

Supplemental Table S1. Validation parameters of the OPLS-DA models

OPLS-DA models for the elicitors treatments (A) and the *nadC* experiment (B) were validated by multivariate statistics using SIMCA (v 13.0.3). Values of R^2 and Q^2 indicate correlation and predictability parameters, respectively, where X represents the variables, and Y the classes. Models were also confirmed by cross-validation ANOVA, with the *P* value given in blue. In all cases, validation parameters were highly satisfactory. ESI⁻ and ESI⁺: negative and positive electrospray ionization, respectively.

	Elicitors (A)		<i>nadC</i> (B)	
	ESI ⁻	ESI ⁺	ESI ⁻	ESI ⁺
Detected metabolic markers	5112	10273	5107	10207
Goodness of prediction, R^2 X	0.78	0.69	0.85	0.86
Goodness of prediction, R^2 Y	0.93	0.97	0.99	1.00
Goodness to fit, Q^2 X	0.64	0.72	0.85	0.89
Cross-validation ANOVA <i>P</i> value	2E-04	1E-06	1E-03	3E-04