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Supplementary material

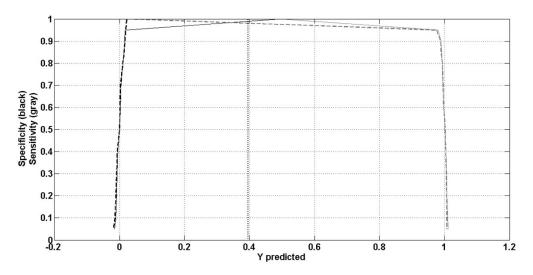


Figure 1S. ROC curve for organic sugar crystal. Solid lines correspond to the predicted values from PLS-DA model. Dashed lines correspond to the cross-validation predicted values (contiguous block of 5 samples). The vertical pointed black bold line corresponds to the threshold value of 0.3953.

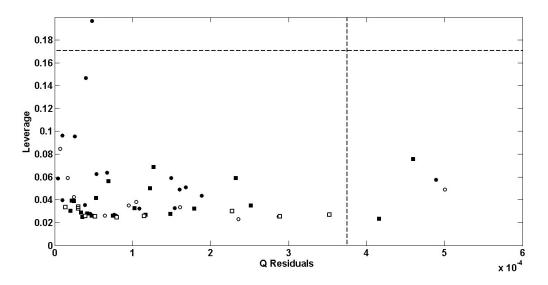


Figure 2S. Q residuals against leverage for the crystal sugar PLS-DA model. (\bullet) organic samples in training (O) organic samples in validation. (\blacksquare) conventional samples in training. (\Box) conventional samples in validation.