# Multivariate statistical models of metabolomic data reveals different metabolite distribution patterns in isonitrosoacetophenone-elicited *Nicotiana tabacum* and *Sorghum bicolor* cells.

Ntakadzeni E Madala[1], Lizelle A Piater[1], Paul A Steenkamp[1,2] and Ian A Dubery[1*].

[1]Department of Biochemistry, University of Johannesburg, Auckland Park, 2006, South Africa

[2]BioSciences, CSIR, Pretoria, 0001, South Africa.

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**Additional file 1:**

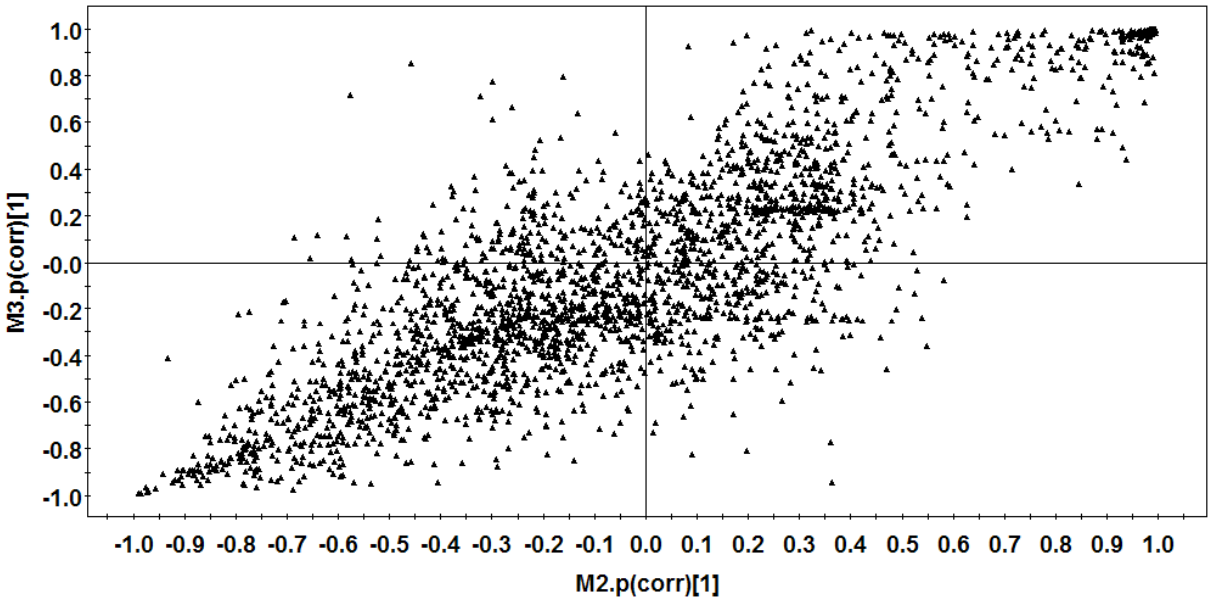
**Figure S1 A-E: OPLS-DA based SUS-plots showing metabolite distribution from different time intervals of INAP elicited tobacco cell suspensions.** For the code description M2 encodes 6 h, M3 12 h, M4 18 h, and M5 24 h.

**Figure S2 A-E: OPLS-DA based SUS-plots showing metabolite distribution from different time intervals of INAP elicited sorghum cell suspensions.** For the code description M2 encodes 6 h, M3 12 h, M4 18 h, and M5 24 h.

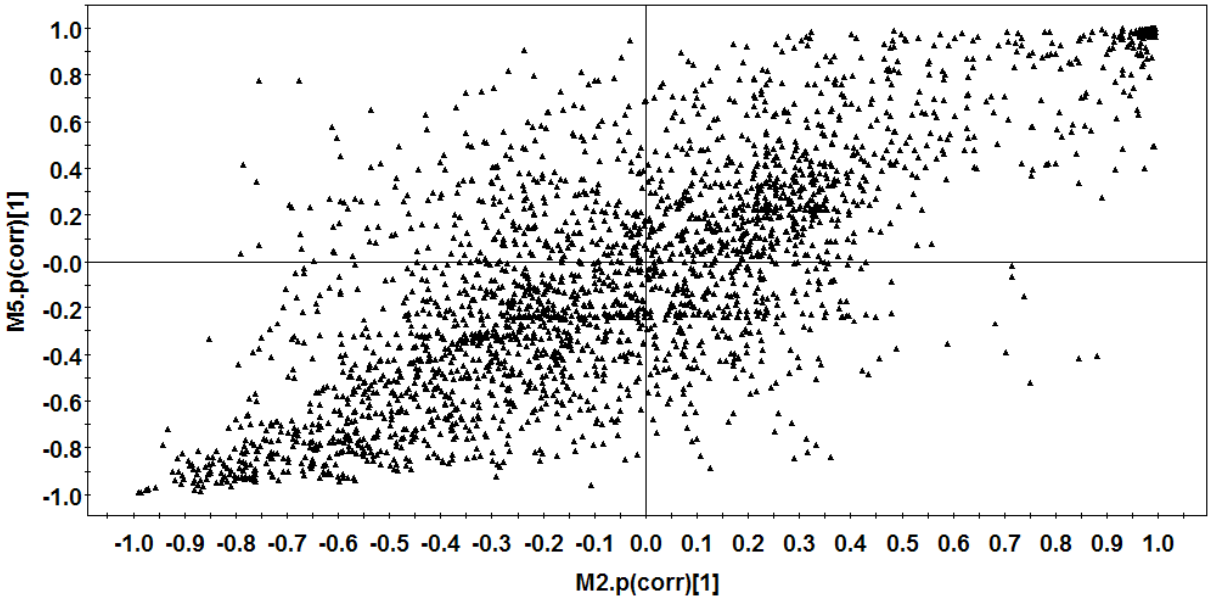
**Tables S1–S2. Cross-validation (CV)-Anova of OPLS-DA-derived SUS plots for tobacco and sorghum.** M2, M3, M4 and M5 refers to Control vs. 6 h, Control vs. 12 h, Control vs. 18 h and Control vs. 24 h respectively.

**Figure S1**: OPLS-DA based SUS-plots showing metabolite distribution from different treatment time intervals, **A** (6 h vs12 h), **B** (6 h vs 24 h), **C** (12 h vs 18 h), **D** (12 h vs 24 h) and **E** (18 h vs 24) of **tobacco cell suspensions** treated with 1 mM isonitrosacetophenone. For keys features, refer to Fig. 4.

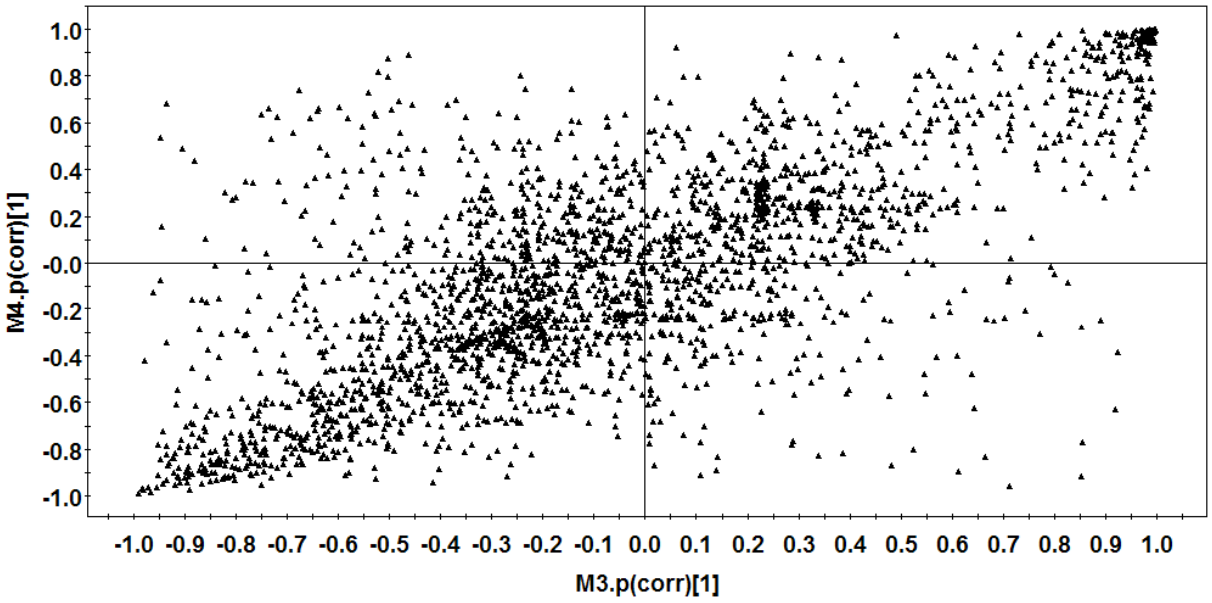
**S1-A.**



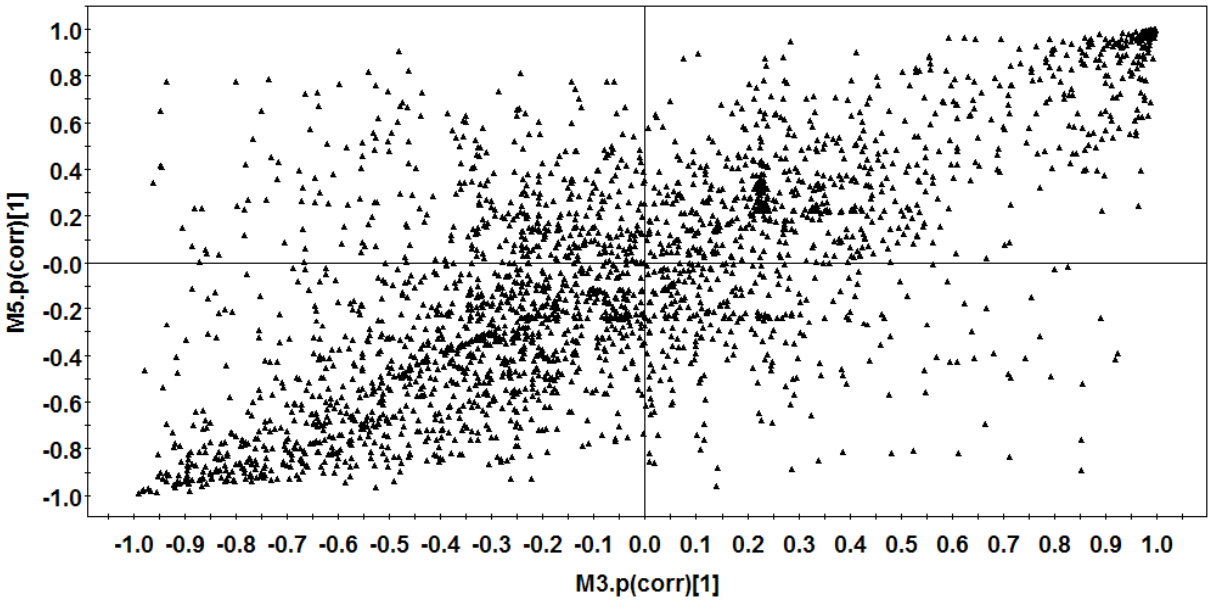

**S1-B.**



**S1-C.**


M4.p(corr)[1]
1.0
0.8
0.6
0.4
0.2
-0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
M3.p(corr)[1]

**S1-D.**


M5.p(corr)[1]
1.0
0.8
0.6
0.4
0.2
-0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
M3.p(corr)[1]

**S1-E.**

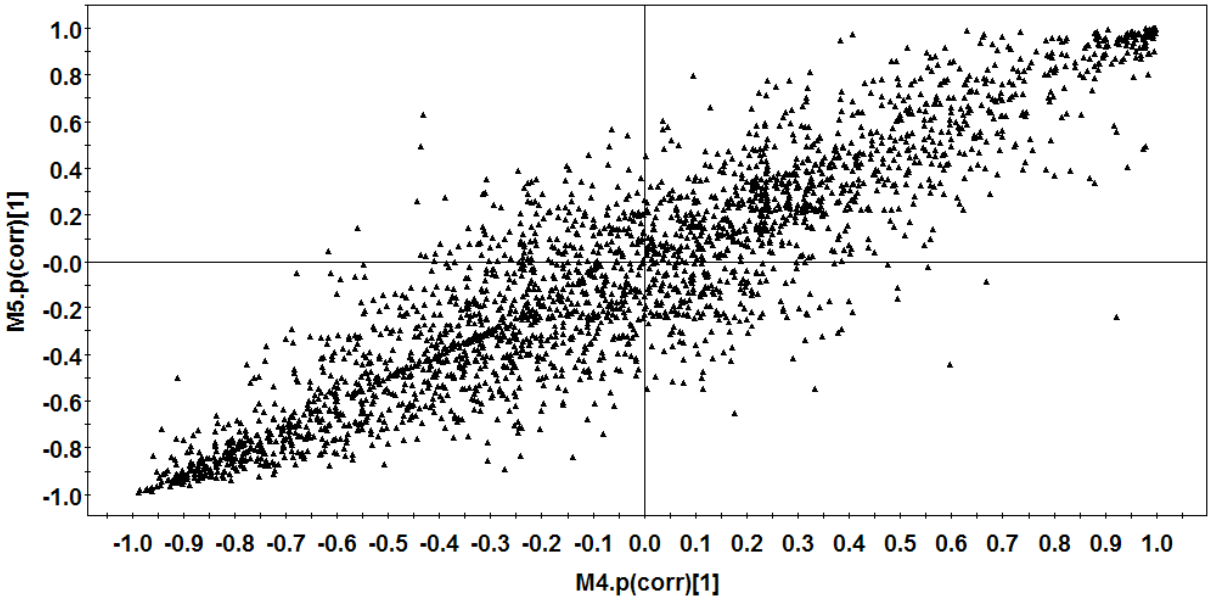
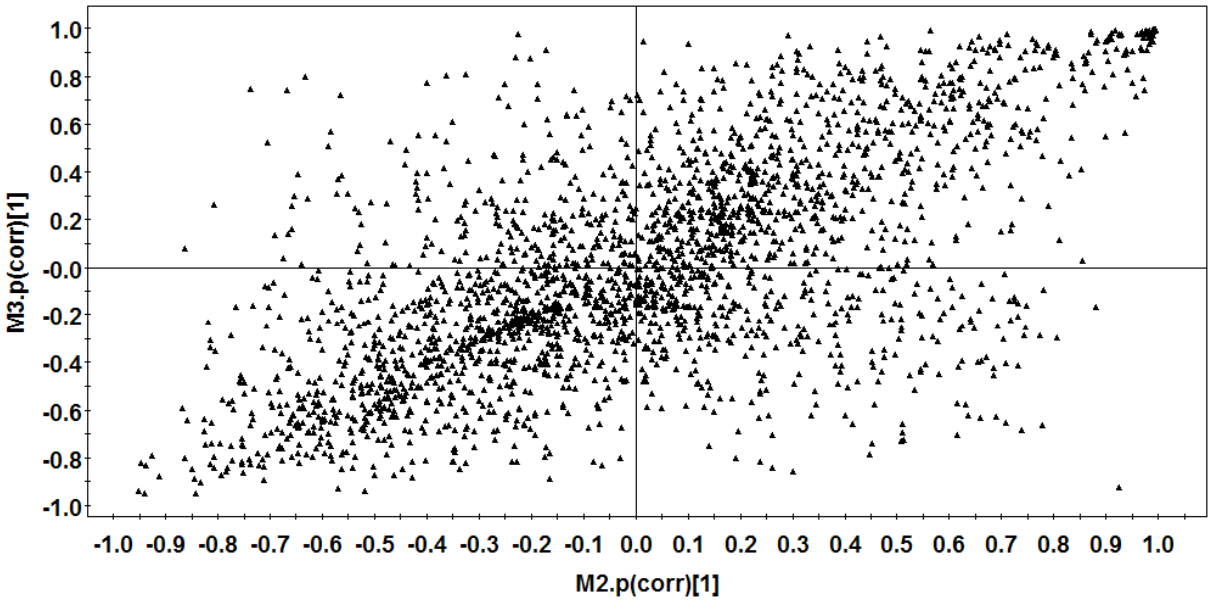
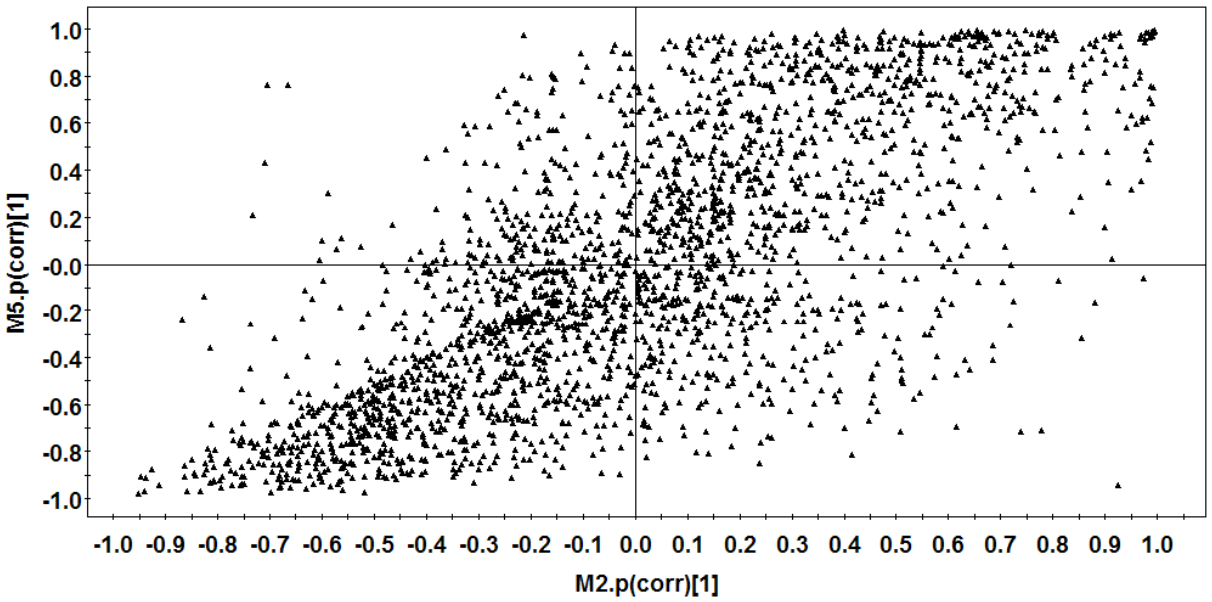

M5.p(corr)[1]
1.0
0.8
0.6
0.4
0.2
-0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
M4.p(corr)[1]

**Figure S2**: OPLS-DA based SUS-plots showing metabolite distribution from different treatment time intervals, **A** (6 h vs.12 h), **B** (6 h vs. 24 h), **C** (12 h vs. 18 h), **D** (12 h vs. 24 h) and **E** (18 h vs. 24) of **sorghum cell suspensions** treated with 1 mM isonitrosacetophenone. For keys features, refer to Fig. 4.

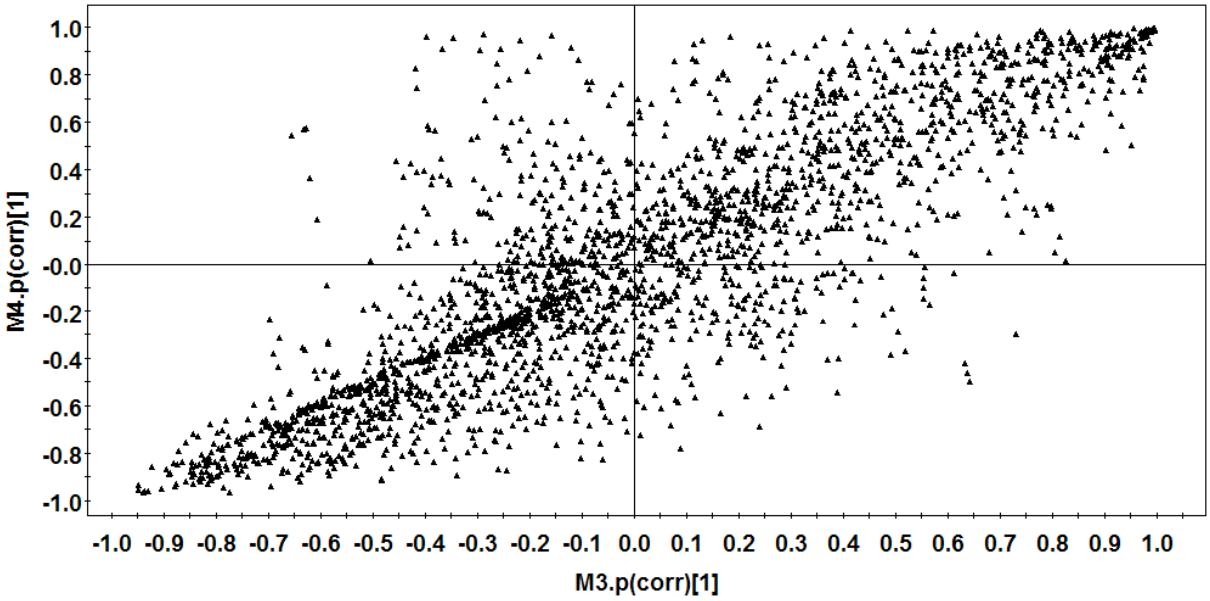
**S2-A.**



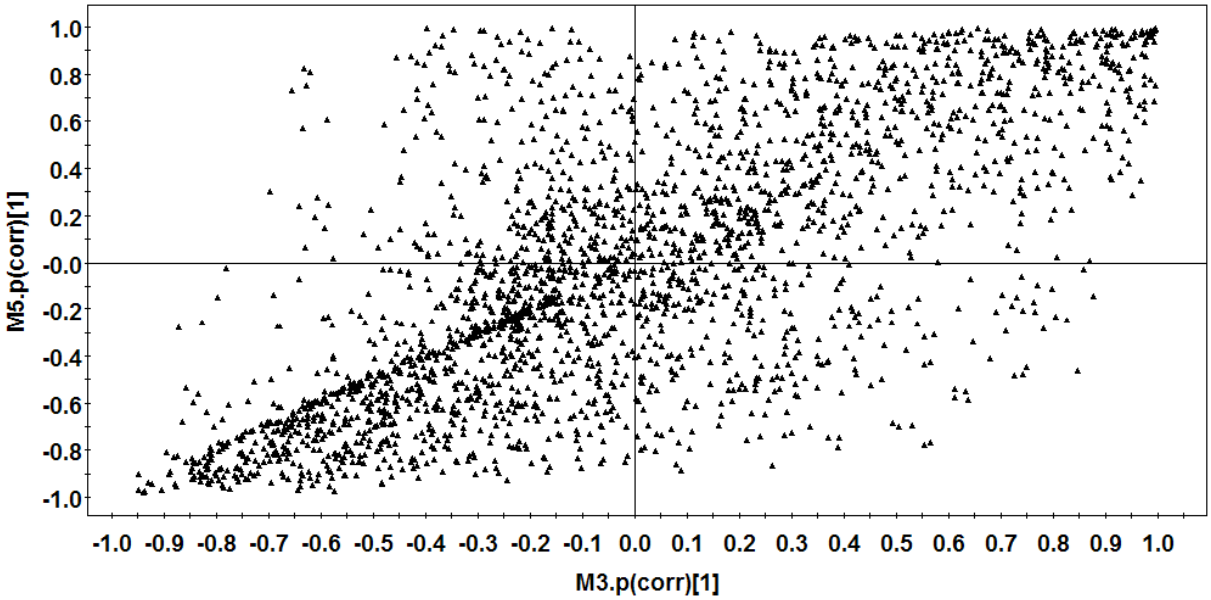

**S2-B.**



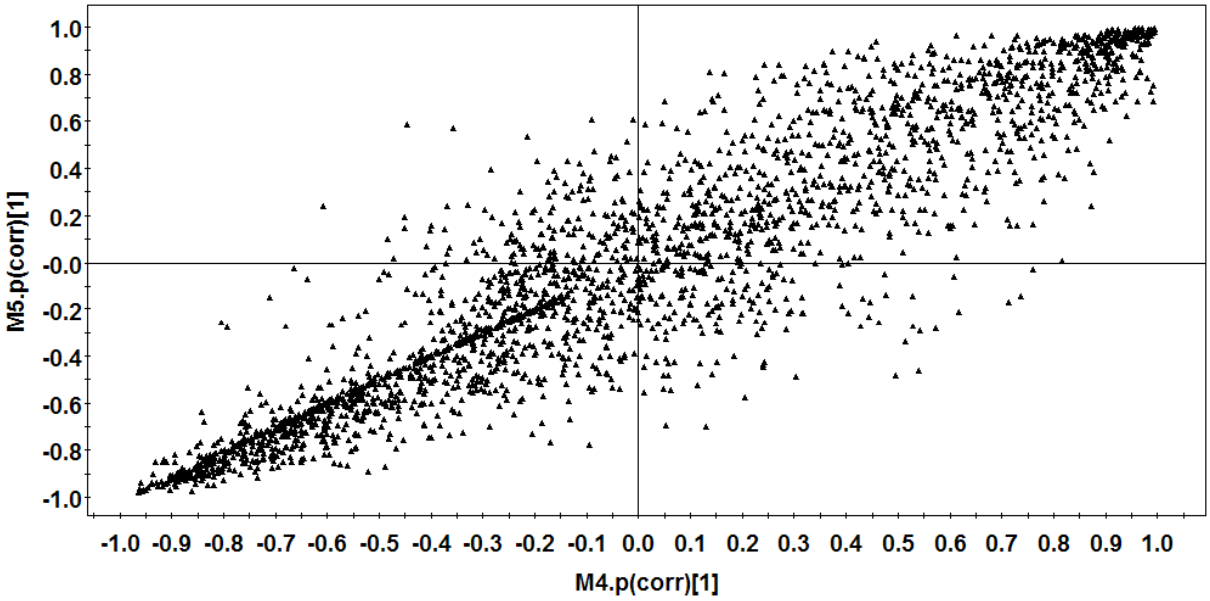
**S2-C.**


M4.p(corr)[1]
1.0
0.8
0.6
0.4
0.2
-0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
M3.p(corr)[1]

**S2-D.**


M5.p(corr)[1]
1.0
0.8
0.6
0.4
0.2
-0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
M3.p(corr)[1]

**S2-E.**


M5.p(corr)[1]
1.0
0.8
0.6
0.4
0.2
-0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
M4.p(corr)[1]

**Tables S1 –S2. CV-Anova validation of OPLS-DA derived SUS plots.** M2, M3, M4 and M5 refers to Control vs. 6 h, Control vs. 12 h, Control vs. 18 h and Control vs. 24 h respectively.

## 1. INAP treated tobacco cells

**a**. CV-anova results for the OPLS model for M2

[$R^2X$ (cum) = 0.390; $R^2Y$ (cum) = 0.995; $Q^2$ (cum) = 0.966].

| M2(Untitled) | SS | DF | MS | F | P | SD |
|---|---|---|---|---|---|---|
| **Total corr.** | 19 | 19 | 1 | | | 1 |
| **Regression** | 18.3612 | 4 | 4.59031 | 107.795 | 7.34028e-011 | 2.1425 |
| **Residual** | 0.638758 | 15 | 0.0425839 | | | 0.206359 |

**b.** CV-anova results for the OPLS model for M3

[$R^2X$ (cum) = 0.493; $R^2Y$ (cum) = 0.998; $Q^2$ (cum) = 0.985].

| M3(Untitled) | SS | DF | MS | F | P | SD |
|---|---|---|---|---|---|---|
| **Total corr.** | 18 | 18 | 1 | | | 1 |
| **Regression** | 17.7266 | 4 | 4.43165 | 226.929 | 1.4723e-012 | 2.10515 |
| **Residual** | 0.273403 | 14 | 0.0195288 | | | 0.139745 |

**c.** CV-anova results for the OPLS model for M4

[$R^2X$ (cum) = 0.444; $R^2Y$ (cum) = 0.998; $Q^2$ (cum) = 0.986].

| M4(Untitled) | SS | DF | MS | F | P | SD |
|---|---|---|---|---|---|---|
| **Total corr.** | 19 | 19 | 1 | | | 1 |
| **Regression** | 18.7399 | 4 | 4.68496 | 270.135 | 8.8637e-014 | 2.16448 |
| **Residual** | 0.260146 | 15 | 0.0173431 | | | 0.131693 |

**d.** CV-anova results for the OPLS model for M5

[$R^2X$ (cum) = 0.486; $R^2Y$ (cum) = 0.999; $Q^2$ (cum) = 0.985].

| M5(Untitled) | SS | DF | MS | F | P | SD |
|---|---|---|---|---|---|---|
| **Total corr.** | 19 | 19 | 1 | | | 1 |
| **Regression** | 18.7138 | 4 | 4.67846 | 245.239 | 1.80922e-013 | 2.16297 |
| **Residual** | 0.286157 | 15 | 0.0190772 | | | 0.13812 |

## 2. INAP treated sorghum cells

**a.** CV-anova results for the OPLS model for M2

[$R^2X$ (cum) = 0.514; $R^2Y$ (cum) = 0.998; $Q^2$ (cum) = 0.985].

| M2(Con vs 6 h) | SS | DF | MS | F | p | SD |
|---|---|---|---|---|---|---|
| **Total corr.** | 39 | 39 | 1 | | | 1 |
| **Regression** | 38.4257 | 6 | 6.40428 | 367.982 | 9.34485e-029 | 2.53067 |
| **Residual** | 0.574325 | 33 | 0.0174038 | | | 0.131923 |

**b.** CV-anova results for the OPLS model for M3

[$R^2X$ (cum) = 0.498; $R^2Y$ (cum) = 0.996; $Q^2$ (cum) = 0.992].

| M3(Con vs 12 h) | SS | DF | MS | F | p | SD |
|---|---|---|---|---|---|---|
| **Total corr.** | 39 | 39 | 1 | | | 1 |
| **Regression** | 38.6956 | 4 | 9.67389 | 1112.15 | 2.40803e-036 | 3.11029 |
| **Residual** | 0.304442 | 35 | 0.00869835 | | | 0.093265 |

**c.** CV-anova results for the OPLS model for M4

[$R^2X$ (cum) = 0.550; $R^2Y$ (cum) = 0.996; $Q^2$ (cum) = 0.993].

| M4(Con vs 18 h) | SS | DF | MS | F | p | SD |
|---|---|---|---|---|---|---|
| **Total corr.** | 39 | 39 | 1 | | | 1 |
| **Regression** | 38.7321 | 4 | 9.68303 | 1265.14 | 2.56831e-037 | 3.11176 |
| **Residual** | 0.267879 | 35 | 0.0076537 | | | 0.0874854 |

**d.** CV-anova results for the OPLS model for M5

[$R^2X$ (cum) = 0.584; $R^2Y$ (cum) = 0.997; $Q^2$ (cum) = 0.994].

| M5(Con vs 24 h) | SS | DF | MS | F | p | SD |
|---|---|---|---|---|---|---|
| **Total corr.** | 39 | 39 | 1 | | | 1 |
| **Regression** | 38.7779 | 4 | 9.69448 | 1527.85 | 0 | 3.1136 |
| **Residual** | 0.222081 | 35 | 0.00634516 | | | 0.0796565 |

**Reference**

L. Eriksson, J. Trygg, S. Wold, CV-ANOVA for significance testing of PLS and OPLS® models, J. Chemometr 22 (2008) 594-600.