1 **Opportunities and limitations of milk mid-infrared spectra based estimation of acetone and**

2 **β-hydroxybutyrate for the prediction of metabolic stress and ketosis in dairy cows**

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8 **SUPPLEMENTARY FILE**

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11 **Supplementary Table S1.** Description of farms enrolled in the field study with information on

12 dairy breeds, number of animals and samples, parity and percentage of positive samples for

13 SCK.

Farm	Breed	No. of animals	No. of samples	Parity[1]	SCK (%)[2]	Blood BHB (mmol/L)[3]
Farm 1	Brown Swiss	37	308	2.9 ± 2.1	5.1	0.53 (± 0.02)
Farm 2	Brown Swiss	35	303	3.8 ± 2.6	4.1	0.55 (± 0.02)
Farm 3	Swiss Fleckvieh/ Holstein	26/ 11	225/ 98	2.9 ± 1.6	7.0	0.63 (± 0.02)
Farm 4	Swiss Fleckvieh	32	257	2.5 ± 2.2	2.4	0.46 (± 0.01)
Farm 5	Holstein	36	299	3.0 ± 2.2	2.4	0.54 (± 0.01)
Farm 6	Holstein	33	276	1.9 ± 1.4	0.7	0.51 (± 0.01)
Total	-	210	1766	2.8 ± 2.0	3.6	0.54 (± 0.01)

14 [1] means ± SD

15 [2] Subclinical ketosis (SCK) was assumed at blood BHB ≥ 1.0 mmol/L.

16 [3] means ± SEM

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19 **Supplementary Table S2**

20 **Comparison of measures of energy status from Experiment 1, field trial**

Measurement methodology	SCK	Non-CK
	mmol/l, mean±se	
MIR spectra-predicted BHB	0.11±0.01	0.02±0.00
MIR spectra-predicted acetone	0.14±0.02	0.01±0.01
Enzymatically determined BHB	1.59±0.08	0.50±0.00
Chemically determined acetone	0.17±0.02	0.05±0.00
	Ratio	
Milk fat-to-protein ratio FPR	1.30±0.05	1.15±0.01

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23 **Supplementary Table S3**

24 **Effects of breed and parity in Experiment 1, field trial**

	Holstein	Swiss Fleckvieh	Brown Swiss
MIR spectra-predicted BHB mmol/l	-0.00±0.00	0.03±0.00	0.03±0.00
MIR spectra-predicted acetone mmol/l	-0.022±0.005	0.06±0.02	0.01±0.00
FPR ratio	1.18±0.01	1.20±0.02	1.07±0.01
Milk yield kg/d	36.1±0.5	34.9±0.6	31.6±0.5
	Primiparous	Multiparous	
Blood BHB mmol/l	0.49±0.01	0.57±0.01	
MIR spectra-predicted BHB mmol/l	0.01±0.00	0.03±0.00	
Blood acetone mmol/l	0.05±0.00	0.05±0.00	
Milk yield kg/d	27.7±0.3	38.0±0.04	

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