

**Supplementary Table S10. Comparison of AUC and NRI between ML models and conventional indicators for bacterial infection in ACLF.**

| <b>Model names</b>    | <b>AUC<br/>(95% CI)</b> | <b><i>P</i>-value vs.<br/>Five-metabolite<br/>model</b> | <b>NRI</b> | <b><i>P</i>-value vs.<br/>Five-metabolite<br/>model</b> |
|-----------------------|-------------------------|---------------------------------------------------------|------------|---------------------------------------------------------|
| Discovery set         |                         |                                                         |            |                                                         |
| Five-metabolite model | 0.881(0.844-0.918)      | -                                                       | -          | -                                                       |
| Combined model        | 0.937(0.913-0.961)      | 0.002                                                   | 0.107      | 0.004                                                   |
| CRP                   | 0.794(0.764-0.843)      | 0.004                                                   | - 0.139    | 0.037                                                   |
| WBC                   | 0.760(0.707-0.812)      | <0.001                                                  | - 0.225    | <0.001                                                  |
| Validation set        |                         |                                                         |            |                                                         |
| Five-metabolite model | 0.835(0.769-0.902)      | -                                                       | -          | -                                                       |
| Combined model        | 0.840(0.774-0.905)      | 0.855                                                   | 0.008      | 0.910                                                   |
| CRP                   | 0.691(0.601-0.780)      | 0.004                                                   | - 0.237    | 0.030                                                   |
| WBC                   | 0.665(0.571-0.759)      | <0.001                                                  | - 0.245    | 0.012                                                   |

Note: ACLF, acute-on-chronic liver failure; AUC, area under the ROC curve; CRP, C-reactive protein; ML, machine learning; NRI, net reclassification improvement ; WBC, white blood cell count.