**S5 Table. Predictive model construction and calculation of risk score (n=89)**

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| **Model 1: ctDNA information only (5 features)** | | | |
| **Feature** | **Coefficient** | **Odds ratio** | **P value** |
| TP53 mutation status | 1.62 | 5.04(0.95-47.96) | 0.09 |
| HRR mutation status | -1.69 | 0.18(0.04-0.75) | 0.02 |
| HMT mutation status | -1.91 | 0.15(0.03-0.62) | 0.01 |
| Acquired mutation status | 1.61 | 5.01(0.7-105.21) | 0.17 |
| T234\_clearance status | -2.28 | 0.1(0.01-0.64) | 0.04 |
| Risk score = 3.31 (intercept)+1.62×TP53 mutation status + (-1.69)×HRR mutation status + (-1.91)×HMT mutation status +1.61×acquire mutation status + (-2.28)×T234\_clearance status | | | |

ctDNA: circulating tumor DNA; HRR: Homologous recombination repair; HMT: Histone methyltransferase family

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| **Model 2: MRI information only (1 features)** | | | |
| **Feature** | **Coefficient** | **Odds ratio** | **P value** |
| mrTRG grade | 1.41 | 4.1(1.90-10.40) | 0.001 |
| Risk score = -1.76 (intercept)+1.41×mrTRG grade | | | |

mrTRG: magnetic resonance imaging tumor regression grade

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| **Model 3: ctDNA+MRI (6 features)** | | | |
| **Feature** | **Coefficient** | **Odds ratio** | **P value** |
| TP53 mutation status | 1.41 | 4.09(0.69-42.46) | 0.16 |
| HRR mutation status | -1.56 | 0.21(0.04-1.04) | 0.06 |
| HMT mutation status | -1.75 | 0.17(0.03-0.83) | 0.04 |
| Acquired mutation status | 1.59 | 4.88(0.65-104.82) | 0.18 |
| T234\_clearance status | -2.71 | 0.07(0-0.52) | 0.03 |
| mrTRG grade | 1.48 | 4.4(1.78-14.19) | 0.004 |
| Risk score = 0.67 (intercept)+1.41×TP53 mutation status + (-1.56)×HRR mutation status + (-1.75)×HMT mutation status +1.59×acquired mutation status + (-2.71)×T234\_clearance status + 1.48×mrTRG grade | | | |

Non-pCR was designated as positive event. ctDNA: circulating tumor DNA; MRI: magnetic resonance imaging; HRR: homologous recombination repair; HMT: histone methyltransferase family; mrTRG: magnetic resonance imaging tumor regression grade