

SUPPORTING INFORMATION

Targeted metabonomics analysis of fatty acid in soybean seed by GC-MS reveal the metabolic manipulation of shading in intercropping system

Cai-qiong Yang,^{a,b,1} Nasir Iqbal,^{a,1} Bao-yu Hu,^a Qi-hui Zhang,^a Hai-jun Wu,^a Xin Liu,^a Jing Zhang,^{a,c} Wei-guo Liu,^{a,b} Wen-yu Yang^{*a} and Jiang Liu^{*a,b}

^a Key Laboratory of Crop Ecophysiology and Farming System in Southwest, Ministry of Agriculture, Chengdu 611130, China

^b Institute of Ecological Agriculture, Sichuan Agricultural University, Chengdu 611130, China

^c College of Horticulture, Sichuan Agricultural University, Chengdu 611130, China

Appendix A. Supplementary data

Table S1 Calibration curve equation of 17 fatty acids

Fig. S1 3D PCA with all groups

Fig. S2 permutation of PLS-DA

* Corresponding author. Tel.: +28 86290960; fax: +28 86290870.

E-mail address: jiangliu@sicau.edu.cn (J. Liu), mssiyangwy@sicau.edu.cn (W.-Y. Yang).

¹ These authors contributed equally to this work.

Table S1 Calibration curve equation of 17 fatty acids

Code	Component	Retention time (min)	Regression equations	Correlation coefficients
1	Lauric acid (C12:0)	7.98	$Y = 1090849X - 281876.0$	$R^2 = 0.9999$
2	Myristic acid (C14:0)	12.39	$Y = 1208393X - 411899.8$	$R^2 = 0.9999$
3	Pentadecanoic acid (C15:0)	15.92	$Y = 616361.4X - 241672.8$	$R^2 = 0.9999$
4	Palmitoleic acid (C16:1)	18.81	$Y = 177704.8X - 66497.0$	$R^2 = 0.9999$
5	Palmitic acid (C16:0)	19.56	$Y = 1872343X - 685370.7$	$R^2 = 0.9999$
6	10-Heptadecenoic acid (C17:1)	22.32	$Y = 199454.7X - 78181.15$	$R^2 = 0.9997$
7	Margaric acid (C17:0)	23.03	$Y = 463079.2X - 202883.2$	$R^2 = 0.9999$
8	Linoleic acid (C18:2n6c)	25.27	$Y = 214703.7X - 97937.54$	$R^2 = 0.9998$
9	Oleic acid (C18:1n9c)	25.48	$Y = 493867.9X - 200863.2$	$R^2 = 0.9999$
10	α -Linolenic acid (C18:3n3)	25.57	$Y = 343718.1X - 132877.8$	$R^2 = 0.9999$
11	Stearic acid (C18:0)	30.42	$Y = 1255501X - 478889.2$	$R^2 = 0.9999$
12	8,11,14-Eicosatrienoic acid (C20:3n6)	31.41	$Y = 160097.3X - 66916.92$	$R^2 = 0.9999$
13	11,14-Eicosadienoic acid (C20:2)	31.74	$Y = 210482.8X - 101018.5$	$R^2 = 0.9997$
14	11-Eicosenoic acid (C20:1)	31.93	$Y = 221147.2X - 80045.54$	$R^2 = 0.9999$
15	Arachidic acid (C20:0)	32.96	$Y = 1191224X - 422994.8$	$R^2 = 0.9999$
16	Heneicosanoic acid (C21:0)	37.58	$Y = 560951.8X - 228357.0$	$R^2 = 0.9999$
17	Lignoceric acid (C24:0)	54.71	$Y = 937515.0X - 305258.9$	$R^2 = 0.9999$

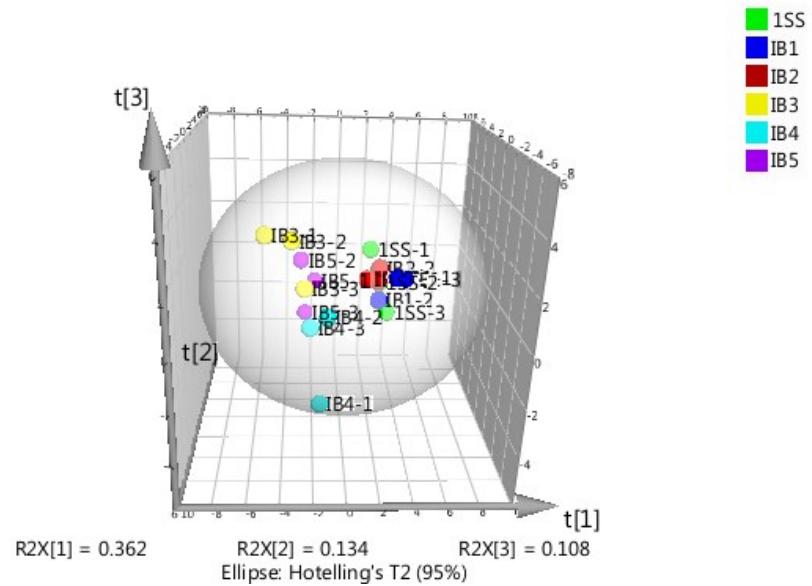


Fig. S1 3D PCA with all groups

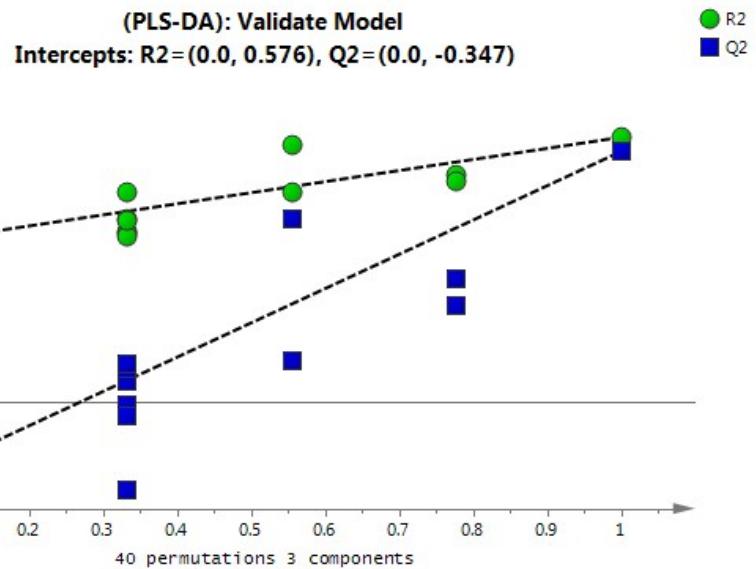


Fig. S2 permutation of PLS-DA.