

SUPPLEMENTARY MATERIAL

to the article N.Yu. Malysheva, T.V. Shelenga, A.E. Solovyeva, T.B. Nagiev, N.V. Kovaleva, L.L. Malyshev
 "Metabolomic approach to investigate *Dactylis glomerata* L. from the VIR collection"

Composition and content of the metabolomes in cocksfoot, mg/100 g
 (Leningrad Research Agriculture Institute Branch of Russian Potato Research Centre, 2018)

Name	$X \pm S_x$	Min-max	CV, %
Free amino acids and nucleoside			
Valine	11.51 ± 1.513	4.79–24.18	50.9
Alanine	15.97 ± 4.282	0.21–48.49	103.9
Leucine	3.64 ± 0.862	0.51–13.40	91.8
Isoleucine	5.03 ± 0.801	0.70–11.02	61.7
Serine	15.07 ± 2.428	0.79–31.76	62.4
Glycine	0.85 ± 0.180	0.00–3.07	82
Asparagine	0.26 ± 0.233	0.00–0.46	341.7
Asparagine acid	16.61 ± 2.677	2.05–46.98	62.4
Pipecolic acid	9.81 ± 11.842	1.19–27.58	72.8
Threonine	5.22 ± 0.852	0.87–12.00	63.2
Phenylalanine	3.61 ± 0.806	0.00–10.37	86.4
Tyrosine	6.24 ± 0.643	2.30–11.09	39.9
Tryptophan	10.69 ± 0.795	5.41–16.08	28.8
Glutamic acid	5.76 ± 2.045	0.62–44.06	137.5
Glutamine	27.53 ± 2.921	0.00–31.86	41.1
Proline	7.24 ± 1.571	3.24–24.27	84.0
Oxyprolinic acid	47.76 ± 2.790	28.06–68.79	22.6
N-Acetylglutamic acid	6.93 ± 1.803	1.51–28.43	100.7
Ornithine	0.31 ± 0.096	0.07–1.59	120.5
Adenosine	7.16 ± 1.160	1.42–17.14	62.7
Sum	207.18 ± 18.987	91.77–346.08	35.5
Organic acids			
Lactic	30.59 ± 1.798	20.12–42.43	22.8
Oxalic	7.68 ± 1.101	2.09–17.40	55.5
Pyruvic	4.72 ± 0.226	3.30–6.30	18.5
Me-malonic	0.02 ± 0.018	0.00–0.25	283.1
Phosphoric	248.64 ± 24.550	140.95–536.97	38.2
Maleic	7.64 ± 0.991	1.25–16.02	50.3
Succinic	75.72 ± 7.338	31.58–123.57	37.5
Glyceric	28.55 ± 1.423	18.10–36.81	19.3
Citraconic	0.11 ± 0.105	0.00–1.58	387.3
Fumaric	102.22 ± 19.994	16.85–269.21	75.8
Malic	1121.50 ± 90.466	265.67–1667.06	31.2
Erythronic	6.21 ± 0.361	2.99–8.63	22.5
Threonic	64.68 ± 5.635	40.02–131.45	33.7
Tartaric	1.50 ± 0.227	0.57–3.51	58.6
Aconitic	1.22 ± 0.494	0.30–8.00	156.9
Ketogluconic	17.82 ± 1.024	9.40–25.13	22.3
Ribonic	31.55 ± 2.798	14.42–50.65	34.4
Azelaic	2.06 ± 0.511	0.71–3.70	95.9
Citric	45.31 ± 9.138	10.55–115.68	78.1

Supplementary Material (continued)

Name	$\bar{X} \pm S_x$	Min–max	CV, %
Gluconic	9.88 ± 0.566	3.63–13.32	22.2
Glucaric	7.64 ± 1.317	0.97–17.59	66.8
DH-abietinic	4.23 ± 0.926	0.00–10.58	84.8
Sum	1819.48 ± 113.934	1074.83–2579.87	24.3
Lactones			
Erythrono-1,4-lactone	7.92 ± 0.622	4.93–11.73	30.4
Glucono-1,4-lactone	118.00 ± 15.039	41.51–211.31	49.4
Glucono-1,5-lactone	1.54 ± 0.691	0.00–6.89	174.0
Sum	127.46 ± 14.947	46.44–220.16	45.4
Phosphates			
Methylphosphate	2.15 ± 0.194	1.10–3.741	35.0
Glycerol-5-phosphate	17.54 ± 1.087	7.25–21.935	24.0
Glucose-1-phosphate	1.13 ± 0.521	0.00–5.510	178.4
Phosphate	7.52 ± 1.697	0.00–24.758	87.5
Gluconic-6-phosphate	2.71 ± 0.491	0.00–6.056	70.2
Myo-inositol-2-phosphate	2.72 ± 0.516	0.00–6.000	73.6
Sum	33.76 ± 2.817	16.68–52.992	32.3
Glycosides			
Methylpentofuranoside	4.06 ± 0.470	0.76–7.83	44.8
Methylmannoside	0.41 ± 0.107	0.00–1.42	101.5
Methylglucofuranoside	330.32 ± 53.359	16.91–734.99	62.6
Antirrinoside	9.63 ± 4.867	0.00–63.48	195.8
Lupeol	1.17 ± 0.978	0.00–14.70	323.8
Sum	346.60 ± 52.814	25.31–761.111	59
Sterols			
Camosterol	7.80 ± 0.608	2.34–11.47	30.2
Stigmasterol	1.65 ± 0.195	0.89–3.41	45.6
β-sitosterol	24.57 ± 1.902	12.14–39.78	30.0
STRSum	34.03 ± 2.560	15.92–53.7	29.1
Alkanes			
Pentacosane nC25	0.75 ± 0.561	0.00–7.992	289.6
Octacosane nC28	7.94 ± 1.071	0.90–14.76	52.2
Nonacosan nC29	9.60 ± 0.459	0.00–6.88	296.2
Hentriacontane nC31	1.57 ± 1.124	0.00–16.95	278.0
Sum	10.86 ± 1.823	3.83–30.07	65.0
Phenolic compounds			
Benzoic	1.37 ± 0.195	0.45–3.183	55.1
Nicotinic	0.55 ± 0.133	0.00–1.682	93.3
H-quinone	1.34 ± 0.190	0.43–2.465	54.8
Resorcinol	1.19 ± 0.226	0.28–3.625	73.7
4-HO-benzoic	0.65 ± 0.139	0.17–1.635	83.3
Pyrogallol	3.04 ± 0.560	1.23–9.693	71.3
Protocatechuic	2.20 ± 0.306	0.00–5.103	53.8
Shikimic	342.76 ± 44.202	32.67–647.955	49.9
Quinic	829.91 ± 77.363	78.41–1267.766	36.1

Supplementary Material (continued)

Name	$X \pm S_x$	Min-max	CV, %
(E)-4-HO-cinnamic	22.85 ± 3.144	7.63–41.288	53.3
Coniferyl alcohol	17.22 ± 2.193	4.56–34.912	49.3
2,3-DHO-benzoic	0.09 ± 0.063	0.00–0.860	278
(E)-Ferulic	6.51 ± 1.165	3.33–18.371	69.3
Caffeic	24.96 ± 2.185	12.78–45.256	33.9
α-tokoferol	1.04 ± 0.139	0.43–2.089	51.8
Chlorogenic	21.05 ± 3.851	1.24–64.437	70.9
C-chlorogenic	4.26 ± 1.096	0.00–13.056	99.6
N-chlorogenic	10.05 ± 2.177	1.20–34.193	83.9
Plumbagin	1.01 ± 0.118	0.13–1.80	45.2
Sum	1292.06 ± 115.766	165.27–1788.160	34.7
Sugars			
Glyceraldehyde	3.65 ± 0.321	1.48–6.44	34.0
Arabinose	2.13 ± 0.601	0.21–8.02	109.6
Lyxose	0.48 ± 0.232	0.00–2.64	188.6
Rhamnose	1.05 ± 0.265	0.09–4.02	98.1
Ribose	1.75 ± 0.163	0.70–3.09	36.2
Xylose	0.38 ± 0.174	0.00–1.95	178.4
Altrose	6.05 ± 0.747	0.00–11.60	47.8
Fructose	1083.73 ± 133.034	307.51–2275.03	47.5
Sorbose	116.41 ± 13.486	35.19–239.39	44.9
Galactose	209.20 ± 27.611	25.80–420.29	51.1
Mannose	523.92 ± 65.932	135.68–1001.43	48.7
Glukosamin	6.23 ± 1.139	0.48–12.28	70.8
Glucose	898.49 ± 97.877	256.50–1755.90	42.2
Monosaccharides	2853.46 ± 309.971	766.94–5481.62	42.1
Sucrose	1132.26 ± 96.207	295.73–1770.49	32.9
Maltose	4.10 ± 0.700	1.23–12.30	66.2
Rutinose	1.34 ± 0.418	0.00–5.72	120.8
Raffinose	8.42 ± 1.600	2.09–27.19	73.5
Oligosaccharides	1146.12 ± 96.014	300.47–1784.41	32.4
Sum	3999.57 ± 378.093	1067.41–7266.02	36.6
Fatty acids			
Pelargonic acid	0.32 ± 0.079	0.00–0.92	96.2
Undecylic acid	0.89 ± 0.177	0.00–1.85	76.7
Palmitic acid	58.79 ± 3.463	31.82–82.52	22.8
Oleic acid	25.60 ± 4.390	7.30–68.90	66.5
Linoleic acid	42.29 ± 3.286	17.90–61.71	30.1
Linolenic acid	31.07 ± 5.373	10.17–78.47	67
Stearic acid	16.43 ± 1.404	8.12–29.45	33.1
Behenic acid	1.88 ± 0.495	0.00–6.81	101.8
Lignoceric acid	0.41 ± 0.314	0.00–4.73	297.7
Hydroxyoctadecadienoic acid	0.82 ± 0.147	0.00–1.33	69.5
Cerotic acid	7.18 ± 1.064	0.69–13.82	57.4

Supplementary Material (end)

Name	$X \pm S_x$	Min-max	CV, %
Monoacylglycerol palmitic acid MAG1-C16:0	10.31 ± 0.644	5.97-15.72	24.2
Monoacylglycerol stearic acid MAG1-C18:0	4.12 ± 0.841	0.00-10.37	79
Sum	185.69 ± 13.295	82.70-297.30	27.7
Alcohols			
Ethanolamin	0.24 ± 0.174	0.00-2.66	276.1
Glycerol	33.52 ± 3.478	16.64-66.37	40.2
Erytritol	3.68 ± 0.593	1.02-9.91	62.5
Trietol	0.35 ± 0.350	0.00-5.25	387.3
Xylitol	4.96 ± 0.341	2.35-8.15	26.6
Arabinitol	24.39 ± 1.663	13.96-37.70	26.4
Sorbitol	10.33 ± 1.453	0.00-20.83	54.5
Dulcitol	7.26 ± 4.201	0.00-63.90	224
H-inositol	0.79 ± 0.788	0.00-11.82	387.3
Me-inositol	12.83 ± 5.912	0.00-89.64	178.5
Myo-inositol	32.29 ± 5.621	16.06-102.28	67.4
Phytol	0.98 ± 0.224	0.00-3.20	88.3
Galactinol	33.82 ± 5.119	6.60-85.80	58.6
Sum	179.87 ± 11.759	119.58-269.02	25.3