

Article

Milk Metabolomics Reveals Potential Biomarkers for Early Prediction of Pregnancy in Buffaloes Having Undergone Artificial Insemination

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SUPPLEMENTARY MATERIALS

Table 1. Secondary metabolites differentially expressed in pregnant and non-pregnant buffaloes at D10 (Figure 2 A).

Table 2. Secondary metabolites differentially expressed in pregnant and non-pregnant buffaloes at D0 (Figure 2B).

Table 3. Secondary metabolites differentially expressed in pregnant and non-pregnant buffaloes at D7 (Figure 2C).

Table 4. Secondary metabolites differentially expressed in pregnant and non-pregnant buffaloes at D18 (Figure 2D).

Table 1. Secondary metabolites differentially expressed in pregnant and non-pregnant buffaloes at D10 (Figure 2A).

Compound	Mass
Acetyl carnitine (3-Acetoxy-4-(trimethylammonio)butanoate)	203.1147
C ₈ H ₂₁ N ₅ O	203.1738
C ₁₇ H ₃₇ N O ₂	287.2821
C ₁₄ H ₁₆ N ₆ O ₂	300.1325
C ₁₇ H ₂₆ O ₅	310.1766
C ₁₉ H ₃₄ O ₃	310.2505
C ₁₅ H ₂₄ N ₇ O ₃	350.1935
C ₁₂ H ₂₂ O ₁₁	364.0980
C ₁₄ H ₂₈ N ₄ O ₅ S	364.1771
Arginine - succinic acid hydrate	364.1805
C ₁₃ H ₁₂ N ₆ O ₈	380.0715
C ₁₁ H ₂₂ N ₇ O ₈	380.1534
C ₁₅ H ₁₆ N ₃ O ₇ S	382.0708
C ₁₂ H ₂₈ C ₁₂ N ₈ O ₂	386.1709
C ₁₉ H ₃₈ N ₄ S ₂	386.2539
C ₁₆ H ₄₀ N ₅ O ₆	398.2991
C ₁₉ H ₃₈ N ₆ O ₃	398.2992
C ₁₉ H ₄₀ N ₉ O ₃	442.3250
C ₂₁ H ₄₂ N ₆ O ₄	442.3253

C ₂₄ H ₅₂ N ₅ O ₂	442.4121
C ₂₂ H ₄₄ N ₆ O ₄	456.3406
C ₂₀ H ₄₂ N ₉ O ₃	456.3410
C ₂₃ H ₅₂ N ₈ O	456.4295
C ₂₅ H ₄₁ N ₃ O ₆	479.2992
C ₁₈ H ₄₇ N ₁₂ O ₃	479.3898
C ₂₁ H ₅₁ N ₇ O ₅	481.3958
C ₂₄ H ₄₉ N ₈ O ₂	481.3959
N-(1-Hydroxy-2-hexadecanyl) pentadecanamide	481.4858
C ₂₀ H ₄₈ N ₅ O ₈	486.3515
C ₂₆ H ₅₈ N ₆ S	486.4432
C ₂₆ H ₄₅ N ₃ O ₆	495.3304
C ₂₂ H ₄₉ N ₁₃	495.4231
C ₂₉ H ₆₃ N ₆ O	511.5001
C ₂₆ H ₄₅ N ₆ O ₅	521.3458
C ₃₀ H ₅₇ N ₄ O ₃	521.4408
C ₂₂ H ₄₉ N ₁₄ O	525.4215
C ₂₆ H ₅₃ N ₈ O ₃	525.4215
C ₂₃ H ₅₅ N ₇ O ₆	525.4220
C ₃₃ H ₆₉ N ₂ S	525.5197
C ₂₂ H ₅₂ N ₅ O ₉	530.3771
C ₂₇ H ₆₀ N ₇ O ₃	530.4744
C ₃₁ H ₆₇ N ₆ O	539.5337
C ₃₄ H ₇₁ N ₂ S	539.5339
C ₃₁ H ₆₇ N ₆ O ₂	555.5318
C ₁₇ H ₃₇ N ₇ O ₁₄	563.2401
C ₂₃ H ₄₇ N ₈ O ₈	563.3520
C ₂₄ H ₄₆ N ₃ O ₁₂	568.3074
C ₂₄ H ₅₃ N ₁₄ O ₂	569.4473
C ₂₈ H ₅₇ N ₈ O ₄	569.4474
C ₃₂ H ₆₉ N ₆ O ₂	569.5490
C ₂₄ H ₅₆ N ₅ O ₁₀	574.4028
C ₂₄ H ₄₆ N ₁₆ O	574.4029
C ₃₃ H ₇₁ N ₆ O ₂	583.5639
C ₃₅ H ₇₃ N ₃ O ₃	583.5643
C ₂₇ H ₅₀ N ₄ O ₁₀	590.3523
C ₃₃ H ₇₁ N ₆ O ₃	599.5608
C ₁₈ H ₃₉ N ₈ O ₁₅	607.2523
C ₂₇ H ₅₃ N ₅ O ₁₀	607.3786
C ₂₈ H ₅₉ N ₁₁ O ₄	613.4737
C ₃₈ H ₇₇ O ₅	613.5773
C ₃₉ H ₇₃ N ₄ O	613.5773
C ₂₅ H ₅₄ N ₁₂ O ₆	618.4295
C ₂₀ H ₃₇ N ₁₃ O ₁₂	651.2650
C ₂₉ H ₅₇ N ₅ O ₁₁	651.4045
C ₂₈ H ₅₄ N ₃ O ₁₄	656.3609
C ₄₀ H ₈₃ N ₃ O ₃ S	657.6069
C ₃₈ H ₈₁ N ₄ O ₂ S	657.6074
C ₃₀ H ₅₅ N ₁₂ O ₇	695.4308
C ₃₉ H ₈₃ N ₅ O ₅	701.6356
C ₂₂ H ₃₈ N ₆ O ₂₀	706.2141
C ₂₅ H ₅₀ N ₆ O ₁₇	706.3231
*	223.6216
*	330.3534
*	495.5052
*	627.5956
*	643.5908
*	1990.5967

*	2235.7114
*	3980.1743
*	4481.3916

*compounds for which the Software Mass Profile Professional, version 13.1.1 (Agilent Technologies) did not generate the molecular formula.

Table 2. Secondary metabolites differentially expressed in pregnant and non-pregnant buffaloes at D0 (Figure 2B).

Compound	Mass
C ₆ H ₉ N ₃	123.0782
Acetyl carnitine (3-Acetoxy-4-(trimethylammonio)butanoate)	203.1147
C ₁₇ H ₃₂ N ₃ O ₂	310.2493
C ₉ H ₂₀ N ₂ O ₁₃	364.0957
C ₁₀ H ₂₄ N ₁₀ O ₃ S	364.1758
Arginine-succinic acid hydrate	364.1805
C ₁₇ H ₄₀ N ₆ O ₃	376.3151
C ₁₁ H ₁₀ N ₉ O ₇	380.0693
C ₁₃ H ₁₂ N ₆ O ₈	380.0719
C ₁₀ H ₂₆ N ₃ O ₁₂	380.1504
C ₂₀ H ₄₃ N ₁₁	437.3671
C ₂₂ H ₅₀ N ₈ O	442.4115
C ₂₀ H ₄₉ N ₇ O ₄	451.3837
C ₂₁ H ₄₅ N ₁₁ O	467.3785
5'-O-[[3-((4-[(3 Aminopropyl)amino]butyl)amino)propyl]carbamoyl]-2'-deoxyadenosine	479.2967
C ₂₀ H ₄₅ N ₁₄	481.3939
N-(1-Hydroxy-2-hexadecanyl)pentadecanamide	481.4858
C ₂₁ H ₄₇ N ₁₄	495.4089
C ₂₂ H ₄₉ N ₁₃	495.4216
C ₂₃ H ₄₉ N ₁₁ O ₂	511.4033
C ₁₉ H ₄₁ N ₁₁ O ₆	519.3266
C ₂₄ H ₅₁ N ₁₁ O ₂	525.4192
C ₃₆ H ₆₅ N ₂	525.5159
C ₃₀ H ₆₄ N ₃ O ₂ S	530.4711
C ₂₃ H ₅₁ N ₁₄ O	539.4344
C ₃₄ H ₇₁ N ₂ S	539.5324
C ₂₃ H ₅₁ N ₁₄ O ₂	555.4318
C ₂₀ H ₃₉ N ₁₈ O ₂	563.3533
C ₂₄ H ₅₃ N ₁₄ O ₂	569.4462
C ₃₂ H ₆₉ N ₆ O ₂	569.5454
C ₂₉ H ₆₄ N ₇ O ₄	574.5012
C ₂₅ H ₅₅ N ₁₄ O ₂	583.4629
C ₃₃ H ₇₁ N ₆ O ₂	583.5625
C ₃₅ H ₇₃ N ₃ O ₃	583.5650
C ₂₇ H ₅₇ N ₁₁ O ₄	599.4550
C ₁₈ H ₃₉ N ₈ O ₁₅	607.2532
C ₂₃ H ₄₉ N ₁₁ O ₈	607.3793
C ₂₈ H ₅₉ N ₁₁ O ₄	613.4725
C ₃₈ H ₇₇ O ₅	613.5751
C ₃₈ H ₇₉ N O ₂ S	613.5784
C ₂₇ H ₅₉ N ₁₄ O ₃	627.4862
C ₂₅ H ₅₇ N ₁₇ O ₃	643.4808
C ₂₄ H ₄₇ N ₁₈ O ₄	651.3994
C ₃₈ H ₈₁ N ₄ O ₂ S	657.6049
C ₄₁ H ₇₇ N ₄ O ₂	657.6049
C ₃₇ H ₇₉ N ₅ O ₄	657.6083
C ₂₇ H ₆₁ N ₁₇ O ₃	671.5122
C ₂₉ H ₆₃ N ₁₄ O ₅	687.5060

C ₂₆ H ₅₁ N ₁₈ O ₅	695.4307
C ₂₉ H ₅₉ N ₂₁	701.5234
C ₂₂ H ₃₈ N ₆ O ₂₀	706.2102
C ₃₀ H ₆₁ N ₂₁ O	731.5362
C ₂₉ H ₆₁ N ₂₄	745.5504
*	223.6216
*	330.3534
*	495.5026
*	495.5052
*	511.5008
*	555.5285
*	599.5585
*	627.5956
*	643.5908
*	662.4501
*	687.5083
*	695.4313
*	706.3176
*	1226.4552

*compounds for which the Software Mass Profile Professional. version 13.1.1 (Agilent Technologies) did not generate the molecular formula.

Table 3. Secondary metabolites differentially expressed in pregnant and non-pregnant buffaloes at D7 (Figure 2C).

Compound	Mass
C ₆ H ₉ N ₃	123.0783
Acetyl carnitine (3-Acetoxy-4-(trimethylammonio)butanoate)	203.1147
C ₈ H ₂₁ N ₅ O	203.1727
C ₁₃ H ₂₂ N ₆ O ₃	310.1753
C ₉ H ₃₀ N ₁₀ O ₂	310.2489
C ₁₉ H ₄₄ N ₃ O	330.3508
C ₂₀ H ₄₁ N ₄	337.3304
C ₉ H ₂₀ N ₂ O ₁₃	364.0954
C ₁₆ H ₂₈ O ₉	364.1734
C ₁₀ H ₂₄ N ₁₀ O ₃ S	364.1754
C ₁₀ H ₁₄ N ₅ O ₁₁	380.0683
C ₁₀ H ₂₆ N ₃ O ₁₂	380.1499
C ₁₇ H ₄₅ N ₁₀ O ₃	437.3670
C ₁₆ H ₄₂ N ₈ O ₆	442.3218
C ₁₅ H ₃₆ N ₁₅ O	442.3228
C ₂₂ H ₅₀ N ₈ O	442.4096
C ₃₁ H ₅₄ O	442.4104
C ₁₈ H ₄₇ N ₁₀ O ₃	451.3824
C ₁₆ H ₃₈ N ₁₅ O	456.3382
C ₂₃ H ₅₂ N ₈ O	456.4279
C ₂₅ H ₅₄ N ₅ O ₂	456.4280
C ₂₀ H ₃₉ N ₅ O ₈	477.2810
5'-O-[[3-((4-[(3-Aminopropyl)amino]butyl)amino)propyl]carbonyl]-2'-deoxyadenosine	479.2967
C ₁₈ H ₄₉ N ₁₃ S	479.3872
C ₁₇ H ₄₇ N ₁₃ O ₃	481.3935
C ₁₉ H ₄₉ N ₁₀ O ₄	481.3935
C ₂₉ H ₆₁ N ₄ O	481.4842
C ₂₈ H ₆₁ N ₆	481.4844
C ₁₇ H ₄₀ N ₁₅ O ₂	486.3482
C ₂₉ H ₅₄ N ₆	486.4402
C ₂₃ H ₅₄ N ₁₀ O	486.4405
C ₁₈ H ₄₉ N ₁₃ O ₃	495.4087

C ₂₇ H ₅₅ N ₆ S	495.4202
C ₂₉ H ₆₃ N ₆	495.5015
C ₁₉ H ₄₈ N ₈ O ₇	500.3634
C ₁₇ H ₄₆ N ₁₁ O ₆	500.3636
C ₁₈ H ₄₉ N ₁₃ O ₄	511.4030
C ₂₉ H ₆₃ N ₆ O	511.4984
C ₃₃ H ₅₅ N ₅	521.4381
C ₂₀ H ₄₇ N ₁₇	525.4192
C ₃₂ H ₆₇ N ₃ O ₂	525.5143
C ₃₆ H ₆₅ N ₂	525.5145
C ₃₄ H ₆₉ O ₃	525.5147
C ₁₇ H ₄₂ N ₁₈ O ₂	530.3744
C ₃₀ H ₆₄ N ₃ O ₂ S	530.4711
C ₂₁ H ₄₉ N ₁₇	539.4334
C ₃₅ H ₇₁ O ₃	539.5312
C ₁₉ H ₅₀ N ₁₁ O ₇	544.3885
C ₁₉ H ₄₇ N ₂₀	555.4282
C ₃₈ H ₆₉ N ₀	555.5342
C ₂₀ H ₄₉ N ₂₀	569.4451
C ₃₂ H ₆₉ N ₆ O ₂	569.5444
C ₃₄ H ₇₃ N ₄ S	569.5519
C ₂₁ H ₅₁ N ₂₀	583.4593
C ₃₅ H ₇₅ N ₄ S	583.5607
C ₂₀ H ₄₈ N ₁₈ O ₃	588.4149
C ₂₁ H ₅₁ N ₂₀ O	599.4550
C ₁₉ H ₂₅ N ₂₃ O ₂	607.2541
C ₂₂ H ₅₃ N ₂₀ O	613.4705
C ₃₄ H ₇₃ N ₆ O ₃	613.5733
C ₃₅ H ₇₅ N ₅ O ₃	613.5754
C ₂₃ H ₅₅ N ₂₀ O	627.4847
C ₂₁ H ₅₃ N ₂₃ O	643.4803
C ₂₀ H ₅₃ N ₂₆	657.4966
C ₄₀ H ₇₇ N ₆ O	657.6028
C ₄₁ H ₇₇ N ₄ O ₂	657.6042
C ₂₁ H ₅₂ N ₂₁ O ₄	662.4512
C ₂₈ H ₆₃ N ₁₇ O ₄	701.5216
C ₂₆ H ₃₆ N ₅ O ₁₈	706.2067
C ₂₈ H ₃₈ N ₂ O ₁₉	706.2090
C ₂₁ H ₄₆ N ₁₂ O ₁₅	706.3182
C ₄₂ H ₇₃ N ₄ O ₇	745.5475
*	495.5050
*	563.3520
*	574.5010
*	607.3780
*	364.0976
*	398.1677
*	398.2968
*	398.3796
*	398.3831
*	467.3766
*	467.4712
*	495.3272
*	495.5054
*	519.3253
*	530.4747
*	544.3891
*	583.5621
*	618.4254

*	618.5341
*	627.5951
*	643.5914
*	662.4501
*	687.5083
*	695.4313
*	706.3176
*	1226.4552
*	2235.7092
*	2236.2046
*	2236.5254
*	3980.1887
*	3980.7107

*compounds for which the Software Mass Profile Professional. version 13.1.1 (Agilent Technologies) did not generate the molecular formula.

Table 4. Secondary metabolites differentially expressed in pregnant and non-pregnant buffaloes at D18 (Figure 2D).

Compound	Mass
C ₆ H ₉ N ₃	123.0791
Acetyl carnitine (3-Acetoxy-4-(trimethylammonio)butanoate)	203.1147
C ₁₇ H ₃₇ N O ₂	287.2828
C ₁₇ H ₂₆ O ₅	310.1774
C ₁₇ H ₃₂ N ₃ O ₂	310.2518
C ₁₇ H ₃₆ N ₃ O ₃	330.2766
C ₂₂ H ₄₃ N O	337.3339
C ₉ H ₂₀ N ₂ O ₁₃	364.0982
C ₁₄ H ₂₈ N ₄ O ₅ S	364.1771
C ₁₈ H ₁₀ N ₈ O ₂	370.0932
C ₁₉ H ₄₂ N ₃ O ₄	376.3191
C ₁₃ H ₂₄ N ₄ O ₉	380.1535
C ₁₈ H ₄₀ N ₂ O ₆	380.2886
C ₁₅ H ₃₈ C ₁₂ N ₇	386.2559
C ₁₈ H ₃₈ N ₂ O ₇	394.2677
C ₁₇ H ₄₄ N ₇ O ₃	394.3516
C ₂₁ H ₄₉ N ₄ O ₅	437.372
C ₂₀ H ₄₆ N ₂ O ₈	442.3271
C ₂₅ H ₅₄ N ₅ O ₂	456.4307
C ₁₈ H ₃₉ N ₉ O ₄ S	477.2844
C ₁₈ H ₄₁ N ₉ O ₄ S	479.3005
C ₂₅ H ₄₉ N ₇ O ₂	479.3916
C ₁₈ H ₄₉ N ₁₃ S	479.3944
C ₁₈ H ₄₃ N ₉ O ₄ S	481.3161
C ₂₃ H ₅₃ N ₄ O ₆	481.3979
C ₂₈ H ₆₁ N ₆	481.4879
C ₁₆ H ₄₆ N ₁₂ O ₃ S	486.3516
C ₂₁ H ₅₂ N ₁₃	486.4438
C ₂₆ H ₅₈ N ₆ S	486.4444
C ₁₄ H ₃₉ N ₁₆ O ₄	495.3321
C ₂₄ H ₅₁ N ₁₀ O	495.4251
C ₂₉ H ₆₃ N ₆ O	511.5022
C ₂₁ H ₅₃ N ₁₃ S	519.4268
C ₂₈ H ₄₇ N ₃ O ₆	521.3475
C ₃₀ H ₅₇ N ₄ O ₃	521.4437
C ₂₄ H ₅₁ N ₁₁ O ₂	525.4229
C ₃₀ H ₆₅ N ₆ O	525.5183
C ₃₁ H ₆₇ N ₆ O	539.5352

N-[2.3-Bis(dodecyloxy)propyl]-L-lysineamide	555.5336
C ₁₈ H ₁₉ N ₁₄ O ₈	559.1506
C ₁₇ H ₃₉ N ₁₀ O ₉ S	559.2625
C ₁₇ H ₃₇ N ₇ O ₁₄	563.2392
C ₂₁ H ₄₅ N ₁₁ O ₇	563.3516
C ₂₆ H ₅₅ N ₁₁ O ₃	569.4496
C ₃₆ H ₇₃ O ₄	569.5513
C ₃₃ H ₆₈ N O ₆	574.5065
C ₃₂ H ₆₂ N ₈ O	574.5068
C ₃₅ H ₇₃ N ₃ O ₃	583.5650
C ₃₅ H ₇₅ N ₄ O S	599.5656
C ₁₈ H ₃₉ N ₈ O ₁₅	607.2532
C ₁₈ H ₃₉ N ₈ O ₁₅	607.2532
C ₂₃ H ₄₉ N ₁₁ O ₈	607.3776
C ₂₉ H ₆₅ N ₄ O ₉	613.4761
C ₃₈ H ₇₉ N O ₂ S	613.5826
C ₁₉ H ₄₁ N ₉ O ₁₆	651.2666
C ₃₀ H ₆₃ N ₁₁ O ₅	657.5014
C ₃₇ H ₇₉ N ₅ O ₄	657.6136
C ₃₉ H ₈₅ N ₆ O ₂ S	701.6413
C ₂₈ H ₃₈ N ₂ O ₁₉	706.209
C ₂₂ H ₃₈ N ₆ O ₂₀	706.2128
C ₂₅ H ₅₀ N ₆ O ₁₇	706.3273
C ₃₅ H ₇₇ N ₄ O ₁₂	745.5547
C ₁₂ H ₁₈ N ₃	364.0992
*	495.5051
C ₁₃ H ₁₂ N ₆	380.0719
*	398.3831
C ₂₉ H ₅₂ N ₃	442.4143
*	467.4712
C ₂₅ H ₄₁ N ₃	479.3007
*	495.5054
C ₃₀ H ₅₇ N ₄	521.4437
*	530.4747
C ₁₇ H ₃₇ N ₇	563.2392
*	618.5341
*	627.5951
*	643.5914
C ₂₆ H ₅₉ N ₄	651.4025
*	2235.7092
*	2236.2046
*	3980.1887
*	3980.7107

*compounds for which the Software Mass Profile Professional. version 13.1.1 (Agilent Technologies) did not generate the molecular formula.