

Article

Supplementary Materials: Andean Blueberry of the Genus *Disterigma*: a High-Resolution Mass Spectrometric Approach for the Comprehensive Characterization of Phenolic Compounds

Sara Elsa Aita ¹, Anna Laura Capriotti ¹, Chiara Cavaliere ¹, Andrea Cerrato ^{1,*}, Benedetta Giannelli Moneta ¹, Carmela Maria Montone ¹, Susy Piovesana ¹ and Aldo Laganà ^{1,2}

¹ Department of Chemistry, Sapienza University of Rome, Piazzale Aldo Moro 5, 00185 Rome, Italy; saraelsa.aita@uniroma1.it (S.E.A.); annalaura.capriotti@uniroma1.it (A.L.C.); chiara.cavaliere@uniroma1.it (C.C.); benedetta.giannellimoneta@uniroma1.it (B.G.M.); carmelamaria.moneta@uniroma1.it (C.M.M.); susy.piovesana@uniroma1.it (S.P.); aldo.lagana@uniroma1.it (A.L.)

² CNR NANOTEC, Campus Ecotekne, University of Salento, Via Monteroni, 73100 Lecce, Italy

* Correspondence: andrea.cerrato@uniroma1.it

Table 1. Detailed identification data for the annotated anthocyanins in *Disterigma alaternoides*.

ID	Name	RT [min]	Formula	Molecular Weight	Adduct	Experimental m/z	Δ (ppm)	Confirming Peak	Main Fragments	Confidence Level	Mean Area
1	Cyanidin O-hexoside	1.63	C ₂₁ H ₂₁ O ₁₁ ⁺	449.1088	[M] ⁺	449.1088	1.5		449.1085; 287.0553; 241.0499; 231.0656; 213.0550; 149.0237; 137.0235; 121.0285	2	4.680 × 10 ⁷
2	Delphinidin O-hexoside	2.79	C ₂₁ H ₂₁ O ₁₂ ⁺	465.1038	[M] ⁺	465.1038	2.1		465.1034; 303.0502; 257.0448; 247.0605; 229.0499; 153.0185; 149.0237; 121.0285	2	8.249 × 10 ⁷
3	Delphinidin O-hexoside	3.77	C ₂₁ H ₂₁ O ₁₂ ⁺	465.1034	[M] ⁺	465.1034	1.4		465.1034; 303.0502; 257.0448; 247.0605; 229.0499; 153.0185; 149.0237; 121.0285	2	8.317 × 10 ⁸
4	Delphinidin O-pentoside	4.98	C ₂₀ H ₁₉ O ₁₁ ⁺	435.0920	[M] ⁺	435.0920	−0.5	303.0497	435.0920; 303.0502; 257.0448; 247.0605; 229.0499; 153.0185; 149.0237; 121.0286	2	5.393 × 10 ⁸

5	Cyanidin O-hexoside	5.07	C ₂₁ H ₂₁ O ₁₁ ⁺	449.1088	[M] ⁺	449.1088	2.1		449.1085; 287.0553; 241.0499; 231.0656; 213.0550; 149.0237; 137.0235; 121.0285	2	2.983 × 10 ¹⁰
6	Delphinidin O-hexoside	5.95	C ₂₁ H ₂₁ O ₁₂ ⁺	465.1038	[M] ⁺	465.1038	2.1		465.1034; 303.0502; 257.0448; 247.0605; 229.0499; 153.0185; 149.0237; 121.0285	2	2.533 × 10 ⁷
7	Pelargonidin O-hexoside	6.25	C ₂₁ H ₂₁ O ₁₀ ⁺	433.1127	[M] ⁺	433.1127	−0.4		433.1127; 271.0608; 215.0707; 197.0601; 149.0237; 121.0285	2	2.177 × 10 ⁸
8	Cyanidin O-deoxyhexoside	6.54	C ₂₁ H ₂₁ O ₁₀ ⁺	433.1126	[M] ⁺	433.1126	1.9		433.1126; 287.0553; 241.0499; 231.0656; 213.0550; 149.0237; 137.0235; 121.0285	2	2.853 × 10 ⁸
9	Cyanidin O-pentoside	6.71	C ₂₀ H ₁₉ O ₁₀ ⁺	419.0976	[M] ⁺	419.0976	0.8	287.0541	419.0976; 287.0553; 241.0499; 231.0656; 213.0550; 149.0237; 137.0235; 121.0285	2	2.859 × 10 ⁹
10	Pelargonidin O-pentoside	7.66	C ₂₀ H ₁₉ O ₉ ⁺	403.1030	[M] ⁺	403.1030	1.6	271.0599	403.1030; 271.0608; 215.0707; 197.0601; 149.0237; 121.0285	2	3.146 × 10 ⁸
11	Cyanidin O-hexoside	7.98	C ₂₁ H ₂₁ O ₁₁ ⁺	449.1088	[M] ⁺	449.1088	2.2	287.0541	449.1085; 287.0553; 241.0499; 231.0656; 213.0550; 149.0237; 137.0235; 121.0285	2	9.304 × 10 ⁷
12	Peonidin 3-O-glucoside	8.34	C ₂₂ H ₂₃ O ₁₁ ⁺	463.1247	[M] ⁺	463.1247	2.7		463.1247; 301.0707; 286.0472;	1	9.522 × 10 ⁶

13	Peonidin O-pento- side	8.75	C ₂₁ H ₂₁ O ₁₀ ⁺	433.1136	[M] ⁺	433.1136	1.5	2	1.221 × 10 ⁸
14	Cyanidin O-hexo- side	8.88	C ₂₁ H ₂₁ O ₁₁ ⁺	449.1088	[M] ⁺	449.1088	2.1	2	9.987 × 10 ⁷
15	Del- phinidin O-di-hexo- side	9.40	C ₂₇ H ₃₁ O ₁₇ ⁺	627.1570	[M] ⁺	627.1570	2.2	2	5.367 × 10 ⁶
16	Cyanidin O-pento- side	9.51	C ₂₀ H ₁₉ O ₁₀ ⁺	419.0976	[M] ⁺	419.0976	0.8	2	9.948 × 10 ⁷
17	Cyanidin	10.23	C ₁₅ H ₁₁ O ₆ ⁺	287.0541	[M] ⁺	287.0541	-3.2	1	1.595 × 10 ⁸
18	Cyanidin isomer	12.06	C ₁₅ H ₁₁ O ₆ ⁺	287.0541	[M] ⁺	287.0541	-3.2	2	2.729 × 10 ⁷

Table 2. Detailed identification data for the annotated flavonoids in *Disterigma alaternoides*.

ID	Name	RT [min]	Formula	Molecular Weight	Adduct	Experi- mental m/z	Δ (ppm)	Confirm- ing Peak	Main Fragments	Confi- dence Level	Mean Area
19	(Epi)cate- chin O- hexoside	3.47	C ₂₁ H ₂₄ O ₁₁	452.1326	[M-H] ⁻	451.1253	1.6		451.1253; 289.0719; 245.0817; 137.0245;	2	1.559 × 10 ⁷

								125.0244; 109.0295		
20	Epicatechin	6.30	C ₁₅ H ₁₄ O ₆	290.0796	[M-H] ⁻	289.0724	1.8	289.0719; 245.0817; 137.0245; 125.0244; 109.0295	1	1.158 × 10 ⁸
21	Taxifolin isomer	7.05	C ₁₅ H ₁₂ O ₇	304.0588	[M-H] ⁻	303.0515	1.7	303.0513; 259.0613; 193.0142; 167.0350; 165.0193; 137.0245; 109.0295	2	7.234 × 10 ⁸
22	Quercetin O-dihexoside	7.05	C ₂₇ H ₃₀ O ₁₇	626.1503	[M-H] ⁻	625.1430	3.1	463.0880; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	4.149 × 10 ⁶
23	Aromaden-drin O-hexoside	7.25	C ₂₁ H ₂₂ O ₁₁	450.1173	[M-H] ⁻	449.1100	2.4	289.0714 449.1100; 287.0561; 269.0456; 177.0194; 151.0036; 125.0244; 107.0139	2	9.806 × 10 ⁶
24	Taxifolin O-hexoside	7.65	C ₂₁ H ₂₂ O ₁₂	466.1130	[M-H] ⁻	465.1057	4.0	465.1057; 303.0512; 285.0407; 241.0407; 177.0194; 151.0036; 125.0244; 107.0140	2	2.687 × 10 ⁷
25	Eriodictyol O-pentoside	8.21	C ₂₀ H ₂₀ O ₁₀	420.1068	[M-H] ⁻	419.0995	2.7	419.0995; 287.0561; 177.0194; 151.0036; 135.0452; 107.0139	2	1.292 × 10 ⁷
26	Quercetin O-hexoside O-deoxyhexoside	8.70	C ₂₇ H ₃₀ O ₁₆	610.1548	[M-H] ⁻	609.1475	2.3	463.0859; 447.0949; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	2.875 × 10 ⁶
27	Taxifolin	9.26	C ₁₅ H ₁₂ O ₇	304.0593	[M-H] ⁻	303.0520	3.3	303.0512; 285.0407; 241.0407; 177.0194;	1	1.255 × 10 ⁷

								151.0036; 125.0244; 107.0140		
28	Quercetin O-dihex- side	9.38	C ₂₇ H ₃₀ O ₁₇	626.1503	[M-H] ⁻	625.1430	3.2	463.0880; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	3.778 × 10 ⁶
29	Myricetin 3-O-hexo- side	9.55	C ₂₁ H ₂₀ O ₁₃	480.0927	[M-H] ⁻	479.0854	2.7	479.0844; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2	1.995 × 10 ⁷
30	Myricetin O-pento- side	9.58	C ₂₀ H ₁₈ O ₁₂	450.0811	[M-H] ⁻	449.0738	2.7	449.0724; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2	2.295 × 10 ⁶
31	Myricetin 3-O-hexo- side	9.86	C ₂₁ H ₂₀ O ₁₃	480.0917	[M-H] ⁻	479.0844	2.6	479.0844; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2	8.087 × 10 ⁶
32	Isorham- netin O- glucu- ronide	9.96	C ₂₂ H ₂₀ O ₁₃	492.0917	[M-H] ⁻	491.0844	2.7	491.0844; 315.0512; 300.0275; 271.0244; 255.0296; 151.0036; 107.0139	2	4.154 × 10 ⁵
33	Naringeni n O-hexo- side	10.03	C ₂₁ H ₂₂ O ₁₀	434.1223	[M-H] ⁻	433.1150	2.2	433.1144; 271.0613; 227.0713; 177.0194; 151.0036; 119.0503; 107.0139	2	1.842 × 10 ⁷
34	Myricetin O-hexo- side O- pentoside	10.04	C ₂₆ H ₂₈ O ₁₇	612.1339	[M-H] ⁻	611.1266	2.0	479.0833; 449.0729; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2	8.979 × 10 ⁶

35	Myricetin O-pento- side	10.07	C ₂₀ H ₁₈ O ₁₂	450.0807	[M-H] ⁻	449.0735	2.0	449.0724; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2	2.516 × 10 ⁶
36	Quercetin O-dihexo- side	10.08	C ₂₇ H ₃₀ O ₁₇	626.1499	[M-H] ⁻	625.1426	2.6	463.0880; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	3.348 × 10 ⁶
37	Myricetin O-pento- side	10.16	C ₂₀ H ₁₈ O ₁₂	450.0808	[M-H] ⁻	449.0736	2.2	449.0724; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2	1.701 × 10 ⁷
					[M+H] ⁺	451.0884	2.9	451.0879; 319.0454; 273.0395; 245.0447; 165.0187; 153.0186; 137.0298		9.708 × 10 ⁶
								319.0453		
38	Quercetin O-hexo- side O- pentoside	10.33	C ₂₆ H ₂₈ O ₁₆	596.1387	[M-H] ⁻	595.1314	1.5	463.0901; 433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	1.569 × 10 ⁷
39	Taxifolin isomer	10.36	C ₁₅ H ₁₂ O ₇	304.0593	[M-H] ⁻	303.0520	3.2	303.0512; 285.0407; 241.0407; 177.0194; 151.0036; 125.0244; 107.0139	2	2.516 × 10 ⁷
40	Quercetin O-hexo- side O- pentoside	10.62	C ₂₆ H ₂₈ O ₁₆	596.1386	[M-H] ⁻	595.1313	1.4	301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	4.757 × 10 ⁶
41	Myricetin isomer	10.63	C ₁₅ H ₁₀ O ₈	318.0381	[M-H] ⁻	317.0308	1.7	317.0303; 271.0259; 178.9985; 151.0036;	2	1.689 × 10 ⁷

								137.0244; 107.0139		
42	Naringenin O-hexoside	10.81	C ₂₁ H ₂₂ O ₁₀	434.1217	[M-H] ⁻	433.1144	0.9	433.1144; 271.0613; 227.0713; 177.0194; 151.0036; 119.0503; 107.0139	2	7.129 × 10 ⁶
43	Eriodictyol O-hexoside	10.84	C ₂₁ H ₂₂ O ₁₁	450.1174	[M-H] ⁻	449.1101	2.7	449.1100; 287.0561; 177.0194; 151.0036; 135.0452; 107.0139	2	1.878 × 10 ⁷
44	Shiikimoyl Kaempferol	11.10	C ₂₂ H ₁₈ O ₁₀	442.0911	[M-H] ⁻	441.0838	2.5	285.0407; 243.0296; 241.0502; 151.0036; 133.0295; 107.01139	2	9.337 × 10 ⁶
45	Myricetin 3-O-pentoside	11.11	C ₂₀ H ₁₈ O ₁₂	450.0808	[M-H] ⁻	449.0735	2.0	449.0724; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2	9.116 × 10 ⁷
					[M+H] ⁺	451.0879	1.8	451.0879; 319.0454; 273.0395; 245.0447; 165.0187; 153.0186; 137.0298		3.828 × 10 ⁷
46	Quercetin O-hexoside O-pentoside	11.18	C ₂₆ H ₂₈ O ₁₆	596.1383	[M-H] ⁻	595.1310	1.0	463.0901; 433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	7.383 × 10 ⁶
47	Myricetin O-pentoside	11.21	C ₂₀ H ₁₈ O ₁₂	450.0797	[M-H] ⁻	449.0724	-0.4	449.0724; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2	9.200 × 10 ⁵
48	Myricetin 3-O-deoxyhexoside	11.25	C ₂₁ H ₂₀ O ₁₂	464.0968	[M-H] ⁻	463.0895	2.8	463.0895; 317.0303; 271.0259; 178.9985; 151.0036;	2	5.408 × 10 ⁶

Number	Compound	Retention Time (min)	Chemical Formula	Mass (Da)	Ionization Mode	m/z	Relative Abundance (%)	Reference	Reference	Reference
49	Quercetin O-hexoside O-pentoside	11.27	C ₂₆ H ₂₈ O ₁₆	596.1388	[M-H] ⁻	595.1315	1.8	137.0244; 107.0139	2	2.274 × 10 ⁷
								463.0901; 433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
50	Quercetin O-hexoside O-pentoside	11.55	C ₂₆ H ₂₈ O ₁₆	596.1394	[M+H] ⁺	597.1461	1.8	465.1045	2	1.697 × 10 ⁷
								597.1385; 465.1026; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
51	Quercetin 3-O-galactoside	11.58	C ₂₆ H ₂₈ O ₁₆	596.1394	[M-H] ⁻	595.1321	2.7	463.0901; 433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	1.517 × 10 ⁶
								463.0883; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
52	Quercetin O-hexoside O-pentoside	11.69	C ₂₆ H ₂₈ O ₁₆	596.1391	[M-H] ⁻	595.1319	2.3	463.0883; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	5.958 × 10 ⁹
								465.1024; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
53	Quercetin O-hexoside O-pentoside	11.84	C ₂₆ H ₂₈ O ₁₆	596.1394	[M+H] ⁺	465.1024	3.7	303.0497	2	3.870 × 10 ⁹
								465.1024; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
54	Quercetin O-hexoside O-pentoside	11.84	C ₂₆ H ₂₈ O ₁₆	596.1394	[M-H] ⁻	595.1321	2.7	463.0901; 433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	8.975 × 10 ⁵
								463.0901; 433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		

								245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
								463.0859; 447.0949; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
					[M-H] ⁻	609.1482	3.5			9.379 × 10 ⁶
54	Rutin	11.90	C ₂₇ H ₃₀ O ₁₆	610.1555					1	
					[M+H] ⁺	611.1602	-0.8			4.554 × 10 ⁶
								611.1602; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
					[M-H] ⁻	463.0884	0.4			3.467 × 10 ⁸
								463.0883; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
55	Quercetin 3-O-gluco- side	12.09	C ₂₁ H ₂₀ O ₁₂	464.0957					1	
					[M+H] ⁺	465.1024	-0.7	303.0497		2.042 × 10 ⁸
								465.1024; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
					[M-H] ⁻	287.0570	3.1		2	2.460 × 10 ⁸
56	Aro- maden- drin	12.15	C ₁₅ H ₁₂ O ₆	288.0643				287.0561; 269.0456; 177.0194; 151.0036; 125.0244; 107.0139		
					[M-H] ⁻	565.1212	2.3		2	1.948 × 10 ⁶
57	Quercetin O-dipen- toside	12.26	C ₂₅ H ₂₆ O ₁₅	566.1285				433.0776; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
					[M-H] ⁻	595.1318	2.3		2	1.241 × 10 ⁷
58	Quercetin O-hexo- side O- pentoside	12.30	C ₂₆ H ₂₈ O ₁₆	596.1391				463.0901; 433.0777; 301.0354; 273.0411; 245.0454; 178.0085;		

59	Quercetin O-hexo- side O- pentoside	12.37	C ₂₆ H ₂₈ O ₁₆	596.1390	[M-H] ⁻	595.1317	2.0	465.1026	151.0036; 121.0295; 107.0139	2	1.072 × 10 ⁸
									463.0901; 433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
									597.1385; 465.1026; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
									447.0944; 285.0403; 257.0457; 229.0504; 151.0036; 107.0139		
60	Kaempfer ol O-hexo- side	12.45	C ₂₁ H ₂₀ O ₁₁	448.1023	[M-H] ⁻	447.0950	3.9	465.1026	433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	5.098 × 10 ⁶
									433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
									435.0918; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
									433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
61	Quercetin 3-O-pento- side	12.62	C ₂₀ H ₁₈ O ₁₁	434.0849	[M-H] ⁻	433.0776	-0.1	435.0920	433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	2.185 × 10 ⁹
									433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
									435.0918; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
									433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
62	Quercetin O-hexo- sypento- side	12.87	C ₂₆ H ₂₈ O ₁₆	596.1392	[M-H] ⁻	595.1320	2.5	465.1026	433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	4.589 × 10 ⁶
									433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
									435.0918; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
									433.0777; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
63	Eriodic- tyol O- hexoside	12.91	C ₂₁ H ₂₂ O ₁₁	450.1173	[M-H] ⁻	449.1100	2.4	465.1026	449.1100; 287.0561; 177.0194; 151.0036; 135.0452; 107.0139	2	4.093 × 10 ⁶
									449.1100; 287.0561; 177.0194; 151.0036; 135.0452; 107.0139		
									449.1100; 287.0561; 177.0194; 151.0036; 135.0452; 107.0139		
									449.1100; 287.0561; 177.0194; 151.0036; 135.0452; 107.0139		

64	Quercetin O-pento- side	12.99	C ₂₀ H ₁₈ O ₁₁	434.0848	[M-H] ⁻	433.0775	-0.2	433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	4.490 × 10 ⁸
					[M+H] ⁺	435.0920	-0.5	303.0497 435.0918; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		
65	Kaempfer ol 3-O- hexoside	13.14	C ₂₁ H ₂₀ O ₁₁	448.1017	[M-H] ⁻	447.0944	2.5	447.0944; 285.0403; 257.0457; 229.0504; 151.0036; 107.0139	2	5.263 × 10 ⁷
					[M+H] ⁺	449.1083	1.0	287.0545 449.1083; 287.0553; 241.0496; 213.0547; 165.0187; 153.0185; 121.0286		
66	Naringeni n O-hexo- side	13.28	C ₂₁ H ₂₂ O ₁₀	434.1219	[M-H] ⁻	433.1146	1.3	433.1144; 271.0613; 227.0713; 177.0194; 151.0036; 119.0503; 107.0139	2	4.847 × 10 ⁷
					[M+H] ⁺	435.1290	1.0	273.0760 435.1290; 273.0761; 255.0648; 179.0340; 153.0185; 147.0444; 119.0494		
67	Quercetin O-dipen- toside	13.36	C ₂₅ H ₂₆ O ₁₅	566.1286	[M-H] ⁻	565.1214	2.6	433.0776; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	5.170 × 10 ⁶
68	Quercetin O-pento- side	13.51	C ₂₀ H ₁₈ O ₁₁	434.0848	[M-H] ⁻	433.0775	-0.3	433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036;	2	6.687 × 10 ⁹

69	Quercetin O-pento- side	13.84	C ₂₀ H ₁₈ O ₁₁	434.0848	[M+H] ⁺	435.0918	-0.9	303.0497	121.0295; 107.0139	2.411 × 10 ⁹
									435.0918; 303.0502; 257.0445;	
									229.0499; 165.0186; 153.0185; 137.0237	
									433.0775; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	
70	Myricetin	13.89	C ₁₅ H ₁₀ O ₈	318.0383	[M-H] ⁻	317.0310	2.2		435.0918; 303.0502; 257.0445;	2.367 × 10 ⁸
									229.0499; 165.0186; 153.0185; 137.0237	
									317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	
									447.0933; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	
71	Quercetin 3-O-deox- yhexoside	14.04	C ₂₁ H ₂₀ O ₁₁	448.1006	[M-H] ⁻	447.0933	0.0		447.0933; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	3.539 × 10 ⁹
									449.1078; 303.0502; 257.0445;	
									229.0499; 165.0186; 153.0185; 137.0237	
									463.0883; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	
72	Quercetin O-hexo- side	14.18	C ₂₁ H ₂₀ O ₁₂	464.0972	[M-H] ⁻	463.0899	3.7		449.1078; 303.0502; 257.0445;	7.593 × 10 ⁸
									229.0499; 165.0186; 153.0185; 137.0237	
									463.0883; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	
									477.1049; 315.0512; 300.0275;	
73	Isorham- netin 3-O- hexoside	14.27	C ₂₂ H ₂₂ O ₁₂	478.1124	[M-H] ⁻	477.1052	2.8		477.1049; 315.0512; 300.0275;	1.619 × 10 ⁷

								271.0244; 255.0296; 151.0036; 107.0139		
					[M+H] ⁺	479.1192	1.7	317.0660	479.1192; 317.0663; 302.0425; 274.0474; 165.0185; 153.0185	1.254 × 10 ⁷
74	Kaempferol O-pentoside	14.40	C ₂₀ H ₁₈ O ₁₀	418.0906	[M-H] ⁻	417.0833	1.4		417.0832; 285.0403; 257.0457; 229.0504; 151.0036; 107.0139	2 3.090 × 10 ⁶
					[M-H] ⁻	477.1049	2.3		477.1049; 315.0512; 300.0275; 271.0244; 255.0296; 151.0036; 107.0139	2 2.640 × 10 ⁷
75	Isorhamnetin 3-O-hexoside	14.71	C ₂₂ H ₂₂ O ₁₂	478.1122					479.1192; 317.0663; 302.0425; 274.0474; 165.0185; 153.0185	1.839 × 10 ⁷
					[M-H] ⁻	417.0834	1.6		417.0832; 285.0403; 257.0457; 229.0504; 151.0036; 107.0139	2 2.928 × 10 ⁷
76	Kaempferol O-pentoside	14.74	C ₂₀ H ₁₈ O ₁₀	418.0907					419.0976; 287.0553; 241.0496; 213.0547; 165.0187; 153.0185; 121.0286	2 1.309 × 10 ⁷
					[M+H] ⁺	419.0979	1.5	287.0546	273.0771; 167.0350; 123.0452	1.425 × 10 ⁷
77	Phloretin O-hexoside	14.95	C ₂₁ H ₂₄ O ₁₀	436.1382	[M-H] ⁻	435.1310	3.0		479.0844; 317.0303; 271.0259; 178.9985; 151.0036; 137.0244; 107.0139	2 1.949 × 10 ⁶
78	Myricetin isomer O-hexoside	15.17	C ₂₁ H ₂₀ O ₁₃	480.0919	[M-H] ⁻	479.0846	3.1		303.0502; 257.0445; 229.0499; 165.0186;	2 1.231 × 10 ⁷
79	Quercetin O-acetylhexoside	15.23	C ₂₃ H ₂₂ O ₁₃	506.1067	[M+H] ⁺	507.1140	1.3			

80	Diosmetin O-hexoside	15.30	C ₂₂ H ₂₂ O ₁₁	462.1175	[M+H] ⁺	463.1248	2.8	153.0185; 137.0237	2	5.356 × 10 ⁶
								463.1248; 301.0715; 286.0479; 258.0530; 153.0185		
81	Kaempferol 3-O-pentoside	15.46	C ₂₀ H ₁₈ O ₁₀	418.0905	[M-H] ⁻	417.0832	1.2	417.0832; 285.0403; 284.0327; 257.0457; 229.0504; 151.0036; 107.0139	2	2.960 × 10 ⁸
								419.0976; 287.0553; 241.0496; 213.0547; 165.0187; 153.0185; 121.0286		
82	Quercetin O-hexoside	15.56	C ₂₁ H ₂₀ O ₁₂	464.0967	[M-H] ⁻	463.0894	2.6	463.0883; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	1.622 × 10 ⁷
								461.0741; 285.0407; 243.0296; 241.0502; 151.0036; 133.0295; 107.01139		
83	Luteolin O-glucuronide	15.67	C ₂₁ H ₁₈ O ₁₂	462.0814	[M-H] ⁻	461.0741	3.3	461.0741; 285.0407; 243.0296; 241.0502; 151.0036; 133.0295; 107.01139	2	9.772 × 10 ⁵
								287.0561; 177.0194; 151.0036; 135.0452; 107.0139		
84	Eriodictyol	15.86	C ₁₅ H ₁₂ O ₆	288.0641	[M-H] ⁻	287.0568	2.5	287.0561; 177.0194; 151.0036; 135.0452; 107.0139	1	1.434 × 10 ⁶
								447.0937; 315.0512; 314.0433; 300.0275; 271.0244; 255.0296; 151.0036; 107.0139		
85	Isorhamnetin 3-O-pentoside	15.86	C ₂₁ H ₂₀ O ₁₁	448.1010	[M-H] ⁻	447.0937	0.9	447.0937; 315.0512; 314.0433; 300.0275; 271.0244; 255.0296; 151.0036; 107.0139	2	9.355 × 10 ⁶
								449.1087; 317.0663; 302.0425; 274.0474; 165.0185; 153.0185		
85	Isorhamnetin 3-O-pentoside	15.86	C ₂₁ H ₂₀ O ₁₁	448.1010	[M+H] ⁺	449.1087	1.9	449.1087; 317.0663; 302.0425; 274.0474; 165.0185; 153.0185	2	5.339 × 10 ⁶
								449.1087; 317.0663; 302.0425; 274.0474; 165.0185; 153.0185		

86	Naringenin O-hexoside	15.88	C ₂₁ H ₂₂ O ₁₀	434.1222	[M-H] ⁻	433.1149	2.0	273.0762	433.1144; 271.0613; 227.0713; 177.0194; 151.0036; 119.0503; 107.0139	2	1.501 × 10 ⁷
87	Kaempferol O-pentoside	15.90	C ₂₀ H ₁₈ O ₁₀	418.0908	[M-H] ⁻	417.0835	1.8		417.0832; 285.0403; 257.0457; 229.0504; 151.0036; 107.0139	2	4.205 × 10 ⁶
88	Kaempferol O-deoxyhexoside	16.11	C ₂₁ H ₂₀ O ₁₀	432.1063	[M+H] ⁺	433.1136	1.5	287.0546	433.1136; 287.0553; 241.0496; 213.0547; 165.0187; 153.0185; 121.0286	2	2.273 × 10 ⁷
89	Isorhamnetin 3-O-pentoside	16.41	C ₂₁ H ₂₀ O ₁₁	448.1010	[M-H] ⁻	447.0937	0.9		447.0937; 315.0512; 314.0437; 300.0275; 271.0244; 255.0296; 151.0036; 107.0139	2	2.657 × 10 ⁷
					[M+H] ⁺	449.1082	0.9	317.0658	449.1082; 317.0663; 302.0425; 274.0474; 165.0185; 153.0185		1.433 × 10 ⁷
90	Quercetin 3-O-malonyldeoxyhexoside	16.64	C ₂₄ H ₂₂ O ₁₄	534.1021	[M-H] ⁻	533.0948	2.0		301.0354; 300.0278; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	1.414 × 10 ⁷
					[M+H] ⁺	535.1090	1.5	303.0498	535.1099; 303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		7.760 × 10 ⁶
91	Quercetin	17.34	C ₁₅ H ₁₀ O ₇	302.0426	[M-H] ⁻	301.0353	-0.1		301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	1	3.608 × 10 ⁸

					[M+H] ⁺	303.0495	-1.5	303.0502; 257.0445; 229.0499; 165.0186; 153.0185; 137.0237		4.159 × 10 ⁸
92	Quercetin 3-O-dihydroxybenzoylpentose	17.68	C ₂₇ H ₂₂ O ₁₄	570.1023	[M-H] ⁻	569.0950	2.3	433.0776; 301.0354; 300.0278; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	1.756 × 10 ⁶
93	Luteolin	17.69	C ₁₅ H ₁₀ O ₆	286.0485	[M-H] ⁻	285.0412	2.7	285.0407; 243.0296; 241.0502; 151.0036; 133.0295; 107.01139	1	3.209 × 10 ⁶
					[M+H] ⁺	287.0552	0.8	287.0554; 269.0452; 241.0498; 153.0185; 137.0237; 135.0443		4.265 × 10 ⁵
94	Quercetin 3-O-coumaroylhexoside	18.05	C ₃₀ H ₂₆ O ₁₄	610.1339	[M-H] ⁻	609.1266	2.7	609.1306; 463.0883; 301.0354; 300.0278; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	1.460 × 10 ⁶
95	Quercetin 3-O-coumaroylhexoside	18.28	C ₃₀ H ₂₆ O ₁₄	610.1335	[M-H] ⁻	609.1262	2.0	609.1306; 463.0883; 301.0354; 300.0278; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139	2	1.060 × 10 ⁶
96	Naringenin isomer	18.41	C ₁₅ H ₁₂ O ₅	272.0687	[M-H] ⁻	271.0614	0.7	271.0613; 227.0713; 177.0194; 151.0036; 119.0503; 107.0139	2	8.259 × 10 ⁵
97	Naringenin	18.76	C ₁₅ H ₁₂ O ₅	272.0687	[M-H] ⁻	271.0614	0.7	271.0613; 227.0713; 177.0194;	1	9.616 × 10 ⁶

								151.0036; 119.0503; 107.0139		
								273.0761; 255.0648; 179.0340; 153.0185; 147.0444; 119.0494		
					[M+H] ⁺	273.0761	1.3			3.056 × 10 ⁶
								433.0776; 301.0354; 300.0278; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
98	Quercetin 3-O-dihydroxybenzoylpentose	19.06	C ₂₇ H ₂₂ O ₁₄	570.1009	[M-H] ⁻	569.0937	0.0		2	1.124 × 10 ⁶
								433.0776; 301.0354; 273.0411; 245.0454; 178.0085; 151.0036; 121.0295; 107.0139		
99	Quercetin O-dihydroxybenzoylpentose	19.25	C ₂₇ H ₂₂ O ₁₄	570.1016	[M-H] ⁻	569.0943	1.2		2	2.613 × 10 ⁶
								301.0716; 286.0480; 242.0581; 177.0195; 164.0115; 151.0036; 107.0139		
100	Hesperetin	19.56	C ₁₆ H ₁₄ O ₆	302.0799	[M-H] ⁻	301.0726	2.7		1	4.739 × 10 ⁵
								269.0455; 225.0557; 151.0036; 117.0346; 107.0139		
101	Apigenin	20.05	C ₁₅ H ₁₀ O ₅	270.0533	[M-H] ⁻	269.0460	1.6		1	7.775 × 10 ⁵
								285.0403; 257.0457; 229.0504; 151.0036; 107.0139		
					[M-H] ⁻	285.0409	1.4			6.323 × 10 ⁶
102	Kaempferol	20.23	C ₁₅ H ₁₀ O ₆	286.0481				287.0553; 241.0496; 213.0547; 165.0187; 153.0185; 121.0286	1	
					[M+H] ⁺	287.0552	0.8			1.641 × 10 ⁶
								299.0562; 284.0327; 257.0411; 255.0303; 151.0036; 107.0139		
103	Diosmetin	20.96	C ₁₆ H ₁₂ O ₆	300.0640	[M-H] ⁻	299.0567	2.1		1	1.006 × 10 ⁶

104	Isorhamnetin	21.13	C ₁₆ H ₁₂ O ₇	316.0590	[M-H] ⁻	315.0517	2.1	315.0512; 300.0275; 271.0244; 255.0296; 151.0036; 107.0139	1	1.950 × 10 ⁶
					[M+H] ⁺	317.0659	1.1	317.0663; 302.0425; 274.0474; 165.0185; 153.0185		6.168 × 10 ⁵
105	Chrysin	25.50	C ₁₅ H ₁₀ O ₄	254.0581	[M-H] ⁻	253.0508	0.8	253.0506; 209.0608; 151.0036; 107.0139	2	4.399 × 10 ⁴

Table 3. Detailed identification data for the annotated phenolic acids in *Disterigma alaternoides*.

ID	Name	RT [min]	Formula	Molecular Weight	Adduct	Experimental m/z	Δ (ppm)	Main Fragments	Confidence Level	Mean Area
106	Quinic acid	0.50	C ₇ H ₁₂ O ₆	192.0628	[M-H] ⁻	191.0555	-3.3	191.0562; 127.0401; 111.0088; 87.0084; 85.0292	2	1.654 × 10 ⁹
107	Gallic acid	0.64	C ₇ H ₆ O ₅	170.0218	[M-H] ⁻	169.0145	1.4	169.0142; 125.0243	2	2.602 × 10 ⁷
108	Methylgallic acid	0.79	C ₈ H ₈ O ₅	184.0372	[M-H] ⁻	183.0300	0.4	183.0300; 139.0302	2	1.516 × 10 ⁷
109	Hydroxybenzoyl hexose (I)	0.82	C ₁₃ H ₁₆ O ₈	300.0849	[M-H] ⁻	299.0776	1.2	137.0244; 93.0343	2	5.929 × 10 ⁷
110	Methylhydroxybenzoic acid	1.04	C ₈ H ₈ O ₄	168.0425	[M-H] ⁻	167.0352	1.3	167.0350; 123.0453	2	4.533 × 10 ⁶
111	Dihydroxybenzoyl hexose (I)	1.08	C ₁₃ H ₁₆ O ₉	316.0799	[M-H] ⁻	315.0727	1.6	315.0727; 153.0194; 109.0296	2	5.830 × 10 ⁸
112	Dihydroxybenzoic acid	1.19	C ₇ H ₆ O ₄	154.0269	[M-H] ⁻	153.0196	1.8	153.0194; 109.0296	2	1.271 × 10 ⁸
113	Phloroglucinol carboxylic acid	1.22	C ₇ H ₆ O ₅	170.0218	[M-H] ⁻	169.0145	1.4	169.0142; 151.0036; 125.0244	2	2.660 × 10 ⁷
114	Hexosyl caffeoyl hexose (I)	1.24	C ₂₁ H ₂₈ O ₁₄	504.1487	[M-H] ⁻	503.1415	1.6	503.1438; 341.0881; 179.0350; 161.0245; 135.0453	2	3.887 × 10 ⁷

115	Hydroxybenzoyl hexose (II)	1.29	C ₁₃ H ₁₆ O ₈	300.0849	[M-H] ⁻	299.0777	1.4	299.0777; 137.0244; 93.0343	2	1.290 × 10 ⁸
116	Methylhydroxybenzoyl hexose	1.38	C ₁₄ H ₁₈ O ₈	314.1009	[M-H] ⁻	313.0936	2.2	151.0401; 107.0502	2	1.198 × 10 ⁸
117	Dihydroxybenzoyl hexose (II)	1.43	C ₁₃ H ₁₆ O ₉	316.0797	[M-H] ⁻	315.0724	0.8	315.0727; 153.0194; 109.0296	2	1.007 × 10 ⁸
118	Hydroxybenzoyl hexose (III)	1.62	C ₁₃ H ₁₆ O ₈	300.0850	[M-H] ⁻	299.0777	1.6	299.0777; 137.0244; 93.0343	2	7.209 × 10 ⁷
119	Neochlorogenic acid	1.68	C ₁₆ H ₁₈ O ₉	354.0956	[M-H] ⁻	353.0884	1.6	353.0879; 191.0562; 179.0350; 145.0452; 135.0453	2	3.622 × 10 ⁸
120	Dihydroxybenzoyl pentose	1.72	C ₁₂ H ₁₄ O ₈	286.0694	[M-H] ⁻	285.0621	1.7	285.0618; 153.0194; 109.0296	2	6.018 × 10 ⁶
121	Chlorogenic acid	1.91	C ₂₂ H ₂₈ O ₁₄	516.1482	[M-H] ⁻	515.1409	0.6	515.1409; 353.0883; 191.0561; 179.0349; 135.0453; 87.0084; 85.0292	2	1.161 × 10 ⁸
122	Hexosyl caffeoyl hexose (I)	2.07	C ₂₁ H ₂₈ O ₁₄	504.1491	[M-H] ⁻	503.1418	2.3	503.1438; 341.0881; 179.0350; 161.0245; 135.0453	2	2.269 × 10 ⁷
123	Caffeoyl hexose (I)	2.10	C ₁₅ H ₁₈ O ₉	342.0955	[M-H] ⁻	341.0883	1.3	341.0881; 179.0350; 135.0453	2	3.060 × 10 ⁸
124	Coumaroyl hexose (I)	2.10	C ₁₅ H ₁₈ O ₈	326.1006	[M-H] ⁻	325.0933	1.3	325.0933; 163.0402; 119.0503	2	1.943 × 10 ⁸
125	Dihydroxybenzoyl hexose (III)	2.14	C ₁₃ H ₁₆ O ₉	316.0798	[M-H] ⁻	315.0725	1.1	315.0727; 153.0194; 109.0296	2	2.806 × 10 ⁷
126	Dihydroxybenzoyl hexose (IV)	2.37	C ₁₃ H ₁₆ O ₉	316.0798	[M-H] ⁻	315.0725	1.1	315.0727; 153.0194; 109.0296	2	8.893 × 10 ⁷
127	Hydroxyferuloyl hexose (I)	2.74	C ₁₆ H ₂₀ O ₁₀	372.1061	[M-H] ⁻	371.0988	1.2	371.0981; 209.0456; 191.0352; 147.0452; 119.0503	2	1.465 × 10 ⁷

128	Quinoyl coumaric acid	2.76	C ₁₆ H ₁₈ O ₈	338.1007	[M-H] ⁻	337.0935	1.7	337.0921; 191.0561; 173.0459; 163.0400; 119.0502	2	1.064 × 10 ⁸
129	Caffeoyl hexose (II)	3.21	C ₁₅ H ₁₈ O ₉	342.0953	[M-H] ⁻	341.0880	0.7	341.0881; 179.0350; 135.0453	2	3.682 × 10 ⁸
130	Caffeoyl hexose (III)	3.49	C ₁₅ H ₁₈ O ₉	342.0951	[M-H] ⁻	341.0879	0.2	341.0881; 179.0350; 161.0244; 135.0453	2	4.820 × 10 ⁷
131	Caffeic acid	3.58	C ₉ H ₈ O ₄	180.0425	[M-H] ⁻	179.0352	1.2	179.0350; 135.0453	2	7.903 × 10 ⁷
132	Feruloyl hexose (I)	3.60	C ₁₆ H ₂₀ O ₉	356.1113	[M-H] ⁻	355.1040	1.5	355.1040; 193.0507; 178.0272; 149.0608; 134.0374	2	1.285 × 10 ⁸
133	Coumaroyl hexose (II)	3.61	C ₁₅ H ₁₈ O ₈	326.1007	[M-H] ⁻	325.0934	1.5	325.0933; 163.0402; 119.0503	2	9.889 × 10 ⁷
134	Chloro- genic acid	3.76	C ₁₆ H ₁₈ O ₉	354.0952	[M-H] ⁻	353.0880	0.4	353.0879; 191.0562; 179.0350; 145.0452	2	4.609 × 10 ⁹
135	Hy- droxyferu- loyl hexose (II)	4.04	C ₁₆ H ₂₀ O ₁₀	372.1061	[M-H] ⁻	371.0988	1.2	371.0981; 209.0456; 191.0352; 147.0452; 119.0503	2	1.132 × 10 ⁷
136	Hy- droxyferu- lic acid	4.82	C ₁₀ H ₁₀ O ₅	210.0531	[M-H] ⁻	209.0458	1.1	209.0456; 191.0352; 147.0452; 119.0503	2	4.604 × 10 ⁷
137	Sinapoyl hexose (I)	5.23	C ₁₇ H ₂₂ O ₁₀	386.1218	[M-H] ⁻	385.1145	1.2	385.1145; 223.0611; 208.0377; 193.0141; 179.0913; 164.0478; 149.0243; 121.0295	2	1.375 × 10 ⁸
138	Feruloyl hexose (II)	5.68	C ₁₆ H ₂₀ O ₉	356.1110	[M-H] ⁻	355.1037	0.7	355.1040; 193.0507; 178.0272; 149.0608; 134.0374	2	1.291 × 10 ⁷
139	Chloro- genic acid isomer	5.93	C ₁₆ H ₁₈ O ₉	354.0959	[M-H] ⁻	353.0886	2.3	353.0879; 191.0562; 179.0350; 145.0452	2	8.869 × 10 ⁷
140	Coumaric acid (I)	6.06	C ₉ H ₈ O ₃	164.0477	[M-H] ⁻	163.0404	2.0	163.0402; 119.0503	2	2.245 × 10 ⁷

141	Coumaroyl quinic acid (I)	6.19	C ₁₆ H ₁₈ O ₈	338.1008	[M-H] ⁻	337.0936	2.0	337.0936; 191.0560; 173.0455; 163.0401; 119.0501	2	7.525 × 10 ⁷
142	Caffeoyl shikimoyl hexose (I)	6.46	C ₂₂ H ₂₆ O ₁₃	498.1380	[M-H] ⁻	497.1307	1.3	497.1300; 335.0773; 179.0349; 135.0451	2	1.002 × 10 ⁷
143	Hy- droxyferu- lic acid iso- mer	6.61	C ₁₀ H ₁₀ O ₅	210.0531	[M-H] ⁻	209.0458	1.1	209.0456; 165.0557; 123.0452; 81.0342	2	1.575 × 10 ⁷
144	Coumaric acid (II)	6.69	C ₉ H ₈ O ₃	164.0477	[M-H] ⁻	163.0404	2.1	163.0402; 119.0503	2	9.255 × 10 ⁵
145	Acetyl di- hy- droxyben- zoic acid	6.71	C ₉ H ₈ O ₅	196.0374	[M-H] ⁻	195.0301	1.2	195.0299; 153.0194; 109.0296	2	6.957 × 10 ⁶
146	Sinapoyl hexose (II)	7.06	C ₁₇ H ₂₂ O ₁₀	386.1218	[M-H] ⁻	385.1146	1.4	385.1145; 223.0611; 208.0377; 193.0141; 179.0913; 164.0478; 149.0243; 121.0295	2	1.013 × 10 ⁷
147	Caffeoyl shikimic acid (I)	7.15	C ₁₆ H ₁₆ O ₈	336.0850	[M-H] ⁻	335.0777	1.3	335.0773; 179.0349; 173.0452; 161.0242; 135.0451	2	5.470 × 10 ⁸
148	Coumaroyl hexose (III)	7.35	C ₁₅ H ₁₈ O ₈	326.1009	[M-H] ⁻	325.0936	2.1	325.0933; 163.0402; 119.0503	2	7.631 × 10 ⁶
149	Feruloyl quinic acid	7.88	C ₁₇ H ₂₀ O ₉	368.1114	[M-H] ⁻	367.1041	1.8	367.1010; 193.0507; 191.0560; 178.0272; 173.0455; 149.0608; 134.0374	2	7.640 × 10 ⁷
150	Coumaroyl quinic acid (II)	8.11	C ₁₆ H ₁₈ O ₈	338.1009	[M-H] ⁻	337.0936	2.0	337.0936; 191.0560; 173.0455; 163.0401; 119.0501	2	5.432 × 10 ⁷
151	Ferulic acid	8.16	C ₁₀ H ₁₀ O ₄	194.0582	[M-H] ⁻	193.0509	1.5	193.0507; 178.0272; 149.0608; 134.0374	1	1.080 × 10 ⁷
152	Feruloyl shikimoyl hexose	8.25	C ₂₃ H ₂₈ O ₁₃	512.1541	[M-H] ⁻	511.1468	2.1	511.1468; 193.0507; 178.0272; 149.0608; 134.0374	2	2.117 × 10 ⁶

153	Caffeoyl hexosyl ar- butin (I)	8.93	C ₂₇ H ₃₂ O ₁₅	596.1756	[M-H] ⁻	595.1683	2.4	595.1700; 433.1143; 323.0779; 179.0348; 161.0245; 135.0454	2	3.357 × 10 ⁷
154	Caffeoyl shiikimic acid (II)	9.01	C ₁₆ H ₁₆ O ₈	336.0853	[M-H] ⁻	335.0780	2.3	335.0773; 179.0349; 173.0452; 161.0242; 135.0451	2	3.548 × 10 ⁶
155	Caffeoyl shiikimoyl hexose (II)	9.29	C ₂₂ H ₂₆ O ₁₃	498.1382	[M-H] ⁻	497.1310	1.8	497.1300; 335.0773; 179.0349; 161.0245; 135.0451	2	2.624 × 10 ⁶
156	Sinapic acid	9.33	C ₁₁ H ₁₂ O ₅	224.0690	[M-H] ⁻	223.0617	2.4	223.0611; 208.0377; 193.0141; 179.0913; 164.0478; 149.0243; 121.0295	2	1.285 × 10 ⁶
157	Coumaroyl shiikimic acid	9.65	C ₁₆ H ₁₆ O ₇	320.0902	[M-H] ⁻	319.0829	1.8	319.0831; 173.0454; 163.0402; 155.0350; 137.0244; 119.0503	2	4.759 × 10 ⁶
158	Acetyl caffeoyl de- oxyhexo- side	9.91	C ₁₇ H ₂₀ O ₉	368.1110	[M-H] ⁻	367.1037	0.6	367.1030; 179.0350; 161.0244; 135.0452	2	8.930 × 10 ⁶
159	Caffeoyl hexosyl ar- butin (II)	9.95	C ₂₇ H ₃₂ O ₁₅	596.1756	[M-H] ⁻	595.1683	2.4	595.1700; 433.1143; 323.0779; 179.0348; 161.0245; 135.0454	2	2.260 × 10 ⁶
160	Caffeoyl hexosyl ar- butin (III)	10.05	C ₂₇ H ₃₂ O ₁₅	596.1758	[M-H] ⁻	595.1686	2.9	595.1700; 433.1143; 323.0779; 179.0348; 161.0245; 135.0454	2	2.115 × 10 ⁷
161	Hy- droxyben- zoyl ar- butin (I)	10.12	C ₁₉ H ₂₀ O ₉	392.1117	[M-H] ⁻	391.1044	2.4	391.1037; 281.0669; 137.0245; 109.0296; 93.0344	2	1.384 × 10 ⁸
162	Caffeoyl hexosyl tri- hy- droxymeth- oxyphenyl	10.16	C ₂₅ H ₂₈ O ₁₄	552.1489	[M-H] ⁻	551.1416	1.8	551.1409; 389.0873; 345.0975; 327.0873; 179.0349; 165.0557;	2	1.494 × 10 ⁷

	propanoic acid							161.0243; 147135.0451 ; 121.0296 433.1138; 323.0778; 179.0351; 161.0244; 135.0453; 133.0295; 109.0295		
163	Caffeoyl arbutin (I)	11.05	C ₂₁ H ₂₂ O ₁₀	434.1212	[M-H] ⁻	433.1139	-0.3	415.1242; 169.0142; 125.0244	2	7.640 × 10 ⁷
164	Galloyl valeryl hexoside	11.26	C ₁₈ H ₂₄ O ₁₁	416.1328	[M-H] ⁻	415.1255	2.2	433.1138; 323.0778; 179.0351; 161.0244; 135.0453; 133.0295; 109.0295	2	4.770 × 10 ⁶
165	Caffeoyl arbutin (II)	11.35	C ₂₁ H ₂₂ O ₁₀	434.1212	[M-H] ⁻	433.1139	-0.3	193.0504; 175.0402; 149.0608	2	4.986 × 10 ⁹
166	Ferulic acid isomer	11.85	C ₁₀ H ₁₀ O ₄	194.0582	[M-H] ⁻	193.0509	1.5	535.1459; 191.0350; 163.0400; 147.0452; 119.0502	2	3.216 × 10 ⁷
167	Coumaroyl iridoid (I)	11.98	C ₂₅ H ₂₈ O ₁₃	536.1533	[M-H] ⁻	535.1460	0.6	535.1459; 191.0350; 163.0400; 147.0452; 119.0502	2	7.940 × 10 ⁶
168	Coumaroyl iridoid (II)	12.04	C ₂₅ H ₂₈ O ₁₃	536.1533	[M-H] ⁻	535.1460	0.6	463.1253; 323.0771; 179.0349; 161.0244; 139.0401; 135.0453; 124.0166	2	4.080 × 10 ⁸
169	Caffeoyl methoxyarbutin	12.31	C ₂₂ H ₂₄ O ₁₁	464.1322	[M-H] ⁻	463.1249	0.7	309.0776; 163.0401; 119.0503	2	7.710 × 10 ⁷
170	Coumaroyl coumaric acid	12.55	C ₁₈ H ₁₄ O ₅	310.0849	[M-H] ⁻	309.0776	2.4	477.0970; 315.0724; 179.0347; 161.0243; 153.0193; 135.0451; 109.0296	2	6.693 × 10 ⁶
171	Caffeoyl dihydroxybenzoyl hexose	13.63	C ₂₂ H ₂₂ O ₁₂	478.1119	[M-H] ⁻	477.1046	1.6	503.1228; 341.0875; 323.0778; 179.0351; 161.0228; 135.0453	2	8.520 × 10 ⁶
172	Dicafeoyl hexoside	14.36	C ₂₄ H ₂₄ O ₁₂	504.1286	[M-H] ⁻	503.1213	3.6		2	3.063 × 10 ⁶

173	Dihydroxybenzoyl valeryl hexose (I)	14.44	C ₁₈ H ₂₄ O ₁₀	400.1375	[M-H] ⁻	399.1303	1.5	399.1290; 153.0193; 109.0294	2	4.330 × 10 ⁷
174	Coumaroyl dihydroxybenzoyl hexose (II)	14.81	C ₂₂ H ₂₂ O ₁₁	462.1174	[M-H] ⁻	461.1101	2.6	461.1108; 315.0741; 153.0195; 109.0296	2	1.254 × 10 ⁶
175	Dihydroxybenzoyl valeryl hexose (II)	14.95	C ₁₈ H ₂₄ O ₁₀	400.1375	[M-H] ⁻	399.1303	1.5	399.1290; 153.0193; 109.0294	2	1.520 × 10 ⁸
176	Coumaroyl coumaric acid	15.14	C ₁₈ H ₁₄ O ₅	310.0850	[M-H] ⁻	309.0777	2.7	309.0776; 163.0401; 119.0503	2	1.134 × 10 ⁷
177	Dihydroxybenzoyl benzoyl hexose (I)	15.15	C ₂₀ H ₂₀ O ₁₀	420.1064	[M-H] ⁻	419.0991	1.8	315.0727; 153.0194; 109.0296	2	2.594 × 10 ⁶
178	Coumaroyl hydroxybenzoyl hexose	15.24	C ₂₂ H ₂₂ O ₁₀	446.1218	[M-H] ⁻	445.1146	1.2	307.0822; 163.0403; 145.0294; 137.0243; 119.0501; 93.0343	2	3.808 × 10 ⁷
179	Sinapoyl coumaroyl hexose	15.31	C ₂₆ H ₂₈ O ₁₂	532.1593	[M-H] ⁻	531.1520	2.3	531.1481; 307.0823; 223.0612; 208.0378; 193.0141; 163.0400; 149.0243; 145.0295; 119.0503	2	1.545 × 10 ⁷
180	Hydroxybenzoyl arbutin (II)	15.52	C ₁₉ H ₂₀ O ₉	392.1117	[M-H] ⁻	391.1044	2.5	391.1047; 281.0669; 137.0244; 93.0343	2	5.623 × 10 ⁶
181	Dihydroxybenzoyl benzoyl hexose (II)	15.58	C ₂₀ H ₂₀ O ₁₀	420.1067	[M-H] ⁻	419.0994	2.5	315.0727; 153.0194; 109.0296	2	1.819 × 10 ⁶
182	Caffeoyl acetyl arbutin (II)	15.71	C ₂₃ H ₂₄ O ₁₁	476.1319	[M-H] ⁻	475.1246	0.0	475.1245; 179.0348; 161.0244; 135.0452; 133.0295	2	4.880 × 10 ⁸
183	Caffeoyl acetyl arbutin (I)	15.84	C ₂₃ H ₂₄ O ₁₁	476.1319	[M-H] ⁻	475.1246	0.0	475.1245; 179.0348; 161.0244; 135.0452; 133.0295	2	2.340 × 10 ⁹

184	Chlorogenic acid derivative (I)	15.85	C ₂₆ H ₂₈ O ₁₂	532.1589	[M-H] ⁻	531.1516	1.5	353.0879; 191.0562; 179.0350; 145.0452	3	1.269 × 10 ⁷
185	Hydroxybenzoyl benzoyl hexose (I)	15.86	C ₂₀ H ₂₀ O ₉	404.1153	[M-H] ⁻	403.1080	2.0	403.1041; 137.0244; 93.0344	2	6.070 × 10 ⁶
186	Caffeoyl coumaroyl hexose	16.06	C ₂₄ H ₂₄ O ₁₁	488.1329	[M-H] ⁻	487.1257	2.2	487.1247; 323.0772; 179.0349; 163.0399; 161.0243; 133.0294; 119.0501	2	1.114 × 10 ⁷
187	Dihydroxybenzoyl valeryl hexose (III)	16.32	C ₁₈ H ₂₄ O ₁₀	400.1375	[M-H] ⁻	399.1303	1.5	399.1290; 153.0193; 109.0294	2	7.360 × 10 ⁷
188	Caffeoyl feruloyl hexose (I)	16.43	C ₂₅ H ₂₆ O ₁₂	518.1431	[M-H] ⁻	517.1358	1.5	517.1358; 337.0929; 179.0349; 175.0399; 135.0452	2	8.930 × 10 ⁶
189	Coumaroyl dihydroxybenzoyl hexose (I)	16.46	C ₂₂ H ₂₂ O ₁₁	462.1174	[M-H] ⁻	461.1101	2.5	461.1108; 315.0741; 153.0195; 109.0296	2	1.264 × 10 ⁷
190	Dihydroxybenzoyl dihydroxybenzoic acid	16.60	C ₁₄ H ₁₀ O ₇	290.0435	[M-H] ⁻	289.0362	2.8	153.0194; 109.0296	2	1.246 × 10 ⁷
191	Caffeoyl feruloyl hexose (II)	16.64	C ₂₅ H ₂₆ O ₁₂	518.1431	[M-H] ⁻	517.1358	1.5	517.1358; 179.0349; 175.0399; 135.0452	2	4.260 × 10 ⁶
192	Dicoumaroyl hexose (I)	16.87	C ₂₄ H ₂₄ O ₁₀	472.1378	[M-H] ⁻	471.1305	1.8	471.1298; 307.0826; 163.0400; 145.0294; 119.0502	2	2.540 × 10 ⁷
193	Feruloyl dihydroxybenzoyl hexose	17.19	C ₂₃ H ₂₄ O ₁₂	492.1277	[M-H] ⁻	491.1204	1.8	491.1197; 315.0724; 193.0505; 175.0401; 160.0165; 153.0192; 134.0371; 109.0294	2	4.180 × 10 ⁶
194	Coumaroyl Feruloyl hexose (I)	17.28	C ₂₅ H ₂₆ O ₁₁	502.1485	[M-H] ⁻	501.1413	2.0	501.1398; 337.0936; 307.0824; 193.0507;	2	1.238 × 10 ⁷

								178.0272; 163.0400; 149.0608; 145.0295; 134.0374; 119.0502		
195	Caffeoyl valeryl hex- ose (I)	17.32	C ₂₀ H ₂₆ O ₁₀	426.1531	[M-H] ⁻	425.1459	1.3	425.1531; 179.0350; 135.0451	3	5.624 × 10 ⁷
196	Caffeoyl valeryl hex- ose (II)	17.39	C ₂₀ H ₂₆ O ₁₀	426.1530	[M-H] ⁻	425.1457	0.9	425.1531; 179.0350; 135.0451	3	1.237 × 10 ⁸
197	Caffeoyl benzoyl hexose (I)	17.40	C ₂₂ H ₂₂ O ₁₀	446.1219	[M-H] ⁻	445.1146	1.3	445.1144; 179.0345; 135.0452; 121.0296	2	1.129 × 10 ⁷
198	Diferuloyl hexose	17.61	C ₂₆ H ₂₈ O ₁₂	532.1594	[M-H] ⁻	531.1521	2.4	531.1520; 337.0936; 193.0507; 178.0272; 149.0608; 134.0374	2	5.227 × 10 ⁶
199	Caffeoyl benzoyl hexose (II)	17.72	C ₂₂ H ₂₂ O ₁₀	446.1222	[M-H] ⁻	445.1149	1.9	445.1144; 179.0345; 135.0452	2	8.108 × 10 ⁶
200	Hy- droxyben- zoyl ben- zoyl hexose (II)	17.84	C ₂₀ H ₂₀ O ₉	404.1153	[M-H] ⁻	403.1080	2.0	403.1041; 137.0244; 93.0344	2	4.350 × 10 ⁶
201	Dicafeoyl shiikimic acid (II)	17.94	C ₂₅ H ₂₂ O ₁₁	498.1153	[M-H] ⁻	497.1080	-1.9	497.1090; 179.0350; 161.0243; 135.0451	2	2.307 × 10 ⁶
202	Coumaroyl methylhy- droxyben- zoyl hexose (I)	17.95	C ₂₃ H ₂₄ O ₁₀	460.1375	[M-H] ⁻	459.1302	1.2	459.1299; 307.0818; 163.0402; 145.0295; 119.0502	2	4.490 × 10 ⁷
203	Coumaroyl valeryl hex- ose (I)	17.96	C ₂₀ H ₂₆ O ₉	410.1586	[M-H] ⁻	409.1513	2.2	409.1500; 163.0399; 119.0501	3	4.709 × 10 ⁷
204	Dicouma- royl hexose (II)	18.04	C ₂₄ H ₂₄ O ₁₀	472.1379	[M-H] ⁻	471.1306	2.0	471.1281; 307.0820; 163.0399; 145.0293; 119.0501	2	7.523 × 10 ⁶
205	Dicafeoyl shiikimic acid (I)	18.06	C ₂₅ H ₂₂ O ₁₁	498.1141	[M-H] ⁻	497.1068	-4.2	497.1090; 179.0350; 161.0243; 135.0451	2	1.114 × 10 ⁶
206	Dihy- droxyben- zoyl ben- zoyl hexose (III)	18.36	C ₂₀ H ₂₀ O ₁₀	420.1065	[M-H] ⁻	419.0992	1.9	419.0981; 153.0194; 109.0295	2	6.094 × 10 ⁶

207	Feruloyl valeryl hex- ose	18.38	C ₂₁ H ₂₈ O ₁₀	440.1691	[M-H] ⁻	439.1618	1.9	439.1609; 193.0507; 178.0272; 149.0608; 134.0374	2	4.270 × 10 ⁷
208	Coumaroyl methylhy- droxyben- zoyl hexose (II)	18.42	C ₂₃ H ₂₄ O ₁₀	460.1375	[M-H] ⁻	459.1302	1.2	459.1299; 307.0818; 163.0402; 145.0295; 119.0502	2	2.050 × 10 ⁸
209	Coumaroyl Feruloyl hexose (II)	18.58	C ₂₅ H ₂₆ O ₁₁	502.1485	[M-H] ⁻	501.1413	2.0	501.1398; 337.0936; 193.0507; 175.0401; 163.0400; 160.0165; 149.0608; 145.0295; 134.0374; 119.0502	2	3.440 × 10 ⁶
210	Chloro- genic acid derivative (II)	19.14	C ₂₆ H ₂₈ O ₁₂	532.1585	[M-H] ⁻	531.1512	0.7	531.0879; 191.0562; 179.0350; 145.0452	2	2.514 × 10 ⁶
211	Caffeoyl di- hy- droxyben- zoyl meva- lonic acid	19.47	C ₂₂ H ₂₂ O ₁₀	446.1221	[M-H] ⁻	445.1149	1.9	445.1144; 179.0345; 153.0194; 135.0452; 109.0296	2	1.629 × 10 ⁶
212	Coumaroyl valeryl hex- ose (II)	19.77	C ₂₀ H ₂₆ O ₉	410.1584	[M-H] ⁻	409.1512	1.8	409.1500; 163.0399; 119.0501	3	2.633 × 10 ⁷
213	Caffeoyl cinnamoyl hexose	20.26	C ₂₄ H ₂₄ O ₁₀	472.1376	[M-H] ⁻	471.1303	1.3	471.1230; 179.0350; 135.0452	2	1.922 × 10 ⁶

Table 4. Detailed identification data for the annotated proanthocyanidins in *Disterigma alaternoides*.

ID	Name	RT [min]	Formula	Molecular Weight	Adduct	Experi- mental m/z	Δ (ppm)	Main Frag- ments	Confidence Level	Mean Area
214	a-Procy- nidin te- tramer (cat- cat-cat-cat)	2.56	C ₆₀ H ₄₈ O ₂₄	1152.2564	[M-2H] ²⁻	575.1209	2.5	981.1918; 863.1859; 829.1519; 693.1247; 573.1050; 451.1032; 425.0874; 411.0724; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	2.091 × 10 ⁷

215	b-Procyanidin dimer (cat-cat)	5.73	C ₃₀ H ₂₆ O ₁₂	578.1438	[M-H] ⁻	577.1365	2.3	577.1334; 451.1032; 425.0874; 407.0772; 289.0720; 287.0568; 245.0828; 137.02443; 125.0244	2	8.073 × 10 ⁷
216	a-Procyanidin pentamer (cat-cat-cat-cat-cat)	5.78	C ₇₅ H ₆₀ O ₃₀	1440.3213	[M-2H] ²⁻	719.1533	3.0	981.1981; 863.1859; 711.1358; 693.1247; 575.1198; 573.1064; 451.1054; 449.0878; 423.0739; 411.0740; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	1.728 × 10 ⁷
217	b-Procyanidin trimer (cat-cat-cat)	5.94	C ₄₅ H ₃₈ O ₁₈	866.2077	[M-H] ⁻	865.2004	2.2	865.2015; 713.1520; 577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	1.323 × 10 ⁷
218	b-Procyanidin tetramer (cat-cat-cat-cat)	7.08	C ₆₀ H ₅₀ O ₂₄	1154.2720	[M-2H] ²⁻	576.1287	2.4	577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	1.146 × 10 ⁷
219	a-Procyanidin trimer (cat-cat-cat)	7.33	C ₄₅ H ₃₆ O ₁₈	864.1919	[M-H] ⁻	863.1846	2.0	863.1859; 711.1358; 693.1247; 573.1050; 451.1032; 425.0874; 411.0724; 407.0772; 289.0720; 285.0406;	2	4.379 × 10 ⁶

									137.0245; 125.0245; 577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244		
220	b-Procyanidin tetramer (cat-cat-cat-cat)	7.59	C ₆₀ H ₅₀ O ₂₄	1154.2727	[M-2H] ²⁻	576.1291	3.0	2	1.925 × 10 ⁷		
									125.0244 693.1247; 573.1050; 451.1032; 425.0874; 411.0724; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245		
221	a-Procyanidin tetramer (cat-cat-cat-cat)	8.14	C ₆₀ H ₄₈ O ₂₄	1152.2571	[M-2H] ²⁻	575.1213	3.2	2	7.635 × 10 ⁶		
									863.1859; 711.1358; 693.1247; 573.1050; 451.1032; 425.0874; 411.0724; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245		
222	a-Procyanidin trimer (cat-cat-cat)	8.38	C ₄₅ H ₃₆ O ₁₈	864.1913	[M-H] ⁻	863.1840	1.3	2	2.909 × 10 ⁸		
									407.0772; 289.0720; 285.0406; 137.0245; 125.0245		
223	b-Procyanidin trimer (cat-cat-cat)	8.71	C ₄₅ H ₃₈ O ₁₈	866.2075	[M-H] ⁻	865.2002	1.9	2	5.503 × 10 ⁷		
									865.2015; 713.1520; 577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244		
224	b-Procyanidin pentamer (cat-cat-cat-cat-cat)	8.92	C ₇₅ H ₆₂ O ₃₀	1442.3367	[M-2H] ²⁻	720.1611	2.9	2	1.491 × 10 ⁷		
									863.1821; 693.1250; 577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828;		

								137.0244; 125.0244 863.1859; 711.1330; 693.1247; 573.1050; 451.1032; 425.0874; 411.0724; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245		
225	a-Procyanidin tetramer (cat-cat-cat-cat)	9.60	C ₆₀ H ₄₈ O ₂₄	1152.2564	[M-2H] ²⁻	575.1209	2.6	577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	5.099 × 10 ⁷
226	b-Procyanidin tetramer (cat-cat-cat-cat)	9.65	C ₆₀ H ₅₀ O ₂₄	1154.2721	[M-2H] ²⁻	576.1288	2.5	591.1118; 465.0753; 439.0693; 303.0506; 285.0406; 137.0245; 125.0245	2	3.123 × 10 ⁷
227	a-Proanthocyanidin dimer (gal-cat-cat)	9.98	C ₃₀ H ₂₄ O ₁₃	592.1224	[M-H] ⁻	591.1151	1.2	863.1821; 737.1509; 693.1250; 577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	2.279 × 10 ⁶
228	b-Procyanidin pentamer (cat-cat-cat-cat-cat)	10.15	C ₇₅ H ₆₂ O ₃₀	1442.3358	[M-2H] ²⁻	720.1606	2.3	863.1859; 711.1358; 693.1247; 575.1198; 449.0878; 423.0739; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	1.471 × 10 ⁷
229	a-Procyanidin trimer (cat-cat-cat)	10.54	C ₄₅ H ₃₆ O ₁₈	864.1916	[M-H] ⁻	863.1844	1.7		2	3.598 × 10 ⁷

230	b-Procyanidin pentamer (cat-cat-cat-cat-cat)	10.61	C ₇₅ H ₆₂ O ₃₀	1442.3351	[M-2H] ²⁻	720.1603	1.7	721.1294; 577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	3.738 × 10 ⁷
231	b-Procyanidin tetramer (cat-cat-cat-cat)	10.75	C ₆₀ H ₅₀ O ₂₄	1154.2725	[M-2H] ²⁻	576.1290	2.9	577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	6.568 × 10 ⁶
232	a-Procyanidin pentamer (cat-cat-cat-cat-cat)	10.82	C ₇₅ H ₆₀ O ₃₀	1440.3239	[M-2H] ²⁻	719.1547	4.9	1115.2210; 861.1715; 719.1268; 577.1363; 451.1054; 449.0878; 425.0880; 411.0740; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	4.323 × 10 ⁶
233	a-Procyanidin tetramer (cat-cat-cat-cat)	10.94	C ₆₀ H ₄₈ O ₂₄	1152.2571	[M-2H] ²⁻	575.1213	3.1	575.1198; 449.0878; 423.0739; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	7.927 × 10 ⁶
234	b-Procyanidin hexamer (cat-cat-cat-cat-cat-cat)	11.07	C ₉₀ H ₇₄ O ₃₆	1730.3911	[M-2H] ²⁻	864.1883	-2.8	1151.2379; 865.1873; 863.1821; 695.1427; 577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	1.438 × 10 ⁷

235	b-Procyanidin hexamer (cat-cat-cat-cat-cat)	11.42	C ₉₀ H ₇₄ O ₃₆	1730.3965	[M-2H] ²⁻	864.1910	0.3	1151.2379; 865.1873; 863.1821; 695.1427; 577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	2.342 × 10 ⁷
236	a-Procyanidin pentamer (cat-cat-cat-cat-cat)	11.87	C ₇₅ H ₆₀ O ₃₀	1440.3200	[M-2H] ²⁻	719.1527	2.1	861.1613; 739.1692; 737.1482; 689.2198; 577.1314; 573.1050; 451.1032; 425.0874; 411.0724; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	1.373 × 10 ⁷
237	a-Procyanidin dimer (cat-cat)	12.02	C ₃₀ H ₂₄ O ₁₂	576.1277	[M-H] ⁻	575.1204	1.5	575.1195; 449.0883; 423.0725; 407.0762; 289.0720; 285.0406; 137.0245; 125.0245	2	4.554 × 10 ⁸
238	a-Procyanidin hexamer (cat-cat-cat-cat-cat)	12.02	C ₉₀ H ₇₂ O ₃₆	1728.3825	[M-2H] ²⁻	863.1840	1.9	863.1859; 575.1198; 539.0993; 449.0878; 423.0739; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	5.899 × 10 ⁶
239	a-Procyanidin pentamer (cat-cat-cat-cat-cat)	12.30	C ₇₅ H ₆₀ O ₃₀	1440.3205	[M-2H] ²⁻	719.1530	2.5	693.1247; 573.1050; 527.1164; 451.1032; 447.0710; 425.0874; 411.0724; 407.0772; 289.0720; 285.0406;	2	1.101 × 10 ⁷

								137.0245; 125.0245 577.1334; 451.1032; 425.0874; 407.0772; 289.0720; 287.0568; 245.0828; 137.02443; 125.0244		
240	b-Procyanidin dimer (cat-cat)	12.35	C ₃₀ H ₂₆ O ₁₂	578.1442	[M-H] ⁻	577.1369	3.0	289.0720; 287.0568; 245.0828; 137.02443; 125.0244	2	1.997 × 10 ⁷
241	a-Procyanidin tetramer (cat-cat-cat-cat)	12.44	C ₆₀ H ₄₈ O ₂₄	1152.2569	[M-2H] ²⁻	575.1212	2.9	863.1859; 711.1358; 693.1247; 575.1198; 449.0878; 423.0739; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	6.703 × 10 ⁶
242	b-Procyanidin hexamer (cat-cat-cat-cat-cat-cat)	12.49	C ₉₀ H ₇₄ O ₃₆	1730.3902	[M-2H] ²⁻	864.1878	-2.8	863.1859; 693.1280; 575.1198; 539.0993; 449.0878; 423.0739; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	1.642 × 10 ⁶
243	a-Procyanidin trimer (cat-afz-galcat)	12.64	C ₄₅ H ₃₆ O ₁₈	864.1893	[M-H] ⁻	863.1820	-1.0	863.1859; 711.1358; 693.1247; 575.1198; 449.0878; 433.0771; 407.0772; 301.0340; 289.0720; 137.0245; 125.0245	2	1.592 × 10 ⁷
244	a-Procyanidin tetramer (cat-cat-cat-cat)	13.15	C ₆₀ H ₄₈ O ₂₄	1152.2566	[M-2H] ²⁻	575.1210	2.7	573.1050; 451.1032; 425.0874; 411.0724; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	8.694 × 10 ⁶
245	b-Procyanidin trimer (cat-cat-cat)	13.21	C ₄₅ H ₃₈ O ₁₈	866.2085	[M-H] ⁻	865.2013	3.4	865.2015; 713.1520; 577.1334; 575.1216;	2	4.968 × 10 ⁶

								451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244		
246	a-Procyanidin trimer (cat-cat-cat)	13.44	C ₄₅ H ₃₆ O ₁₈	864.1882	[M-H] ⁻	863.1809	-2.3	863.1859; 711.1358; 693.1247; 575.1198; 449.0878; 433.0771; 423.0739; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	2.176 × 10 ⁷
247	a-Procyanidin pentamer (cat-cat-cat-cat-cat)	14.11	C ₇₅ H ₆₀ O ₃₀	1440.3198	[M-2H] ²⁻	719.1526	2.0	863.1859; 711.1358; 693.1247; 575.1198; 449.0878; 423.0739; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	1.293 × 10 ⁷
248	a-Procyanidin hexamer (cat-cat-cat-cat-cat-cat)	14.80	C ₉₀ H ₇₂ O ₃₆	1728.3836	[M-2H] ²⁻	863.1845	1.9	863.1859; 693.1280; 575.1198; 539.0993; 449.0878; 423.0739; 407.0772; 289.0720; 285.0406; 137.0245; 125.0245	2	1.168 × 10 ⁷
249	b-Procyanidin tetramer (cat-cat-cat-cat)	15.14	C ₆₀ H ₅₀ O ₂₄	1154.2732	[M-2H] ²⁻	576.1293	3.5	577.1334; 575.1216; 451.1032; 425.0874; 407.0772; 289.0720; 287.0562; 245.0828; 137.0244; 125.0244	2	5.320 × 10 ⁶