## **Supporting Information**

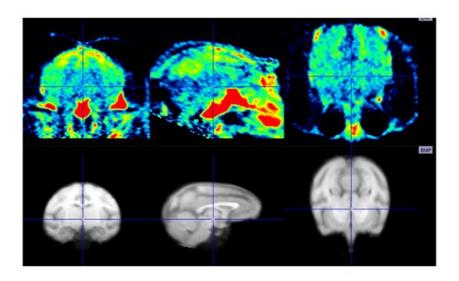
## 3-Substituted 1,5-Diaryl-1*H*-1,2,4-triazoles as Prospective PET Radioligands for Imaging Brain COX-1 in Monkey. Part 2: Selection and Evaluation of [<sup>11</sup>C]PS13 for Quantitative Imaging

Stal Shrestha,<sup>†</sup> Prachi Singh,<sup>†</sup> Michelle Y. Cortes-Salva,<sup>†</sup> Kimberly J. Jenko,<sup>†</sup> Masamichi Ikawa,<sup>†</sup> Min-Jeong Kim,<sup>†</sup> Masato Kobayashi,<sup>†</sup> Cheryl L. Morse,<sup>†</sup> Robert L. Gladding,<sup>†</sup> Jeih-San Liow,<sup>†</sup> Sami S. Zoghbi,<sup>†</sup> Masahiro Fujita,<sup>†</sup> Robert B. Innis<sup>†</sup> and Victor W. Pike<sup>†\*</sup>

<sup>&</sup>lt;sup>†</sup>Molecular Imaging Branch, National Institute of Mental Health, National Institutes of Health, Building 10, Room B3 C346A, 10 Center Drive, Bethesda, Maryland 20892, United States

## Contents

Figure S1. PET images of brain radioactivity (SUV) in normal rhesus monkey							
after intravenous injection of [ <sup>2</sup> H <sub>2</sub> , <sup>18</sup> F]PS2 (top row). The images show undesirable							
radioactivity uptake in skull. The bottom row shows the MRI.							
Figure S2. Time courses of parent radioligand concentration in monkey arterial							
plasma for [11C]PS1, [2H2,18F]PS2, and [11C]PS13. Plasma curves were fitted as a							
triexponential. The inset shows the data up to about 5 min.	S3						
<b>Figure S3.</b> Regional $V_T$ for (panel <b>A</b> ) and $V_T/f_P$ (panel <b>B</b> ) for [ $^{11}$ C] <b>PS13</b> in one							
Rhesus monkey at baseline and under self-block condition (1 mg/kg, i.v.); regional							
$V_{\rm T}$ (panel C) and $V_{\rm T}/f_{\rm P}$ (panel D) for [11C]PS13 in another monkey at baseline and							
under pre-block with <b>KTP-Me</b> (3 mg/kg, i.v.); regional $V_T$ (panel <b>E</b> ) and $V_T/f_P$							
(panel F) for [11C]PS13 in another monkey at baseline and after pre-administration							
of MC1 (0.3 mg/kg, i.v.).	S4						
<b>Table S1.</b> Regional $V_T$ for [ $^{11}$ C] <b>PS13</b> in rhesus monkeys before (baseline) and after							
self-treatments (i.v.) with 1) PS13 (1 mg/kg), 2) KTP-Me (3 mg/kg); and 3) MC1							
(0.3 mg/kg).	S5						



**Figure S1.** PET images of brain radioactivity (SUV) in normal rhesus monkey after intravenous injection of  $[^2H_{25}^{18}F]PS2$  (top row). The images show undesirable radioactivity uptake in skull. The bottom row shows the MRI.

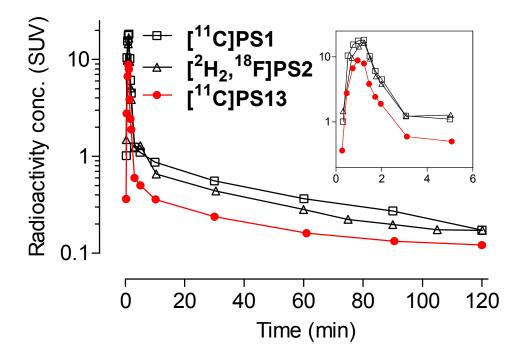
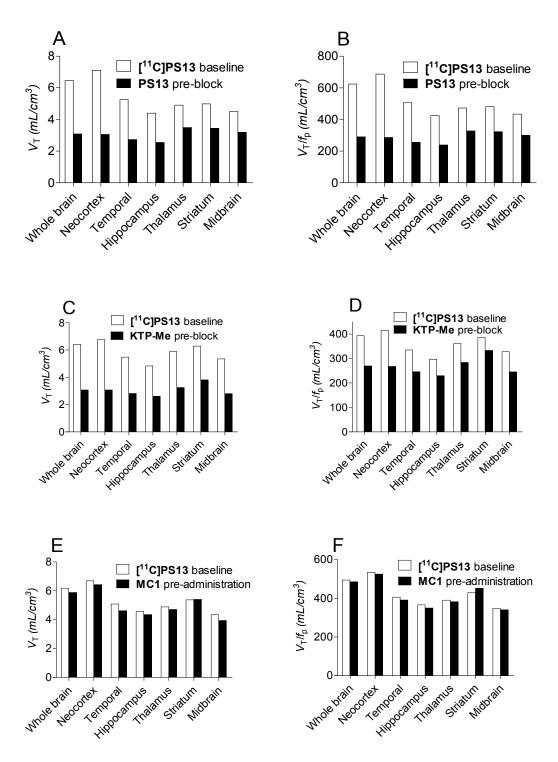


Figure S2. Time courses of parent radioligand concentration in monkey arterial plasma for [\frac{11}{C}]PS1, [\frac{2}{H\_2}, \frac{18}{F}]PS2, and [\frac{11}{C}]PS13. Plasma curves were fitted as a triexponential. The inset shows the data up to about 5 min.



**Figure S3.** Regional  $V_T$  for (panel **A**) and  $V_T/f_P$  (panel **B**) for [ $^{11}$ C]PS13 in one rhesus monkey at baseline and under self-block condition (1 mg/kg, i.v.); regional  $V_T$  (panel **C**) and  $V_T/f_P$  (panel **D**) for [ $^{11}$ C]PS13 in another monkey at baseline and under pre-block with **KTP-Me** (3 mg/kg, i.v.); regional  $V_T$  (panel **E**) and  $V_T/f_P$  (panel **F**) for [ $^{11}$ C]PS13 in another monkey at baseline and after pre-administration of **MC1** (0.3 mg/kg, i.v.).

**Table S1.** Regional  $V_T$  for [ $^{11}$ C]PS13 in rhesus monkeys before (baseline) and after self-treatments (i.v.) with 1) PS13 (1 mg/kg), 2) KTP-Me (3 mg/kg); and 3) MC1 (0.3 mg/kg).

	$V_{\rm T}~({\rm mL/cm}^3)$								
Regions	Baselines			Study 1		Study 2		Study 3	
	mean		SD	Baseline	PS13	Baseline	KTP- Me	Baseline	MC1
Whole brain	6.45	土	0.24	6.76	3.09	6.41	3.07	6.18	5.88
Neocortex	6.97	$\pm$	0.34	7.44	3.13	6.77	3.07	6.69	6.42
Temporal	5.33	$\pm$	0.18	5.43	3.04	5.47	2.82	5.08	4.61
Hippocampus	4.59	$\pm$	0.19	4.37	2.54	4.83	2.62	4.58	4.35
Thalamus	5.22	$\pm$	0.48	4.88	3.49	5.89	3.25	4.88	4.71
Striatum	5.59	$\pm$	0.50	5.11	3.21	6.28	3.81	5.37	5.40
Midbrain	4.73	$\pm$	0.44	4.49	3.19	5.35	2.80	4.34	3.94