

Supplementary material for *Chenopodium quinoa* Willd. and *Amaranthus hybridus* L.: Ancestral Andean Food Safety and Modern Anticancer and Anti-microbial Activity

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Table S1 : Phytochemicals from *Chenopodium quinoa* Willd.

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
Benzoic acid analogues							
1	Benzoic acid	x		Leaves and flour	N.D.	HPLC-DAD	[1,2]
2	4-hydroxybenzoic acid	x		Leaves and seeds	Antimicrobial	HPLC-DAD	[3]
3	2,4 -dihydroxybenzoic acid	x		Seeds	N.D.	HPLC-DAD	[3]
4	2,5 dihydroxybenzoic acid	x		Seeds	N.D.	HPLC-DAD-MS	[4]
5	3,4 dihydroxybenzoic acid	x		Seeds	N.D.	HPLC-DAD	
6	Canthoside	x		Flour	N.D.	HPLC-DAD	
7	<i>m</i> - Ethyl digallate	x		Flour	N.D.	HPLC-DAD	[2]
8	Gallic acid	x		Leaves, stems and seeds	Antibacterial Antioxidant	HPLC-DAD	[1,5]
9	1- O- Galloyl- β -D-glucose	x		Seeds	N.D.	HPLC-DAD	[2]
10	Protocatechuic acid	x		Stems and seeds	Anticancer Antibacterial Antioxidant	HPLC-DAD	[6,7]
11	Protocatechuic acid 4- O-glucoside	x		Flour	Antioxidant	HPLC-DAD	[2]
12	Syringic acid	x		Leaves and seeds	Antioxidant	HPLC DAD	[3,7]
13	Vanillic acid	x		Leaves and seeds	hepatoprotective Anti-inflammatory	HPLC DAD	[3,7,8]
14	Vanillic acid glycosidic ester	x		Seeds	N.D.	HPLC-UV-VIS	[9]
15	Vanillic acid 4- O-glucoside	x		Seeds	N.D.	HPLC-DAS-MS	[4]

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
16	Vanillin	x		Seeds	Antioxidant	HPLC-DAS-MS	[2,4,7]
Cinnamic acid analogues							
17	Caffeic acid	x		Seeds	Antioxidant	HPLC-DAD	[3,7]
18	Chlorogenic acid	x		Leaves and seeds	Antidiabetic	HPLC-DAD	[3,10]
19	Cinnamic acid	x		Stems and seeds	N.D.	HPLC-DAD	[11]
20	<i>o</i> - coumaric acid	x		Leaves and seeds	Antioxidant	HPLC-DAD	[3,7]
21	<i>p</i> - coumaric acid	x		Leaves and seeds	Antimicrobial	HPLC-DAD	[1,12]
22	<i>p</i> - coumaric acid glucoside	x		Seeds	N.D.	HPLC-DAS-MS	[4]
23	8,5'- diferulic acid	x		Seeds	N.D.	HPLC and LC-MS	[3]
24	Ferulic acid	x		Leaves, stems and seeds	Antibacterial Anticancer	HPLC-DAD-MS	[3,11,13]
25	Ferulic acid 4- O- glucoside	x		Flour	N.D.	HPLC-DAD	[2]
26	Isoferulic acid	x		Seeds	Antioxidant	HPLC-DAD	[4,14]
27	4' geranyloxyferulic acid	x		Seeds	N.D.	HPLC-DAD	[15]
28	Rosmarinic acid	x		Seeds	Antiviral Anti-inflammatory Antioxidant	HPLC-DAD	[3,16,17]
29	Sinapinic acid	x		Leaves and seeds	Antioxidant	HPLC-DAD	[1,18]
Flavones							
30	Acacetin	x		Flour	Anticancer Anti-inflammatory Contraceptive	HPLC-DAD	[2,19,20]
31	Isovitexin	x		Stems and seeds	Antioxidant Anti-inflammatory Antitumor	HPLC-DAD	[11,21]
32	Orientin	x		Seeds	Anticancer(Esmail et al., 2013)	HPLC-DAD	[11,22]
33	Vitexin	x		Stems and seeds	Antithrombotic Anticancer Anti-inflammatory	HPLC-DAD	[11,23,24]
Flavonols							
34	Kaempferol	x		Leaves and seeds	Antioxidant Antibacterial	HPLC -DAD- MS	[3,25]

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
35	Kaempferol -3-glucoside	x		Seeds	N.D.	HPLC-DAD-MS	[4,9]
36	Kaempferol -3-galactoside	x		Seeds	N.D.	HPLC-DAD-MS	[4,9]
37	Kaempferol 3-O-(2,6 di- α -L rhamnopyranosyl) β -D-galactopyranoside	x		Seeds	Antioxidant	HPLC-DAD-MS	[4,9]
38	Kaempferol 3- O- β -D apiofuranosyl (1 \rightarrow 2)-O- α -L rampyranosyl (1 \rightarrow 6)- β -D- galactopyran or been	x		Seeds	Antioxidant	HPLC-UV-VIS	[9]
39	Kaempferol 3- O- β -D apiofuranosyl (1 \rightarrow 2)- β -D-galactopyran or been	x		Seeds	Antioxidant	HPLC-UV-VIS	[9,26]
40	Kaempferol 3- O- α -L rhamnopyranosyl (1 \rightarrow 2)- β -D-galactopyran or been	x		Seeds	Antioxidant	HPLC-UV-VIS	[26]
41	Kaempferol 3- O- β -D glucuronic acid	x		Seeds	Antioxidant	HPLC-UV-VIS	[9]
42	Kaempferol 3,7 dirhamnoside	x		Seeds	N.D.	HPLC-DAD-MS	[4]
43	Isoharmentin	x		Leaves	Antitumor Anti-inflammatory Anticoagulant	HPLC-DAD	[11,27–29]
44	Quercetin	x		Leaves and seeds	Cytotoxic Antioxidant	HPLC-DAD-MS	[4,25,30]
45	Quercetin 3- O- glucoside	x		Flour	N.D.	HPLC-DAD	[2]
46	Quercetin 3 rutinoside	x		Seeds	N.D.	HPLC-DAD-MS	[4]
47	Quercetin 3 arabinoside	x		Seeds	N.D.	HPLC-DAD-MS	
48	Quercetin 3-O- β -D- apiofuranosyl-(1 \rightarrow 2) - α -L- rhamnopyranosyl -(1 \rightarrow 6)- β - D galactopyran or idoarabin or been	x		Seeds	Antioxidant	HPLC-UV-VIS	[26,31]
49	Quercetin 3- O- (2,6 di- α -L- rhamnopyranosyl) β -D galactopyranoside	x		Seeds	Antioxidant	HPLC-UV-VIS	[9,26]
50	Quercetin 3- O - (2,6 di- O - α rhamnopyranosyl) β -glucopyranoside	x		Seeds	N.D.	HPLC-UV-VIS	[31]
51	Quercetin 3- O- β -D- apiofuranosyl (1 \rightarrow 2) O- α -L-rhamnoporanosyl (1 \rightarrow 6)- β -D- galactopyran	x		Seeds	Antioxidant	HPLC- UV- Vis	[9]

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
	or been 3,4,5 dimethyl ether						
52	Rutin	x		Leaves, stems and seeds	Antidiabetic Antioxidant	HPLC-DAD	[10,11,32]
53	Morin	x		Stems and seeds	Anti-inflammatory Antitumor	HPLC-DAD-MS	[4,11,26]
54	Myricetin	x		Seeds	Apoptosis Antimicrobial Antihyperglycemic	HPLC	[33,34]
Flavanones							
55	Hesperidin	x		Seeds	Antitumor Antifungal Antioxidant	HPLC-DAD	[11,35,36]
56	Neohesperidin	x		Seeds	Cytotoxic Antifungal Anti-inflammatory	HPLC-DAD	[11,37]
57	Naringin	x		Seeds	Antioxidant Antifungal	HPLC-DAD-MS	[4,38,39]
Flavanols							
58	Catechin	x		Seeds	Antioxidant	HPLC-DAD	[3,40]
59	Epicatechin	x		Seeds	Antioxidant	HPLC-DAD-MS	[4,41]
60	Epigallocatechin	x		Seeds	Antioxidant	HPLC-DAD-MS	[4,42]
Isoflavones							
61	Biochanin A	x		Seeds		HPLC-DAD	[4]
62	Daidzein	x		Seeds	Antioxidant Antithroimbotic Antiproliferative	HPLC-UV-VIS	[43–45]
63	Genistein	x		Seeds	Antioxidant Anti-inflammatory Neuroprotective	HPLC-UV-VIS	[43,46,47]
64	Prunetin	x		Seeds	Anti-inflammatory	HPLC and LC-MS	[3,48]
65	Puerarin	x		Seeds	Anti-inflammatory	HPLC-DAD-MS	[4,49]
Monoterpenes							
66	<i>cis</i> - Ascaridol	x		Leaves	N.D.	GC-MS	
67	<i>cis</i> - Isoascaridol	x		Leaves	N.D.	GC-MS	[50]
68	Camphene	x		Leaves	N.D.	GC-MS	
69	Camphor	x		Leaves	N.D.	GC-MS	

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
70	<i>trans</i> - carveol	x		Leaves	N.D.	GC-MS	
71	<i>p</i> - Cimene	x		Leaves	N.D.	GC-MS	
72	<i>p</i> - menta 1(7), 8 diene	x		Leaves	N.D.	GC-MS	
73	<i>trans-p</i> - menta- 2 in- 1-ol	x		Leaves	N.D.	GC-MS	
74	Pentebioside	x		Flour	N.D.	HPLC-DAD	[2]
75	β- Pinene	x		Leaves	N.D.	GC-MS	
76	Pinocarvone	x		Leaves	N.D.	GC-MS	
77	α-Terpinene	x		Leaves	N.D.	GC-MS	[50]
78	γ-Terpinene	x		Leaves	N.D.	GC-MS	
79	Terpine-1-ol	x		Leaves	N.D.	GC-MS	
80	α-terpinyl acetate	x		Leaves	N.D.	GC-MS	
Sesquiterpenes							
81	Caryophyllene	x		Leaves	N.D.	GC-MS	[50]
Triterpenes							
Hederagenin and its derivatives							
82	Hederagenin	x		Seeds and bran	Cytotoxic Immunomodulator	GC-MS	[51,52]
83	3- O- α-L- Abinopyranosyl hederagenin		x	Seeds	Cytotoxic	HPLC-NMR	[53,54]
84	3- O- α-L- Abinopyranosyl hederagenin 28-O-β-D glucopyranosyl ester		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	[55]
85	3- O -β-D- glucopyranosyl (1 → 3)- α-L- arabinopyranosyl hederagenin	x		Seeds and bran	Cytotoxic	HPLC-NMR	[56,57]
86	3- O -β-D- glucopyranosyl (1 → 3)- β-D-galactopyranosyl hederagenin	x		Saved	N.D.	HPLC-NMR	[56]
87	3- O -β-D- glucopyranosyl (1 → 3)- α-L- arabinopyranosyl hederagenin 28-O-β-D glucopyranosyl ester	x		Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	[55]

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
88	3- O - β -D-glucopyranosyl (1 \rightarrow 3)-O- β -D- galactopyranosyl hederagenin 28-O- β -D glucopyranosyl ester	x		Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	
89	3- O - β -D-glucopyranosyl (1 \rightarrow 4)- β -D- glucopyranosyl hederagenin (1 \rightarrow 4)- β -D-glucopyranosyl hederegenin	x		Seeds	N.D.	HPLC-UV-VIS	[9]
90	3,23 Bis (O - β -D-glucopyranosyloxy) acid olean 12- en- 28-oic-28-O- β -D glucopyranosyl (1 \rightarrow 3)- α -L-arabinopyranosyl ester	x		Seeds	N.D.	GC-MS	[58]
91	3- O - β -D-glucopyranosyl hederagenin 28-O- β -D glucopyranosyl ester		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	[55]
92	3- O - β -D- xylopyranosyl (1 \rightarrow 3)- β -D-glucopyranosyl hederagenin ester 28-O- β -D glucopyranosyl		x	Saved	N.D.	HPLC-NMR	[56]
Spergulgagenic acid and its derivatives							
93	Spergulgagenic acid	x					
94	3- O - α -L-arabinopyranosyl- (1 \rightarrow 3)- β -D-acid gluciciranosyl spergulgagenic ester-28-O- β -D glucopyranosyl	x		Seeds	N.D.	HPLC-UV-VIS	[59]
95	3- O - β -D-glucopyranosyl (1 \rightarrow 2)- β -D-glucopyranosyl (1 \rightarrow 3) - α -L-arabinopyranosyl spergulgagenic acid	x		Saved	N.D.	HPLC-NMR	[56]
96	3- O - β -D-glucopyranosyl (1 \rightarrow 2)- β -D-glucopyranosyl (1 \rightarrow 3) - α -L-arabinopyranosyl acid spergulgagenic ester 28-O- β -D glucopyranosyl	x		Seeds	N.D.	HPLC-UV-VIS	[9]

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
Serjanic acid and its derivatives							
97	Serjanic acid		x	Flowers, fruits, seeds and bran	Cytotoxic	HPLC-NMR	[55,60]
98	3-O-β-D glucopyranosyl ester 3-O- α-L arabinopyranosyl serjanic acid		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	
99	3-O-β-D-glucopyranosyl- (1 → 3)- α -L- acid arabinopyranosyl serjanic 28 -O- β -D glucopyranosyl ester		x	Flowers, fruits, seeds and bran.	N.D.	HPLC-NMR	[55]
100	3-O-β-D- glucopyranosyl (1 → 2)- β-D- glucopyranosyl (1 → 3) - α-L-arabinopyranosyl ester		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	
101	3-O-β-D-glucopyranosyl serjanic 28-O—β-D glucopyranosyl ester		x	Flowers, fruits, seeds and bran	Cytotoxic	HPLC-NMR	
Phytolacagenic acid and its derivatives							
102	Phytocagenic acid		x	Saved	N.D.	HPLC-NMR	
103	3-O-α-L- arabinopyranosyl photolacagenic acid 28- O- β-D glucopyranosyl ester		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	[56]
104	3-O-α-L- arabinopyranosyl-(1 → 3)- β -D- acid glucopyranosyl phytolactide 28 -O- β -D glucopyranosyl ester	x		Seeds	N.D.	HPLC-UV-VIS	[9]
105	3-O-β-D galactopyranosyl- (1 → 3)- β -D acid glucopyranosyl phytolacagenic 28- O-β- D glucopyranosyl ester		x	Seeds	N.D.	MRI-MS	[26]
106	3-O - β-D glucopyranosyl (1 → 3)- α -L acid arabinopyranosyl phytolactide		x	Seeds	N.D.	HPLC-NMR	[53]

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
107	3-O-β-D glucopyranosyl (1 → 3)- α -L acid arabinopyranosyl phytolactide 28 -O- β -D glucopyranosyl ester	x		Flowers, fruits, seeds and bran	N.D.	HPLC-UV-VIS	
108	3-O-β-D glucopyranosyl (1 → 3)- β -D phytocaginic acid galactopyranoside ester 28-O-β-D glucopyranosyl ester	x		Flowers, fruits, seeds and bran	N.D.	HPLC-UV-VIS	
109	3-O-β-D glucopyranosyl (1 → 2)- β -D glucopyranosyl (1 → 3)- α -L phytocag onic acid arabinopyran or 28-O- β -D glucopyranosyl ester	x		Flowers, fruits, seeds and bran	N.D.	HPLC-UV-VIS	[9]
110	3-O-β-D glucopyranosyl (1 → 4)- β -D glucopyranosyl acid phytolacagenic 28-O-β-D glucopyranosyl ester	x		Flowers, fruits, seeds and bran	N.D.	HPLC-UV-VIS	
111	3-O-β-D glucopyranosyl (1 → 3)- β -D xylopyranosyl (1 → 2)- β -D glucopyranosyl acid phytocag enic 28-O- β -D glucopyranosyl ester	x		Seeds	N.D.	HPLC-UV-VIS	
112	Gypsogenin		x	Gypsogenin and its derivatives Flowers, fruits, seeds and bran	Cytotoxic	HPLC-NMR	
113	3-O-β-D- glucopyranosyl (1 → 3)- α -L arabinopyranosyl 23-oxo-olean-12-en-28-oic ester 28-O-β-D glucopyranosyl		x	Flowers, fruits, seeds and bran	Cytotoxic	HPLC-NMR	[55,61]
114	3- β- hydroxy 27- oxo- olean- 12- en- 28-oic acid		x		Cytotoxic	HPLC-NMR	
115	3-O-β-D- glucopyranosyl (1 → 3)- α -L arabinopyranosyl 27-oxo-olean-12-en-28-oic ester 28-O- β -D glucopyranosyl		x	Flowers, fruits, seeds and bran	Cytotoxic	HPLC-NMR	[55]

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
3- β ,23,30 trihydroxy oleanane 12- en-c 28- oic acid triterpenoids							
116	3- β ,23,30 trihydroxy oleanane 12- en-c 28- oic acid		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	
117	3-O- β -D- glucopyranosyl (1 \rightarrow 3)- α -L arabinopyranosyl acid 3- β ,23,30 - trihydroxyoleanane- 12-2n- 28-oic 28-O- β -D glucopyranosyl ester		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	[55]
Oleanolic acid and its derivatives							
118	Oleanolic acid		x	Seeds	Anticancer Anti-inflammatory Antimicrobial Antioxidant	HPLC-NMR	[56,62–65]
119	Methyl oleanate		x	Saved	Anti-inflammatory	HPLC-NMR	[56,66]
120	3-O- α -Arabinopyranosyl (1 \rightarrow 3) β -D- acid 28-O- β -D- glucopyranosyl ester glucopyranosyl olean olic ester	x		Seeds	N.D.	HPLC-UV-VIS	[59]
121	3- O- β -D- glucopyranosyl oleanolic acid		x	Seeds	Antidibaetic	TLC-MRI	[67,68]
122	3-O- β -D glucopyranosyl (1 \rightarrow 3) α -L acid arabinopyranosyl olean olic ester 28- O- β -D glucopyranosyl		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	[55]
123	3-O- β -D glucopyranosyl (1 \rightarrow 2) β -D glucopyranosyl (1 \rightarrow 3) α -L acid arabinopyranosyl olean olic 28- O- β -D glucopyranosyl ester		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	
124	Oleanolic acid 3- O- β -D glucopyranosyl		x	Seeds	N.D.	TLC-MRI	[67]
125	Oleanolic acid 3- O- β -D glucopyranosyl 28- O- D glucopyranosyl ester		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	[55]
126	3- O- D xylopyranosil (1 \rightarrow 3)- β -D glucopyranosyl oleanolic acid		x	Seeds	N.D.	TLC-MRI	[67]
127	3- O- D xylopyranosyl (1 \rightarrow 3)-6- methyl β -D		x	Seeds	N.D.	TLC-MRI	

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
128	glucopyranosyl oleanolic acid 3- O- β -D xylopyranosyl (1 \rightarrow 3)- β -D- glucopyranosyl acid oleanolic ester 28- O- β -D glucopyranosyl		x	Flowers, fruits, seeds and bran	N.D.	HPLC-NMR	[55]
Tetracyclic triterpenes							
129	Citrostadienol	x		Seeds	Anticomplementary activity	GC-MS	[69,70]
130	Gramisterol	x		Seeds	Anticancer	GC-MS	[69,71]
131	24-methylene cycloartenol	x		Seeds	N.D.	GC-MS	[69]
Pentacyclic triterpenes							
132	α - Amirin	x		Seeds	Antibacterial Antioxidant	GC-MS	[51,72,73]
133	β -Amyrin	x		Seeds	Antibacterial Antioxidant	GC-MS	
134	Erythrodiol	x		Seeds	N.D.	GC-MS	[51]
135	Echinocystic acid	x		Seeds	N.D.	GC-MS	
136	3 β , 23 Dihydroxy- oleano-12-en 28,30- dioic acid		x	Seeds	N.D.	HPLC-NMR	[53]
137	2 β , 3 β , 23 trihydroxy- olean-12-ene-acid 28,30- dioic 30- methyl ester		x	Saved	N.D.	HPLC-NMR	[56]
138	Queretaroic acid	x		Seeds	N.D.	GC-MS	[51]
139	Ursolic acid	x		Seeds	Antispasmodic Contraceptive anticarcinogen	GC-MS	[14,51,74]
Meroterpenoids							
140	α -Tocopherol	x		Seeds	Antioxidant Antihypercholesterolemic Anticancer Neuroprotect Antioxidant	HPLC-DAD	[6,75]
141	β -Tocopherol	x		Seeds	Antihypercholesterolemic Anticancer Neuroprotect Antioxidant	HPLC-DAD	
142	γ -Tocopherol	x		Seeds	Antihypercholesterolemic Antioxidant	HPLC-DAD	
143	δ -Tocopherol	x		Seeds	Antihypercholesterolemic Antioxidant	HPLC-DAD	
144	α Tocotrienol	x		Seeds	Antioxidant	HPLC-DAD	[4]

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
Anti-inflammatory							
145	β Tocotrienol	x		Seeds	Antioxidant Anti-inflammatory	HPLC-DAS	
Steroids							
Steroids C ₂₇							
146	Cholesterol	x		Seeds		GC-MS	[9]
147	20- Hydroxyecdysone	x		Seeds	Antioxidant	HPLC-UV-VIS	[76,77]
148	20,26- Dihydroxyecdysone	x		Seeds	Antioxidant	HPLC-UV-VIS	[26,77]
149	2-Deoxy-20- hydroxyecdysone		x	Seeds	N.D.	HPLC-NMR	
150	3-epi-2-Deoxy 20-26- hydroxyecdysone		x	Seeds	N.D.	HPLC-NMR	[78]
151	2-Deoxy 20,26 dihydroxyecdysone		x	Seeds	N.D.	HPLC-NMR	
152	22-Hydroxyecdysone 22- Glycolate		x	Seeds	Antioxidant	TLC- NMR	[77,79]
153	24.25 Dehydroinokosterone		x	Seeds	N.D.	HPLC-NMR	
154	25.27 Dehydroinokosterone		x	Seeds	N.D.	HPLC-NMR	[78]
155	Lanosterol	x		Seeds	N.D.	HPLC-MS	[69]
156	Polypodin B		x	Seeds	N.D.	HPLC-NMR	[78]
Steroids C ₂₈							
157	Brassicasterol	x		Seeds	N.D.	HPLC-MS	[80]
158	Campestanol	x		Seeds	N.D.	HPLC-MS	
159	Campesterol	x		Seeds	N.D.	HPLC-MS	[69]
160	Δ^7 Campesterol	x		Seeds	N.D.	HPLC-MS	
161	Dacristerone		x	Seeds	N.D.	HPLC-NMR	[78]
162	Episterol	x		Seeds	N.D.	HPLC-MS	[69]
163	Ergost-7-en-3-ol	x		Seeds	N.D.	HPLC-MS	[69]
164	Cancholesterone	x		Seeds	N.D.	HPLC-UV-VIS	[9]
165	Makisterone A	x		Seeds	Antioxidant	HPLC-UV-VIS	
166	24- <i>epi</i> - Makisterone A	x		Seeds	Antioxidant	HPLC-UV-VIS	[26,77]
167	24-Methyl-20,26 Dihydroxyecdysone		x	Seeds	Antioxidant	HPLC-NMR	

No.	Compound	Id	Is	PO	Biological activity	Identification method	Ref.
168	24(28) Dehydromakisterone A	x		Seeds	Antioxidant	HPLC-UV-VIS	
169	26-Hydroxy 24(28) dehygromakisterone		x	Seeds	N.D.	TLC- NMR	[79]
170	5- β Hydroxy 24(28) dehydromakisterone A	x		Seeds	N.D.	HPLC-NMR	[78]
Steroids C ₂₉							
171	Δ^5 Avenasterol	x		Seeds	N.D.	GC-MS	[81]
172	Δ^7 Avenasterol	x		Seeds	N.D.	HPLC-MS	
173	Makisterone C	x		Seeds	N.D.	HPLC-MS	[69]
174	Sitostanol	x		Seeds	N.D.	HPLC-MS	
175	β Sitosterol	x		Seeds	Antioxidant Antimutagenic Apoptotic	GC-MS	[81,82]
176	Δ^7 Stigmastenol	x		Seeds	Antitumor Cytotoxic Antihypercholesterolemic	HPLC-MS	[69,83,84]
177	Δ^7 Stigmasterol	x		Seeds	N.D.	GC-MS	[81]
Nitrogen-containing metabolites							
178	Amaranthine	x		Seeds	N.D.	HPLC-PDA	[85]
179	Betanin	x		Seeds	Antioxidant	HPLC-DAD	[4,86]
180	Isobetanine	x		Seeds	N.D.	HPLC-DAD	[4]
181	Betaine	x		Seeds	N.D.	HPLC-DAD	[4]
182	3-Carboxy-1(2- sulfoethyl)pyridine	x		Seeds	N.D.	HPLC-DAD	
183	Dopaxanthin	x		Seeds	N.D.	HPLC-PDA	
184	Indicaxanthin	x		Seeds	N.D.	HPLC-PDA	[85]
185	Miraxanthin V	x		Seeds	N.D.	HPLC-PDA	
186	Trigonelline	x		Seeds	Antiinvasive activity in cell lines Hypoglycemic	HPLC-UV-VIS	[9,87,88]
187	Trigoneline glucosyl ester	x		Seeds	N.D.	HPLC-UV-VIS	[9]
188	Trigoneline methyl ester	x		Seeds	N.D.	HPLC-UV-VIS	

Note: Is: Isolated; DAD: Diode Array Detector; PO: Plant organ; GC: Gas chromatography; HPLC: High Performance Liquid Chromatography; Id: Identified; MS: Mass spectrometry; ND: Not determined; PDA: Photodiode

array detector; NMR: Nuclear magnetic resonance; TLC: Thin layer chromatography; UV: Ultraviolet; VIS: Visible.

Table S2 : Phytochemicals from *Amaranthus hybridus* L.

No.	Compound	Id	Is	PO	Bioactivity	Method	Refs
Hydroxybenzoic acid analogues							
1	Ellagic acid	x		Leaves	Antioxidant Anticancer Anti-inflammatory	HPLC-DAD	[89–92]
2	Gallic acid	x		Leaves	Antibacterial Antioxidant	HPLC-DAD	[5,89]
Hydroxycinnamic acid analogues							
3	Caffeic acid	x		Leaves	Antioxidant	HPLC-DAD	[7,89]
4	Citric acid-2-caffeoyl	x		Leaves	N.D.	HPLC-DAD	[93]
5	Chlorogenic acid	x		Leaves	Antidiabetic	HPLC-DAD	[10,89]
Flavonols							
6	Kaempferol	x		Dried and cooked leaves	Antioxidant Antibacterial	HPLC-DAD	[3,94]
7	Myricetin	x		Dried and cooked leaves	Apoptosis of breast cancer cells Antihyperglycemic Antibacterial	HPLC-DAD	[33,34,94]
8	Quercetin	x		Leaves, flowers, stems	Cytotoxic in the A549 cell line Antioxidant	HPLC-DAD	[30,94,95]
9	Rutin	x		Leaves Seeds	Antioxidant Antidiabetic	HPLC-DAD	[10,32,89,96]
Flavones							
10	Vitexin	x		Leaves	Anticancer Antioxidant	HPLC-DAD	[23,24,89]
12	Apigenin	x		Leaves	Breast cancer Anti-inflammatory	HPLC-DAD	[89,97]
Carotenoids							
13	β -carotene	x		Raw and boiled leaves	Antioxidant	HPLC-DAD	[98,99]
14	Lutein	x		Raw and boiled leaves	Antioxidant	HPLC-DAD	[98,100]
Nitrogen-containing compounds							
15	Amaranthine	x		Seeds	Antioxidant	HPLC-MS	[101,102]
16	Isoamaranthine	x		Seeds	Antioxidant	HPLC-MS	

Note: Is: Isolated; DAD: Diode Array Detector; PO: Plant organ; GC: Gas chromatography; HPLC: High Performance Liquid Chromatography; Id: Identified; MS: Mass spectrometry; ND: Not determined; PDA: Photodiode array detector; NMR: Nuclear magnetic resonance; TLC: Thin layer chromatography; UV: Ultraviolet; VIS: Visible.

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