Figure S1 – Image preprocessing

Before feature extraction, several steps were involved to preprocess images: (1) use threshold to exclude voxels that didn't have an intensity within the range of (mean-standard deviation, mean+8*standard deviation), to remove the noise; (2) normalize images using z-score normalization with z=100; (3) resample images to 1*1*1 mm^3; (4) discretize images by a fixed bin width of 5. Below image shows the distribution of intensity range of each patient after completing image preprocessing. The intensity range had a mean of 710 and standard deviation of 203.

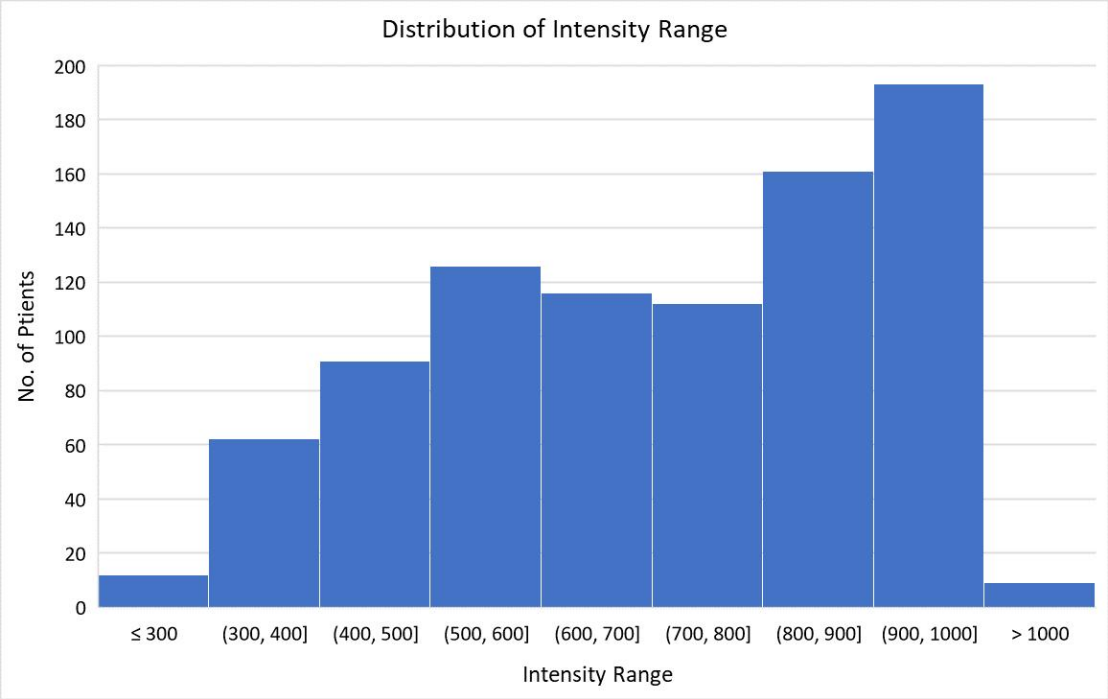
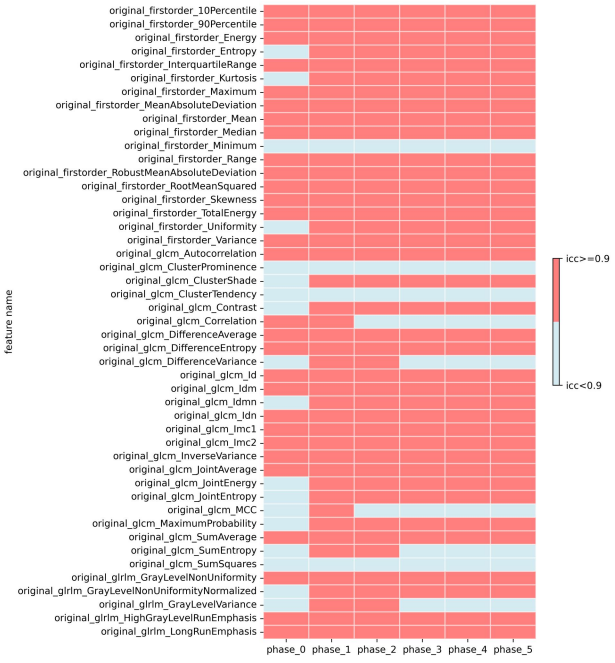


Figure S2. Feature repeatability of different DCE-MRI phases.

The repeatability of extracted radiomics features was assessed by single rater intraclass correlation coefficient (ICC) (1,1). The ICC for each feature was calculated under 30-time perturbations which involved random translation, rotation, as well as contour randomization. The formula for ICC calculation is:

$$\frac{MS_R - MS_W}{MS_R + (k+1)MS_W}$$

where MS_R is the mean square for all the features, MS_W is the mean square for the residual sources of variance, and k is the number of measurements. The calculation of ICC was performed using python package pingouin (version 0.5.2). An ICC >= 0.9 was determined as high-repeatable. Below figures shown the feature repeatability at different DCE-MRI phases.



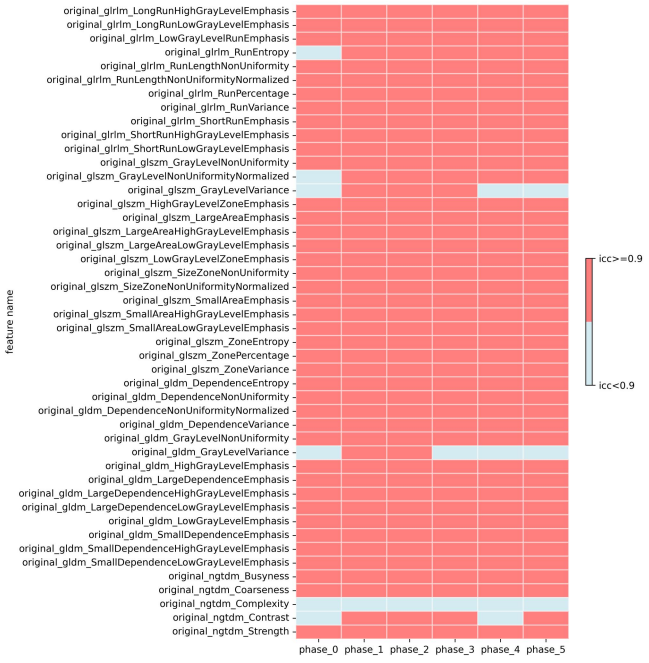


Figure S3. Feature change across different DCE-MRI phases.
The assessment of feature change across different DCE-MRI phases involved evaluating whether the feature change calculated by subtraction was significantly different from zero. It was conducted by performiang a single-sample t test. A t test p value smaller than 0.05 was determined as 'change'. Below figures shown the feature change across different phases. The coordinate of x-axis n/m referred to feature change = feature at phase n – feature at phase m, and 0-5 denoted pre-contrast phase and 1st to 5th post-contrast phase.

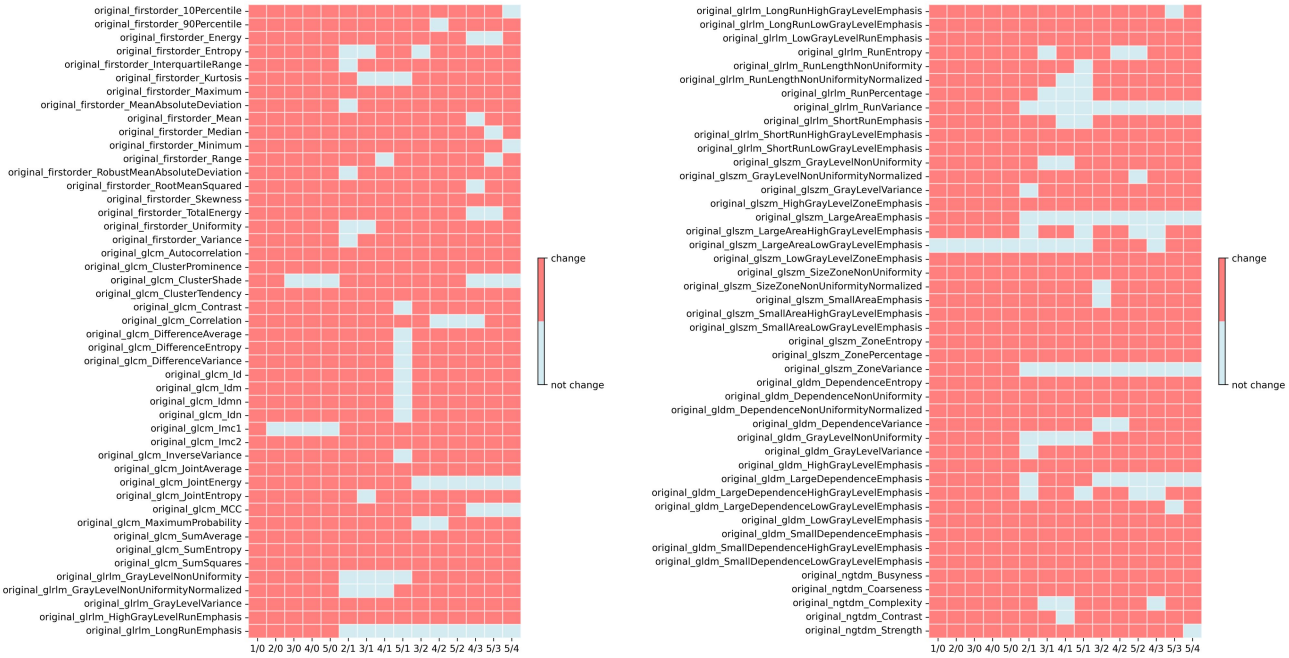


Table S1. DCE-MRI parameters

Parameter	Value
Scanner Manufacturer	GE / Philips / SIEMENS
Magnetic Field Strength	1.5T / 3.0T
Fat Suppression	Required
Slice Orientation	Axial
Slice Thickness	0.8 - 3 mm
Pixel Size	0.3 - 1.4 mm
Slice Number	56 - 256
Repetition Time	3.8 - 9.3 s
Echo Time	1.3 - 4.8 s
Number of averages	0.7 - 3
Spacing Between Slices	0.8 - 2.6 mm
Flip Angle	10 - 20 degrees
Total Phase	6 - 11
Sequence Acquisition Time	80 - 100 s
Total Acquisition Time	At least 8 min after contrast agent injection

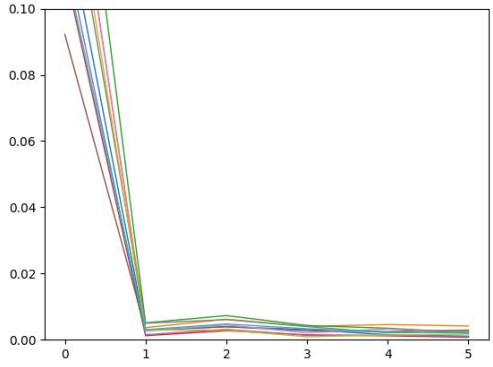
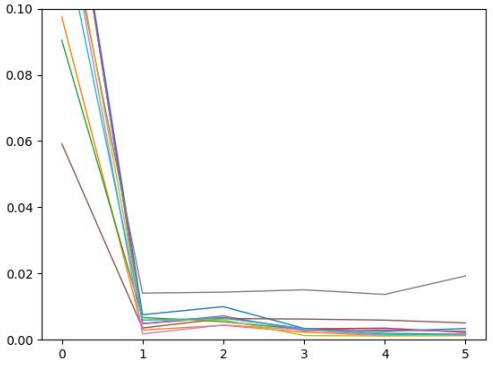
Table S2. Patient characteristics of pCR and non-pCR.

		non-pCR	pCR	P-value
Treatment	Paclitaxel	114	28	<0.001
	Paclitaxel + ABT 888 + Carboplatin	36	21	
	Paclitaxel + AMG 386	67	29	

	Paclitaxel + AMG 386 + Trastuzumab	10	6	
	Paclitaxel + Ganetespib	58	20	
	Paclitaxel + Ganitumab	69	20	
	Paclitaxel + MK-2206	32	14	
	Paclitaxel + MK-2206 + Trastuzumab	15	15	
	Paclitaxel + Neratinib	54	31	
	Paclitaxel + Pembrolizumab	29	25	
	Paclitaxel + Pertuzumab + Trastuzumab	13	20	
	Paclitaxel + Trastuzumab	17	3	
	T-DM1 + Pertuzumab	17	22	
HR	negative	201	153	<0.001
	positive	330	101	
HER2	negative	432	169	<0.001
	positive	99	85	
MP	negative	312	94	<0.001
	positive	219	160	
Age(mean,range)		49 (23-77)	49 (25-73)	0.530
Race	American Indian or Alaska Native	3	1	0.791
	American Indian or Alaska Native;White	0	1	
	Asian	39	18	
	Asian;White	3	1	
	Black or African American	63	30	
	Native Hawaiian or Pacific Islander	2	2	
	Native Hawaiian or Pacific Islander;White	0	1	
	White	419	199	
	N/A	2	1	
Menopausal status	Premenopausal	259	111	0.291
	Perimenopausal	18	10	
	Postmenopausal	152	89	
	N/A	102	44	
Ethnicity	Hispanic or Latino	66	38	0.573
	Not Hispanic or Latino	464	216	
	N/A	1	0	

Table S3 – Example of visualizing dynamic features

The table gives an example of how a dynamic feature quantify the change of a radiomics feature. The selected radiomics feature is original_glszm_LowGrayLevelZone_Emphasis. The dynamic feature is MD_hrv_classic_pnn40. It calculates the proportion of differences magnitude that is greater than 4% of standard deviation of the time series. In these figures, the x-axis denotes the phase of DCE-MRI and y-axis denotes the value of radiomics feature. And each line denotes one patient. Those have a relatively constant radiomics feature value after contrast agent injection (phase1 to phase5) were given lower dynamic feature value. This table also shows that patients with different dynamic feature value has d0i00fferent pCR rate.

		
Feature value	-3.53	-1.91

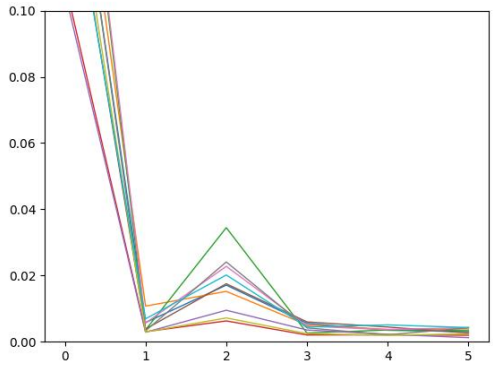
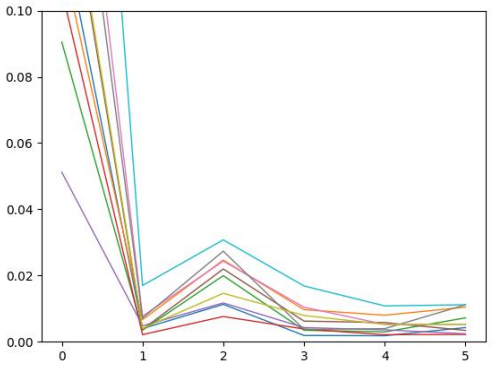
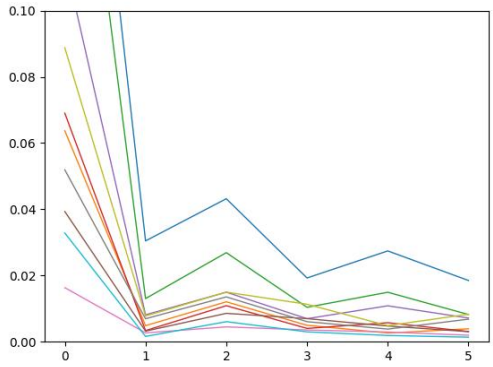
pCR rate (pCR / total)	0.2 (2/10)	0.25 (8/32)
		
Feature value	-0.29	1.33
pCR rate (pCR / total)	0.32 (185/582)	0.38 (50/133)
		
Feature value	2.95	
pCR rate (pCR / total)	0.30 (9/30)	

Table S4 Performance of models with different feature number.

Dynamic model feature No.	Training AUC	Internal Validation AUC	Radiomic model feature No.	Training AUC	Internal Validation AUC
1	0.571	0.560	1	0.595	0.564
2	0.600	0.634	2	0.621	0.535
3	0.607	0.635	3	0.650	0.637
4	0.643	0.649	**4**	**0.650**	**0.640**
5	0.650	0.675	5	0.650	0.634
6	0.660	0.643	6	0.650	0.635
7	0.664	0.673	7	0.666	0.603
8	0.675	0.667	8	0.672	0.603
9	0.682	0.660	9	0.673	0.589
10	**0.688**	**0.680**	10	0.690	0.570
11*	0.698	0.651			

*As the 10-feature dynamic model achieved the highest internal validation AUC. We further explored whether adding more dynamic features can obtain better performance. Therefore, the results of 11-feature dynamic model is also listed here.

Table S5 Odds ratios showing the significance of dynamic features in the dynamic model.

Dynamic feature name	Odds ratio
original_firstorder_RootMeanSquared_SP_Summaries_welch_rect_centroid	1.098
original_firstorder_Mean_FC_LocalSimple_mean3_stderr	0.795
original_glrlm_ShortRunLowGrayLevelEmphasis_SP_Summaries_welch_rect_centroid	0.807
original_glszm_GrayLevelNonUniformity_CO_HistogramAMI_even_2_5	0.780
original_glszm_LowGrayLevelZoneEmphasis_MD_hrv_classic_pnn40	1.161
original_glcm_Id_SB_MotifThree_quantile_hh	0.793
original_glcm_DifferenceEntropy_CO_HistogramAMI_even_2_5	1.193
original_firstorder_90Percentile_FC_LocalSimple_mean1_tauresrat	1.248
original_glcm_Imc1_CO_f1ecac	0.868
original_firstorder_InterquartileRange_DN_HistogramMode_10	0.833

Table S6 Odds ratios showing the significance of radiomic features in the radiomic model.

Radiomic feature name	Odds ratio
original_shape_Maximum2DDiameterColumn_phase0	0.793
original_glcm_Imc2_phase1	1.345
original_glszm_ZoneEntropy_phase0	0.772
original_ngtdm_Busyness_phase1	0.973

Table S7 Coefficients and p valus of variables in the CRD model

Variable	coefficient	P value
HR	-1.076	<0.001
HER2	0.837	<0.001
Dynamic	4.879	<0.001
Radiomic	4.169	<0.001