

Table S1. Confusion matrices obtained in calibration and external validation for the six algorithms performed using NIRS spectra of faeces samples. 1

Algorithm	Mathematical treatment	Model calibration				Model validation						
		Groups	Model prediction		Classifica- tion %	Groups	Model prediction		Classifica- tion %			
			Graz- ing	Intensive feeding			Graz- ing	Intensive feeding				
PLS2	1,5,1,1 no scatter	Real classi- fication	Grazing	26	100%	Real classi- fication	Grazing	3	81.8%			
			Intensive feeding	0			29	Intensive feeding		0	6	
	2,5,1,1 no scatter		Grazing	26	100%		Grazing	5	100%			
			Intensive feeding	0			29	Intensive feeding		0	6	
	1,5,1,1 SNV+DT		Grazing	26	100%		Grazing	5	100%			
			Intensive feeding	0			29	Intensive feeding		0	6	
	2,5,1,1 SNV+DT		Grazing	25	96.4%		Grazing	4	90.9%			
			Intensive feeding	1			28	Intensive feeding		0	6	
	Correlation		1,5,1,1 no scatter	Real classi- fication	Grazing		21	87.3%	Real classi- fication	Grazing	4	90.9%
					Intensive feeding		2			27	Intensive feeding	
			2,5,1,1 no scatter		Grazing		24	90.9%		Grazing	3	81.8%
					Intensive feeding		3			26	Intensive feeding	
1,5,1,1 SNV+DT		Grazing	21		87.3%	Grazing	4	90.9%				
		Intensive feeding	2			27	Intensive feeding			0	6	

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		Grazing	24	2	90.9%	Grazing	3	2	81.8%	
2,5,1,1 SNV+DT		Intensive feeding	3	26		Intensive feeding	0	6		
Maximum distance	Real classification	Groups	Model prediction		Classification %	Groups	Model prediction		Classification %	
			Graz-ing	Intensive feeding			Graz-ing	Intensive feeding		
		1,5,1,1 no scatter	Grazing	25	1	94.5%	Grazing	3	2	81.8%
			Intensive feeding	2	27		Intensive feeding	0	6	
		2,5,1,1 no scatter	Grazing	26	0	96.4%	Grazing	3	2	81.8%
			Intensive feeding	2	27		Intensive feeding	0	6	
		1,5,1,1 SNV+DT	Grazing	26	0	96.4%	Grazing	2	3	72.7%
			Intensive feeding	2	27		Intensive feeding	0	6	
		2,5,1,1 SNV+DT	Grazing	25	1	94.5%	Grazing	1	4	54.5%
			Intensive feeding	2	27		Intensive feeding	1	5	
Mahalanobis distance	Real classification	Groups	Model prediction		Classification %	Groups	Model prediction		Classification %	
			Graz-ing	Intensive feeding			Graz-ing	Intensive feeding		
		1,5,1,1 no scatter	Grazing	26	0	89.1%	Grazing	4	1	90.9%
			Intensive feeding	6	23		Intensive feeding	0	6	
		2,5,1,1 no scatter	Grazing	25	1	89.1%	Grazing	4	1	90.9%
			Intensive feeding	5	24		Intensive feeding	0	6	

		Grazing	26	0	87.3%	Grazing	5	0	100%
1,5,1,1 SNV+DT		Intensive feeding	7	22		Intensive feeding	0	6	
		Grazing	25	1	87.3%	Grazing	1	4	54.5%
2,5,1,1 SNV+DT		Intensive feeding	6	23		Intensive feeding	1	5	
		Groups	Model prediction		Classifica- tion %	Groups	Model prediction		Classifica- tion %
			Graz- ing	Intensive feeding			Graz- ing	Intensive feeding	
		Grazing	26	0	100%	Grazing	4	1	90.9%
1,5,1,1 no scatter		Intensive feeding	0	29		Intensive feeding	0	6	
		Grazing	26	0	100%	Grazing	5	0	100%
X-residuals	2,5,1,1 no scatter	Intensive feeding	0	29		Intensive feeding	0	6	
	Real classi- fication	Grazing	26	0	100%	Grazing	5	0	100%
		Intensive feeding	0	29		Intensive feeding	0	6	
		Grazing	26	0	100%	Grazing	5	0	100%
		Intensive feeding	0	29		Intensive feeding	0	6	
	1,5,1,1 SNV+DT	Grazing	26	0	100%	Grazing	5	0	100%
		Intensive feeding	0	29		Intensive feeding	0	6	
		Grazing	26	0	100%	Grazing	5	0	100%
2,5,1,1 SNV+DT		Intensive feeding	0	29		Intensive feeding	0	6	
		Groups	Model prediction		Classifica- tion %	Groups	Model prediction		Classifica- tion %
			Graz- ing	Intensive feeding			Graz- ing	Intensive feeding	
		Grazing	25	1	96.4%	Grazing	4	1	90.9%
Maximum X- residuals	1,5,1,1 no scatter	Intensive feeding	1	28		Intensive feeding	0	6	

2,5,1,1 no scatter	Grazing	26	0	98.2%	Grazing	4	1	90.9%
	Intensive feeding	1	28		Intensive feeding	0	6	
1,5,1,1 SNV+DT	Grazing	25	1	96.4%	Grazing	5	0	100%
	Intensive feeding	1	28		Intensive feeding	0	6	
2,5,1,1 SNV+DT	Grazing	26	0	100%	Grazing	5	0	100%
	Intensive feeding	0	29		Intensive feeding	0	6	

No scatter: no scatter effect correction performed; SNV + DT: Standard Normal Variate and De-trending transformation.

Table 2. Confusion matrices obtained in calibration and external validation for the six algorithms performed using NIRS spectra of milk samples.

Algorithm	Mathematical treatment	Model calibration				Model validation			
		Groups	Model prediction		Classifica- tion %	Groups	Model prediction		Classifica- tion %
			Graz- ing	Intensive feeding			Graz- ing	Intensive feeding	
PLS2	1,5,1,1 no scatter	Real classi- fication	Grazing	18	78.6%	Grazing	7	0	100%
			Intensive feeding	5		Intensive feeding	0	8	
	2,5,1,1 no scatter		Grazing	22	94.6%	Grazing	7	0	100%
			Intensive feeding	0		Intensive feeding	0	8	
	1,5,1,1 SNV+DT		Grazing	24	98.2%	Grazing	4	3	73.3%
			Intensive feeding	0		Intensive feeding	1	7	
	2,5,1,1 SNV+DT		Grazing	18	80.4%	Grazing	4	3	73.3%
			Intensive feeding	4		Intensive feeding	1	7	
		Groups	Model prediction		Classifica- tion %	Groups	Model prediction		Classifica- tion %
			Graz- ing	Intensive feeding			Graz- ing	Intensive feeding	
Correlation	1,5,1,1 no scatter	Real classi- fication	Grazing	21	87.5%	Grazing	6	1	93.3%
			Intensive feeding	3		Intensive feeding	0	8	
	2,5,1,1 no scatter		Grazing	22	92.9%	Grazing	7	0	100%
			Intensive feeding	1		Intensive feeding	0	8	
	1,5,1,1 SNV+DT		Grazing	22	85.7%	Grazing	6	1	93.3%
			Intensive feeding	5		Intensive feeding	0	8	

2,5,1,1 SNV+DT			Grazing	22	3	87.5%		Grazing	7	0	100%			
			Intensive feeding	4	27			Intensive feeding	0	8				
		Groups	Model prediction		Classifica- tion %			Groups	Model prediction		Classifica- tion %			
			Graz- ing	Intensive feeding		Graz- ing	Intensive feeding							
Maximum dis- tance	1,5,1,1 no scatter	Real classi- fication	Grazing	24	1	94.6%	Real classi- fication	Grazing	7	0	100%			
			Intensive feeding	2	29			Intensive feeding	0	8				
	2,5,1,1 no scatter		Grazing	23	2	78.6%		Grazing	7	0	80%			
			Intensive feeding	10	21			Intensive feeding	3	5				
	1,5,1,1 SNV+DT		Grazing	24	1	98.2%		Grazing	7	0	100%			
			Intensive feeding	0	31			Intensive feeding	0	8				
	2,5,1,1 SNV+DT		Grazing	24	1	94.6%		Grazing	6	1	80%			
			Intensive feeding	2	29			Intensive feeding	2	6				
			Groups	Model prediction		Classifica- tion %				Groups	Model prediction		Classifica- tion %	
		Graz- ing		Intensive feeding	Graz- ing		Intensive feeding							
Mahalanobis distance	1,5,1,1 no scatter	Real classi- fication	Grazing	25	0	87.5%	Real classi- fication	Grazing	7	0	80%			
			Intensive feeding	7	24			Intensive feeding	3	5				
	2,5,1,1 no scatter		Grazing	23	2	76.8%		Grazing	7	0	73.3%			
			Intensive feeding	11	20			Intensive feeding	4	4				
	1,5,1,1 SNV+DT		Grazing	25	0	92.9%		Grazing	7	0	93.3%			

2,5,1,1 SNV+DT			Intensive feeding	4	27	85.7%	Intensive feeding	1	7	73.3%		
			Grazing	24	1		Grazing	7	0			
			Intensive feeding	7	24		Intensive feeding	4	4			
X-residuals	Real classification		Groups	Model prediction		Classification %	Groups	Model prediction		Classification %		
				Grazing	Intensive feeding			Grazing	Intensive feeding			
			1,5,1,1 no scatter	Grazing	21	4	92.9%	Grazing	4	3	73.3%	
				Intensive feeding	0	31		Intensive feeding	1	7		
			2,5,1,1 no scatter	Grazing	22	3	89.3%	Grazing	7	0	100%	
				Intensive feeding	3	28		Intensive feeding	0	8		
			1,5,1,1 SNV+DT	Grazing	24	1	98.2%	Grazing	7	0	100%	
				Intensive feeding	0	31		Intensive feeding	0	8		
			2,5,1,1 SNV+DT	Grazing	25	0	98.2%	Grazing	7	0	93.3%	
				Intensive feeding	1	30		Intensive feeding	1	7		
			Maximum X-residuals	Real classification		Groups	Model prediction		Classification %	Groups	Model prediction	
Grazing	Intensive feeding	Grazing					Intensive feeding					
1,5,1,1 no scatter	Grazing	25				0	100%	Grazing	5	2	86.7%	
	Intensive feeding	0				31		Intensive feeding	0	8		
2,5,1,1 no scatter	Grazing	24				1	96.4%	Grazing	6	1	93.3%	

	Intensive feeding	1	30		Intensive feeding	0	8	
	Grazing	25	0		Grazing	6	1	
1,5,1,1 SNV+DT	Intensive feeding	0	31	100%	Intensive feeding	0	8	93.3%
	Grazing	24	1		Grazing	5	2	
2,5,1,1 SNV+DT	Intensive feeding	0	31	98.2%	Intensive feeding	1	7	80%

No scatter: no scatter effect correction performed; SNV + DT: Standard Normal Variate and De-trending transformation.

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