SUPPLEMENTAL MATERIAL



Supplemental Figure 1. Linear correlations within quadrants obtained from sections (Pearson R for Q1=0.5605, Q2=0.6979, Q3=-0.3358 and Q4=0.8150). We found that variance in the model is attributed to random errors from the four image quadrants (87.58% of total variance, Supplementary Table 1). Therefore, we calculated Pearson's R within the four quadrants, respectively (Fig. 4F). Quadrant 3 (Q3) shows a negative correlation, while the other quadrants show positive correlations between the signals. We speculated that histological section 6 (S6) is an outlier causing a negative correlation (Fig. 4F). We conducted Jackknife resampling and calculated Pearson's R to test if S6 is an outlier in Q3 (Supplementary Table 2). The resampled correlation coefficients without S6 (r = -0.3798 ~ 0.8611) are much higher than ones with S6 (r = -0.6819 ~ -0.3141), indicating that S6 is an influential outlier causing a negative correlation in Q3. These findings demonstrate the presence of microcalcifications in areas identified as PET-positive and CT-negative during *ex vivo* PET/CT imaging of explanted specimens.

Supplemental Table 1. Variance component analysis results. We conducted variance component analysis (VCA) for a mixed model for a correlational analysis between NIRF signal and ¹⁸F-fluoride autoradiography signal. CV: Coefficient of variation.

	Variance component	Percent to total (%)	CV (%)
Total	23.3549	100	41.449
Quadrant	20.4531	87.5753	38.7886
Histological Sections	1.5833	6.7792	10.792
Error	1.3185	5.6455	9.8484

Supplemental Table 2. Pearson's R in quadrants with Jackknife resampling. We conducted Jackknife resampling for all six sections with or without section 6 (S6) in quadrant 3 and calculated Pearson's r for signals between NIRF and 18F-fluoride. S6: Histological section 6.

Quadrant	Excluded section	Pearson's r with S6	Pearson's r without S6
3	1	-0.4208	0.3239
3	2	-0.6819	-0.3798
3	3	-0.3786	0.8611
3	4	-0.3141	0.2372
3	5	-0.3372	0.2348