

Table S4. Putative identification of core compounds detected in chickpea grains

RT	m/z	Compound	Adduct	Adduct m/z	Error	Chemical group
Carbohydrates						
0.43	391.1015	Galactopinitol	[M+Cl] ⁻	391.1013	0.5	Hexose derivative
0.46	563.1846	Xylopyranosyl-arabinose	[M-H] ⁻	563.1829	3.0	Oligosaccharide
0.49	503.1636	Oligosaccharide	[M-H] ⁻	503.1618	3.6	Oligosaccharide
1.84	863.4269	Amylopectin	[M+Cl] ⁻	863.2441	3.2	Polysaccharide
Organic acids						
0.71	191.0196	Citric acid	[M-H] ⁻	191.0197	-0.5	Organic acid
Nitrogen Containing Compounds						
1.70	309.1088	Glutamyltyrosine	[M-H] ⁻	309.1092	-1.3	Amino acid derivative
2.28	203.0822	Tryptophan	[M-H] ⁻	203.0826	-2.0	Amino acid
2.81	293.1154	Glutamylphenylalanine	[M-H] ⁻	293.1143	3.8	Amino acid derivative
Phenolics						
0.48	381.0972	Genistein-rhamnoside	[M-2H ₂ O+H] ⁺	381.0980	-2.1	Isoflavonoid glucoside
0.49	711.2227	Trihydroxy-heptamethoxy-biflavan	[M+Cl] ⁻	711.2214	1.8	Biflavonoid
1.72	315.0721	Protocatechuic acid glucoside	[M-H] ⁻	315.0722	-0.3	Dihydrobenzoic acid glucoside
2.27	188.0750	Pentamethoxyflavanone	[M+2H] ²⁺	188.0756	-3.2	Polymethoxyflavone
Terpenoids						
1.72	311.1304	Gibberellin	[M-2H ₂ O+H] ⁺	311.1289	4.8	Diterpenoid
2.80	295.1340	Gibberellin A5	[M-2H ₂ O+H] ⁺	295.1340	0.0	Diterpenoid
3.47	281.1389	Dihydrophaseic acid	[M-H] ⁻	281.1394	-1.8	Sesquiterpenoid
9.85	941.5111	Soyasaponin I	[M-H] ⁻	941.5115	-0.4	Triterpenoid saponin
10.09	795.4521	Soyasaponin III	[M-H] ⁻	795.4536	-1.9	Triterpenoid saponin
Lipids						
12.93	478.2926	Lysophospholipid	[M+H] ⁺	478.2928	-0.4	Lysophospholipid
13.00	520.3401	Lysolecithin	[M+H] ⁺	520.3398	0.6	Phosphatidylcholine derivative
13.26	478.2927	Lysophospholipid	[M+H] ⁺	478.2928	-0.2	Lysophospholipid
13.32	520.3400	Lysolecithin	[M+H] ⁺	520.3398	0.4	Phosphatidylcholine derivative
13.38	313.2743	Glycerolipid	[M-H ₂ O+H] ⁺	313.2743	0.0	Glycerolipid
13.60	496.3402	Lysolecithin	[M+H] ⁺	496.3398	0.8	Phosphatidylcholine derivative
13.92	454.2928	Lysophospholipid	[M+H] ⁺	454.2928	0.0	Lysophospholipid
13.99	496.3402	Lysolecithin	[M+H] ⁺	496.3398	0.8	Phosphatidylcholine derivative
14.09	522.3556	Lysolecithin	[M+H] ⁺	522.3554	0.4	Phosphatidylcholine derivative
14.38	480.3084	Lysophospholipid	[M+H] ⁺	480.3085	-0.2	Lysophospholipid
14.45	522.3562	Lysolecithin	[M+H] ⁺	522.3554	1.5	Phosphatidylcholine derivative

RT: Retention time in minutes; m/z in Daltons; Error in ppm.