

Qualitative Summary Report

Lab Name:

Instrument:

User:

Batch:

Plant Sciences  
Thermo Scientific Instrument  
ISQ140326  
snow\_batch2\_4ml

Method:

Call File:

snow\_batch2\_4ml\_GCMS\_FAME\_METABOLOMICS  
GCMS\_FAME\_METABOLOMICS  
snow\_batch2\_4ml.calx

| <u>Vial Pos</u> | <u>Sample ID</u> | <u>File Name</u> | <u>Level</u> | <u>Sample Name</u> | <u>File Date</u>     | <u>Comment</u> |
|-----------------|------------------|------------------|--------------|--------------------|----------------------|----------------|
| 13              | Site_9_a_Red     | Site_9_a_Red     | N/A          | Site_9_a_Red       | 10/6/2015 3:16:50 AM |                |

Internal Standards

| Internal Standard | ISTD# | RT | Response | Injected |       | Sample |       |
|-------------------|-------|----|----------|----------|-------|--------|-------|
|                   |       |    |          | Conc     | Units | Conc   | Units |



Qualitative Summary Report

|             |                              |            |  |
|-------------|------------------------------|------------|--|
| Lab Name:   | Plant Sciences               |            |  |
| Instrument: | Thermo Scientific Instrument | Method:    | snow_batch2_4ml_GCMS_FAME_METABOLOMICS |
| User:       | ISQ140326                    |            | GCMS_FAME_METABOLOMICS                 |
| Batch:      | snow_batch2_4ml              | Call File: | snow_batch2_4ml.calx                   |

Qualitatively-identified Compounds

| Compound   | Uses ISTD# | RT    | Response    | Injected |       | Sample |       | Flag |
|--|------------|-------|-------------|----------|-------|--------|-------|------|
|  |            |       |             | Conc     | Units | Conc   | Units |      |
| Tris(trimethylsilyl)borate   |            | 4.27  | 24992969633 | 0.000    |       | 0.000  |       |      |
| Pyridine, 3-trimethylsiloxy-   |            | 4.85  | 1985822012  | 0.000    |       | 0.000  |       |      |
| Acetamide, 2,2,2-trifluoro-N-methyl-N-(trimethylsilyl)-                    |            | 5.11  | 3268923470  | 0.000    |       | 0.000  |       |      |
| Hexanoic acid, trimethylsilyl ester  |            | 5.23  | 988995977   | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_LJALD_1099.5_2236BG34_L-Alanine (2TMS)                         |            | 5.65  | 4604700813  | 0.000    |       | 0.000  |       |      |
| Tris(trimethylsilyl)hydroxylamine  |            | 5.82  | 11026896484 | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_NID1_1139.3_1267BK12_[NA]                                      |            | 6.12  | 9511276755  | 0.000    |       | 0.000  |       |      |
| Pentasiloxane, dodecamethyl-   |            | 6.56  | 2490322324  | 0.000    |       | 0.000  |       |      |
| EITTMS_N12C_ATHR_1436.4_1135EC44_  |            | 7.06  | 2186395497  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_SD1_1256.5_3035BB03_Urea (2TMS)                                |            | 7.42  | 13274778795 | 0.000    |       | 0.000  |       |      |
| Carbamic acid,(trimethylsilyl)[(trimethylsilyl)oxy] trimethylsilyl ester   |            | 7.57  | 3191649690  | 0.000    |       | 0.000  |       |      |
| Octanoic acid, trimethylsilyl ester  |            | 7.79  | 1273661264  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_LJARL_1284.6_2236BN14_Glycerol (3TMS)                          |            | 8.08  | 23207444494 | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_LJALM_1304.1_2236BN40_L-Proline (2TMS)                         |            | 8.45  | 3658478911  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_ATHL_1310.2_3161BN21_Glycine (3TMS)                            |            | 8.63  | 1847384547  | 0.000    |       | 0.000  |       |      |
| Cyclohexasiloxane, dodecamethyl-   |            | 8.75  | 382940755   | 0.000    |       | 0.000  |       |      |
| EITTMS_N12C_ATHR_1358.9_1135EC06_  |            | 9.10  | 1258009833  | 0.000    |       | 0.000  |       |      |
| 5-Keto-2,2-dimethylheptanoic acid, ethyl(ester)                            |            | 9.42  | 7567812992  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_ATHL_1367.4_3161BN33_L-Serine (3TMS)                           |            | 9.59  | 2105800860  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_LJAF_1394.7_2236BN50_L-Threonine (3TMS)                        |            | 10.10 | 971151554   | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_LJAF_1431.9_2236BN50_beta-Alanine (3TMS)                       |            | 10.79 | 235037678   | 0.000    |       | 0.000  |       |      |
| Glycine, N-[α-[(tert-butyl)dimethylsilyl]oxy]benzylidene]-, tert-butylidin |            | 11.46 | 617463778   | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_ATHL_1491.4_3161BN27_Malic acid (3TMS)                         |            | 12.07 | 2178153761  | 0.000    |       | 0.000  |       |      |
| 3,6,9,12-Tetraoxa-2,13-disilatetradecane, 2,2,13,13-tetramethyl-           |            | 12.25 | 289225230   | 0.000    |       | 0.000  |       |      |
| (Trimethylsilyl)methyl octanoate   |            | 12.39 | 3230230779  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_LJARP_1527.6_2236BN20_Pyroglutamic acid (2TMS)                 |            | 12.66 | 8081437825  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_SD1_1567.6_3196BU28_Threonic acid (4TMS)                       |            | 13.71 | 2042073985  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_ATHL_1630.5_3161BN27_L-Glutamic acid (3TMS)                    |            | 14.74 | 6833663428  | 0.000    |       | 0.000  |       |      |
| Dodecanoic acid, trimethylsilyl ester                                      |            | 15.15 | 562604943   | 0.000    |       | 0.000  |       |      |
| EITTMS_N12C_SD2_1681.5_1179EK03_L-Asparagine (3TMS)                        |            | 15.81 | 194605161   | 0.000    |       | 0.000  |       |      |
| EITTMS_N12C_STUL_1681.2_1135EC28_Ribose methoxyamine (4TMS)                |            | 16.26 | 263425697   | 0.000    |       | 0.000  |       |      |
| 2-[1-[2-(tert-Butyl-dimethyl-siloxy)methyl]-pyrrolidino]ethyl]-5-phenyl-   |            | 16.65 | 640769063   | 0.000    |       | 0.000  |       |      |
| EITTMS_N12C_SD1_1886.0_1344EC16_2-Ketogluconic acid methyl ester           |            | 16.82 | 299036926   | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_SD1_1716.4_3196BU17_Xylitol (5TMS)                             |            | 17.14 | 2603921280  | 0.000    |       | 0.000  |       |      |
| EITTMS_N12C_SD1_1862.2_2011EC39_2-Keto-L-gulonic acid methyl ester         |            | 17.36 | 573864390   | 0.000    |       | 0.000  |       |      |
| 5,8,11,14-Eicosatetraynoic acid, trimethylsilyl ester                      |            | 17.58 | 587746537   | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_ATHL_1784.8_3038BN18_L-Glutamine (3TMS)                        |            | 17.88 | 4033403861  | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_OARPLAS_1827.4_3350DF05_Citric acid (4TMS)                     |            | 19.02 | 10626369468 | 0.000    |       | 0.000  |       |      |
| N-Acetyl glucosamine methoxime, tetrakis(trimethylsilyl)                   |            | 19.37 | 553299468   | 0.000    |       | 0.000  |       |      |
| EIQTMS_N12C_SD1_1878.2_3035BB03_Sorbose methoxyamine (4TMS)                |            | 20.30 | 1422416885  | 0.000    |       | 0.000  |       |      |
| EITTMS_N12C_NTAR_2690.8_1135EC08_Lactose methoxyamine (4TMS)               |            | 20.61 | 3468037413  | 0.000    |       | 0.000  |       |      |

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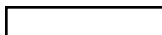
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**Lab Name:** Plant Sciences  
**Instrument:** Thermo Scientific Instrument  
**User:** ISQ140326  
**Batch:** snow\_batch2\_4ml

**Method:** snow\_batch2\_4ml\_GCMS\_FAME\_METABOLOMICS  
GCMS\_FAME\_METABOLOMICS  
**Call File:** snow\_batch2\_4ml.calx

|  |       |             |       |       |
|--|-------|-------------|-------|-------|
| d-Glucose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxyme, (1   | 20.79 | 4307276600  | 0.000 | 0.000 |
| EITTMS_N12C_SD2_1889.9_1135EC00_Glucose methoxyamine (5                | 21.09 | 2157397570  | 0.000 | 0.000 |
| D-Mannitol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-                    | 21.42 | 8361945175  | 0.000 | 0.000 |
| D-Mannitol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-                    | 21.56 | 328831142   | 0.000 | 0.000 |
| EITTMS_N12C_SD2_1728.8_1164EK02_Ribitol (5TMS)                         | 21.66 | 1761505843  | 0.000 | 0.000 |
| α-D-Galactopyranoside, methyl 2,3-bis-O-(trimethylsilyl)-, cyclic met  | 22.26 | 1334176668  | 0.000 | 0.000 |
| EITTMS_N12C_STUF_1968.0_1135EC32_G                                     | 22.37 | 204788873   | 0.000 | 0.000 |
| EIQTMS_N12C_LJAF_2051.5_2236BN50_Hexadecanoic acid (1TM                | 22.89 | 17533098540 | 0.000 | 0.000 |
| EITTMS_N12C_ATHR_2027.2_1135EC44_                                      | 23.29 | 474146826   | 0.000 | 0.000 |
| EITTMS_N12C_SD1_2089.0_1288EC05_Allantoin (3TMS)                       | 23.71 | 2244945976  | 0.000 | 0.000 |
| α-D-Glucopyranoside, methyl 2-(acetylamino)-2-deoxy-3-O-(trimeth       | 23.99 | 132025130   | 0.000 | 0.000 |
| α-D-Glucopyranoside, methyl 2-(acetylamino)-2-deoxy-3-O-(trimeth       | 24.20 | 232701439   | 0.000 | 0.000 |
| EIQTMS_N12C_SD1_2111.3_1325BK16_Uric acid (4TMS)                       | 24.44 | 4272334819  | 0.000 | 0.000 |
| Heptadecanoic acid, trimethylsilyl ester                               | 24.66 | 233568323   | 0.000 | 0.000 |
| trans-9-Octadecenoic acid, trimethylsilyl ester                        | 25.94 | 3050857258  | 0.000 | 0.000 |
| EIQTMS_N12C_SCA_2246.9_3147BF23-Octadecanoic acid (1TMS                | 26.37 | 12541367562 | 0.000 | 0.000 |
| EITTMS_N12C_ATHL_2309.5_1135EC24_[Galactosylglycerol (6TM              | 27.42 | 846852532   | 0.000 | 0.000 |
| EITTMS_N12C_ATHL_3035.3_1135EC05_[952; Sucrose (8TMS)]                 | 27.64 | 12148141071 | 0.000 | 0.000 |
| EITTMS_N12C_ATHL_2309.5_1135EC24_[Galactosylglycerol (6TM              | 27.74 | 334403736   | 0.000 | 0.000 |
| EITTMS_N12C_SD1_2322.8_1344EC17_Galactose-6-phosphate m                | 28.01 | 404469096   | 0.000 | 0.000 |
| Oleamide, N-trimethylsilyl-  | 28.19 | 5457764053  | 0.000 | 0.000 |
| α-D-Galactopyranose, 6-O-(trimethylsilyl)-, cyclic 1,2:3,4-bis(butylbc | 28.41 | 179800117   | 0.000 | 0.000 |
| EITTMS_N12C_SD1_2640.8_1194EK21_Sucrose (8TMS); alpha-D                | 29.16 | 8459331475  | 0.000 | 0.000 |
| EIQTMS_N12C_ATHL_2651.2_3161BN21_Sucrose (8TMS); alpha-                | 30.02 | 42244822653 | 0.000 | 0.000 |
| 4β-Methylandrosterane2,3-diol-1,17-dione                               | 31.07 | 3931401473  | 0.000 | 0.000 |
| β-D-Galactopyranoside, methyl 2,3-bis-O-(trimethylsilyl)-, cyclic met  | 31.62 | 239441589   | 0.000 | 0.000 |
| D-(+)-Cellobiose, octakis(trimethylsilyl) ether, methyloxime (isomer   | 32.02 | 1594889261  | 0.000 | 0.000 |
| EIQTMS_N12C_LJAN_3180.9_2233BN14_[NA]                                  | 32.93 | 11169855840 | 0.000 | 0.000 |
| 1-Monolinoleoylglycerol trimethylsilyl ether                           | 34.44 | 226045780   | 0.000 | 0.000 |

Manually integrated



Flag legend: P = Library entry selected manually