

Anion	SCN ⁻	PO ₃ F ₂ ⁻	I ⁻	SO ₃ F ⁻	BF ₄ ⁻	ReO ₄ ⁻	TcO ₄ ⁻	PF ₆ ⁻	ClO ₄ ⁻	Br ⁻	CN ⁻	NO ₃ ⁻	N ₃ ⁻
Anion volume (A ³)	71 ± 3	90 ± 6	72 ± 16	88 ± 4	73 ± 9	86 ± 13	93 ± 2	109 ± 8	82 ± 13	56 ± 14	50 ± 6	64 ± 11	58 ± 14
IC ₅₀ vs. ^{99m} TcO ₄ ⁻ uptake, 3E.Δ-NIS cells	8.3 (K)	3.9 (NH ₄)	2.7 (K)	0.56 (K)	0.29 (K)	0.15 (K)	0.07 (NH ₄)	0.021 (K)	N/D	N/D	N/D	N/D	N/D
IC ₅₀ vs. ^{99m} TcO ₄ ⁻ uptake, HCT116-C19 cells	8.5 (K)	6.9 (NH ₄)	4.7 (Na)	0.55 (K)	4.5 (Na)	N/D	N/D	0.026 (K)	N/D	N/D	N/D	755 (Na)	N/D
IC ₅₀ vs. ¹²⁷ I ⁻ uptake, FRTL5 cells (1)	12 (Na)	N/D	N/D	N/D	1.2 (Na)	N/D	N/D	0.015 (K)	0.1 (Na)	3300 (Na)	1900 (K)	800 (Na)	2200 (Na)
IC ₅₀ vs. ¹²⁵ I ⁻ uptake, FRTL5 cells (1)	14 (Na)	N/D	N/D	N/D	0.75 (Na)	N/D	N/D	0.009 (K)	0.14 (Na)	1400 (Na)	1700 (K)	250 (Na)	1200 (Na)
IC ₅₀ vs. ¹²⁵ I ⁻ uptake, CHO-hNIS cells (2)	19.3	N/D	33.9 (Na)	N/D	N/D	N/D	N/D	N/D	1.27	N/D	N/D	297	N/D
IC ₅₀ vs. ¹²⁵ I ⁻ uptake, FRTL5 cells (3)	N/D	N/D	N/D	N/D	0.7 (K)	N/D	N/D	N/D	0.4 (K)	N/D	N/D	N/D	N/D
IC ₅₀ vs. ¹⁸ F-BF ₄ ⁻ uptake, HCT116-C19 cells (4)	N/D	N/D	N/D	N/D	1.6 (Na)	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
IC ₅₀ vs. ^{99m} TcO ₄ ⁻ uptake, HCT116-C19 cells (4)	N/D	N/D	N/D	N/D	0.74 (Na)	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
IC ₅₀ vs. ¹⁸ F-BF ₄ ⁻ uptake, HCT116-C19 cells (5)	N/D	N/D	N/D	N/D	4.8 (Na)	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
IC ₅₀ vs. ¹⁸ F-SO ₃ F uptake, HCT116-C19 cells	N/D	N/D	N/D	1.6 (K)	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D

Supplemental Table 1. IC₅₀ values (μM) against anion transport in various cell lines and corresponding volumes (b) for univalent anions. Counter-cation is given in brackets after IC₅₀ value (if known). N/D = not determined.

Entry	Base	Precursor (mg)	Temp. (°C)	Time (min)	Radiochemical yield (%)*
1	KHCO ₃	5	80	15	38
2	KHCO ₃	5	30	15	7
3	K ₂ CO ₃	5	80	15	50
4	K ₂ CO ₃	0.5	80	15	14

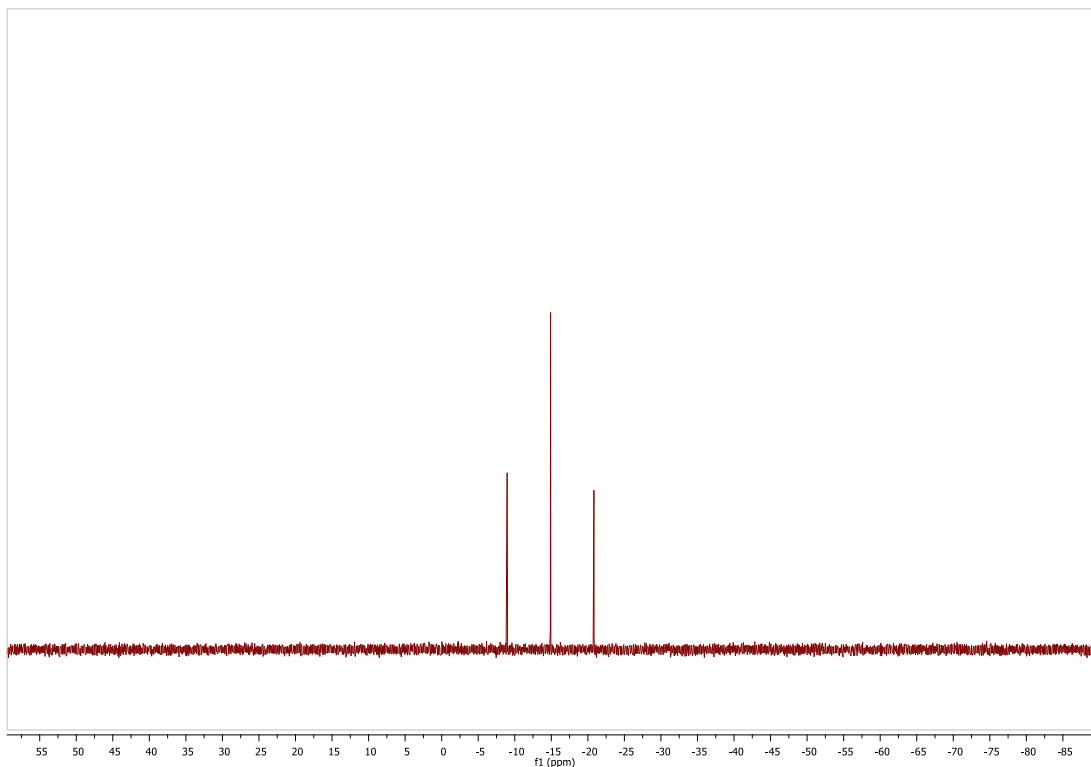
5	K ₂ CO ₃	5	80	10	65
6	K ₂ CO ₃	5	80	20	38
7	K ₂ CO ₃	5	80	5	25

Supplemental Table 2. Radiochemical yield values for reaction of ¹⁸F-KF with SO₃-pyridine under varying conditions, as determined by ion chromatography (details in main manuscript)

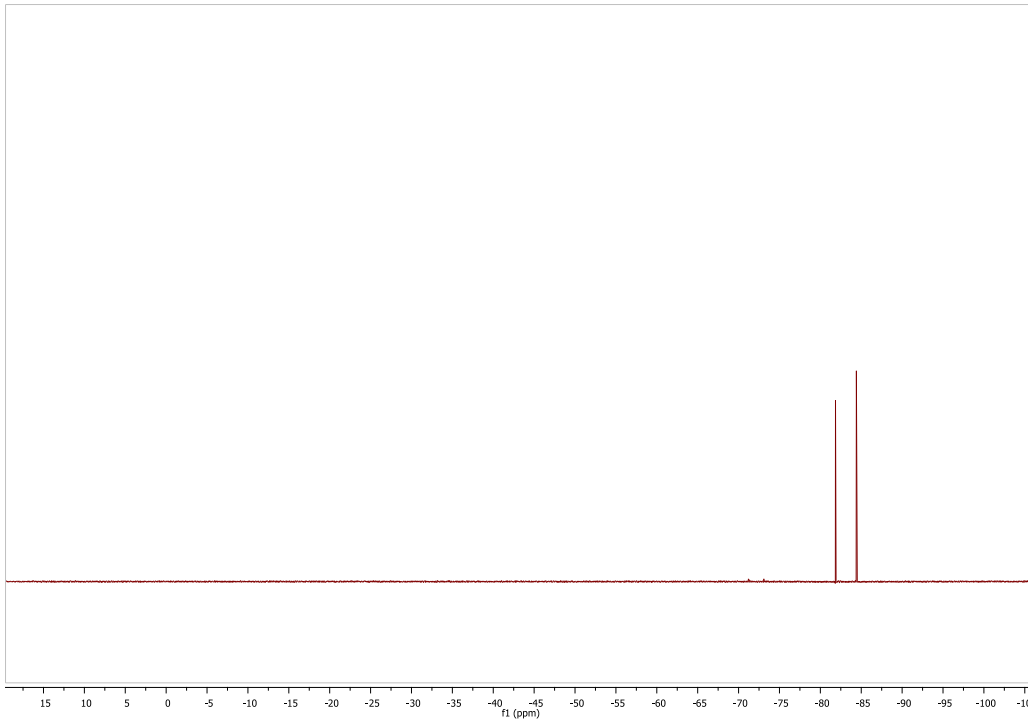
*Pre-purification yield in crude reaction mixture

	0.9% NaCl @ 25°C	Human serum @ 37°C	HCl/glycine buffer (pH 3.0) @ 37°C
0 h	99	99	95
1 h	ND	98	95
2 h	ND	98	95
3 h	ND	98	95
4 h	99	98	94

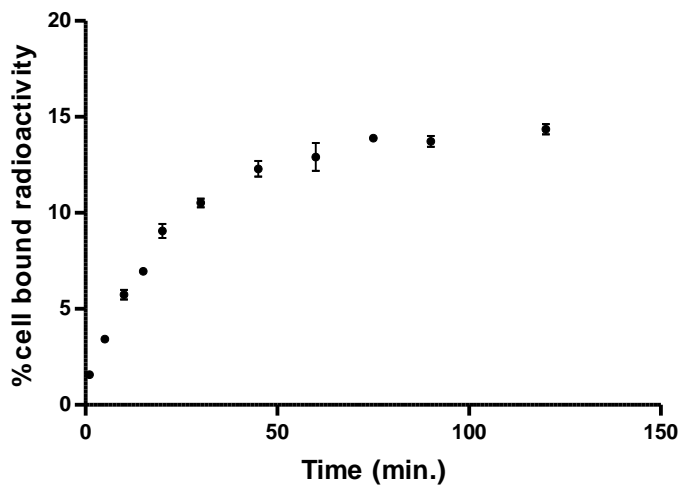
Supplemental Table 3. Radiochemical purity (%) of ¹⁸F-SO₃F⁻ incubated in saline, serum or acidic buffer over a 4 hour time period, as determined by ion chromatography (0.9% NaCl) and TLC (human serum and HCl/Glycine buffer). Details of analytical methods are given in main manuscript.



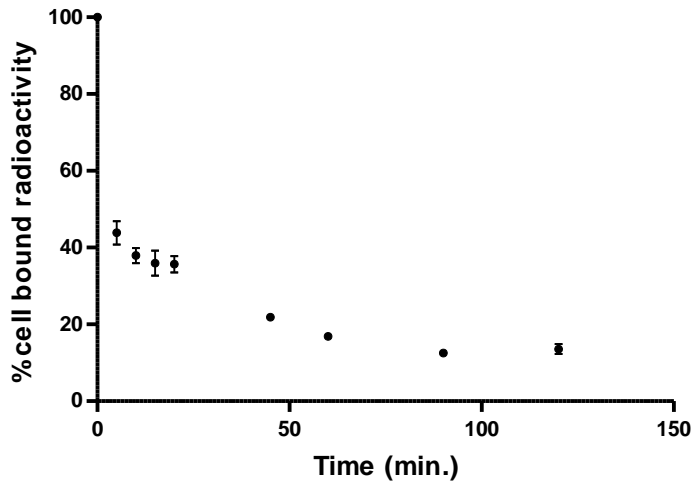
Supplemental Figure 1. ³¹P NMR spectrum of NH₄PO₂F₂ showing a triplet at δ 14.89 ($J = 962.1$ MHz) owing to coupling to two ¹⁹F nuclei. Data collected using Bruker Ultrashield 400WB PLUS 9.4 T spectrometer operating at a frequency of 161.976 MHz. The compound was analyzed as a solution (5 mg/mL) in D₂O. Data were analyzed using MestReNova LITE (v5.2.5-5780).



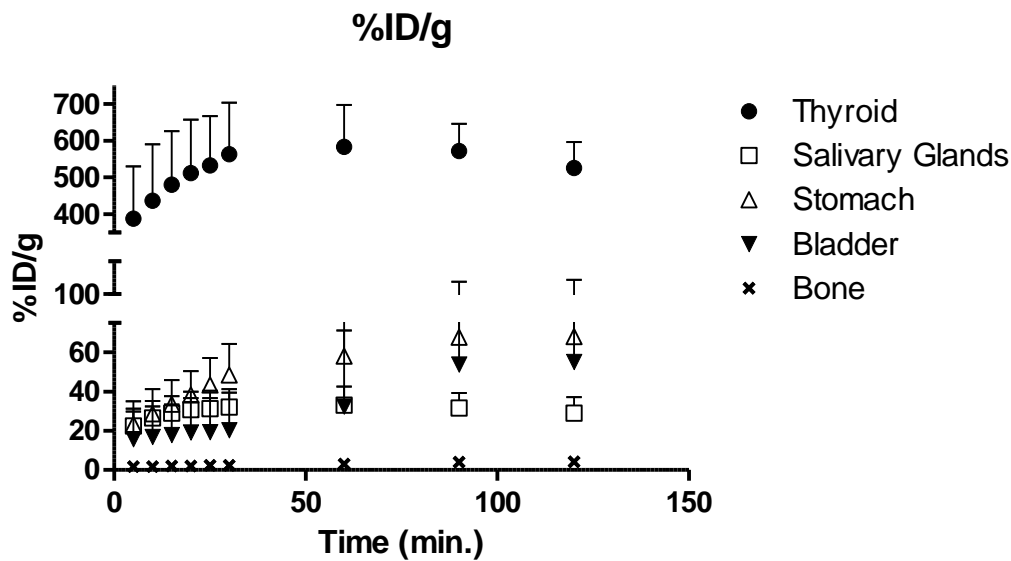
Supplemental Figure 2. ^{19}F NMR spectrum of $\text{NH}_4\text{PO}_2\text{F}_2$ showing a doublet at $\delta -83.14$ ($J = 971.4$ MHz) owing to coupling to a single ^{31}P nucleus. Data collected using Bruker Ultrashield 400WB PLUS 9.4 T spectrometer operating at a frequency of 376.461 MHz respectively. The compound was analyzed as a solution (5 mg/mL) in D_2O . Data were analyzed using MestReNova LITE (v5.2.5-5780).



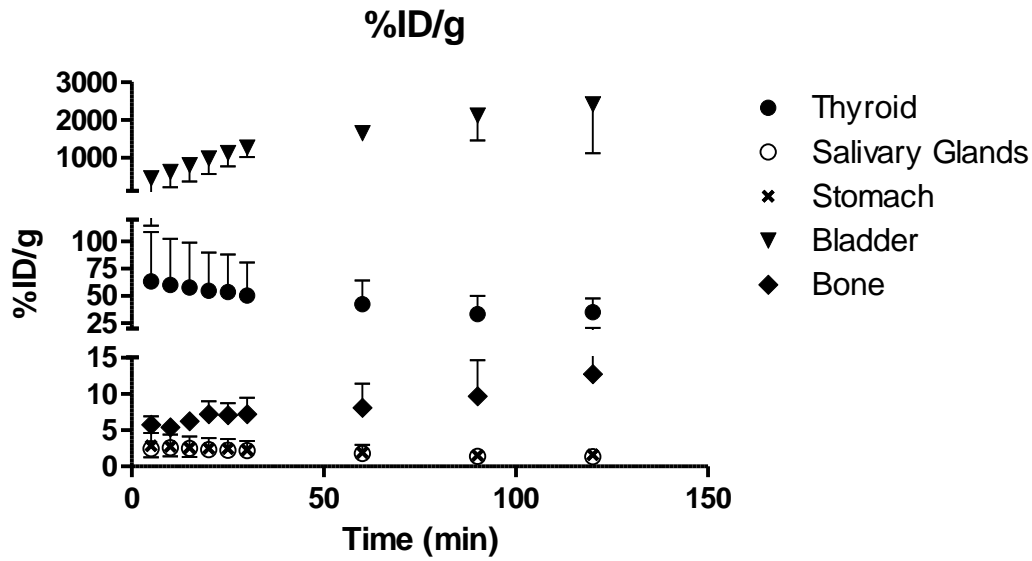
Supplemental Figure 3. Uptake of $^{18}\text{F}\text{-SO}_3\text{F}^-$ in HCT116-C19 cells over a 2 h time period, assessed as % radioactivity bound to cells. Error bars represent 1 S.D.



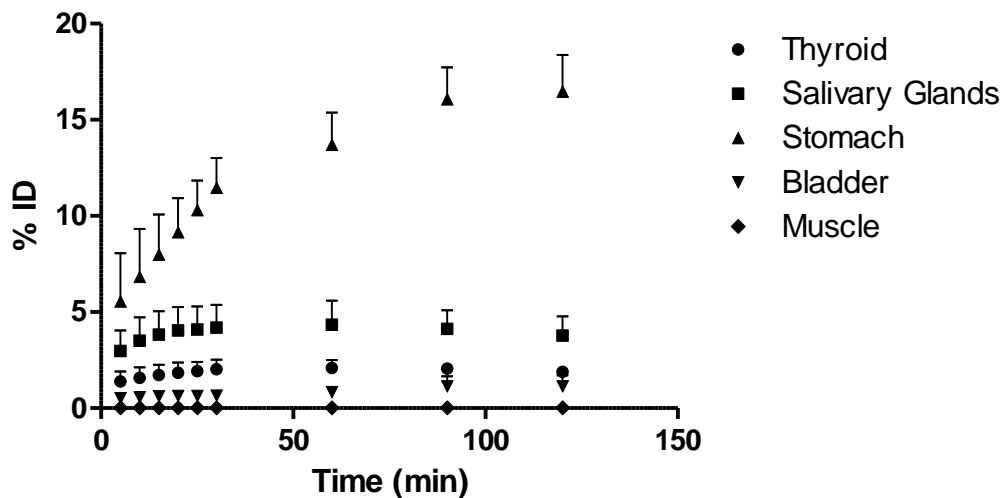
Supplemental Figure 4. Efflux of $^{18}\text{F-SO}_3\text{F}^-$ from HCT116-C19 cells over a 2 h time period, displayed as % remaining cell bound radioactivity. At $t = 0$ min it was assumed that all remaining activity was cell bound following the washing protocol and that this represented maximal cell bound activity (100%). Error bars represent 1 S.D.



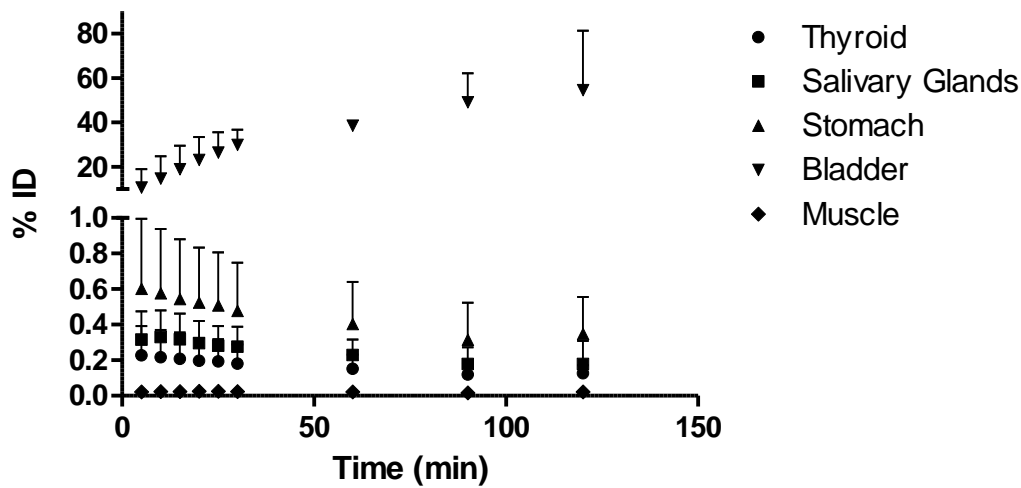
Supplemental Figure 5. Time-activity curve displaying %ID/g values calculated from PET/CT images for thyroid, salivary glands, stomach, and bladder over a 2 h time period in BALB/c mice without NaClO_4 inhibition ($n = 3$).



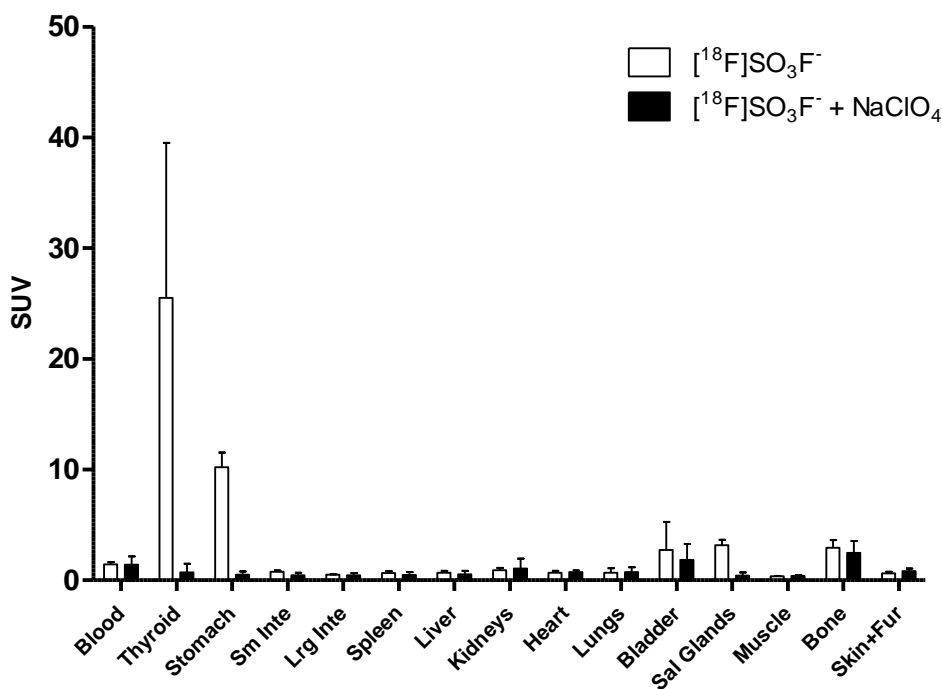
Supplemental Figure 6. Time-activity curve displaying %ID/g values calculated from PET/CT images for thyroid, salivary glands, stomach, and bladder over a 2 h time period in BALB/c mice with NaClO₄ inhibition (n = 3).



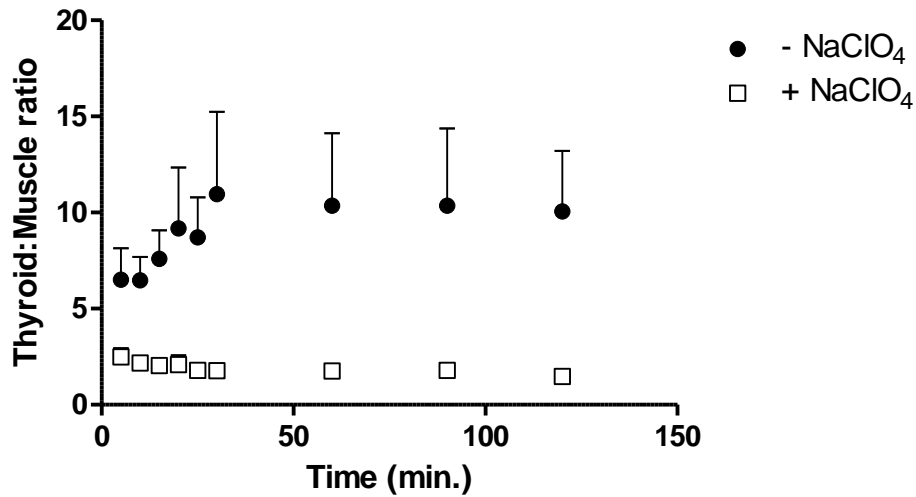
Supplemental Figure 7. Time-activity curve displaying %ID values calculated from PET/CT images for thyroid, salivary glands, stomach, bladder, and muscle over a 2 h time period in BALB/c mice without NaClO₄ inhibition (n = 3)



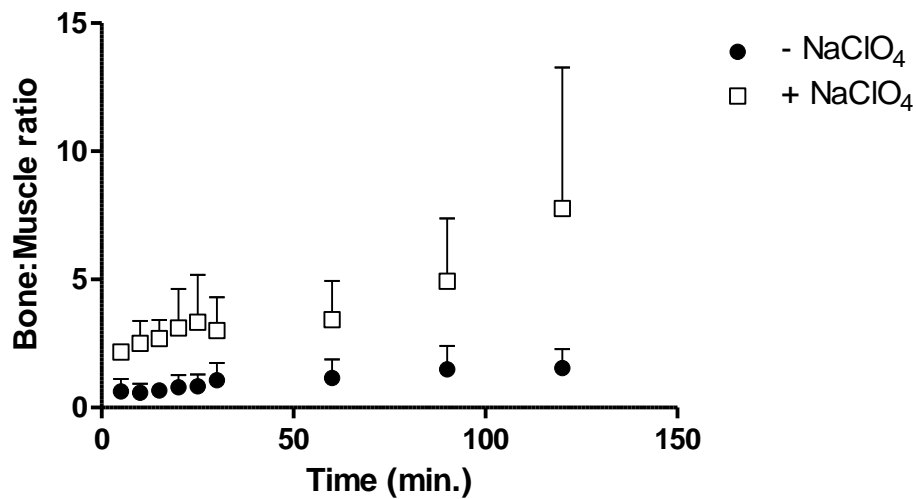
Supplemental Figure 8. Time-activity curve displaying %ID values calculated from PET/CT images for thyroid, salivary glands, stomach, bladder, and muscle over a 2 h time period in BALB/c mice with NaClO₄ inhibition (n = 3).



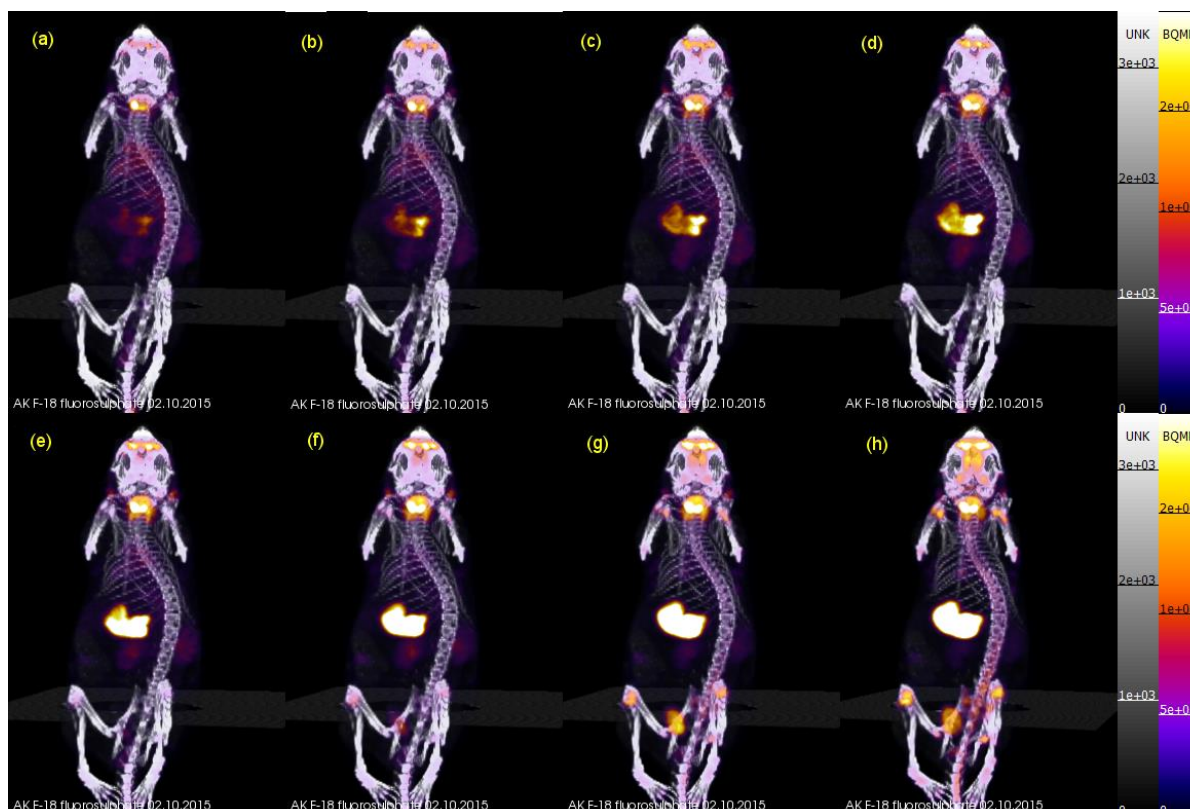
Supplemental Figure 9. *Ex vivo* biodistribution data for ¹⁸F-SO₃F⁻ in BALB/c mice 2.25 h post-injection at (n = 3). Uptake is reported as a standardized uptake value (SUV), which was determined as the ratio of radioactivity in each tissue (MBq) per gram of organ tissue (weighed post-mortem) and radioactivity in the whole body (MBq) per gram of whole body weight (excluding tail). Error bars represent 1 SD.



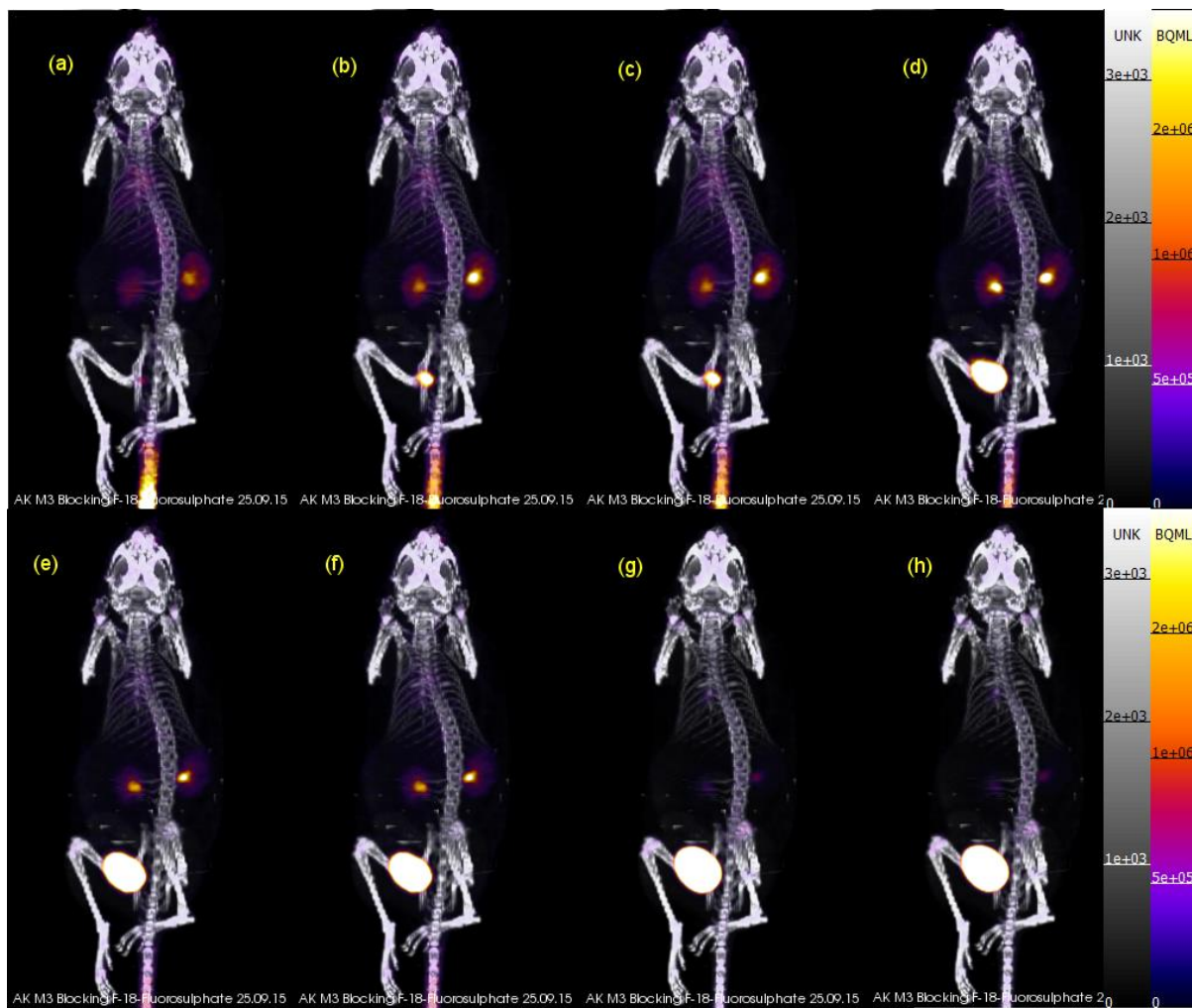
Supplemental Figure 10. Change in ratio of thyroid uptake to muscle uptake (%ID/mL) over time in presence and absence of NaClO₄ inhibition (n = 3 per group).



Supplemental Figure 11. Change in ratio of bone uptake to muscle uptake (%ID/mL) over time in presence and absence of NaClO₄ inhibition (n = 3 per group).



Supplemental Figure 12. PET/CT images of BALB/c mouse following administration of $^{18}\text{F}\text{-SO}_3\text{F}^-$ at (a) 5 min, (b) 10 min, (c) 15 min, (d) 20 min, (e) 30 min, (f) 60 min, (g) 90 min and (h) 120 min post-injection



Supplemental Figure 13. PET/CT images of BALB/c mouse following administration of ^{18}F - SO_3F^- and NaClO_4 (250 mg/kg) at (a) 5 min, (b) 10 min, (c) 15 min, (d) 20 min, (e) 30 min, (f) 60 min, (g) 90 min and (h) 120 min post-injection.

References

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