Distinguishing Infested Flour from Un-infested Flour Through Chemometric Processing of DART-HRMS Data - Revealing the Presence of *Tribolium castaneum,* the red flour beetle

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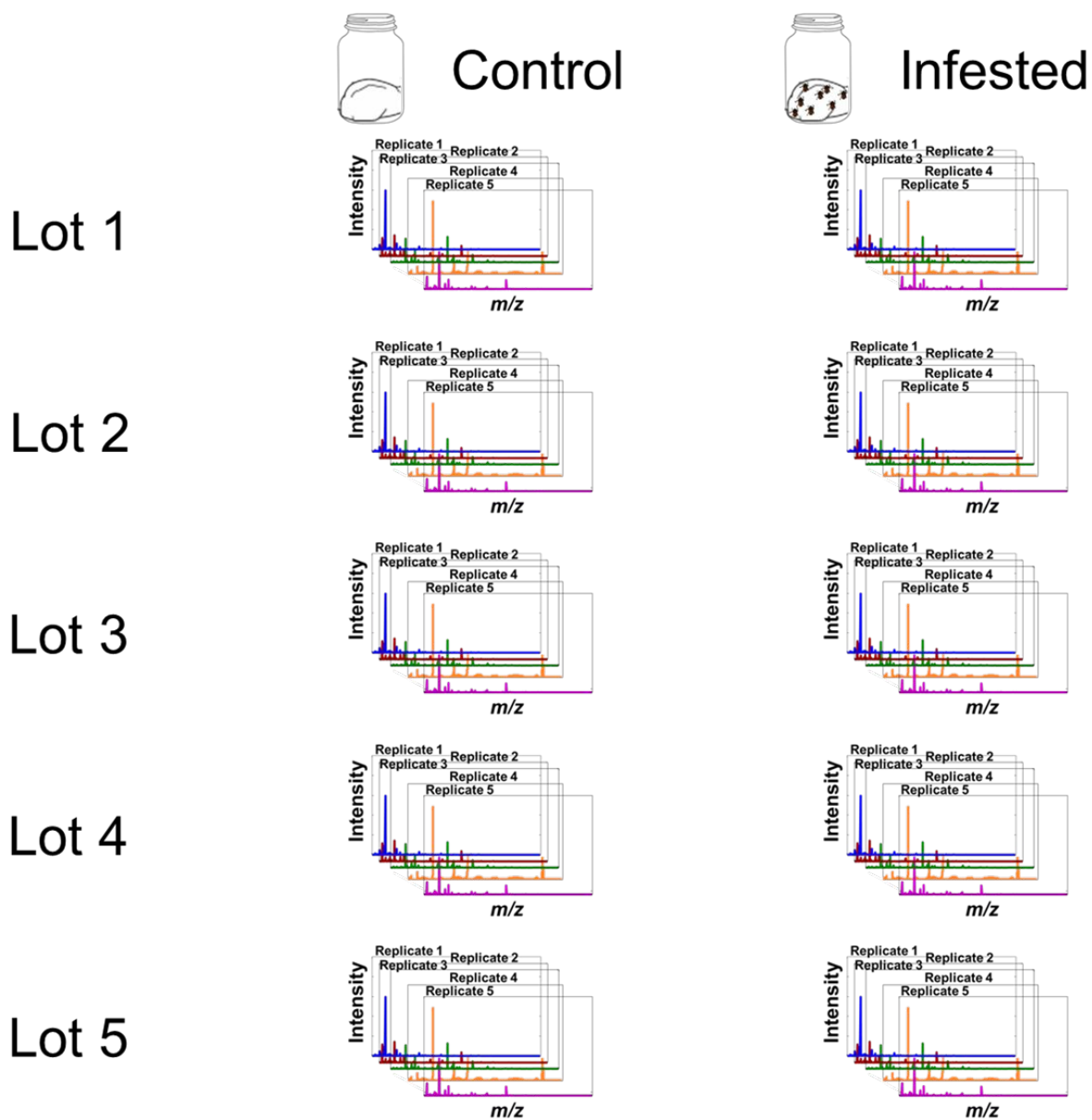# Supporting Information

Contents

Supporting Figures

Figure S1. Five replicate spectra obtained for each of the five flour lots, resulting in 25 spectra for the control flour samples and 25 spectra for the infested flour samples for each day of sampling. This resulted in a data matrix of 50 total spectra with 1191 total *m/z* values.
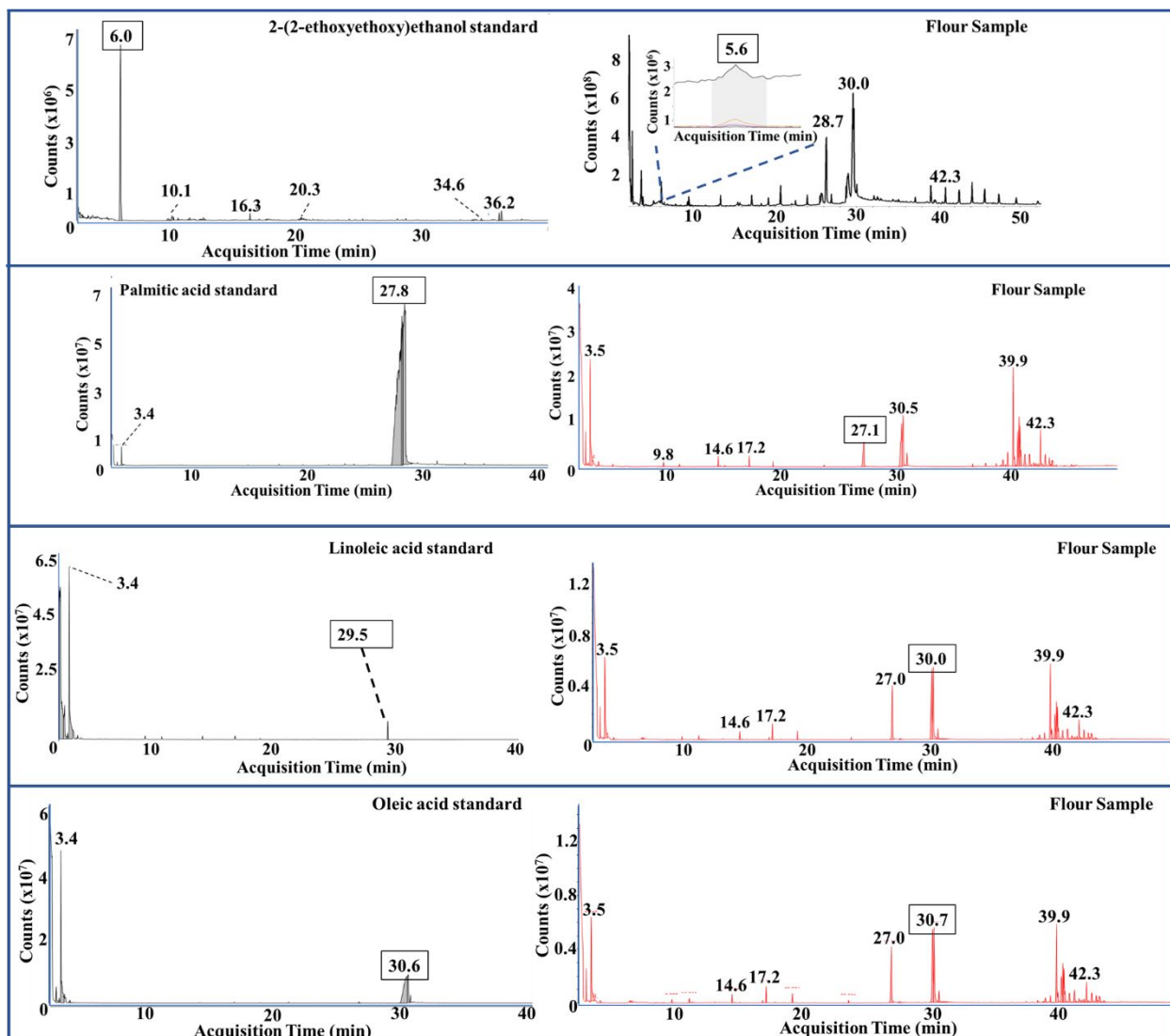
Figure S2. Chromatograms of standards (left) and flour samples (right). The standards tested include from top to bottom 2-(2-ethoxyethoxy)ethanol, palmitic acid, linoleic acid, and oleic acid, which correspond to the nominal *m/z* values 135, 257, 281, and 283 (highlighted in Figure 2B)

Supporting Tables

Table S1. The *m/z* values extracted by EDR analysis of flour data collected on day 21-43.

73.026, 83.086, 87.051, 89.061, 95.086, 97.106, 101.061, 109.101, 114.091, 114.176, 115.063, 115.119, 124.041, 127.041, 133.061, 135.106, 136.066, 137.136, 144.051, 145.051, 152.131, 163.061, 171.151, 180.091, 183.081, 211.126, 211.171, 227.176, 228.211, 257.246, 263.236, 279.231, 280.241, 281.246, 283.261, 295.231, 297.246, 298.276, 306.281, 324.296, 337.276, 338.341, 354.336, 355.291, 371.106, 371.316, 372.316, 394.364, 397.386, 429.358, 519.456, 519.511.

Table S2. Performance results of the EDR-MCR model, which was generated for discrimination of infested and control flour in prediction of test and external validation samples.

	Test set	External validation
Accuracy	0.79	0.83
Sensitivity	0.83	0.79
Specificity	0.76	0.86
Precision	0.73	0.86