Supplementary

Appendix 1

Supplementary Data S1

PET acquisition

^{18}F-PSMA-1007 images were acquired from a body PET/CT scanner (Gemini 64 TF, Philips Medical Systems, Best, The Netherlands) and were performed approximately 120 minutes after IV injection of 4.0 MBq/kg ^{18}F-PSMA-1007 (median activity: 282.7 MBq; range: 170.2–366.3 MBq). For attenuation correction, a low-dose unenhanced CT scan was performed from the skull base to the middle of the thigh, with the following parameters: tube voltage of 140 Kvp, tube current of 110 mA, detector collimation of 64 × 0.625 mm, pitch of 0.829, a tube rotation speed of 0.5 s, section thickness of 5 mm and reconstruction thickness of 2.5 mm, and was followed by the PET scan that matched the CT section thickness. A three-dimensional model was used to obtain PET images with the following parameters: field of view, 576 mm; matrix of 144 × 144; slice thickness and interval, 5 mm. The emission scan time for each bed position was 1.5 min and the overlap between two adjacent bed positions was 50%. PET images with CT attenuation correction were reconstructed using the time-of-flight algorithm.

Supplementary Data S2

MRI acquisitionMRI was performed by 3.0 T-MR-scanner (Signa HDxt × t3.0 T, GE, USA; Achieva3.0 T, Philips, Netherlands). The mpMRI scan sequence consisted of transverse T2-weighted fast spin-echo images, diffusion-weighted imaging (DWI) sequence, and apparent diffusion coefficient (ADC) maps. DWI sequence was scanned with b-values (b=0, 1000 s/mm2), and ADC maps were calculated from DWI using b values.

The signal intensity on DWI is written in a mono-exponential model as follows

$$\frac{S_b}{S_0} = e^{-b*ADC} \qquad [1]$$

where S_b and S_0 are the signal intensities at b values of b and 0, respectively. The ADC value can be calculated from two signal intensities at b values of b_1 and b_2, which is given by

$$ADC = \frac{\ln\left(\frac{S_{b1}}{S_{b2}}\right)}{\left(b_2 - b_1\right)} \qquad [2]$$

Details of the scanning parameters of MRI are shown in S2 *Table 1*. To reduce the heterogeneity between images, all Original MR images were preprocessed by resampling into voxel sizes of 1×1×1 mm^3 and gray level discretization.

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Table S1 Details of the scanning parameters of MRI

Parameters	Achieva, Philips		Signa HDxt	
	T2WI	DWI	T2WI	DWI
Sequence	TSE/FS	SE	FRFSE	SE-EPI
TR (ms)	4900	2500	3800	5600
TE (ms)	90	70	110	70
Flip angle (degree)	90	90	90	90
Echo train length	19	61	32	1
Field of view (mm)	220×220	320×320	260×260	320×320
Acquisition matrix	220×220	160×157	320×224	256×128
Slice thickness (mm)	3.5	3.5	3.5	4.0
Other		b=1000 mm^2/sec		b=1000 mm^2/sec

Table S2 Performance of PET models based on different VOI

Models	Training cohort					Validation cohort				
	AUC	ACC	SEN	SPE	F1	AUC	ACC	SEN	SPE	F1
$VOI_{40\%}$	0.819	0.810	0.737	0.827	0.596	0.794	0.707	0.714	0.706	0.455
VOI_{Whole}	0.791	0.760	0.737	0.765	0.538	0.731	0.659	0.571	0.676	0.364

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Appendix 2

Supplementary Data S1

The details of each radiomic model containing the features

Models	mRMR(n=15)	LASSO
PET VOI$_{40\%}$	GLSZM_LargeAreaHighGrayLevelEmphasis; GLCM_fointEntropy; SHAPE_Sphericity; SHAPE_Volume; GLSZM_GrayLevelNonUniformityNormalized; GLCM_LargeAreaHighGrayLevelEmphasis; GLSZM_SmallAreaLowGrayLevelEmphasis; GLDM_LargeDependenceLowGrayLevelEmphasis; SHAPE_Compacity.onlyFor3DROI; GLRLM_LRLGE; CONVENTIONAL_SUVbwmin; GLCM_Entropy_log2..JointEntropy; CONVENTIONAL_SUVbwSkewness; GLCM_Energy.AngularSecondMoment; CONVENTIONAL_TLG.mL;	(n=8) GLSZM_LargeAreaHighGrayLevelEmphasis; GLCM_fointEntropy; SHAPE_Sphericity; SHAPE_Volume; GLSZM_GrayLevelNonUniformityNormalized; GLCM_LargeAreaHighGrayLevelEmphasis; GLSZM_SmallAreaLowGrayLevelEmphasis; GLDM_LargeDependenceLowGrayLevelEmphasis;
PET VOI$_{Whole}$	GLRLM_LargeAreaHighGrayLevelEmphasis; GLSZM_LargeAreaHighGrayLevelEmphasis; SHAPE_Sphericity; GLSZM_GrayLevelNonUniformityNormalized; GLSZM_SmallAreaLowGrayLevelEmphasis; GLDM_DependenceNonUniformityNormalized; GLDM_LargeDependenceLowGrayLevelEmphasis; CONVENTIONAL_TLG.mL; DISCRETIZED_HISTO_Skewness; CONVENTIONAL_TLG.mL; GLCM_Correlation; SHAPE_Sphericity.onlyFor3DROI; SHAPE_Volume.vx; CONVENTIONAL_SUVbwQ1; CONVENTIONAL_SUVbwSkewness;	(n=7) GLRLM_LargeAreaHighGrayLevelEmphasis; GLSZM_LargeAreaHighGrayLevelEmphasis; SHAPE_Sphericity; GLSZM_GrayLevelNonUniformityNormalized; GLSZM_SmallAreaLowGrayLevelEmphasis; GLDM_DependenceNonUniformityNormalized; GLDM_LargeDependenceLowGrayLevelEmphasis;
M-model	DWI_glcm_Imc2; DWI_firstorder_Median; DWI_firstorder_90Percentile; DWI_firstorder_Mean; DWI_glszm_GrayLevelNonUniformity; ADC_glszm_GrayLevelNonUniformityNormalized; ADC_glszm_SizeZoneNonUniformity; ADC_glszm_SmallAreaHighGrayLevelEmphasis; T2WI_firstorder_Variance; T2WI_glszm_SizeZoneNonUniformityNormalized; T2WI_firstorder_Kurtosis; ADC glcm_ClusterProminence; DWI firstorder_Entropy; DWI_glcm_Correlation; ADC_GLDM_SmallDependenceHighGrayLevelEmphasis;	(n=11) DWI_glcm_Imc2; DWI_firstorder_Median; DWI_firstorder_90Percentile; DWI_firstorder_Mean; DWI_glszm_GrayLevelNonUniformity; ADC_glszm_GrayLevelNonUniformityNormalized; ADC_glszm_SizeZoneNonUniformity; ADC_glszm_SmallAreaHighGrayLevelEmphasis; T2WI_firstorder_Variance; T2WI_glszm_SizeZoneNonUniformityNormalized; T2WI_firstorder_Kurtosis;

PM-model	DWI_glcm_Imc2; DWI glszm_SizeZoneNonUniformity; DWI_firstorder_90Percentile; DWI_glcm_Imc2; DWI_firstorder_Mean; ADC_glrlm_ShortRunHighGrayLevelEmphasis; ADC_glcm_Contrast; ADC_glszm_GrayLevelNonUniformityNormalized; ADC_firstorder_Minimum; ADC glcm_ClusterProminence; T2WI_firstorder_Median; T2WI_glszm_SizeZoneNonUniformityNormalized; PET_glszm_LargeAreaHighGrayLevelEmphasis; PET_gldm_LargeDependenceLowGrayLevelEmphasis; PET_SHAPE_Volume;	(n=12) DWI_glcm_Imc2; DWI glszm_SizeZoneNonUniformity; DWI_firstorder_90Percentile; DWI_glcm_Imc2; ADC_glrlm_ShortRunHighGrayLevelEmphasis; ADC_glcm_Contrast; ADC_glszm_GrayLevelNonUniformityNormalized; ADC_firstorder_Minimum; T2WI_firstorder_Median; T2WI_glszm_SizeZoneNonUniformityNormalized; PET_glszm_LargeAreaHighGrayLevelEmphasis; PET_gldm_ LargeDependenceLowGrayLevelEmphasis;

Supplementary Data S2

Implementation and parameter settings of logistic regression model

Logistic regression is a widely used statistical model for binary classification problems. This model predicts the probability of an event occurring by modeling the relationship between the features and the target variable. In this study, the logistic regression model was implemented using the R package “glm”, with the parameter ‘family’ set to ‘binomial(link = “logit”)’ to specify a binary classification problem and utilize the logit link function. For feature selection, LASSO regression was applied, which incorporates an L1 regularization term to shrink the coefficients of less important features to zero. This process identifies the most relevant features for predicting the target variable.

The LASSO regression was performed with the glmnet function, and a 10-fold cross-validation (default in the cv.glmnet function) was used to select the optimal regularization parameter, ‘lambda’. The parameter ‘lambda.min’ was chosen, which corresponds to the value of ‘lambda’ that minimizes the cross-validated mean squared error. This optimal value of ‘lambda’ was then used to fit the logistic regression model.

During the training process, the logistic regression model was fitted using a dataset that had been preprocessed with SMOTE to address class imbalance, and standardized to ensure that the features were on the same scale. The final model, with selected features and regularization, was used for prediction.