molecules

MDPI

Supplementary Materials for

Composition of Primary and Secondary Metabolite Compounds in Seeds and Pods of Asparagus Bean (*Vigna unguiculata* (L.) Walp.) from China

Table S1. The content of primary and secondary metabolite compounds in *Vigna unguiculata* (L.) Walp. seeds (ppm (mg/kg)/ dry matter).

Metabolite compound	Mean	Minimum	Maximum	Standard Error
Oxalate	35	22	57	11
Lactic acid	120	85	150	19
Pyruvic acid	22	10	30	6
Glyceric acid	18	18	18	0
Succinic acid	13	6	20	4
Malic acid	95	56	133	22
Citric acid	436	268	665	119
Nicotinic acid	10	6	16	3
Azelaic acid	34	17	45	9
4-Hydroxybenzoic acid	4	3	6	2
Protocatechuic acid	31	21	46	8
Fumaric acid	6			
Valine	9	5	15	3
Leucine	6	4	7	1
Isoleucine	2			
Threonine	18	5	43	12
Phenylalanine	79	30	111	25
Tryptophan	21	4	37	9
α-Alanine	16	10	23	4
Glycine	62	21	98	22
Proline	10	5	15	5
Serine	16			
Tyrosine	9	5	11	2
Aspartic acid	57	29	84	28
Asparagine	42	11	67	17
Glutamic acid	50	39	57	5
Oxoproline	62	30	95	19
Ornithine lactam	12	6	15	3
Glycerol-3-phosphate	12	11	13	1
Fructose	15	9	24	5
Sorbose	9	6	13	2
Mannose	19	10	27	5
Glucose	20	15	29	4
Sucrose	13509	11807	15281	1003
Raffinose	2013	862	2794	588
Xylitol	6			
Glycerol	112	80	145	19
Arabinitol	19	6	39	10
Sorbitol	55	39	67	8
Myo-inositol	216	73	448	117
Galactinol	452	373	599	74
Methyl-inositol	205	164	242	23

Myo-inositol-2-phosphate	65	58	77	6
4-Hydroxybenzoic acid	4	3	6	2
Protocatechuic acid	31	21	46	8
Nicotinic acid	10	6	16	3
Pyrogallol	15			
Catechin+epi-Catechin	14	11	19	3
Undecylic acid	26	21	32	3
Palmitic acid	359	261	471	61
Stearic acid	94	91	97	2
Arachidic acid	17	16	18	1
Behenic acid	45	26	75	15
Lignoceric acid	20	15	27	4
Lignoceric asid-methyl-ester	20	19	21	1
Oleic acid	245	65	502	132
Linoleic acid	469	322	701	117
Linolenic acid	162	95	228	66
Linolenic acid-methyl-ester	431	48	1117	344
Acylglycerols	129	111	153	12
Cholesterol	23			
Isofucosterol	162			
Campesterol	107	31	182	44
Stigmasterol	217	195	232	12
β-Sitosterol	198	151	223	23
Cycloartenol	110	43	204	48
Adenosine	27	6	50	13
Urea	289	271	319	15
Methyl-phosphate	8	4	11	2
Phosphoric acid	2407	2127	2885	240
Protein*	27,10	26,75	27,51	0,22

* - content in %/ dry matter

Table S2. The content of primary and secondary metabolite compounds in *Vigna unguiculata* (L.) Walp. pods of old Chinese landraces and the modern cultivars 'Yunanskaya' and 'Sibirskiy razmer' (ppm (mg/kg)/ dry matter).

Organic compound	Mean	Minimum	Maximum	Standard Error
Oxalate	57	10	85	14
Lactic acid	294	134	808	130
3-Hydroxypropionic acid	21	10	39	5
Pyruvic acid	26	22	30	1
Glyceric acid	53	20	75	10
Succinic acid	397	78	1055	183
Malic acid	472	272	9209	117
Fumaric acid	7	4	10	1
Tartaric acid	14	6	26	4
Citric acid	257	101	367	52
2-Ketoglutaric acid	23			
Threonic acid	171	34	338	50
Erythronic acid	55	15	110	17
Ribonic acid	40	2,18	6,51	0,79
Gluconic acid	350	206	501	55
Saccharic acid	22	15	28	6
Nicotinic acid	24	17	30	2
Benzoic acid	13			
Azelaic acid	50	23	112	17

4-Hydroxybenzoic acid	51	27	115	16
Protocatechuic acid	7	4	9	3
4-Hydroxycinnamic acid	104	59	162	24
Erythrono-1,4-lactone	28			
Valine	720	504	912	79
Leucine	112	27	301	49
Threonine	313	150	545	64
Methionine	58	9	96	14
Phenylalanine	616	401	873	79
Tryptophan	420	351	538	31
Arginine	63	17	153	24
α-Alanine	951	783	1147	68
Glycine	3705	1333	5684	841
Proline	4889	3665	7372	672
Serine	1069	801	1349	97
Tyrosine	262	142	560	76
Aspartic acid	212	152	308	26
Asparagine	2598	817	4892	712
Glutamic acid	239	130	427	55
Glutamine	1002	147	1955	367
Ornithine	140	32	218	30
β-Alanine	66	25	131	21
GABA	1493	828	2481	310
Hydroxyproline	234	197	272	37
Oxoproline	733	137	1584	236
Norleucine	268	238	290	16
Pipecolic acid	19	14	26	2
Ornithine lactam	500	233	786	109
Glycerol-3-phosphate	249	51	404	104
Ribose	52	3	174	32
Fructose	2090	280	7451	1360
Altrose	23	11	47	6
Sorbose	490	128	1325	213
Galactose	53	10	199	37
Mannose	728	162	2207	374
Glucose	813	155	3051	561
Rhamnose	10	6	16	2
Sucrose	31519	25953	37615	1907
Raffinose	1083	320	3249	548
Methylglucoside	24	17	37	4
Glucosamine	17	6	29	4
Galactose MeOX	49	47	51	2
Glycerol	9848	499	1973	279
Arabinitol	218	113	490	71
Erythritol	100	38	238	36
Mannitol	753	341	1761	264
Dulcitol	1330	549	3096	458
Myo-inositol	1338	358	3261	569
Ononitol	29	16	35	3
Galactinol	624	240	906	109
Methyl-inositol	37	13	57	7
Desoxyglucitol	55	39	83	8

Myo-inositol-2-phosphate	11	8	15	3
Ethanolamine	65	44	101	10
Phytol	104	80	157	14
Phytosphingosine	37	10	51	8
Salicylic acid	16	14	18	2
4-Hydroxybenzoic acid	51	27	115	16
Protocatechuic acid	7	4	9	3
4-Hydroxycinnamic acid	104	59	162	24
Catechin+epi-Catechin	67	17	108	21
Gallocatechin	21	13	29	8
Baicalein	17	5	24	6
Undecylic acid	30	24	35	3
Palmitic acid	1009	609	1787	234
Stearic acid	308	209	528	58
Arachidic acid	49	15	72	10
Behenic acid	36	25	48	4
Lignoceric acid	66	32	98	13
Hydroxybehenic acid	8			
Hydroxylignoceric acid	33	17	67	9
Oleic acid	147	85	226	25
Linoleic acid	1016	412	2194	319
Linolenic acid	906	336	1987	305
Acylglycerols	196	55	439	69
Campesterol	336	219	444	37
Stigmasterol	956	743	1265	98
β-Sitosterol	1681	980	2076	195
α-Amyrin	60	16	121	20
β-Amyrin	294	196	523	62
Adenosine	127	46	250	34
Guanosine	79	54	104	25
Neophytadiene	94	73	115	21
Urea	446	181	780	102
Methyl-phosphate	20	16	27	2
Phosphoric acid	1667	1037	2274	236
Protein*	29,98	26,90	33,50	1,10

* - content in %/ dry matter

Table S3. The content of primary and secondary metabolite compounds in *Vigna unguiculata* (L.) Walp. pods of old Chinese landraces (ppm (mg/kg)/ dry matter).

Organic compound	Mean	Minimum	Maximum	Standard Error
Oxalate	71	47	85	12
Lactic acid	145	134	152	6
3-Hydroxypropionic acid	14	10	20	3
Pyruvic acid	24	22	25	1
Glyceric acid	39	20	51	10
Succinic acid	135	78	245	55
Malic acid	359	272	480	63
Fumaric acid	6	4	10	2
Tartaric acid	16	7	26	5
Citric acid	284	168	367	60
Threonic acid	102	34	137	34

Erythronic acid	33	15	57	12
Ribonic acid	46	25	65	12
Gluconic acid	302	206	441	71
Saccharic acid	22	15	28	6
Nicotinic acid	23	17	30	4
Azelaic acid	28	23	36	4
4-Hydroxybenzoic acid	32	27	39	4
Protocatechuic acid	7	4	9	3
4-Hydroxycinnamic acid	99	67	162	32
Leucine	49	27	61	11
Threonine	383	301	545	81
Methionine	74	62	96	111
Phenylalanine	564	401	668	83
Tryptophan	429	351	538	56
Arginine	33	17	48	9
α-Alanine	912	783	1076	86
Glycine	4471	2354	5684	1062
Proline	3977	3665	4426	230
Serine	1130	906	1349	128
Tyrosine	189	142	227	25
Aspartic acid	225	152	308	45
Asparagine	3182	1444	4892	996
Glutamic acid	183	130	284	50
Glutamine	1498	766	1955	370
Ornithine	149	137	161	7
β-Alanine	32	25	44	6
GABA	1025	828	1299	141
Hydroxyproline	272			
Oxoproline	986	636	1584	300
Norleucine	238			
Pipecolic acid	21	14	26	4
Ornithine-lactam	452	233	728	146
Glycerol-3-phosphate	51			
Ribose	8	3	13	3
Fructose	464	280	637	103
Altrose	15	10	18	2
Sorbose	243	128	311	58
Galactose	13	10	18	2
Mannose	309	162	402	74
Glucose	205	155	278	37
Rhamnose	10	7	14	2
Sucrose	29344	25953	32439	1878
Raffinose	439	320	547	66
α-Methylglucoside	28	19	37	5
Glucosamine	15	6	26	6
Glycerol	575	499	682	55
Arabinitol	124	113	146	11
Erythritol	54	38	70	9
Mannitol	416	341	565	75
Dulcitol	781	549	1085	159
Myo-inositol	467	358	618	78
Ononitol	26	16	32	5

Galactinol	658	614	736	39
Methyl-inositol	26	13	35	7
Desoxyglucitol	47	39	58	6
Myo-inositol-2-phosphate	11	8	15	3
Ethanolamine	59	44	70	8
Phytol	85	80	92	4
Phytosphingosine	31	10	51	12
4-Hydroxybenzoic acid	32	27	39	4
Protocatechuic acid	7	4	9	3
4-Hydroxycinnamic acid	99	67	162	32
Catechin+epi-Catechin	83	49	109	18
Baicalein	17	5	24	6
Undecylic acid	30	24	35	3
Palmitic acid	647	609	682	21
Stearic acid	243	209	297	27
Arachidic acid	34	15	47	10
Behenic acid	39	31	48	5
Lignoceric acid	68	32	98	19
Hydroxybehenic acid	8			
Hydroxylignoceric acid	38	21	67	15
Oleic acid	157	116	226	35
Linoleic acid	594	412	848	131
Linolenic acid	478	336	736	129
Acylglycerols	96	55	139	24
Campesterol	333	219	444	65
Stigmasterol	1026	755	1265	148
β-Sitosterol	1683	980	2076	352
α-Amyrin	85	43	121	23
β-Amyrin	352	203	523	93
Adenosine	87	46	115	21
Guanosine	54			
Urea	563	354	780	123
Methyl-phosphate	21	16	27	3
Phosphoric acid	1959	1448	2274	258
Protein*	31,33	29,50	33,50	1,17

* - content in %/ dry matter