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| --- | --- | --- |
| **PCA Model** | **R2X(cum) (# of components)** | **Q2(cum)** |
| Figure 1A: Durum vs. HBW vs. SBW (3-Class) | 68.6% (7) | 38.9% |
| Figure 2A: HBW Subclasses (4-Class) | 40.3% (3) | 10.8% |
| Figure 3A: SBW Subclasses (3-Class) | 48.9% (2) | 4.9% |
| Figure 4: (scatter plot not shown) DW vs. All BW (2-Class) | 68.6% (7) | 38.9% |
| Supplemental Figure 2A: HBW vs. SBW (2-Class) | 64.8% (7) | 27.6% |
|  | **X** | **Y** |  |
| **OPLS-DA Model** | **R2Xp (number of components)** | **R2Xo (number of components)** | **R2X(cum)** | **R2Y(cum)** | **Q2Y(cum)** | **Wheat Lines Misclassified** |
| Figure 1B: Durum vs. HBW vs. SBW (3-Class) | 22.0% (2) | 37.7% (4) | 59.7% | 93.2% | 71.0% | 0/45 |
| Figure 2B: HBW Subclasses (4-Class) | 9.7% (1) | 11.4% (1) | 21.1% | 36.6% | 17.3% | 10/27 |
| Figure 3B: SBW Subclasses (3-Class) | 32.1% (2) | 40.0% (3) | 72.1% | 99.1% | 64.9% | 0/12 |
| Figure 4 (scatter plot not shown): DW vs. All BW (2-Class) | 12.6% (1) | 38.9% (3) | 51.5% | 95.4% | 82.1% | 0/45 |
| Supplemental Figure 2A: HBW vs. SBW (2-Class) | 12.8% (1) | 30.7% (3) | 43.5% | 95.0% | 64.2% | 0/39 |

**Table S1. Model fit summaries of unsupervised and supervised analyses.**