

## Supplementary Material

### **A Comparative Metabolomic Study on Desi and Kabuli Chickpea (*Cicer arietinum* L.) genotypes under Rainfed and Irrigated Field Conditions**

Zaib Un Nisa<sup>a</sup>, Anjuman Arif<sup>c</sup>, Muhammad Qandeel Waheed<sup>c</sup>, Tariq Mahmood Shah<sup>c</sup>, Ayesha Iqbal<sup>b</sup>, Amna Jabbar Siddiqui<sup>b</sup>, Muhammad Iqbal Choudhary<sup>a,b,d</sup>, Hesham R. El-Seedi<sup>e,f</sup>, Syed Ghulam Musharraf<sup>a,b\*</sup>

<sup>a</sup> *H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan*

<sup>b</sup> *Dr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan*

<sup>c</sup> *Nuclear Institute for Agriculture & Biology (NIAB), Faisalabad-38000, Pakistan*

<sup>d</sup> *Department of Biochemistry, Faculty of Science, King Abdulaziz University, Jeddah-21589, Saudi Arabia*

<sup>e</sup> *Pharmacognosy Group, Department of Medicinal Chemistry, Uppsala University, Biomedical Centre, Box 574, 75 123 Uppsala, Sweden*

<sup>f</sup> *Alrayan Medical College, Medina 42541, Kingdom of Saudi Arabia*

\* Corresponding author. Tel.: +92 21 34824924-5; 34819010; fax: + 92 21 34819018-9.

E-mail address: musharraf1977@yahoo.com

**Table S1:** Environment description of control and drought experiments during October 2016 to March 2017.

Experiment	Environment	October	November	December	January	February	March	Average
<b>Control (Irrigated):</b>								
<i>Faisalabad</i>	<b>Temp (min)</b>	23	17	13	10	13	17	15
Latitude: 31.450	<b>Temp (max)</b>	37	29	24	24	26	32	29
Longitude: 73.135	<b>Sunny days</b>	31	28	31	31	25	22	28
Soil type: Silt loam or very fine sandy loam*	<b>Rain fall</b>	0	0	0	13	84	32	22
	<b>Humidity</b>	17	23	24	26	35	33	26
<b>Drought (Rainfed):</b>								
<i>Kallur kot</i>	<b>Temp (min)</b>	25	17	13	11	13	20	16
Latitude: 32.156	<b>Temp (max)</b>	36	27	23	22	24	31	27
Longitude: 71.272	<b>Sunny days</b>	31	29	30	31	22	20	27
Soil type: Sandy loam**	<b>Rain fall</b>	0	2	0	0	5	9	2
	<b>Humidity</b>	15	23	21	22	34	34	25

Temperature is measured in °C (minimum and maximum), average rainfall in mm and humidity in %.

\*Silt soils are fertile, light but moisture-retentive and easily compacted.

\*\*Sandy loams are capable of quickly draining excess water and usually deficient in micronutrients, especially zinc and iron.

**Table S2:** Confusion matrix of model generated on data of rainfed and control desi type of plants (26 lines).

	Control Predicted	Rainfed predicted	Accuracy
True control	26	0	100.00
True drought	0	25	100.00
Overall Accuracy			100.00

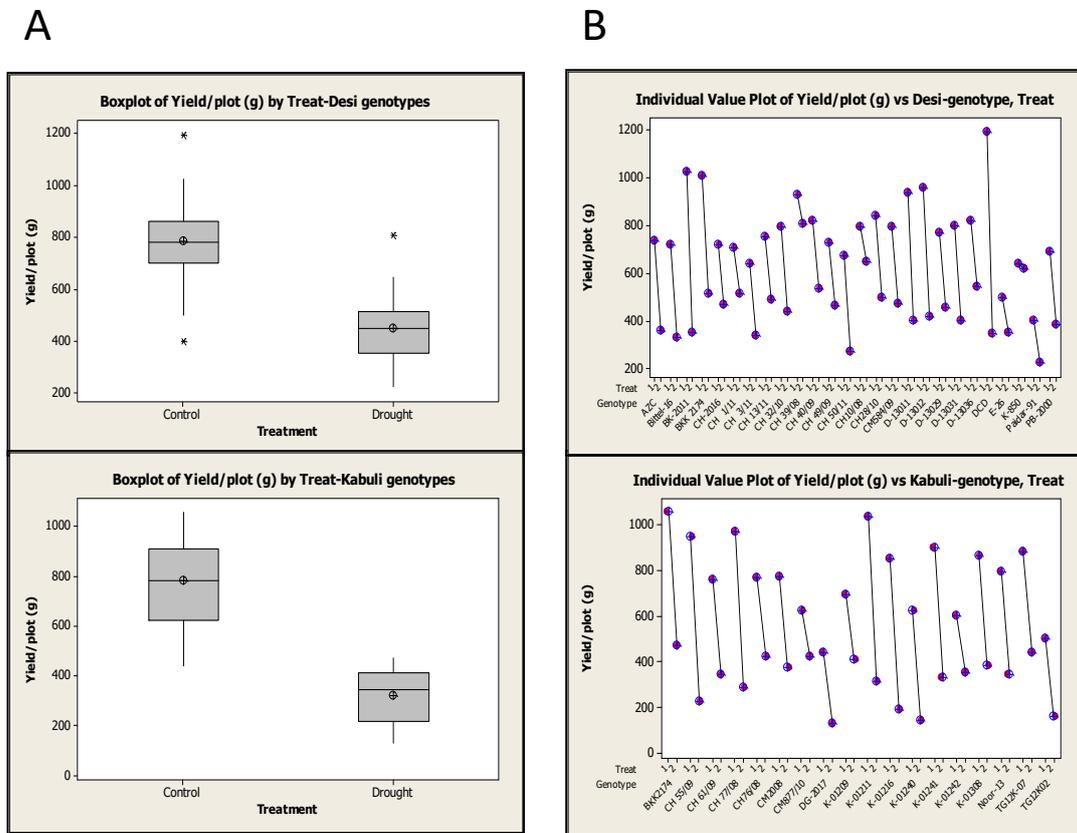
**Table S3:** Confusion matrix of model generated on data of rainfed and control kabuli type of plants (18 lines).

	Control Predicted	Rainfed predicted	Accuracy
True control	16	1	94.11
True drought	0	18	100.00
Overall Accuracy			97.14

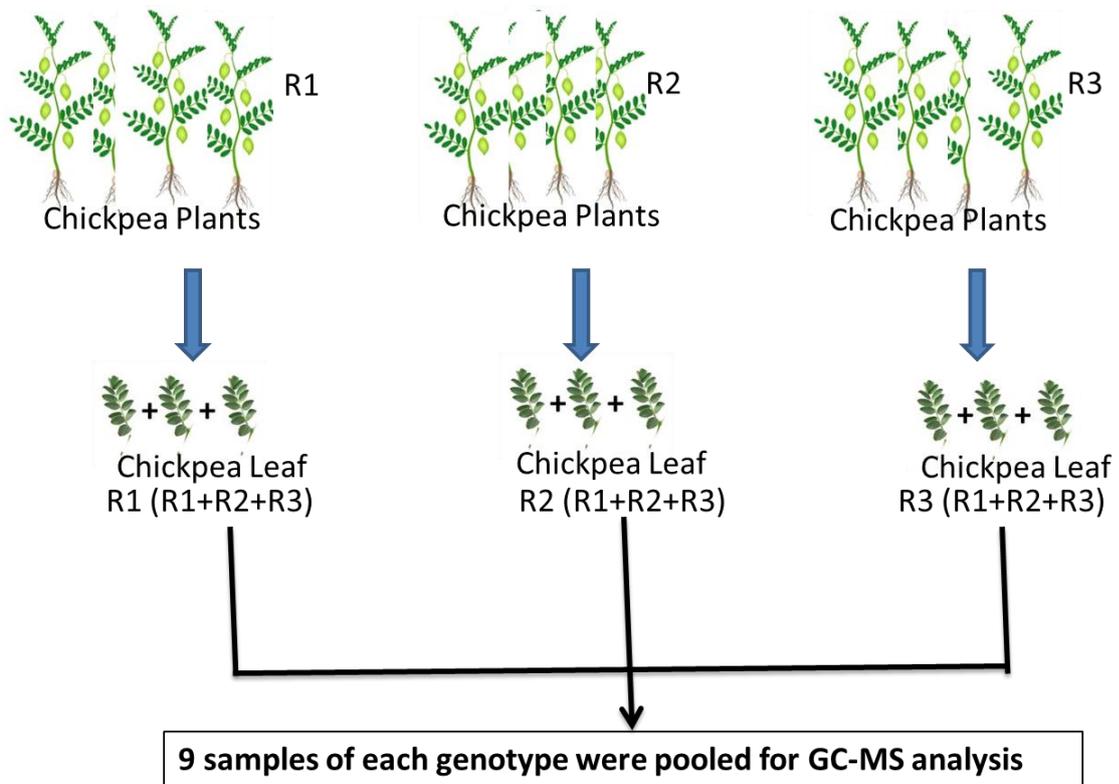
**Table S4.** List of altered metabolites in desi and kabuli groups of chickpea plant samples under rainfed condition *versus* irrigated control.

Cluster name	Cluster size	p-values	FDR	Key compound	Altered metabolites	Increased	Decreased	Increased ratio	Altered Ratio
<b>Cluster level enrichment result of desi chickpea genotype</b>									
Dicarboxylic Acids	4	2.2E-20	3.3E-20	Threonic acid	4	1	3	0.2	1
Sugar Alcohols	4	2.2E-20	3.3E-20	Xylitol	4	2	2	0.5	1
Hexoses	4	6.3E-14	6.3E-14	$\alpha$ -D-Glucopyranoside	4	3	1	0.8	1
<b>Cluster level enrichment result of kabuli chickpea genotypes</b>									
Monosaccharides	4	3.2E-09	9.5E-09	Mannofuranoside	4	0	4	0	1
Disaccharides	3	1.10E-08	1.60E-08	Maltose	3	0	3	0	1
Dicarboxylic Acids	4	8.40E-08	8.40E-08	Oxalic acid	4	0	4	0	1

**Figure S1:** Box plot of mean (A) and individual value (B) of chickpea genotypes in non-stressed (control) and stressed (drought) conditions

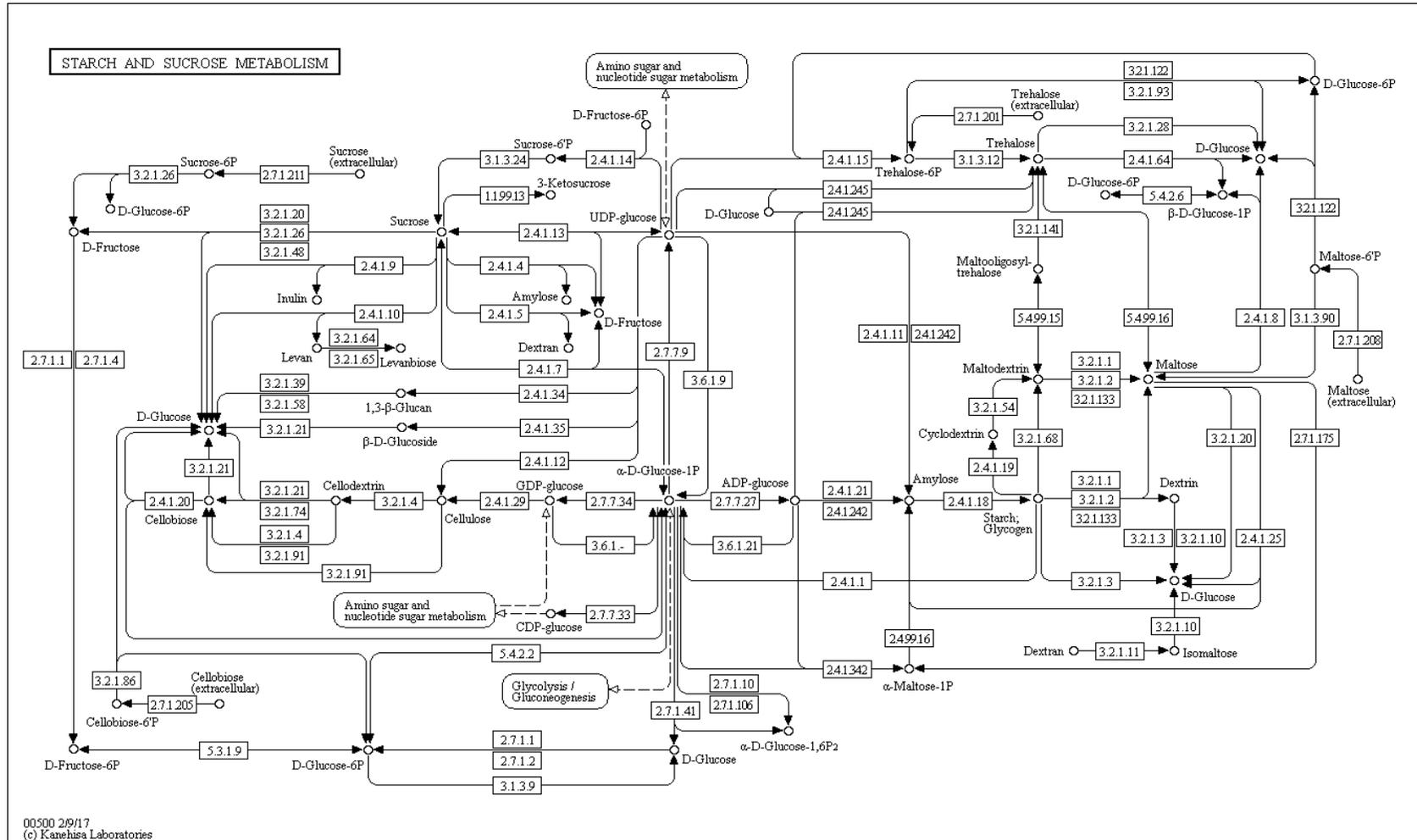


**Figure S2:** A diagrammatic representation of sample collection for metabolite analysis



**Figure S3:** Pathways generated by list of metabolites discriminating between irrigated controls and drought stressed samples of chickpea plants.

Starch and sucrose metabolism [1]



**Figure S4:** Citrate cycle (TCA cycle) [1].

