

Table 1S The MS/MS fragment of CGAs in *D. nervosa*

Peak	t_R	Theoretical Mass m/z	Experimental Mass m/z	Error (ppm)	Formula [M-H]	MS/MS fragment	Identification
1	1.64	353.10894	353.10833	-1.71	$C_{13}H_{21}O_{11}$	$MS^2[353]:101.0593(100), 129.0542(10), 191.0548(5), 173.0443(2)$	QA-hexoside
2	1.64	677.19345	677.19128	-3.20	$C_{28}H_{37}O_{19}$	$MS^2[677]:341.0865(100), 179.0335(84), 191.0548(36), 173.0442(28), 134.9742(25)$	CQA-Dihexoside
3	1.81	353.10894	353.10812	-2.31	$C_{13}H_{21}O_{11}$	$MS^2[353]:101.0593(100), 129.0542(15), 191.0548(7), 173.0443(3)$	QA-hexoside
4	1.93	353.10894	353.10845	-1.37	$C_{13}H_{21}O_{11}$	$MS^2[353]:101.0593(100), 129.0542(37), 191.0548(9), 173.0443(3)$	QA-hexoside
5	2.06	677.19345	677.19312	-0.49	$C_{28}H_{37}O_{19}$	$MS^2[677]:191.0548(100), 515.1394(42), 353.0868(37), 323.0763(22), 516.1425(13)$	CQA-Dihexoside
6	2.10	353.10894	353.10825	-1.94	$C_{13}H_{21}O_{11}$	$MS^2[353]:191.0548(100), 129.0542(97), 115.0386(73), 85.0279(51), 101.0593(32), 173.0443(10)$	QA-hexoside
7	2.30	353.10894	353.10848	-1.29	$C_{13}H_{21}O_{11}$	$MS^2[353]:191.0548(100), 129.0542(88), 115.0386(67), 101.0593(55), 173.0443(8)$	QA-hexoside

8	2.31	677.19345	677.19269	-1.12	C ₂₈ H ₃₇ O ₉	MS ² [677]:173.0442(100), 155.0336(65), 341.0869(21), 209.0292(15), 129.0543(14)	CQA-Dihexoside
9	2.40	353.10894	353.10822	-2.02	C ₁₃ H ₂₁ O ₁₁	MS ² [353]:191.0549(100), 129.0542(93), 115.0385(81), 101.0593(37), 85.0279(19), 173.0443(18)	QA-hexoside
10	2.65	353.08781	353.08707	-2.08	C ₁₆ H ₁₇ O ₉	MS ² [353]:191.0548(100), 85.0279(10), 135.0435(1), 173.0442(1)	Cis-3-CQA
11	2.99	677.19345	677.19263	-1.21	C ₂₈ H ₃₇ O ₉	MS ² [677]:173.0442(100), 315.0714(63), 341.0868(24), 191.0548(17), 179.0335(15)	CQA-Dihexoside
12	3.04	529.15628	529.15509	-2.25	C ₂₃ H ₂₉ O ₁₄	MS ² [529]:193.0494(100), 191.0547(7)	3-FQA-hexoside
13	3.08	677.19345	677.19180	-2.44	C ₂₈ H ₃₇ O ₉	MS ² [677]:265.0924(100), 266.0955(12), 265.1071(12), 96.9586(11), 191.0549(9)	CQA-Dihexoside
14	3.2	515.14063	515.13934	-2.50	C ₂₂ H ₂₇ O ₁₄	MS ² [515]:191.0548(100), 179.0338(39), 341.0869(6), 173.0441(6)	CQA-4'-hexoside
15	3.27	353.08781	353.08682	-2.79	C ₁₆ H ₁₇ O ₉	MS ² [353]:191.0548(100), 135.0437(81), 179.0336(40), 173.0440(3)	Trans-3-CQA
16	3.35	499.14571	499.14459	-2.25	C ₂₂ H ₂₇ O ₁₃	MS ² [499]:173.0442(100), 93.0330(91), 191.0548(45), 163.0387(14), 337.0919(5)	4-pCoQA-hexoside

17	3.49	341.08781	341.08701	-2.33	C ₁₅ H ₁₇ O ₉	MS ² [341]:135.0437(100), 161.0230(66), 179.0337(49)	CA-hexoside
18	3.64	341.08781	341.08691	-2.63	C ₁₅ H ₁₇ O ₉	MS ² [341]:135.0438(100), 179.0337(49), 161.0231(29)	CA-hexoside
19	3.72	499.14571	499.14536	-0.71	C ₂₂ H ₂₇ O ₁₃	MS ² [499]:173.0442(100), 163.0387(29), 191.0548(21), 337.0921(2)	4- <i>p</i> CoQA-hexoside
20	3.80	515.14063	515.13959	-2.02	C ₂₂ H ₂₇ O ₁₄	MS ² [515]: 173.0441(100), 179.0336(91), 323.0764(9), 341.0869(9)	CQA-3'-hexoside
21	4.14	529.15628	529.15521	-2.02	C ₂₃ H ₂₉ O ₁₄	MS ² [529]:173.0442(100), 93.0330(80), 191.0548(35), 87.0072(20), 111.0436(19), 193.0494(16), 367.1024(5)	4-FQA-hexoside
22	4.19	515.14063	515.13954	-2.11	C ₂₂ H ₂₇ O ₁₄	MS ² [515]:191.0548(100), 173.0442(57), 179.0336(24), 353.1077(18)	CQA-4'-hexoside
23	4.20	341.08781	341.08734	-1.36	C ₁₅ H ₁₇ O ₉	MS ² [341]:135.0437(100), 161.0231(75), 179.0337(60)	CA-hexoside
24	4.21	499.14571	499.14407	-3.29	C ₂₂ H ₂₇ O ₁₃	MS ² [499]:191.0548(100), 135.0436(19), 337.0920(16)	5- <i>p</i> CoQA-hexoside
25	4.48	353.08781	353.08701	-2.25	C ₁₆ H ₁₇ O ₉	MS ² [353]:173.0442(100), 179.0335(65), 191.0547(48), 135.0436(37)	Cis-4-CQA
26	4.50	337.09289	337.09232	-1.69	C ₁₆ H ₁₇ O ₈	MS ² [337]: 163.0387(100), 119.0488(45), 191.0549(37), 135.0437(5)	Tran-3- <i>p</i> CoQA

27	4.50	397.11402	397.11374	-0.70	C ₁₈ H ₂₁ O ₁₀	MS ² [397]:191.0548(100), 179.0338(49), 205.0496(39), 173.0442(28)	3-SQA
28	4.5 1	515.14063	515.13947	-2.25	C ₂₂ H ₂₇ O ₁₄	MS ² [515]:191.0549(100), 323.0765(49), 161.0230(15)	CQA-3'-hexoside
29	4.68	341.08781	341.08688	-2.71	C ₁₅ H ₁₇ O ₉	MS ² [341]:135.0438(100), 179.0337(89), 161.0230(35)	CA-hexoside
30	4.69	337.09289	337.09225	-1.90	C ₁₆ H ₁₇ O ₈	MS ² [337]:163.0388(100)	Cis-3- <i>p</i> CoQA
31	4.6 9	397.11402	397.11395	-0.18	C ₁₈ H ₂₁ O ₁₀	MS ² [397]:173.0442(100), 179.0701(31), 191.0548(14), 205.0497(4)	4-SQA
32	4.69	499.14571	499.14447	-2.49	C ₂₂ H ₂₇ O ₁₃	MS ² [499]:179.0337(100), 191.0548(98)	CQA-pentoside
33	4.7 4	397.11402	397.11322	-1.99	C ₁₈ H ₂₁ O ₁₀	MS ² [397]:205.0496(100), 191.0550(64), 173.0442(2)	5-SQA
34	4.75	529.15628	529.15594	-0.64	C ₂₃ H ₂₉ O ₁₄	MS ² [529]:173.0442(100), 193.0494(19)	4-FQA-hexoside
35	4.8 0	515.14063	515.13916	-2.85	C ₂₂ H ₂₇ O ₁₄	MS ² [515]:191.0548(100), 179.0336(34), 323.0764(30), 161.0230(27), 173.0442(24)	CQA-3'-hexoside
36	4.83	499.14571	499.14526	-0.91	C ₂₂ H ₂₇ O ₁₃	MS ² [499]:179.0337(100), 191.0548(32), 173.0441(16)	CQA-pentoside

37	4.84	341.08781	341.08685	-2.80	C ₁₅ H ₁₇ O ₉	MS ² [341]:135.0437(100), 179.0337(65), 161.0230(15)	CA-hexoside
38	4.95	497.13006	497.12930	-1.54	C ₂₂ H ₂₅ O ₁₃	MS ² [497]:179.0337(100), 335.0765(27), 135.0437(21), 161.0230(11), 191.0549(6)	CSA-hexoside
39	5.10	353.08781	353.08682	-2.79	C ₁₆ H ₁₇ O ₉	MS ² [353]:191.0547(100)	Trans-5-CQA
40	5.1 1	515.14063	515.13910	-2.97	C ₂₂ H ₂₇ O ₁₄	MS ² [515]:179.0336(100), 173.0442(66), 341.0868(21), 191.0548(20), 161.0229(17)	CQA-4'-hexoside
41	5.25	341.08781	341.08710	-2.07	C ₁₅ H ₁₇ O ₉	MS ² [341]:135.0437(100), 179.0337(77), 161.0231(21)	CA-hexoside
42	5.3 9	839.22515	839.22614	1.18	C ₃₇ H ₄₃ O ₂₂	MS ² [839]:353.0869(100), 173.0442(28), 354.0904(17), 179.0337(16)	DiCQA-Dihexoside
43	5.42	367.10346	367.10273	-1.98	C ₁₇ H ₁₉ O ₉	MS ² [367]:193.0494(100), 191.0548(8), 173.0442(4)	Tran-3-FQA
44	5.43	353.08781	353.08682	-2.79	C ₁₆ H ₁₇ O ₉	MS ² [353]:173.0441(100), 179.0336(73), 191.0547(50), 135.0436(33)	Trans-4-CQA
45	5.51	515.14063	515.13995	-1.32	C ₂₂ H ₂₇ O ₁₄	MS ² [515]:191.0548(100), 179.0337(19)	CQA-4'-hexoside
46	5.61	499.14571	499.14488	-1.67	C ₂₂ H ₂₇ O ₁₃	MS ² [499]:191.0548(100), 173.0445(38), 163.0387(24), 337.0919(6)	5-pCQA-hexoside

47	6.00	337.09289	337.09229	-1.78	C ₁₆ H ₁₇ O ₈	MS ⁺ [337]:191.0548(100), 119.0487(24), 163.0387(19), 173.0442(18)	Tran-5- <i>p</i> CoQA
48	6.08	529.15628	529.15546	-1.55	C ₂₃ H ₂₉ O ₁₄	MS ⁺ [529]:173.0442(100), 191.0548(32), 367.1024(28), 337.0349(9)	4-FQA-hexoside
49	6.31	497.13006	497.12994	-0.25	C ₂₂ H ₂₅ O ₁₃	MS ⁺ [497]:179.0337(100), 193.0494(40), 341.0869(8), 135.0437(8), 335.0769(2)	CSA-hexoside
50	6.31	839.22515	839.22431	-1.00	C ₃₇ H ₄₃ O ₂₂	MS ⁺ [839]:357.1183(100), 341.0870(57), 259.0716(35), 179.0337(31), 358.1212(29), 301.0233(16), 260.0760(13), 261.1348(12)	DiCQA-Dihexoside
51	6.38	337.09289	337.09229	-1.78	C ₁₆ H ₁₇ O ₈	MS ⁺ [337]:173.0442(100), 135.0437(89), 119.0487(51), 191.0549(27), 163.0387(17)	Cis-4- <i>p</i> CoQA
52	6.51	497.13006	497.12903	-2.08	C ₂₂ H ₂₅ O ₁₃	MS ⁺ [497]:335.0762(100), 161.0230(82), 179.0337(73), 191.0549(16), 135.0437(17)	CQL-hexoside
53	6.55	367.10346	367.10239	-2.90	C ₁₇ H ₁₉ O ₉	MS ⁺ [367]:193.0494(100)	Cis-3-FQA
54	6.65	529.15628	529.15540	-1.66	C ₂₃ H ₂₉ O ₁₄	MS ⁺ [529]:337.0346(100), 191.0548(72), 173.0442(16), 367.1024(4)	5-FQA-hexoside
55	6.76	839.22515	839.22369	-1.73	C ₃₇ H ₄₃ O ₂₂	MS ⁺ [839]:341.0868(100), 515.1396(88), 371.0610(77),	DiCQA-Dihexoside

									209.0291(35), 179.0336(33)	
56	6.80	497.13006	497.12918	-1.78	$C_{22}H_{25}O_{13}$	$MS^2[497]:179.0337(100), 335.0765(29), 135.0437(18), 161.0230(10)$				CSA-hexoside
57	6.85	529.15628	529.15594	-0.64	$C_{23}H_{29}O_{14}$	$MS^2[529]:173.0442(100), 191.0549(70), 337.0348(40), 367.1025(24)$				4-FQA-hexoside
58	6.90	353.08781	353.08694	-2.45	$C_{16}H_{17}O_9$	$MS^2[353]:191.0548(100)$				Cis-5-CQA
59	7.18	335.07724	335.07678	-1.37	$C_{16}H_{15}O_8$	$MS^2[335]:135.0438(100), 161.0231(65), 93.0331(47), 179.0338(29)$				5-CSA
60	7.26	335.07724	335.07687	-1.11	$C_{16}H_{15}O_8$	$MS^2[335]:135.0436(100), 93.0330(46), 179.0337(33), 161.0230(8)$				4-CSA
61	7.40	337.09289	337.09222	-1.99	$C_{16}H_{17}O_8$	$MS^2[337]:173.0442(100), 191.0550(28), 135.0437(18), 163.0387(7)$				Tran-4- <i>p</i> CoQA
62	7.69	337.09289	337.09210	-2.35	$C_{16}H_{17}O_8$	$MS^2[337]:191.0549(100), 173.0443(5)$				Cis-5- <i>p</i> CoQA
63	7.73	367.10346	367.10264	-2.20	$C_{17}H_{19}O_9$	$MS^2[367]:173.0442(100), 85.0279(88), 134.0358(62), 191.0548(34), 161.0230(23)$				Cis-4-FQA
64	8.08	335.07724	335.07654	-2.09	$C_{16}H_{15}O_8$	$MS^2[335]:135.0437(100), 179.0337(30), 161.0231(26),$				3-CSA

								93.0330(14), 173.0443(5)	
65	8.09	515.11950	515.11835	-2.23	$C_{23}H_{33}O_{12}$	$MS^2[515]:191.0548(100), 179.0336(94), 135.0436(15), 353.0869(11), 161.0227(6), 173.0443(6)$			1,3-DiCQA
66	8.23	335.07724	335.07663	-1.82	$C_{16}H_{15}O_8$	$MS^2[335]:161.0231(100), 173.0443(62), 135.0438(61), 179.0337(24), 93.0331(16)$			3-CQL
67	8.47	367.10346	367.10242	-2.82	$C_{17}H_{19}O_9$	$MS^2[367]:173.0442(100), 93.0330(35), 134.0358(32), 193.0494(13), 111.0072(10)$			Tran-4-FQA
68	8.62	367.10346	367.10242	-2.82	$C_{17}H_{19}O_9$	$MS^2[367]:191.0548(100), 93.0330(54), 134.0358(18), 87.0072(16), 173.0442(9), 111.0436(9)$			Tran-5-FQA
69	8.69	335.07724	335.07645	-2.36	$C_{16}H_{15}O_8$	$MS^2[335]:161.0230(100), 135.0437(49), 133.0281(14), 179.0337(10), 173.0442(8)$			1-CQL
70	9.35	335.07724	335.07687	-1.11	$C_{16}H_{15}O_8$	$MS^2[335]:161.0231(100), 133.0281(14), 135.0437(3), 173.0442(6), 179.0338(6)$			4-CQL
71	9.80	367.10346	367.10257	-2.41	$C_{17}H_{19}O_9$	$MS^2[367]:191.0549(100), 134.0358(6)$			Cis-5-FQA
72	9.83	677.17232	677.17023	-3.09	$C_{31}H_{33}O_{17}$	$MS^2[677]:353.0868(100), 191.0547(85), 179.0336(58), 173.0441(28), 335.0764(28), 515.1166(16), 161.0229(16)$			DiCQA-hexoside

73	9.98	839.22515	839.22376	-1.65	C ₃₇ H ₄₃ O ₂₂	MS ² [839]:515.1392(100), 293.0119(21), 191.0548(10), 179.0534(10)	DiCQA-Dihexoside
74	10.10	677.17232	677.17297	0.96	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:179.0336(100), 515.1393(51), 341.0866(23), 191.0547(23), 173.0441(10)	DiCQA-hexoside
75	10.28	677.17232	677.16852	-5.62	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:353.0868(100), 191.0547(36), 179.0336(32), 515.1166(27), 89.0228(25), 173.0441(24)	DiCQA-hexoside
76	10.58	677.17232	677.16992	-3.55	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:353.0868(100), 191.0549(25), 173.0442(21), 179.0336(21), 263.1281(21)	DiCQA-hexoside
77	10.8 9	677.17232	677.16980	-3.71	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:515.1393((100), 353.0863(88), 217.1070(56), 191.0547(54), 179.0336(45)	DiCQA-hexoside
78	11.0 5	677.17232	677.16913	-4.72	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:353.0868(100), 173.0442(76), 191.0547(50), 179.0336(45)	DiCQA-hexoside
79	11.0 9	559.14571	559.14508	-1.13	C ₂₇ H ₂₇ O ₁₃	MS ² [559]:179.0336(100), 191.0548(70), 205.0495(37), 397.1128(23), 173.0442(19)	SCQA
80	11.2 0	559.14571	559.14429	-2.55	C ₂₇ H ₂₇ O ₁₃	MS ² [559]:191.0548(100), 179.0336(82), 173.0442(32), 397.1128(24), 205.0495(23)	SCQA
81	11.2 2	677.17232	677.16962	-3.99	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:353.0868(100), 191.0548(25), 179.0336(25)	DiCQA-hexoside

82	11.4 7	677.17232	677.16974	-3.81	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:353.0868(100), 191.0547(35), 179.0336(18)	DiCQA-hexoside
83	11.56	515.11950	515.11835	-2.23	C ₂₃ H ₂₃ O ₁₂	MS ² [515]:173.0441(100), 179.0337(73), 203.0338(42), 191.0542(27), 255.0655(21), 353.0869(14), 135.0436(12)	1,4-DiCQA
84	11.83	515.11950	515.11829	-2.35	C ₂₅ H ₂₃ O ₁₂	MS ² [515]:173.0442(100), 179.0336(87), 191.0549(37), 135.0437(14), 161.0231(14), 353.0870(12)	3,4-DiCQA
85	11.8 9	677.17232	677.17023	-3.09	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:353.0869(100), 173.0442(43), 179.0336(32), 191.0548(27)	DiCQA-hexoside
86	11.9 1	559.14571	559.14441	-2.33	C ₂₇ H ₂₇ O ₁₃	MS ² [559]:173.0442(100), 191.0548(38), 179.0336(25), 335.0768(11), 397.1126(8)	SCQA
87	11.99	515.11950	515.11792	-3.07	C ₂₃ H ₂₃ O ₁₂	MS ² [515]:191.0548(100), 179.0336(42), 135.0437(6), 353.0872(6)	3,5-DiCQA
88	12.0 9	677.17232	677.17346	1.68	C ₃₁ H ₃₃ O ₁₇	MS ² [677]:353.0868(100), 191.0548(65), 341.0867(54), 179.0336(50), 515.1408(46), 173.0441(33)	DiCQA-hexoside
89	12.2 1	559.14571	559.14463	-1.94	C ₂₇ H ₂₇ O ₁₃	MS ² [559]:191.0548(100), 179.0337(75), 205.0493(34), 173.0442(22), 397.1128(16)	SCQA
90	12.25	677.15119	677.14978	-2.09	C ₃₄ H ₃₉ O ₁₅	MS ² [677]:191.0548(100), 353.0869(95), 179.0336(42), 173.0442(28), 335.0761(18)	Cis-TriCQA

91	12.3 5	559.14571 559.14441	-2.33	C ₂₇ H ₂₇ O ₁₃	MS ² [559]:173.0442(100), 191.0550(71), 179.0337(20), 397.1128(12)	SCQA
92	12.47	515.11950 515.11853	-1.88	C ₂₃ H ₂₃ O ₁₂	MS ² [515]:191.0548(100), 179.0337(58), 173.0440(20), 161.0230(12), 353.0867(11), 135.0437(11)	1,5-DiCQA
93	12.6 5	559.14571 559.14392	-3.02	C ₂₇ H ₂₇ O ₁₃	MS ² [559]:179.0336(100), 191.0548(77), 173.0443(42), 205.0495(34), 397.1128(20)	SCQA
94	12.84	677.15119 677.15101	-0.27	C ₃₄ H ₂₉ O ₁₅	MS ² [677]:179.0337(100), 161.0231(79), 335.0761(76), 173.0442(68), 191.0548(59), 353.0869(46), 515.1121(22)	Cis-TriCQA
95	12.94	515.11950 515.11804	-2.83	C ₂₅ H ₂₃ O ₁₂	MS ² [515]:173.0441(100), 179.0336(69), 191.0548(25), 353.0870(14), 135.0436(10)	4,5-DiCQA
96	13.0 7	499.12458 499.12323	-2.71	C ₂₅ H ₂₃ O ₁₁	MS ² [499]:163.0387(100), 173.0442(80), 179.0336(72), 191.0548(48), 335.0761(11), 353.0868(5)	Cis-3-pCo, 5CQA
97	13.24	721.17741 721.17786	0.63	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:179.0337(100), 191.0549(50), 397.1128(46), 559.1448(32), 379.1024(10)	DiCSQA
98	13.2 9	499.12458 499.12363	-1.91	C ₂₅ H ₂₃ O ₁₁	MS ² [499]:163.0387(100), 173.0442(32), 191.0548(11), 119.0487(6), 337.0920(4)	3-pCo, 5CQA
99	13.35	529.13515 529.13409	-2.00	C ₂₆ H ₂₃ O ₁₂	MS ² [529]:173.0442(100), 193.0494(90), 179.0337(61), 155.0336(21), 161.0230(20), 135.0437(14), 335.0765(14)	3F,4CQA

10	13.4	499.12458	499.12363	-1.91	C ₂₅ H ₂₃ O ₁₁	MS ² [499]:191.0548(100), 179.0336(39), 173.0442(10), 135.0437(10), 353.0869(4)	3C, 5- <i>p</i> CoQA
0	3						
101	13.45	721.17741	721.17828	1.97	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:179.0336(100), 191.0548(73), 397.1127(50), 559.1435(21)	DiCSQA
102	13.61	529.13515	529.13428	-1.64	C ₂₆ H ₂₅ O ₁₂	MS ² [529]:173.0442(100), 193.0493(18)	3C,4FQA
10	13.6	499.12458	499.12341	-2.35	C ₂₅ H ₂₃ O ₁₁	MS ² [499]:173.0442(100), 191.0548(22), 179.0336(19), 163.0387(18), 337.0923(4)	4- <i>p</i> Co, 5CQA
3	6						
104	13.78	529.13515	529.13391	-2.34	C ₂₆ H ₂₅ O ₁₂	MS ² [529]:193.0494(100), 161.0230(24), 367.1024(12), 173.0443(8)	3F,5CQA
105	13.78	677.15119	677.14990	-1.91	C ₃₄ H ₂₉ O ₁₅	MS ² [677]:353.0869(100), 179.0336(22), 335.0765(20), 191.0548(17), 497.1075(8), 161.0230(6)	1,3,5-TriCQA
106	13.81	497.10893	497.10910	0.33	C ₂₅ H ₂₁ O ₁₁	MS ² [497]:161.0230(100), 173.0442(74) 335.0765(74), 179.0337(52), 119.0487(42), 135.0437(27)	DiCQL
107	13.92	529.13515	529.13416	-1.87	C ₂₆ H ₂₅ O ₁₂	MS ² [529]:191.0549(100), 179.0336(39), 173.0443(14), 135.0437(10), 353.0871(6)	3C,5FQA
108	13.93	497.10893	497.10834	-1.20	C ₂₅ H ₂₁ O ₁₁	MS ² [497]:179.0337(100), 161.0230(67), 135.0437(39), 335.0765(10)	DiCSA

109	14.07	721.17741	721.17737	-0.05	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:397.1128(100), 353.0868(96), 191.0548(67), 179.0336(45)	DiCSQA
110	14.15	497.10893	497.10867	-0.53	C ₂₃ H ₂₁ O ₁₁	MS ² [497]:161.0230(100), 179.0337(60), 203.0338(34), 135.0437(22)	DiCQL
111	14.17	677.15119	677.14978	-2.09	C ₃₄ H ₂₉ O ₁₅	MS ² [677]:353.0869(100), 179.0337(90), 161.0230(84), 515.1182(61), 355.0765(28), 497.1074(19), 191.0548(11)	1,3,4-TriCQA
11 2	14.2 8	499.12458	499.12402	-1.13	C ₂₅ H ₂₃ O ₁₁	MS ² [499]:173.0442(100), 163.0387(21), 337.0920(6)	Cis-4-pCo, 5CQA
113	14.29	721.17741	721.18115	5.95	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:397.1129(100), 179.0337(53), 191.0548(46), 335.0776(33), 353.0868(17)	DiCSQA
114	14.41	515.11950	515.11847	-2.00	C ₂₅ H ₂₃ O ₁₂	MS ² [515]:173.0440(100), 179.0337(81), 191.0548(61), 353.0867(16), 135.0436(14)	Tran-4-Cis-5-DiCQA
115	14.53	529.13515	529.13422	-1.76	C ₂₆ H ₂₅ O ₁₂	MS ² [529]:173.0442(100), 161.0230(40), 367.1024(17), 193.0494 (17), 179.0337(15), 135.0437(5)	4F,5CQA
11 6	14.5 5	499.12458	499.12378	-1.61	C ₂₅ H ₂₃ O ₁₁	MS ² [499]:173.0442(100), 179.0336(59), 191.0548(37), 353.0868(11), 135.0436(9)	4C, 5-pCoQA
117	14.58	497.10893	497.10822	-1.44	C ₂₅ H ₂₁ O ₁₁	MS ² [497]:179.0337(100), 247.0789(65), 135.0437(44),	DiCSA

					161.0230(26)			
118	14.68	721.17741	721.18005	4.42		$C_{36}H_{33}O_{16}$	MS ² [721]:191.0548(100), 161.0230(52), 173.0441(44), 179.0335(37), 353.0868(31), 559.1431(27)	DiCSQA
119	14.72	677.15119	677.14984	-2.00		$C_{34}H_{29}O_{15}$	MS ² [677]:353.0869(100), 179.0336(29), 191.0548(20), 335.0765(19), 161.0230(15), 515.1180(9), 497.1074(7)	1,4,5-TriCQA
120	14.73	529.13515	529.13446	-1.30		$C_{36}H_{25}O_{12}$	MS ² [529]:173.0442(100), 179.0336 (61), 191.0548(44), 353.08661(10)	4C,5FQA
121	14.78	497.10893	497.10852	-0.83		$C_{25}H_{21}O_{11}$	MS ² [497]:161.0230(100), 179.0336(86), 135.0437(52), 273.0762(41)	DiCQL
122	14.91	721.17741	721.18073	5.37		$C_{36}H_{33}O_{16}$	MS ² [721]:179.0337(100), 191.0548(84), 151.0387(80), 193.0493(72), 173.0442(52), 397.1128(49), 559.1447(38), 353.0868(37)	DiCSQA
123	15.10	661.15628	661.15533	-1.44		$C_{34}H_{29}O_{14}$	MS ² [661]:353.0870(100), 179.0336 (39), 191.0548(20), 335.0765(18), 354.0904(16)	<i>p</i> CoDiCQA
124	15.12	691.16684	691.16681	-0.05		$C_{35}H_{31}O_{15}$	MS ² [691]:353.0868(100), 179.0337(43), 367.1189(21), 335.0763(17), 191.0549(15), 529.1346(5)	DiCFQA
125	15.12	721.17741	721.17316	-5.13		$C_{36}H_{33}O_{16}$	MS ² [721]:341.1020(100), 285.0397(90), 307.1179(84), 191.0549(53), 559.1443(40)	DiCSQA

126	15.23	691.16684	691.16638	-0.67	C ₃₅ H ₃₁ O ₁₅	MS ² [69]:367.1189(100), 193.0493(34), 179.0337(34), 353.0868(26), 161.0229(23), 515.1175(9)	DiCFQA
127	15.28	661.15628	661.15533	-1.44	C ₃₄ H ₂₉ O ₁₄	MS ² [66]:337.0922(100), 163.0387(51), 353.0870(34), 179.0337(32), 161.0231(28)	<i>p</i> CoDiCQA
128	15.40	661.15628	661.15485	-2.16	C ₃₄ H ₂₉ O ₁₄	MS ² [66]:307.1077(100), 337.0914(23), 338.1111(20), 173.0442(15), 179.0337(14)	<i>p</i> CoDiCQA
129	15.54	497.10893	497.10815	-1.58	C ₃₅ H ₃₁ O ₁₁	MS ² [49]:161.0230(100), 335.0765(53), 179.0336(29), 137.0229(28), 135.0437(19)	DiCQL
130	15.58	721.17741	721.17554	-2.59	C ₃₆ H ₃₃ O ₁₆	MS ² [72]:559.1442(100), 173.0442(86), 191.0549(84), 397.1128(72), 353.0868(21)	DiCSQA
131	15.62	661.15628	661.15473	-2.34	C ₃₄ H ₂₉ O ₁₄	MS ² [66]:353.0869(100), 161.0230(95), 179.0337(95), 173.0443(71), 155.0336(5)	<i>p</i> CoDiCQA
132	15.62	691.16684	691.16608	-1.10	C ₃₅ H ₃₁ O ₁₅	MS ² [69]:367.1189(100), 179.0337(90), 353.0868(72), 173.0442(48), 529.1337(41), 161.0229(45), 191.0549(24), 193.0493(23), 335.0776(23)	DiCFQA
133	15.92	677.15119	677.14996	-1.82	C ₃₄ H ₂₉ O ₁₅	MS ² [67]:353.0869(100), 515.1179(62), 173.0442(30), 179.0337(23), 335.0765(14), 191.0548(9)	3,4,5-TriCQA

134	16.29	721.17741	721.17627	-1.58	C ₃₆ H ₃₃ O ₁₆	MS ² [72]:329.1021(100), 353.0868(89), 191.0549(74), 179.0336(58), 173.0441(41), 559.1442(15)	DiCSQA
135	16.35	497.10893	497.10785	-2.18	C ₂₃ H ₂₁ O ₁₁	MS ² [497]:179.0337(100), 161.0230(71), 335.0763(40), 135.0437(36), 191.0551(23)	DiCSA
136	16.99	661.15628	661.15466	-2.45	C ₃₄ H ₂₉ O ₁₄	MS ² [661]:499.1239(100), 179.0337(94), 353.0870(91), 173.0443(84), 191.0549(65), 337.0922(57)	pCoDiCQA
137	17.01	721.17741	721.17603	-1.15	C ₃₆ H ₃₃ O ₁₆	MS ² [72]:353.0869(100), 191.0548(69), 179.0336(34), 559.1439(30), 367.0810(18)	DiCSQA
138	17.13	661.15628	661.15479	-2.25	C ₃₄ H ₂₉ O ₁₄	MS ² [661]:353.0869(100), 179.0337(33), 173.0442(31), 191.0548(30), 515.1184(22), 337.0917(11)	pCoDiCQA
139	17.22	691.16684	691.16644	-0.58	C ₃₅ H ₃₁ O ₁₅	MS ² [691]:529.1338(100), 179.0337(65), 367.1189(60), 353.0868(59), 173.0442(50), 193.0493(46), 335.0776(23), 161.0229(14)	DiCFQA
140	17.31	661.15628	661.15453	-2.65	C ₃₄ H ₂₉ O ₁₄	MS ² [661]:337.0921(100), 173.0442(70), 499.1239(35), 283.1544(21), 353.0866(19), 191.0550(19), 179.0337(16)	pCoDiCQA
141	17.36	691.16684	691.16632	-0.76	C ₃₅ H ₃₁ O ₁₅	MS ² [691]:353.0868(100), 173.0442(33), 179.0337(30), 367.1189(25), 515.1175(18), 191.0549(17), 529.1338(17), 335.0776(14), 161.0229(14), 161.0229(14), 193.0493(7)	DiCFQA

142	17.36	721.17741	721.17743	0.03	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:353.0868(100), 179.0336(52), 191.0549(32), 173.0442(25), 559.1439(20)	DiCSQA
143	17.49	691.16684	691.16628	-0.81	C ₃₃ H ₃₁ O ₁₅	MS ² [691]:367.1024(100), 173.0442(63), 529.1338(41), 335.0776(14), 179.0337(14), 553.0868(11)	DiCFQA
144	17.87	721.17741	721.17682	-0.06	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:353.0868(100), 173.0442(55), 515.1181(47), 191.0549(45), 233.0808(42), 179.0337(38)	DiCSQA
145	18.34	691.16684	691.16608	-1.10	C ₃₅ H ₃₁ O ₁₅	MS ² [691]:161.0230(100), 529.1338(56), 179.0337(49), 367.1029(30)	DiCFQA
146	18.49	721.17741	721.17639	-1.41	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:353.0869(100), 179.0336 (22), 191.0549(20), 559.1442(19)	DiCSQA
147	18.82	721.17741	721.17578	-1.50	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:353.0868(100), 191.0547(34), 179.0336(34), 173.0441(21), 559.1442(10)	DiCSQA
148	19.07	721.17741	721.17584	-2.17	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:353.0868(100), 559.1442(38), 191.0548(23), 179.0336(17)	DiCSQA
149	19.17	721.17741	721.17761	1.04	C ₃₆ H ₃₃ O ₁₆	MS ² [721]:353.0868(100), 191.0548(22), 179.0336(18), 559.1442(9), 173.0442(9)	DiCSQA