

## Monitoring the Transition Period in Dairy Cows through $^1\text{H}$ NMR-Based Untargeted Metabolomics

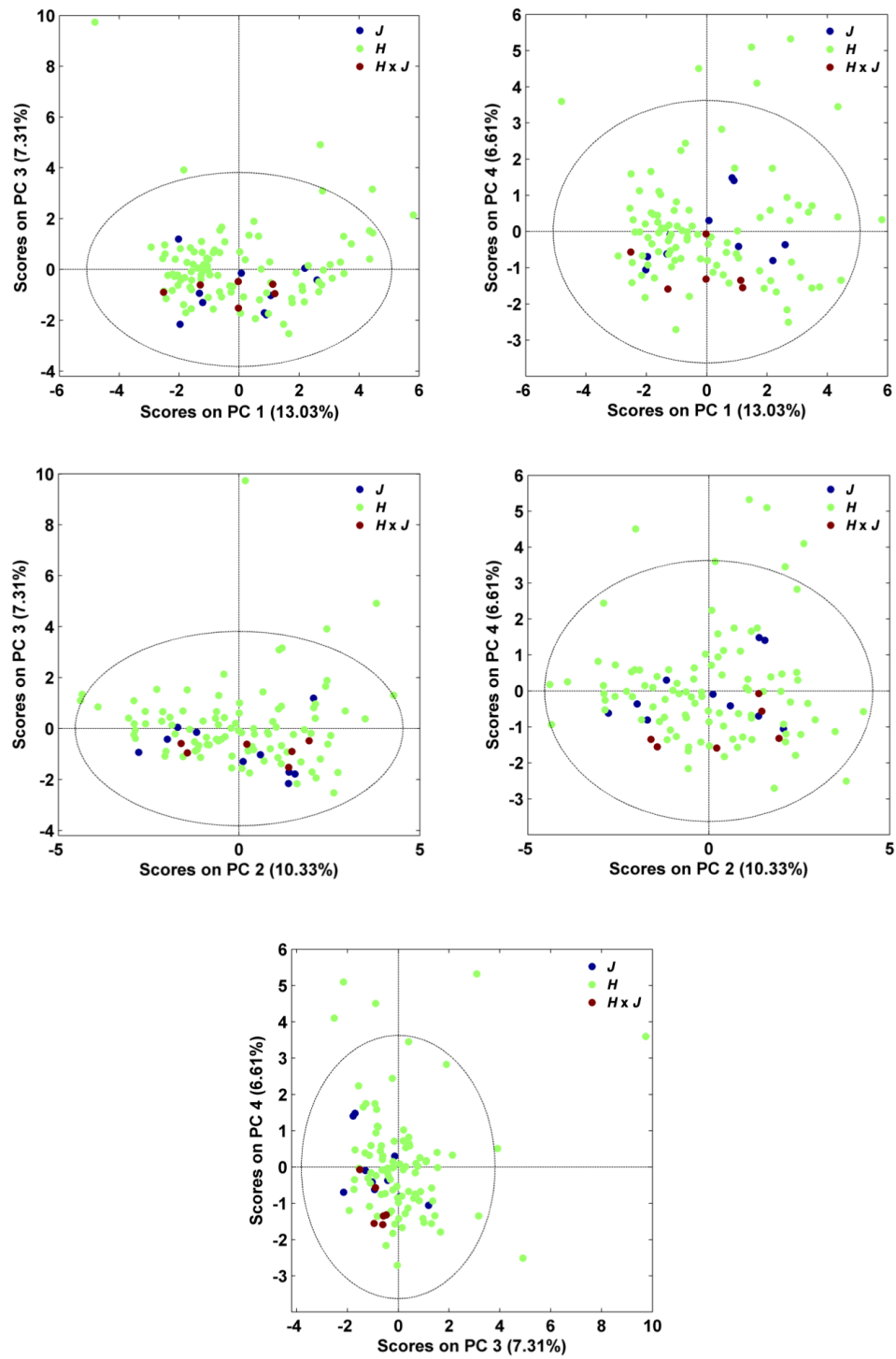
*Andrés López Radcenco, María de Lourdes Adrien, Gretel Ruprecht, Elena de Torres, Ana Meikle, and Guillermo Moyna*

### Supplementary Materials

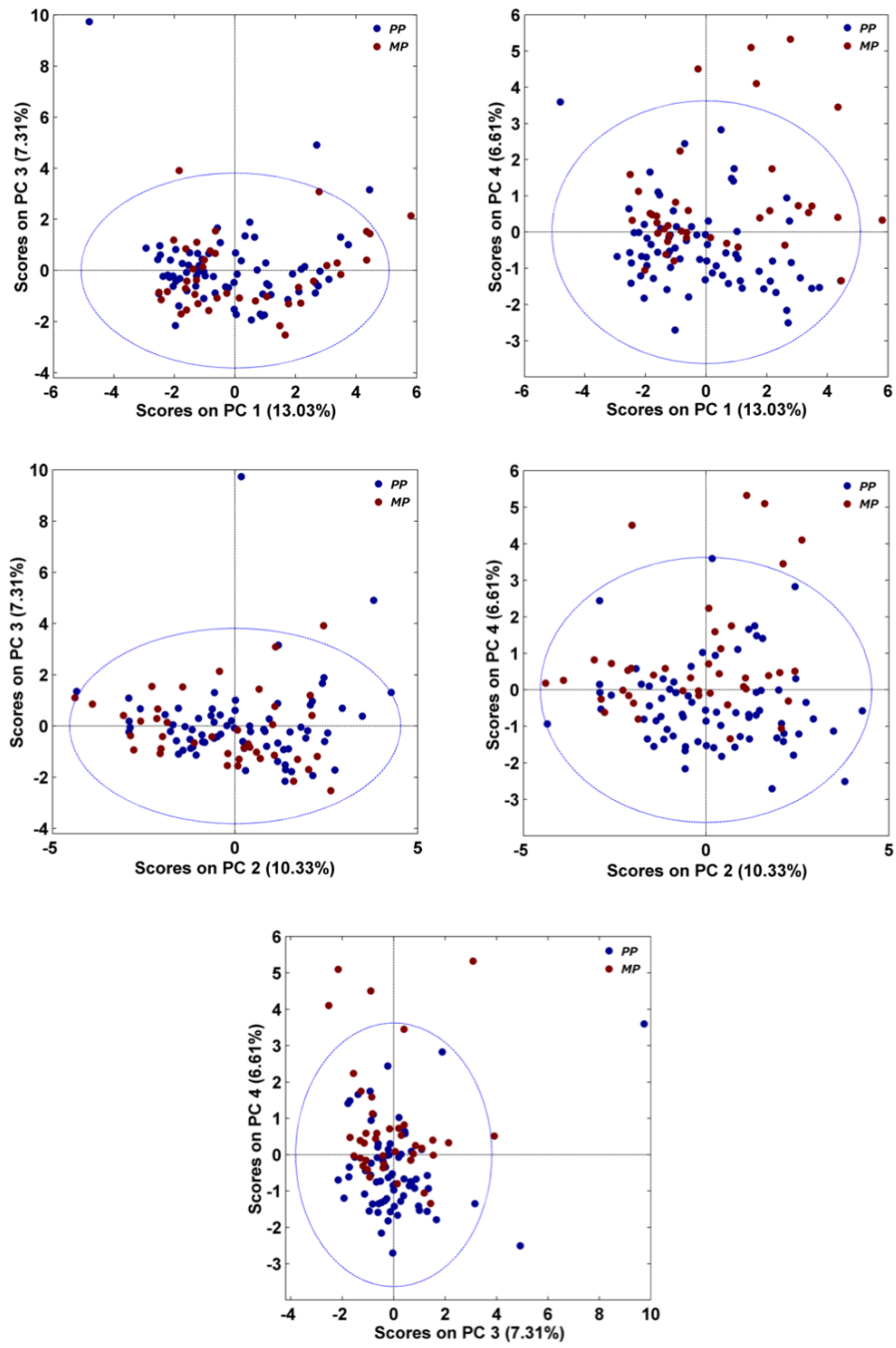
**Table S1.** Monthly postpartum diet composition estimate.

Month	Components <sup>a</sup>			Total offered
	Soybean hull	Maize silage	Pasture	
February	5	2	11	18
March	5	11	2	18
April	5	9	5	19
May	6	11	2	19
June	6	11	2	19

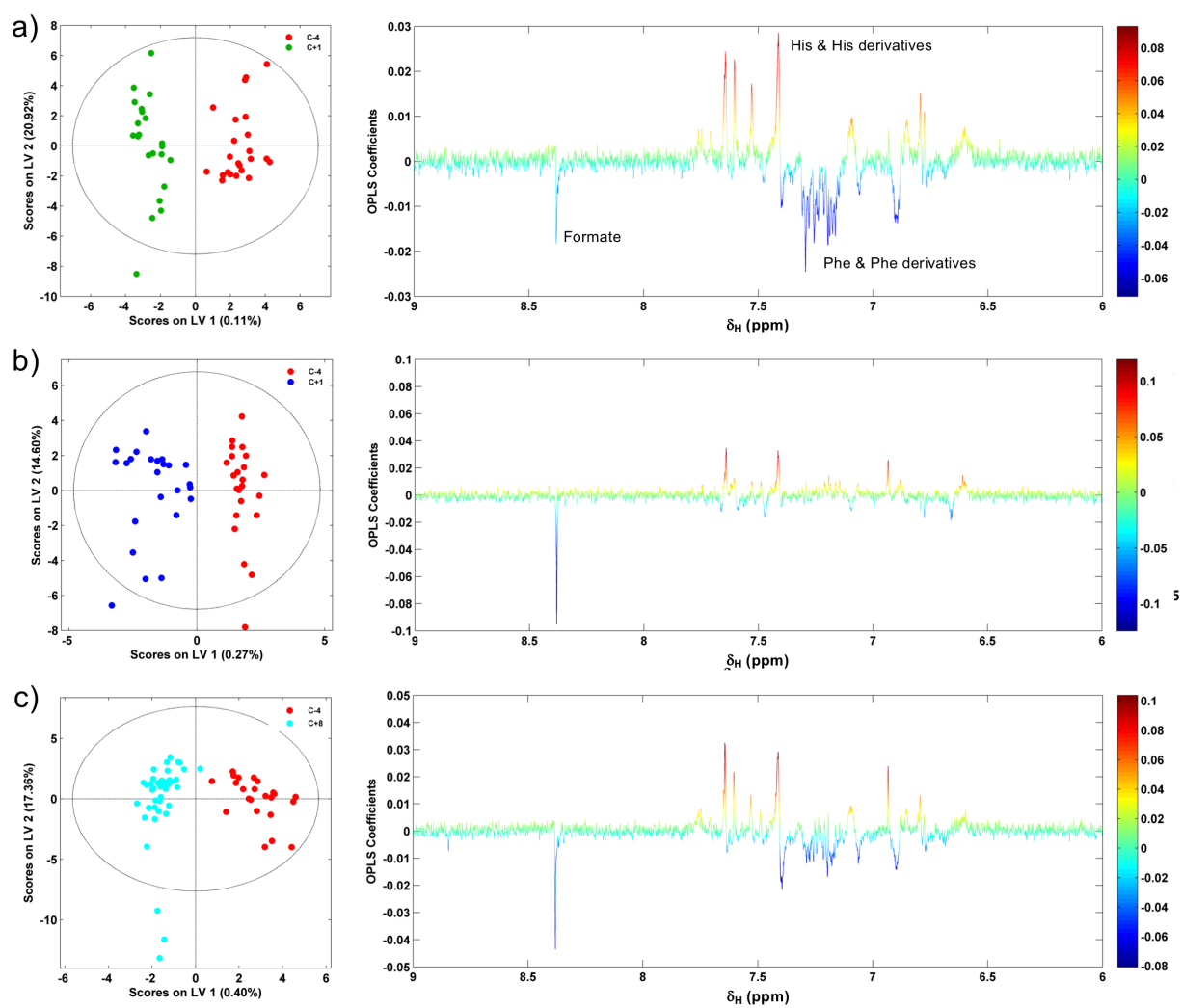
<sup>a</sup> Kg of dry matter per cow per day.



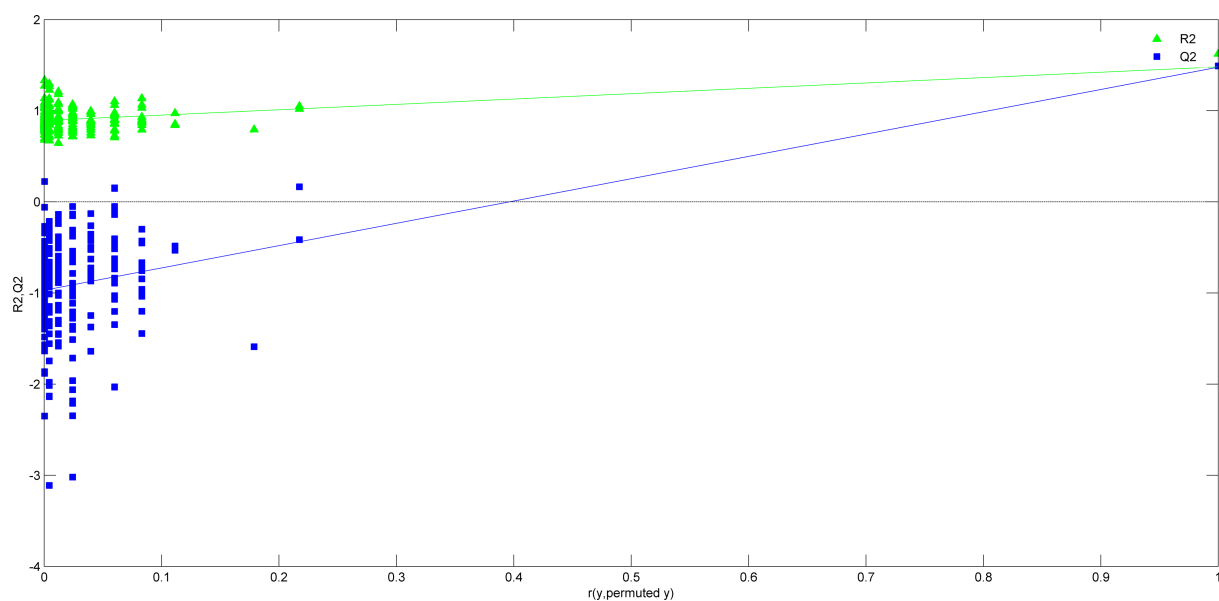
**Figure S1.** Additional PCA score plots colored according to breed.



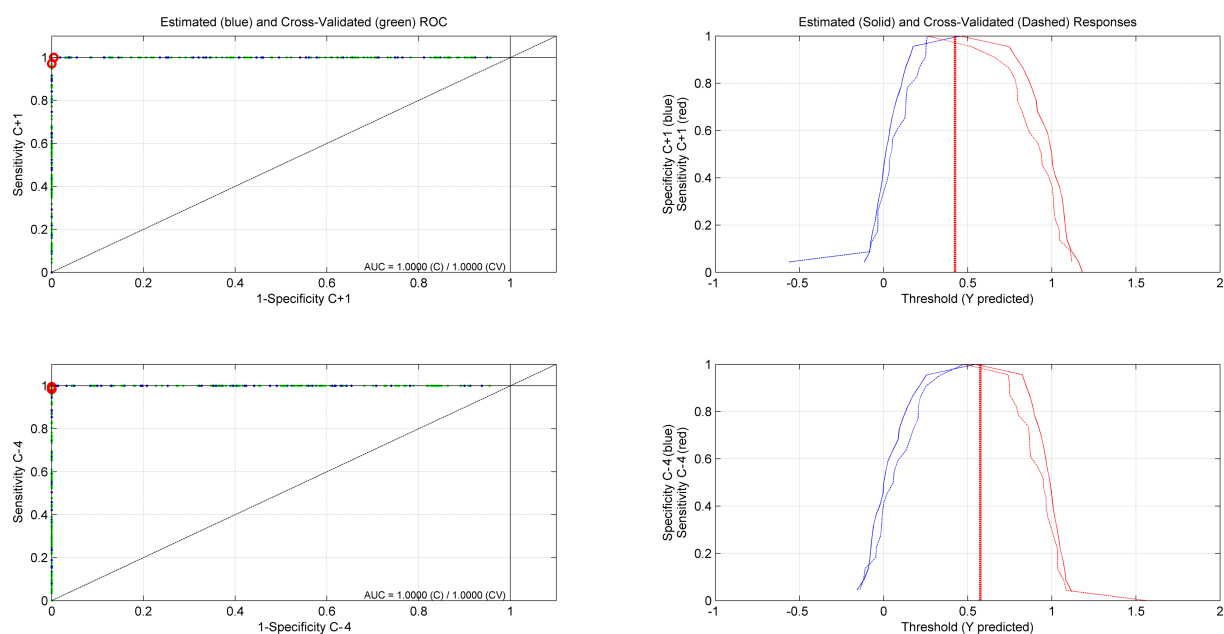
**Figure S2.** Additional PCA score plots colored according to parity.



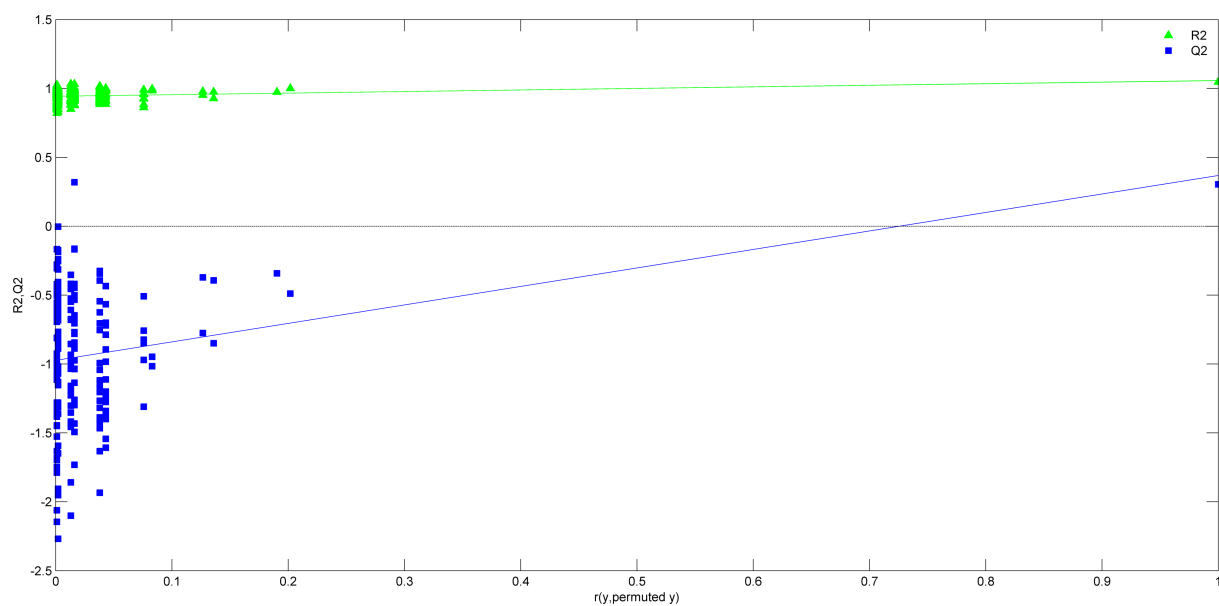
**Figure S3.** Score and loading factor plots obtained from the OPLS-DA for data in the 6.0 to 9.0 ppm range comparing prepartum (C-4) and first (C+1) (a), second (C+4) (b), and third (C+8) (c) postpartum groups. Validations of these models are detailed in Figures S10-S15.



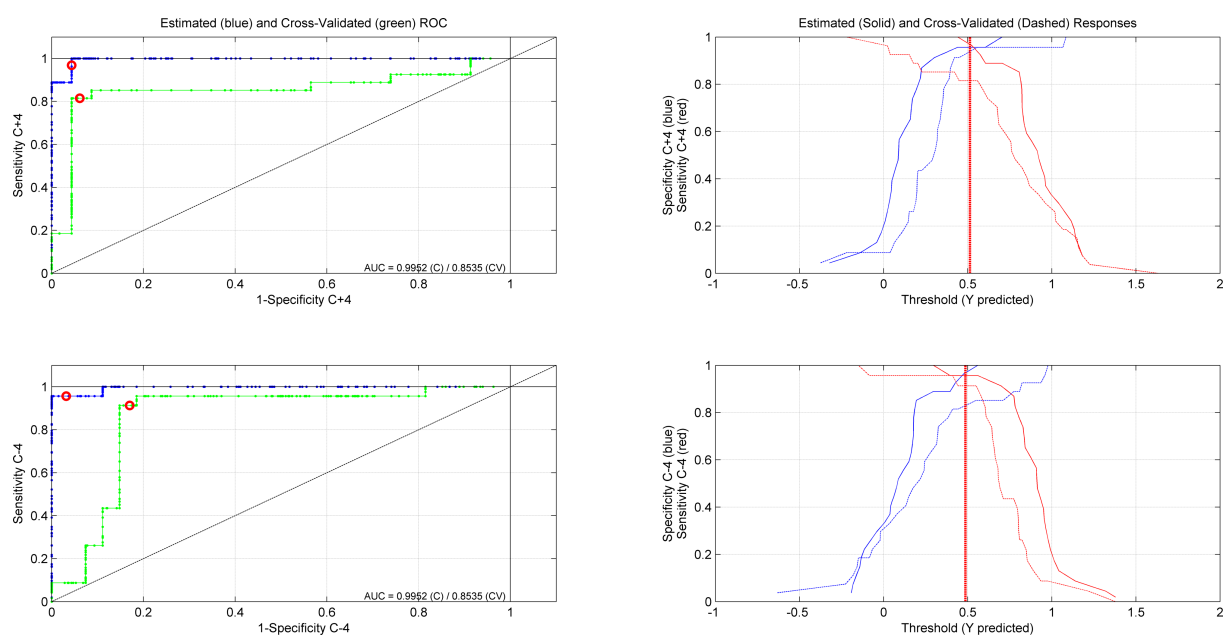
**Figure S4.** Permutation test plots for the OPLS-DA model comparing the C-4 and the C+1 stages ( $R^2Y = 0.80$  and  $Q^2Y = 0.72$ ).



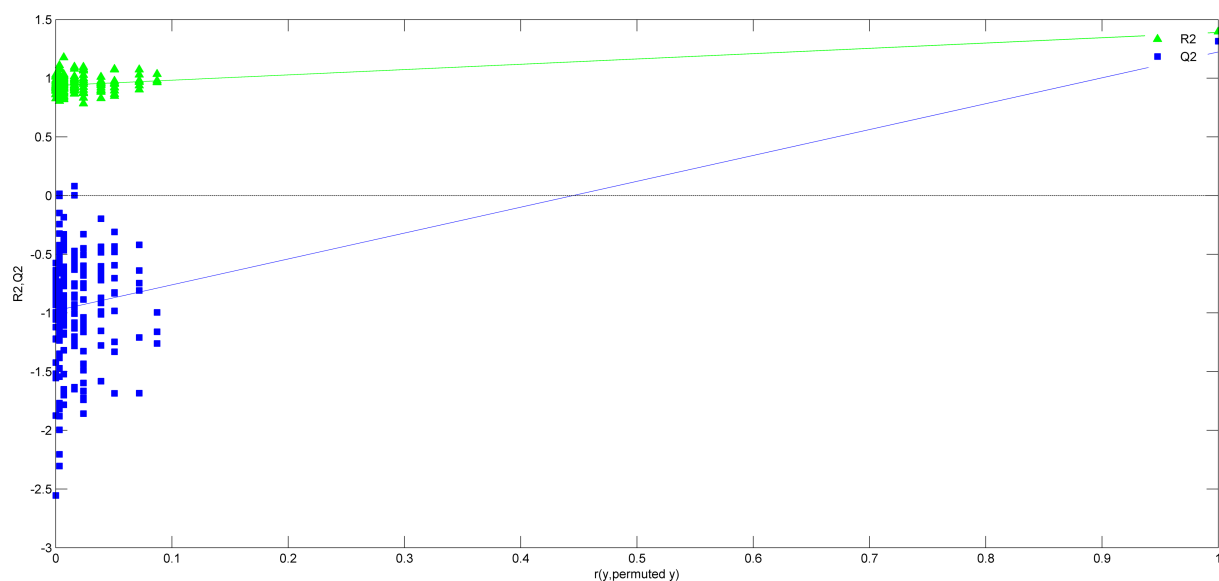
**Figure S5.** ROC analysis curves derived from the OPLS-DA model comparing the C-4 and the C+1 stages (AUC = 1.00).



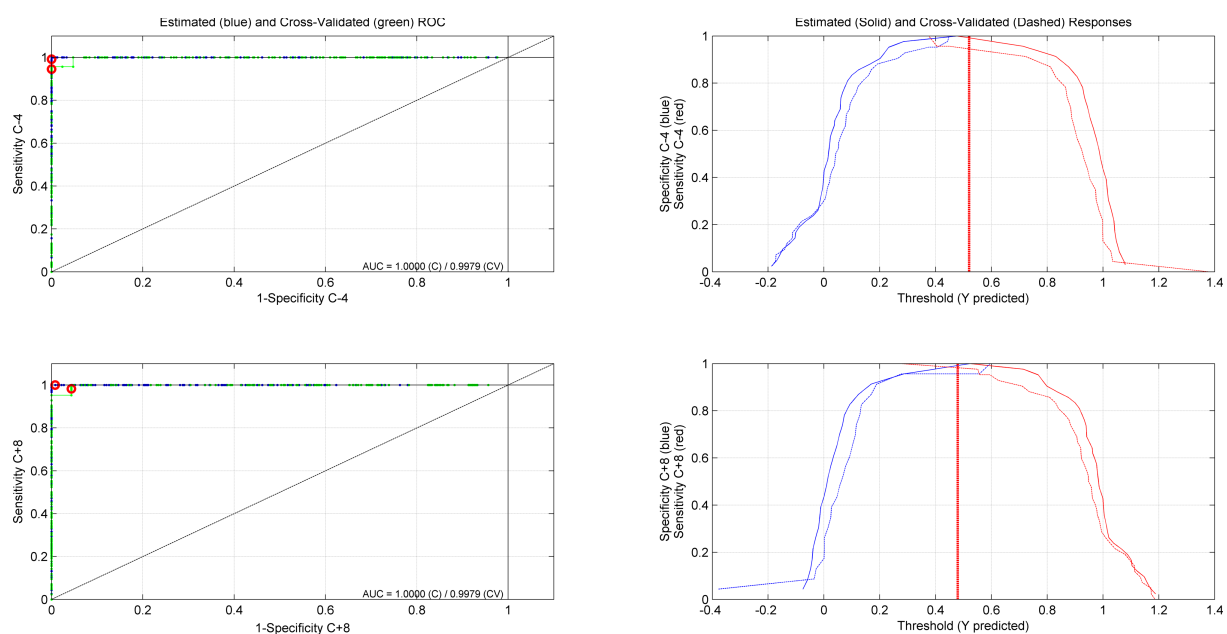
**Figure S6.** Permutation test plots for the OPLS-DA model comparing the C-4 and the C+4 stages ( $R^2Y = 0.89$  and  $Q^2Y = 0.37$ ).



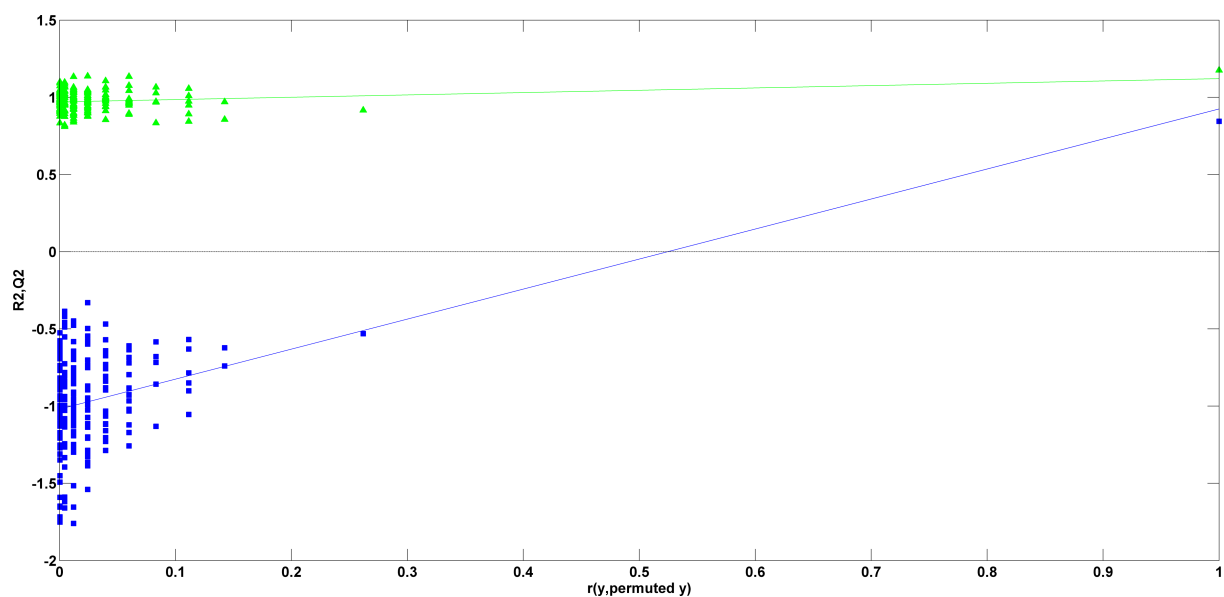
**Figure S7.** ROC analysis curves derived from the OPLS-DA model comparing the C-4 and the C+4 stages (AUC = 0.85).



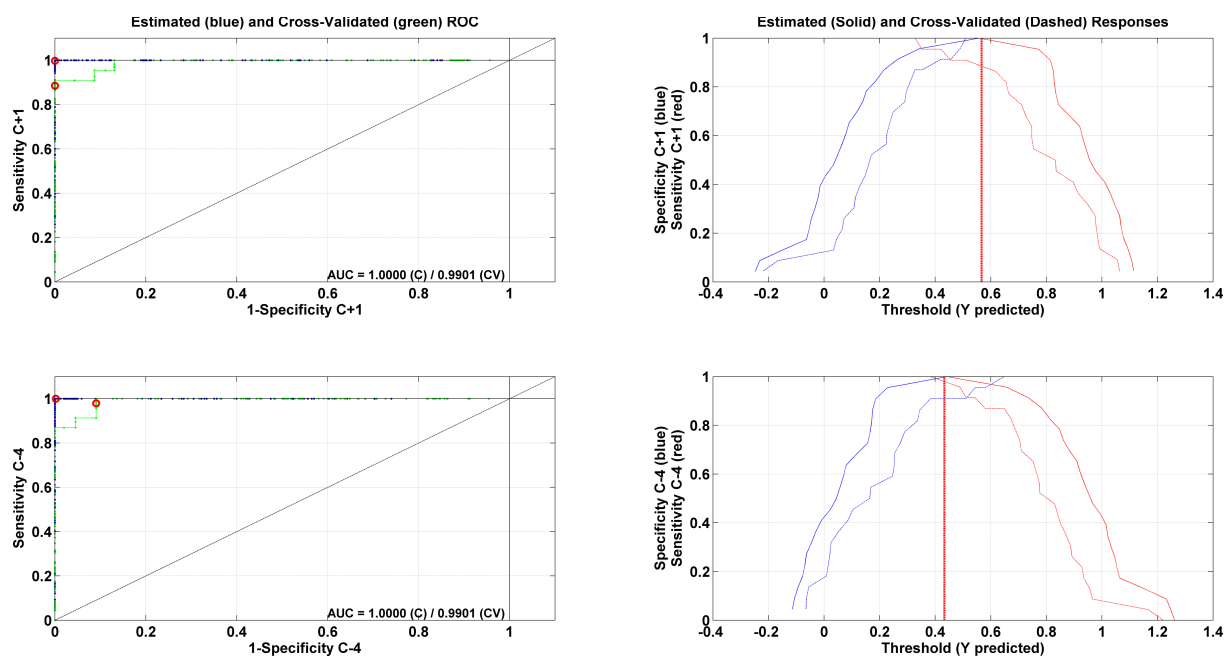
**Figure S8.** Permutation test plots for the OPLS-DA model comparing the C-4 and the C+8 stages ( $R^2Y = 0.94$  and  $Q^2Y = 0.87$ ).



**Figure S9.** ROC analysis curves derived from the OPLS-DA model comparing the C-4 and the C+8 stages ( $AUC = 0.99$ ).

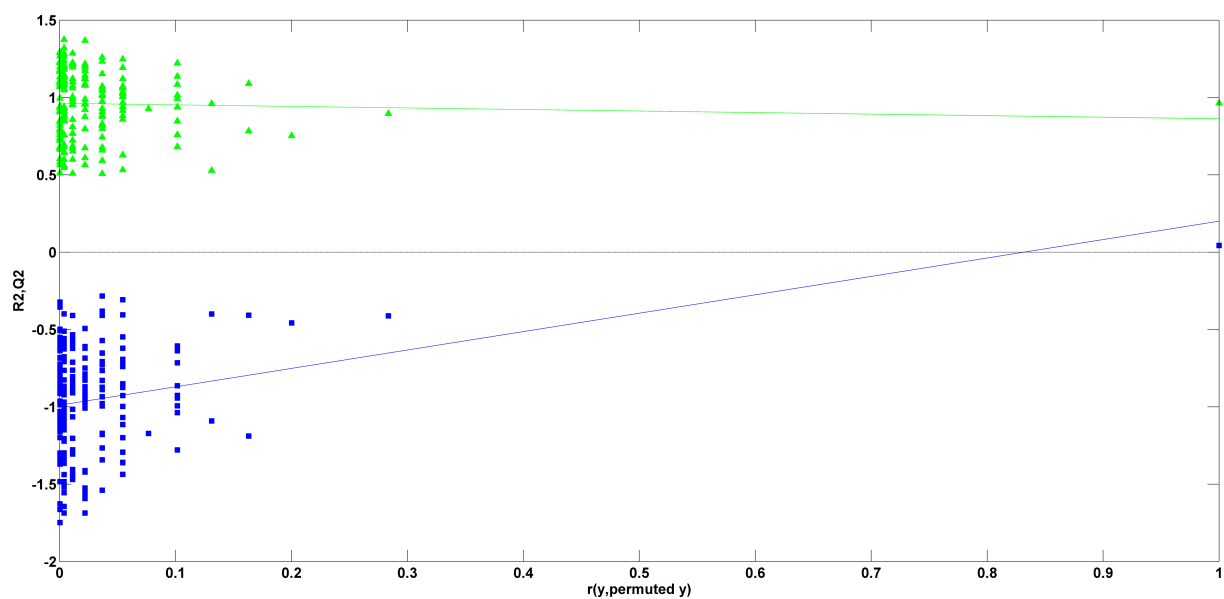


**Figure S10.** Permutation test plots for the OPLS-DA model for data in the 6.0 to 9.0 ppm range comparing the C-4 and the C+1 stages ( $R^2Y = 0.84$  and  $Q^2Y = 0.66$ ).

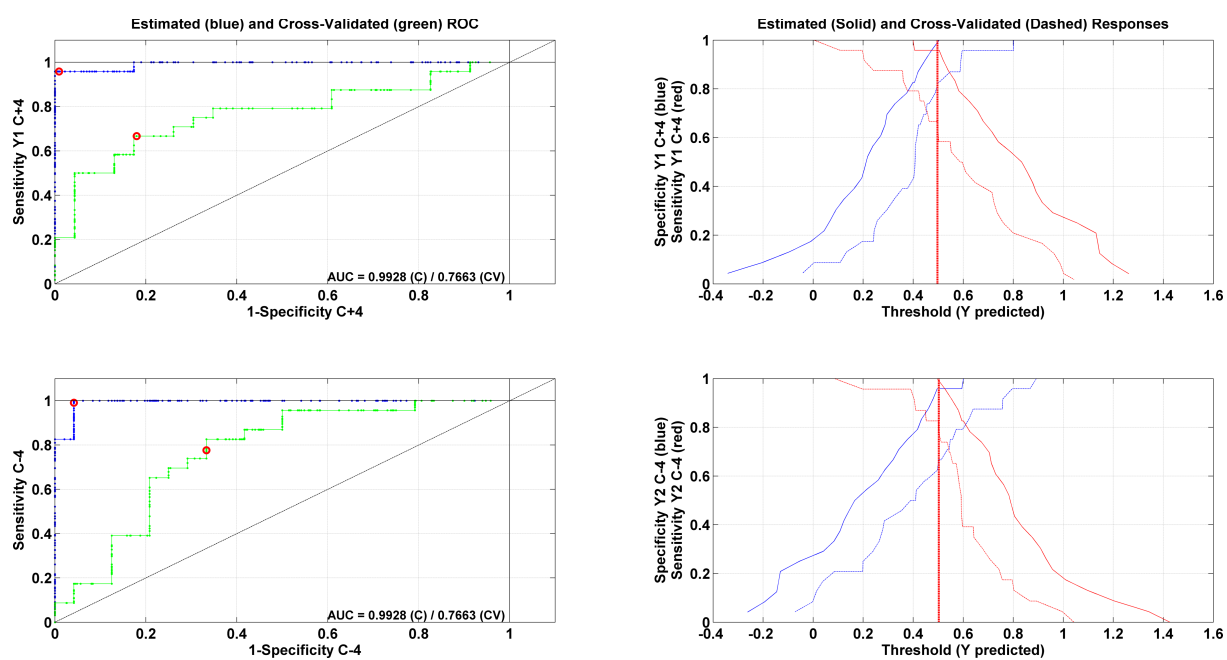


**Figure S11.** ROC analysis curves derived from the OPLS-DA model for data in the 6.0 to 9.0 ppm range comparing the C-4 and the C+1 stages ( $AUC = 0.99$ ).

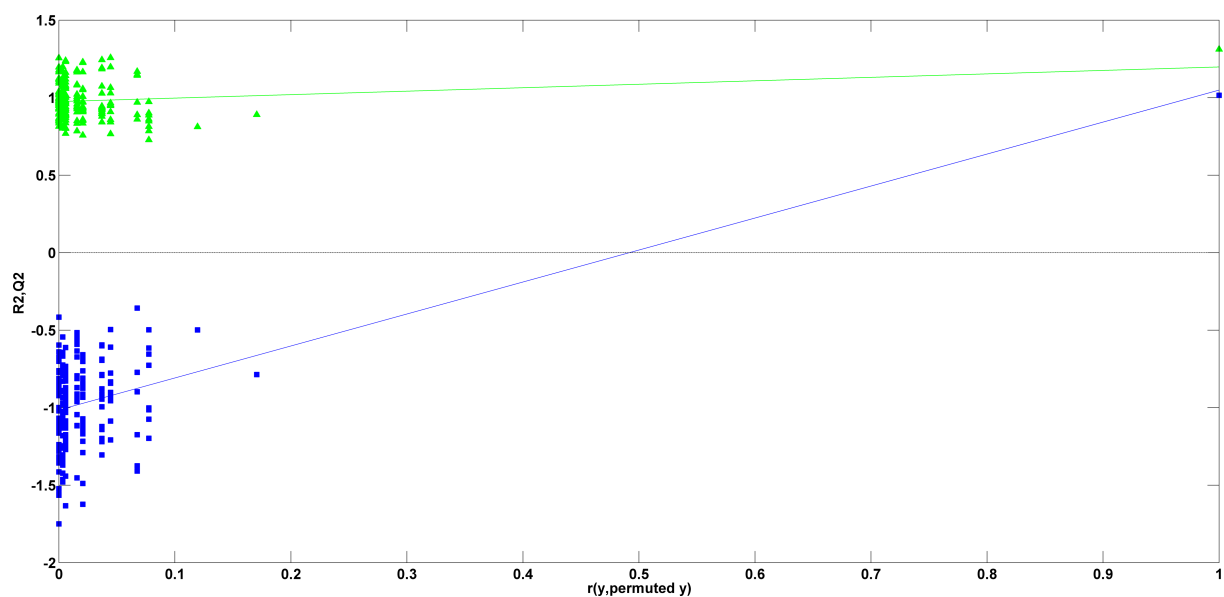




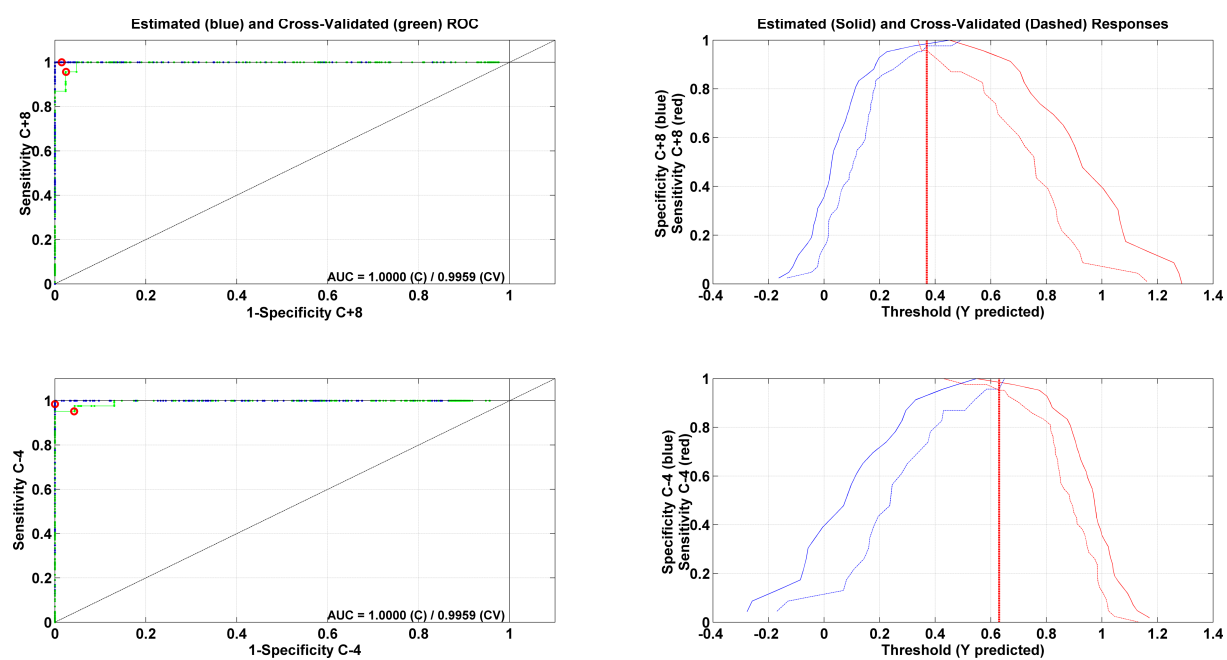
**Figure S12.** Permutation test plots for the OPLS-DA model for data in the 6.0 to 9.0 ppm range comparing the C-4 and the C+4 stages ( $R^2Y = 0.66$  and  $Q^2Y = 0.20$ ).



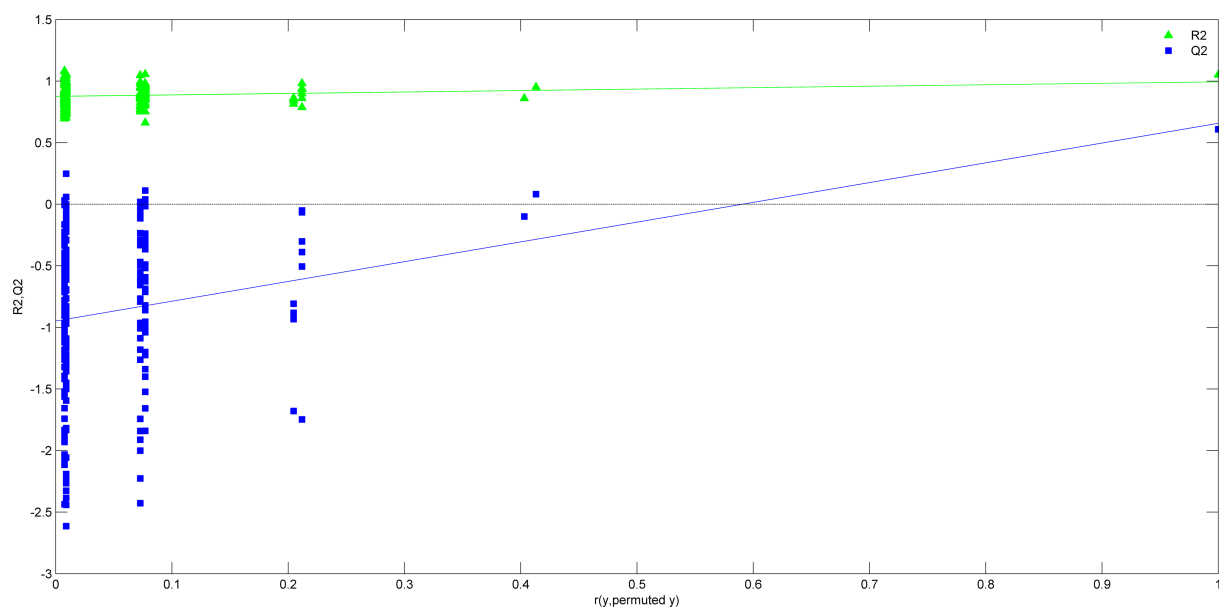
**Figure S13.** ROC analysis curves derived from the OPLS-DA model for data in the 6.0 to 9.0 ppm range comparing the C-4 and the C+4 stages ( $AUC = 0.77$ ).



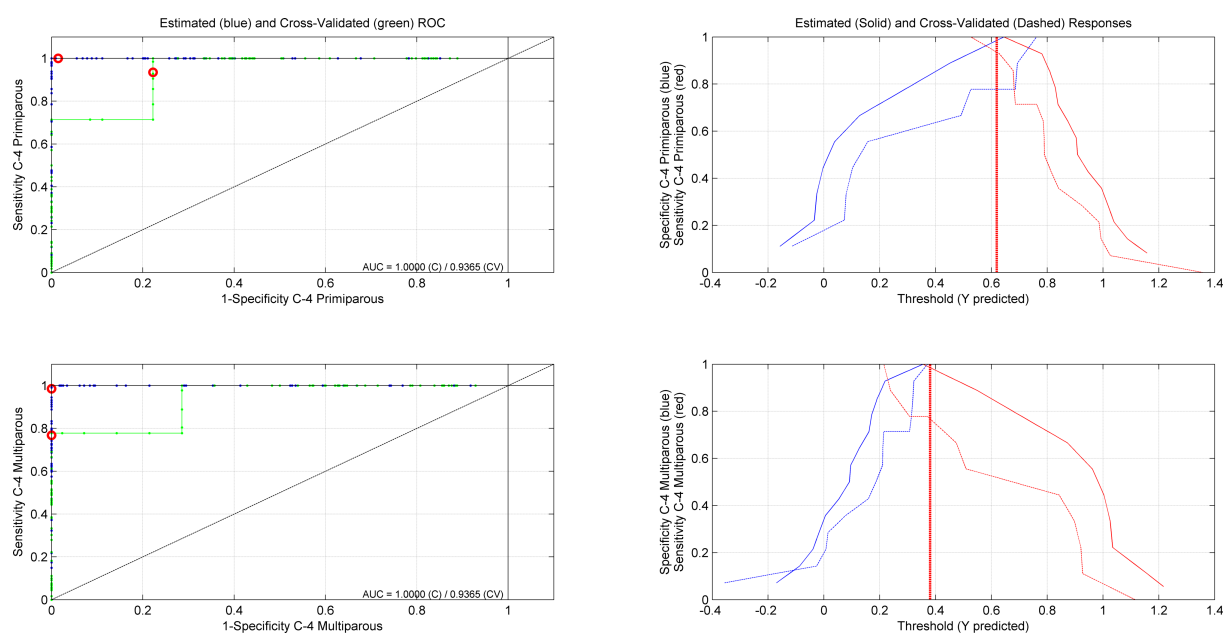
**Figure S14.** Permutation test plots for the OPLS-DA model for data in the 6.0 to 9.0 ppm range comparing the C-4 and the C+8 stages ( $R^2Y = 0.78$  and  $Q^2Y = 0.66$ ).



**Figure S15.** ROC analysis curves derived from the OPLS-DA model for data in the 6.0 to 9.0 ppm comparing the C-4 and the C+8 stages ( $AUC = 0.99$ ).



**Figure S16.** Permutation test plots for the OPLS-DA model comparing primiparous and multiparous dairy cows within the C-4 stage ( $R^2Y = 0.82$  and  $Q^2Y = 0.56$ ).



**Figure S17.** ROC analysis curves derived from the OPLS-DA model comparing primiparous and multiparous dairy cows within the C-4 stage (AUC = 0.93).