

Table S1. Metabolites and their chemical formulas from *A. sativa* leaves

№	tr, min	Compound	Chemical formula
1	7.01	Alanine	C ₃ H ₇ NO ₂
2	9.37	Valine	C ₅ H ₁₁ NO ₂
3	10.59	Leucine	C ₆ H ₁₃ NO ₂
4	10.69	Phosphoric acid	H ₃ PO ₄
5	11.06	Proline	C ₅ H ₉ NO ₂
6	11.44	Succinic acid	C ₄ H ₆ O ₄
7	11.95	Glyceric acid	C ₃ H ₆ O ₄
8	12.09	Itaconic acid	C ₅ H ₆ O ₄
9	12.57	Serine	C ₃ H ₇ NO ₃
10	13.15	Threonine	C ₄ H ₉ NO ₃
11	15.25	Malic acid	C ₄ H ₆ O ₅
12	15.79	5-Oxoproline	C ₅ H ₇ NO ₃
13	15.93	Aminobutyric acid	C ₄ H ₉ NO ₂
14	16.45	Erythronic acid	C ₄ H ₈ O ₅
15	17.79	Glutamic acid	C ₅ H ₉ NO ₄
16	19.30	Xylose	C ₅ H ₁₀ O ₅
17	19.89	Ribitol	C ₅ H ₁₂ O ₅
18	19.99	Adonitol	C ₅ H ₁₂ O ₅
19	20.15	Aconitic acid	C ₆ H ₆ O ₆
20	21.55	Fructose	C ₆ H ₁₂ O ₆
21	22.11	Allose	C ₆ H ₁₂ O ₆
22	22.34	Quinic acid	C ₁₁ H ₉ NO ₃
23	22.88	Mannose	C ₆ H ₁₂ O ₆
24	23.65	Ascorbic acid	C ₆ H ₈ O ₆
25	24.38	Glucose	C ₆ H ₁₂ O ₆
26	24.82	Palmitic Acid	C ₁₆ H ₃₂ O ₂
27	25.99	Myo-Inositol	C ₆ H ₁₂ O ₆
28	27.29	Linoleic acid	C ₁₈ H ₃₂ O ₂
29	27.40	Linolenic acid	C ₁₈ H ₃₀ O ₂
30	27.75	Stearic acid	C ₁₈ H ₃₆ O ₂
31	29.41	Glyceryl-glycoside	C ₉ H ₁₈ O ₈
32	32.02	Maltose	C ₁₂ H ₂₂ O ₁₁
33	33.80	Sucrose	C ₁₂ H ₂₂ O ₁₁
34	35.00	Mannobiose	C ₁₂ H ₂₂ O ₁₁
35	36.34	Melibiose	C ₁₂ H ₂₂ O ₁₁
36	37.42	3-O-Feruloylquinic acid	C ₁₇ H ₂₀ O ₉
37	37.84	Galactinol	C ₁₂ H ₂₂ O ₁₁
38	38.34	3-O-Coumaroyl-D-quinic acid	C ₁₆ H ₁₈ O ₈
39	39.64	5-O-Feruloylquinic acid	C ₁₇ H ₂₀ O ₉
40	39.82	Chlorogenic acid	C ₁₆ H ₁₈ O ₉
41	42.22	Raffinose	C ₁₈ H ₃₂ O ₁₆