Supplemental Table 1. Indicators of all developed models for buffalo raw milk.

	Pre-		Indicators						
Algorithm	processed of MIR ¹	Dataset	Accuracy	Sensitivity	Specificity	AUC ²	F1 score	MCC	
Partial least	Original	Calibration	0.95	0.94	1.00	0.99	0.98	0.82	
	Original	Validation	0.85	0.82	1.00	0.96	0.97	0.67	
	Diff	Calibration	0.93	0.92	1.00	0.99	0.98		
squares	Dili	Validation	0.80	0.76	1.00	0.94	0.94		
discriminant	SNV	Calibration	0.94	0.93	1.00	0.99	0.97		
analysis		Validation	0.88	0.85	1.00	0.94	0.95	0.71	
(PCs: 20) ³	MSC	Calibration	0.95	0.94	1.00	0.99	0.99	0.84	
(FCS. 20)	MSC	Validation	0.83	0.79	1.00	0.95	0.95	0.63	
	SG(13,4)	Calibration	0.96	0.96	1.00	1.00	0.99	0.87	
	30(13,4)	Validation	0.85	0.82	1.00	0.97	0.98	0.67	
	Original	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
	Original	Validation	1.00	1.00	1.00	1.00	1.00	00 1.00 96 0.68	
Support vector machine ⁴	Diff	Calibration	0.93	0.98	0.63	0.95	0.96		
	Dili	Validation	0.86	0.92	0.50	0.93	0.92	.00	
	SNV	Calibration	1.00	1.00	1.00	1.00	1.00		
		Validation	0.93	0.97	0.67	0.88	0.96		
macinic	MSC	Calibration	0.98	0.99	0.88	0.98	0.99		
		Validation	0.90	0.94	0.67	0.96	0.94		
	SG(17,2)	Calibration	0.99	1.00	0.96	1.00	1.00		
	30(17,2)	Validation	0.98	0.97	1.00	1.00	0.99	0.91	
	Original	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
Random forest	Original	Validation	0.83	0.86	0.67	0.88	0.90	0.45	
	Diff	Calibration	1.00	1.00	1.00	1.00	1.00		
		DIII	Validation	0.86	0.92	0.50	0.87	0.92	0.42
	SNV	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
	DIN V	Validation	0.83	0.92	0.33	0.83	0.90	0.27	
	MSC	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
	MISC	Validation	0.81	0.86	0.50	0.88	0.89	0.32	
	SG(17,2)	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
		Validation	0.83	0.89	0.50	0.90	0.90	0.37	

Validation 0.83 0.89 0.50 0.90 0.90 0.37

1: MIR: mid-infrared spectra; Diff: first-order difference; SNV: standardized normal variation; MSC: multiplicative scatter correction; SG: Savitzky-Golag (window length, poly order)

2: AUC: area under curve

^{3:} PCs: number of principal components used by partial least squares discriminant analysis 4: Bold indicates the optimal model for this type of milk

Supplemental Table 2. Indicators of all developed models for bovine raw milk.

	Pre-		Indicators						
Algorithm	processed of MIR ¹	Dataset	Accuracy	Sensitivity	Specificity	AUC^2	F1 score	MCC	
	Original	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
Partial least	Original	Validation	0.96	0.94	1.00	0.99	0.99	0.90	
	Diff	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
squares	Dili	Validation	0.92	1.00	0.67	0.98	0.98	0.77	
discriminant	SNV	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
analysis	514 4	Validation	0.96	0.94	1.00	0.99	0.99	0.90	
(PCs: 20) ^{3,4}	MSC	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
(FCS. 20)	MSC	Validation	0.96	0.94	1.00	0.99	0.99	0.90	
	SG(13,7) Original Diff	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
		Validation	0.92	0.94	0.83	0.98	0.98	0.78	
	Original	Calibration	0.99	0.99	1.00	1.00	0.99	0.97	
	Original	Validation	0.96	1.00	0.83	1.00	0.97	0.89	
	Diff	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
Support	Dill	Validation	1.00	1.00	1.00	1.00	1.00	1.00	
vector	SNV	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
machine	SINV	Validation	0.79	0.89	0.50	0.84	0.86	0.41	
macmie	MSC	Calibration	0.98	0.99	0.96	1.00	0.99	0.94	
		Validation	0.83	0.89	0.67	0.90	0.89	0.56	
	SG(17,2)	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
	30(17,2)	Validation	0.88	1.00	0.50	0.84	0.92	0.65	
Random forest	Original	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
	Original	Validation	0.79	0.94	0.33	0.69	score MCC 1.00 1.00 0.99 0.90 1.00 1.00 0.98 0.77 1.00 1.00 0.99 0.90 1.00 1.00 0.99 0.90 1.00 1.00 0.98 0.78 0.99 0.97 0.97 0.89 1.00 1.00 1.00 1.00 0.86 0.41 0.99 0.94 0.89 0.56 1.00 1.00 0.87 0.36 1.00 1.00 0.87 0.36 1.00 1.00 0.83 -0.12 1.00 1.00 0.74 -0.26 1.00 1.00 0.74 -0.26 1.00 1.00	0.36	
	Diff	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
	DIII	Validation	0.83	1.00	0.33	0.80	0.90	0.52	
	SNV	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
	SINV	Validation	0.71	0.94	0.00	0.28	0.83	-0.12	
	MSC	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
	MSC	Validation	0.58	0.78	0.00	0.31	0.74	-0.26	
	SG(17,2)	Calibration	1.00	1.00	1.00	1.00	1.00	1.00	
		Validation	0.79	0.94	0.33	0.82	0.87	0.36	

Validation 0.79 0.94 0.33 0.82 0.87 0.36

1: MIR: mid-infrared spectra; Diff: first-order difference; SNV: standardized normal variation; MSC: multiplicative scatter correction; SG: Savitzky-Golag (window length, poly order)

2: AUC: area under curve

3: PCs: number of principal components used by partial least squares discriminant analysis

4: Bold indicates the optimal model for this type of milk

Supplemental Table 3. Indicators of all developed models for bovine pasteurized milk.

	Pre-				Indicators		
Algorithm	processed of MIR ¹	PCs ²	Dataset	Accuracy	kappa	F1 score	
	Original	5	Calibration	0.15	-0.10	0.10	
	Original		Validation	0.18	-0.10	0.11	
	Diff	3	Calibration	0.14	-0.09	0.09	
Partial least	DIII	3	Validation	0.16	-0.11	0.09	
squares	SNV	2	Calibration	0.29	0.04	0.20	
discriminant	DIA A		Validation	0.32	0.04	0.18	
analysis	MSC	2	Calibration	0.21	-0.04	0.15	
	MISC	2	Validation	0.24	-0.02	0.15	
	SG(27,2)	2	Calibration	0.20	-0.03	0.11	
	50(21,2)		Validation	0.26	0.01	0.13	
	Original		Calibration	0.96	0.95	0.96	
	Originar		Validation	0.75	0.63	0.75	
	Diff	NA^3	Calibration	0.86	0.79	0.86	
Support	Dili		Validation	0.72	0.58	0.71	
Support vector	SNV		Calibration	0.91	0.87	0.91	
machine			Validation	0.59	0.39	0.58	
macmine	MSC		Calibration	0.84	0.76	0.84	
			Validation	0.59	0.39	0.58	
	CC(27.2)		Calibration	0.82	0.73	0.82	
	SG(27,3)		Validation	0.77	0.65	0.75	
Random forest ⁴	Oni sin al		Calibration	1.00	1.00	1.00	
	Original		Validation	0.84	0.77	0.84	
	Diff	NA	Calibration	1.00	1.00	1.00	
	DIII		Validation	0.86	0.79	0.86	
	SNV		Calibration	1.00	1.00	1.00	
			Validation	0.39	0.08	0.39	
	MSC		Calibration	1.00	1.00	1.00	
	MISC		Validation	tion 0.34 0.02		0.34	
	SG(27,3)		Calibration	1.00	1.00	1.00	
	56(21,5)		Validation	0.94	0.91	0.94	

^{1:} MIR: mid-infrared spectra; Diff: first-order difference; SNV: standardized normal variation; MSC: multiplicative scatter correction; SG: Savitzky-Golag (window length, poly order)
2: PCs: number of principal components used by partial least squares discriminant analysis

^{3:} NA: not applicable
4: Bold indicates the optimal model for this type of milk

Supplemental Table 4. Indicators of all developed models for bovine ultra-high temperature sterilized (UHT) milk.

	Pre-	PCs ²		Indicators			
Algorithm	processed of MIR ¹		Dataset	Accuracy	kappa	F1 score	
	Original	2	Calibration	0.21	-0.10	0.10	
	Original		Validation	0.24	-0.05	0.15	
	Diff	2	Calibration	0.27	0.05	0.15	
Partial least	Dill	2	Validation	0.30	0.08	0.16	
squares	SNV	2	Calibration	0.15	-0.04	0.10	
discriminant	511 4		Validation	0.19	-0.01	0.12	
analysis	MSC	5	Calibration	0.18	-0.03	0.13	
	MSC		Validation	0.22	0.01	0.16	
	SG(21,2)	2	Calibration	0.30	0.07	0.17	
	50(21,2)		Validation	0.31	0.09	0.17	
	Original		Calibration	0.99	0.99	1.00	
			Validation	0.92	0.89	0.93	
	Diff		Calibration	1.00	1.00	1.00	
Commont			Validation	0.90	0.86	0.91	
Support	SNV	NA ³	Calibration	0.97	0.95	0.97	
vector machine			Validation	0.87	0.82	0.87	
macmine	MSC		Calibration	0.96	0.94	0.96	
			Validation	0.87	0.82	0.87	
	90(21.2)		Calibration	1.00	1.00	1.00	
	SG(21,2)		Validation	0.88	0.83	0.88	
Random forest ⁴	0.5.5		Calibration	1.00	1.00	1.00	
	Original		Validation	0.88	0.84	0.88	
	D:cc	NA	Calibration	1.00	1.00	1.00	
	Diff		Validation	0.92	0.89	0.93	
	SNV		Calibration	1.00	1.00	1.00	
	SINV		Validation	0.51	0.31	0.50	
	MSC		Calibration	1.00	1.00	1.00	
	MSC		Validation	0.45	0.21	0.35	
	SG(21,2)		Calibration	1.00	1.00	1.00	
	3G(41,4)		Validation	0.95	0.92	0.95	

¹: MIR: mid-infrared spectra; Diff: first-order difference; SNV: standardized normal variation; MSC: multiplicative scatter correction; SG: Savitzky-Golag (window length, poly order)

²: PCs: number of principal components used by partial least squares discriminant analysis

³: NA: not applicable

^{4:} Bold indicates the optimal model for this type of milk