## Supplementary document 1

### 1. Treatment protocol

Patients who met the criteria were scheduled to begin NAC within a week. The NAC regimen was determined according to the guidelines outlined by the Chinese Society of Clinical Oncology (CSCO). The treatment protocol was mainly TEC (docetaxel 75 mg/m2, epirubicin 75 mg/m2, and cyclophosphamide 500 mg/m2), TCbHP (docetaxel 75 mg/m2; trastuzumab, a loading dose of 8 mg/kg with a maintenance dose of 6 mg/kg; and pertuzumab, a loading dose of 840 mg with a maintenance dose of 420 mg), or THP (docetaxel 75 mg/m2; carboplatin, area under curve = 6; trastuzumab, a loading dose of 8 mg/kg with a maintenance dose of 6 mg/kg; and pertuzumab, a loading dose of 840 mg with a maintenance dose of 420 mg). The drugs were administered in 21-day cycles. Following completion of 4–8 cycles of NAC, the treatment response was assessed by both clinicians and pathologists. Afterwards, either mastectomy or breast-conserving surgery along with axillary lymphadenectomy was conducted. Additionally, the systemic therapy procedures were as follows: 1) Patients with an IHC score of 3+ or 2+ with positive fluorescence in situ hybridization (FISH) should receive anti-HER2 targeted therapy. 2) Patients positive for estrogen receptor (ER) or progesterone receptor (PR) required hormone therapy. Finally, all the patients receive PMRT to the chest wall.

### 2. Pathological evaluation

The pathological diagnosis was established through interpretation of pathological slides, complemented by the immunohistochemistry (IHC) index derived from the tumor's core needle biopsy. ER, PR, or P53 positivity was characterized by the presence of cells expressing at a percentage greater than 1% on IHC. HER2 status was classified according to the IHC score and the result of FISH. A score

of 0 indicated HER2 negative, whereas a score of 1+ or 2+ without ERBB2 gene amplification was classified as HER2-low expression. Conversely, a score of 3+ or 2+ with ERBB2 gene amplification was categorized as HER2-positive. These evaluations were conducted independently and blindly by two pathologists. Moreover, the absence of residual invasive tumor in both the breast and axillary lymph nodes (ypT0ypN0) was regarded as achieving pathological complete response (pCR) following NAC.

**Supplementary document 2**

## 1. Image evaluation

An 8-channel dedicated phased-array surface coil in conjunction with either the 3.0T GE SimgaHDx or Siemens 3.0T Skyra superconducting MRI scanner. Patients were positioned supine with both breasts placed simultaneously within the coil, naturally hanging, and aligned with the coil center. Sequential scans were conducted, including axial T1-weighted imaging (T1WI), T2-weighted imaging (T2WI) with fat suppression, and diffusion-weighted imaging (DWI) with b values of 0 - 800 s/mm2. Subsequently, dynamic contrast-enhanced MRI (DCE-MRI) scans were performed following contrast agent injection. Gadopentetate dimeglumine was administered at a dose of 0.1-0.2 mmol/kg at a rate of 2 ml/s, followed by a 20 ml saline flush at the same rate. The pre-contrast scan served as the baseline, followed by continuous scanning for 6 or 7 phases post-contrast injection to obtain dynamic enhancement images.

## 2. Preprocessing of image

Firstly, bias field correction was applied to the MRI images by using Histogram-Based methods. Subsequently, the images were resampled to a voxel size of 1x1x1 $mm^3$ to standardize the voxel spacing. Following this, the images were normalized, with the signal intensity (SI) adjusted to a range of 1 to 100 SI. This step helps to minimize the differences in SI that may arise from images collected using different machines. Finally, Z-score normalization was employed to standardize the

gray values of the images, thereby reducing the impact of inconsistencies in image parameters on the variation of image omics features.

**3. Segmentation of volume of interest (VOI) and extraction of radiology features**

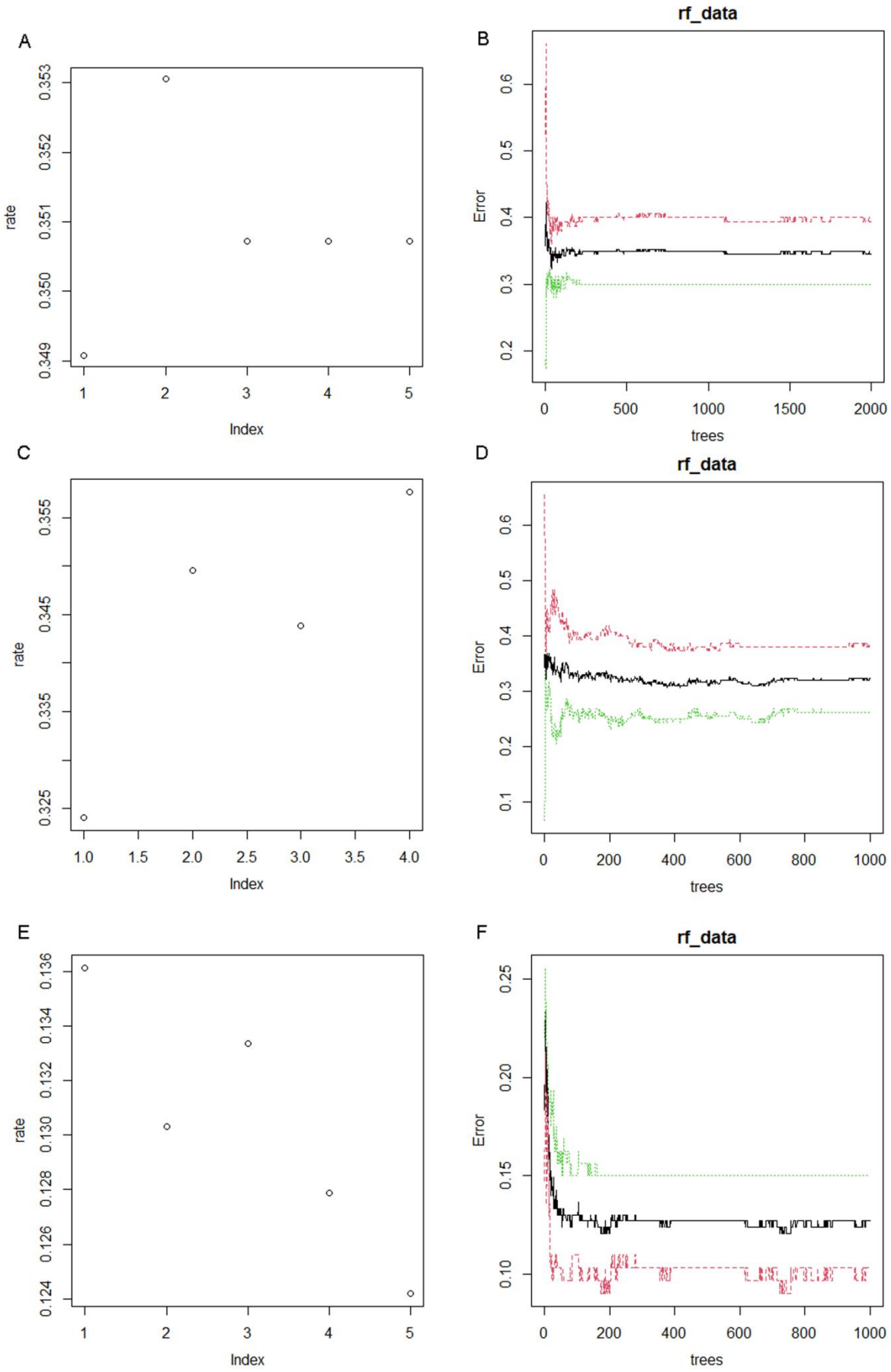
Utilizing the Darwin research platform (http://premium.darwin.yizhun-ai.com), we conducted semi-automated manual contouring of the tumor region. Two experienced radiologists independently and blindly delineated the tumor on the T1-DCE sequence of the MRI. Inter-observer variability was assessed, and only radiomics features with an intraclass correlation coefficient (ICC) greater than 0.9 were retained. All delineated target areas were confirmed by a third senior radiologist.

**4. Data preprocessing of the radiomics features**

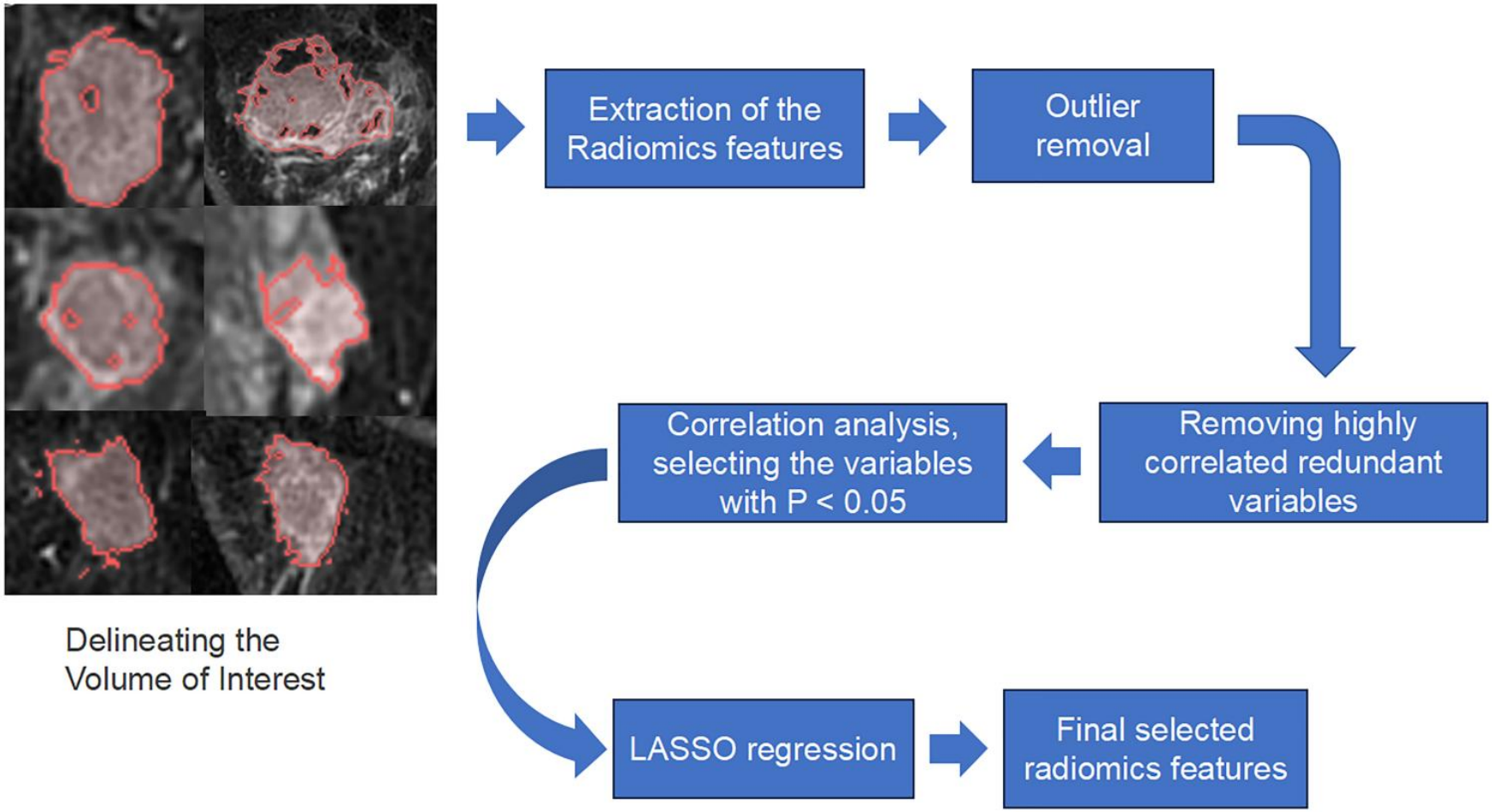
For the radiomic features, data preprocessing includes the following steps: 1) Outlier removal: calculation of the first quartile (Q1) and third quartile (Q3) of the data, and use Interquartile range IQR (Q3-Q1) to determine the outlier, where the lower limit = Q1-1.5*(Q3-Q1); Upper bound = Q3 + 1.5*(Q3-Q1) Data points beyond these bounds are considered outliers. 2) Based on Pearson correlation coefficient, features with absolute values greater than 0.9 were deleted; 3) Correlation analysis: t test was employed to identify variables with a significance level of $P < 0.05$ that were strongly associated with axillary pCR following NAC. 4) Variables associated with axillary LN pCR were selected using LASSO regression. 5) Weighted linear combination of selected features: $rad\_score = W_1 \times \text{Feature}_1 + W_2 \times \text{Feature}_2 +$

$W_3$×Feature$_3$ + ... + $W_n$×Feature$_n$, where W was LASSO-derived coefficients, and Feature was normalized feature values.

**Supplementary Figure 1.** Adjustments of the parameters of the random forest model. A-B for the Clinical model, C-D for the Clinical-Radiomics model; E-F for the Clinical-DLR model. For the figure B, D, and F, the red line was for error rate of predicting “pCR”; green line was for error rate of predicting “Non-pCR”; black line was for out of bag error rate.



**Supplementary Figure 2.** Selection process of the radiomics features.



**Supplementary Figure 3.** We selected images from several patients with higher prediction accuracy, showing that the peritumoral region appears to be a key area requiring focused attention.