**Prediction of methane emission from dairy cows and a novel approach to identify high emitter cases based on milk fatty acid profiles**

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**Supplementary Table S1** *Summary statistics of variables included in the analyses of the study*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Variable | Mean | SD | Minimum | Maximum |
| CH4 (g/d) | 357.5 | 70.63 | 198.4 | 547.0 |
| CH4 (g/kg DMI) | 18.2 | 3.01 | 12.3 | 26.8 |
| CH4 (g/kg milk) | 16.4 | 4.65 | 9.0 | 44.3 |
| Dry matter intake (kg/d) | 19.7 | 3.05 | 13.5 | 24.9 |
| Milk yield (kg/d) | 22.8 | 5.59 | 8.36 | 37.8 |
| Forage proportion | 0.67 | 0.12 | 0.46 | 0.83 |
| Concentrate intake (kg DM/d) | 6.68 | 3.11 | 2.58 | 13.43 |
| *Milk Fatty Acids (g/100 g Fat)* | |  |  |  |
| C4:0 | 3.32 | 0.251 | 2.59 | 4.13 |
| C5:0 | 0.03 | 0.009 | 0.01 | 0.06 |
| C6:0 | 2.18 | 0.213 | 1.50 | 2.54 |
| C7:0 | 0.02 | 0.007 | 0.00 | 0.04 |
| C8:0 | 1.28 | 0.203 | 0.62 | 1.61 |
| C9:0 | 0.03 | 0.010 | 0.00 | 0.06 |
| C10:0 | 2.85 | 0.593 | 1.11 | 4.04 |
| C10:1 | 0.31 | 0.069 | 0.11 | 0.45 |
| C11:0 | 0.04 | 0.018 | 0.01 | 0.11 |
| C12:0 | 3.32 | 0.731 | 1.22 | 4.90 |
| C12:1 | 0.09 | 0.028 | 0.02 | 0.15 |
| *Iso* C14:0 | 0.08 | 0.029 | 0.01 | 0.31 |
| C14:0 | 11.4 | 1.61 | 6.2 | 13.9 |
| *Iso* C15:0 | 0.22 | 0.038 | 0.12 | 0.29 |
| *Anteiso* C15:0 | 0.40 | 0.057 | 0.24 | 0.51 |
| C14:1 | 1.09 | 0.256 | 0.50 | 1.78 |
| C15:0 | 0.97 | 0.132 | 0.57 | 1.27 |
| *Iso* C16:0 | 0.21 | 0.038 | 0.09 | 0.29 |
| C16:0 | 36.3 | 5.35 | 28.9 | 54.0 |
| *Trans*-9 C16:1 | 0.06 | 0.016 | 0.02 | 0.10 |
| *Iso* C17:0 | 0.28 | 0.083 | 0.14 | 0.53 |
| *Cis*-7 C16:1 | 0.21 | 0.088 | 0.03 | 0.40 |
| *Cis*-9 C16:1 | 1.85 | 0.409 | 1.20 | 3.38 |
| *Anteiso* C17:0 | 0.40 | 0.057 | 0.22 | 0.58 |
| *Cis*-11 C16:1 | 0.04 | 0.014 | 0.01 | 0.13 |
| *Trans*-14 C16:1 | 0.03 | 0.018 | 0.01 | 0.10 |
| *Cis*-13 C16:1 | 0.19 | 0.090 | 0.01 | 0.52 |
| C17:0 | 0.55 | 0.117 | 0.25 | 0.83 |
| *Iso* C18:0 | 0.05 | 0.025 | 0.01 | 0.14 |
| *Cis*-9 C17:1 | 0.19 | 0.073 | 0.07 | 0.54 |
| C18:0 | 8.50 | 1.412 | 4.76 | 12.35 |
| *Trans*-6 + 7 + 8 C18:1 | 0.22 | 0.057 | 0.12 | 0.41 |
| *Trans*-9 C18:1 | 0.17 | 0.037 | 0.11 | 0.27 |
| *Trans*-10 C18:1 | 0.30 | 0.093 | 0.13 | 0.68 |
| *Trans*-11 C18:1 | 0.87 | 0.279 | 0.28 | 1.69 |
| *Trans*-12 C18:1 | 0.28 | 0.126 | 0.06 | 0.46 |
| *Trans*-13 C18:1 | 0.50 | 0.216 | 0.10 | 0.82 |
| *Cis*-9 C18:1 | 16.1 | 2.57 | 7.41 | 27.83 |
| *Trans*-15 C18:1 | 0.26 | 0.086 | 0.08 | 0.63 |
| *Cis*-11 C18:1 | 0.38 | 0.173 | 0.12 | 1.27 |
| *Cis*-12 C18:1 | 0.24 | 0.072 | 0.13 | 0.45 |
| *Cis*-13 C18:1 | 0.06 | 0.025 | 0.02 | 0.24 |
| *Cis*-14 + *trans*-16 C18:1 | 0.37 | 0.080 | 0.16 | 0.67 |
| *Cis*-15 C18:1 | 0.16 | 0.174 | 0.05 | 1.52 |
| *Trans*-11, *cis*-15 C18:2 | 0.09 | 0.062 | 0.03 | 0.58 |
| *n-6* C18:2 | 1.33 | 0.205 | 0.99 | 1.86 |
| *n-6* C18:3 + C20:0 | 0.12 | 0.036 | 0.01 | 0.18 |
| *n-3* C18:3 | 0.39 | 0.068 | 0.28 | 0.62 |
| *Cis*-9, *trans*-11 CLA | 0.42 | 0.127 | 0.16 | 0.80 |
| *n-6* C20:3 | 0.07 | 0.018 | 0.04 | 0.11 |
| *n-3* C20:3 | 0.15 | 0.264 | 0.01 | 1.30 |
| *n-6* C20:4 | 0.26 | 0.297 | 0.01 | 1.12 |
| *n-3* C20:5 | 0.05 | 0.022 | 0.01 | 0.11 |
| *n-6* C22:5 | 0.04 | 0.028 | 0.01 | 0.14 |
| *n-3* C22:5 | 0.08 | 0.055 | 0.01 | 0.26 |
| *n-3* C22:6 | 0.04 | 0.024 | 0.01 | 0.15 |

**Supplementary Table S2** Average milk fatty acid proportion (g/100 g fat) for observations classified into HIGH, MEDIUM or LOW CH4 emissions (g/d). Results presented only for those cases where statistical differences were found between the categories.

|  |  |  |  |
| --- | --- | --- | --- |
| Milk fatty  acid | Milk fatty acid proportions for categories according to daily CH4 (g/d) | | |
| HIGH | MEDIUM | LOW |
| C9:0 | 0.03a | 0.02b | 0.02b |
| C10:1 | 0.34a | 0.30b | 0.29b |
| C11:0 | 0.05a | 0.04a | 0.03b |
| C12:0 | 3.55a | 3.36ab | 3.03b |
| C12:1 | 0.10a | 0.08b | 0.07b |
| C16:0 | 38.9a | 35.8b | 34.5b |
| *Trans*-9 C16:1 | 0.04a | 0.05b | 0.06b |
| *Iso* C17:0 | 0.23a | 0.27ab | 0.31b |
| *Cis*-9 C16:1 | 2.07a | 1.81b | 1.72b |
| *Cis*-13 C16:1 | 0.18a | 0.15a | 0.25b |
| C17:0 | 0.49b | 0.58a | 0.54ab |
| *Iso* C18:0 | 0.02a | 0.05b | 0.06c |
| *Cis*-9 C17:1 | 0.12a | 0.19b | 0.23c |
| C18:0 | 7.61a | 8.57b | 9.13b |
| *Trans*-6 + 7 + 8 C18:1 | 0.19b | 0.23a | 0.22ab |
| *Trans*-9 C18:1 | 0.15b | 0.17a | 0.17ab |
| *Trans*-10 C18:1 | 0.25b | 0.31a | 0.30ab |
| *Trans*-11 C18:1 | 0.72a | 0.89b | 0.96b |
| *Trans*-12 C18:1 | 0.16a | 0.31b | 0.33b |
| *Trans*-13 C18:1 | 0.29a | 0.54b | 0.60b |
| *Cis*-9 C18:1 | 14.8a | 15.8a | 17.7b |
| *Trans*-15 C18:1 | 0.30a | 0.25b | 0.23b |
| *Cis*-11 C18:1 | 0.23a | 0.39b | 0.46b |
| *Cis*-12 C18:1 | 0.20a | 0.25b | 0.26b |
| *Cis*-13 C18:1 | 0.04a | 0.06b | 0.07c |
| *Cis*-14 + *trans*-16 C18:1 | 0.31a | 0.37b | 0.40b |
| *Trans*-11, *cis*-15 C18:2 | 0.05a | 0.07a | 0.13b |
| *n-6* C18:2 | 1.21b | 1.40a | 1.29b |
| *n-6* C18:3 + C20:0 | 0.10a | 0.11ab | 0.13b |
| *n-3* C18:3 | 0.35a | 0.39b | 0.41b |
| *Cis*-9, *trans*-11 CLA | 0.35a | 0.41a | 0.48b |
| *n-6* C20:3 | 0.05a | 0.07b | 0.07b |
| *n-3* C20:3 | 0.03b | 0.20a | 0.15ab |
| *n-6* C20:4 | 0.13b | 0.30a | 0.29ab |
| *n-6* C22:5 | 0.02b | 0.05a | 0.03b |
| *n-3* C22:5 | 0.11a | 0.06b | 0.07b |
| *n-3* C22:6 | 0.03ab | 0.04b | 0.02a |
| *SFA* | 74.5a | 72.3b | 70.5c |
| *UFA* | 24.8a | 27.0b | 29.0c |
| *MUFA* | 22.3a | 23.7a | 25.9b |
| *PUFA* | 2.53a | 3.20b | 3.16b |
| *Trans C18:1* | 2.10a | 2.73b | 2.84b |
| *Cis-C18:1* | 15.8a | 17.1a | 19.0b |

**Supplementary Table S3** Average milk fatty acid proportion (g/100 g fat) for observations classified into HIGH, MEDIUM or LOW CH4 emissions relative to dry matter intake (g/kg DMI). Results presented only for those cases where statistical differences were found between the categories.

|  |  |  |  |
| --- | --- | --- | --- |
| Milk fatty  acid | Milk fatty acid proportions for categories according to daily CH4 (g/kg DMI) | | |
| HIGH | MEDIUM | LOW |
| C6:0 | 2.07a | 2.19b | 2.21b |
| C8:0 | 1.18a | 1.29b | 1.31b |
| C14:0 | 10.1a | 11.7b | 11.9b |
| *Iso* C15:0 | 0.20b | 0.22a | 0.21ab |
| *Anteiso* C15:0 | 0.37b | 0.40a | 0.39ab |
| C14:1 | 1.00b | 1.14a | 1.07ab |
| *Iso* C16:0 | 0.18b | 0.21a | 0.20ab |
| C16:0 | 41.4a | 34.7b | 34.8b |
| *Trans*-9 C16:1 | 0.04b | 0.05a | 0.05ab |
| *Iso* C17:0 | 0.22a | 0.27b | 0.32c |
| *Cis*-7 C16:1 | 0.23a | 0.21a | 0.16b |
| *Cis*-9 C16:1 | 2.18a | 1.80b | 1.66b |
| *Anteiso* C17:0 | 0.35a | 0.41b | 0.40b |
| *Cis*-11 C16:1 | 0.02a | 0.03b | 0.03b |
| *Trans*-14 C16:1 | 0.03b | 0.02a | 0.02ab |
| *Cis*-13 C16:1 | 0.15b | 0.20a | 0.19ab |
| C17:0 | 0.43a | 0.56b | 0.63c |
| *Iso* C18:0 | 0.02a | 0.05b | 0.06b |
| *Cis*-9 C17:1 | 0.13a | 0.19b | 0.21b |
| C18:0 | 7.61a | 8.64b | 8.94b |
| *Trans*-11 C18:1 | 0.74b | 0.91a | 0.90ab |
| *Trans*-12 C18:1 | 0.17a | 0.30b | 0.33b |
| *Trans*-13 C18:1 | 0.31a | 0.52b | 0.61c |
| *Cis*-11 C18:1 | 0.27a | 0.39b | 0.42b |
| *Cis*-13 C18:1 | 0.04a | 0.06b | 0.06b |
| *Cis*-14 + *trans*-16 C18:1 | 0.32a | 0.37b | 0.38b |
| *Cis*-15 C18:1 | 0.29a | 0.12b | 0.12b |
| *n-6* C18:3 + C20:0 | 0.08a | 0.12b | 0.13b |
| *n-3* C18:3 | 0.35a | 0.39b | 0.42b |
| *Cis*-9, *trans*-11 CLA | 0.36b | 0.44a | 0.41ab |
| *n-6* C20:3 | 0.05a | 0.07b | 0.08c |
| *n-3* C20:3 | 0.01a | 0.16b | 0.22b |
| *n-6* C20:4 | 0.10a | 0.27b | 0.37b |
| *n-3* C20:5 | 0.05a | 0.05ab | 0.04b |
| *n-6* C22:5 | 0.02a | 0.04b | 0.05c |
| *n-3* C22:5 | 0.08ab | 0.08b | 0.05a |
| *n-3* C22:6 | 0.03ab | 0.03b | 0.04a |
| *SFA* | 74.4a | 71.5b | 72.3b |
| *UFA* | 25.2a | 27.6b | 27.2b |
| *MUFA* | 22.7b | 24.5a | 23.9ab |
| *PUFA* | 2.52a | 3.13b | 3.27b |
| *OBCFA* | 2.95a | 3.40b | 3.52b |
| *Trans C18:1* | 2.18a | 2.71b | 2.77b |

**Supplementary Table S4** Average milk fatty acid proportion (g/100 g fat) for observations classified into HIGH, MEDIUM or LOW CH4 emissions relative to milk yield (g/kg milk). Results presented only for those cases where statistical differences were found between the categories.

|  |  |  |  |
| --- | --- | --- | --- |
| Milk fatty  acid | Milk fatty acid proportions for categories according to daily CH4 (g/kg milk) | | |
| HIGH | MEDIUM | LOW |
| C4:0 | 3.23a | 3.30a | 3.43b |
| C6:0 | 2.09b | 2.21a | 2.16ab |
| C10:0 | 2.77ab | 2.97b | 2.65a |
| C14:0 | 10.7b | 11.8a | 11.3ab |
| C16:0 | 39.3a | 35.2b | 35.5b |
| *Cis*-9 C16:1 | 2.11a | 1.74b | 1.82b |
| *Anteiso* C17:0 | 0.37a | 0.40b | 0.42b |
| *Trans*-14 C16:1 | 0.03a | 0.02b | 0.02b |
| C17:0 | 0.49b | 0.58a | 0.54ab |
| *Cis*-9 C17:1 | 0.15a | 0.19b | 0.19b |
| *Trans*-13 C18:1 | 0.42b | 0.54a | 0.49ab |
| *Cis*-9 C18:1 | 15.0a | 16.1ab | 17.1b |
| *Cis*-13 C18:1 | 0.04a | 0.06b | 0.07b |
| *Cis*-15 C18:1 | 0.25a | 0.13b | 0.13b |
| *Trans*-11, *cis*-15 C18:2 | 0.06a | 0.08ab | 0.10b |
| *n-6* C18:3 + C20:0 | 0.10a | 0.12b | 0.12b |
| *n-3* C18:3 | 0.36b | 0.40a | 0.39ab |
| *n-6* C22:5 | 0.03ab | 0.04b | 0.03a |
| *n-3* C22:5 | 0.05a | 0.08ab | 0.09b |
| *n-3* C22:6 | 0.04a | 0.03ab | 0.02b |
| *SFA* | 73.9a | 72.2b | 71.3b |
| *UFA* | 25.7a | 27.0ab | 28.1b |
| *MUFA* | 22.8a | 23.9ab | 25.0b |
| *OBCFA* | 3.14b | 3.40a | 3.37ab |
| *Cis-C18:1* | 16.2a | 17.3ab | 18.3b |

**Supplementary Table S5** Average Gini coefficients for observations classified into HIGH, MEDIUM or LOW CH4 emissions relative to dry matter intake (g/kg DMI) and milk yield (g/kg milk). Results presented only for those cases where statistical differences were found between the categories.

|  |  |  |  |
| --- | --- | --- | --- |
| CH4 (g/kg DMI) | | | |
| Group | HIGH | MEDIUM | LOW |
| All MFA | 0.86a | 0.85b | 0.84b |
| SFA | 0.81a | 0.79b | 0.79b |
| UFA | 0.82a | 0.81b | 0.80b |
| PUFA | 0.69a | 0.67b | 0.65c |
| OBCFA | 0.41a | 0.40b | 0.39b |
| MFA < 0.2 g/100 g Fat | 0.50a | 0.47b | 0.44c |
| MFA > 1 g/100 g Fat | 0.61a | 0.57b | 0.58b |
| CH4 (g/kg Milk) | | | |
|  | HIGH | MEDIUM | LOW |
| All MFA | 0.86b | 0.85a | 0.85ab |
| SFA | 0.80b | 0.79a | 0.80ab |
| MFA > 1 g/100 g Fat | 0.59b | 0.58a | 0.58ab |