

Supporting information for:

From Structure-Activity Relationships on Thiazole Derivatives to the *In Vivo* Evaluation of a
New Radiotracer for Cannabinoid Subtype 2 PET Imaging

Fabien Caillé^{†, 1}, Fanny Cacheux^{†, 1}, Marie-Anne Peyronneau,¹ Emilie Jaumain,¹ Benoît Jégou,¹
Géraldine Pottier,¹ Christoph Ullmer,² Uwe Grether,² Alexandra Winkeler,¹ Frédéric Dollé,¹
Annelaure Damont¹ and Bertrand Kuhnast^{*,1}

¹UMR 1023 IMIV, Service Hospitalier Frédéric Joliot, CEA, Inserm, Université Paris Sud,
CNRS, Université Paris-Saclay, Orsay, France

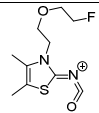
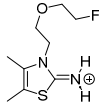
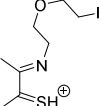
²Roche Innovation Center Basel, F. Hoffmann-La Roche Ltd., Basel, Switzerland

*corresponding author: bertrand.kuhnast@cea.fr

ORCID iD Bertrand Kuhnast : 0000-0002-5035-4072

[†] these authors contributed equally to this work

Table S1. Positive ion ESI-MS [M+H⁺] and predominant MS² and MS³ fragments obtained for **2f** and its main metabolites.

Compound	2f	M1	M2	M3	M4	M5	M6
[M+H ⁺]	343	359	359	375	297	359	375
RT	6.41	5.78	5.48	5.28	5.29	4.55	3.90
	245			261		245	261
	219	235	235	235	173	219	251
	192		208				
	155	171	171		156	155	155
	129	127	146		130		
	91	91	91			91	91

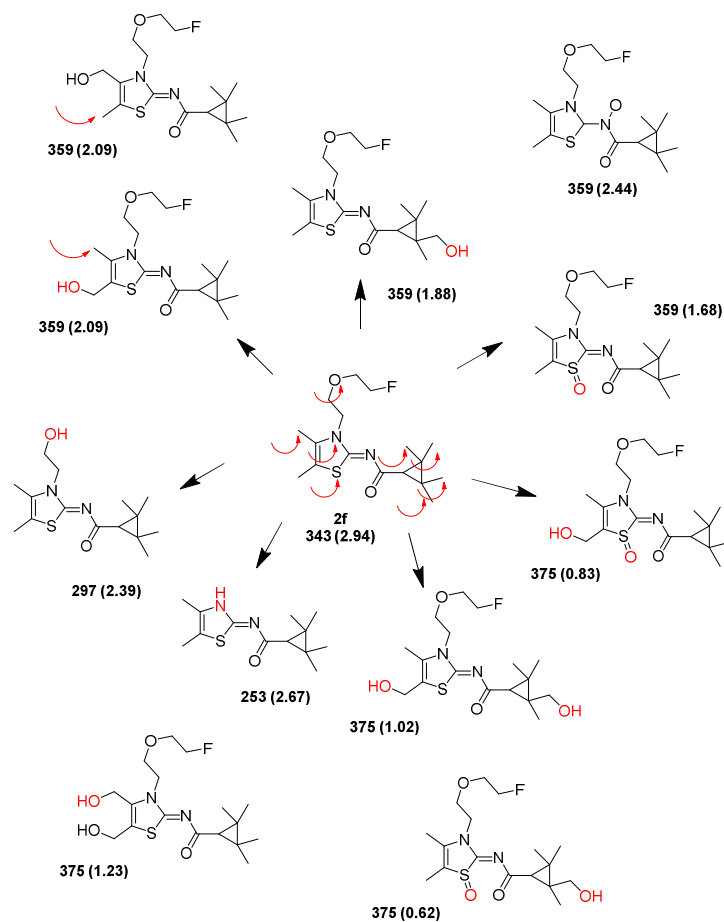


Figure S1. Proposed metabolic pathways for **2f** with potential sites of oxidation (red arrows). The numbers between brackets represent the lipophilicity (logP).

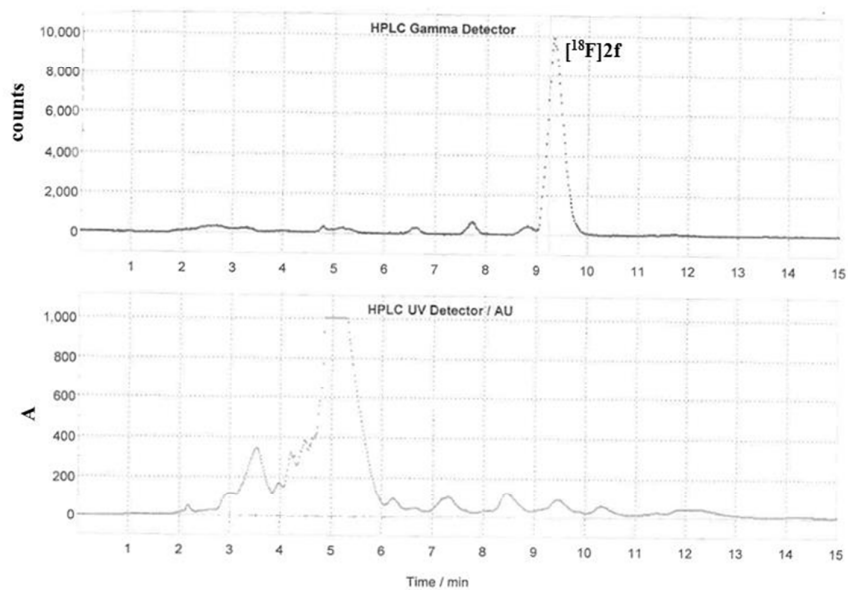


Figure S2. Semi-preparative HPLC with gamma detection (top) and UV detection (bottom) for purification of $[^{18}\text{F}]\mathbf{2f}$.

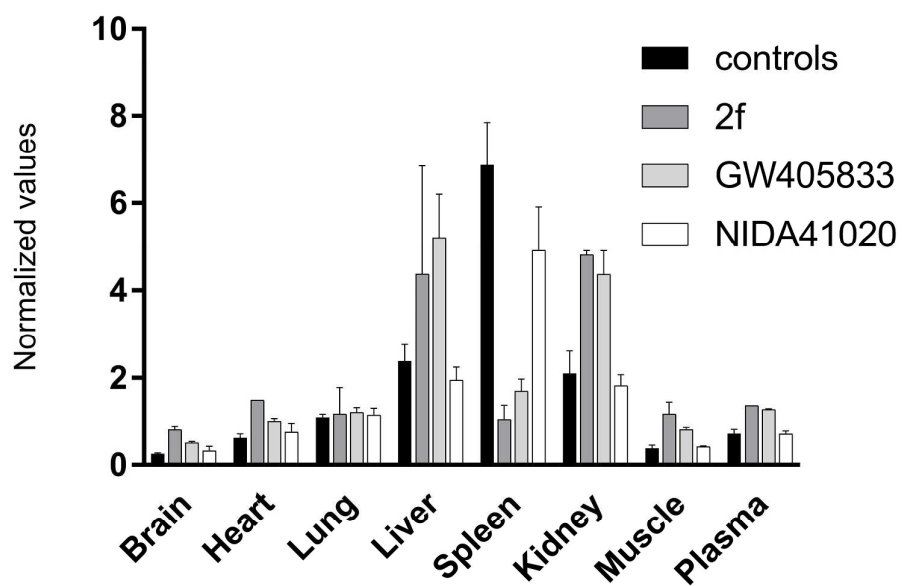


Figure S3. Biodistribution of $[^{18}\text{F}]\mathbf{2f}$ on healthy rats with or without presaturation.