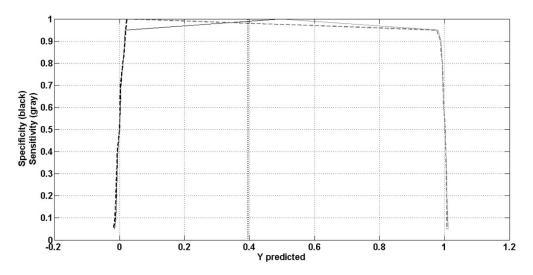
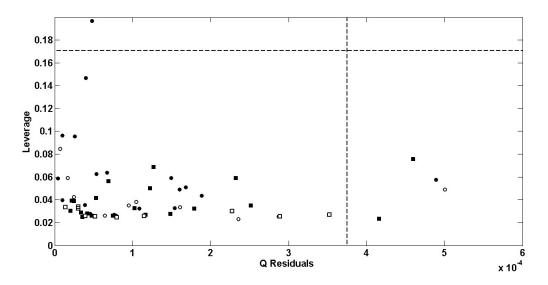
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## Supplementary material



**Figure 1S.** ROC curve for organic sugar crystal. Solid lines correspond to the predicted values from PLS-DA model. Dashed lines correspond to the cross-validation predicted values (contiguous block of 5 samples). The vertical pointed black bold line corresponds to the threshold value of 0.3953.



**Figure 2S.** Q residuals against leverage for the crystal sugar PLS-DA model. ( $\bullet$ ) organic samples in training (O) organic samples in validation. ( $\blacksquare$ ) conventional samples in training. ( $\Box$ ) conventional samples in validation.