

Fig. 1 Suppl. Comparison of control and chlorsulfuron-exposed (0.005 mg kg⁻¹) maize seedlings. A - PCA score plot. B - Validate mode, $R^2 = 0.999$, $Q^2 = 0.987$. R^2 - the predictable variables of the model, Q^2 - the predictive degree of the model. C - OPLS-DA loading plot. OSC is orthogonal signal correction, and the numbers at peaks represent the corresponding metabolites, which can be found in Table 1.

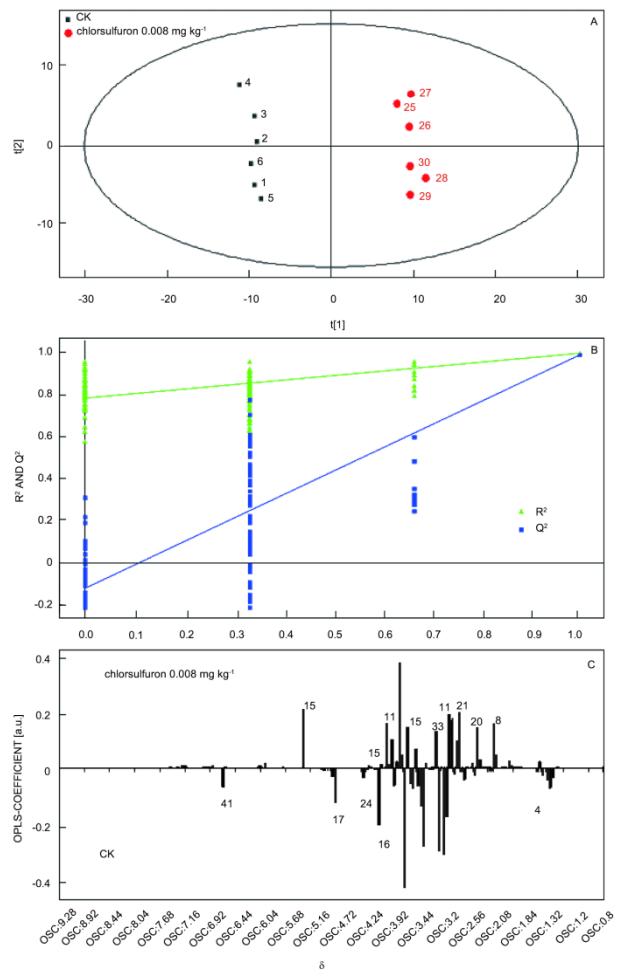


Fig. 2 Suppl. Comparison of control and chlorsulfuron-exposed (0.008 mg kg^{-1}) maize seedlings. A - PCA score plot. B - Validate mode, $R^2 = 0.999$, $Q^2 = 0.991$. R^2 - the predictable variables of the model, Q^2 - the predictive degree of the model. C - OPLS-DA loading plot. OSC is orthogonal signal correction, and the numbers at peaks represent the corresponding metabolites, which can be found in Table 1.

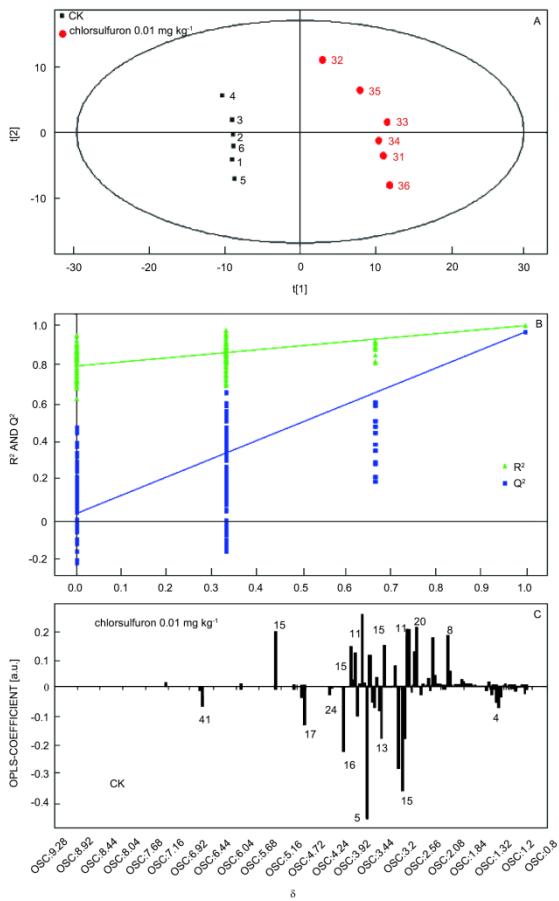


Fig. 3 Suppl. Comparison of control and chlorsulfuron-exposed (0.01 mg kg^{-1}) maize seedlings. A - PCA score plot. B - Validate mode, $R^2 = 0.995$, $Q^2 = 0.964$. R^2 - the predictable variables of the model, Q^2 - the predictive degree of the model. C - OPLS-DA loading plot. OSC is orthogonal signal correction, and the numbers at peaks represent the corresponding metabolites, which can be found in Table 1.

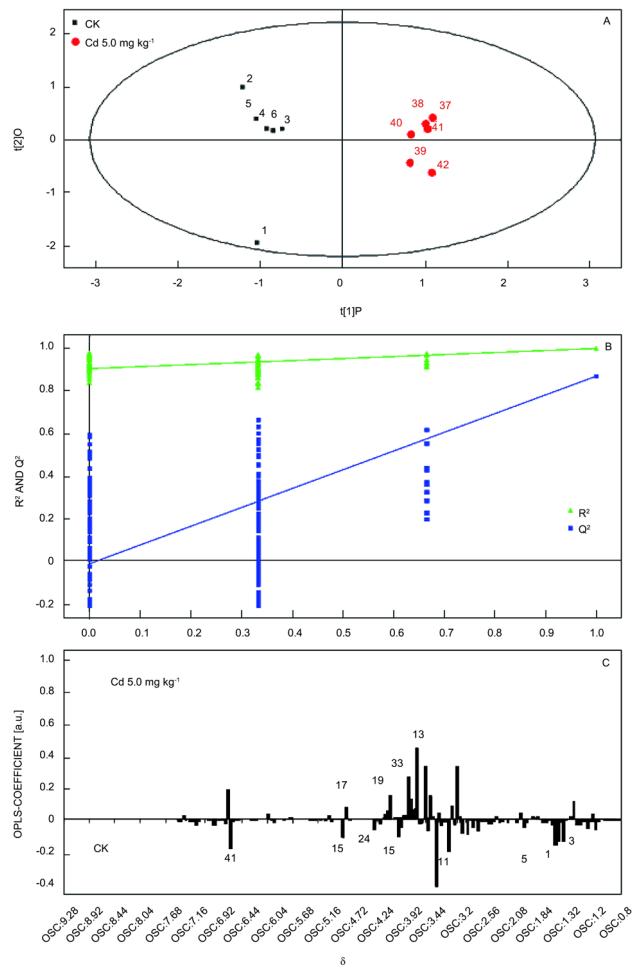


Fig. 4 Suppl. Comparison of control and Cd-exposed (5.0 mg kg^{-1}) maize seedlings. A - PCA score plot. B - Validate mode, $R^2 = 0.995$, $Q^2 = 0.866$. R^2 - the predictable variables of the model, Q^2 - the predictive degree of the model. C - OPLS-DA loading plot. OSC is orthogonal signal correction, and the numbers at peaks represent the corresponding metabolites, which can be found in Table 1.

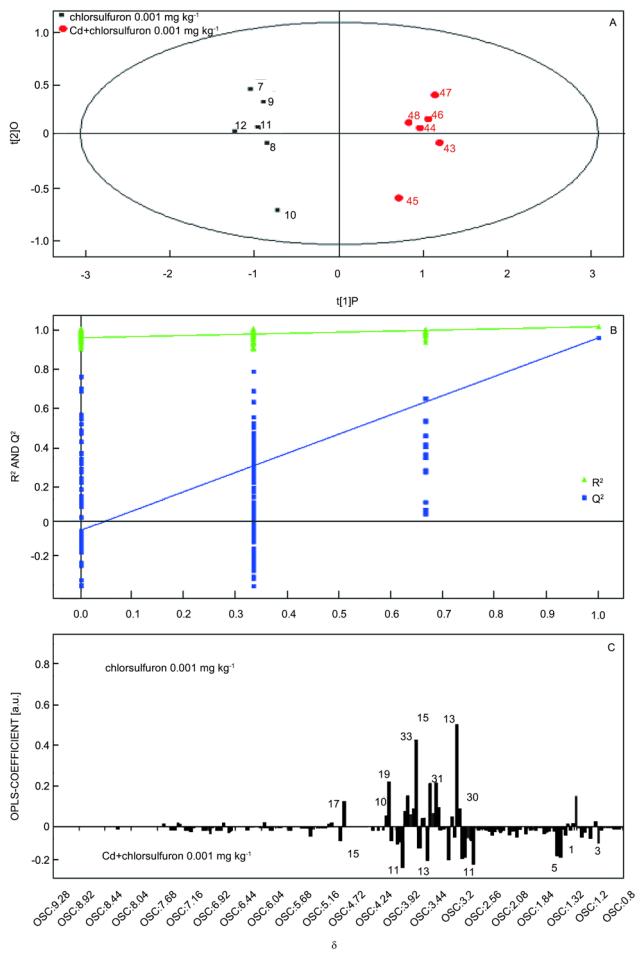


Fig. 5 Suppl. Comparison of chlorsulfuron-exposed (0.001 mg kg^{-1}) and mixture-exposed maize seedlings. A - PCA score plot. B - Validate mode, $R^2 = 0.996$, $Q^2 = 0.943$. R^2 - the predictable variables of the model, Q^2 - the predictive degree of the model. C - OPLS-DA loading plot. OSC is orthogonal signal correction, and the numbers at peaks represent the corresponding metabolites, which can be found in Table 1.

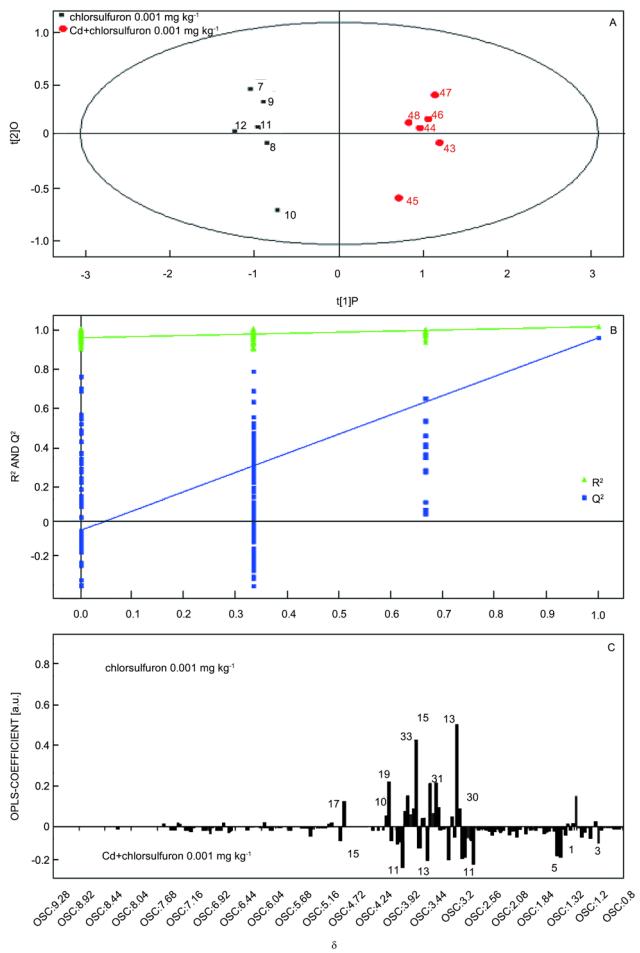


Fig. 6 Suppl. Comparison of chlorsulfuron-exposed (0.003 mg kg^{-1}) and mixture-exposed maize seedlings. A - PCA score plot. B - Validate mode, $R^2 = 0.993$, $Q^2 = 0.892$. R^2 - the predictable variables of the model, Q^2 - the predictive degree of the model. C - OPLS-DA loading plot. OSC is orthogonal signal correction, and the numbers at peaks represent the corresponding metabolites, which can be found in Table 1.