

Table S2. Resume of the Hierarchical Models

Hierarchical Model	Training Set Age	Training Set Spectra		1 st Decision Rule	2 nd Decision Rule
		HB	AB		
HM1.a	6 days	365	168	SIMCA_Q	SIMCA_Q
HM1.b	(6 + 0) days	721	338		
HM1.c	(6 + 1) days	716	323		
HM1.d	(6 + 0 + 1) days	1072	493		
HM2.a	6 days	365	168	SIMCA_Q	SIMCA
HM2.b	(6 + 0) days	721	338		
HM2.c	(6 + 1) days	716	323		
HM2.d	(6 + 0 + 1) days	1072	493		
HM3.a	6 days	365	168	SIMCA_Q	PLS-DA
HM3.b	(6 + 0) days	721	338		
HM3.c	(6 + 1) days	716	323		
HM3.d	(6 + 0 + 1) days	1072	493		

The first number of the models refers to the technique used as second rule (HM1 – SIMCA_Q, HM2 – SIMCA and HM3 – PLS-DA). The letter refers to the training set age used (HM*.a – samples with 6 days; HM*.b - 6 days and fresh samples (6 + 0); HM*.c – six and one days samples (6 + 1) days); HM*.d – six, zero and one days samples (6 + 0 + 1) days.