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DATA PAPER OPEN ACCESS

Leaf metabolomic data of eight sunflower lines and their sixteen hybrids under water deficit☆

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Abstract – This article describes how metabolomic data were produced on sunflower plants subjected to water deficit. Twenty-four sunflower (*Helianthus annuus* L.) genotypes were selected to represent genetic diversity within cultivated sunflower and included both inbred lines and their hybrids. Drought stress was applied at the vegetative stage to plants cultivated in pots using the high-throughput phenotyping facility Heliaphen. Here, we provide untargeted and targeted metabolomic data of sunflower leaves. These compositional data differentiate both plant water status and different genotype groups. They constitute a valuable resource for the community to study the adaptation of crops to drought and the metabolic bases of heterosis.

Keywords: *Helianthus* / abiotic stress / drought stress / LC-MS / metabolomic profiling

Résumé – Données métabolomiques foliaires de huit lignées de tournesol et de leurs seize hybrides sous déficit hydrique. Cet article décrit comment les données métabolomiques ont été produites sur des plants de tournesol soumis à un déficit hydrique. Vingt-quatre génotypes de tournesol (*Helianthus annuus* L.) ont été sélectionnés pour représenter la diversité génétique du tournesol cultivé et comprennent à la fois des lignées consanguines et leurs hybrides. Une limitation hydrique a été appliquée au stade végétatif aux plantes cultivées en pots à l'aide de la plateforme de phénotypage à haut débit Heliaphen. Ici, nous mettons à disposition des données métabolomiques non ciblées et ciblées de feuilles de tournesol. Ces données de composition permettent de différencier l'état hydrique des plantes et différents groupes de génotypes. Elles constituent une ressource précieuse pour la communauté afin d'étudier l'adaptation des cultures à la sécheresse et les bases métaboliques de l'hétérosis.

Mots clés : *Helianthus* / stress abiotique / stress hydrique / LC-MS / profils métabolomiques

Highlights

Leaf metabolomic data were produced on sunflower plants of inbred lines and their hybrids subjected to water deficit at the vegetative stage.

They differentiate both plant water status and different genotype groups.

They constitute a valuable resource to be combined with other omics data and study the adaptation to drought and the bases of heterosis.

☆ Contribution to the Topical Issue "Sunflower / Tournesol".

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1 Specifications table

Subject area	Biology
More specific subject area	Metabolomic data
Type of data	LC-MS: LC-MS acquisition files, R command text file for spectra processing, LC-MS/MS acquisition files, Word file for LC-MS annotation table, tab file for calculated data table Targeted analyses: tab file for calculated data table
How data was acquired	The Heliaphen robot and targeted robotized analyses of major compounds or LC-MS analyses of polar extracts
Data format	Targeted-analyses processed data: txt LC-MS data, metadata, raw and processed data: tab, mzML, docx, tab, txt
Experimental factors	24 genotypes of *Helianthus annuus* in two environmental conditions (irrigated or not) with three replicates
Experimental features	Absolute contents of major compounds of sunflower leaf Relative contents of LC-MS based metabolite signatures of sunflower leaf
Data source location	The outdoor Heliaphen phenotyping platform at INRAE station, Auzeville-Tolosane, France (43°31'41.8"N, 1°29'58.6"E) Bordeaux Metabolome Facility, https://doi.org/10.15454/1.5572412770331912E12
Data accessibility	The LC-MS data are publicly available in Data INRAE repository (https://data.inrae.fr/dataverse/sunflodry, https://doi.org/10.15454/2KOXOH) under license etalab-2.0 The targeted analyses data are publicly available in Data INRAE repository (https://data.inrae.fr/dataverse/sunflodry, https://doi.org/10.15454/STJH47) under license etalab-2.0
Related research article	(Blanchet *et al.*, 2018; Gody *et al.*, 2020; Balliau *et al.*, 2021)

2 Value of the data

Drought stress is a crucial issue for crop adaptation to climate change and sunflower is particularly impacted as it is mostly cultivated in marginal lands (Debaeke *et al.*, 2017). In the present experiment, plants were subjected to two treatments (Well-Watered or Water-Deficit) during the vegetative stage. This experiment was performed in the outdoor high-throughput, semi-automated phenotyping facility Heliaphen (https://www6.inrae.fr/phenotoul_eng/WHO-we-are/PhenoToul/HeliaPhen).

Heterosis is an outstanding phenomenon involved in natural selection and used in crop breeding to adapt plants to environmental constraints. Twenty-four genotypes of cultivated sunflower consisting in four maintainer lines, four restorer lines and their 16 corresponding hybrids are included in this experiment which allows studying heterosis effect on metabolism.

This dataset provides metabolomic data of sunflower leaves of lines and hybrids under control and water deficit conditions.

These data consist in unique untargeted and targeted metabolomic profiles of sunflower responses to drought based on a large genetic variability.

3 Data

Climate change is affecting plant biodiversity, and crop choice and yields. A better knowledge of plant adaptation mechanisms to this recent phenomenon is, therefore, of major interest for crop science, agriculture and for feed and food security (Porter *et al.*, 2019). *Helianthus annuus* L., the domesticated sunflower, is the fourth most important oilseed crop in the world (USDA, 2019). It seems promising for agriculture adaptation to global change because it can maintain stable yields across a range of environmental conditions, especially during stress induced by water limitation (Debaeke *et al.*, 2017). It can be considered as an archetypical systems biology model with large drought stress response which involves many molecular pathways (Moschen *et al.*, 2017) and subsequent metabolic and physiological processes.

In this data article, we are sharing the metabolomic data of 24 sunflower genotypes grown in two environmental conditions in an outdoor phenotyping facility. This dataset is part of a larger project that integrates other omics data (Blanchet *et al.*, 2018; Gody *et al.*, 2020; Balliau *et al.*, 2021).

The LC-MS data and metadata associated with this article were deposited in the Data INRAE repository. The targeted analyses data were deposited in the Data INRAE repository.

4 Experimental design, plant material and growth conditions

The experiment was performed from May to July 2013 on the outdoor Heliaphen phenotyping facility at the Institut National de Recherche pour l'Agriculture, l'Alimentation et l'Environnement (INRAE) station, Auzeville, France (43°31'41.8"N, 1°29'58.6"E) as previously described (Blanchet *et al.*, 2018; Gosseau *et al.*, 2019). Briefly, germinated plantlets were transplanted into individual pots filled with 15-l potting soil and covered with a 3-mm-thick polystyrene sheet to prevent soil water evaporation. Plants were fertilized with Peters Professional fertilizer (17-07-27, 500 mL, 0.6 g/L) and an oligo-element mixture solution (Hortilon, 0.46 g/L) at 17 days after germination (DAG), and treated with Polyaxe (5 mg/L applied on foliage) against thrips at 21 DAG.

In total, 144 plants, corresponding to 24 genotypes, four maintainer (SF009, SF092, SF109 and SF193) and four restorer (SF279, SF317, SF326 and SF342) lines and their corresponding hybrids obtained by crossing, were grown in two conditions: well-watered (WW) and water-deficit (WD) with three biological replicates (Blanchet *et al.*, 2018; Gody *et al.*, 2020). Before the beginning of the water deficit application at 35 DAG, pots were saturated with water and excessive water was drained. Pots were weighed to obtain the full soil water retention mass. At 38 DAG, irrigation was stopped (approximately 20-leaf stage) for WD plants as described previously (Gosseau *et al.*, 2019). Plants were weighed by the Heliaphen robot to estimate transpiration (Gosseau *et al.*, 2019). WW plants were re-watered at each weighing to reach soil water full retention capacity. Pairs of WD and WW plants were harvested when the fraction of transpirable soil water of the stressed plant reached 0.1 (occurring between 42 and 47 DAG). Two out of the three SF342 line plants died under the WW condition. The corresponding plant samples could not be harvested and data could not be obtained.

At harvest, leaves for metabolome analyses were cut without their petiole and immediately frozen in liquid nitrogen from 11 a.m. to 1 p.m. The harvested leaf was the leaf above the leaf that had reached its maximum size the most recently, as for the proteomic and transcriptomic studies (Blanchet *et al.*, 2018; Gody *et al.*, 2020; Balliau *et al.*, 2021).

5 Metabolite analyses

5.1 Metabolite extraction

Leaf sample grinding was performed using a ZM200 grinder (Retsch, Haan, Germany) as described for transcriptome analysis (Gody *et al.*, 2020). Fresh-frozen powdered samples were then lyophilized. Aliquots of about 10 ± 2 mg of dry powder were weighed in 1.1 mL MicronicTM tubes (Lelystad, The Netherlands) and extracted with a robotized Star/Starlet platform (Hamilton, Villebon sur Yvette, France) using ethanol/water (80:20, v/v) added with 0.1% formic acid as solvent at room temperature. Methyl vanillate was used as internal standard to check for the quality of injection for LC-MS. Two successive extractions consisting in 1 min vigorous shaking followed by 15 min ultrasonication were performed with 300 μL of extraction solvent. The two supernatants were combined and filtered with 0.22 µm hydrophilic Durapore filtering microplates (Merck Millipore, Carrightwohill, Ireland). Nine blank extracts from the same procedure, but without sample powder, were also prepared. A QC sample was produced for LC-MS by pooling 10 μL of each sample extract.

5.2 Targeted analyses of major compounds

The targeted analyses of major compound in all samples were performed as done previously for the parents only (Fernandez *et al.*, 2019) and as previously described (Biais *et al.*, 2014) using enzymatic analyses and colorimetric assays performed using a robotic Star/Starlet platform (Hamilton, Villebon-sur-Yvette, France) and spectrophotometers. Glucose, fructose and sucrose were determined in the ethanolic supernatant obtained as described above (Stitt *et al.*, 1989) and expressed in µmol per g dry weight (DW). Total free amino acids were determined in the supernatant with a fluorescamine-based assay (Bantan-Polak *et al.*, 2001) and expressed as glutamate equivalents. Protein content was determined (Bradford, 1976) on the pellet re-suspended in 100 mM NaOH and heated at 95 °C for 20 min and expressed as mg bovine serum albumine equivalents per g DW. After neutralisation of the suspended pellet, starch was determined and expressed in glucose equivalents per g DW (Hendriks *et al.*, 2003). Absorbencies were read at 340 or 595 nm using an MP96 microplate reader (SAFAS, Monaco). For fluorescence, 405 nm excitation and 485 nm emission were used with a Xenius multifunction microplate reader (SAFAS, Monaco). All chemicals and substrates for targeted analyses were purchased from Sigma-Aldrich Ltd. (Gillingham, United Kingdom). All enzymes were purchased from Roche Applied Science (Meylan, France).

5.3 LC-MS based metabolomic profiling

LC-MS-based metabolomic profiling of extracts was performed using the same extracts as for targeted analyses. The sample injection order was randomized. The QC sample was injected every 12 samples to correct for mass spectrometer signal drift. The extracts were analysed using LC-MS (Ultimate 3000 – LTQ-Orbitrap Elite, ThermoScientific, Bremen, Germany), using a C18 chromatographic column (C18-Gemini 2.0×150 mm, 3 µm, 110 Å, Phenomenex, Torrance, CA, USA), a 18 min acetonitrile gradient in acidified water (solvent A: ultrapure water + 0.1% formic acid, solvent B: LC-MS grade acetonitrile) with a 300 μL.min^{-1} flow rate and the following elution gradient: 0-0.5 min, 3% B; 0.5-1 min, 3-10% B; 1-9 min, 10-50% B; 9-13 min, 50-100% B; 13-14 min, 100% B; 14-14.5 min 100-3% B; 14.5-18 min, 3% B. The column temperature was 30 °C. The injection volume was 5 μL. The LC-MS instrument was equipped with an HESI source operated in the positive-ion mode. Source parameters were the following: source voltage, 3.2 kV; sheath gas, 45 arbitrary units (a.u.); auxiliary gas, 15 a.u.; sweep gas, 0 a.u.; capillary temperature, 350 °C; heater temperature, 350 °C. Full Scan MS spectra were acquired at 240k resolution power with a 50-1000 mass range. Data dependent MS/MS spectra were acquired at 60k resolution power. The selected ions were fragmented in CID mode at a 35% normalized collision energy. The MS data were processed using R (R Core Team, 2018) with XCMS (Smith *et al.*, 2006) and MetNormalizer (Shen *et al.*, 2016) packages. Briefly, the corresponding MS-based variables were named using their nominal masses in Da and retention time in s (MxxxTyyy). Variables detected in blank extracts were filtered out. Variables with m/z values varying by more than 0.005 Da or with retention time varying by more than 20 s between different samples were also filtered out. Variables with intensity coefficients of variation in QC greater than 20% were also removed. This resulted in a data matrix of 4843 variables. Intensity drift was corrected using support vector regression. Finally, intensities were normalized according to the sample powder mass used for extraction. Annotation of intense ions

Table 1. Annotation of LC-MS signatures of sunflower leaf ethanolic extracts with LC-MS and LC-MS/MS data in positive ionization mode.

Variable	Metabolite Rt [a] (min)	Metabolite $[M+H]^+$ [a] *m/z*	LC-MS/MS fragments *m/z* [a,b]	Putative name	Metabolite ID	Class	Neutral molecular formula	Calculated molecular formula $[M+H]^+$ *m/z*	MSI level[c]
M284T195	3.26	284.0997	152.0568	Guanosine	CHEBI:16750	Nucleosides	$C_{10}H_{13}N_5O_5$	284.09894	2
M166T209	3.30	166.0864	120.0806	Phenylalanine	CHEBI:28044	Amino acids	$C_9H_{11}NO_2$	166.08626	2
M382T210	3.50	382.1730	220.1195; 202.1091; 136,0618	Pantothenic acid-hexose	–	Amino compounds	$C_{15}H_{27}NO_{10}$	382.17077	3
M285T209	3.50	285.0837	ND	Xanthosine	CHEBI:18107	Nucleosides	$C_{10}H_{12}N_4O_6$	285.08296	3
M356T275 [d]	4.60	355.1024	ND	5-O-Caffeoylquinic acid	CHEBI:16384	Cinnamic acids	$C_{16}H_{18}O_9$	355.10236	2
M342T281 [d]	4.68	341.0869	179.0340	Esculin	CHEBI:4853	Coumarins	$C_{15}H_{16}O_9$	341.08671	2
M356T315_1 [d]	5.25	355.1017	163.0392; 145.0286	3-O-Caffeoylquinic acid	CHEBI:16112	Cinnamic acids	$C_{16}H_{18}O_9$	355.10236	2
M356T341 [d]	5.68	355.1023	ND	4-O-Caffeoylquinic acid	CHEBI:75491	Cinnamic acids	$C_{16}H_{18}O_9$	355.10236	2
M340T362 [d]	6.04	339.1080	321.1128; 147.0442	Coumaroylquinic acid	CHEBI:1945	Cinnamic acids	$C_{16}H_{18}O_8$	339.10744	2
M611T367	6.10	611.1630	465.1028; 303.0502	Rutin	CHEBI:28527	Flavonoids	$C_{27}H_{30}O_{16}$	611.16066	2
M465T374	6.21	465.1034	303.0503	Quercetin hexoside	–	Flavonoids	$C_{21}H_{20}O_{12}$	465.10275	3
M370T374 [d]	6.22	369.1179	207.0995; 177.0550; 145.0286	Feruloylquinic acid	CHEBI:86388	Cinnamic acid	$C_{17}H_{20}O_9$	369.11800	2
M642T389 [d]	6.47	641.1736	495.1133; 333.0603	Pentahydroxy, methoxyflavone hexoside-deoxyhexoside	–	Flavonoids	$C_{28}H_{32}O_{17}$	641.17122	3
M518T468 [d]	7.74	517.1334	ND	3,4-Dicaffeoylquinic acid	CID: 5281780	Cinnamic acids	$C_{25}H_{24}O_{12}$	517.13405	3
M549T502_2	8.36	549.1256	ND	Trihydroxy,methoxyflavone malonylhexoside	–	Flavonoids	$C_{25}H_{24}O_{14}$	549.12388	3
M379T524	8.71	379.1747	ND	Niveusin C or Hydroxyleptocarpin	–	Sesquiterpenoids	$C_{20}H_{26}O_7$	379.17513	3
M274T582	9.68	273.0759	255.0655; 163.0392; 137.0234	Butein	CHEBI:3237	Flavonoids	$C_{15}H_{12}O_5$	273.07574	2
M409T617	10.28	409.1862	ND	3-O-Methylniveusin A	CID: 131752540	Sesquiterpenoids	$C_{21}H_{28}O_8$	409.18569	3

[a] Rt and *m/z* measured with the raw data files. Only the $[M+H]^+$ ion was considered as it was the most abundant ion in each acquired MS spectrum.
[b] MS/MS fragmentation data from data dependent scan in CID mode at a 35% normalized collision energy value; ND: spectrum was not acquired.
[c] Level of metabolite identification (Sumner *et al.*, 2007).
[d] This variable corresponds to M1 of the $[M+H]^+$ ion.

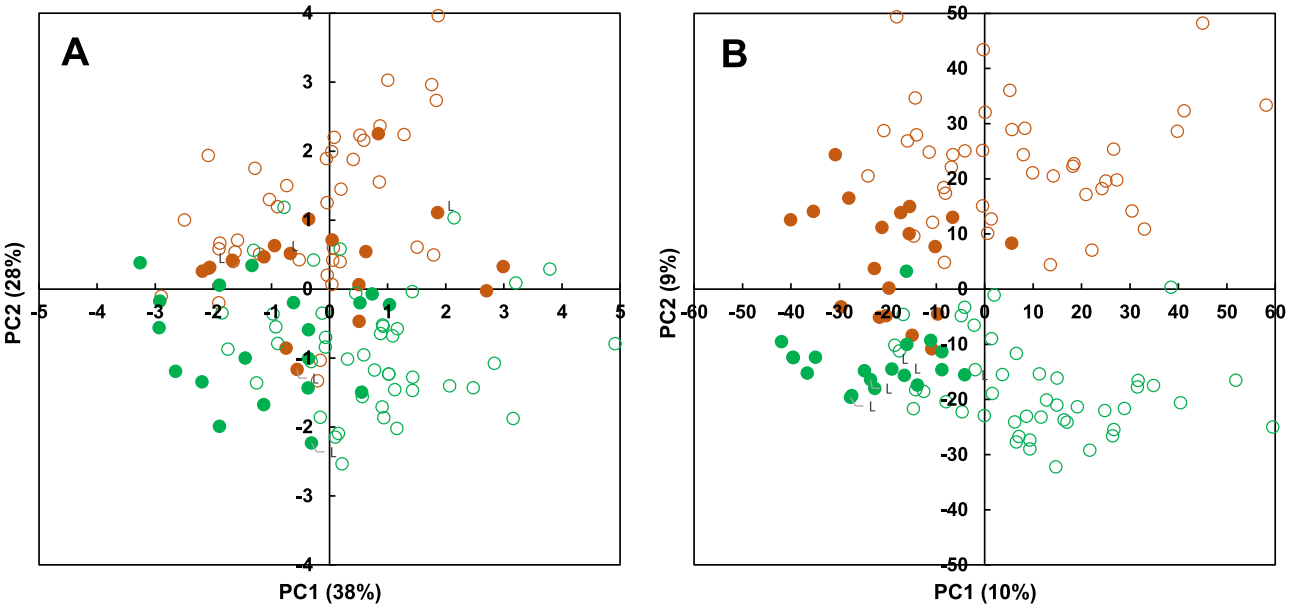

Fig. 1. Principal component analysis of sunflower leaf metabolomic data obtained using targeted measurements of major compounds and untargeted LC-MS-Orbitrap analyses of ethanolic extracts. Leaves were harvested on parental lines (closed symbols) and their hybrids (open symbols) cultivated in Heliaphen phenotyping facility in well-watered or water-deficit conditions. A. Scores plot on the PC1 × PC2 plan for targeted measurements (6 variables). B. Scores plot on the PC1 × PC2 plan for LC-MS profiles (4843 variables). Green, well-watered; Orange, water-deficit.

(Fernandez *et al.*, 2019; Stelzner *et al.*, 2019) was performed using RT, accurate m/z and fragment ions from an MS/MS acquisition of an aliquot of the QC sample. This resulted in the annotation of 18 compounds belonging to eight compound families (Tab. 1). All chemicals for LC-MS analyses were purchased from Sigma Aldrich (Saint-Quentin Fallavier, France) and Extrasynthèse (Genay, France).

Finally, due to plant death or the lack of leaf material for several plants, 121 and 125 samples out of the 144 initial ones were analysed by the targeted (6 variables) and LC-MS based metabolomic (4843 variables) approaches, respectively. To get an overview of each data set, a principal component analysis (PCA) was performed using BioStatFlow web tool (Jacob *et al.*, 2020) on data mean-centred and scaled to unit variance. The two treatments tended to separate along PC2 explaining about 28% of total variability for the targeted analyses (Fig. 1A) and about 9% for the LC-MS based data (Fig. 1B). The lines and hybrids tended to separate along PC1 explaining about 10% of total variability for the LC-MS based data (Fig. 1B). These metabolome data can be combined with other omic and phenotypic data of the same samples (Blanchet *et al.*, 2018; Gody *et al.*, 2020; Balliau *et al.*, 2021) to get deeper insights into drought effects and heterosis.

Supplementary material

DATA-TargetedAnalyses-SunflowerLeaf.txt: This file contains targeted measurements of major compounds for each genotype and their three biological replicates (in columns) for WW and WD conditions.

DATA-LCMS-SunflowerLeaf.txt: This file contains the intensities of LC-MS-Orbitrap metabolite signatures for each genotype and their three biological replicates (in columns) for WW and WD conditions.

The Supplementary Material is available at http://www.ocl-journal.org//10.1051/ocl/2021029/olm.

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Conflicts of interest. The authors declare that they have no conflicts of interest in relation to this article.

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