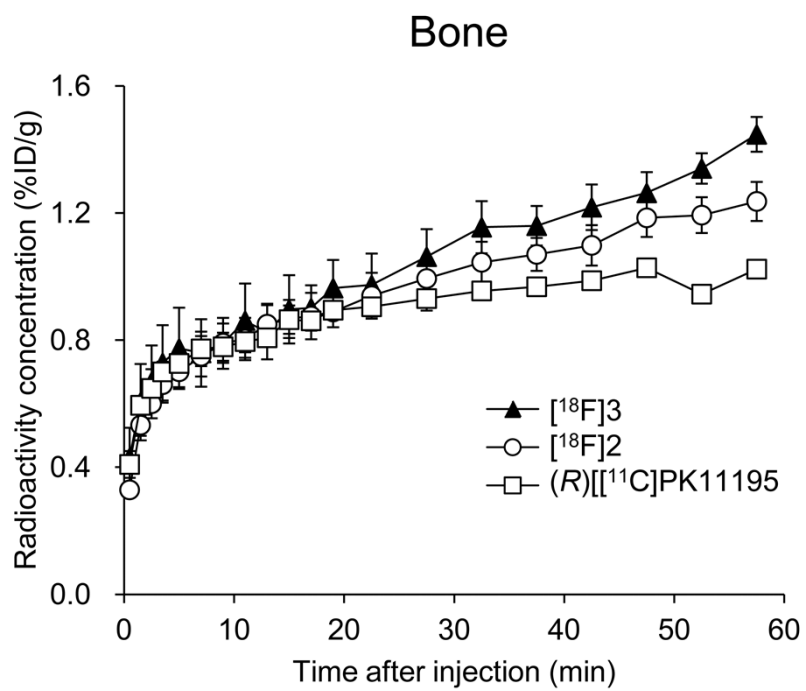
HPLC (Capcell Pack UG80 C₁₈ column (4.6 mm i.d. × 250 mm). MeCN/H₂O/ Et₃N, 65/35/0.01 (v/v/v), flow rate = 1.0 mL/min, λ_{uv} = 254 nm)

Detector: UV-254 nm (Green) and RI (red)



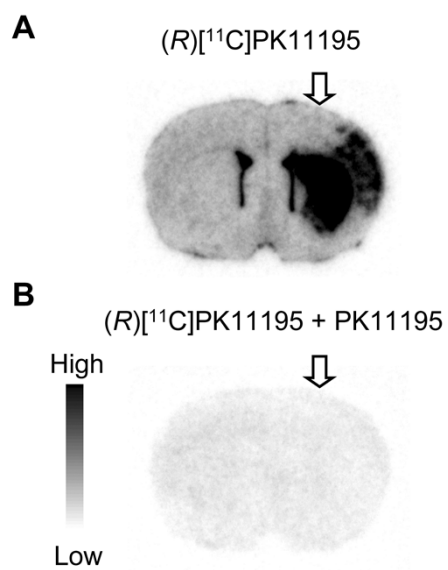
Supplemental Figure 2. HPLC analytical charts [¹⁸F]2 and [¹⁸F]3

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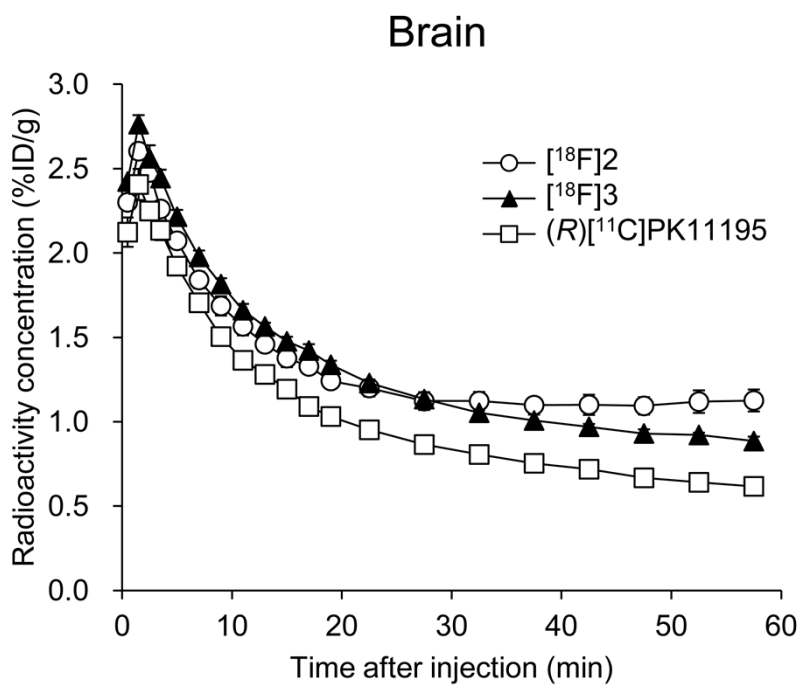
Supplemental Figure 3. Time-activity curves for bone uptake.

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Supplemental Figure 4. Representative in vitro autoradiograms of $(R)[^{11}\text{C}]PK11195$ in ischemic rat brains ($n = 4$). Arrows indicate ischemic areas. (A) $(R)[^{11}\text{C}]PK11195$ only; (B) Incubation with unlabelled PK11195.

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Supplemental Figure 5. Time-activity curves for brain uptake.