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| **S5 Table. Classification Comparisons of Preliminary and Final Biomarker Panels Between Athlete and External Cohorts, without and with Batch Correction Adjustment** |
| **Feature Selection Method Defining Panel** | **No. of analytes in panel** | **Athlete Cohort Training/Discovery** **ROC AUC****(95% CI)**(sens/spec) | **Athlete Cohort** **Internal Validation****ROC AUC****(95% CI)**(sens/spec) | **External Cohort****Replication** **ROC AUC****(95% CI)**(sens/spec) | **Hanley-McNeil Test Results****(z, p)** |
| **Linear SVM** | 6 | **0.913** **(0.888-0.938)** (0.835/0.907) | **0.851** **(0.745-0.957)** (0.815/0.861) | **0.830** **(0.798-0.861)**(0.817/0.715) | **0.293, 0.770** |
| 6 (with batch correction) | **0.911****(0.886-0.936)**(0.774/0.944) | **0.859****(0.755-0.963)**(0.778/0.944) | **0.758****(0.719-0.796)**(0.724/0.751) | **1.325, 0.185** |
| **LASSO** | 8 | **0.948** **(0.930-0.965)** (0.852/0.914) | **0.848** **(0.746-0.949)**(0.741/0.861) | **0.811** **(0.781-0.841)**(0.778/0.686) | **0.502, 0.616** |
| 8 (with batch correction) | **0.938****(0.919-0.957)**(0.704/0.991) | **0.828****(0.718-0.938)**(0.741/0.889) | **0.763****(0.729-0.796)**(0.642/0.736) | **0.822, 0.411** |
| **MS/MS** | 6 | **0.847** **(0.815-0.879)** (0.770/0.784) | **0.791** **(0.677-0.905)** (0.741/0.778) | **0.738** **(0.703-0.773)** (0.695/0.644) | **0.633, 0.527** |
| 6(with batch correction) | **0.845****(0.811-0.879)**(0.823/0.787) | **0.775****(0.656-0.893)**(0.741/0.750) | **0.768****(0.735-0.801)**(0.659/0.665) | **0.839, 0.933** |
| Gray shaded areas depict comparison values, within the same row, for testing the null hypothesis via Hanley-McNeil test between the Athlete and External cohort ROC AUC results. **ROC AUC** = receiver operating characteristic area under the curve. **SVM** = support vector machine. **LASSO**  = least absolute shrinkage and selection operator. **sens/spec** = sensitivity/specificity. **Training/Discovery** = uses logistic regression analysis. **Internal Validation** = uses logistic regression with 10-fold cross validation analysis. **Replication** = uses logistic regression analysis. **z** = Hanley-McNeil statistic. **p** = 2-tailed level of significance.**MS/MS** = Resulting 6 metabolites confirmed via tandem mass spectrometry (MS/MS). Statistical significance considered if p <0.05. |