**Supplementary Information:**

**Direct Analysis Real Time-High Resolution Mass Spectrometry to discriminate *Triticum* species.**



Figure 1S. Comparison of metabolic fingerprinting obtained using different extraction procedures and DART–HRMS analysis. PCA scores plot for methanol/water extract analyzed in positive (A) and negative (B) ionization modes; ethyl acetate extract run in positive (C) and negative (D) modes.

Table 1S. Summary of parameters considered in the evaluation of the four models built. R2X (cum) represent the variance of the x variable explained by the model, while Q2 is the cumulative predicted variation in the Y matrix.

|  |  |  |  |
| --- | --- | --- | --- |
| **Considered parameters** | **Positive ionization mode** |  | **Negative ionization mode** |
| **Ethyl Acetate**  | **MeOH/Water**  |  | **Ethyl Acetate**  | **MeOH/Water**  |
| Aligned metabolites | 4537 | 3648 |   | 4846 | 3295 |
| R2X (cum) PCA | 0.482 | 0.497 |  | 0.454 | 0.444 |
| Q2 (cum) PCA | 0.392 | 0.373 |   | 0.305 | 0.322 |