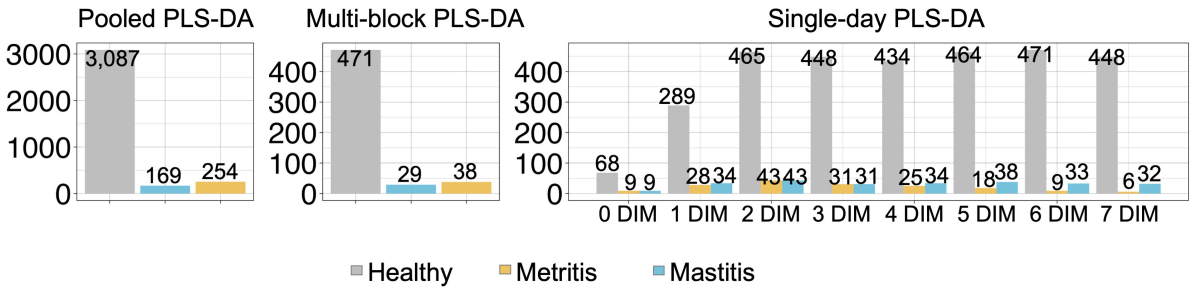
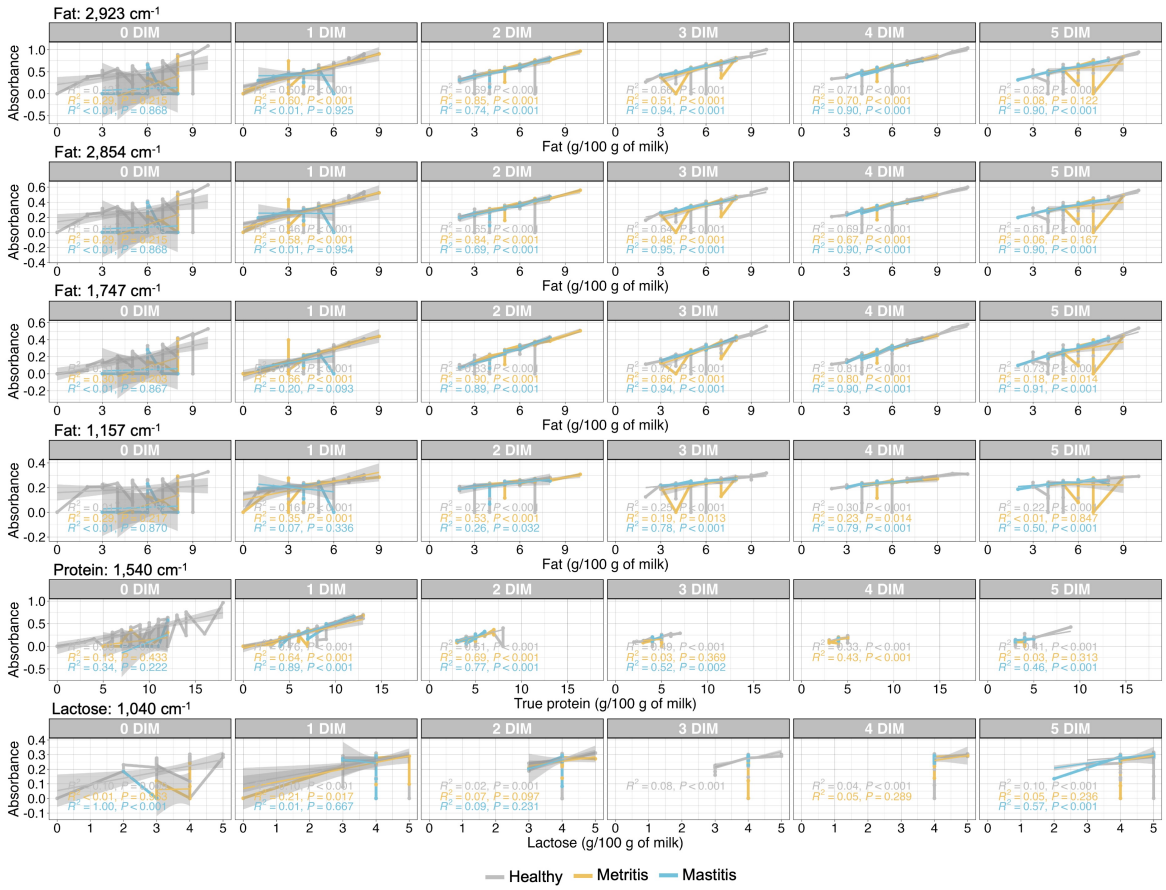
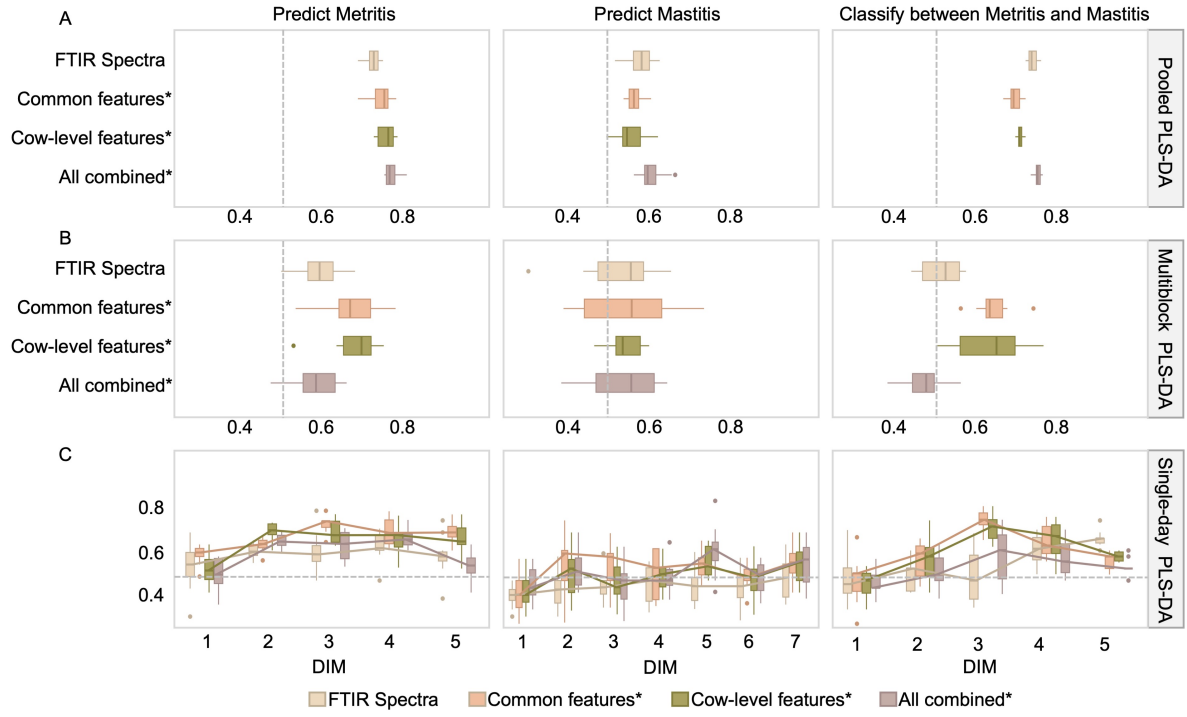
Supplemental Figure 1. The sample size used for three PLS-DA-based modeling strategies.



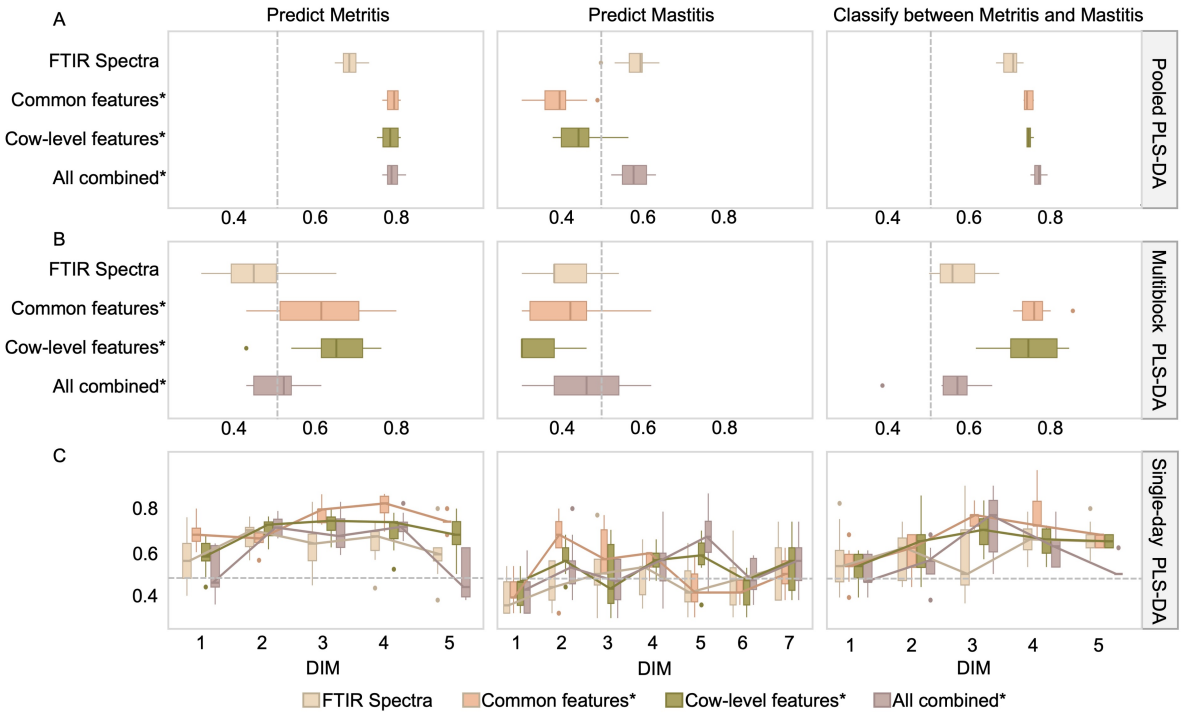
Supplemental Figure 2. Line plots with 95% confident interval showing the linear relationship between the predictive milk components and the absorption peaks of these components (fat, true protein and lactose) at different DIM. Coefficient of determination (R2) which represents the percentage of the variance in the absorption peaks that the predictive milk components explain collectively, and P-value which indicates overall significance of the regression model were present.



Supplemental Figure 3. Comparison of model performance (average Accuracy from repeated LOOCV; mean ± 95% CI) for predicting and classifying metritis and mastitis across modeling strategies using milk FTIR spectra various feature combinations (DIM, milk yield, SCC, parity, and spectra-predicted milk fat, protein and lactose). A. Predictive performance under Pooled PLS-DA strategy. B. Predictive performance under Multi-block PLS-DA strategy. C. Predictive performance under Single-day PLS-DA strategy. Time points with fewer than 10 samples per group were not included in modeling.

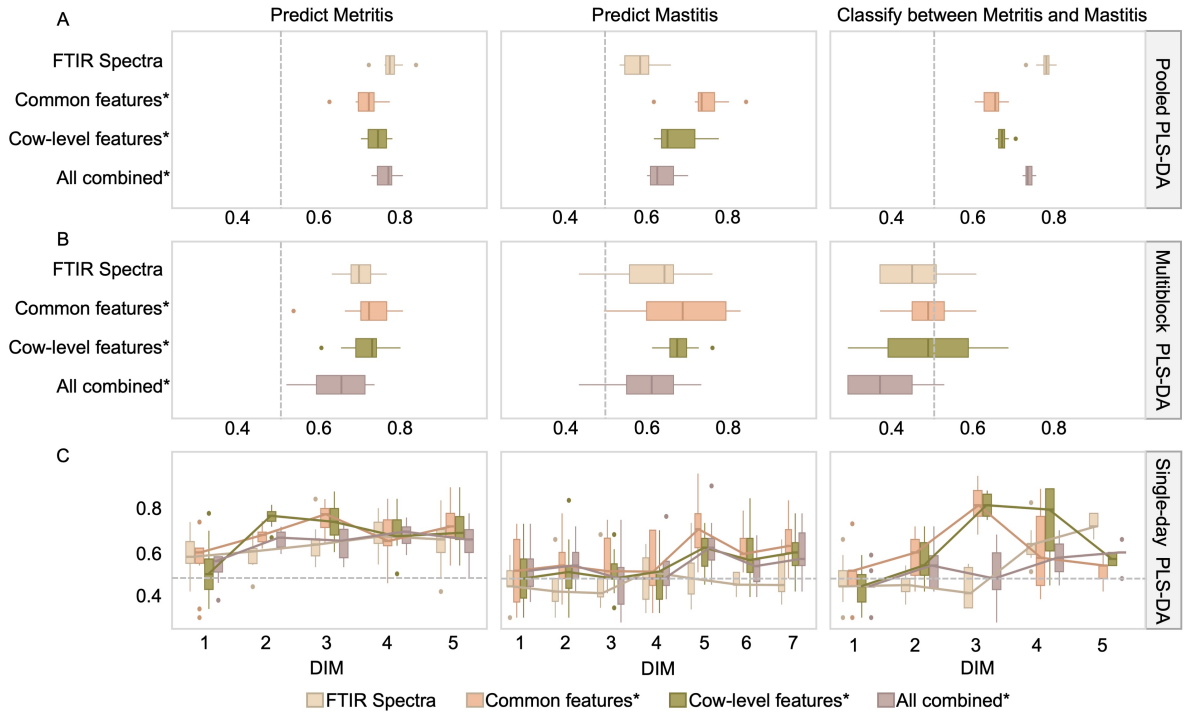


Supplemental Figure 4. Comparison of model performance (average Sensitivity from repeated LOOCV; mean ± 95% CI) for predicting and classifying metritis and mastitis across modeling strategies using milk FTIR spectra various feature combinations (DIM, milk yield, SCC, parity, and spectra-predicted milk fat, protein and lactose). A. Predictive performance under Pooled PLS-DA strategy. B. Predictive performance under Multi-block PLS-DA strategy. C. Predictive performance under Single-day PLS-DA strategy. Time points with fewer than 10 samples per group were not included in modeling.

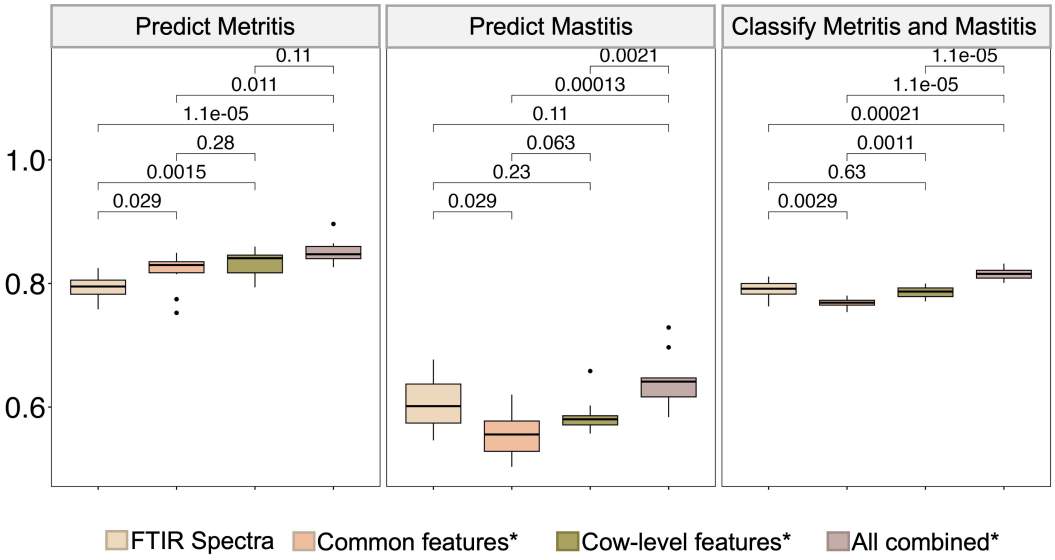


*Common features: DIM, parity, milk yield, SCC
*Cow-level features: DIM, parity, milk yield, SCC, fat%, protein%, lactose%
*All combined: DIM, parity, milk yield, SCC, fat%, protein%, lactose% and spectra

Supplemental Figure 5. Comparison of model performance (average Specificity from repeated LOOCV; mean ± 95% CI) for predicting and classifying metritis and mastitis across modeling strategies using milk FTIR spectra various feature combinations (DIM, milk yield, SCC, parity, and spectra-predicted milk fat, protein and lactose). A. Predictive performance under Pooled PLS-DA strategy. B. Predictive performance under Multi-block PLS-DA strategy. C. Predictive performance under Single-day PLS-DA strategy. Time points with fewer than 10 samples per group were not included in modeling.

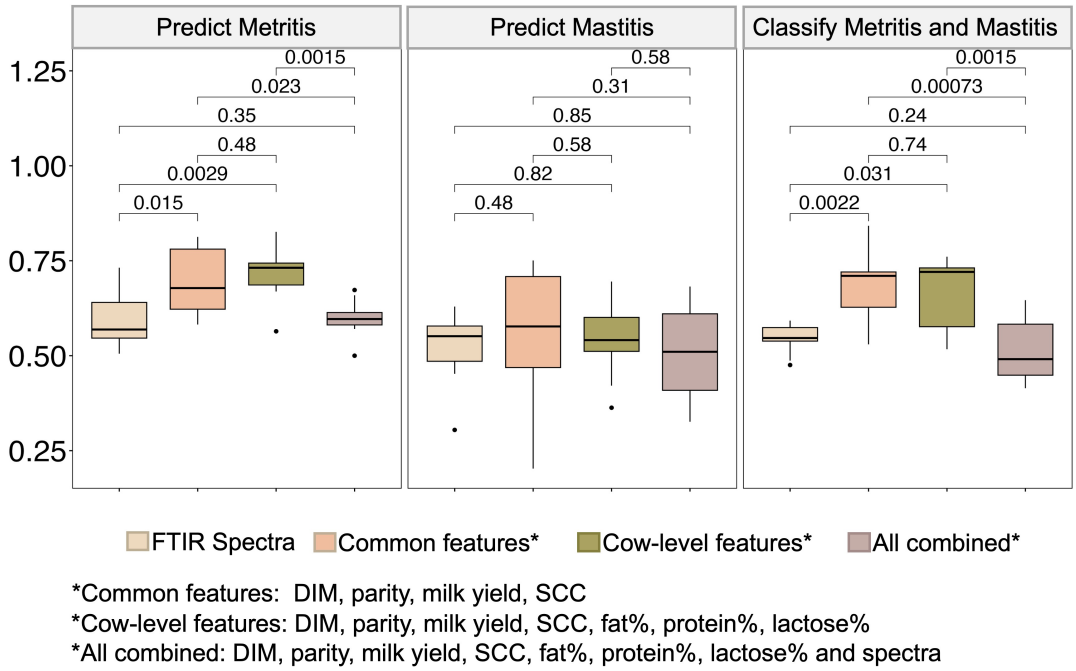


Supplemental Figure 6. Comparisons of predictive performance (AUROCs) for predicting and classifying metritis and mastitis under Pooled PLS-DA strategy using milk FTIR spectra and various feature combinations (DIM, parity, milk yield, SCC, spectra-predicted fat%, protein% and lactose%). * adjusted $P < 0.05$. ** adjusted $P < 0.01$. *** adjusted $P < 0.001$.



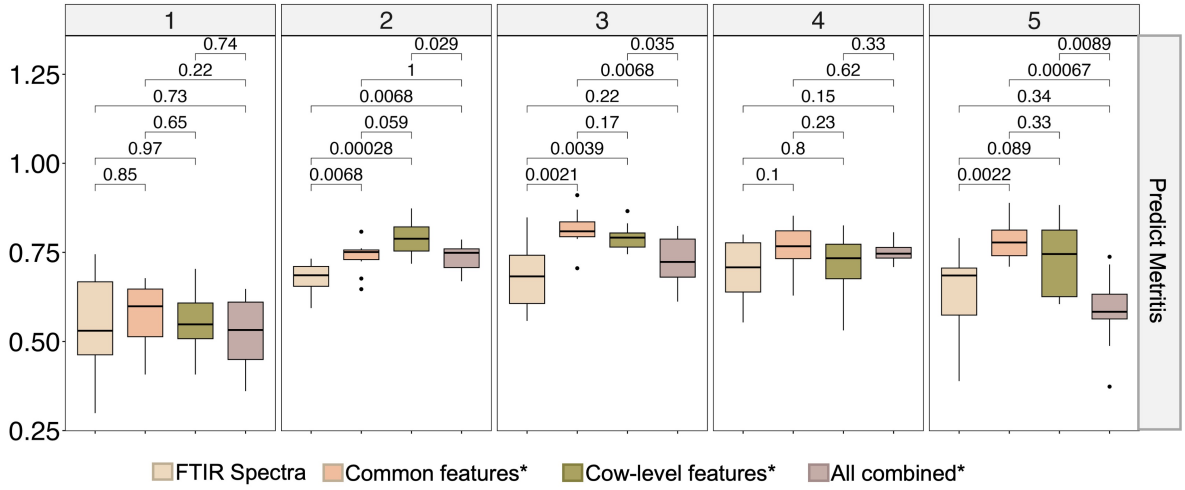
*Common features: DIM, parity, milk yield, SCC
*Cow-level features: DIM, parity, milk yield, SCC, fat%, protein%, lactose%
*All combined: DIM, parity, milk yield, SCC, fat%, protein%, lactose% and spectra

Supplemental Figure 7. Comparisons of predictive performance (AUROCs) for predicting and classifying metritis and mastitis under Multi-block PLS-DA strategy using milk FTIR spectra and various feature combinations (DIM, parity, milk yield, SCC, spectra-predicted fat%, protein% and lactose%). * adjusted $P < 0.05$. ** adjusted $P < 0.01$. *** adjusted $P < 0.001$.



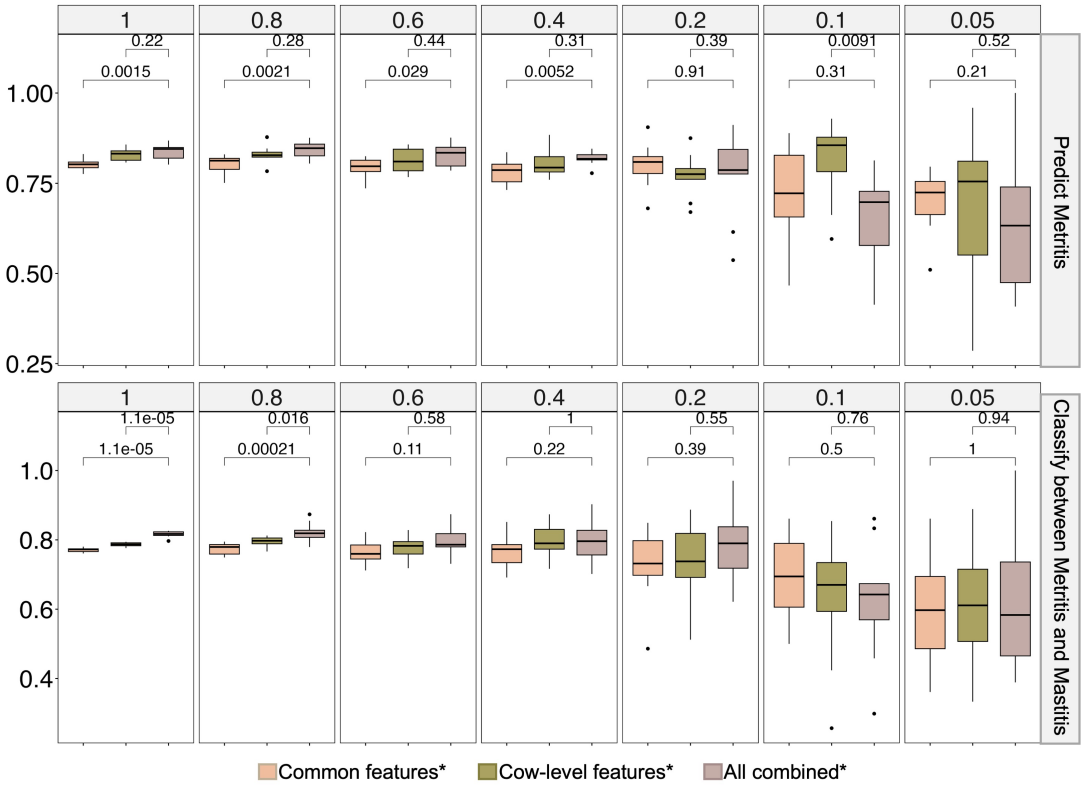
*Common features: DIM, parity, milk yield, SCC
*Cow-level features: DIM, parity, milk yield, SCC, fat%, protein%, lactose%
*All combined: DIM, parity, milk yield, SCC, fat%, protein%, lactose% and spectra

Supplemental Figure 8. Comparisons of predictive performance (AUROCs) for predicting metritis under Single-day PLS-DA strategy using milk FTIR spectra and various feature combinations (DIM, parity, milk yield, SCC, spectra-predicted fat%, protein% and lactose%). * adjusted $P < 0.05$. ** adjusted $P < 0.01$. *** adjusted $P < 0.001$.



*Common features: DIM, parity, milk yield, SCC
*Cow-level features: DIM, parity, milk yield, SCC, fat%, protein%, lactose%
*All combined: DIM, parity, milk yield, SCC, fat%, protein%, lactose% and spectra

Supplemental Figure 9. Comparisons of predictive performance (AUROCs) for predicting and classifying metritis under Pooled PLS-DA strategy using milk FTIR spectra and various feature combinations (DIM, parity, milk yield, SCC, spectra-predicted fat%, protein% and lactose%) at different down-sampled thresholds. * adjusted $P < 0.05$. ** adjusted $P < 0.01$. *** adjusted $P < 0.001$.



*Common features: DIM, parity, milk yield, SCC
*Cow-level features: DIM, parity, milk yield, SCC, fat%, protein%, lactose%
*All combined: DIM, parity, milk yield, SCC, fat%, protein%, lactose% and spectra