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Electronic Supplementary Information (ESI)

An untargeted metabolomics approach to determine component differences and variation in their *in vivo* distribution between Kuqin and Ziqin, two commercial specifications of Scutellaria Radix†

Zhi-Wei Yang[a], Feng Xu[b,*], Xin Liu[c], Yi Cao[a], Qi Tang[a], Qian-Yu Chen[a], Ming-Ying Shang[b], Guang-Xue Liu[b], Xuan Wang[a,*], Shao-Qing Cai[b]

[a] *Department of Chemical Biology, School of Pharmaceutical Sciences, Peking University, No. 38 Xueyuan Road, Beijing 100191, PR China.*

[b] *State Key Laboratory of Natural and Biomimetic Drugs, Peking University, No. 38 Xueyuan Road, Beijing 100191, PR China.*

[c] *Technical Center, Beijing Entry-Exit Inspection and Quarantine Bureau, No. 6 Tianshuiyuan Street, Beijing, 100026, PR China.*

†Electronic supplementary information (ESI) available.

* **Corresponding author:**

Dr. Feng Xu. State Key Laboratory of Natural and Biomimetic Drugs, Peking University, No. 38 Xueyuan Road, Haidian District, Beijing 100191, PR China. Tel: +86-10-82802534; E-mail: xufeng76@bjmu.edu.cn.

Dr. Xuan Wang (responsible for all correspondence during review and processing of the manuscript), Department of Chemical Biology, School of Pharmaceutical Sciences, Peking University, No. 38 Xueyuan Road, Haidian District, Beijing 100191, PR China. Tel: +86-10-82806818; E-mail: xuanwang6818@bjmu.edu.cn.

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Part B: MS² and proposed fragmentation pathways of constituents in SR, colon and lungs tissues

PART A

Table S1 Information of 51 Kuqin (KQ) and Ziqin (ZQ) samples

NO.	Sample ID	Specification	Collection Date	Region
1	KQ-6590	Kuqin	2010/10	Inner Mongolia
2	KQ-6613	Kuqin	2010/11	Hebei province
3	KQ-6616-1	Kuqin	2010/11	Hebei province
4	KQ-6616-2	Kuqin	2010/11	Hebei province
5	KQ-6618	Kuqin	2010/11	Hebei province
6	KQ-6620	Kuqin	2010/11	Hebei province
7	KQ-6626-1	Kuqin	2010/11	Hebei province
8	KQ-6626-2	Kuqin	2010/11	Hebei province
9	KQ-6628	Kuqin	2010/11	Hebei province
10	KQ-6629	Kuqin	2010/11	Hebei province
11	KQ-6697	Kuqin	2010/12	Shandong Province
12	KQ-70002	Kuqin	2014/10	Inner Mongolia
13	KQ-7486-1	Kuqin	2014/07	Inner Mongolia
14	KQ-7486-2	Kuqin	2014/07	Inner Mongolia
15	KQ-7486-3	Kuqin	2014/07	Inner Mongolia
16	KQ-7591	Kuqin	2014/09	Inner Mongolia
17	KQ-7591-1	Kuqin	2014/09	Inner Mongolia
18	KQ-7591-L1	Kuqin	2014/09	Inner Mongolia
19	KQ-7591-L2	Kuqin	2014/09	Inner Mongolia
20	KQ-7591-L3	Kuqin	2014/09	Inner Mongolia
21	KQ-7591-M1	Kuqin	2014/09	Inner Mongolia
22	KQ-7591-M2	Kuqin	2014/09	Inner Mongolia
23	KQ-7591-M3	Kuqin	2014/09	Inner Mongolia
24	KQ-7591-PS-1	Kuqin	2014/09	Inner Mongolia
25	KQ-7591-PS-2	Kuqin	2014/09	Inner Mongolia
26	KQ-7591-PS-3	Kuqin	2014/09	Inner Mongolia
27	KQ-7591-PS-4	Kuqin	2014/09	Inner Mongolia
28	KQ-7591-PS-5	Kuqin	2014/09	Inner Mongolia
29	ZQ-5773	Ziqin	2007/07	Shandong Province
30	ZQ-5797	Ziqin	2007/10	Gansu province
31	ZQ-6580	Ziqin	2010/10	Gansu province
32	ZQ-6596	Ziqin	2010/10	Inner Mongolia
33	ZQ-6614	Ziqin	2010/11	Hebei province
34	ZQ-6619	Ziqin	2010/11	Hebei province
35	ZQ-6624	Ziqin	2010/11	Hebei province
36	ZQ-6630	Ziqin	2010/11	Hebei province
37	ZQ-6633	Ziqin	2010/11	Yanqing County, Beijing
38	ZQ-6636	Ziqin	2010/11	Hebei Province
39	ZQ-6697	Ziqin	2010/12	Shandong Province
40	ZQ-6701	Ziqin	2010/01	Henan province

41	ZQ-70001	Ziqin	2014/10	Inner Mongolia
42	ZQ-7487-1	Ziqin	2014/07	Inner Mongolia
43	ZQ-7487-2	Ziqin	2014/07	Inner Mongolia
44	ZQ-7593	Ziqin	2014/09	Inner Mongolia
45	ZQ-7593-1	Ziqin	2014/09	Inner Mongolia
46	ZQ-7593-L1	Ziqin	2014/09	Inner Mongolia
47	ZQ-7593-L2	Ziqin	2014/09	Inner Mongolia
48	ZQ-7593-L3	Ziqin	2014/09	Inner Mongolia
49	ZQ-7593-M1	Ziqin	2014/09	Inner Mongolia
50	ZQ-7593-M2	Ziqin	2014/09	Inner Mongolia
51	ZQ-7593-S	Ziqin	2014/09	Inner Mongolia

Table S2. Peak areas of the main active constituents in six batches of KQ and ZQ crude drug samples. (ZQ samples batch No. were 7593, 6616, 6620, 70002, and 7486; KQ samples batch No. were 7591, 6619, 6614, 70001, and 7487; Peak area unit, mAU·s)

ID	Compounds	KQ-G1&G2	KQ-G3	KQ-G4	KQ-G5	KQ-G6	ZQ-G1&G2	ZQ-G3	ZQ-G4	ZQ-G5	ZQ-G6
		No.7591	No.6616	No.6620	No.70002	No.7486	No.7593	No.6619	No.6614	No.70001	No.7487
S40	Chrysin 6-*C*-arabinoside 8-*C*-glucoside	3282.4	2896.8	2276.9	2156.7	3685.8	2531.3	3281.1	2512.8	2804.9	3720.7
S46	Chrysin 6-*C*-glucoside 8-*C*-arabinoside	2516.8	1688.9	1424.3	1285.6	2189.0	1760.9	2055.3	1511.7	1705.1	2300.9
S39	Baicalin	70110.8	46159.5	40624.6	46798.9	84945.1	54239.5	74453.6	56288.9	63557.1	89242.1
S25	Wogonoside	19619.0	12814.9	12765.8	11536.8	23661.9	14572.0	21983.8	15610.8	16614.7	22611.1
S21	Oroxylin A 7-*O*-glucuronide	8986.9	5781.5	1631.6	5036.8	8177.6	4828.2	8260.9	3953.5	8804.1	8475.2
S59	Baicalein	4599.4	7592.1	3430.1	4858.5	7286.8	3558.1	4160.2	4755.3	4121.5	5845.2
S60	Wogonin	1035.3	2841.9	2317.0	2559.1	2847.3	868.1	2470.3	2599.3	1903.1	2413.4
S62	Oroxylin A	657.1	947.2	591.0	1314.6	1183.5	321.4	999.1	806.9	1133.6	979.5
S78	Chrysin	211.4	113.4	246.0	158.4	234.2	126.0	111.8	289.0	143.5	144.3

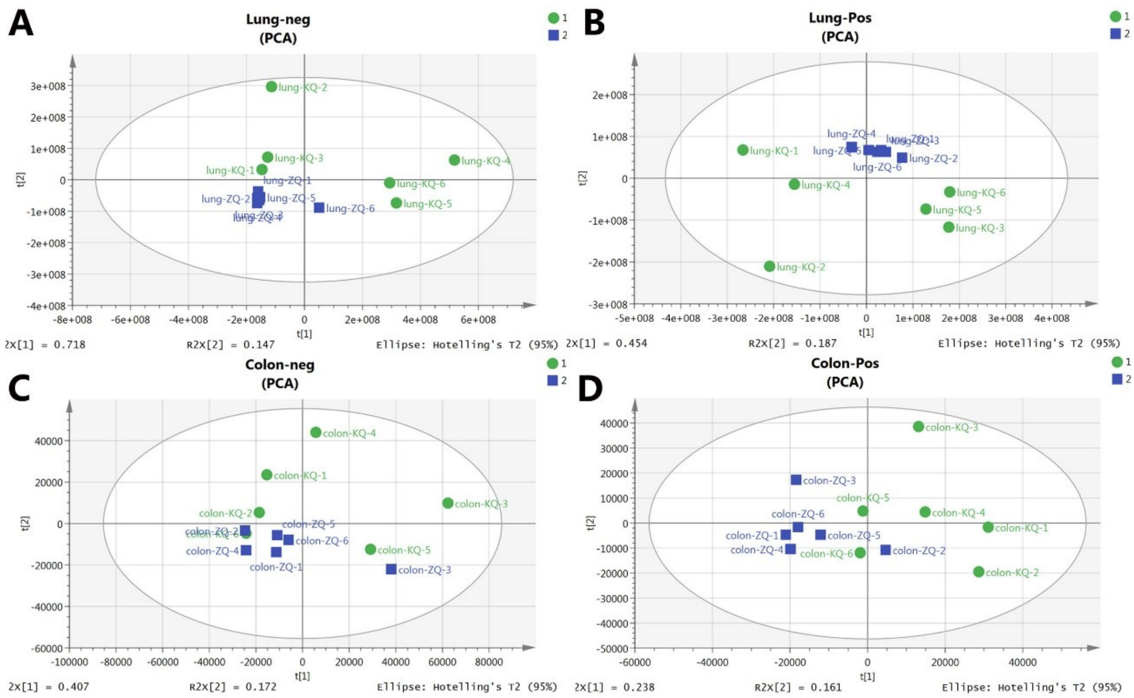


Figure S1. Pattern analysis scores scatter plots between KQ (●1) and ZQ (■2) in colon and lungs. For lungs, PCA in negative (A) and positive (B) ion modes; For colon, PCA in negative (C) and positive (E) ion modes.

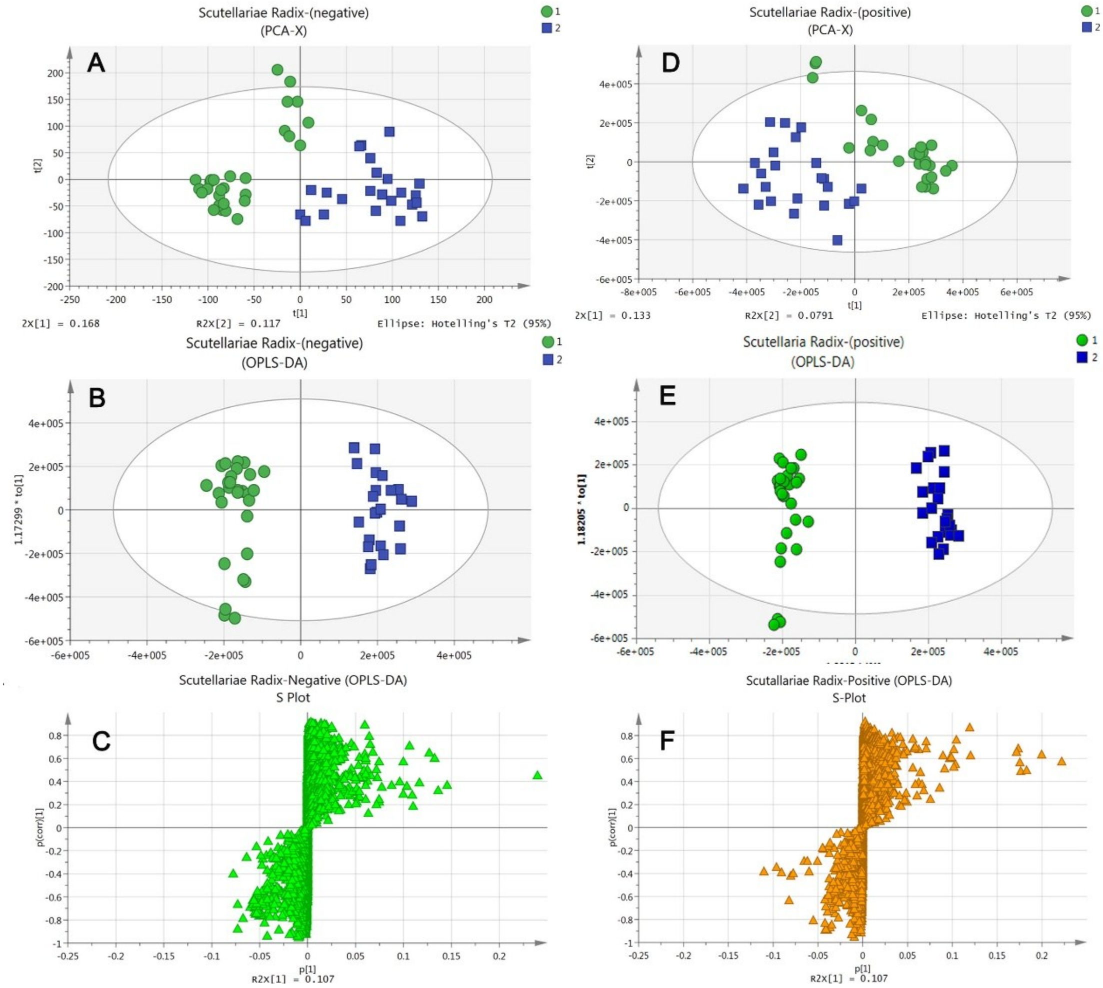


Figure S2. Pattern analysis scores scatter plots between KQ (●1) and ZQ (■2) crude drug samples: PCA in negative (A) and positive (D) ion modes; OPLS-DA in negative (B) and positive (E) ion modes. S-plot of OPLS-DA model both in negative (C) and positive (F) ion modes.

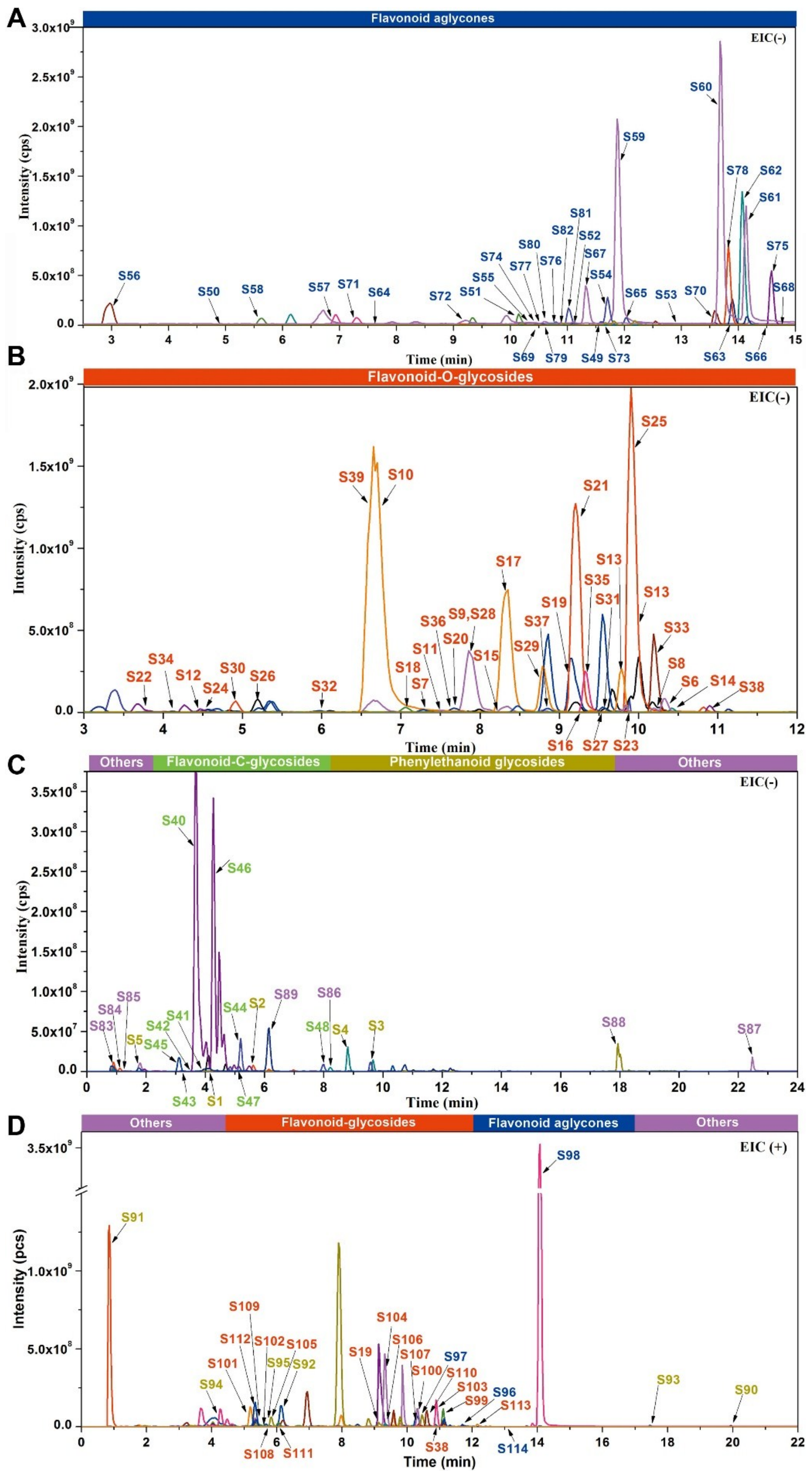


Figure S3. Extracted ion chromatograms of the constituents of Scutellariae Radix. (A) flavonoid aglycones, (B) flavonoid *O*-glycosides, (C) flavonoid *C*-glycosides, phenylethanoid glycosides, and other types in negative ion mode, and (D) flavonoid glycoside, flavonoid aglycones and other types in positive ion mode (samples No. 7593).

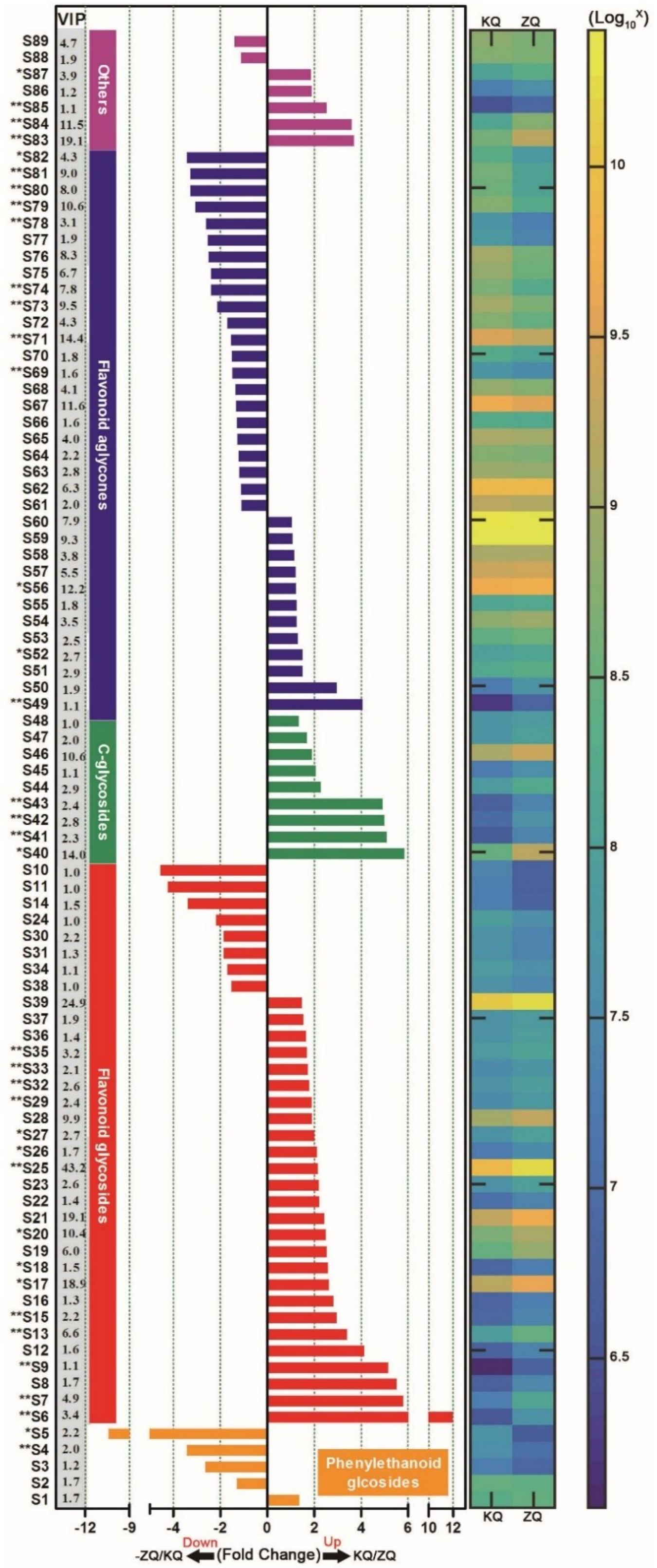


Figure S4. Chemical difference between KQ (SR sample No. 7591) and ZQ (SR sample No. 7593) in negative ion mode for group one. The heat map represented relative content of components in KQ (left) and ZQ (right); Sn, prototype components in SR, n = N; Down (Fold change < 0) = lower content in ZQ; Up (Fold Change > 0) = higher content in ZQ; * $p \leq 0.05$, ** $p \leq 0.01$.

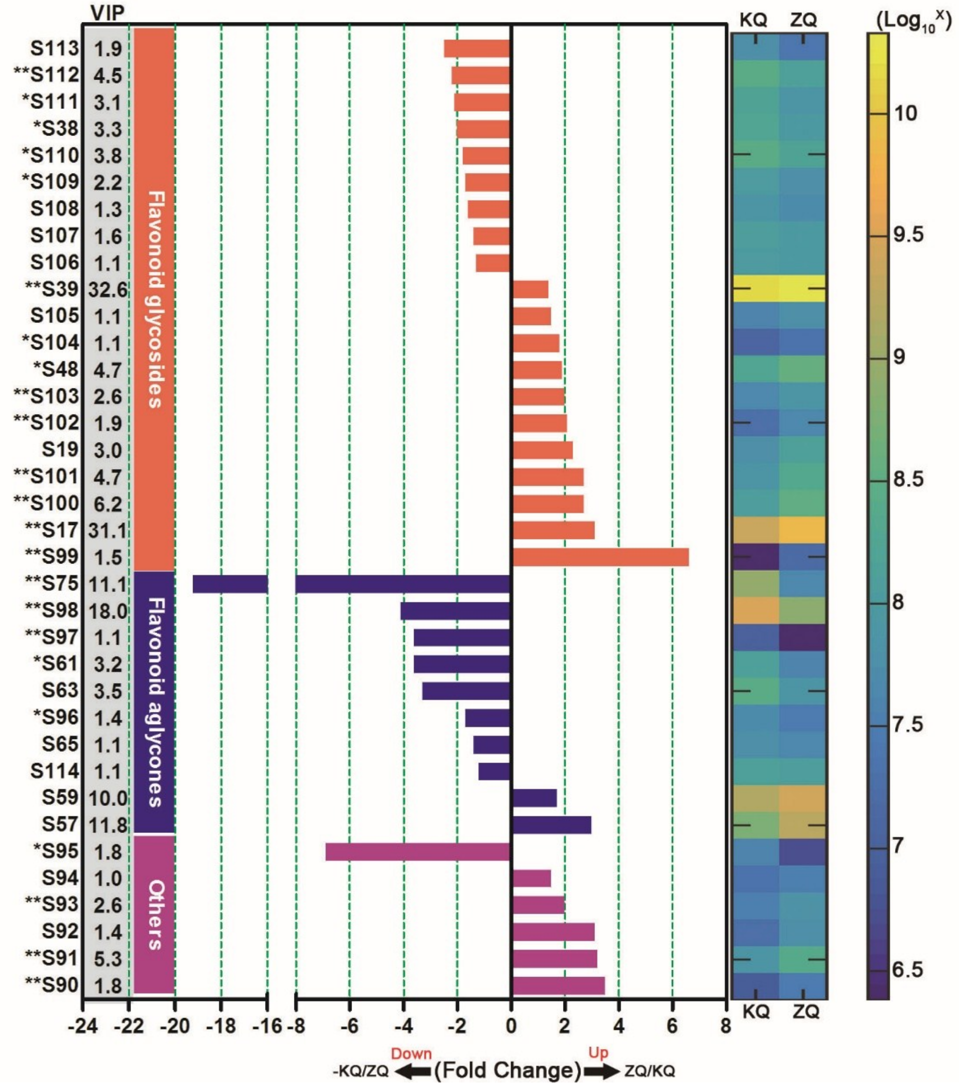


Figure S5. Chemical difference between KQ (SR sample No. 7591) and ZQ (SR sample No. 7593) in positive ion mode for group one. The heat map represented relative content of components in KQ (left) and ZQ (right); Sn, prototype components in SR, n = N; Down (Fold Change < 0) = lower content in ZQ; Up (Fold Change > 0) = higher content in ZQ; * p ≤ 0.05, ** p ≤ 0.01.

Table S3. Characterization of constituents with content difference between KQ and ZQ

ID	t_R (min)	$[M\pm H]^{\pm}$	ion mode	Predicted Formula	Diff (ppm)	ESI-MS^2 *m/z*（% Relative）	Identification	Stucture Type	Note*
S1	4.03	623.19869	−	$C_{29}H_{36}O_{15}$	0.877	461.16760(6),415.10431(27),179.03514(3),161.02452(100), 135.04463(8)	Acteoside	Phenylethanoid glcosides	/
S2	5.56	637.21439	−	$C_{30}H_{38}O_{15}$	0.936	461.16754(9),315.11038(5),193.05070(18),175.04005(100),160.01636(22),153.05603(10),135.04518(17),113.02439(27)	Leucosceptoside A	Phenylethanoid glcosides	/
S3	9.71	651.23014	−	$C_{31}H_{40}O_{15}$	1.069	636.66242(0.7),193.05060(24),175.03962(100),160.01694(20),149.06090(5),134.03725(5),113.02420(18)	Isomartynoside	Phenylethanoid glcosides	F.I#
S4	8.84	651.23018	−	$C_{31}H_{40}O_{15}$	1.131	329.12497(1),299.05658(1),193.05080(13),175.04013(100),167.07126(3),160.01660(28),149.06087(3),134.03743(8),119.03503(2),113.02441(15),101.02448(2)	Martynoside	Phenylethanoid glcosides	/
S5	1.78	475.18188	−	$C_{21}H_{32}O_{12}$	−0.462	329.12436(2),311.11435(1),167.07141(2),149.06070(4),134.03731(4),113.02430(100),101.02428(17),95.01369(9)	Darendoside A	Phenylethanoid glcosides	/
S6	10.31	459.0938	−	$C_{22}H_{20}O_{11}$	1.123	283.06140(36),268.03796(100),113.02448(12),99.01(7),99.0882.01(5),85.02940(13)	Isomer of S21	Flavone-*O*-glycosides	/
S7	7.25	445.07798	−	$C_{21}H_{18}O_{11}$	0.776	269.04590(100)	Isomer of S39	Flavone-*O*-glycosides	/
S8	10.27	503.12007	−	$C_{24}H_{24}O_{12}$	1.134	459.13107(3),428.07468(4),299.05685(61),284.03314(100),255.06674(33),211.04065(4),151.00386(3)	6''-*O*-acetyl homoplantaginin OR Ladanetin-6-*O*-β-(6''-*O*-acetyl)glucoside	Flavone-*O*-glycosides	F.I
S9	7.86	907.19435	−	$C_{43}H_{40}O_{22}$	0.556	676.36243(4),547.01318(4),388.12686(4),345.12686(4),299.05661(100),284.03271(9),269.04614(12),256.09375(4),267.03131(10)	Isomer of Solanoflavone	Flavone-*O*-glycosides	F.I
S10	6.61	731.12622	−	$C_{36}H_{28}O_{17}$	1.159	285.04032(0.6),269.04575(100),267.02943(0.4),251.22560(2),113.02448(8).	5,7,4',5'',3''',4'''-hexahydroxy-3''-*O*-β-glucosyl-3',7''-*O*-biflavone OR isomer	Flavone-*O*-glycosides	F.I
S11	7.51	491.11986	−	$C_{23}H_{24}O_{12}$	0.734	329.06747(42),314.04388(100),299.02063(18),269.04602(2)	Trihydroxy-dimethoxyflavone *O*-glucoside	Flavone-*O*-glycosides	/
S12	4.56	607.13127	−	$C_{27}H_{28}O_{16}$	1.338	431.09888(3),269.04596(100),251.03477(0.4),175.0	Trihydroxyflavone *O*-	Flavone-*O*-glycosides	F.I

						2(1),113.02452(5),95.01376(1),85.02924(3)	glucoside-(1→2)-*O*-glucuronide		
S13	9.88	445.07796	−	$C_{21}H_{18}O_{11}$	0.325	269.04587(100),251.03519(0.3),241.05064(0.1),225.05563(0.1),223.04022(0.3),113.02444(4),99.00870(2),85.02940(4)	Baicalein 6-*O*-glucuronide	Flavone-*O*-glycosides	/
S14	10.47	637.15677	−	$C_{32}H_{30}O_{14}$	0.771	283.06235(0.5),269.04596(100),251.03542(0.3),230.95995(1),223.06(1),205.05(2)	Isomer of chrysoeriol-7-*O*-[2''-*O*-E-feruloyl]-β-D-glucoside	Others	F.I
S15	8.26	863.20450	−	$C_{42}H_{40}O_{20}$	0.56	271.06174(50),269.04608(100),211.07(2),165.62(0.4),113.02454(5)	Unknow	/	/
S16	9.32	473.10911	−	$C_{23}H_{22}O_{11}$	0.371	283.06165(33),269.04611(100),268.03824(45),161.00911(6)	Baicalein 7-*O*-ethylglucuronide OR isomer	Flavone-*O*-glycosides	/
S17	8.49	445.07793	−	$C_{21}H_{18}O_{11}$	0.295	269.04596(100),251.03575(0.1),241.05104(0.6),225.05591(2),197.06102(2),113.02441(4),99.00877(2),85.02941(4)	Norwogonin 7-*O*-glucuronide	Flavone-*O*-glycoside	/
S18	7.13	505.09920	−	$C_{23}H_{22}O_{13}$	0.864	329.06656(28),314.04343(100),299.02014(27),269.04565(5),196(3),113.02434(11),85.02942(13)	Isomer of viscidulin II 2'-*O*-glucuronide	Flavone-*O*-glycosides	/
S19	9.21	431.09677	+	$C_{21}H_{18}O_{10}$	−1.167	271.05957(6),255.06471(100)	Chrysin 7-*O*-glucuronide	Flavone-*O*-glycoside	/
S20	7.7	445.07795	−	$C_{21}H_{18}O_{11}$	0.709	269.04611(100)	Isomer of S39	Flavone-*O*-glycosides	/
S21	9.13	459.09374	−	$C_{22}H_{20}O_{11}$	0.992	283.06149(47),268.03806(100),239.07167(0.3),211.03976(0.1),175.02492(1.0),139.00372(0.4),129.01933(2),117.01934(3),113.02438(17),99.00875(7),85.02939(23),71.01373(7)	Oroxylin A 7-*O*-glucuronide	Flavone-*O*-glycosides	RS
S22	3.86	461.07327	−	$C_{21}H_{18}O_{12}$	1.564	371.07819(6),341.06790(20),299.05603(12),285.04077(100),271.06216(3),245.05(3),227.07204(4),211.04077(3)	Tetrahydroxyflavone *O*-glucuronide (Isomer of Scutellarin)	Flavone-*O*-glycosides	/
S23	9.77	461.10910	−	$C_{22}H_{22}O_{11}$	0.359	299.05609(38),284.03268(83),283.02502(100),269.04312(2),268.03726(1),253.05077(20),211.04008(9),173.06068(2)	Trihydroxy-methoxyflavone-*O*-glucoside	Flavone-*O*-glycosides	/
S24	4.61	477.10424	−	$C_{22}H_{22}O_{12}$	0.819	301.07242(70),286.04889(100),181.01442(21),165.99094(13)	5,7,2'-Trihydroxy-6-methoxyflavanone 7-*O*-glucuronide	Flavanone-*O*-glycosides	/
S25	9.84	459.09363	−	$C_{22}H_{20}O_{11}$	0.752	283.06149(75),268.03806(100),239.07164(0.3),175.02492(1),139.00372(0.4),129.01933(2),113.02438(24),99.00875(12),85.02939(22),71.01373(7)	Wogonoside	Flavone-*O*-glycosides	RS
S26	5.27	475.08834	−	$C_{22}H_{20}O_{12}$	0.296	299.05655(58),284.03311(100)	Isomer of 37 (trihydroxy-methoxyflavone *O*-glucuronide)	Flavone-*O*-glycosides	/

S27	9.47	475.08809	−	$C_{22}H_{20}O_{12}$	−0.23	299.05637(50),284.03305(100),270.04959(5)	Isomer of 37 (trihydroxy-methoxyflavone O-glucuronide)	Flavone-*O*-glycosides	/
S28	7.98	447.09353	−	$C_{21}H_{20}O_{11}$	0.549	271.06250(100),253.05099(8),243.06644(25)	Dihydrobaicalin	Flavanone-*O*-glycosides	/
S29	8.78	445.07795	−	$C_{21}H_{18}O_{11}$	0.709	269.04596(100),268.03815(3),267.03036(1),241.05142(0.5),225.05623(1),197.06119(1),113.02449(3),99.00886(1),85.02956(3),71.01391(2)	Norwogonin 8-*O*-glucuronide	Flavone-*O*-glycosides	/
S30	4.89	621.14659	−	$C_{28}H_{30}O_{16}$	0.776	445.11441(70),430.09079(59),283.06143(49),268.03781(100),267.03018(93),239.03525(2),175.02502(3),117.02(3),113.02444(25),103.00378(3),99.00882(7),95.01390(7),85.02956(21)	Dihydroxy-methoxyflavone *O*-glucuronide-(1→6)-*O*-glucoside	Flavone-*O*-glycosides	F.I
S31	9.61	415.10355	−	$C_{21}H_{20}O_9$	0.228	295.06122(3),269.04590(2),253.05075(100),224.04839(0.2),209.06085(2)	Chrysin 7-*O*-glucoside or isomer	Flavone-*O*-glycosides	F.I
S32	6.02	607.13129	−	$C_{27}H_{28}O_{16}$	1.371	445.18335(1),269.04572(100),113.02447(1)	Trihydroxyflavone *O*-glucuronide-(1→2)-*O*-glucoside	Flavone-*O*-glycosides	F.I
S33	10.27	489.10403	−	$C_{23}H_{22}O_{12}$	0.37	313.07257(24),298.04871(100),283.02521(29),281.04529(4),269.04565(2),239.03593(2),211.04042(5)	5,7-Dihydroxy-8,2'-dimethoxyflavone 7-*O*-glucuronide	Flavone-*O*-glycosides	/
S34	4.13	507.11461	−	$C_{23}H_{24}O_{13}$	0.387	492.09247(1),345.06189(15),330.03836(100),315.01505(14)	Viscidulin III 2'-*O*-glucoside	Flavone-*O*-glycosides	/
S35	9.35	445.11423	−	$C_{22}H_{22}O_{10}$	0.472	285.07462(100),270.05118(17),241.04947(0.1)	Wogonin 5-glucoside	Flavone-*O*-glycosides	/
S36	7.59	475.08836	−	$C_{22}H_{20}O_{12}$	0.339	299.05658(100),284.03305(59),270.10849(0.5)	Isomer of 37 (trihydroxy-methoxyflavone *O*-glucuronide)	Flavone-*O*-glycosides	/
S37	8.84	475.08832	−	$C_{22}H_{20}O_{12}$	0.254	299.05643(30),284.03299(100),267.02997(0.3),239.03540(0.2),228.04262(0.4),200.04805(1),153.01936(1),129.01955(1),113.02440(6),85.02940(7)	5,7,2'-Trihydroxy-6-methoxyflavone 7-*O*-glucuronide	Flavone-*O*-glycosides	/
S38	10.95	551.13891	+	$C_{25}H_{26}O_{14}$	−1.128	375.10657(100),360.08340(9),345.05960(13),342.07269(3),329.06488(0.3),327.04913(4),227.05461(3),177.05432(1)	Dihydroxy-tetramethoxyflavone *O*-glucuronide	Flavone-*O*-glycoside	/
S39	6.59	445.07991	−	$C_{21}H_{18}O_{11}$	2.275	269.04605(100),251.03560(1),241.05084(1),225.05608(0.4),197.06128(0.5),129.01952(1),117.01965(1),113.02452(6),99.00889(3),85.02959(7)	Baicalin	Flavone-*O*-glycoside	RS
S40	3.7	547.14611	−	$C_{26}H_{28}O_{13}$	0.724	547.14618(30),529.13562(3),487.12500(2),469.11435(4),457.11453(40),439.10385(4),427.10352(66),409.09323(4),397.09296(9),367.08243(64),349.07202(7),337.07214(100)	Chrysin 6-*C*-arabinoside 8-*C*-glucoside	Flavone-*C*-glycosides	RS

S41	3.87	565.15757	−	$C_{26}H_{30}O_{14}$	2.285	367.08337(1),337.07230(2),329.08737(8),299.07730(9),269.6674(40),239.05615(97),209.04556(100)	Isomer of Pinobanksin 8-*C*-arabinoside 6-*C*-glucoside	Flavanonol-*C*-glycosides	F.I
S42	3.57	565.15700	−	$C_{26}H_{30}O_{14}$	1.276	329.08783(4),299.07840(10),269.06689(41),239.05627(100),209.04572(95)	Isomer of Pinobanksin 8-*C*-arabinoside 6-*C*-glucoside	Flavanone-*C*-glycosides	F.I
S43	3.24	565.15653	−	$C_{26}H_{30}O_{14}$	0.445	329.08795(7),299.07770(10),269.06622(43),239.05637(100),209.04559(89)	Isomer of Pinobanksin 8-*C*-arabinoside 6-*C*-glucoside	Flavanone-*C*-glycosides	F.I
S44	5.18	415.10373	−	$C_{21}H_{20}O_9$	0.662	325.07175(4),307.06094(2),295.06113(100),277.05060(1),267.06644(32),253.05106(0.5),227.07188(0.5),179.03456(0.6),149.02438(2)	Isomer of S48 (Dihydroxyflavone *C*-glucoside)	Flavone-*C*-glycosides	/
S45	3.13	577.15683	−	$C_{27}H_{30}O_{14}$	0.955	577.15729(14),487.12531(11),457.11462(32),439.10440(3),397.09293(6),367.08258(58),337.07224(100)	Chrysin 6,8-di-*C*-glucopyranoside	Flavone-*C*-glycosides	/
S46	4.25	547.14609	−	$C_{26}H_{28}O_{13}$	0.687	547.14642(17),529.13593(3),487.12570(14),457.11465(22),427.10376(15),409.09360(10),397.09317(8),367.08258(83),337.07224(100)	Chrysin 6-*C*-glucoside 8-*C*-arabinoside	Flavone-*C*-glycosides	RS
S47	5.1	547.14620	−	$C_{26}H_{28}O_{13}$	0.888	547.14624(16),487.12512(17),457.11450(23),427.10364(40),397.09360(31),367.08234(100),337.07205(70),309.07745(6)	6-hexosyl-8-*C*-pentosyl chrysin	Flavone-*C*-glycosides	/
S48	8.03	417.11762	+	$C_{21}H_{20}O_9$	−0.932	325.07217(33),295.06152(100),267.06662(25),253.05095(3),223.07791(0.5),151.05568(0.1)	Chrysin 6-*C*-glucoside	Flavone-*C*-glycoside	/
S49	11.52	343.08222	−	$C_{18}H_{16}O_7$	−0.309	328.06003(12),313.03540(100),298.01190(16),270.01706(2)	Skullcapflavone	Flavones	/
S50	4.91	409.02370	−	$C_{17}H_{14}O_{10}S$	0.512	329.06705(100),314.04361(62),299.01993(27),195.03003(2),180.00662(3),164.98241(1),133.02942(2)	2',5,6-Trihydroxy-7,8-dimethoxyflavone 6-*O*-sulfate	Flavones	/
S51	10.23	329.06682	−	$C_{17}H_{14}O_7$	0.438	314.04337(49),299.01974(100),285.04105(2),271.02505(2),255.02969(0.9),227.03496(0.3),180.00645(9),164.98270(6),133.02942(7)	Isomer of S54 (Trihydroxy-dimethoxyflavone)	Flavones	/
S52	11.16	313.07190	−	$C_{17}H_{14}O_6$	0.443	298.04861(100),283.02521(85),255.03027(2),239.03503(2),211.04025(19),173.06067(5)	Isomer of S63 (Dihydroxy-dimethoxyflavone)	Flavones	/
S53	12.95	329.06680	−	$C_{17}H_{14}O_7$	0.377	314.04309(61),299.01953(100),285.04083(3),271.02472(2),255.02936(0.3),227.0.462(0.3),205.01410(0.8),180.00636(2),152.01122(2),133.02835(0.5)	5,8,2'-Trihydroxy-6,7-dimethoxyflavone	Flavones	/
S54	11.7	329.06679	−	$C_{17}H_{14}O_7$	0.346	314.04349(100),299.01993(80),255.02878(0.7),180.00696(2),165.99080(12),137.99586(6)	5,7,6'-Trihydroxy-8,2'-dimethxoyflavone	Flavones	/
S55	10.26	313.07188	−	$C_{17}H_{14}O_6$	0.379	298.04871(100),283.02530(87),269.04614(78),255.12172(4),211.04001(18),167.04(5),145.02962(15),91.02(28)	Isomer of 6-Methoxywogonin (Dihydroxy-dimethoxyflavone)	Flavones	/

S56	2.89	303.05117	−	$C_{15}H_{12}O_7$	0.475	285.04059(2),241.05075(2),217.05060(9),193.05551(4),177.01930(30),149.02429(10),125.02426(100)	5,7,3,2',6'-Pentahydroxyflavanone	Flavanones	/
S57	6.95	347.07574	+	$C_{17}H_{14}O_8$	−1.164	347.07541(63),332.05203(100),314.04147(35),286.04645(2),183.02850(3),169.01292(7),142.02594(3)	Viscidulin III	Flavones	RS
S58	5.62	285.04059	−	$C_{15}H_{10}O_6$	0.452	285.04077(100),267.03012(3),241.05083(20),217.05066(10),199.04018(15),197.06(2),175.04(5),173.06079(2),169.01425(3),151.00365(80),133.02959(11),107.01385(8)	Scutellarein	Flavones	RS
S59	11.86	271.05975	+	$C_{15}H_{10}O_5$	−1.291	271.05942(100),253.04897(1),225.05417(0.2),169.01289(0.2),153.01797(4)	Baicalein	Flavones	RS
S60	13.72	283.06125	−	$C_{16}H_{12}O_5$	0.188	268.03809(100),240.04349(1),239.03520(1),224.04802(1),212.04816(0.3),211.04041(0.3),198.03249(1),196.05321(1),184.05307(1),165.99049(1),163.00372(2),137.02448(1),110.00012(0.4)	Wogonin	Flavones	RS
S61	14.19	313.07224	−	$C_{17}H_{14}O_6$	0.479	298.04852(100),283.02515(87),269.04590(21),255.03026(2),239.03487(0.3),211.04027(18),195.03015(0.3),180.00664(5),173.06090(0.3),164.98279(2),152.01154(3),117.03396(0.2)	5,8-Dihydroxy-6,7-dimethoxyflavone	Flavones	/
S62	14.15	283.06129	−	$C_{16}H_{12}O_5$	0.33	268.03809(100),240.04308(0.4),239.03503(0.7),224.04767(0.4),212.04845(0.4),211.03987(0.2),198.03233(1),196.05310(1),184.05318(1),165.99036(0.3),163.00372(2),137.02437(0.6),110.00023(0.4)	Oroxylin A	Flavones	RS
S63	13.9	315.08592	+	$C_{17}H_{14}O_6$	−1.253	298.04868(68),283.02527(100),255.03012(2),211.04028(2),183.04514(2),173.06091(4),164.98(2),155.05032(3)	Skullcapflavone I	Flavones	/
S64	7.67	287.05625	−	$C_{15}H_{12}O_6$	0.483	287.05701(4),269.04599(3),225.05568(1),215.03513(9),201.05588(9),177.06(2),173.06(1),161.02443(17),151.00369(3),133.02956(4),125.02438(100)	Isomer of S71 (Tetrahydroxyflavanone)	Flavanones	/
S65	12.06	299.05618	−	$C_{16}H_{12}O_6$	0.23	284.03296(100),256.03872(2),255.03044(0.2),227.03548(0.1),200.04811(2),165.99077(8),137.99599(4),110.00093	Trihydroxy-methoxyflavone	Flavones	/
S66	14.5	373.09289	−	$C_{19}H_{18}O_8$	−0.002	358.06985(22),343.04617(100),328.02286(23),325.03555(2),315.05099(1),313.03574(0.6),300.02783(5),285.00458(1),227.03514(4),194.99355(6),169.01425(3),133.02936(1)	Scullcapflavone II	Flavones	/
S67	11.38	269.04552	−	$C_{15}H_{10}O_5$	−0.099	269.04584(100),241.05078(4),225.05591(8),213.05597(3),197.06100(12),181.06610(2),169.06595(3)	Apigenin	Flavones	RS
S68	14.75	283.06122	−	$C_{16}H_{12}O_5$	0.082	268.03796(100),240.04321(1),239.03526(1),224.04819(0.4),212.04845(0.4),211.04047(0.6),198.03242(	Isomer of S60 (Dihydroxy-methoxyflavone)	Flavones	/

						0.6),196.05336(0.4),184.05302(0.6),171.04515(0.2),165.99080(0.5),137.02440(0.4)			
S69	10.5	313.0719	−	$C_{17}H_{14}O_6$	0.443	298.04874(100),283.02530(87),269.04593(21),255.03079(4),211.04013(18),173.06114(3),145.02940(3),91.02199(8)	Isomer of 6-Methoxywogonin (Dihydroxy-dimethoxyflavone)	Flavones	F.I
S70	13.67	537.08295	−	$C_{30}H_{18}O_{10}$	0.428	391.04648(76),373.03580(10),347.05630(16),335.05679(5),319.06134(7),291.06656(2),245.00926(100),239.03531(1),217.01433(3)	8,8'-Biapigenin	Flavones	/
S71	7.24	287.05622	−	$C_{15}H_{12}O_6$	0.379	269.04581(0.6),243.06630(0.1),225.05594(0.1),179.0350(0.1),161.02428(25),151.00359(1),135.04514(2),125.02432(100)	Eriodictyol	Flavanone	/
S72	9.29	349.00236	−	$C_{15}H_{10}O_8S$	−0.003	269.04593(100),241.05110(0.3),225.05605(1),225.05605(0.9),197.06(1),181.06602(0.2),139.00328(0.1)	Baicalein 6-*O*-sulfate	Flavones	/
S73	11.61	299.05616	−	$C_{16}H_{12}O_6$	0.163	299.06(100),284.03290(49),267.03012(11),255.06651(24),240.04300(12),231.07(7),227.07092(0.5),212.04813(4),153.01930(0.2),151.00368(82),107.01389(8)	Trihydroxy-methoxyflavone (trihydoxy and methoxy on A ring)	Flavones	/
S74	10.27	283.06137	−	$C_{16}H_{12}O_5$	0.612	268.03815(100),255.03041(1),239.03531(1),224.04813(1),211.04037(1),198.03255(1),196.05328(1),184.05304(1),183.04530(0.3),173.06088(1),163.00375(2),137.02452(1),110.00090(0.3)	Isomer of S60 (Dihydroxy-methoxyflavone)	Flavones	/
S75	14.6	345.09647	+	$C_{18}H_{16}O_7$	−1.186	345.09631(100),330.07288(34),315.04938(92),312.06241(18),297.03891(31)	Tenaxin I	Flavones	/
S76	10.72	299.05611	−	$C_{16}H_{12}O_6$	−0.004	284.03275(100),271.06204(6),255.06720(2),227.07127(9),212.04810(12),211.03995(17),183.02997(2),165.01932(6),153.01926(36),133.02950(20)	4'-hydroxy wogonin	Flavones	RS
S77	10.47	315.05119	−	$C_{16}H_{12}O_7$	0.521	300.06476(69),284.02829(19),253.01425(30),227.03526(100),212.04431(7),165.99086(58),137.99605(11),110.00083(9)	Neptin	Flavones	F.I
S78	13.75	253.05057	−	$C_{15}H_{10}O_4$	−0.245	253.05109(100),209.15495(3),151.00400(0.2),143.05037(1),107.01380(1)	Chrysin	Flavones	RS
S79	10.53	283.06165	−	$C_{16}H_{12}O_5$	1.601	268.03815(100),255.03064(0.1),224.04797(1),212.04796(0.3),211.04030(1),198.03264(1),196.05330(1),184.05304(1),165.99068(0.4),163.00375(2),137.02444(1),110.00021(0.3)	Isomer of S60 (Dihydroxy-methoxyflavone)	Flavones	/
S80	10.65	301.07175	−	$C_{16}H_{14}O_6$	−0.038	286.04865(100),283.02444(4),268.03766(),255.23323(10),185.06107(5),180.00667(16),165.99078(45),152.01132(5),137.99594(9),119.05031(8)	Trihydroxy-methoxyflavanone	Flavanones	F.I

S81	11.09	283.06149	−	$C_{16}H_{12}O_5$	1.036	268.04(100),255.03041(),224.04813(0.5),212.04037(0.4),211.04037(0.2),198.03255(1),196.05328(1),184.05(1),165.99072(1),163.00375(2),137.02438(1),110.00014(0.4)	Isomer of S60 (Dihydroxy-methoxyflavone)	Flavones	/
S82	10.87	329.06678	−	$C_{17}H_{14}O_7$	0.316	314.04358(62),299.01959(81)283.26471(26),268.03827(25)	Isomer of S54 (Trihydroxy-dimethoxyflavone)	Flavones	/
S83	0.81	191.0197	−	$C_6H_8O_7$	−0.135	173.00926(3),147.03001(1),129.01953(8),111.00883(4),103.00378(4),85.03(100),72.99311(10)	D-Galactaric acid, 1,5-lactone OR isomer	Others	F.I
S84	1.04	191.01969	−	$C_6H_8O_7$	−0.135	173.00949(4),129.01956(8),117.01949(2),111.00882(100),87.00871(42),85.02947(34)	Isomer of D-Galactaric acid, 1,5-lactone	Others	F.I
S85	1.27	503.14106	−	$C_{21}H_{28}O_{14}$	0.857	341.08823(),323.07770(13),281.06732(20),251.05649(10),223.97(2),221.04567(14),179.03532(44),161.02457(100),135.04533(12)	1-caffeyllaminaribiose	Others	F.I
S86	8.29	417.11947	−	$C_{21}H_{22}O_9$	0.874	255.06686(10),211.07681(100),197.06166(0.2),169.06604(5),112.98558(2)	Gaylussacin	Stilbene (芪类)	/
S87	22.48	255.23276	−	$C_{16}H_{32}O_2$	−0.758	255.23302(100),237.22174(0.2),211.20708(0.2)	Isomer of Hexadecanoic acid	Alkane	F.I
S88	17.94	295.22773	−	$C_{18}H_{32}O_3$	−0.468	277.21747(25),211.13409(1),195.13907(2),183.13905(100)	Isomer of 10-Hydroxyoctadecadienoic acid	Alkane	F.I
S89	6.12	301.07177	−	$C_{16}H_{14}O_6$	0.029	161.02446(23),139.04013(100),135.04533(22),133.00966(16),124.01660(11),107.05027(10)	3-Hydroxy-4-*O*-glucosylbenzyl alcohol OR isomer	Others	F.I
S90	19.97	324.28931	+	$C_{20}H_{37}O_2N$	−1.221	306.27869(6),219.05690(6),147.11668(2),123.11678(5),109.10135(7),95.08574(14),81.07028(17),62.06064(100)	Isomer of Linoleoyl Ethanolamide	Others	F.I
S91	0.87	381.07891	+	$C_{17}H_{16}O_{10}$	−7.12	381.08(100),219.02664(30),201.01584(25)	Isomer of 5-*O*-β-D-glucopyranosyl-6-hydroxyangelicin	Others	F.I
S92	6.17	303.08598	+	$C_{16}H_{14}O_6$	−1.104	285.07507(15),267.06482(1),257.08026(32),242.05684(8),229.08551(57),179.03380(2),167.03363(100),163.03865(3),133.02831(24),123.04404(69),107.04928(44)	3,4-Dihydroxy-7-*O*-caffeoylbenzyl alcohol or isomer	Others	F.I
S93	17.49	701.37151	+	$C_{35}H_{56}O_{14}$	−3.953	701.37067(100),539.31824(96),191.09856(1),105.03367(7)	Isomer of sileneoside H	/	/
S94	4.17	445.07617	+	$C_{21}H_{16}O_{11}$	−0.826	427.06525(4),409.05493(9),381.05975(1),343.04465(6),319.04428(23),287.05(10),275.05447(7),263.05466(5),153.01807(100),141.01810(22)	Benzoic acid, 3,4,5-trihydroxy-,1,1'-(2-methoxy-1,4-phenylene) ester OR isomer	Others	F.I

S95	5.67	339.10696	+	$C_{16}H_{18}O_8$	−1.427	321.07611(3),234.03915(37),177.05437(100),145.02809(31),105.03366(13)	Unknown	/	F.I
S96	11.77	555.09167	+	$C_{30}H_{18}O_{11}$	−0.933	453.04468(11),435.03403(20),419.03882(10),269.03884(18),241.04912(12),121.02847(19),105.03368(34)	Isomer of hegoflavone A	Flavones	/
S97	10.39	347.07572	+	$C_{17}H_{14}O_8$	−1.221	347.07565(100),332.05206(26),317.02866(28),314.04156(37)	Isomer of S57 (Tetrahydroxy-dimethoxyflavone)	Flavones	/
S98	14	375.10704	+	$C_{19}H_{18}O_8$	−1.077	360.08298(30),345.05960(100),342.07272(15),327.04913(16),227.05446(8),213.03889(9)	5,6’-Dihydroxy-6,7,8,2’-tetramethoxyflavone	Flavones	/
S99	11.14	563.13929	+	$C_{26}H_{26}O_{14}$	−0.429	315.08569(100),300.06229(19),285.03885(13),282.05182(7)	Dihydroxy-dimethoxyflavone *O*-6"-malonyl glucoside	Flavone-*O*-glycoside	F.I
S100	10.35	549.12346	+	$C_{25}H_{24}O_{14}$	−0.768	301.06992(100),286.04651(16)	Trihydroxy-methoxyflavone *O*-6"-malonyl glucoside	Flavone-*O*-glycoside	F.I
S101	5.22	417.11739	+	$C_{21}H_{20}O_9$	−1.483	325.07217(5),295.06152(100),267.06662(31),245.04578(1),223.07791(0.5),187.07007(0.5),149.02457(2)	Chrysin 8-*C*-glucoside	Flavone-*C*-glycoside	/
S102	5.51	771.19748	+	$C_{33}H_{38}O_{21}$	−0.46	285.07526(21),271.05966(100),159.02872(0.8),127.03899(3),85.02879(6)	Baicalein 7-*O*-β-D-glucuronide-(1→3)[β-D-glucoside-(1→6)]-β-D-glucoside	Flavone-*O*-glycoside	F.I
S103	10.93	519.11305	+	$C_{24}H_{22}O_{13}$	−0.515	343.08023(10),315.08505(69),311.05420(10),301.07013(20),283.05975(29),271.05951(100),231.06464(5),201.09091(7)	Trihydroxyflavone *O*-6"-malonyl glucoside (Isomer of Apigenin 7-6"-malonyl glucoside)	Flavone-*O*-glycoside	F.I
S104	9.49	433.11257	+	$C_{21}H_{20}O_{10}$	−0.816	271.05969(100)	Isomer of Baicalein 7-*O*-glucoside (Trihydroxyflavone *O*-glucoside)	Flavone-*O*-glycoside	/
S105	5.72	523.14417	+	$C_{24}H_{26}O_{13}$	−0.855	361.09100(100),346.06732(8),331.04391(8),328.05756(3),313.03406(3)	Trihydroxy-trimethoxyflavone-*O*-glucoside	Flavone-*O*-glycoside	/
S106	9.38	519.1129	+	$C_{24}H_{22}O_{13}$	−0.803	337.06061(2),297.07465(7),285.07510(10),271.05954(73),255.06462(10),239.06934(1),231.06471(2),215.07065(1),174.55710(1),156.26376(1),105.03371(7),59.06100(100)	Isomer of S103 (Trihydroxyflavone *O*-6"-malonyl glucoside)	Flavone-*O*-glycoside	F.I
S107	10.34	447.12802	+	$C_{22}H_{22}O_{10}$	−1.237	285.07468(100),270.05124(15)	Oroxylin A 7-*O*-glucoside	Flavanone-*O*-glycoside	RS

S108	5.77	433.11249	+	$C_{21}H_{20}O_{10}$	−1	271.05957(100),169.01288(0.1)	Isomer of Baicalein 7-*O*-glucoside (Trihydroxyflavone *O*-glucoside)	Flavone-*O*-glycoside	/
S109	5.41	595.16536	+	$C_{27}H_{30}O_{15}$	−0.649	271.05954(100),127.03880(1)	Isomer of Apigenin 7-*O*-sophoroside	Flavone-*O*-glycoside	F.I
S110	10.63	533.12852	+	$C_{25}H_{24}O_{13}$	−0.839	285.07535(100),270.05191(18),267.06497(0.3),253.04749(0.1),239.06937(0.1)	Dihydroxy-methoxyflavone *O*-6''-malonyl glucoside	Flavone-*O*-glycoside	F.I
S111	5.97	623.12372	+	$C_{27}H_{26}O_{17}$	−0.892	285.07532(100),271.05948(68),270.05182(15)	Isomer of Clerodendrin	Flavone-*O*-glycoside	F.I
S112	5.36	609.18105	+	$C_{28}H_{32}O_{15}$	−0.569	285.07538(100),271.05981(15),270.05107(6)	Isomer of Acacetin 7-*O*-β-sophoroside	Flavone-*O*-glycoside	F.I
S113	12.17	489.13876	+	$C_{24}H_{24}O_{11}$	−0.773	285.07523(100),270.05176(18),175.07506(1),165.09137(0.2),105.03358(2)	Dihydroxy-methoxyflavone *O*-glucuronide ethyl ester	Flavone-*O*-glycoside	/
S114	12.57	539.09695	+	$C_{30}H_{18}O_{10}$	−0.599	521.08783(3),503.0761(1),493.09171(4),465.0969(2),449.1020(1),437.04977(100),419.03888(71),401.02802(10),391.04047(5),375.05029(8),363.0499(3),347.0550(2),323.05453(50),297.03854(6),271.05960(58),270.04407(24),269.04407(70),241.04915(62),225.05426(4)	8,8'-Bibaicalein	Flavones	/

#, F.I, represented as first report of compound in SR.

ᖻ, RS, represented as identification result obtained by comparing the retention time, UV spectra, and MS data with authentic standards.

Table S4. Literature reported biological activities of anti-inflammation, inhibiting of lungs and colon related diseases of 114 constituents in SR. (UP, ZQ group was higher than KQ group; DOWN, KQ group was higher than ZQ group)

ID	Identification	Up-Down	anti-inflammatory *in vitro*	anti-colitis *in vivo*	anti-pneumonia *in vivo*	Ref.
S1	Acteoside	UP	☑	☑	☑	1, 2 3, 4
S2	Leucosceptoside A	DOWN	☑	/	/	5
S3	Isomartynoside	DOWN	☑	/	/	6
S4	Martynoside	DOWN	☑	/	/	5, 7
S5	Darendoside A	DOWN	☑	/	/	8-11
S17	Norwogonoside	UP	☑	/	/	12
S19	Chrysin 7-*O*-glucuronide	UP	☑	/	/	13
S21	Oroxylin A 7-*O*-glucuronide	UP	☑	/	/	14, 15
S22	Scutellarin	UP	☑	/	☑	16, 17
S23	Dinatin 7 O-glucoside	UP	☑	/	/	18
S24	5,7,2'-Trihydroxy-8-methoxyflavanone 7-*O*-glucuronide	DOWN	☑	/	/	19, 20
S25	Wogonoside	UP	☑	☑	☑	21-24
S39	Baicalin	UP	☑	☑	☑	25-29 27 30
S40	Chrysin-6-*C*-arabinoside-8-*C*-glucoside	UP	☑	/	/	12 31
S45	Chrysin 6,8-di-*C*- glucoside	UP	☑	/	/	31
S46	Chrysin-6-*C*- glucoside-8-*C*-arabinoside	UP	☑	/	/	12
S56	5,7,3,2',6'-Pentahydroxyflavanone	UP	☑	/	/	32
S57	Viscidulin III	UP	☑	/	/	33
S58	Scutellarein	UP	☑	/	☑	34, 35
S59	Baicalein	UP	☑	☑	☑	36-42, [419-421
S60	Wogonin	UP	☑	☑	☑	43, 44 45-47
S62	Oroxylin A	DOWN	☑	☑	☑	48-51
S63	Skullcapflavone I	DOWN	☑	/	/	52
S66	Scullcapflavone II	DOWN	☑	/	/	33
S67	Apigenin	DOWN	☑	☑	☑	53, 54
S71	Eriodictyol	DOWN	☑	/	/	55
S77	Nepetin	DOWN	☑	/	☑	56, 57
S78	Chrysin	DOWN	☑	☑	☑	58
S104	Apigenin 7-*O*-glucoside	UP	☑	/	/	59
S114	8,8''-Bibaicalein	DOWN	☑	/	/	60

Table S5. Peak area ratios of different constituents of KQ and ZQ samples

EIC peak area ratio	Ratio range	Recognition rate for known samples		Prediction accuracy and false negative rate for unknown samples**			
		KQ recognition rate（%）*	ZQ recognition rate（%）*	KQ prediction accuracy（%）**	KQ false negative rate（%）**	ZQ prediction accuracy（%）**	ZQ false negative rate（%）**
S40/S78#	**< 1.0**	75.0		95.5	24.1		
	> 1.0		95.7			75.9	4.5
S78/S46	**> 1.4**	75.0		91.3	25.0		
	< 1.4		91.3			75.0	8.7
（S46+S40）/S78	**< 1.6**	75.0		100.0	23.3		
	> 1.6		100.0			76.7	0.0
S39/S59	**< 1.1**	82.1		88.5	20.0		
	> 1.1		87.0			80.0	11.5
S25/S60	**< 0.9**	89.3		78.1	23.8		
	> 0.9		69.6			76.2	21.9
S21/S62	**< 1.6**	82.1		85.2	22.7		
	> 1.6		82.6			77.3	14.8
（S25+S46+S40）/（S60+S78）	**< 1.1**	82.1		85.2	20.8		
	> 1.1		82.6			79.2	14.8
S13/S67	**< 0.6**	71.4		71.4	34.8		
	> 0.6		65.2			65.2	28.6
S59/S28	**> 5.1**	89.3		89.3	13.0		
	< 5.1		87.0			87.0	10.7
（S39+S28）/S59	**< 1.4**	85.7		85.7	17.4		
	> 1.4		82.6			82.6	14.3
（S17+S25）/S60	**< 1.3**	75.0		84.0	26.9		
	> 1.3		82.6			73.1	16.0

S25/S71	**< 6.5**	92.9		89.7	9.1		
	> 6.5		87.0			90.9	10.3
S39/S71	**< 9.0**	96.4		96.4	4.3		
	> 9.0		95.7			95.7	3.6
（S25+S39）/（S60+S71）	**< 1.8**	85.7		96.0	15.4		
	> 1.8		95.7			84.6	4.0
S28/S71	**< 2.0**	96.4		93.1	4.5		
	> 2.0		91.3			95.5	6.9
S13/S71	**< 1.0**	89.3		89.3	13.0		
	> 1.0		87.0			87.0	10.7
S27/S71	**< 1.4**	92.9		96.3	8.3		
	> 1.4		95.7			91.7	3.7
S29/S71	**< 1.0**	89.3		89.3	13.0		
	> 1.0		87.0			87.0	10.7
S27/S5	**< 30.0**	85.7		88.9	16.7		
	> 30.0		87.0			83.3	11.1

*****, KQ recognition rate (%)=Identified amount of KQ samples/28 KQ samples; ZQ recognition rate (%)=Identified amount of ZQ samples/23 ZQ samples.

**, KQ prediction accuracy (%)=Actual amount of KQ samples in unknown samples/identified amount of unknown samples; ZQ prediction accuracy (%)=Actual amount of ZQ samples in unknown samples/identified amount of unknown samples; KQ false negative rate (%)=1−ZQ prediction accuracy; ZQ false negative rate (%)=1−KQ prediction accuracy.

Table S6. Peak areas of the main active constituents in colon calculated from extracted ion chromatograms in six repeated experiments. Avg1, Avg2, Avg3, Avg4, Avg5, and Avg6 was the average content in G1, G2, G3, G4, G5, and G6 (n=6 in each group). $KQ_{Avg1\sim6}$, $ZQ_{Avg1\sim6}$, SEM_{KQ}, SEM_{ZQ} represented mean ± SEM in KQ groups (n=36) and ZQ groups (n=36).

ID	KQ-G1	KQ-G2	KQ-G3	KQ-G4	KQ-G5	KQ-G6	ZQ-G1	ZQ-G2	ZQ-G3	ZQ-G4	ZQ-G5	ZQ-G6	$KQ_{Avg1\sim6}$	SEM_{KQ}	$ZQ_{Avg1\sim6}$	SEM_{ZQ}
	KQ_{Avg1}	KQ_{Avg2}	KQ_{Avg3}	KQ_{Avg4}	KQ_{Avg5}	KQ_{Avg6}	ZQ_{Avg1}	ZQ_{Avg2}	ZQ_{Avg3}	ZQ_{Avg4}	ZQ_{Avg5}	ZQ_{Avg6}				
S13#	1.33E+06	1.10E+06	3.00E+06	5.21E+05	2.23E+06	2.78E+06	9.85E+05	6.57E+05	3.23E+06	1.60E+06	3.36E+06	3.34E+06	1.83E+06	3.06E+05	2.19E+06	2.75E+05
S21	3.94E+06	4.36E+06	1.26E+07	1.34E+06	8.22E+06	6.82E+06	1.67E+06	1.68E+06	1.09E+07	5.19E+06	1.18E+07	1.05E+07	6.22E+06	1.13E+06	6.95E+06	1.00E+06
S25	1.98E+06	4.66E+06	1.86E+07	4.33E+06	8.71E+06	1.02E+07	5.16E+05	1.32E+06	1.34E+07	9.63E+06	1.20E+07	1.66E+07	8.09E+06	1.76E+06	8.89E+06	8.08E+05
S39	8.35E+05	4.78E+06	1.58E+07	3.03E+06	9.46E+06	9.76E+06	5.19E+05	2.04E+06	1.40E+07	7.79E+06	1.17E+07	1.49E+07	7.29E+06	1.55E+06	8.48E+06	2.21E+08
S40	1.47E+07	1.96E+06	6.61E+06	2.25E+06	5.71E+06	6.50E+06	1.04E+07	2.63E+06	1.07E+07	5.08E+06	7.13E+06	4.59E+06	6.29E+06	1.50E+06	6.76E+06	1.55E+07
S46	7.47E+06	9.71E+05	4.45E+06	1.17E+06	3.94E+06	4.53E+06	7.47E+06	1.53E+06	8.02E+06	4.53E+06	4.62E+06	3.54E+06	3.76E+06	8.26E+05	4.95E+06	4.92E+05
S59	1.95E+08	8.30E+07	4.70E+08	1.14E+08	4.65E+08	7.45E+08	1.32E+08	8.92E+07	8.62E+08	5.59E+08	8.77E+08	1.95E+09	3.45E+08	6.48E+07	7.45E+08	7.91E+06
S60	1.25E+08	2.98E+07	1.14E+08	3.01E+07	1.13E+08	1.35E+08	4.73E+07	1.88E+07	1.85E+08	9.07E+07	1.65E+08	1.80E+08	9.12E+07	1.55E+07	1.14E+08	9.04E+06
S61	1.47E+06	8.61E+05	2.86E+06	3.69E+05	5.77E+06	8.64E+06	1.05E+06	4.05E+05	4.27E+06	3.24E+06	6.35E+06	5.47E+06	3.33E+06	7.97E+05	3.46E+06	2.63E+06
S62	5.38E+07	9.45E+06	5.75E+07	6.57E+06	5.14E+07	4.76E+07	1.72E+07	6.52E+06	9.51E+07	2.98E+07	1.02E+08	7.48E+07	3.77E+07	6.44E+06	5.42E+07	1.53E+07
S65	1.67E+07	4.17E+06	2.50E+07	5.08E+06	2.41E+07	3.94E+07	7.25E+06	4.10E+06	5.91E+07	2.47E+07	3.93E+07	1.44E+08	1.91E+07	3.68E+06	4.64E+07	1.60E+06
S66	7.47E+06	2.77E+06	2.57E+07	5.23E+06	1.26E+07	4.56E+07	4.72E+06	2.98E+06	3.84E+07	1.65E+07	2.06E+07	2.24E+07	1.66E+07	3.40E+06	1.76E+07	1.01E+06
S67	5.09E+07	2.00E+07	9.81E+07	3.15E+07	9.19E+07	1.47E+08	3.96E+07	2.89E+07	2.42E+08	9.37E+07	1.55E+08	1.33E+08	7.32E+07	1.22E+07	1.15E+08	1.38E+06
M2	2.90E+06	2.05E+06	1.07E+07	1.76E+05	7.52E+06	7.37E+06	4.67E+06	1.96E+06	1.26E+07	4.56E+06	1.04E+07	9.36E+06	5.11E+06	1.04E+06	7.24E+06	1.09E+06
M3	1.92E+07	4.05E+06	2.03E+07	2.43E+06	1.00E+07	1.54E+07	1.73E+07	1.51E+07	1.73E+07	9.69E+06	1.89E+07	1.88E+07	1.19E+07	1.76E+06	1.62E+07	2.18E+06
M9	1.76E+06	3.69E+05	6.87E+06	4.97E+05	8.55E+06	4.97E+06	1.78E+06	1.04E+06	1.66E+07	5.12E+06	1.37E+07	6.90E+06	3.84E+06	9.47E+05	7.53E+06	1.32E+06
M10	3.21E+06	7.11E+05	2.12E+06	1.47E+05	2.87E+06	7.46E+06	9.61E+05	5.82E+05	4.53E+06	1.72E+06	4.62E+06	3.88E+06	2.75E+06	6.17E+05	2.72E+06	4.04E+05
M12	1.68E+07	6.89E+05	3.33E+06	1.20E+06	6.74E+06	1.27E+06	5.61E+06	9.64E+05	1.27E+07	2.57E+06	1.01E+07	1.06E+06	5.00E+06	1.52E+06	5.50E+06	1.04E+06
M14	1.53E+06	1.77E+05	7.76E+05	1.47E+05	6.17E+05	6.19E+05	1.58E+06	1.52E+05	1.86E+06	5.27E+05	1.20E+06	4.97E+05	6.45E+05	1.64E+05	9.70E+05	2.15E+05

Table S7. Peak areas of the main active constituents in lungs calculated from extracted ion chromatograms in six repeated experiments. Avg1, Avg2, Avg3, Avg4, Avg5, and Avg6 was the average content in G1, G2, G3, G4, G5, and G6 (n=6 in each group). $KQ_{Avg1\sim6}$/ $ZQ_{Avg1\sim6}$ and SEM_{KQ}/ SEM_{ZQ} represented mean ± SEM in KQ groups (n=36) and ZQ groups (n=36).

ID	KQ-G1	KQ-G2	KQ-G3	KQ-G4	KQ-G5	KQ-G6	ZQ-G1	ZQ-G2	ZQ-G3	ZQ-G4	ZQ-G5	ZQ-G6	$KQ_{Avg1\sim6}$	SEM_{KQ}	$ZQ_{Avg1\sim6}$	SEM_{ZQ}
	KQ_{Avg1}	KQ_{Avg2}	KQ_{Avg3}	KQ_{Avg4}	KQ_{Avg5}	KQ_{Avg6}	ZQ_{Avg1}	ZQ_{Avg2}	ZQ_{Avg3}	ZQ_{Avg4}	ZQ_{Avg5}	ZQ_{Avg6}				
S13[#]	1.65E+06	1.31E+06	1.16E+06	2.95E+05	1.00E+06	1.21E+06	9.18E+05	7.78E+05	1.51E+06	7.33E+05	1.27E+06	1.34E+06	1.10E+06	1.05E+05	1.09E+06	2.88E+05
S21	2.30E+06	1.47E+06	1.16E+06	2.58E+05	1.19E+06	1.71E+06	7.12E+05	6.67E+05	1.39E+06	7.84E+05	4.29E+06	8.49E+05	1.35E+06	1.60E+05	1.45E+06	1.08E+05
S25	2.76E+06	2.18E+06	2.05E+06	6.91E+05	1.71E+06	3.06E+06	8.02E+05	8.86E+05	2.45E+06	1.37E+06	4.07E+06	1.48E+06	2.08E+06	2.10E+05	1.84E+06	2.46E+05
S39	2.50E+06	1.20E+06	1.09E+06	8.94E+04	9.26E+05	8.50E+05	1.42E+06	5.10E+05	1.16E+06	3.78E+05	1.49E+06	9.05E+05	1.11E+06	1.55E+05	9.78E+05	1.00E+05
S59	1.71E+06	1.68E+06	1.21E+06	3.77E+05	1.62E+06	1.64E+06	9.51E+05	1.89E+06	1.14E+06	4.41E+05	3.20E+06	6.26E+06	1.37E+06	2.01E+05	2.31E+06	6.35E+05
S60	1.05E+07	1.57E+06	9.08E+05	3.10E+05	1.47E+06	2.14E+06	3.35E+06	1.43E+06	1.22E+06	4.84E+05	2.86E+06	1.92E+06	2.82E+06	6.95E+05	1.88E+06	2.64E+05
S62	2.63E+06	5.35E+05	3.96E+05	8.07E+04	6.04E+05	7.66E+05	1.21E+06	6.54E+05	4.53E+05	1.36E+05	1.53E+06	6.59E+05	8.35E+05	1.73E+05	7.74E+05	1.35E+05
S67	4.85E+05	1.75E+05	5.05E+04	1.26E+05	1.82E+05	8.40E+05	2.93E+05	3.98E+05	1.61E+05	1.02E+05	5.57E+05	1.14E+06	3.10E+05	7.48E+04	4.41E+05	1.47E+05
S78	2.41E+06	5.66E+05	6.76E+05	2.44E+05	1.16E+06	9.80E+05	1.27E+06	5.87E+05	1.40E+06	4.81E+05	1.57E+06	1.40E+06	1.01E+06	1.52E+05	1.12E+06	1.58E+05
M1	4.14E+06	1.12E+06	5.77E+05	2.21E+05	6.82E+05	1.48E+06	9.64E+05	5.80E+05	2.44E+06	1.28E+06	2.14E+06	7.90E+05	1.37E+06	2.82E+05	1.37E+06	2.48E+05
M2	3.18E+06	9.73E+05	9.58E+05	2.24E+05	8.12E+05	1.48E+06	1.19E+06	6.95E+05	1.28E+06	5.57E+05	4.77E+06	1.21E+06	1.27E+06	1.96E+05	1.62E+06	3.41E+05
M3	3.75E+06	5.76E+05	7.95E+05	3.74E+05	5.86E+05	2.36E+06	1.08E+06	4.69E+05	1.59E+06	6.18E+05	4.79E+06	1.04E+06	1.41E+06	2.98E+05	1.60E+06	3.39E+05
M4	8.08E+07	2.10E+07	1.49E+07	7.36E+06	1.67E+07	3.27E+07	1.36E+07	1.50E+07	3.13E+07	1.78E+07	6.90E+07	1.35E+07	2.89E+07	5.30E+06	2.67E+07	4.35E+06

Part B: MS^2 and proposed fragmentation pathways of constituents in SR, colon and lungs tissues

S2

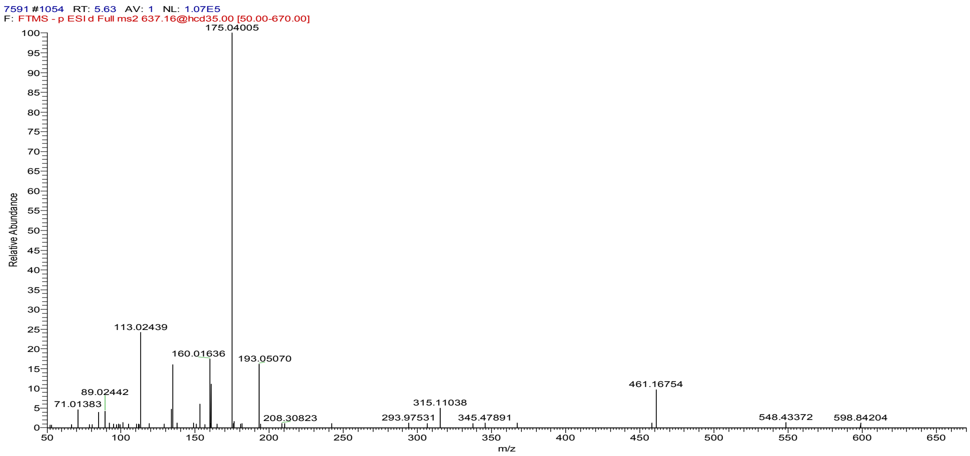
Leucosceptoside A (t_R=5.63 min)[61]

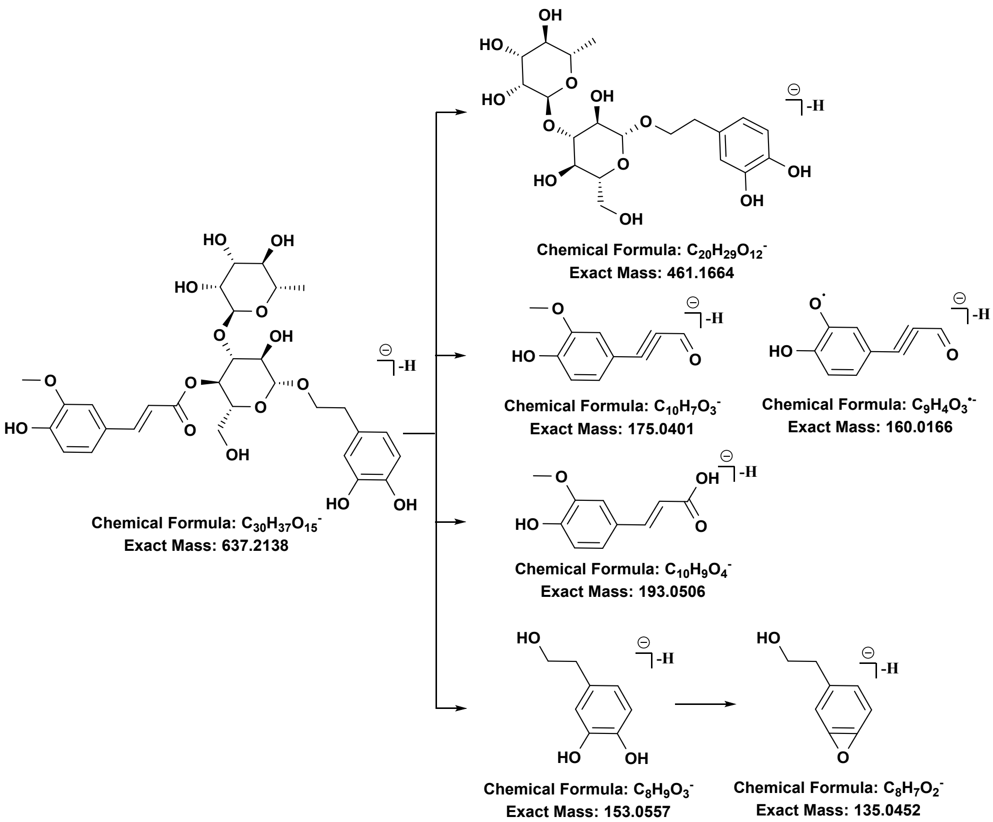
MS^1(−):

637.2141

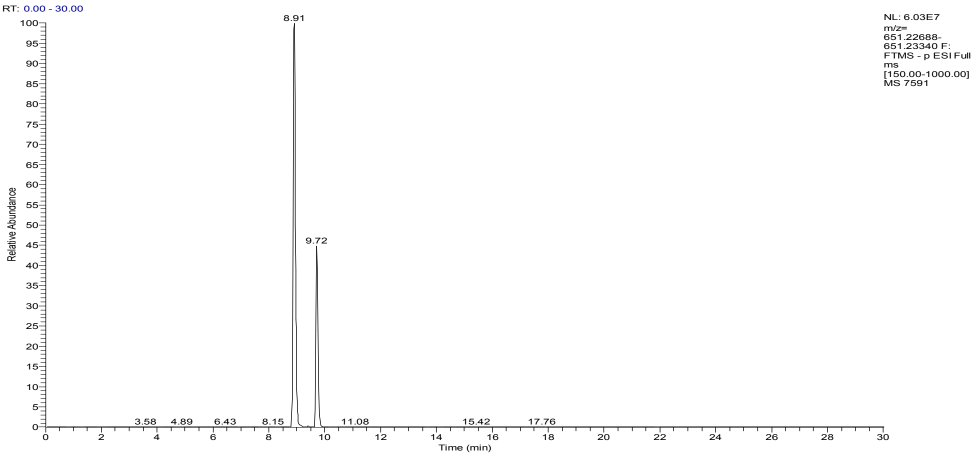
MS^2(−):

461.16754(9),315.11038(5),193.05070(18),175.04005(100),160.01636(22),153.05603(10),135.04518(17),113.02439(27)





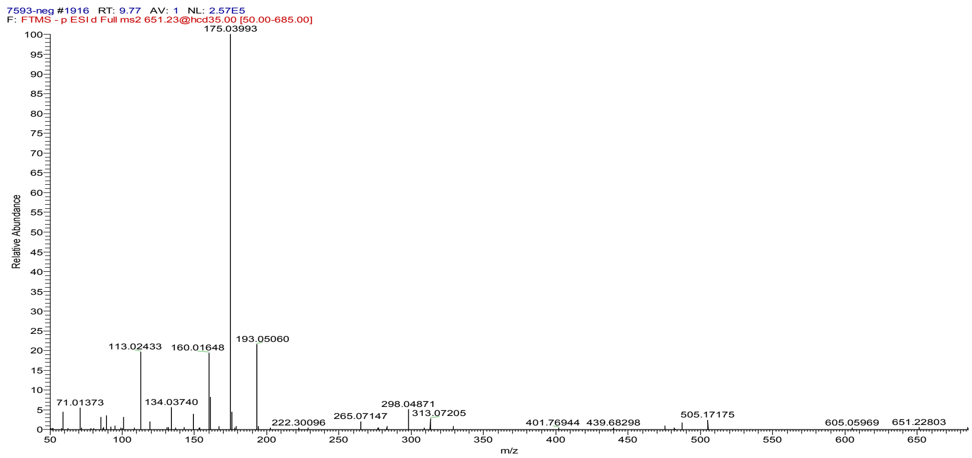
S3, and S4

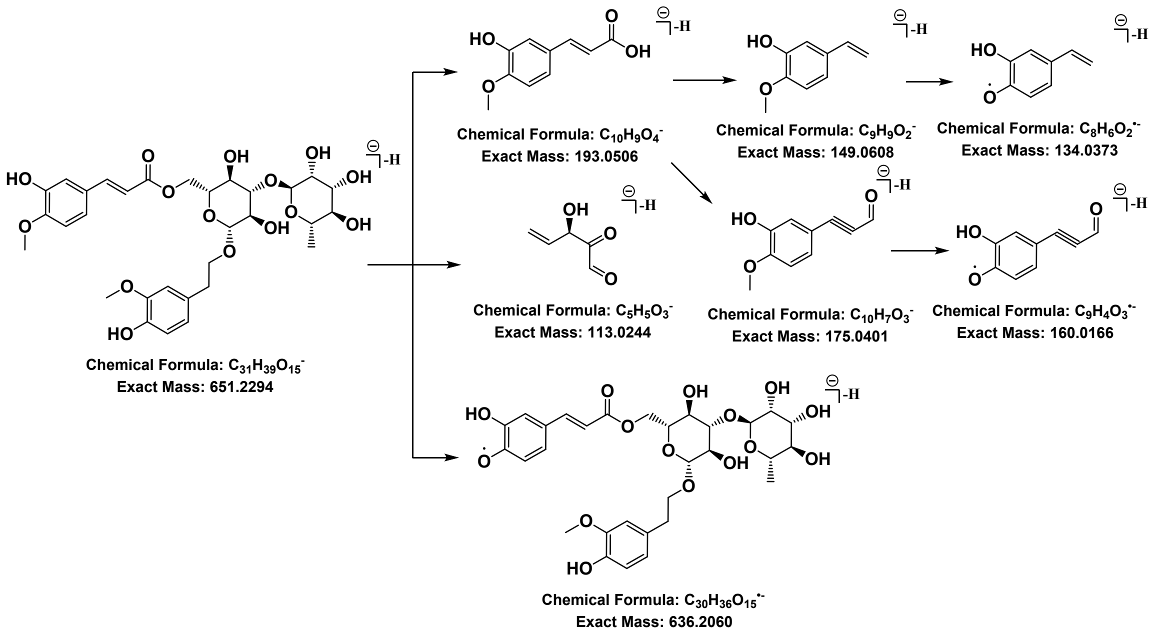


S3 Isomartynoside (t_R=9.74 min)[62]

MS^1(−):651.23014

MS^2(−):636.66242(0.7),193.05060(24),175.03962(100),160.01694(20),149.06090(5),134.03725(5),113.02420(18)





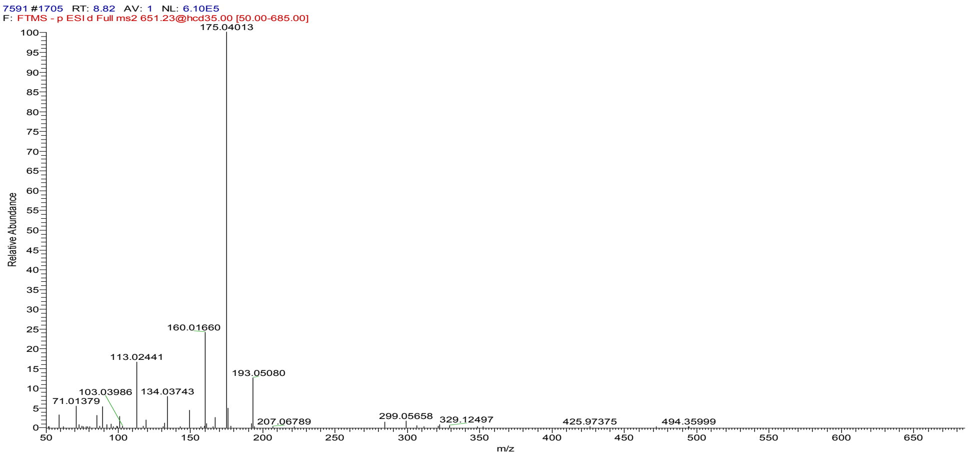
S4 Martynoside (t_R=8.91 min)[62]

MS^1(−):

651.23018

MS^2(−):

329.12497(1),299.05658(1),193.05080(13),175.04013(100),167.07126(3),160.01660(28),149.06087(3),134.03743(8),119.03503(2),113.02441(15),101.02448(2)



S5

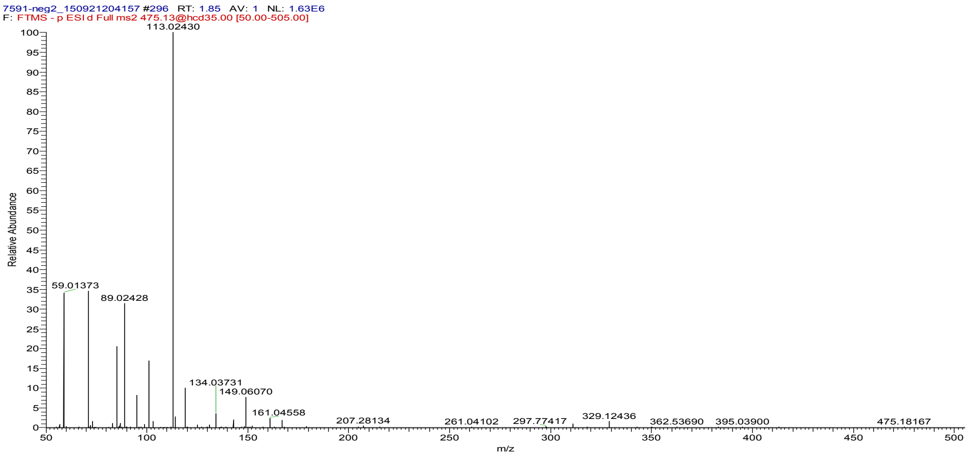
Darendoside A[62]

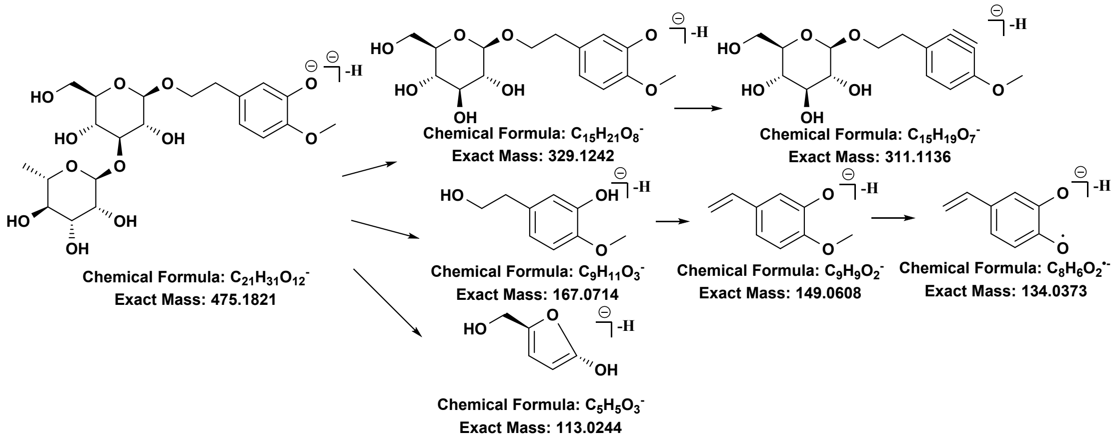
MS[1](−):

475.18188

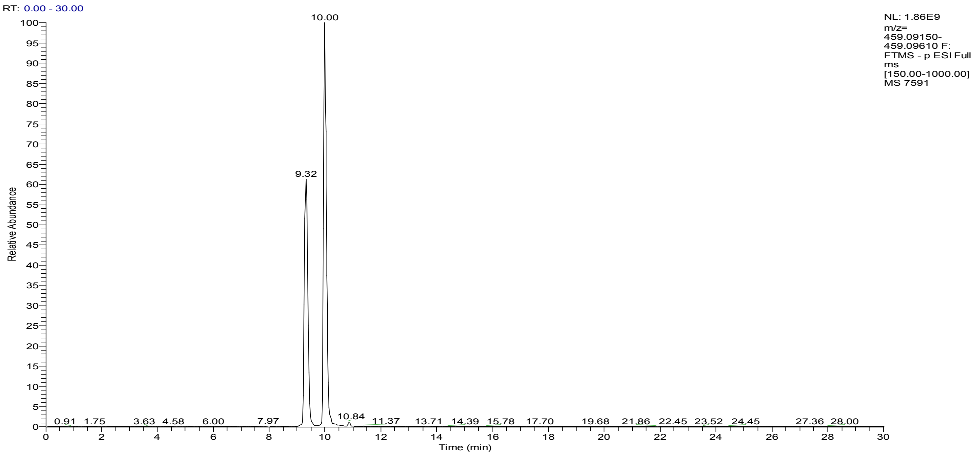
MS[2](−):

329.12436(2),311.11435(1),167.07141(2),149.06070(4),134.03731(4),113.02430(100),101.02428(17),95.01369(9)





S6, S21, and S25



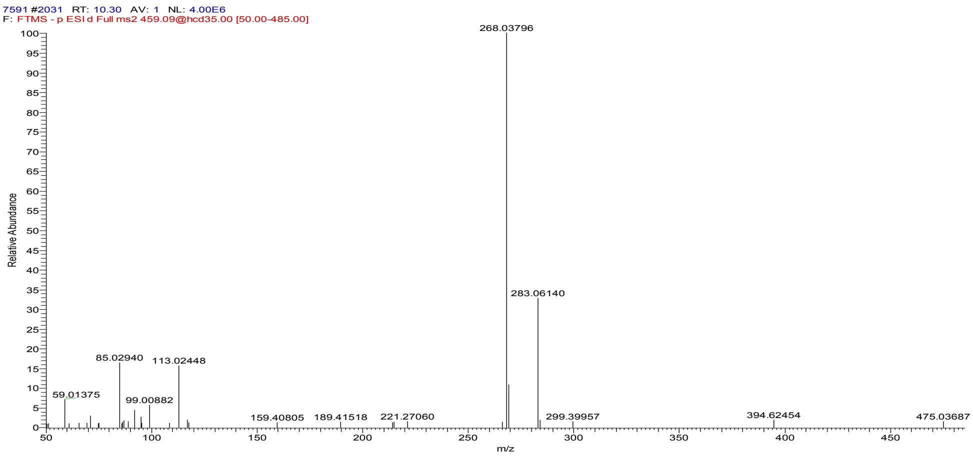
S6 Isomer of S21 (t_R=10.31 min)

MS[1](−):

459.0938

MS[2](−):

283.06140(36),268.03796(100),113.02448(12),99.01(7),99.0882.01(5),85.02940(13)



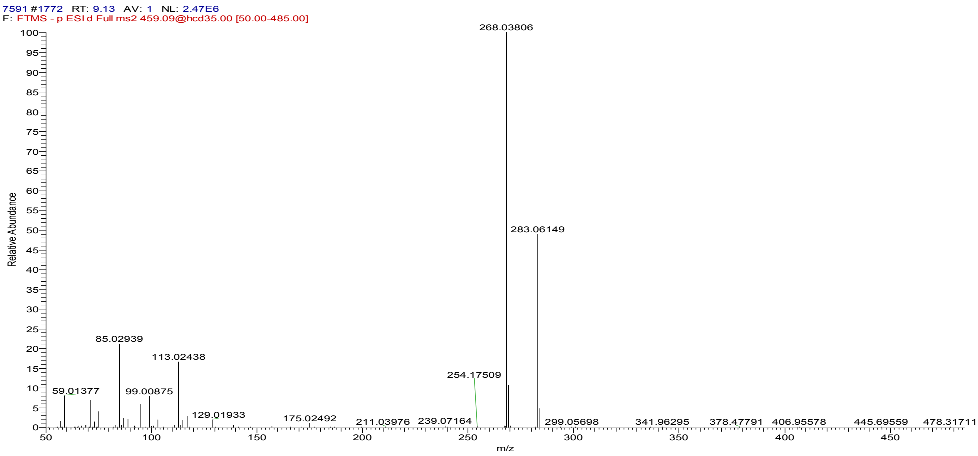
S21 Oroxylin A 7-glucuronide (t_R=9.32 min)

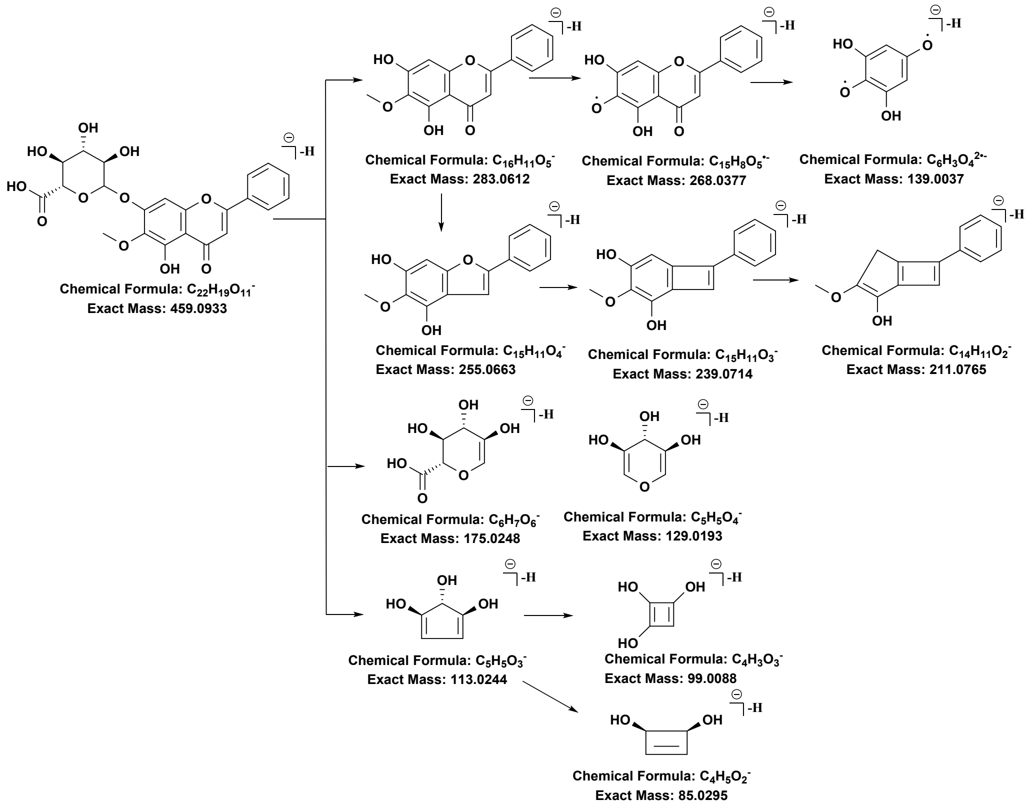
MS[1](−):

459.09374

MS[2](−):

283.06149(47),268.03806(100),239.07167(0.3),211.03976(0.1),175.02492(1.0),139.00372(0.4),129.01933(2),117.01934(3),113.02438(17),99.00875(7),85.02939(23),71.01373(7)





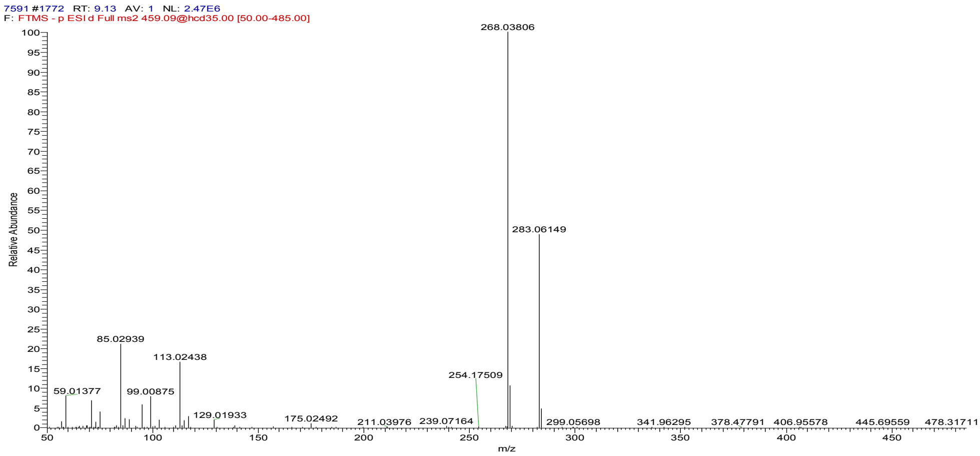
S25 Wogonoside (t_R=10.00 min)

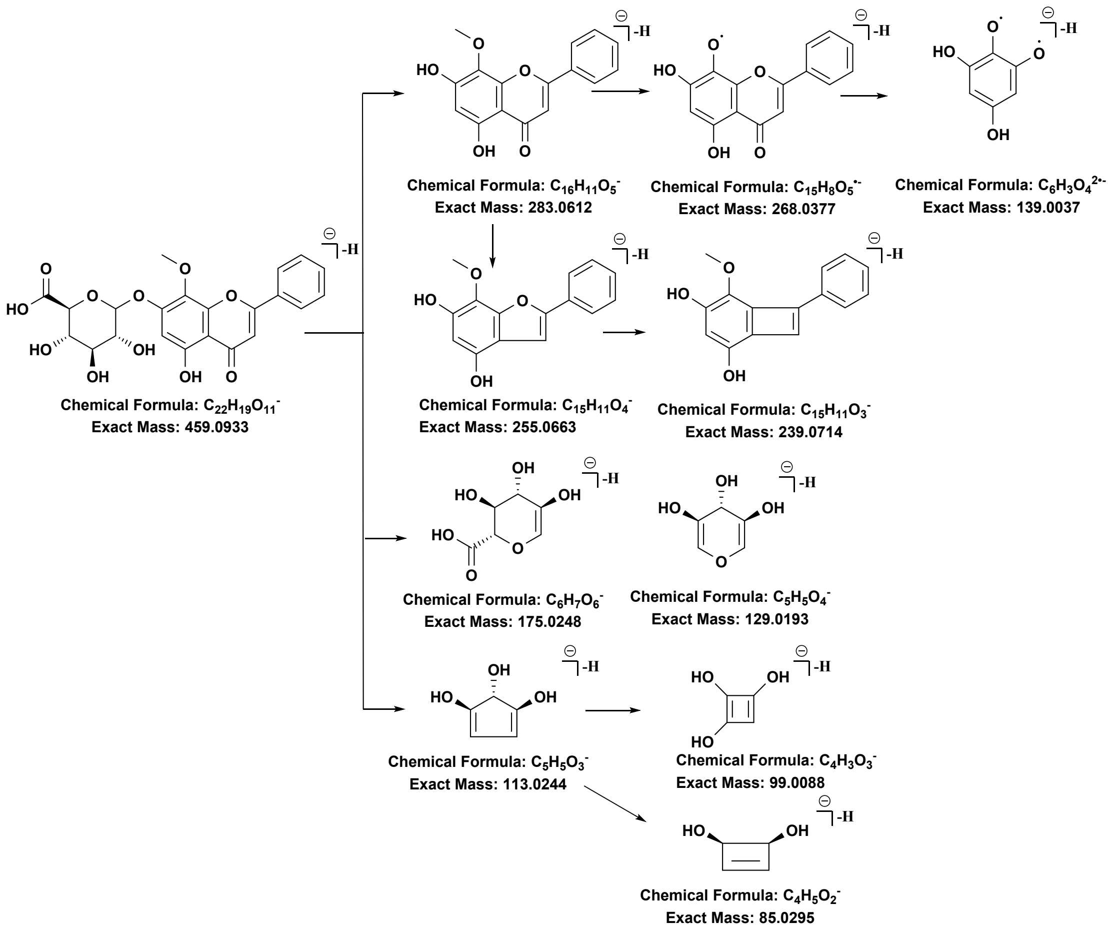
$MS^1(-)$:

459.09363

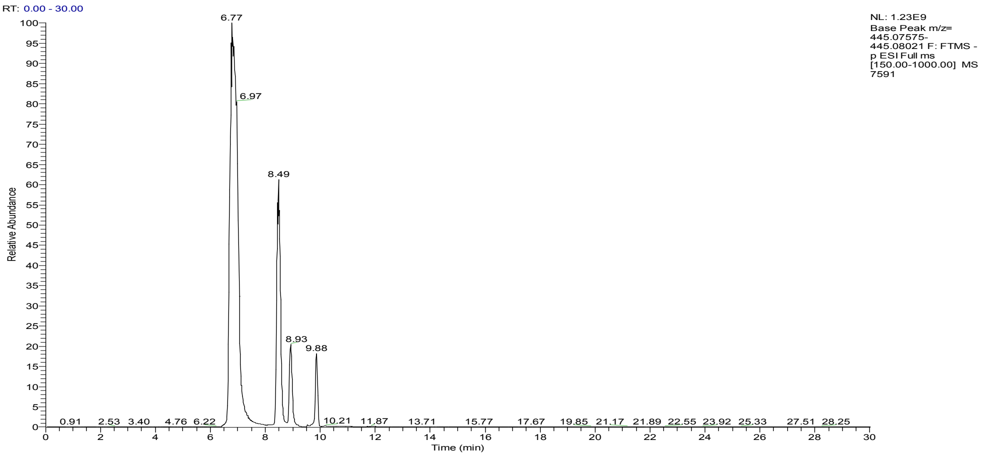
$MS^2(-)$:

283.06149(75),268.03806(100),239.07164(0.3),175.02492(1),139.00372(0.4),129.01933(2),113.02438(24),99.00875(12),85.02939(22),71.01373(7)





S7, S13, S17, S20, S29, and S39



S7 Isomer of S39 (t_R=7.25 min)

MS[1](−):445.07798

MS[2](−):269.04590(100)

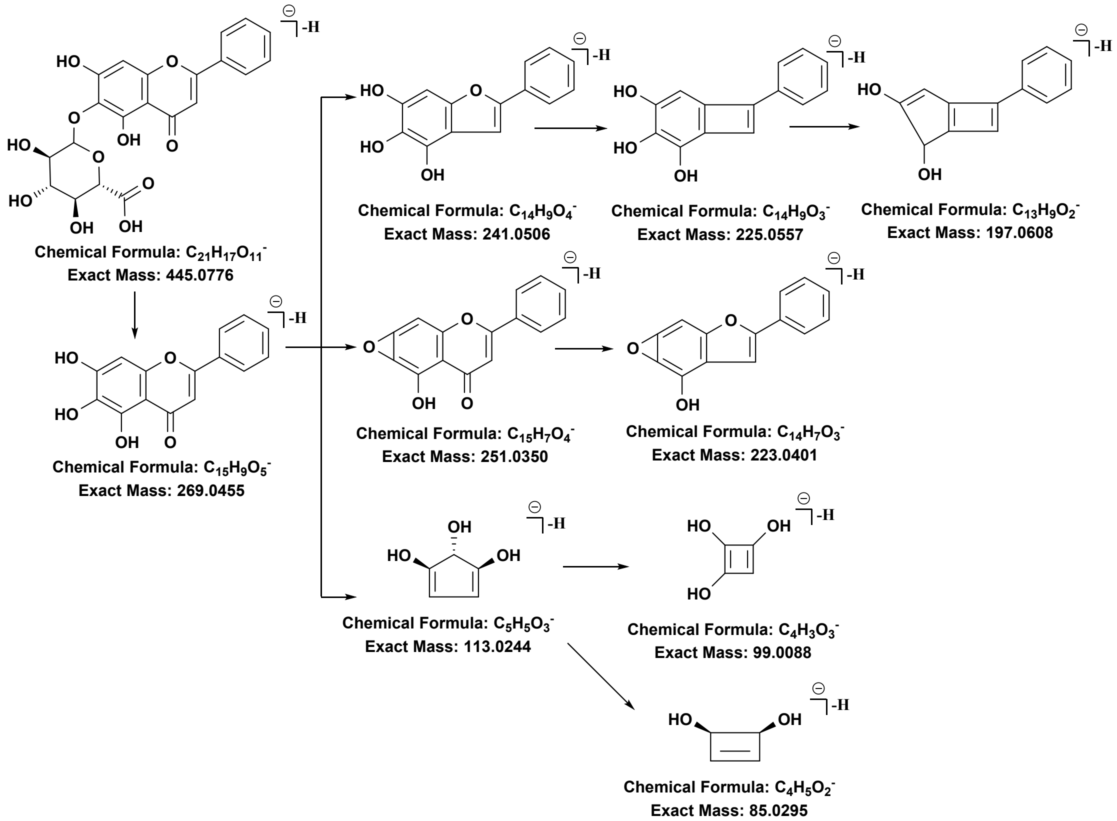
S13 Baicalein 6-*O*-glucuronide (t_R=9.88 min)[61]

MS[1](−):

445.07796

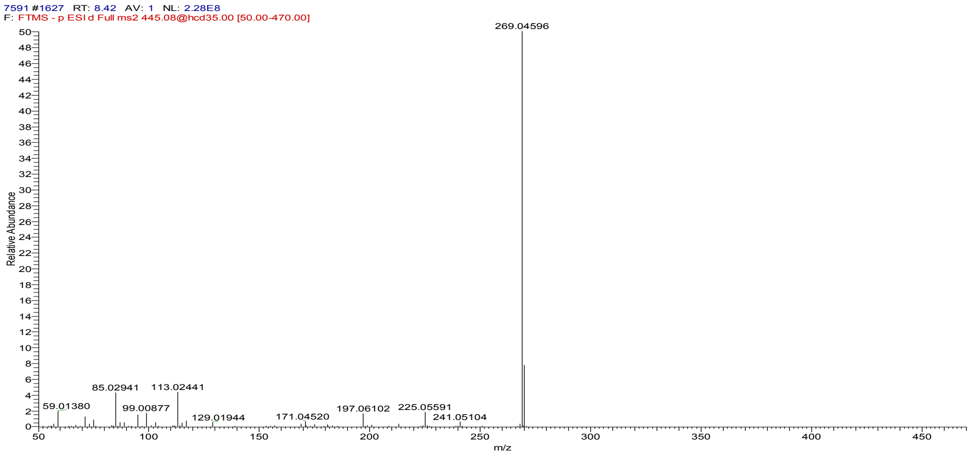
MS[2](−):

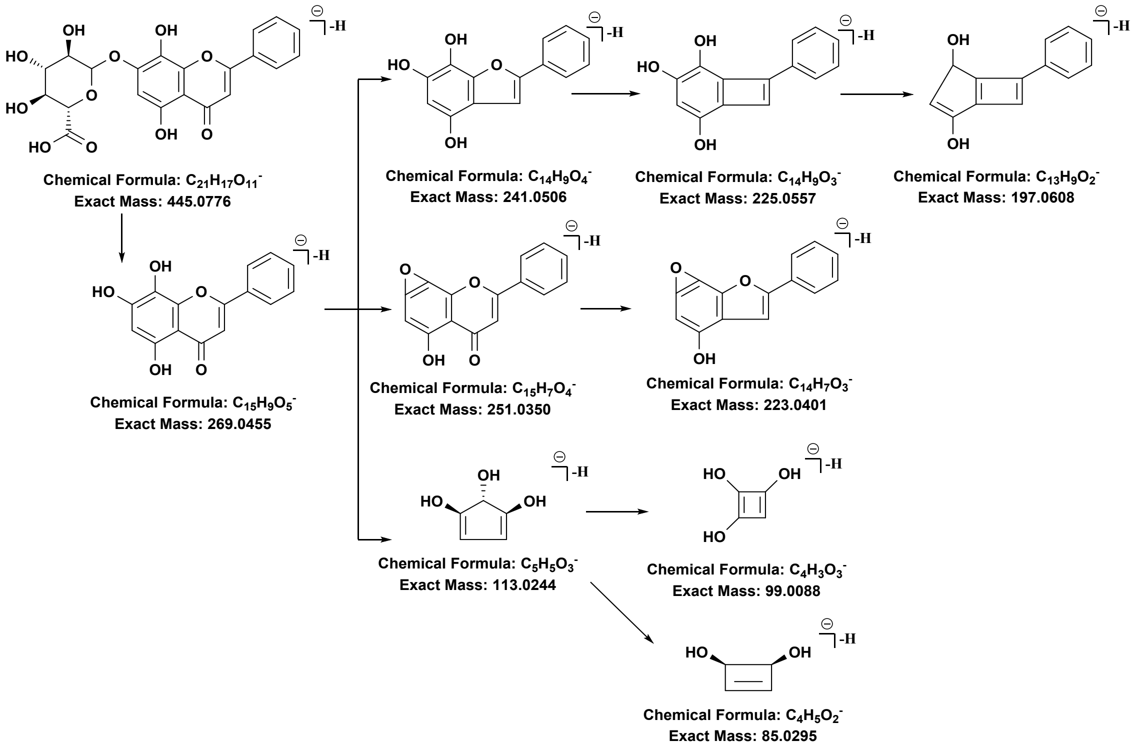
269.04587(100),251.03519(0.3),241.05064(0.1),225.05563(0.1),223.04022(0.3),113.02444(4),99.00870(2),85.02940(4)



S17 Norwogonin 7-*O*-glucuronide(norwogonoside) (t_R=8.49 min)[61]

MS¹(−):
445.07793
MS²(−):
269.04596(100),251.03575(0.1),241.05104(0.6),225.05591(2),197.06102(2),113.02441(4),99.00877(2),85.02941(4)





S20 Isomer of S39 (t_R 7.70)
MS¹(−): 445.07795
MS²(−): 269.04611(100)

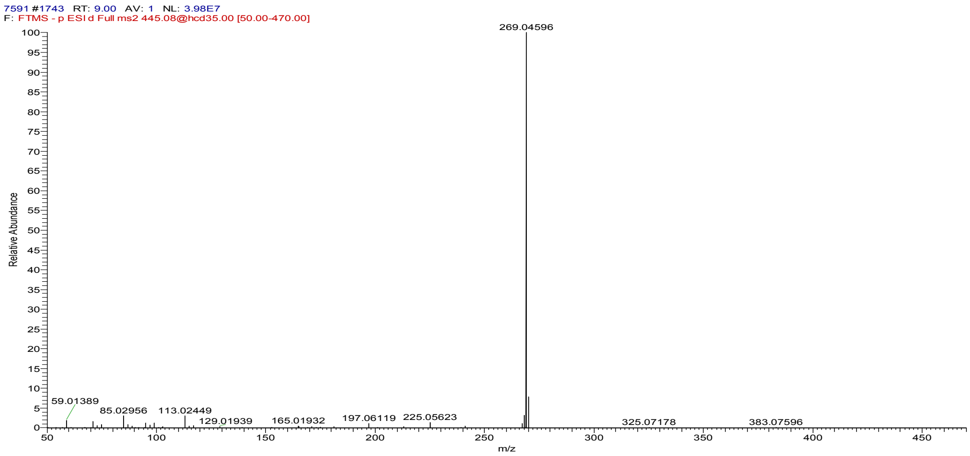
S29 Norwogonin 8-*O*-glucuronide (t_R=8.93 min)[61]

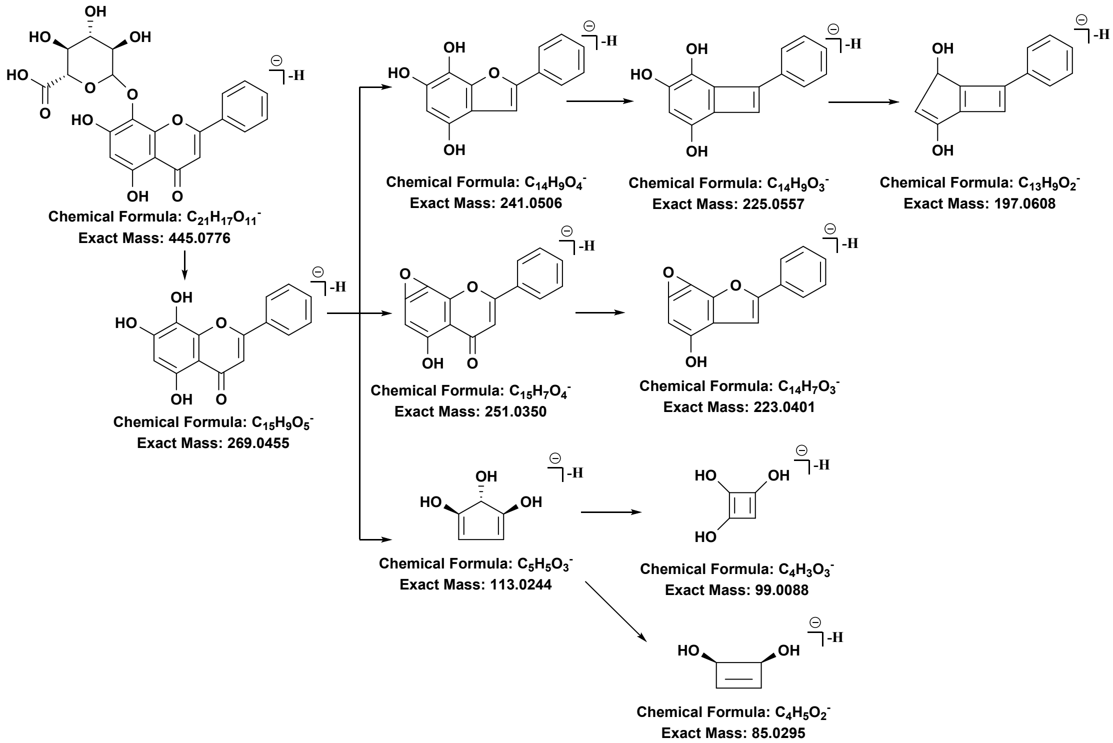
MS[1](−):

445.07795

MS[2](−):

269.04596(100),268.03815(3),267.03036(1),241.05142(0.5),225.05623(1),197.06119(1),113.02449(3),99.00886(1),85.02956(3),71.01391(2)





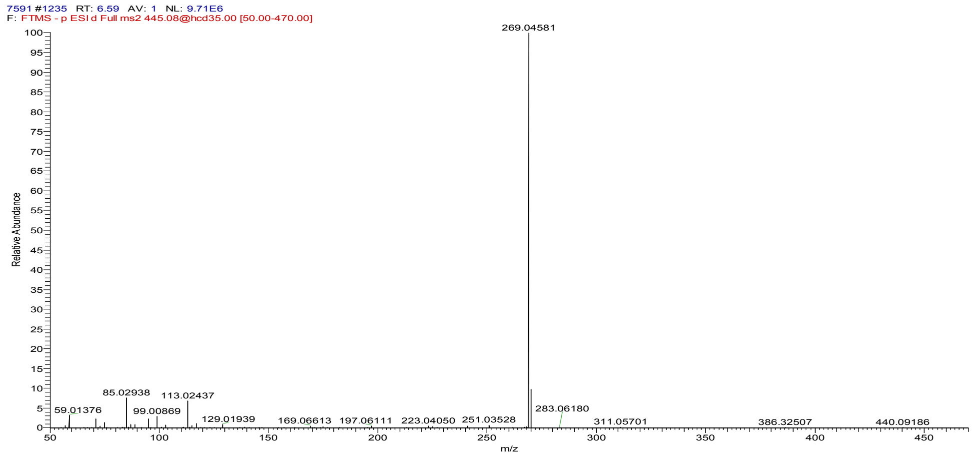
S39 Baicalin (t_R=6.77 min)

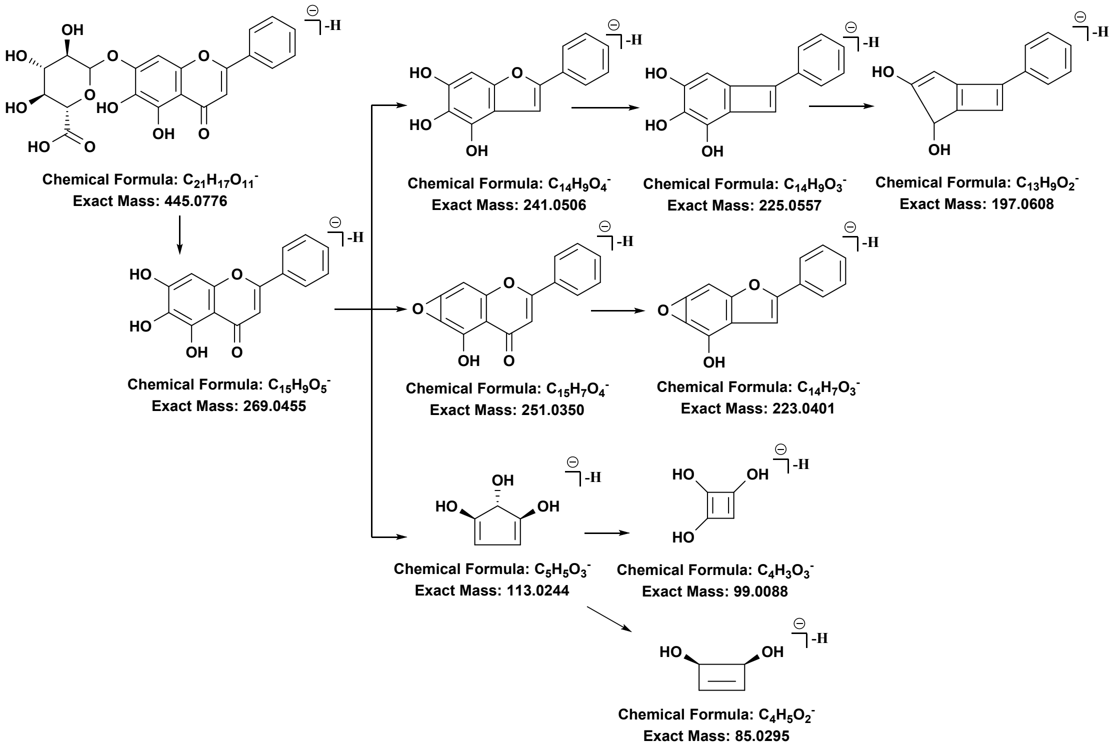
MS^1(−):

445.07991

MS^2(−):

269.04605(100),251.03560(1),241.05084(1),225.05608(0.4),197.06128(0.5),129.01952(1),117.01965(1),113.02452(6),99.00889(3),85.02959(7)





S8

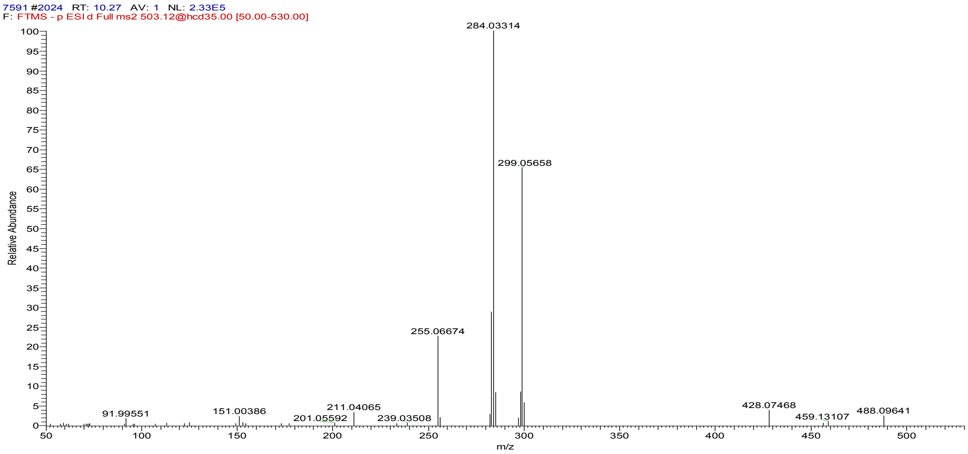
6''-*O*-acetyl homoplantaginin OR Ladanetin-6-*O*-β-(6''-*O*-acetyl)glucoside (t_R=10.39 min)[63]

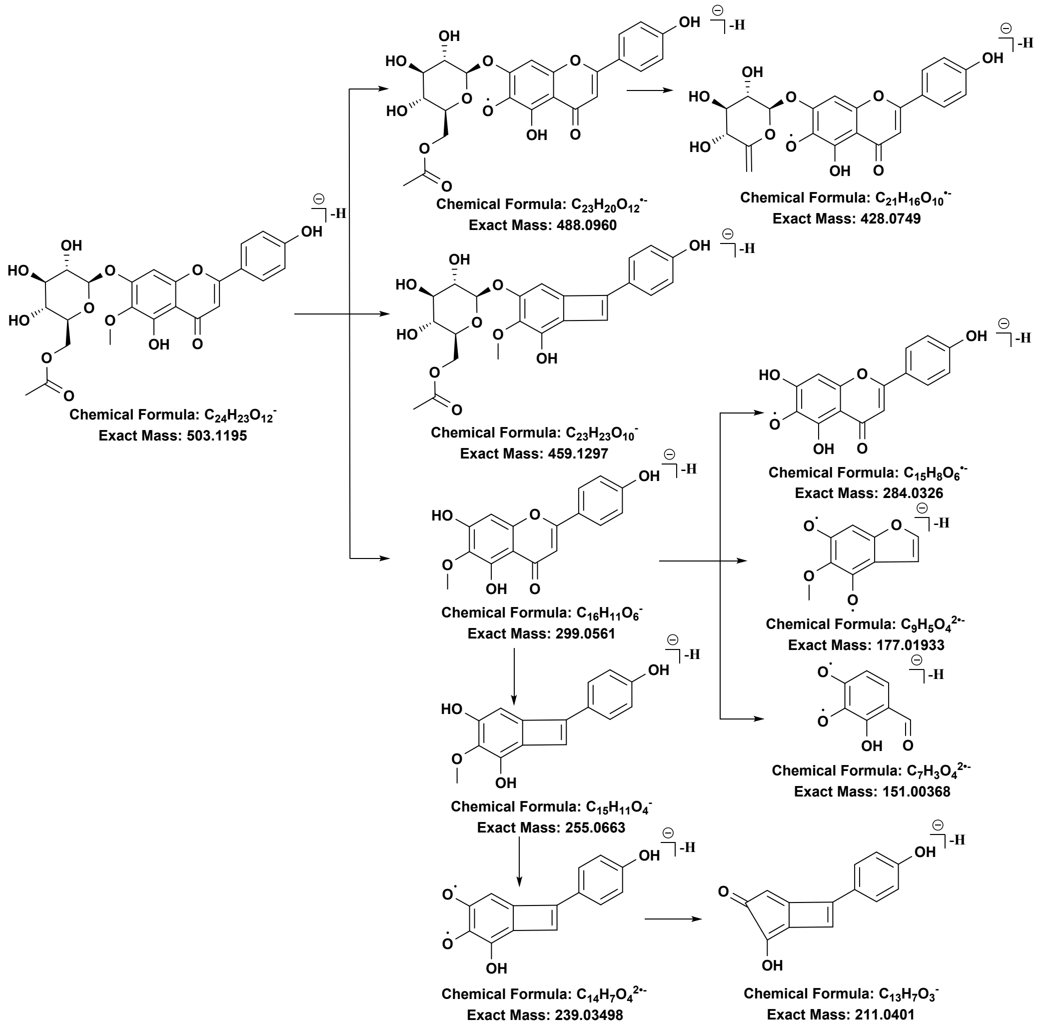
MS^1(−):

503.12007

MS^2(−):

459.13107(3),428.07468(4),299.05685(61),284.03314(100),255.06674(33),211.04065(4),151.00386(3)





S9

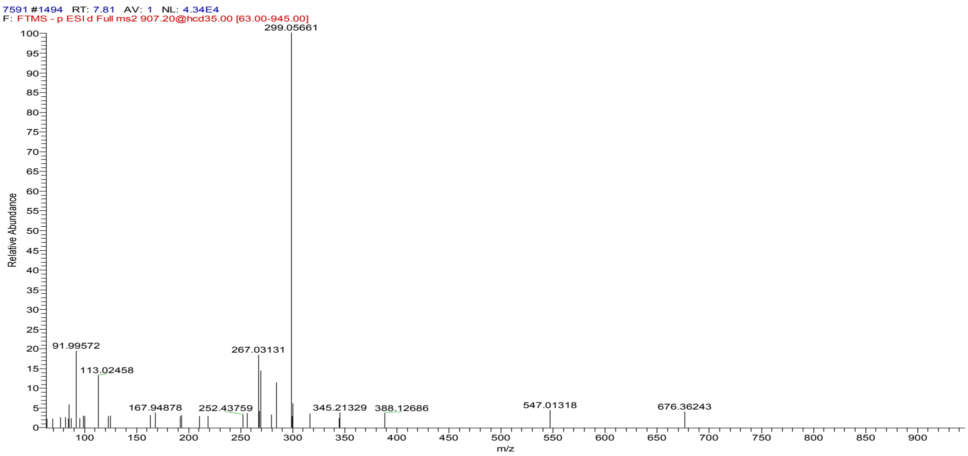
Isomer of Solanoflavone (t_R=7.81 min)[64]

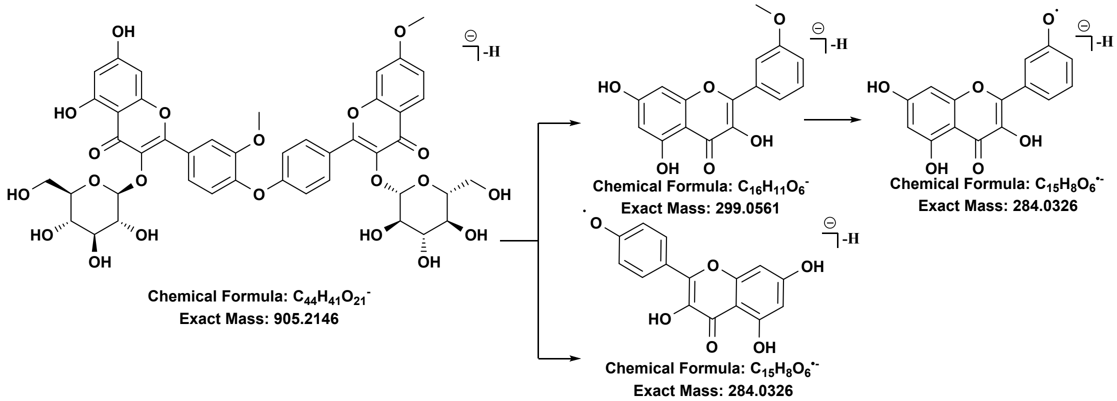
MS[1](−):

907.19435

MS[2](−):

676.36243(4),547.01318(4),388.12686(4),345.12686(4),299.05661(100),284.03271(9),269.04614(12),256.09375(4),267.03131(10)





S10

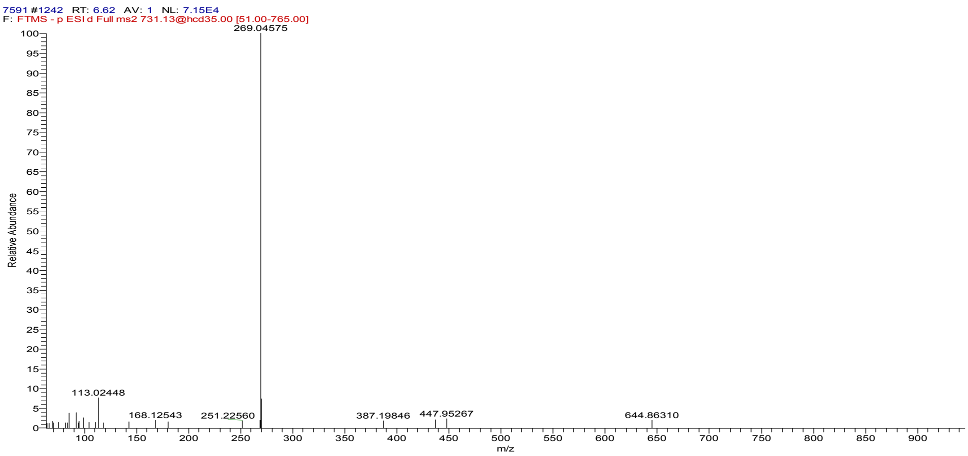
5,7,4',5'',3''',4''''-hexahydroxy-3''-*O*-β-glucosyl-3',7''-*O*-biflavone OR isomer (t_R=6.62 min)[65]

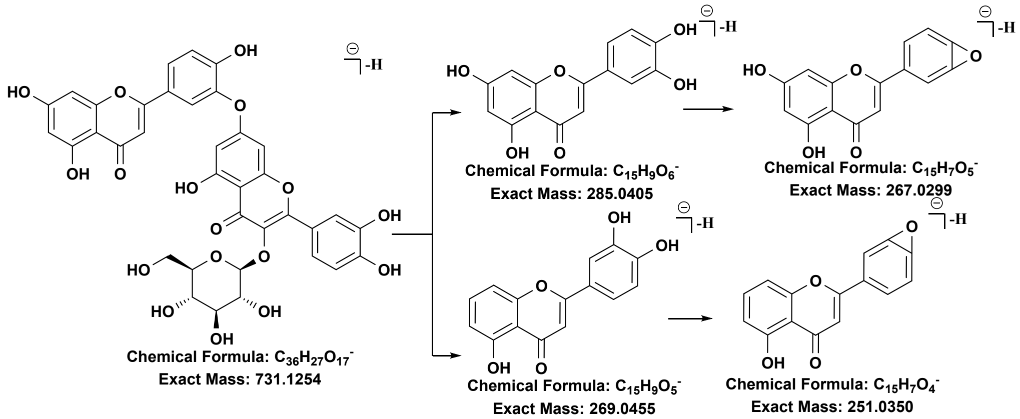
MS[1](−):

731.12622

MS[2](−):

285.04032(0.6),269.04575(100),267.02943(0.4),251.22560(2),113.02448(8).





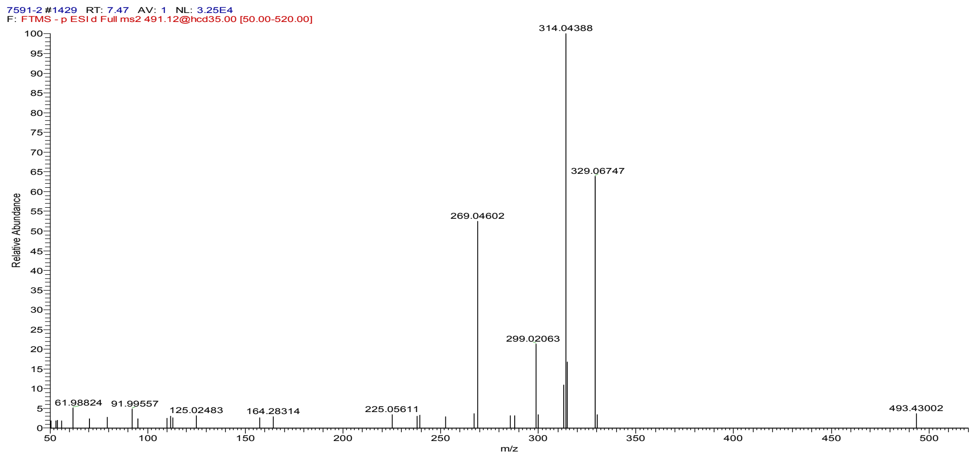
Trihydroxy-dimethoxyflavone *O*-glucoside (t_R=7.51 min)[61]

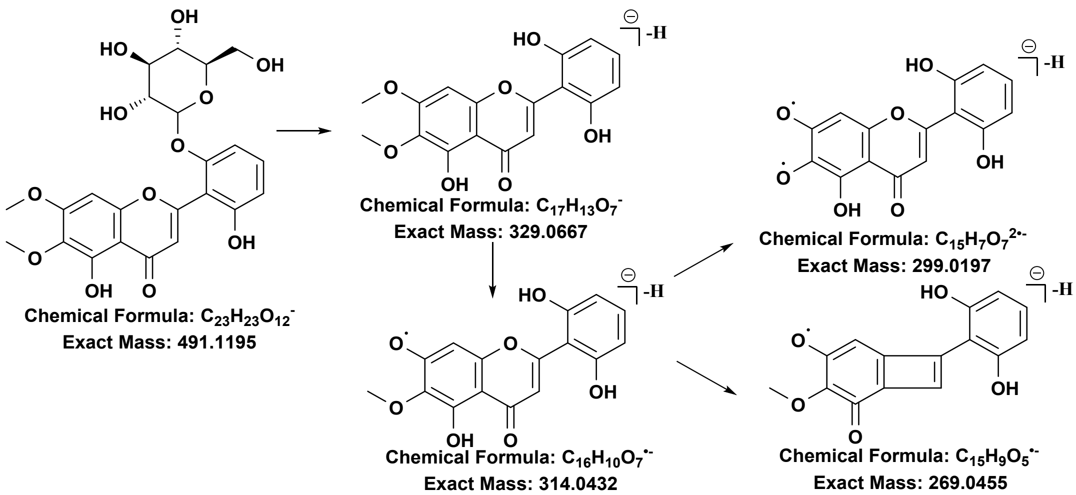
MS[1](−):

491.11986

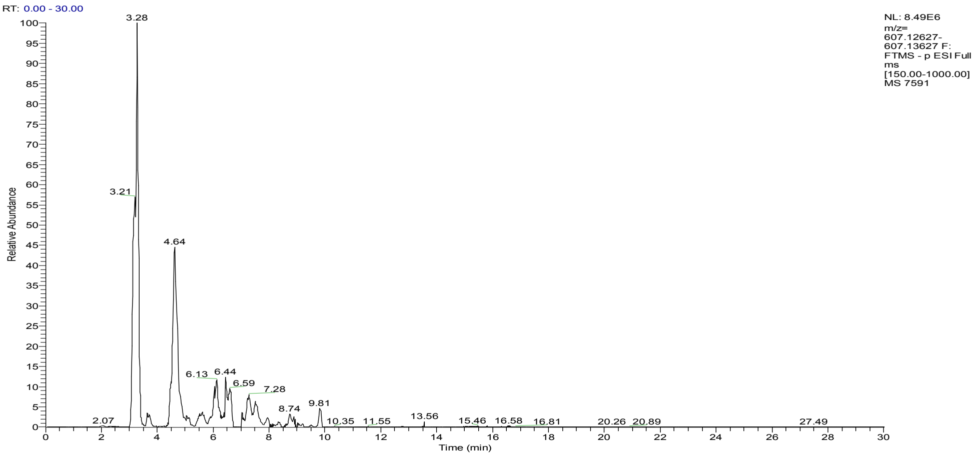
MS[2](−):

329.06747(42),314.04388(100),299.02063(18),269.04602(2)





S12, and S32



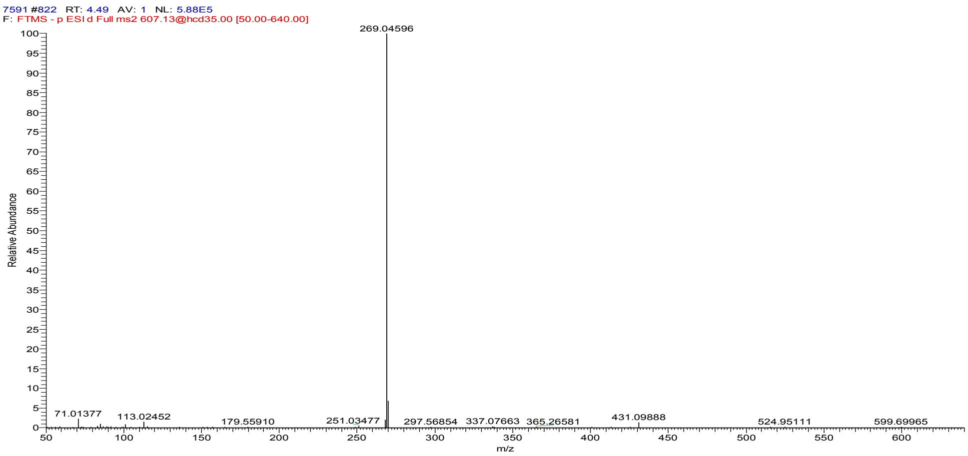
S12 Trihydroxyflavone *O*-glucoside-(1→2)-*O*-glucuronide (t_R=4.56 min)[66]

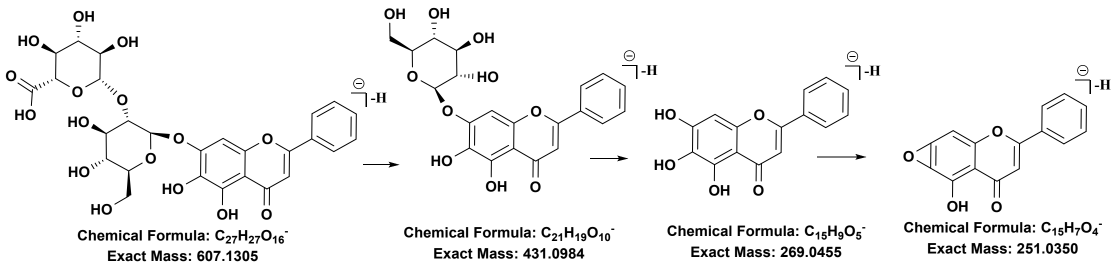
MS^1(−):

607.13127

MS^2(−):

431.09888(3),269.04596(100),251.03477(0.4),175.02(1),113.02452(5),95.01376(1),85.02924(3)





S14

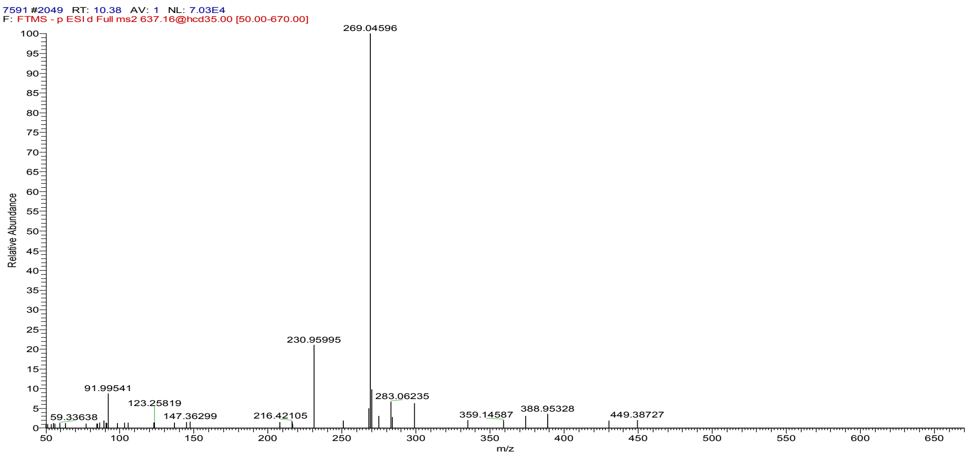
Isomer of chrysoeriol-7-*O*-[2''-*O*-E-feruloyl]-β-D-glucoside (t_R=10.39 min)

MS[1](−):

637.15677

MS[2](−):

283.06235(0.5),269.04596(100),251.03542(0.3),230.95995(1),223.06(1),205.05(2)

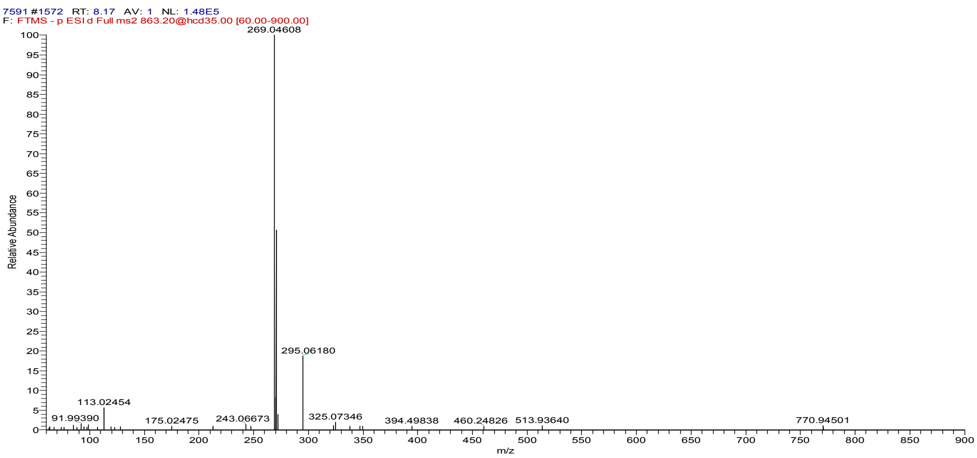


S15

Unknow (t_R=8.17 min)

MS[1](−): 863.20450

MS[2](−): 271.06174(50),269.04608(100),211.07(2),165.62(0.4),113.02454(5)



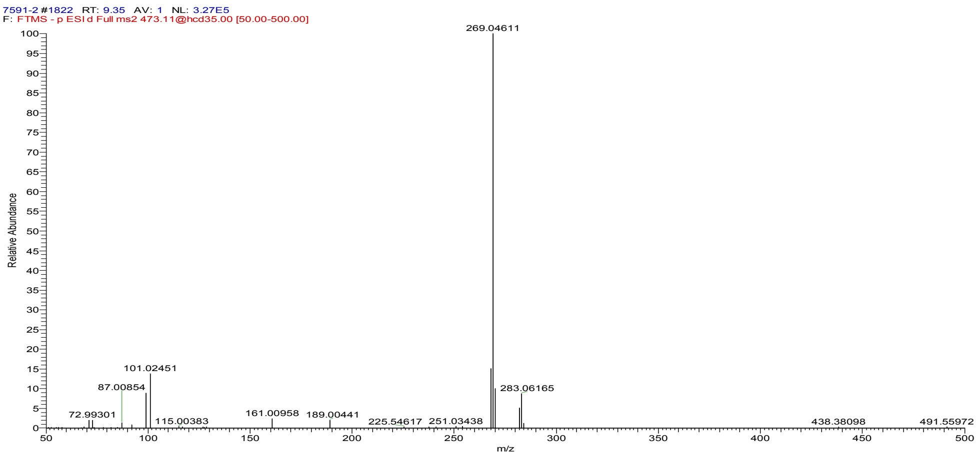
Baicalein 7-*O*-ethylglucuronide OR isomer (t_R=9.32 min)[67, 68]

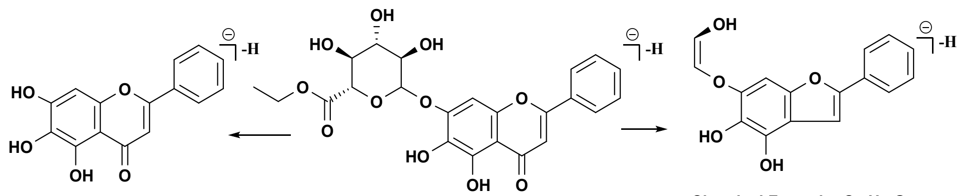
MS[1](−):

473.10911

MS[2](−):

283.06165(33),269.04611(100),268.03824(45),161.00911(6)





S18

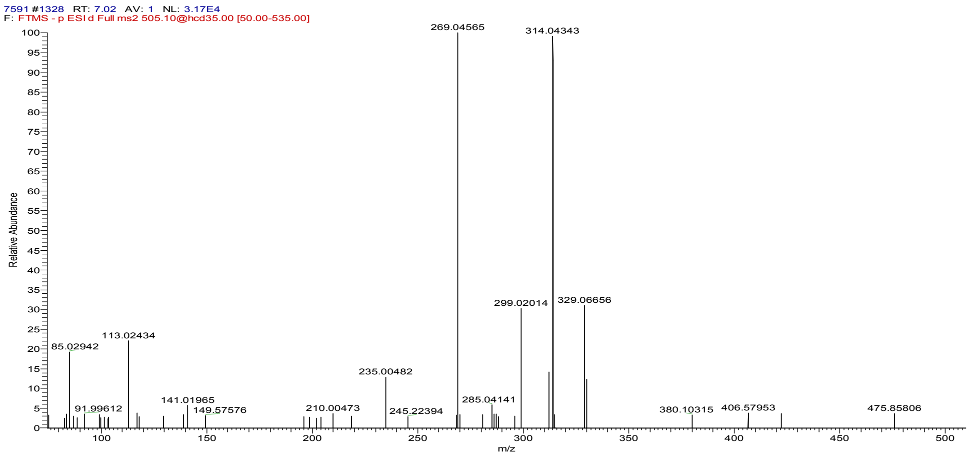
Isomer of viscidulin II 2'-*O*-glucuronide (t_R=7.13 min)

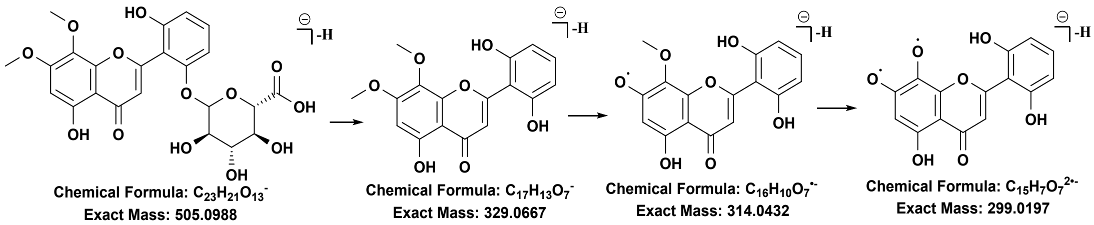
MS^1(−):

505.09920

MS^2(−):

329.06656(28),314.04343(100),299.02014(27),269.04565(5),196(3),113.02434(11),85.02942(13)



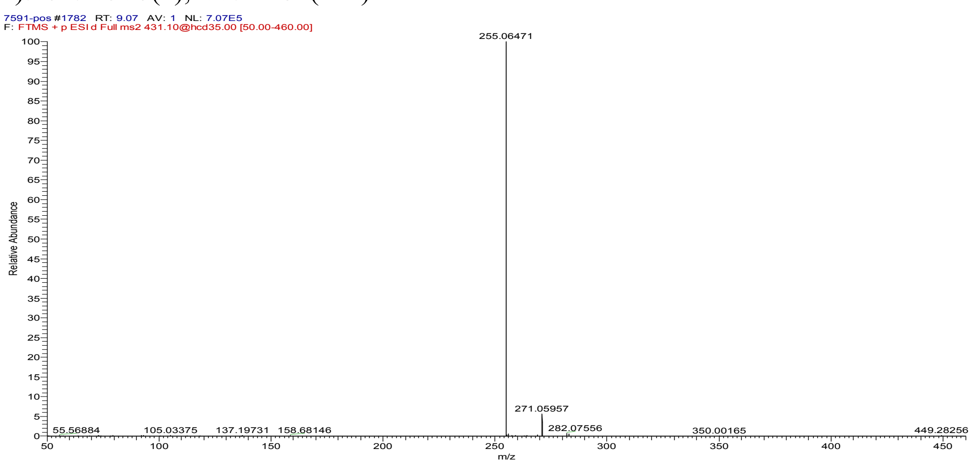


S19

Chrysin 7-*O*-glucuronide (t_R=9.21 min)[61, 62]

MS^1(+):431.09677

MS^2(+):271.05957(6),255.06471(100)



S22

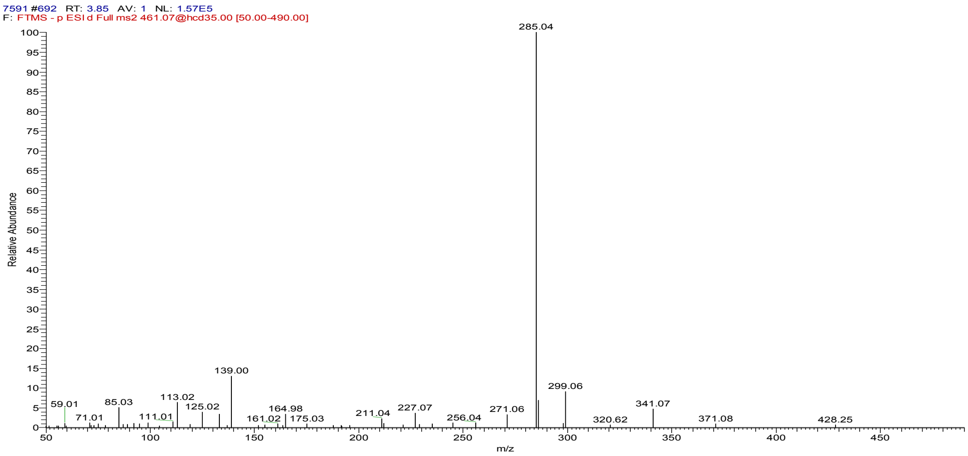
Scutellarin (tR=3.86 min)[61]

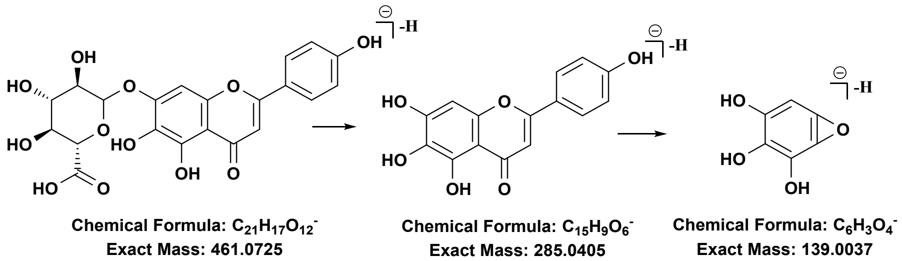
MS[1](−):

461.07327

MS[2](−):

371.07819(6),341.06790(20),299.05603(12),285.04077(100),271.06216(3),245.05(3),227.07204(4),211.04077(3)





S23

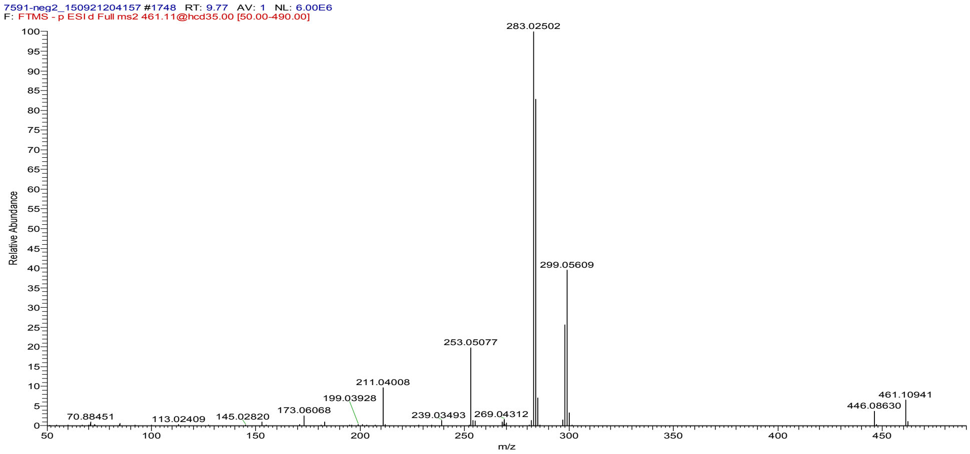
Trihydroxy-methoxyflavone-*O*-glucoside (t_R=9.77 min)[61]

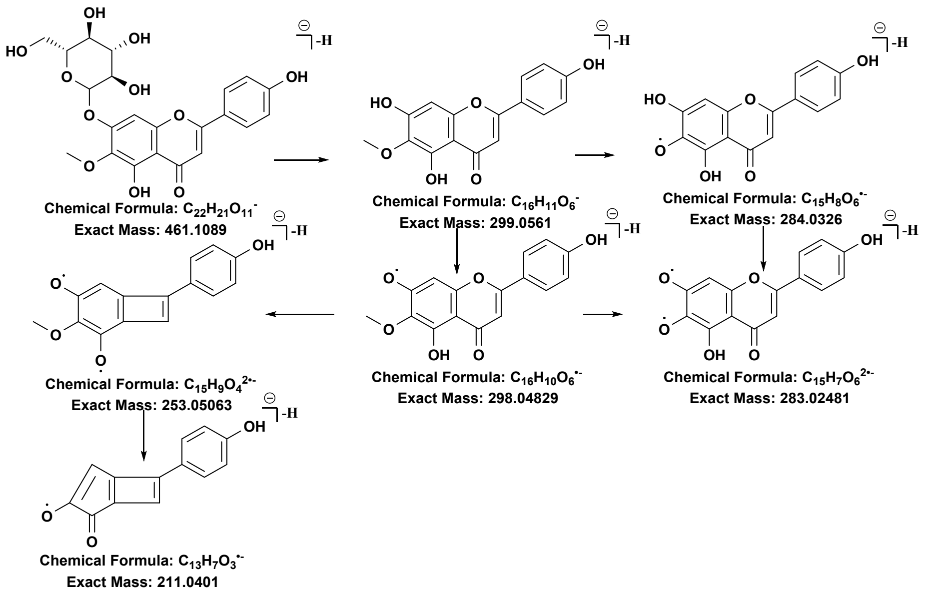
MS[1](−):

461.1091

MS[2](−):

299.05609(38),284.03268(83),283.02502(100),269.04312(2),268.03726(1),253.05077(20),211.04008(9),173.06068(2)





S24

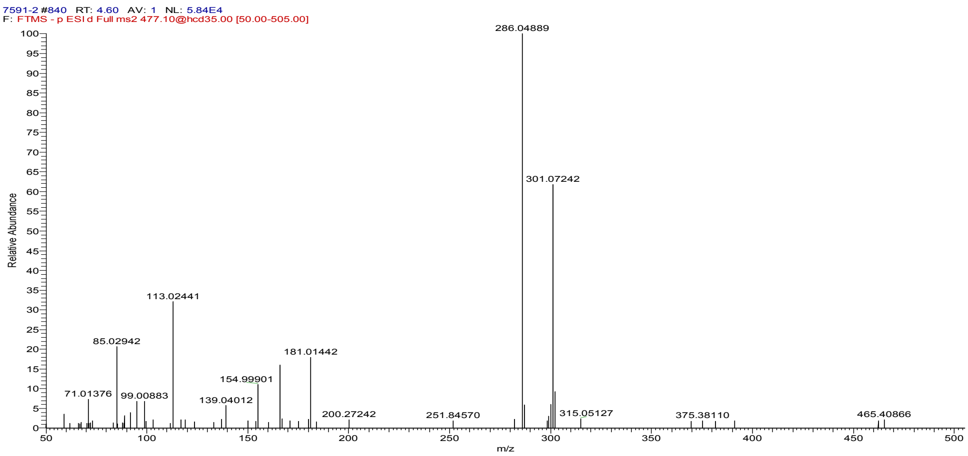
5,7,2'-Trihydroxy-6-methoxyflavanone 7-*O*-glucuronide (t_R=4.60 min)[61]

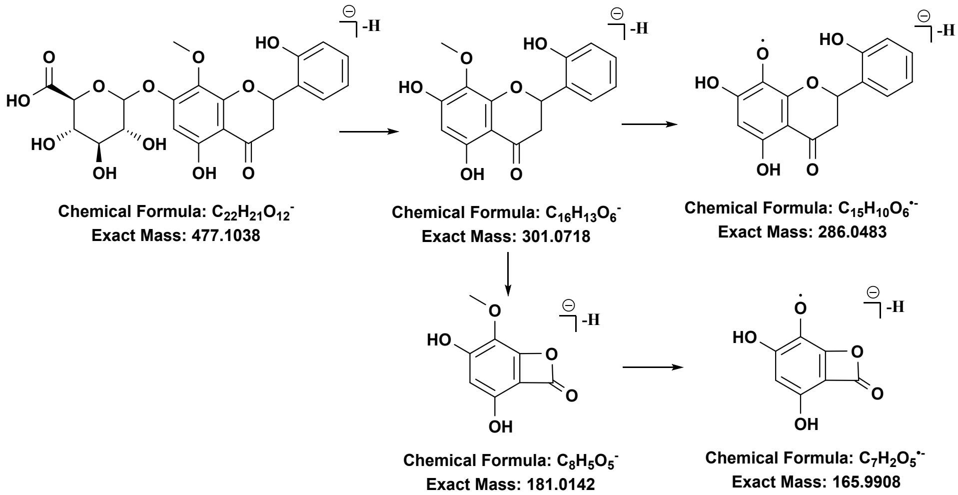
MS[1](−):

477.10424

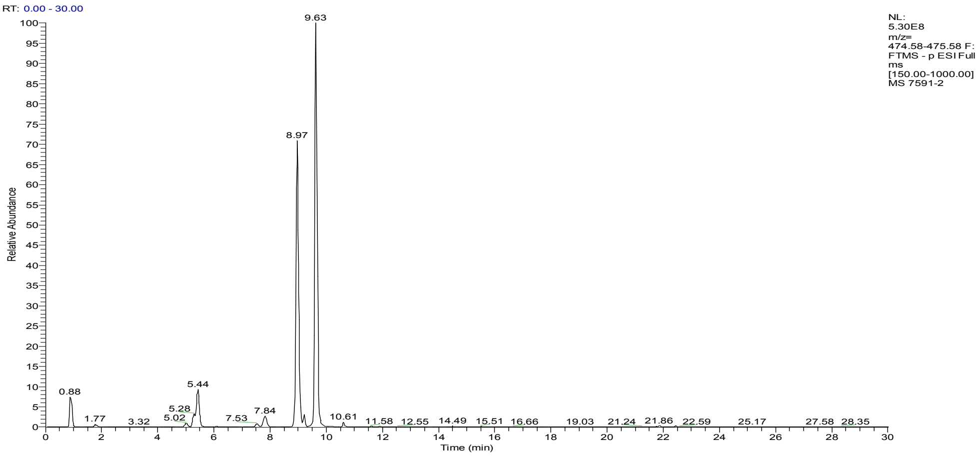
MS[2](−):

301.07242(70),286.04889(100),181.01442(21),165.99094(13)





S26, S27, S36, and S37



S26 Isomer of 37 (trihydroxy-methoxyflavone *O*-glucuronide) (t_R=5.27 min)

MS[1](−):

475.08834

MS[2](−):

299.05655(58),284.03311(100)

S27 Isomer of 37 (trihydroxy-methoxyflavone *O*-glucuronide) (t_R=9.47 min)

MS[1](−):

475.08809

MS[2](−):

299.05637(50),284.03305(100),270.04959(5)

S36 Isomer of 37 (trihydroxy-methoxyflavone *O*-glucuronide) (t_R=7.59 min)

MS[1](−):

475.08836

MS[2](−):

299.05658(100),284.03305(59),270.10849(0.5)

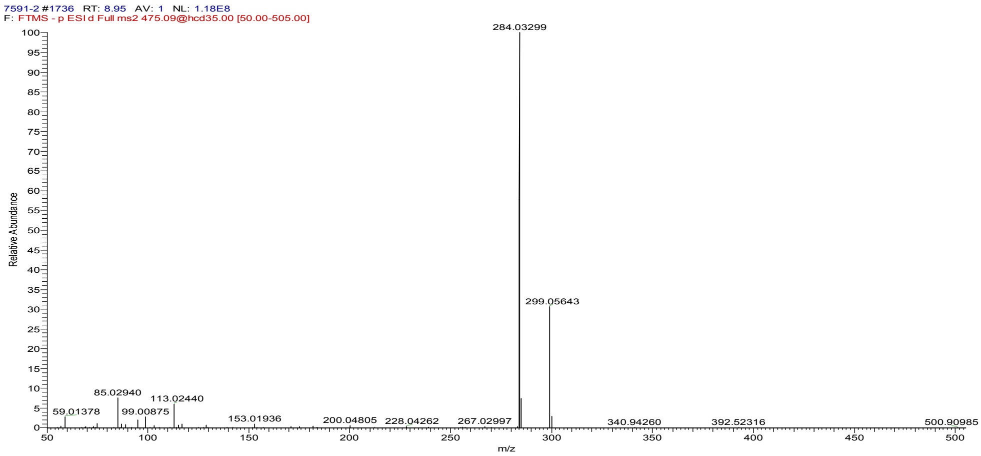
S37 5,7,2'-Trihydroxy-6-methoxyflavone 7-*O*-glucuronide (t_R=8.84 min)[61]

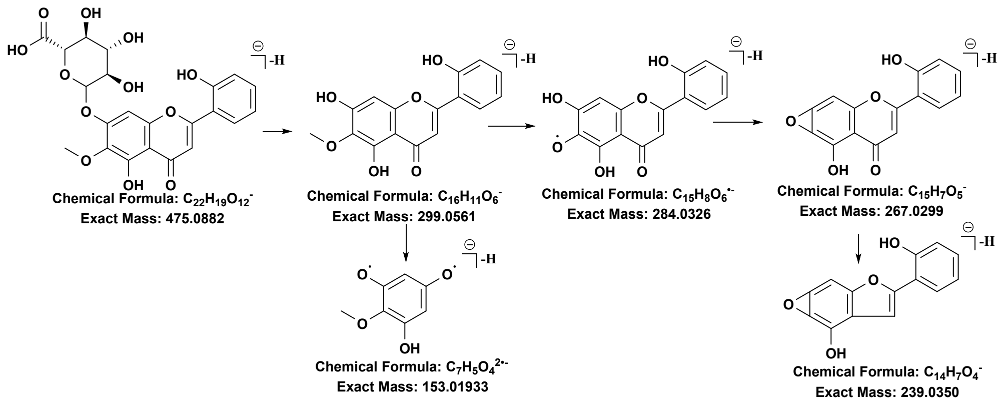
MS[1](−):

475.08832

MS[2](−):

299.05643(30),284.03299(100),267.02997(0.3),239.03540(0.2),228.04262(0.4),200.04805(1),153.01936(1),129.01955(1),113.02440(6),85.02940(7)





S28

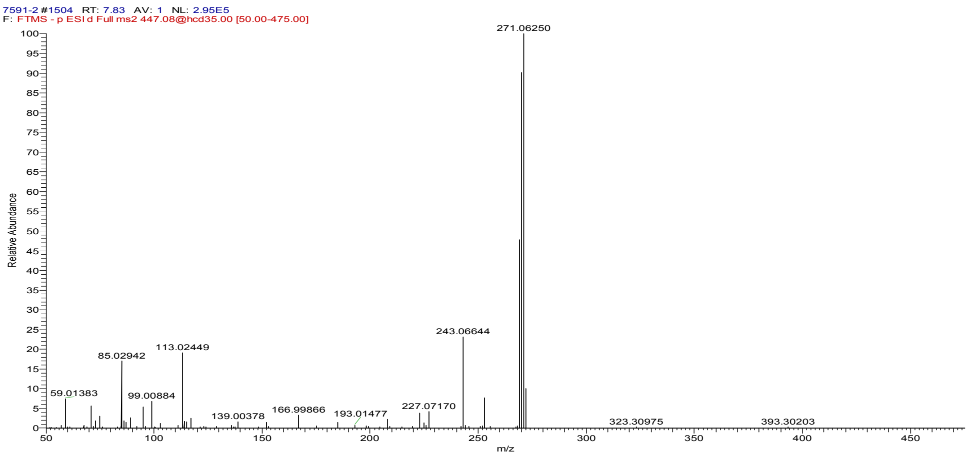
Dihydrobaicalin (tR 7.98)[61, 62]

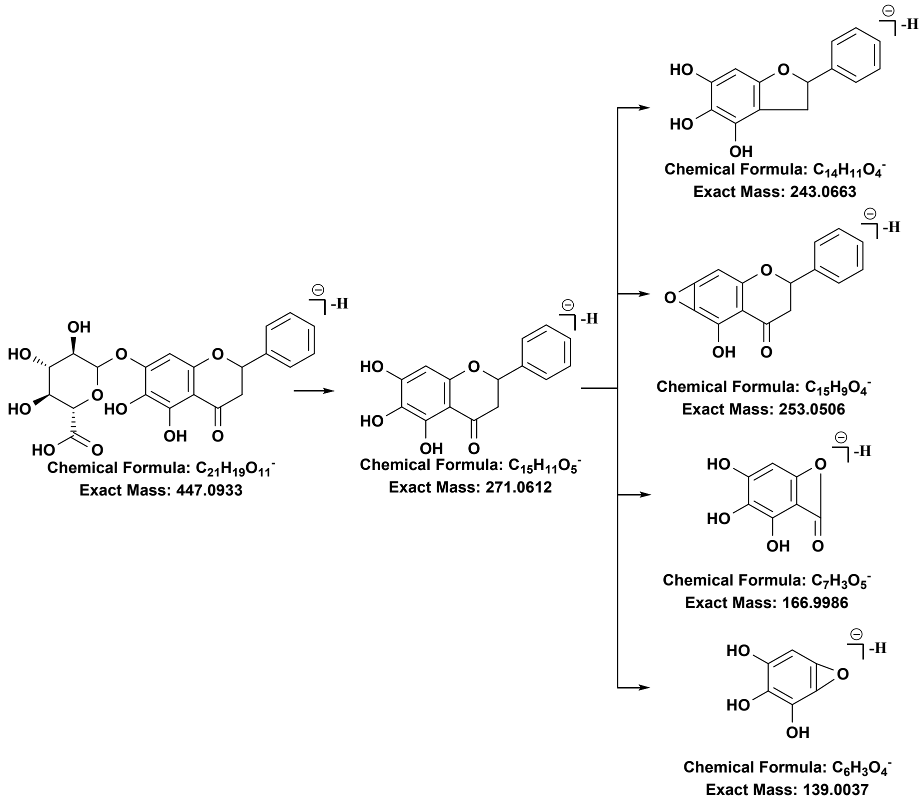
MS^1(−):

447.07795

MS^2(−):

271.06250(100),253.05099(8),243.06644(25)





S30

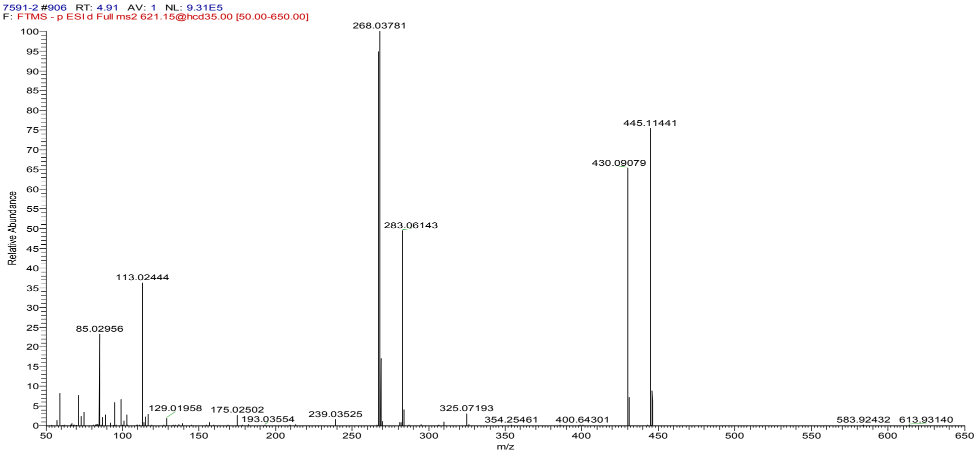
Dihydroxy-methoxyflavone *O*-glucuronide-(1→6)-*O*-glucoside (t_R=4.91 min)

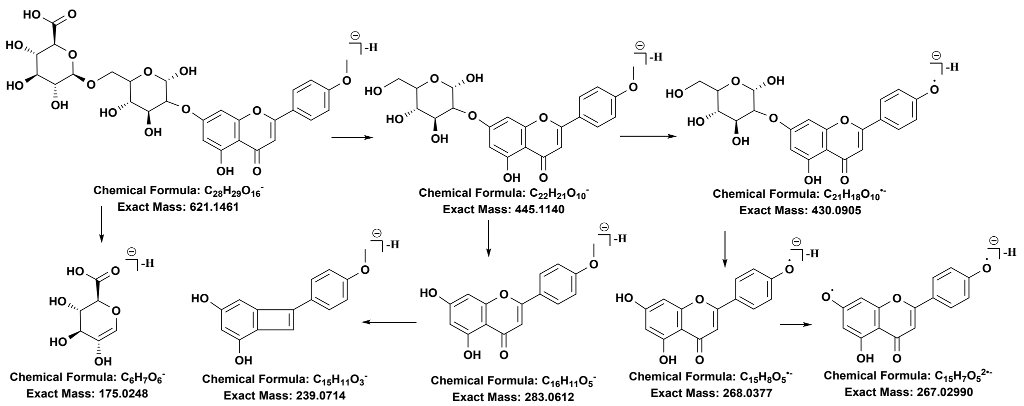
MS[1](−):

621.14659

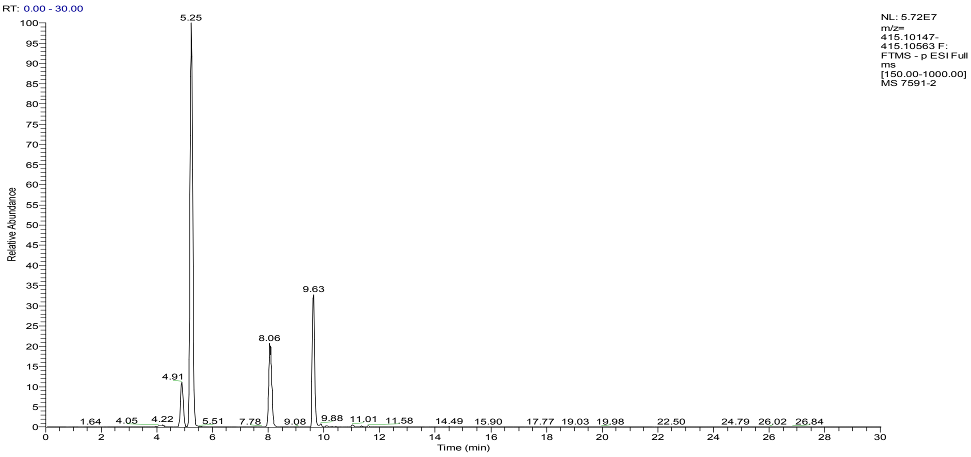
MS[2](−):

445.11441(70),430.09079(59),283.06143(49),268.03781(100),267.03018(93),239.03525(2),175.02502(3),117.02(3),113.02444(25),103.00378(3),99.00882(7),95.01390(7),85.02956(21)





S31, S44, S48, and S101



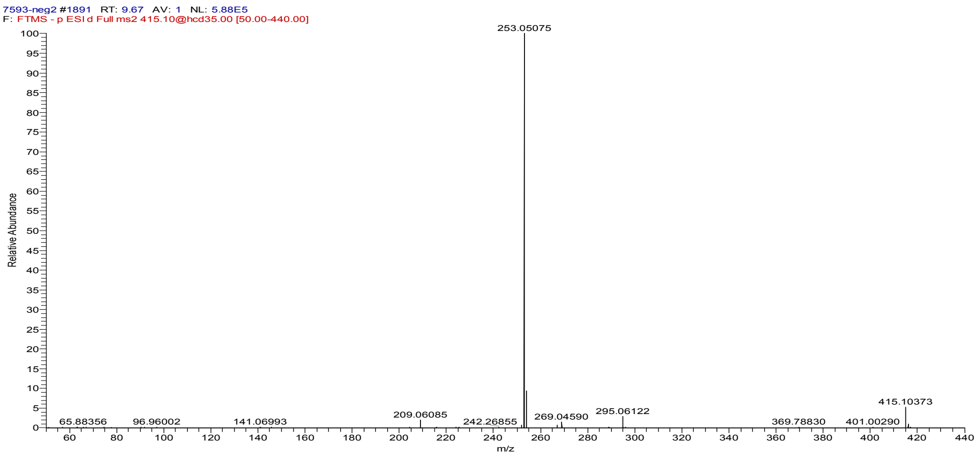
S31 Chrysin 7-*O*-glucoside OR isomer (Trihydroxyflavone *O*- glucoside) (t_R=9.61 min)[69, 70]

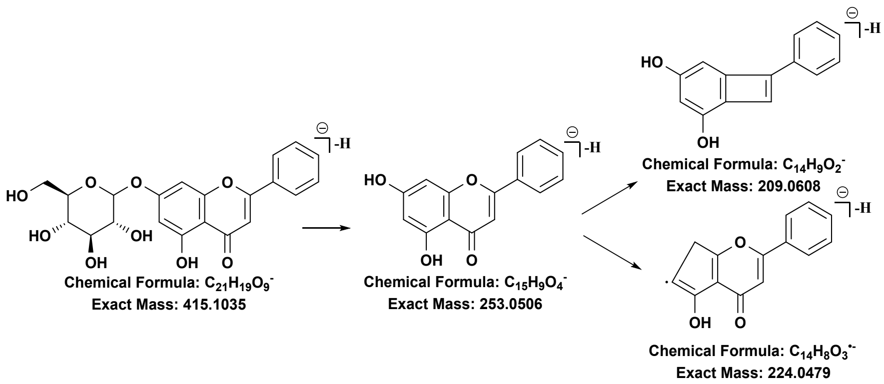
MS[1](−):

415.10355

MS[2](−):

295.06122(3),269.04590(2),253.05075(100),224.04839(0.2),209.06085(2)

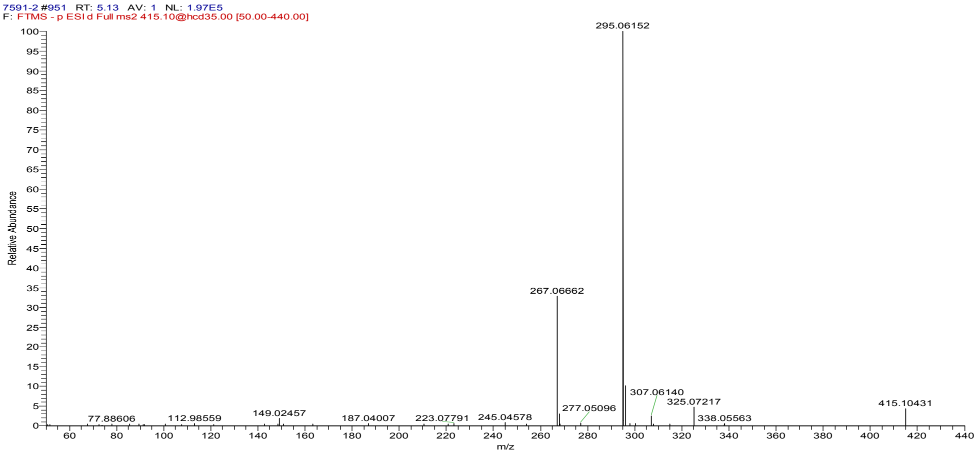




S44 Isomer of S48 (Dihydroxyflavone *C*-glucoside) (t_R=5.12 min)

MS[1](−):415.10373

MS[2](−):325.07175(4),307.06094(2),295.06113(100),277.05060(1),267.06644(32),253.05106(0.5),227.07188(0.5),179.03456(0.6),149.02438(2)



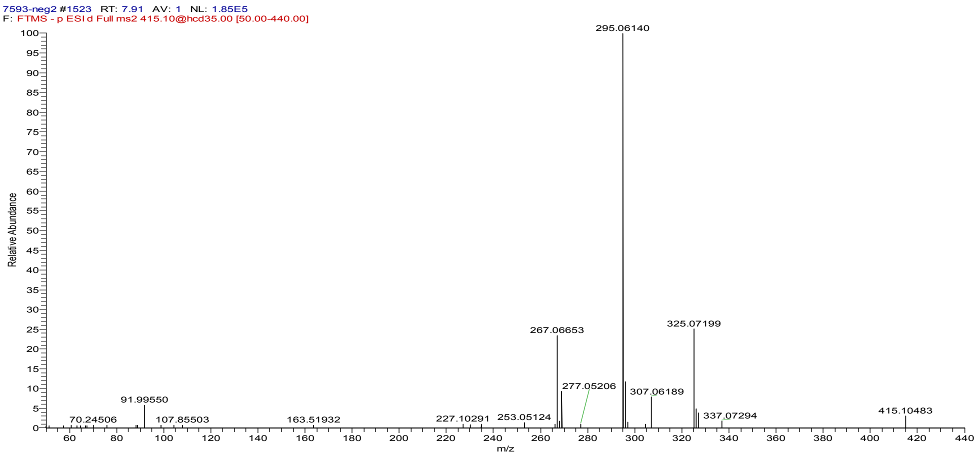
S48 Chrysin 6-*C*-glucoside (t_R=8.03 min)[61]

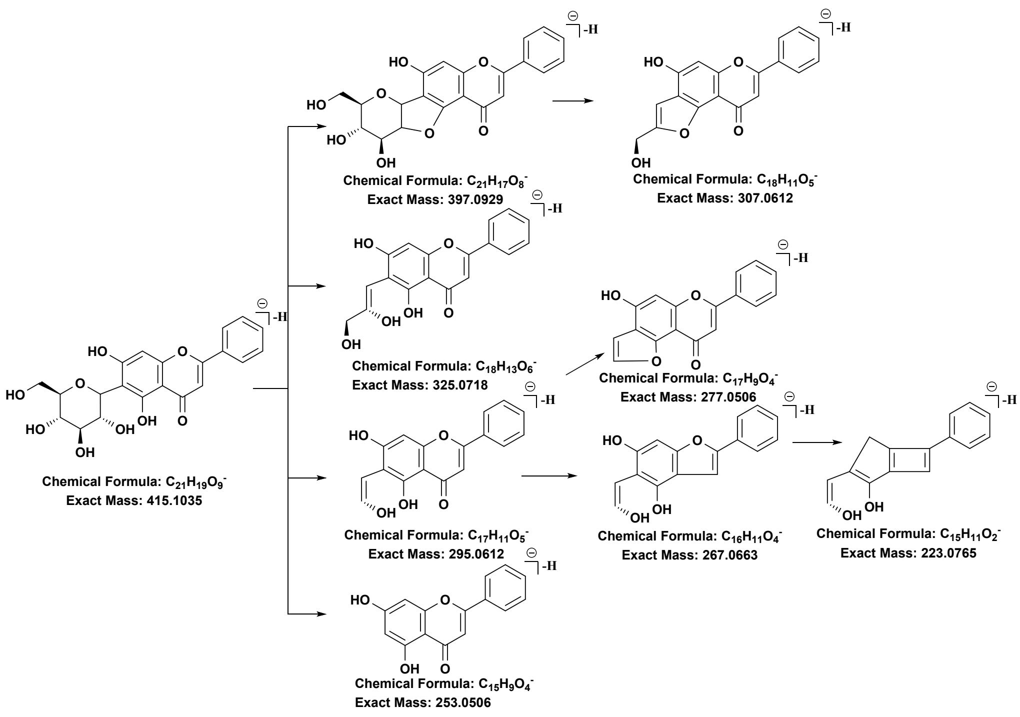
MS[1](+):

415.10413 (positive)

MS[2](+):

325.07217(33),295.06152(100),267.06662(25),253.05095(3),223.07791(0.5),151.05568(0.1)





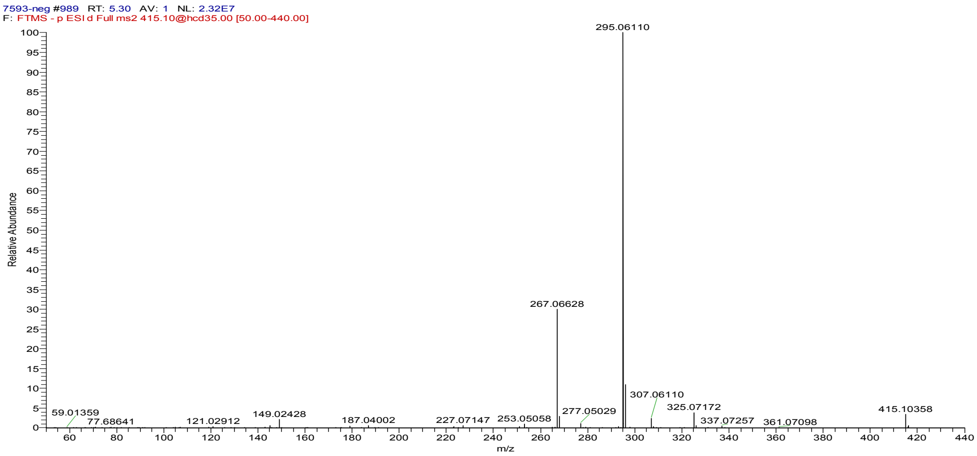
S101 Chrysin 8-*C*-glucoside (t_R=5.22 min)[61]

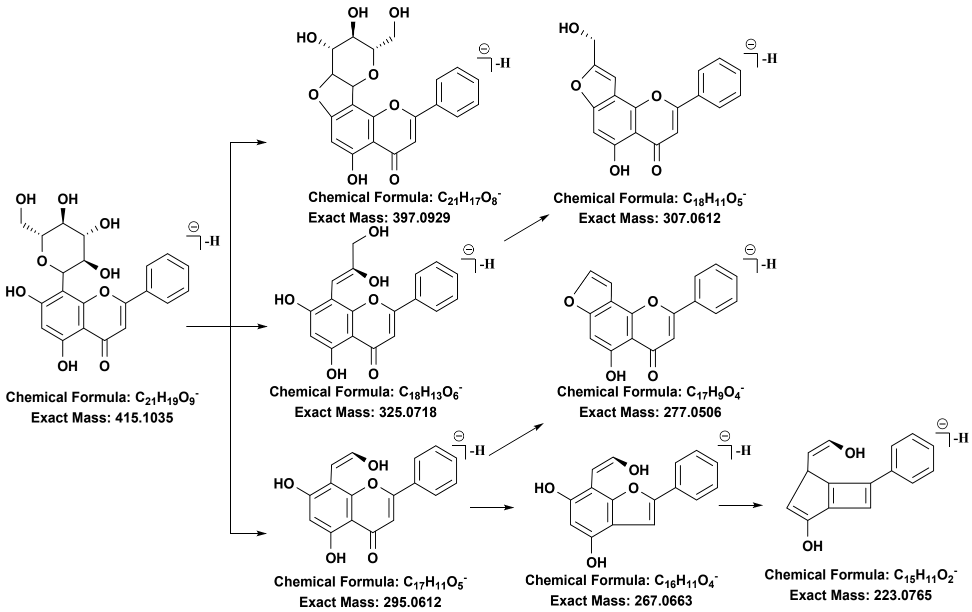
MS[1](+):

415.10431

MS[2](+):

325.07217(5),295.06152(100),267.06662(31),245.04578(1),223.07791(0.5),187.07007(0.5),149.02457(2)





S32

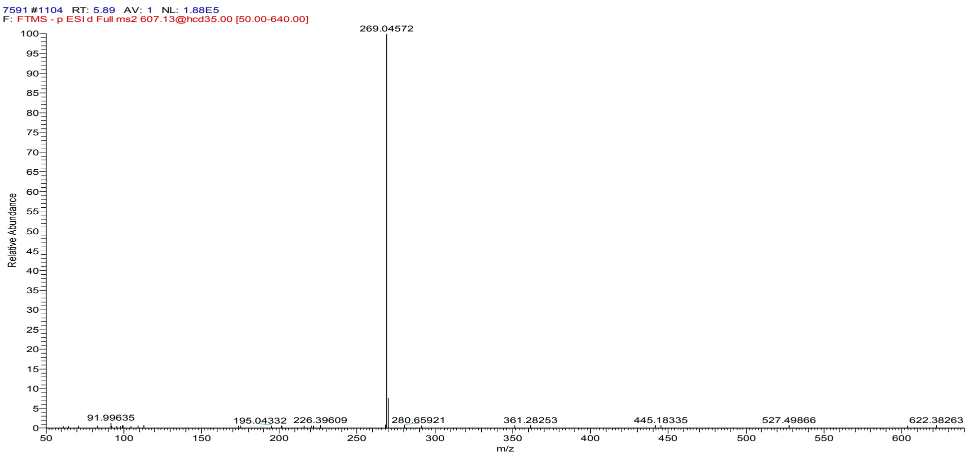
Trihydroxyflavone *O*-glucuronide-(1→2)-*O*-glucoside (t_R=6.02 min)[66]

MS^1(−):

607.13129

MS^2(−):

445.18335(1),269.04572(100),113.02447(1)



S33

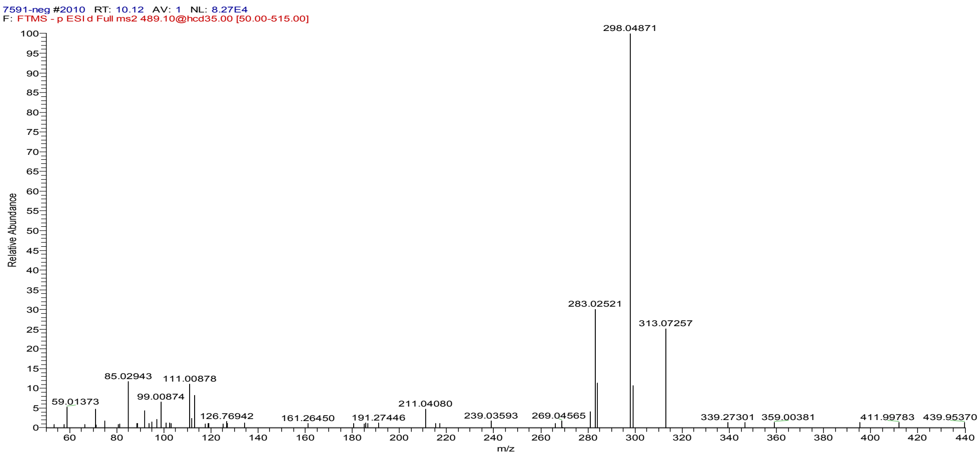
5,7-Dihydroxy-8,2'-dimethoxyflavone 7-*O*-glucuronide (t_R=10.27 min)[61, 62]

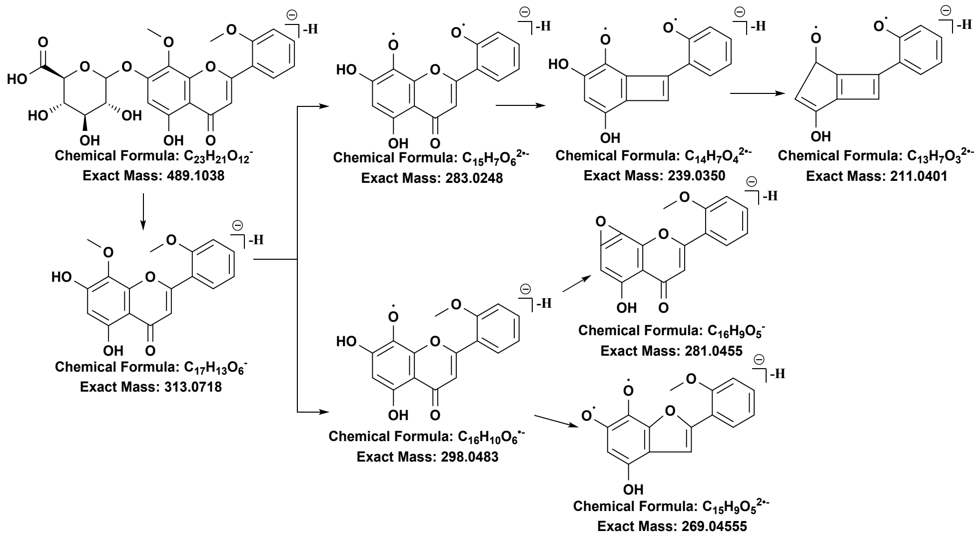
MS[1](−):

489.10400

MS[2](−):

313.07257(24),298.04871(100),283.02521(29),281.04529(4),269.04565(2),239.03593(2),211.04042(5)





S34

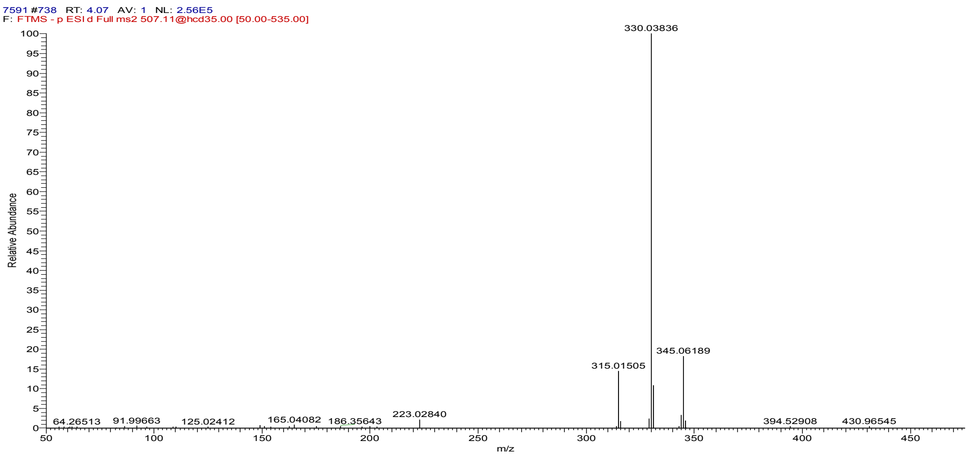
Viscidulin III 6'-*O*-glucoside (t_R=4.13 min)[61]

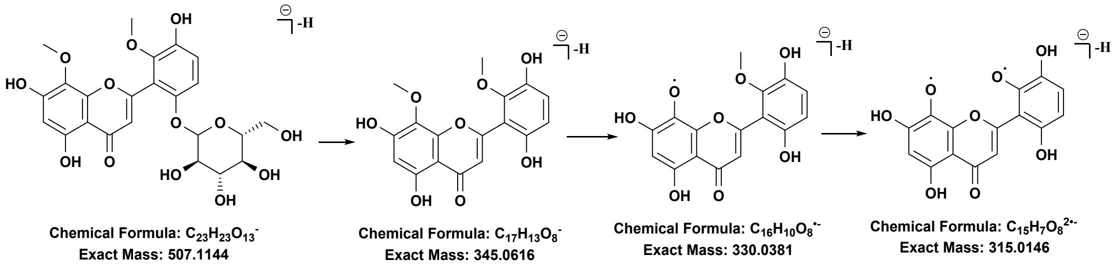
$MS^1(-)$:

507.11461

$MS^2(-)$:

492.09247(1),345.06189(15),330.03836(100),315.01505(14)



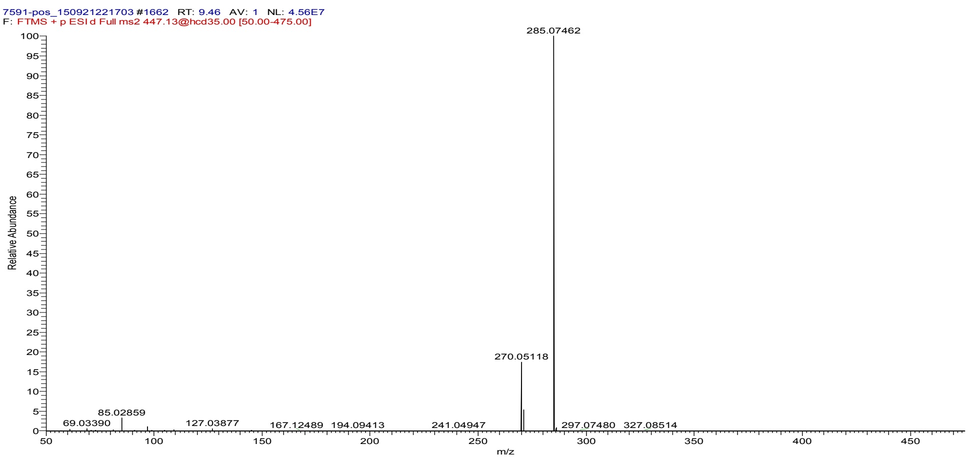


S35

Wogonin 5-glucoside (t_R=9.35 min)[61]

$MS^1(+)$:447.12802

$MS^2(+)$:285.07462(100),270.05118(17),241.04947(0.1)



S38

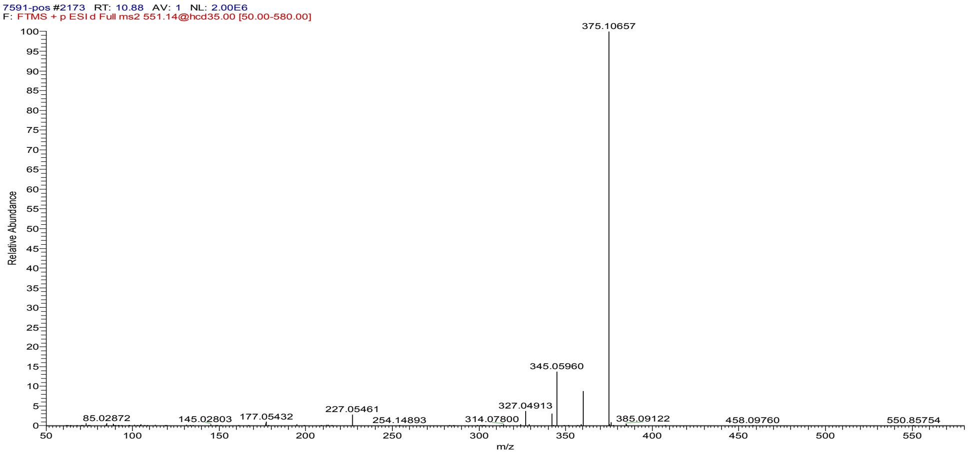
Dihydroxy-tetramethoxyflavone *O*-glucuronide (t_R=10.95 min)

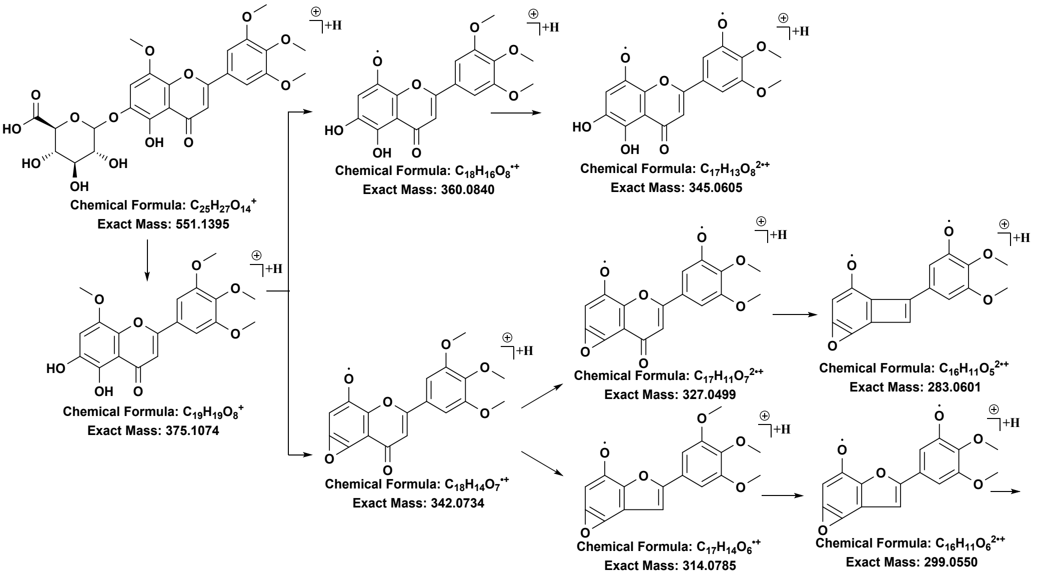
MS[1](+):

551.13891

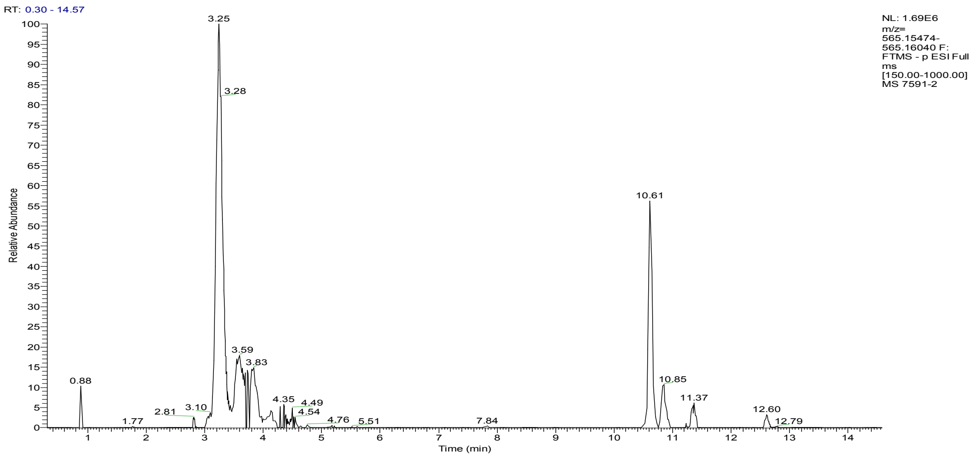
MS[2](+):

375.10657(100),360.08340(9),345.05960(13),342.07269(3),329.06488(0.3),327.04913(4),227.05461(3),177.05432(1)





S41, S42, and S43



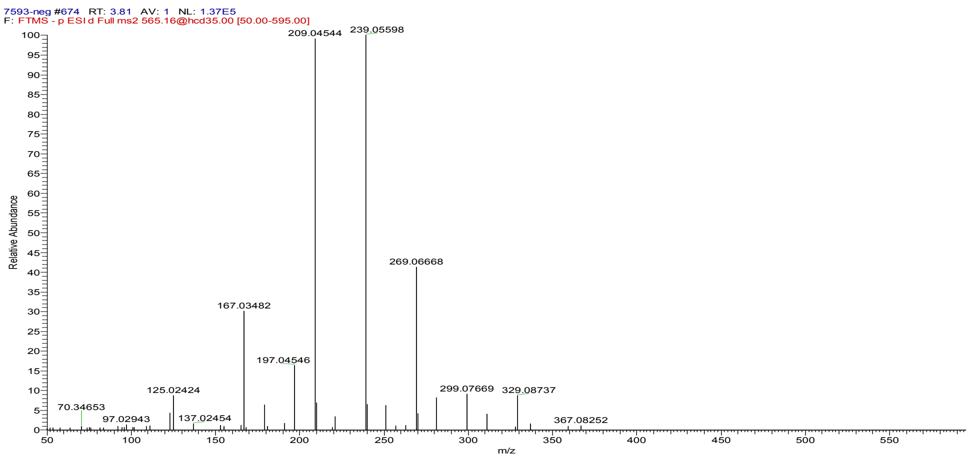
S41 Isomer of Pinobanksin 8-*C*-arabinoside 6-*C*-glucoside (Containing *C*-glycosides) (t_R=3.87 min)

MS[1](−):

565.15757

MS[2](−):

367.08337(1),337.07230(2),329.08737(8),299.07730(9),269.6674(40),239.05615(97),209.04556(100)



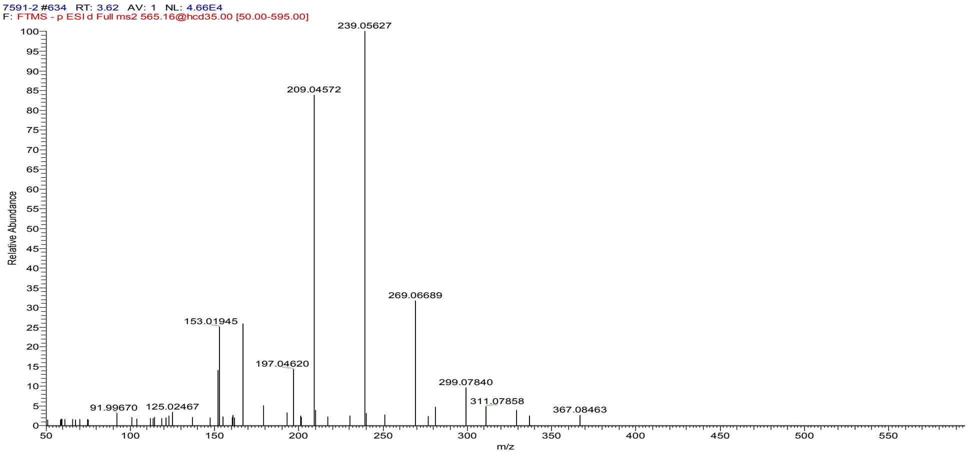
S42 Isomer of Pinobanksin 8-*C*-arabinoside 6-*C*-glucoside (containing *C*-glycosides) (t_R=3.57 min)

MS[1](−):

565.15700

MS[2](−):

329.08783(4),299.07840(10),269.06689(41),239.05627(100),209.04572(95)



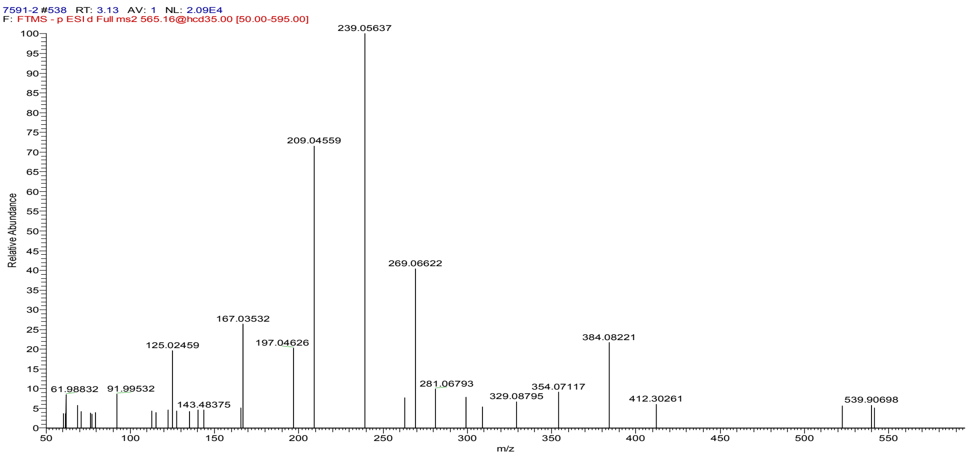
S43 Isomer of Pinobanksin 8-*C*-arabinoside 6-*C*-glucoside (Containing *C*-glycosides) (t_R=3.24 min)

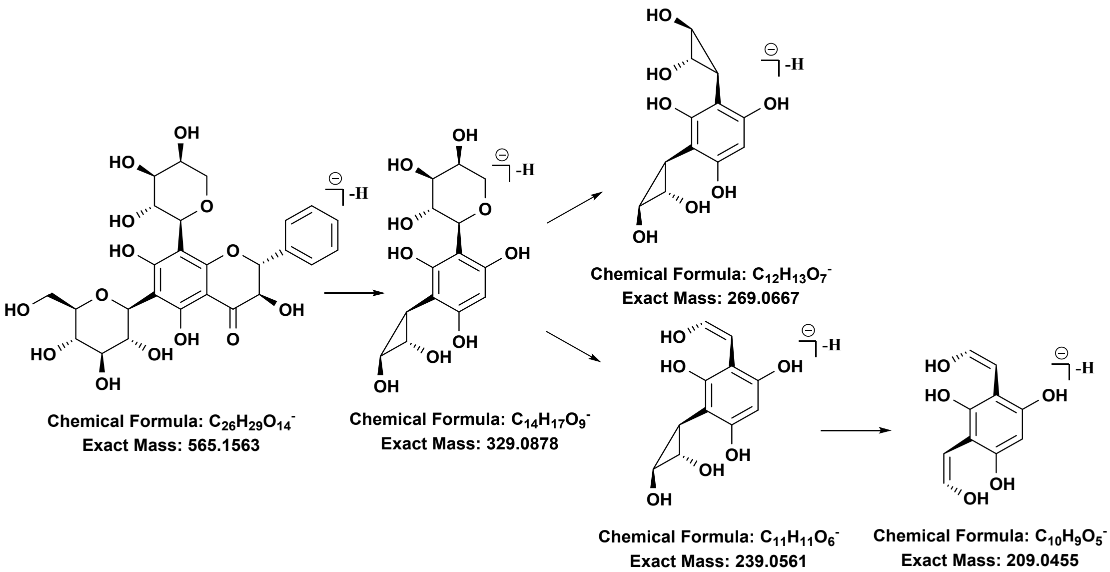
$MS^1(-)$:

565.15653

$MS^2(-)$:

329.08795(7),299.07770(10),269.06622(43),239.05637(100),209.04559(89)





S45

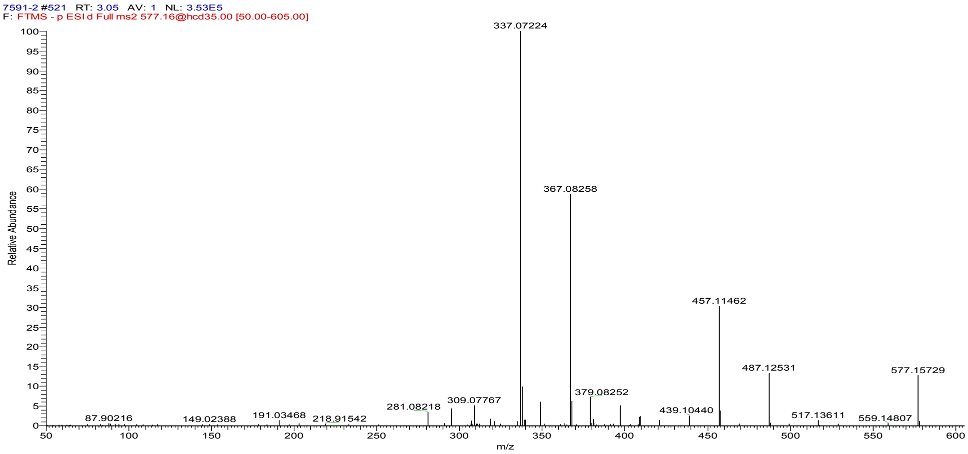
Chrysin 6,8-di-*C*-glucopyranoside (t_R=3.13 min)[71]

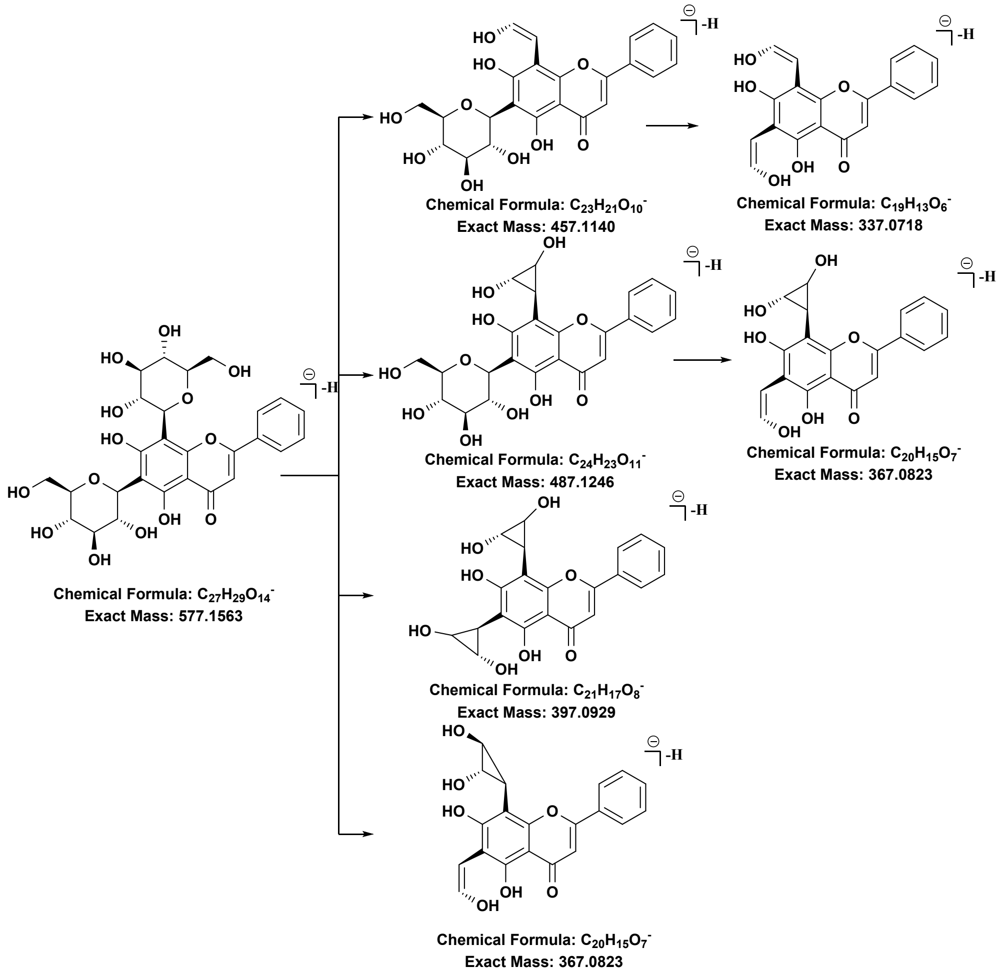
MS^1(−):

577.15683

MS^2(−):

577.15729(14),487.12531(11),457.11462(32),439.10440(3),397.09293(6),367.08258(58),337.07224(100)



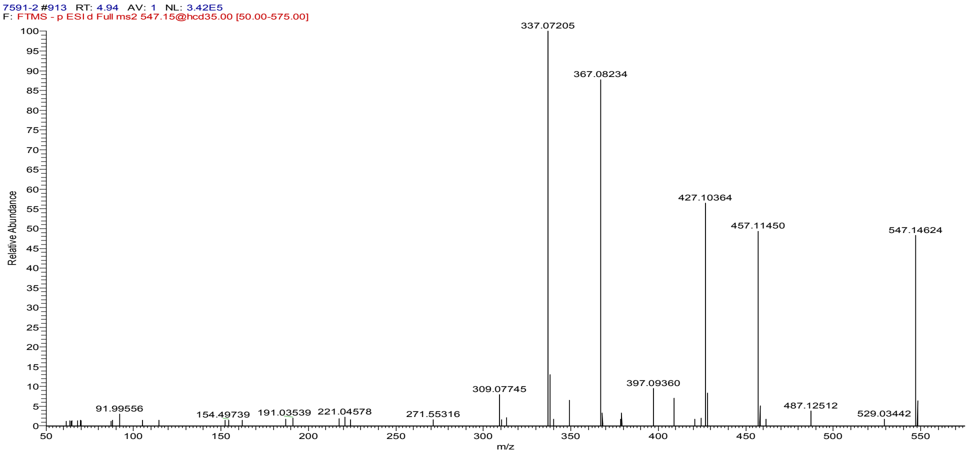


S47

6-hexosyl-8-*C*-pentosyl chrysin (t_R=5.10 min)[61]

MS[1](−):547.1462

MS[2](−):547.14624(16),487.12512(17),457.11450(23),427.10364(40),397.09360(31),367.08234(100),337.07205(70),309.07745(6)

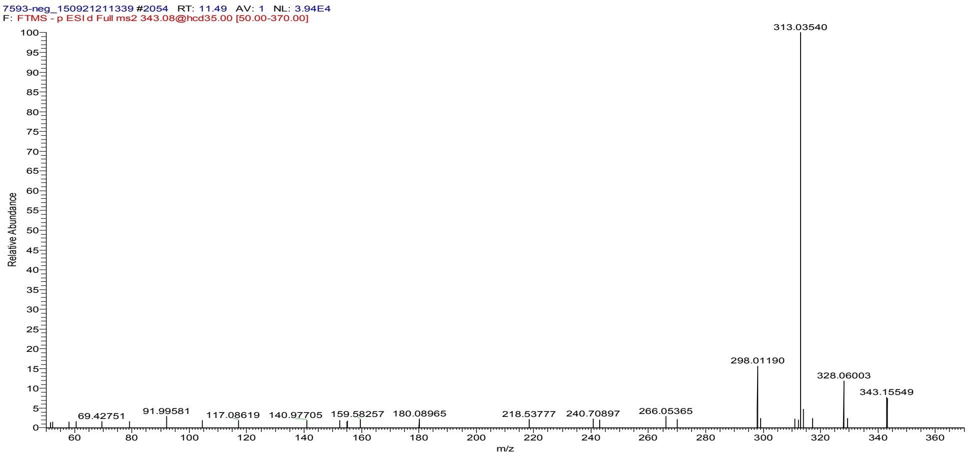


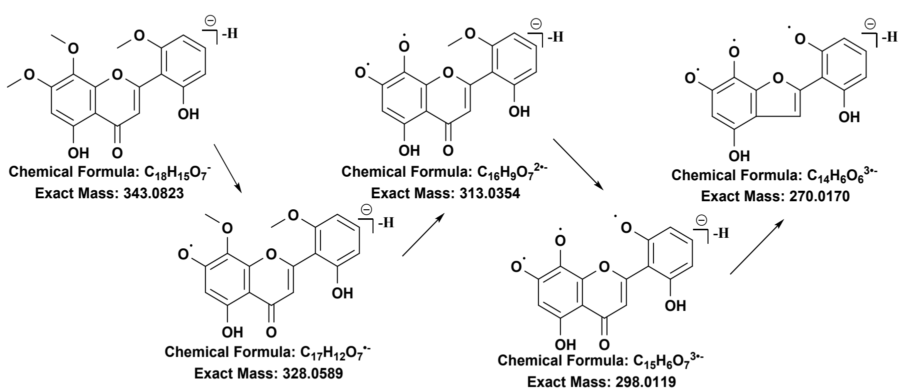
S49

Skullcapflavone (t_R=14.60 min)[61]

MS[1](−):343.08222

MS[2](−):328.06003(12),313.03540(100),298.01190(16),270.01706(2)

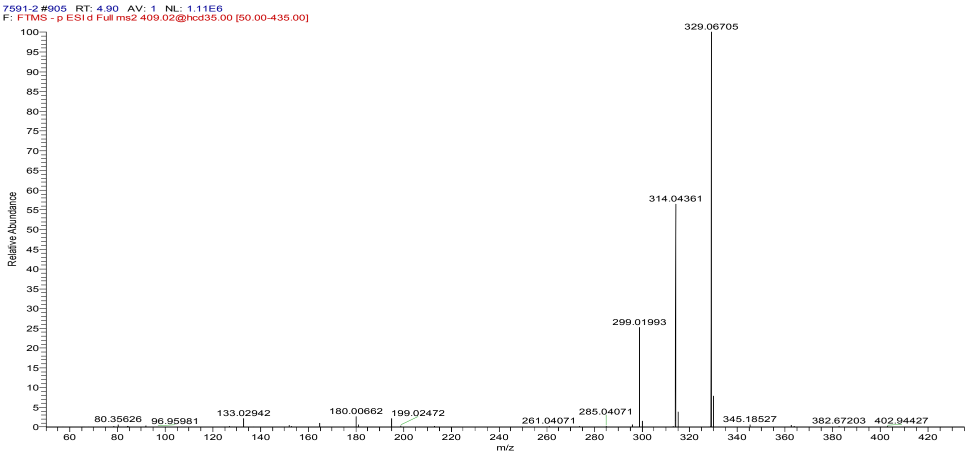


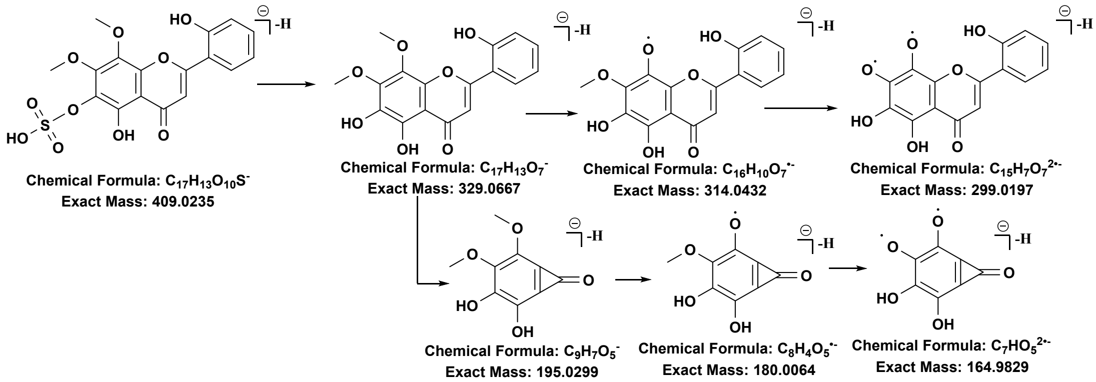


2',5,6-Trihydroxy-7,8-dimethoxyflavone 6-*O*-sulfate (t_R=4.91 min)[70]

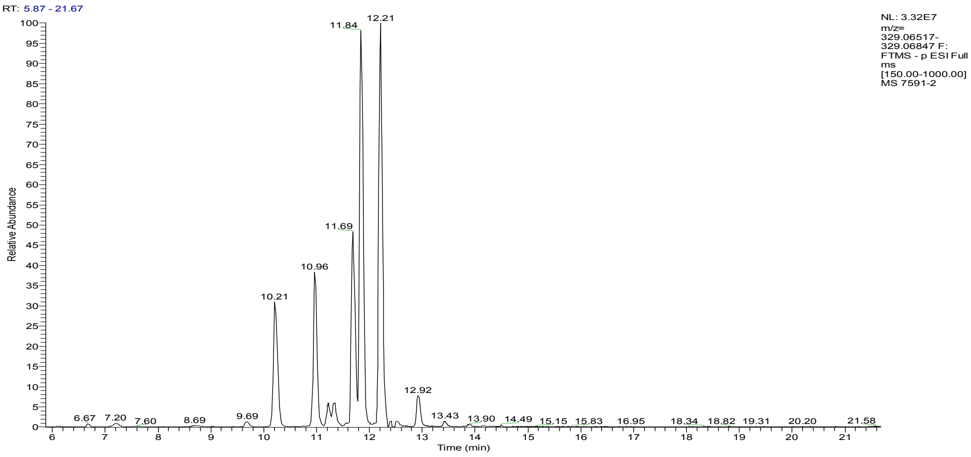
MS[1](−):409.0237

MS[2](−):329.06705(100),314.04361(62),299.01993(27),195.03003(2),180.00662(3),164.98241(1), 133.02942(2)





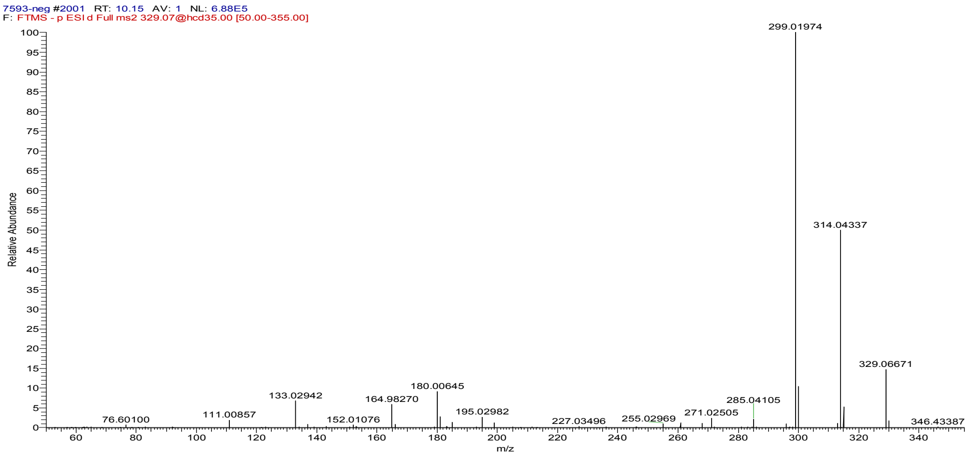
S51, S53, S54, and S82



S51 Isomer of S54 (Trihydroxy-dimethoxyflavone) (t_R=10.23 min)

MS[1](−):329.06682

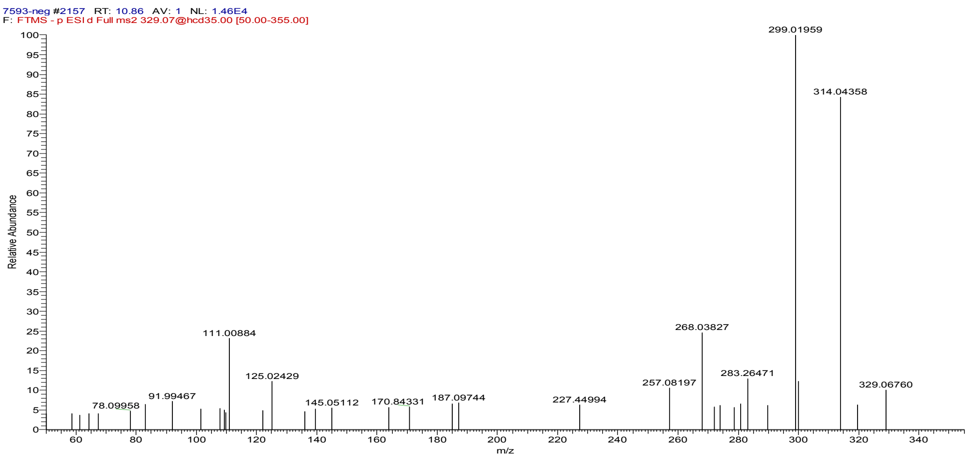
MS[2](−):314.04337(49),299.01974(100),285.04105(2),271.02505(2),255.02969(0.9),227.03496(0.3),180.00645(9),164.98270(6),133.02942(7)



S82 Isomer of S54 (Trihydroxy-dimethoxyflavone) (t_R=10.87 min)

MS[1](−):329.06778

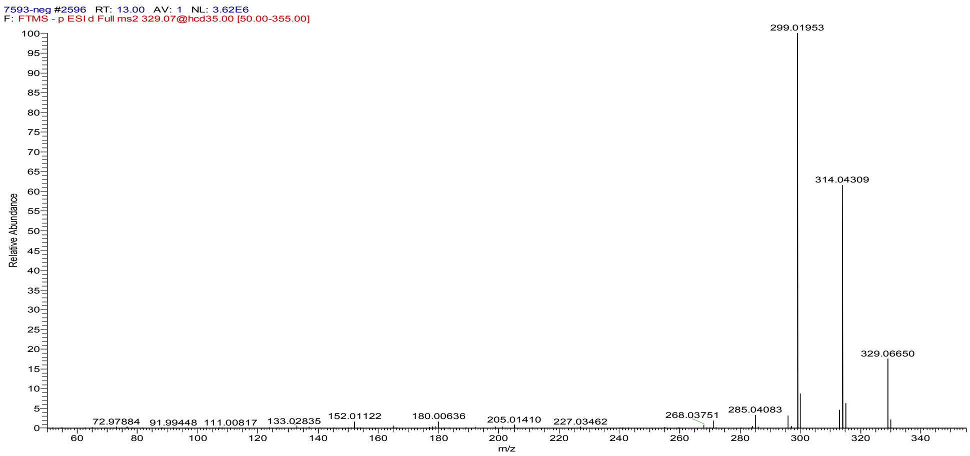
MS[2](−):314.04358(62),299.01959(81)283.26471(26),268.03827(25)

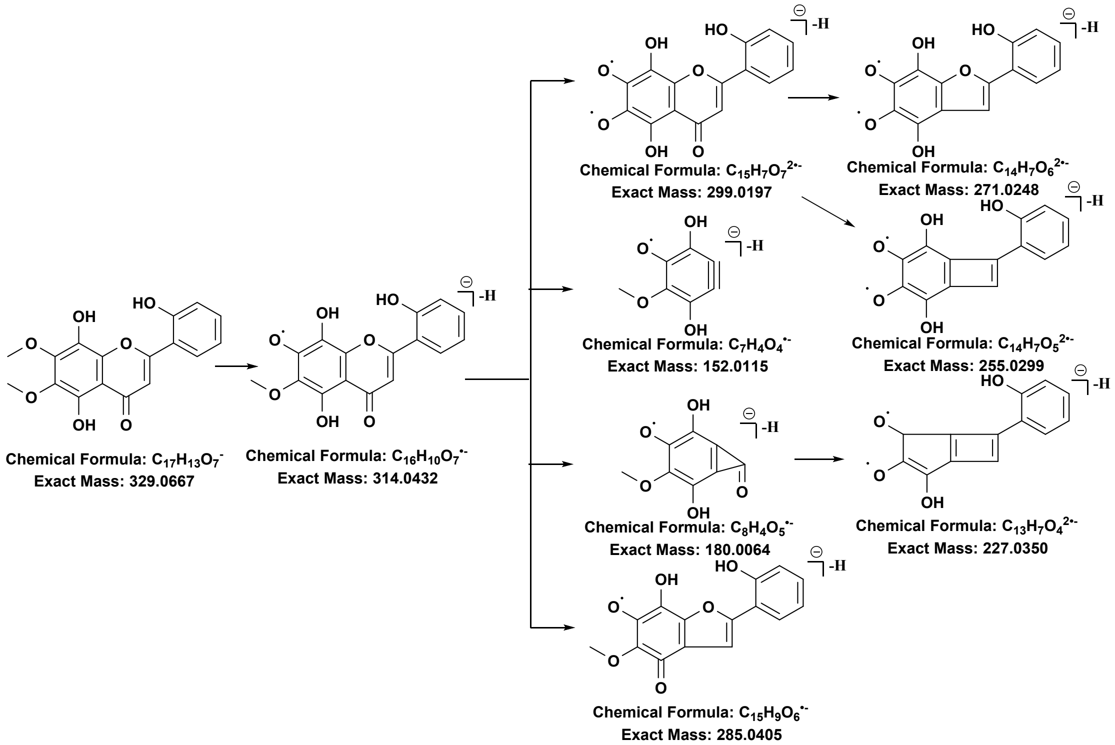


S53 5,8,2'-Trihydroxy-6,7-dimethoxyflavone (t_R=12.95 min)[61]

MS^1(−):329.06680

MS^2(−):314.04309(61),299.01953(100),285.04083(3),271.02472(2),255.02936(0.3),227.0.462(0.3), 205.01410(0.8),180.00636(2),152.01122(2),133.02835(0.5)





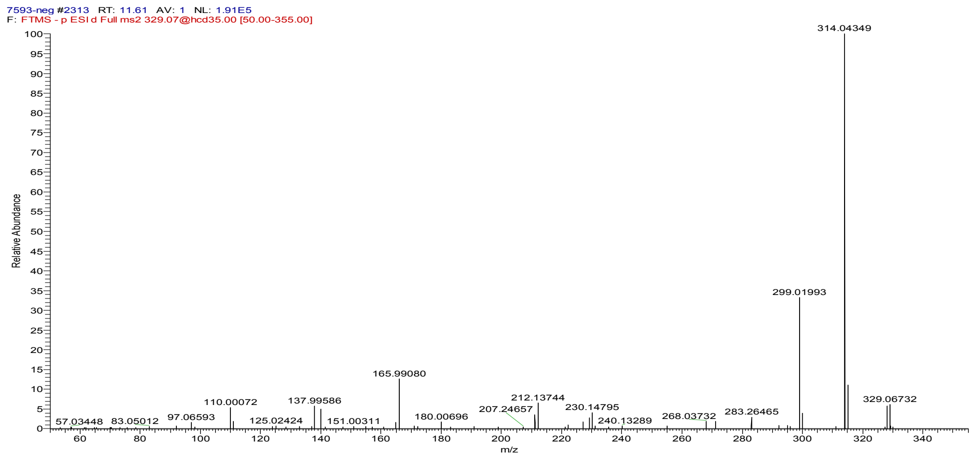
S54 5,7,6'-Trihydroxy-8,2'-dimethxoyflavone (t_R=11.74 min)[61]

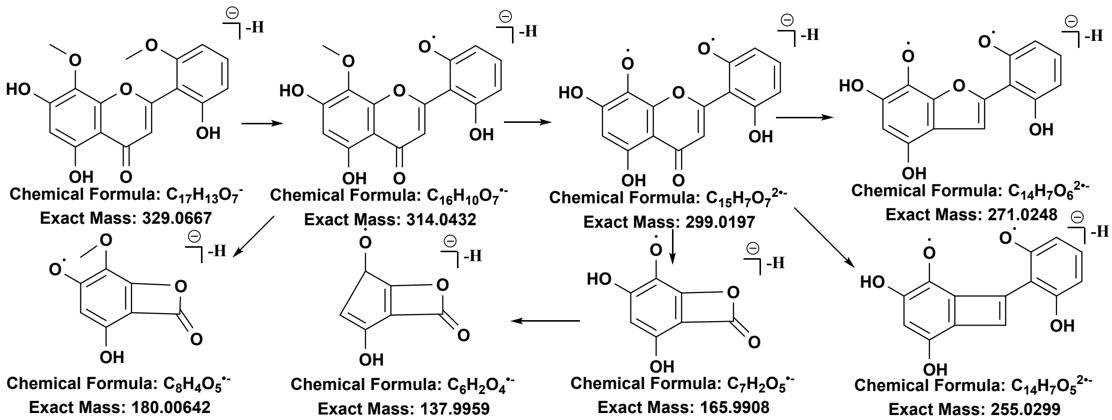
MS^1(−):

329.06679

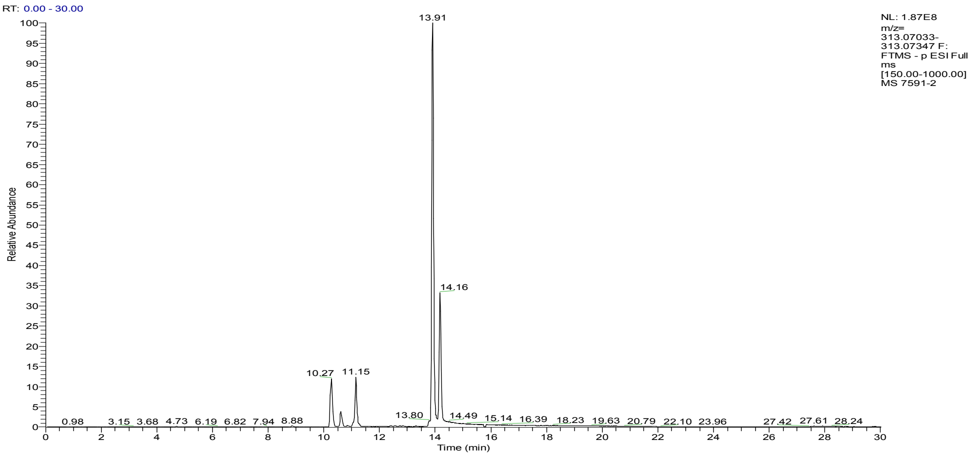
MS^2(−):

314.04349(100),299.01993(80),255.02878(0.7),180.00696(2),165.99080(12),137.99586(6)





S52, S55, S61, S63, and S69



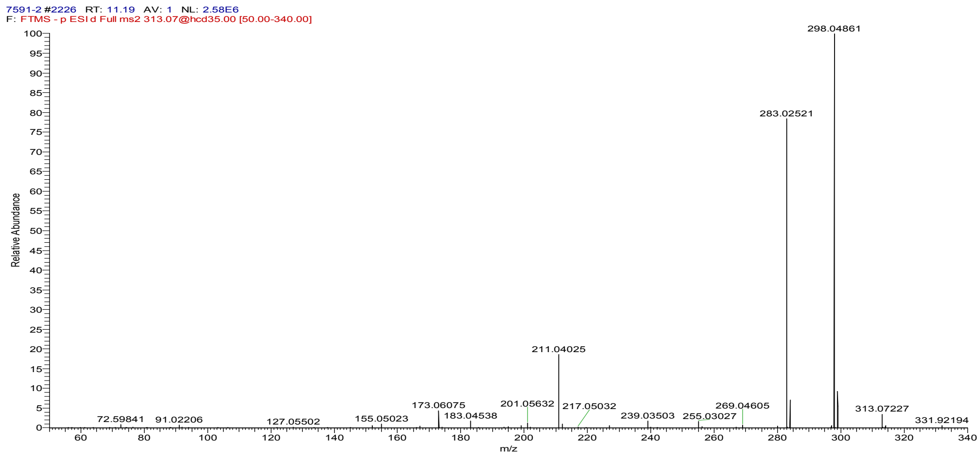
S52 Isomer of S63 (Dihydroxy-dimethoxyflavone) (t_R=11.16 min)

MS[1](−):

313.07190

MS[2](−):

298.04861(100),283.02521(85),255.03027(2),239.03503(2),211.04025(19),173.06067(5)



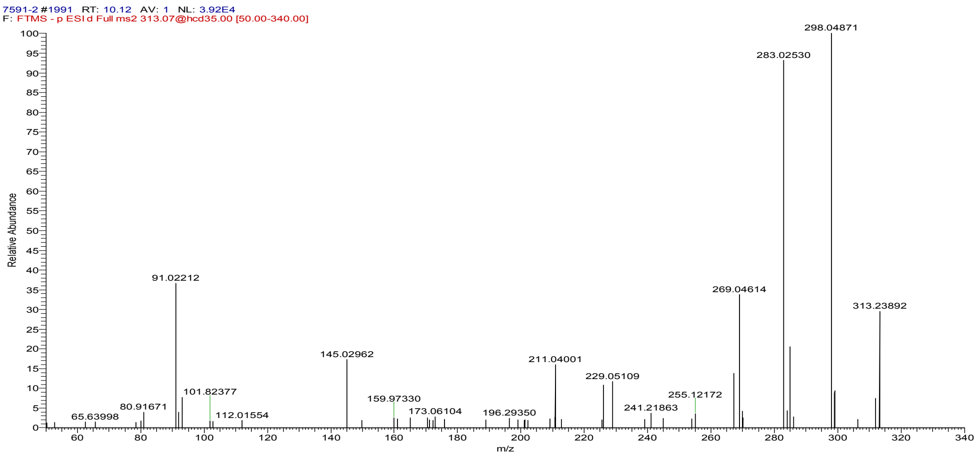
S55 Isomer of 6-Methoxywogonin (Dihydroxy-dimethoxyflavone) (t_R=10.27 min)

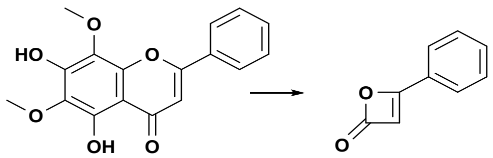
MS[1](−):

313.07188

MS[2](−):

298.04871(100),283.02530(87),269.04614(78),255.12172(4),211.04001(18),167.04(5),145.02962 (15),91.02(28)





Chemical Formula: $C_{17}H_{13}O_6^-$ Exact Mass: 313.0718

Chemical Formula: $C_9H_5O_2^-$ Exact Mass: 145.0295

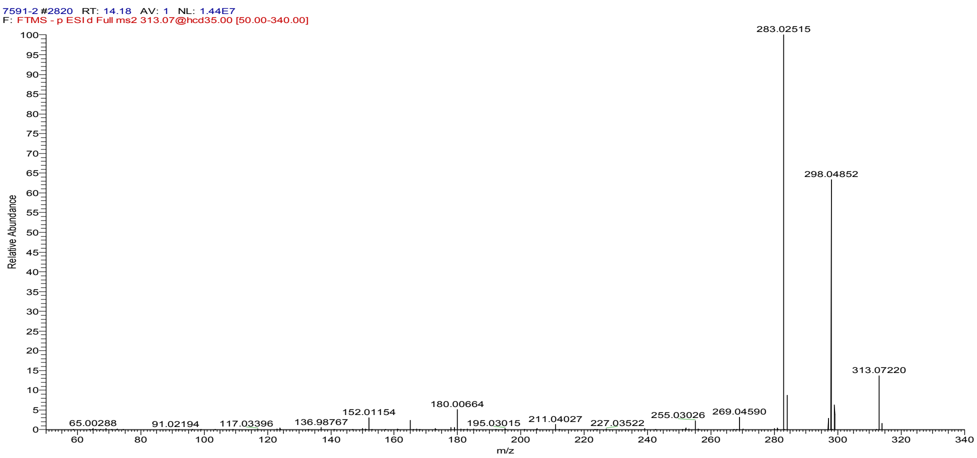
S61 5,8-Dihydroxy-6,7-dimethoxyflavone (t_R=14.19)[61, 62]

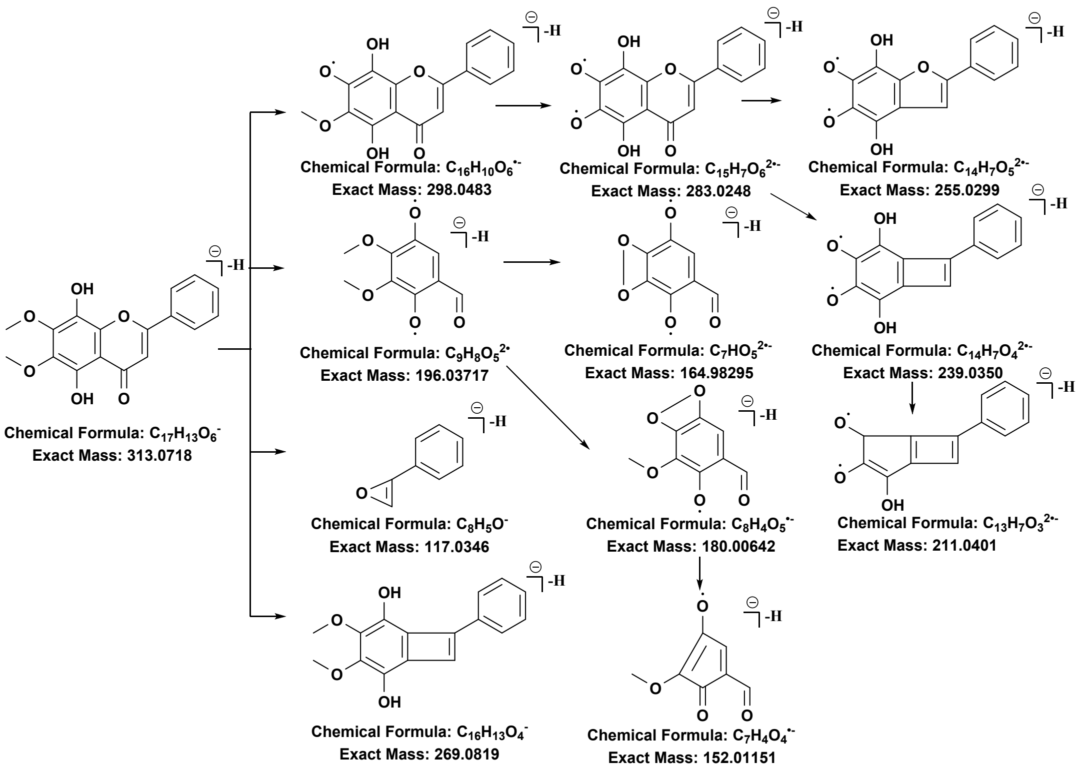
MS^1(−):

313.07224

MS^2(−):

298.04852(100),283.02515(87),269.04590(21),255.03026(2),239.03487(0.3),211.04027(18),195.03015(0.3),180.00664(5),173.06090(0.3),164.98279(2),152.01154(3),117.03396(0.2)





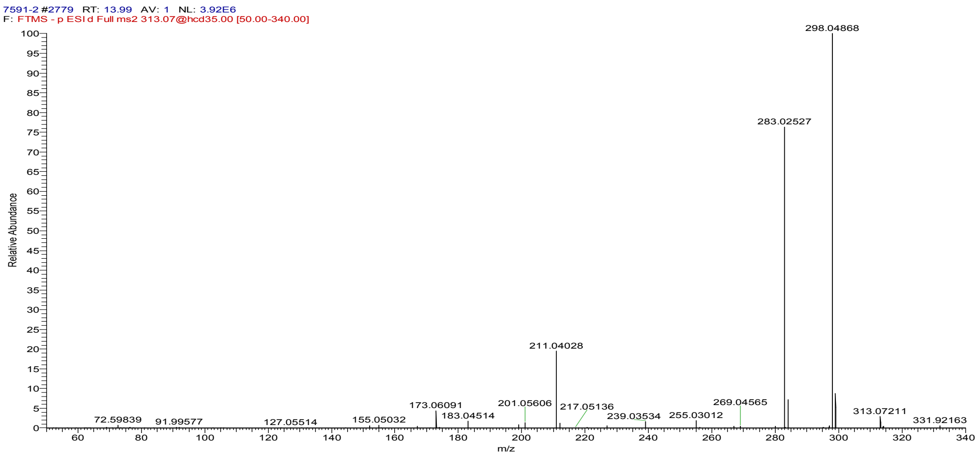
S63 Skullcapflavone I (t_R=13.90 min)[62]

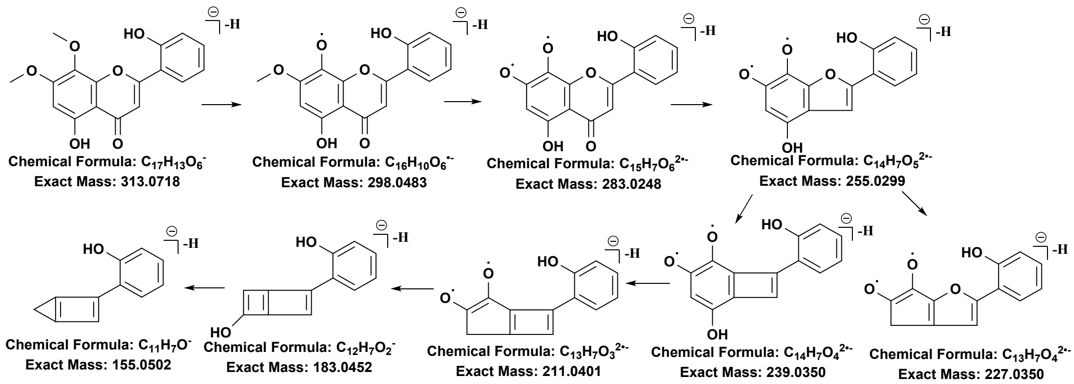
MS[1](−):

313.07211

MS[2](−):

298.04868(68),283.02527(100),255.03012(2),211.04028(2),183.04514(2),173.06091(4),164.98(2),155.05032(3)





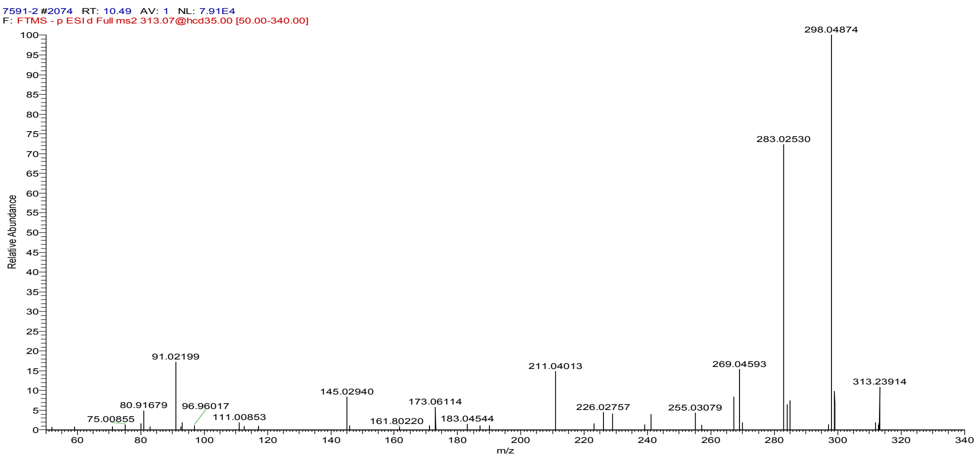
S69 Isomer of 6-Methoxywogonin (Dihydroxy-dimethoxyflavone) (t_R=10.50 min)[72]

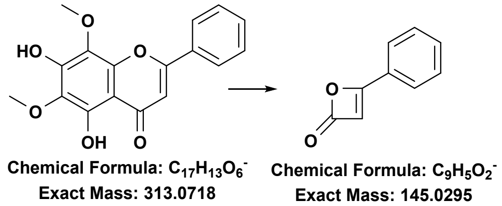
MS[1](−):

313.07190

MS[2](−):

298.04874(100),283.02530(87),269.04593(21),255.03079(4),211.04013(18),173.06114(3),145.02940(3),91.02199(8)





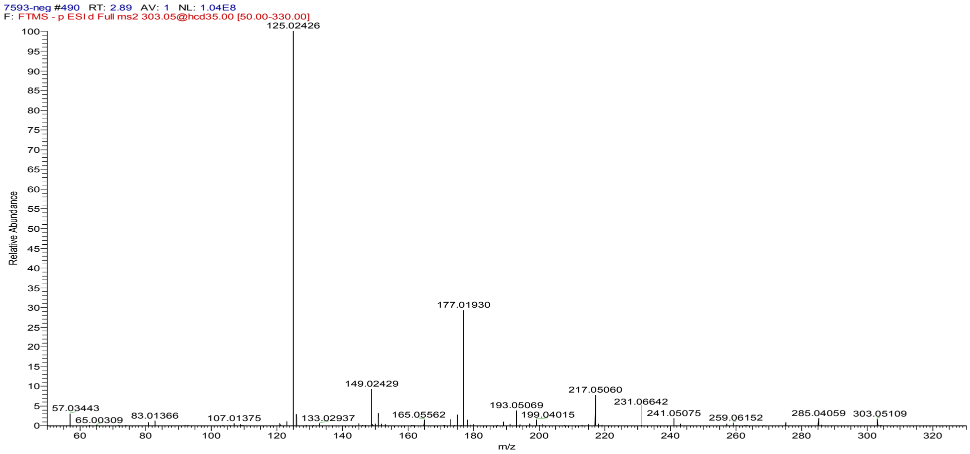
5,7,3,2',6'-Pentahydroxyflavanone (t_R=2.89 min)[61]

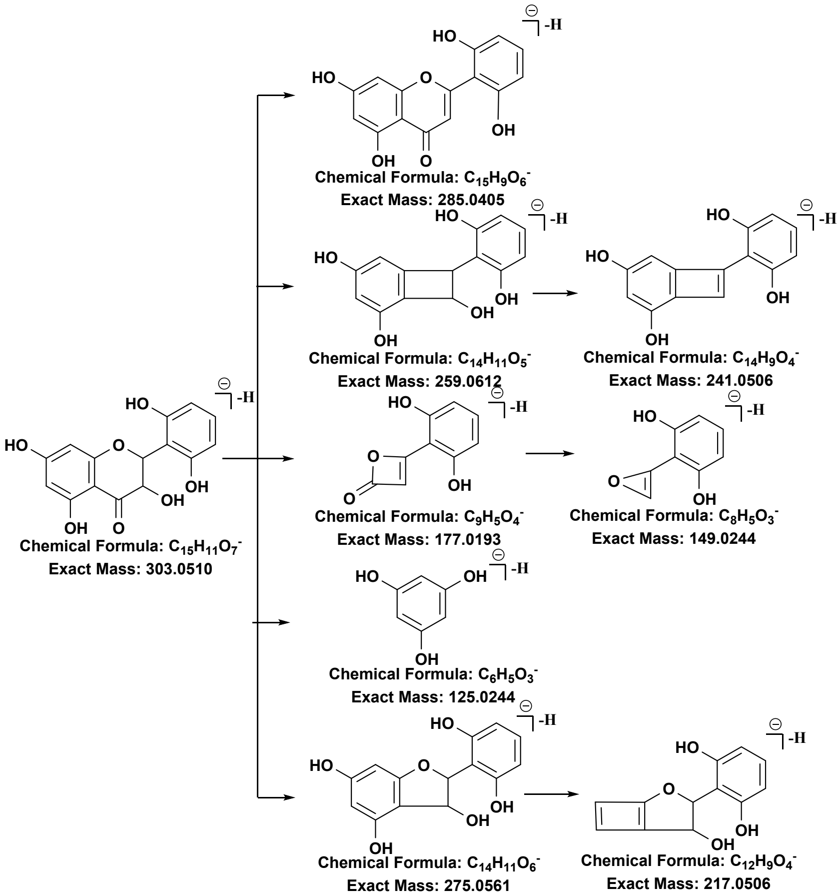
MS[1](−):

303.05117

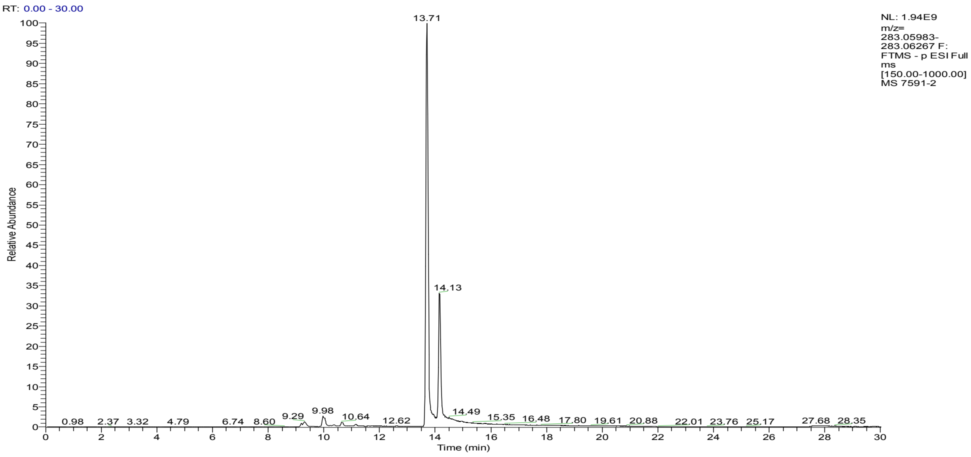
MS[2](−):

285.04059(2),241.05075(2),217.05060(9),193.05551(4),177.01930(30),149.02429(10),125.02426 (100)





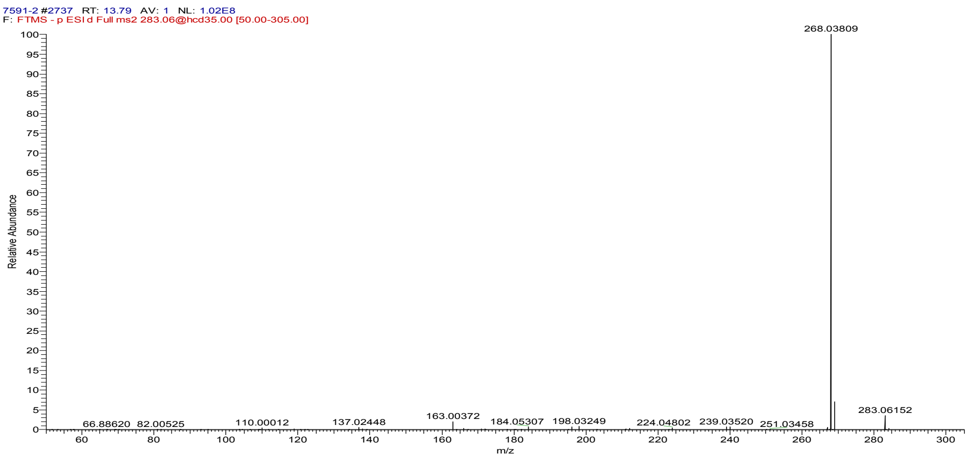
S60, S62, S68, S74, S79, and S81

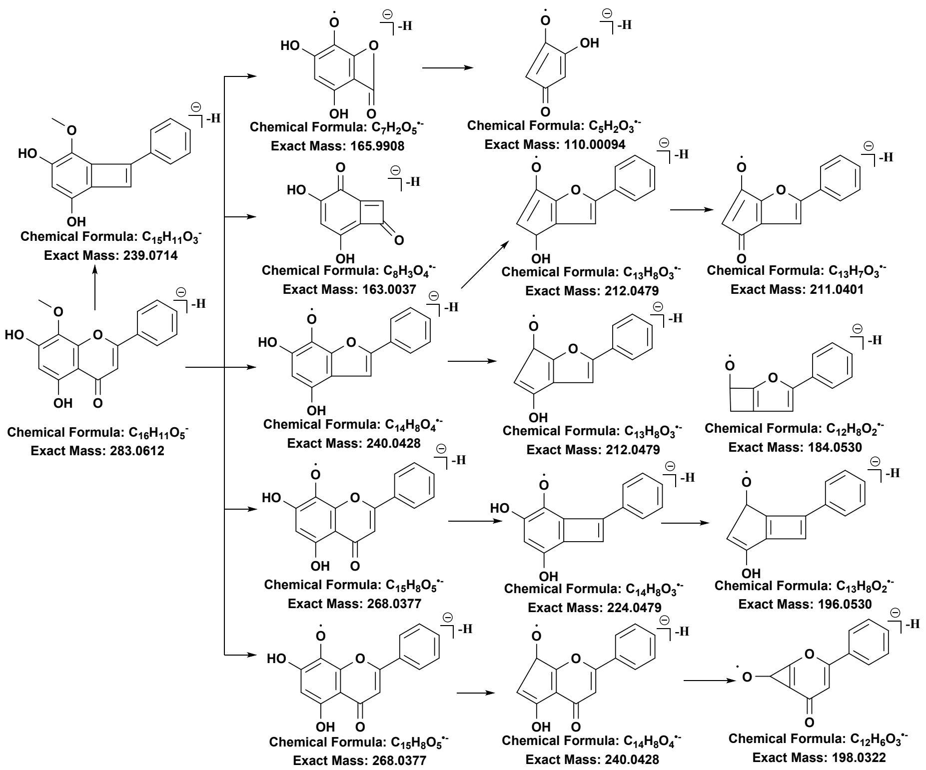


S60 Wogonin (t_R=13.71 min)

MS^1(−): 283.06125

MS^2(−):268.03809(100),240.04349(1),239.03520(1),224.04802(1),212.04816(0.3),211.04041(0.3),198.03249(1),196.05321(1),184.05307(1),165.99049(1),163.00372(2),137.02448(1),110.00012(0.4)





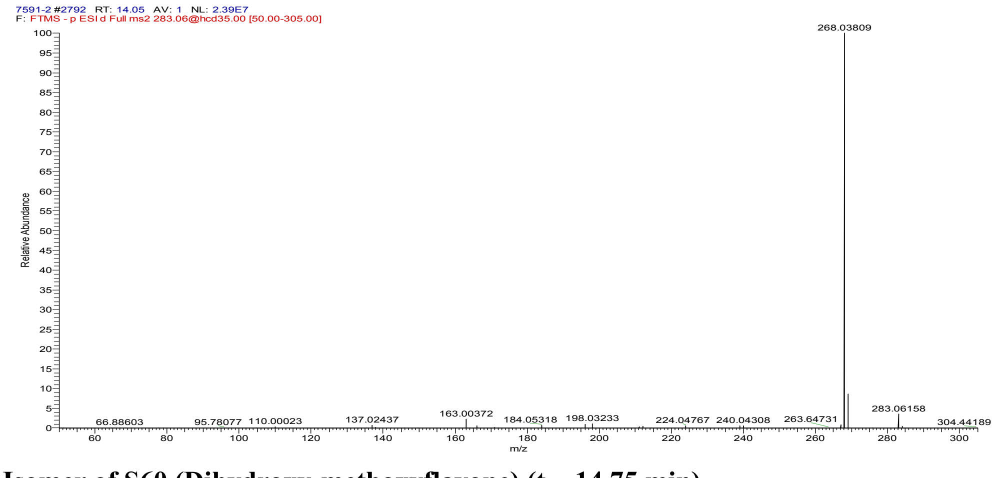
S62 Oroxylin A (t_R=13.91 min)

MS[1](−):

283.06129

MS[2](−):

268.03809(100),240.04308(0.4),239.03503(0.7),224.04767(0.4),212.04845(0.4),211.03987(0.2),198.03233(1),196.05310(1),184.05318(1),165.99036(0.3),163.00372(2),137.02437(0.6),110.00023(0.4)



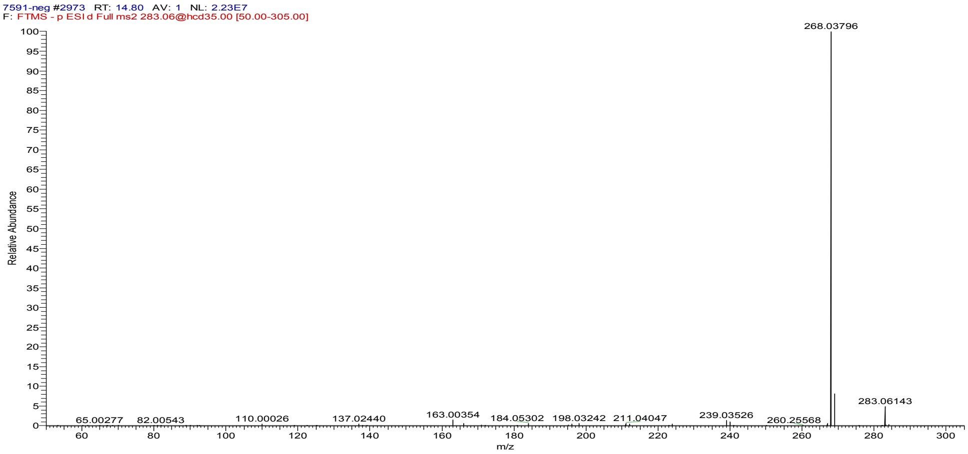
S68 Isomer of S60 (Dihydroxy-methoxyflavone) (t_R=14.75 min)

MS[1](−):

283.06122

MS[2](−):

268.03796(100),240.04321(1),239.03526(1),224.04819(0.4),212.04845(0.4),211.04047(0.6),198.03242(0.6),196.05336(0.4),184.05302(0.6),171.04515(0.2),165.99080(0.5),137.02440(0.4)

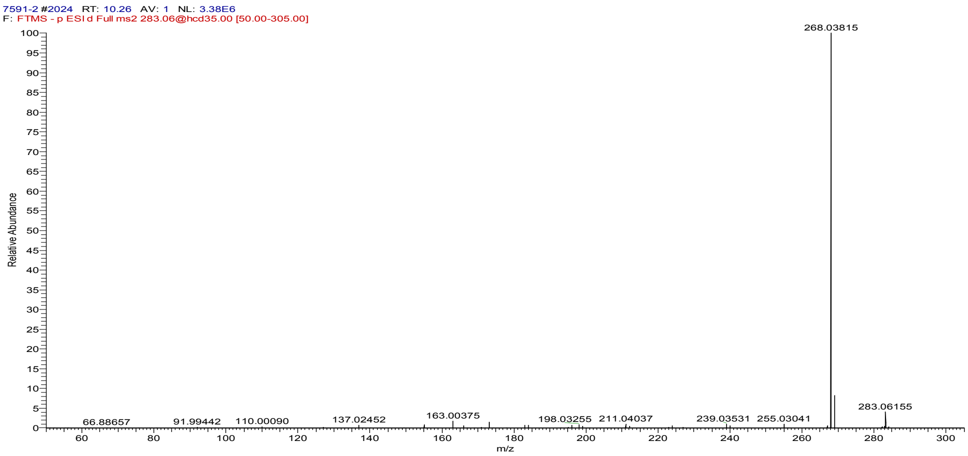


S74 Isomer of S60 (Dihydroxy-methoxyflavone) (t_R=10.27 min)

MS[1](−):283.06137

MS[2](−):

268.03815(100),255.03041(1),239.03531(1),224.04813(1),211.04037(1),198.03255(1),196.05328(1),184.05304(1),183.04530(0.3),173.06088(1),163.00375(2),137.02452(1),110.00090(0.3)



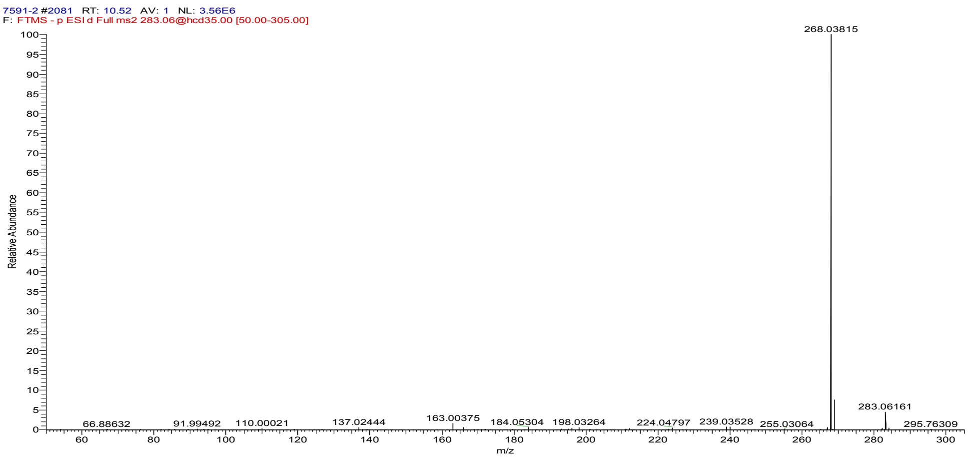
S79 Isomer of S60 (Dihydroxy-methoxyflavone) (t_R=10.53 min)

MS[1]:

283.06165

MS[2]:

268.03815(100),255.03064(0.1),224.04797(1),212.04796(0.3),211.04030(1),198.03264(1),196.05330(1),184.05304(1),165.99068(0.4),163.00375(2),137.02444(1),110.00021(0.3)



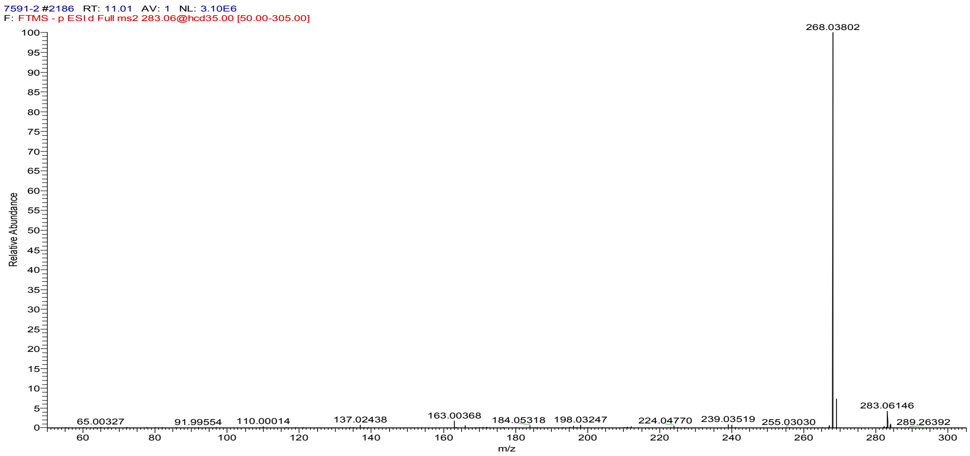
S81 Isomer of S60 (Dihydroxy-methoxyflavone) (t_R=11.09 min)

MS[1](−):

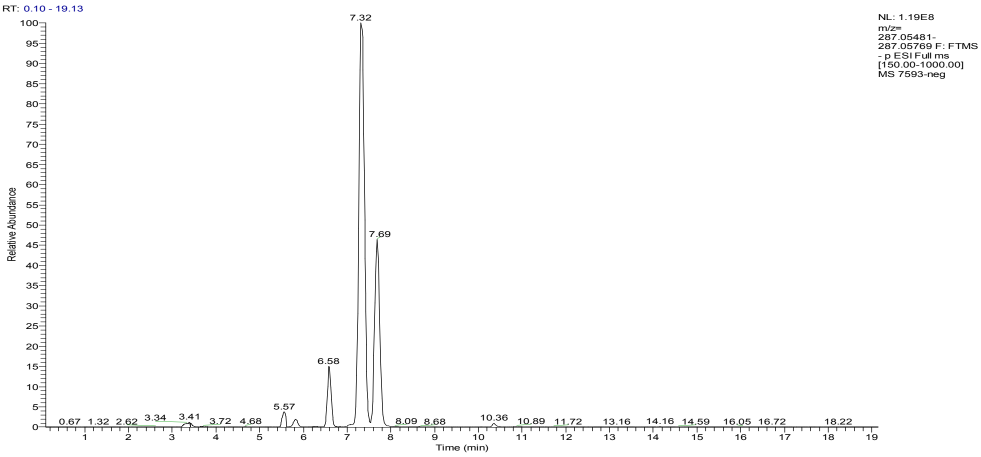
283.06149

MS[2](−):

268.04(100),255.03041(0.2),224.04813(0.5),212.04037(0.4),211.04037(0.2),198.03255(1),196.05328(1),184.05(1),165.99072(1),163.00375(2),137.02438(1),110.00014(0.4)



S64, S71



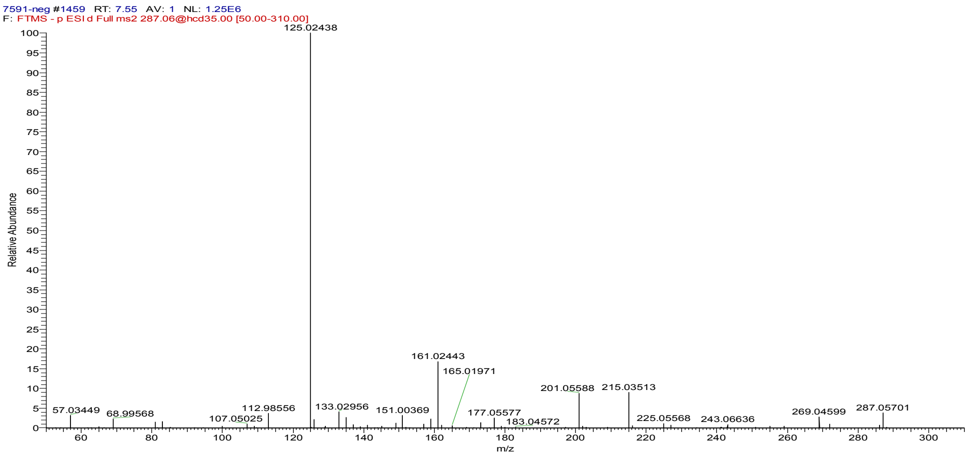
S64 Isomer of S71 (Tetrahydroxyflavanone) (t_R=7.67 min)

MS^1(−):

287.05625

MS^2(−):

287.05701(4),269.04599(3),225.05568(1),215.03513(9),201.05588(9),177.06(2),173.06(1),161.02443(17),151.00369(3),133.02956(4),125.02438(100)



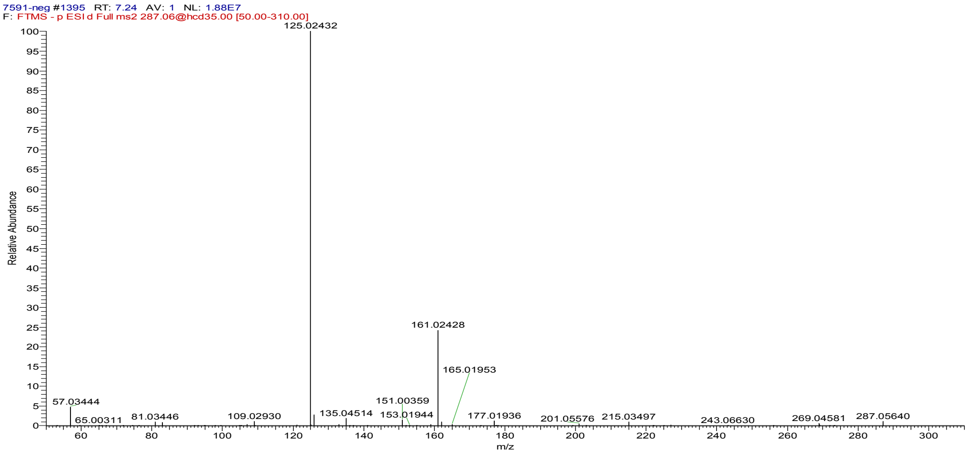
S71 Eriodictyol (t_R=7.24 min)[62, 73]

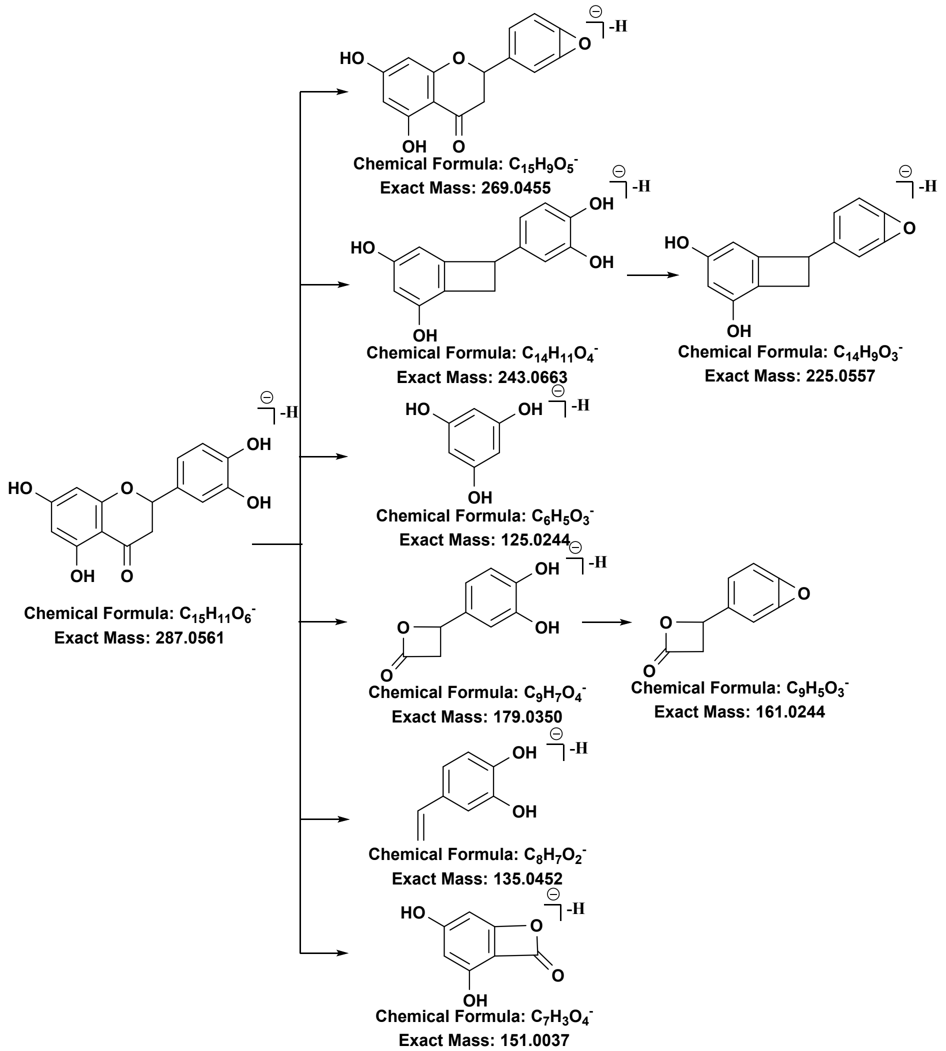
MS^1(−):

287.05622

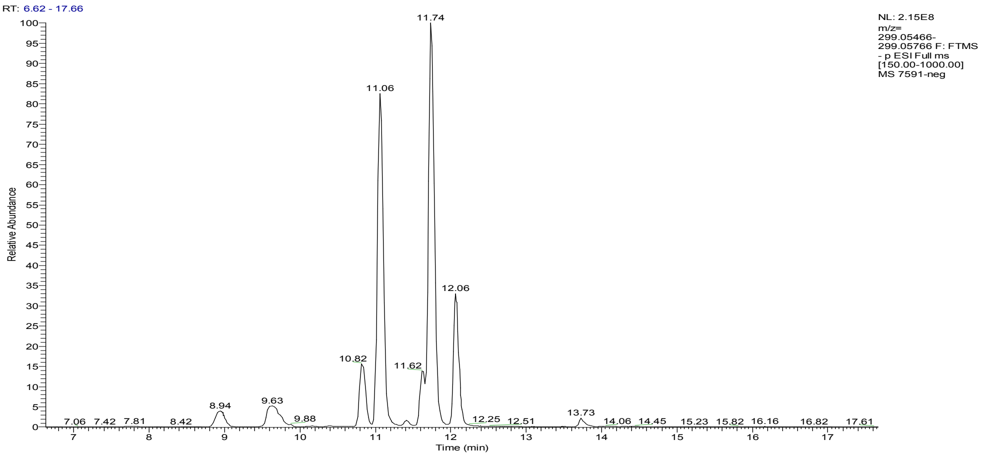
MS^2(−):

269.04581(0.6),243.06630(0.1),225.05594(0.1),179.0350(0.1),161.02428(25),151.00359(1),135.04514(2),125.02432(100)


7591-neg #1395 RT: 7.24 AV: 1 NL: 1.88E7
F: FTMS - p ESI d Full ms2 287.06@hcd35.00 [50.00-310.00]
Relative Abundance
m/z
125.02432
161.02428
165.01953
57.03444
65.00311
81.03446
109.02930
135.04514
151.00359
153.01944
177.01936
201.05576
215.03497
243.06630
269.04581
287.05640


Chemical Formula: $C_{15}H_{11}O_6^-$
Exact Mass: 287.0561
Chemical Formula: $C_{15}H_9O_5^-$
Exact Mass: 269.0455
Chemical Formula: $C_{14}H_{11}O_4^-$
Exact Mass: 243.0663
Chemical Formula: $C_{14}H_9O_3^-$
Exact Mass: 225.0557
Chemical Formula: $C_6H_5O_3^-$
Exact Mass: 125.0244
Chemical Formula: $C_9H_7O_4^-$
Exact Mass: 179.0350
Chemical Formula: $C_9H_5O_3^-$
Exact Mass: 161.0244
Chemical Formula: $C_8H_7O_2^-$
Exact Mass: 135.0452
Chemical Formula: $C_7H_3O_4^-$
Exact Mass: 151.0037

S65, S73, and S76



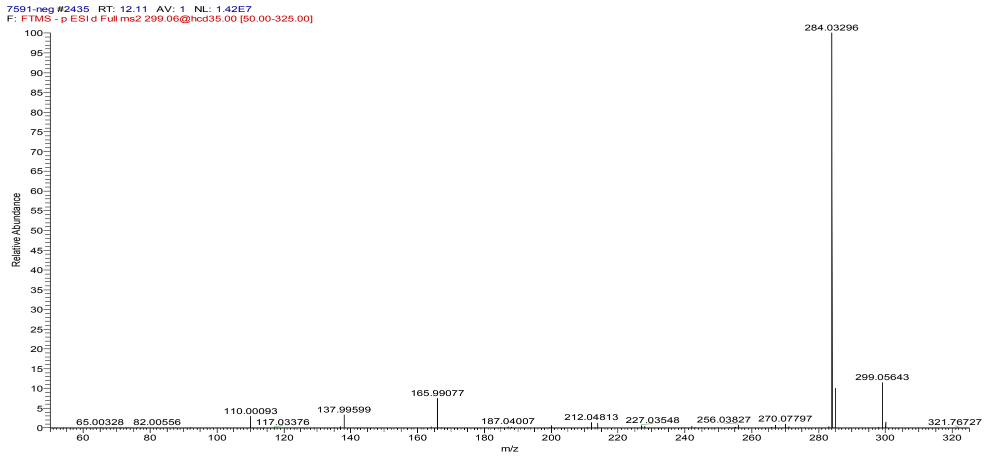
S65 Trihydroxy-methoxyflavone (t_R=12.06 min)

MS^1(−):

299.05618

MS^2(−):

284.03296(100),256.03872(2),255.03044(0.2),227.03548(0.1),200.04811(2),165.99077(8),137.99599(4),110.00093



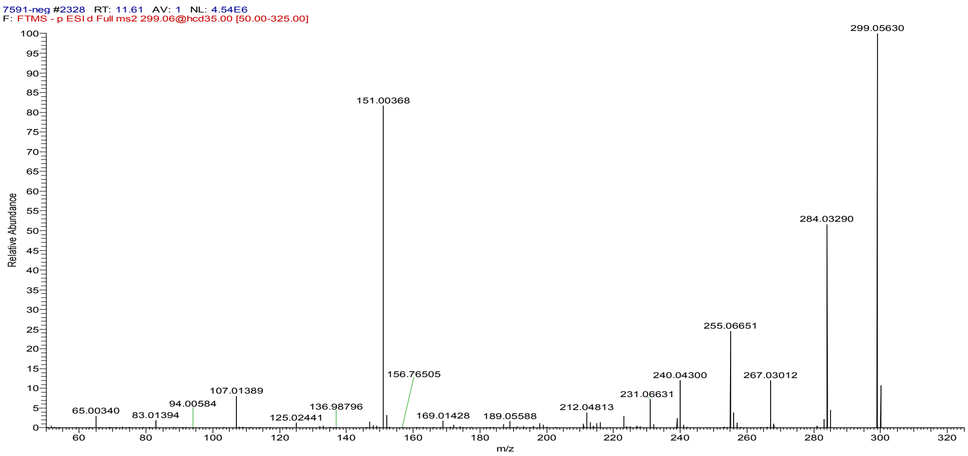
S73 5,6,7-Trihydroxy-8-methoxyflavone OR isomer (trihydoxy and methoxy on A ring) (t_R=11.61 min)

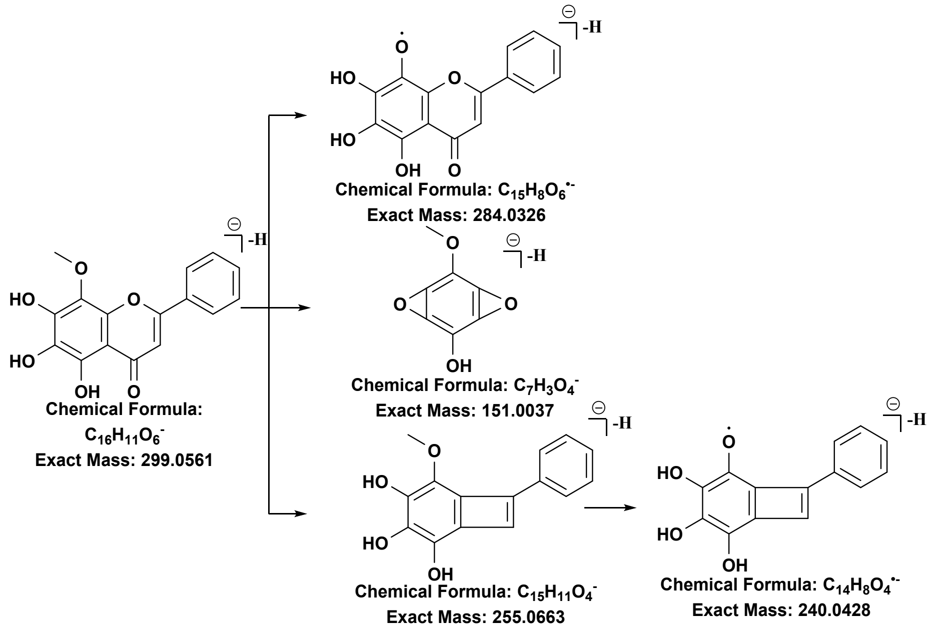
MS^1(−):

299.05616

MS^2(−):

299.06(100),284.03290(49),267.03012(11),255.06651(24),240.04300(12),231.07(7),227.07092(0.5),212.04813(4),153.01930(0.2),151.00368(82),107.01389(8)





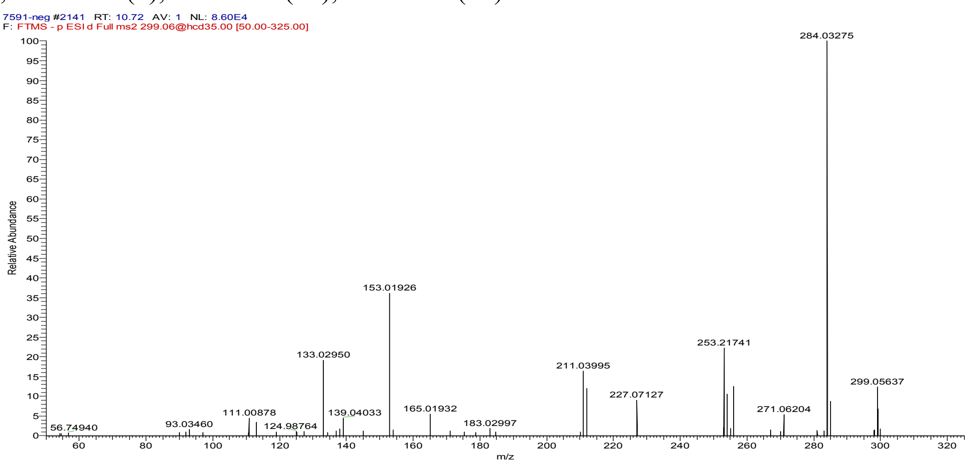
S76 4'-hydroxy wogonin (t_R=10.72 min)

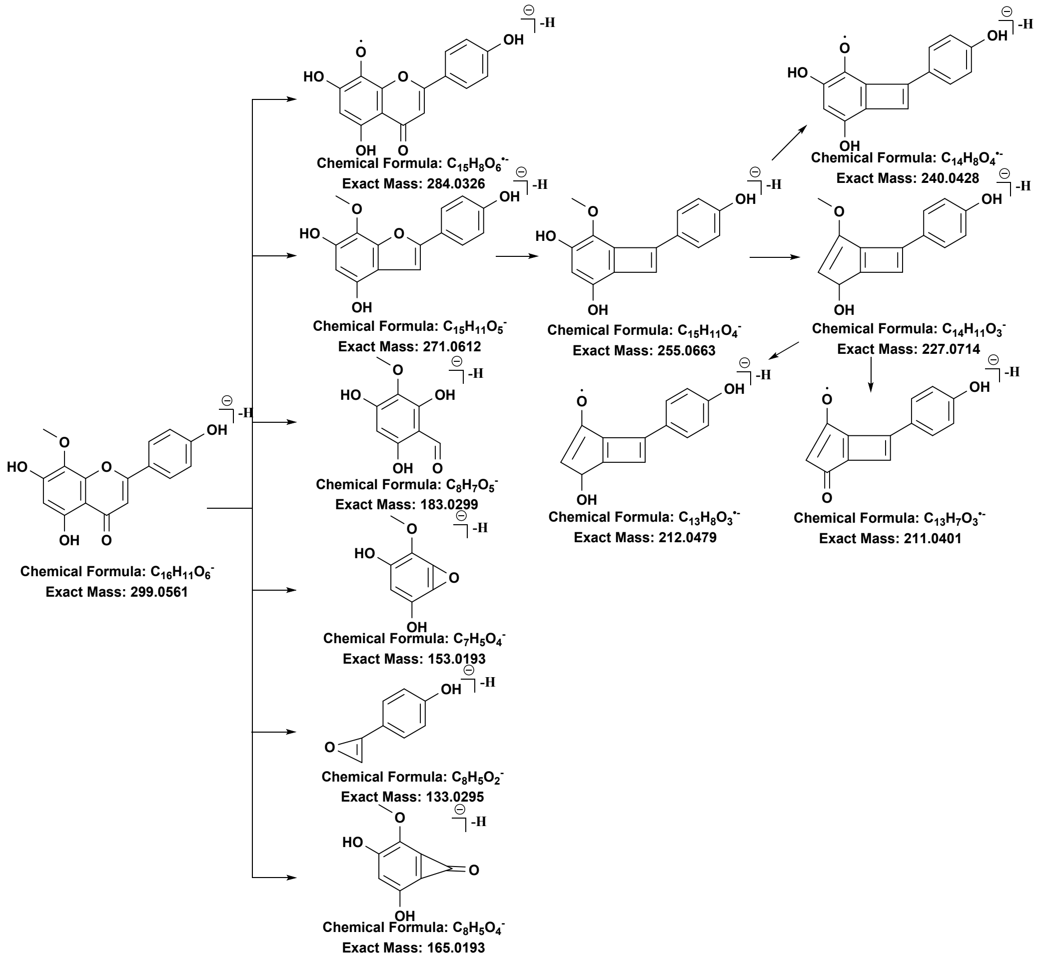
MS[1](−):

299.05611

MS[2](−):

284.03275(100),271.06204(6),255.06720(2),227.07127(9),212.04810(12),211.03995(17),183.02997(2),165.01932(6),153.01926(36),133.02950(20)




Chemical Formula: C16H11O6-
Exact Mass: 299.0561
Chemical Formula: C15H8O6•-
Exact Mass: 284.0326
Chemical Formula: C15H11O5-
Exact Mass: 271.0612
Chemical Formula: C8H7O5-
Exact Mass: 183.0299
Chemical Formula: C7H5O4-
Exact Mass: 153.0193
Chemical Formula: C8H5O2-
Exact Mass: 133.0295
Chemical Formula: C8H5O4-
Exact Mass: 165.0193
Chemical Formula: C15H11O4-
Exact Mass: 255.0663
Chemical Formula: C14H8O4•-
Exact Mass: 240.0428
Chemical Formula: C14H11O3-
Exact Mass: 227.0714
Chemical Formula: C13H8O3•-
Exact Mass: 212.0479
Chemical Formula: C13H7O3•-
Exact Mass: 211.0401

S66

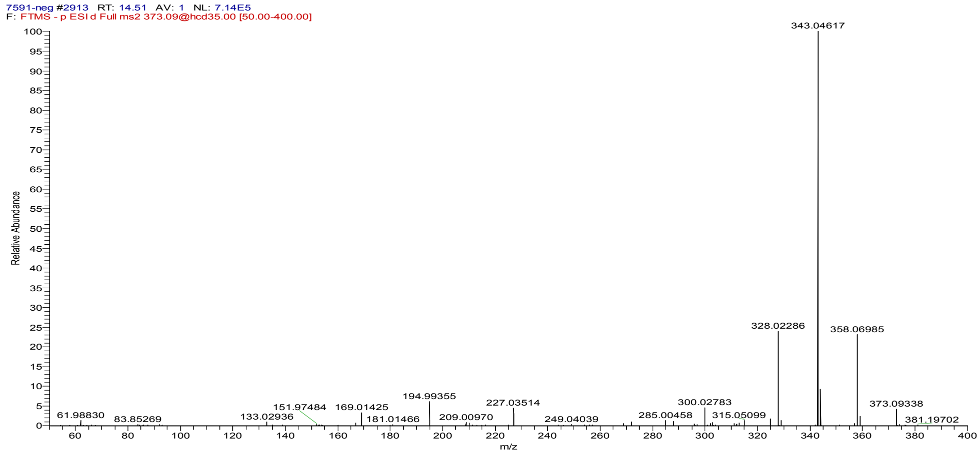
Scullcapflavone II (t_R=14.50 min)[61]

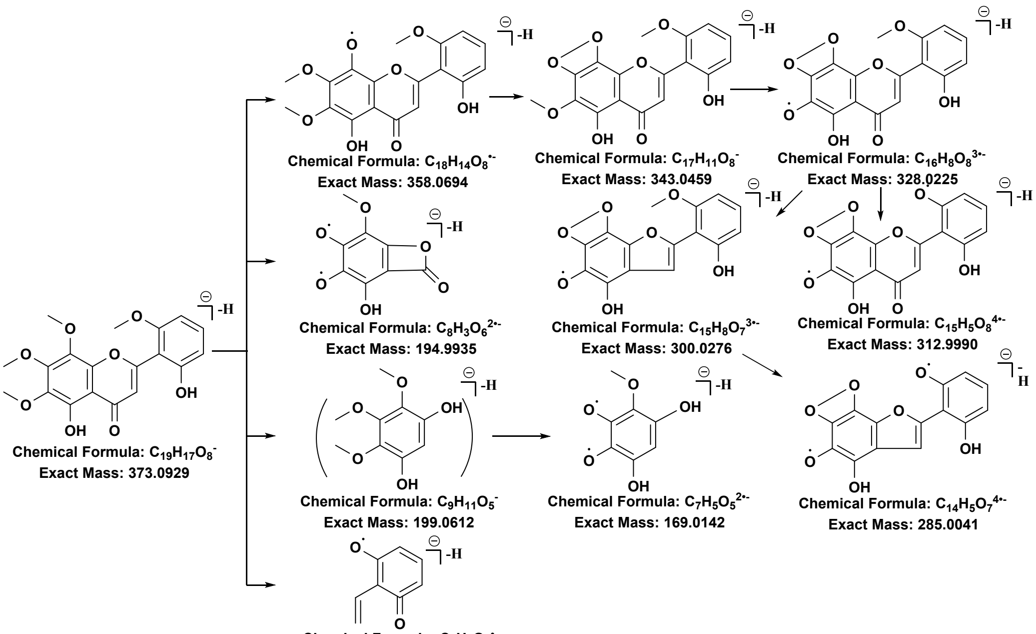
$MS^1(-)$:

373.09289

$MS^2(-)$:

358.06985(22),343.04617(100),328.02286(23),325.03555(2),315.05099(1),313.03574(0.6),300.02783(5),285.00458(1),227.03514(4),194.99355(6),169.01425(3),133.02936(1)



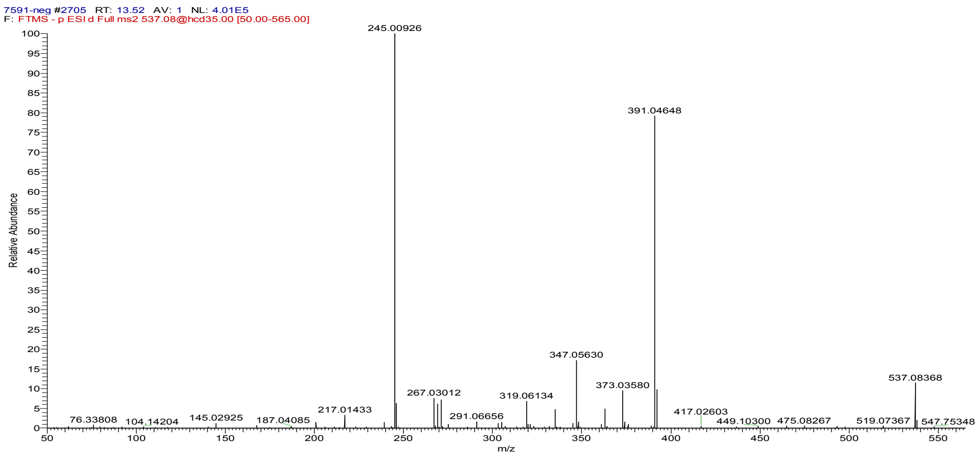


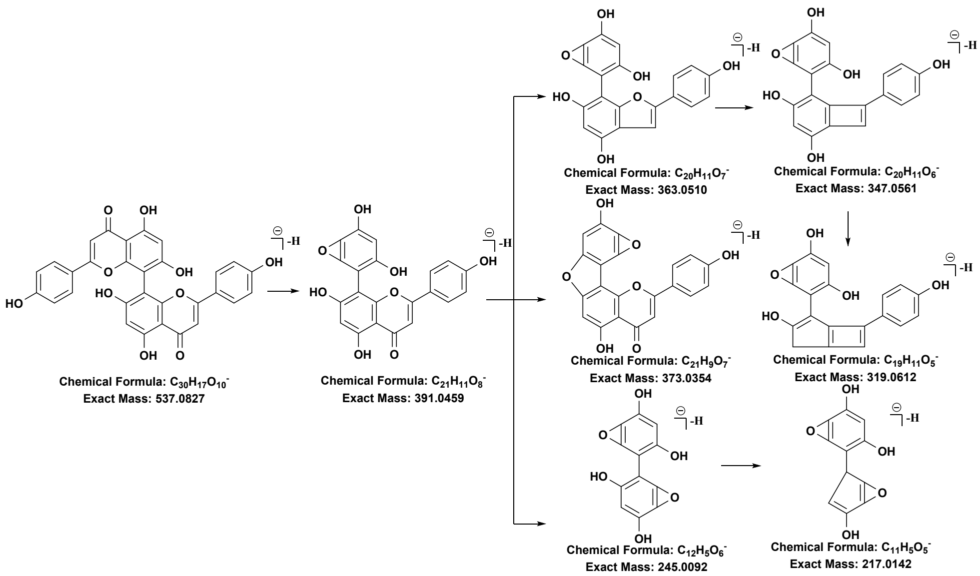
8,8'-Biapigenin (t_R=13.67 min)[62]

MS[1](−):

537.08295

MS[2](−):391.04648(76),373.03580(10),347.05630(16),335.05679(5),319.06134(7),291.06656(2),245.00926(100),239.03531(1),217.01433(3)





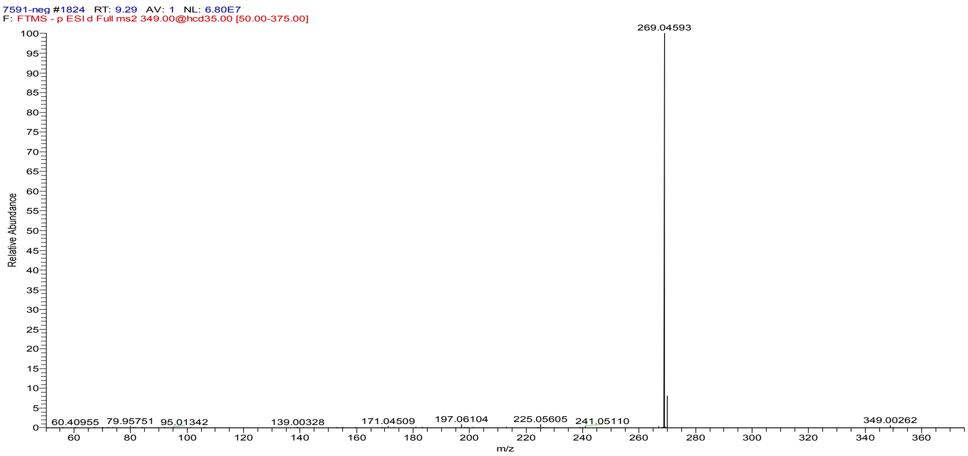
Baicalein 6-*O*-sulfate (t_R=9.29 min)[70]

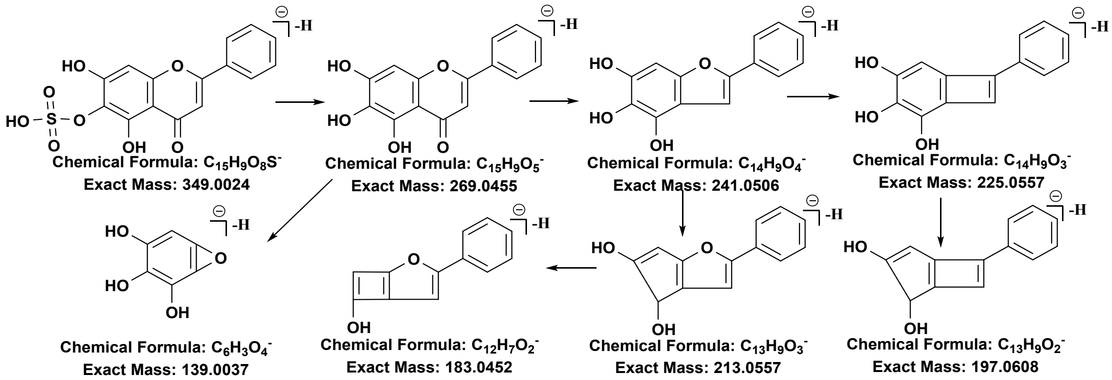
MS[1](−):

349.00236

MS[2](−):

269.04593(100),241.05110(0.3),225.05605(1),225.05605(0.9),197.06(1),181.06602(0.2),139.00328(0.1)





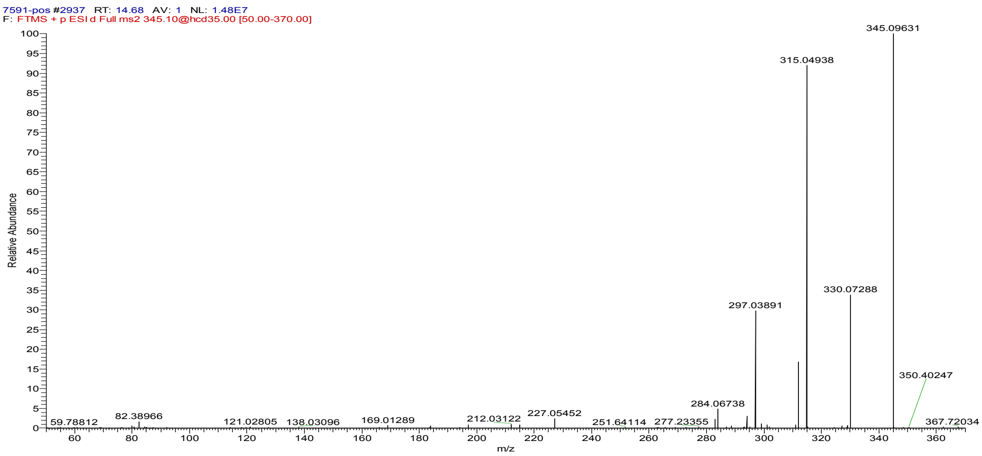
Tenaxin I (t_R=14.60 min)[61]

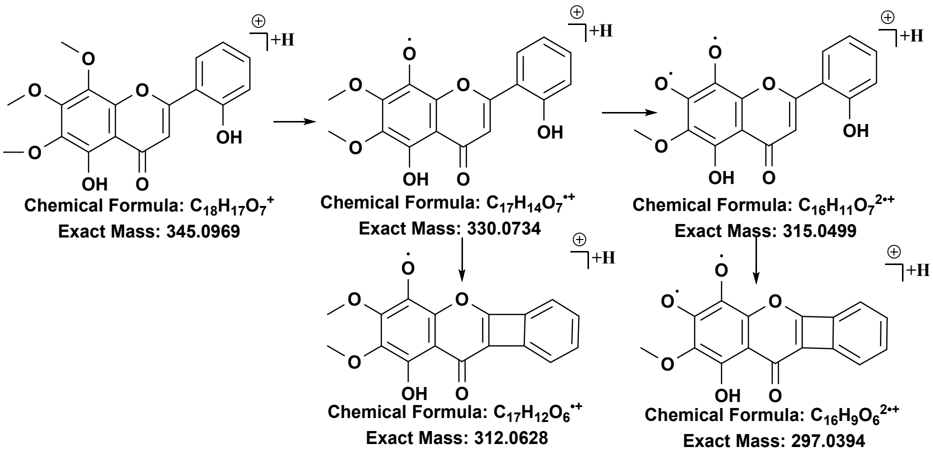
MS[1](+):

345.09647

MS[2](+):

345.09631(100),330.07288(34),315.04938(92),312.06241(18),297.03891(31)





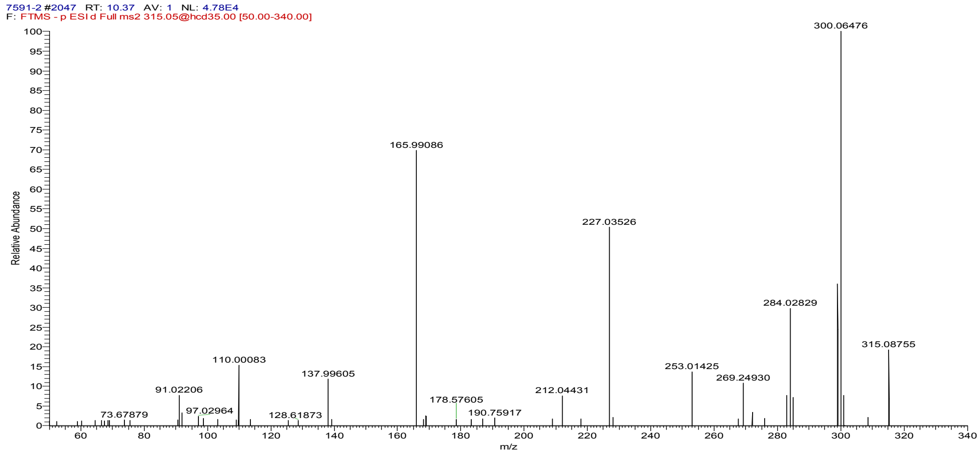
Neptin (t_R=10.47 min)[72]

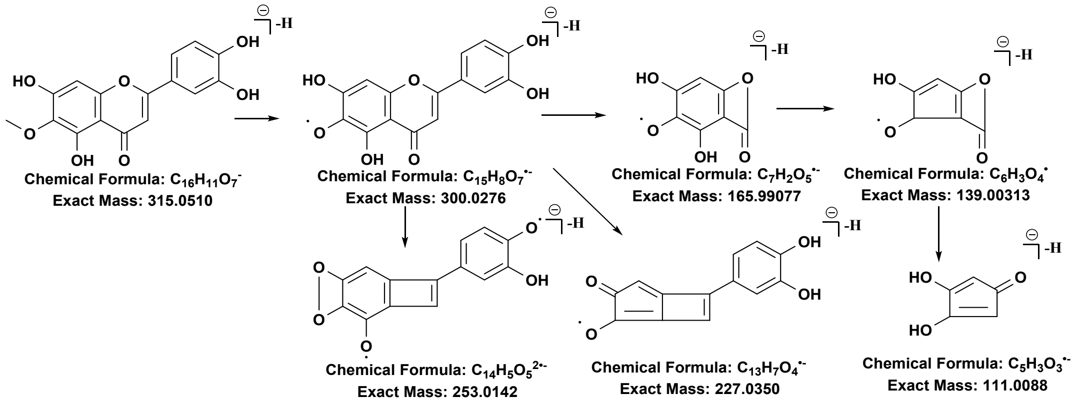
MS[1](−):

315.05119

MS[2](−):

300.06476(69),284.02829(19),253.01425(30),227.03526(100),212.04431(7),165.99086(58),137.99605(11),110.00083(9)





S80

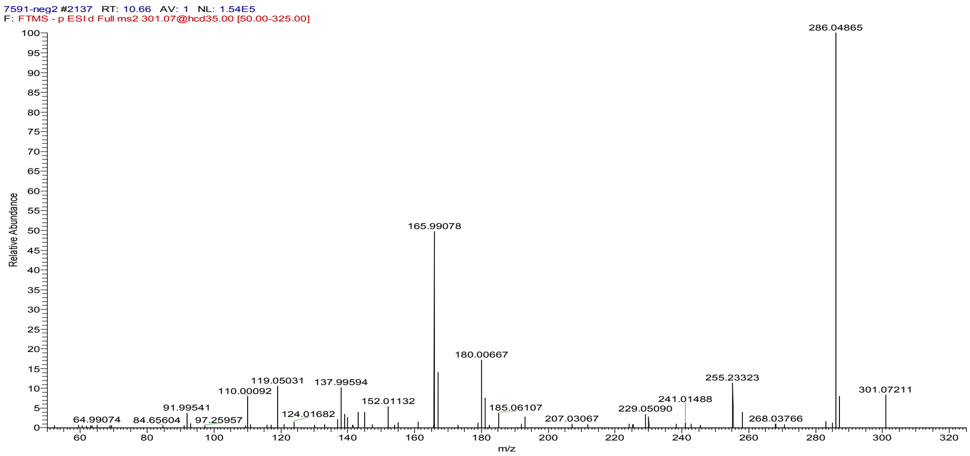
Trihydroxy-methoxyflavanone (dihydroxy and methoxy on A ring, monhydroxy on B ring) (t_R=10.65 min)

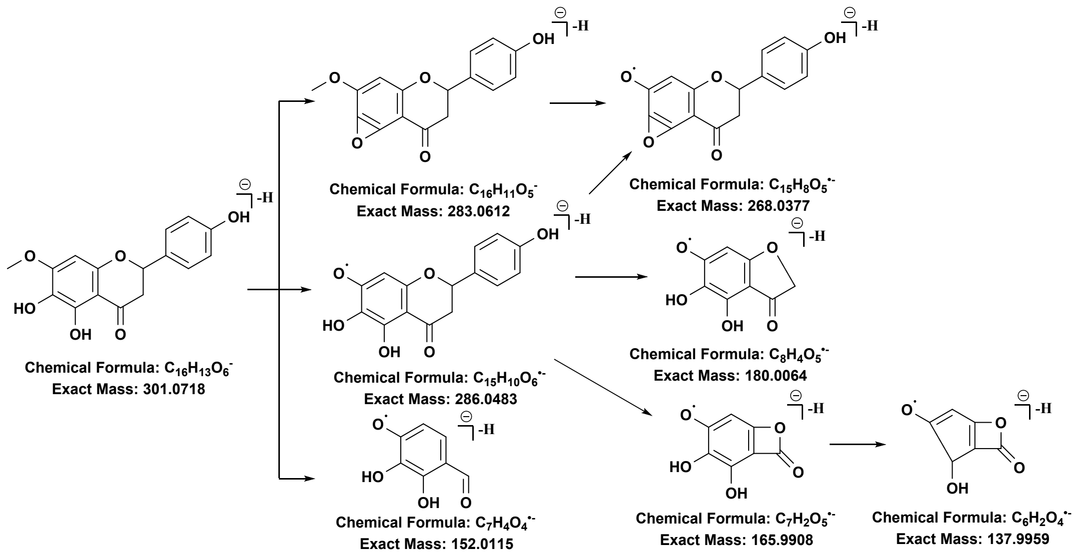
MS^1(−):

301.07175

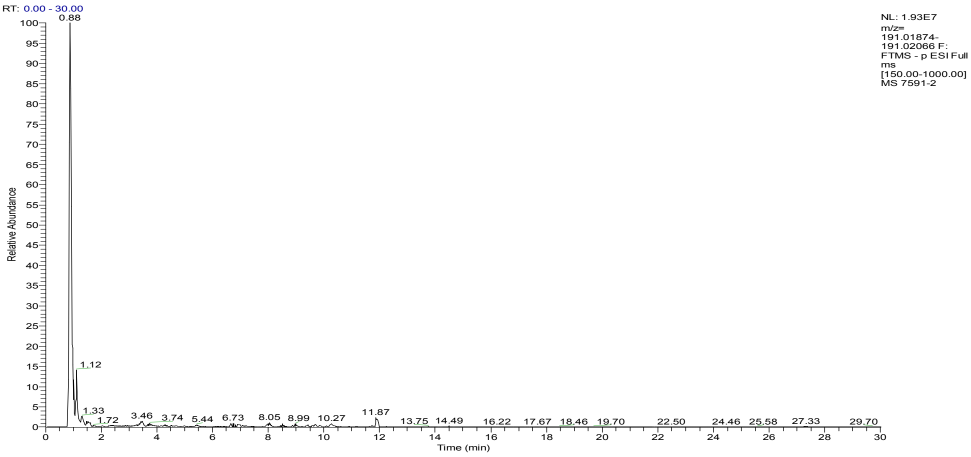
MS^2(−):

286.04865(100),283.02444(4),268.03766(),255.23323(10),185.06107(5),180.00667(16),165.99078(45),152.01132(5),137.99594(9),119.05031(8)





S83, S84



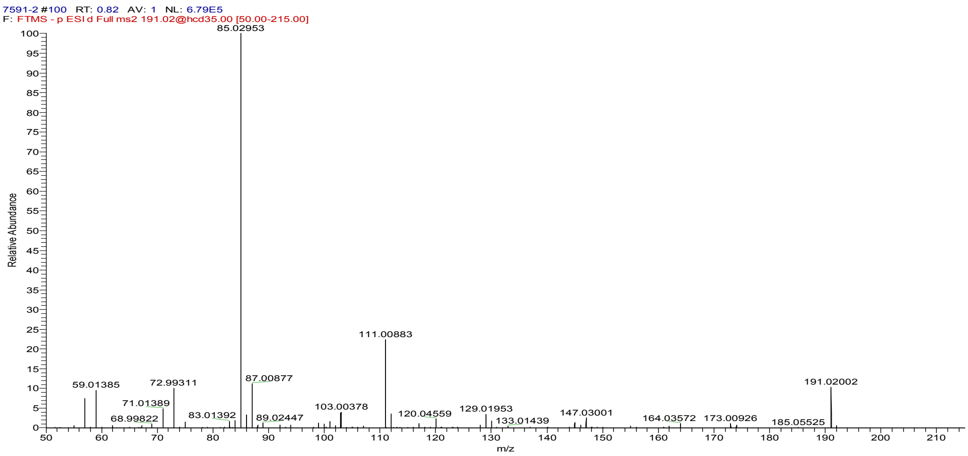
S83 D-Galactaric acid, 1,5-lactone OR isomer (t_R=0.81 min)

MS[1](−):

191.01970

MS[2](−):

173.00926(3),147.03001(1),129.01953(8),111.00883(4),103.00378(4),85.03(100),72.99311(10)



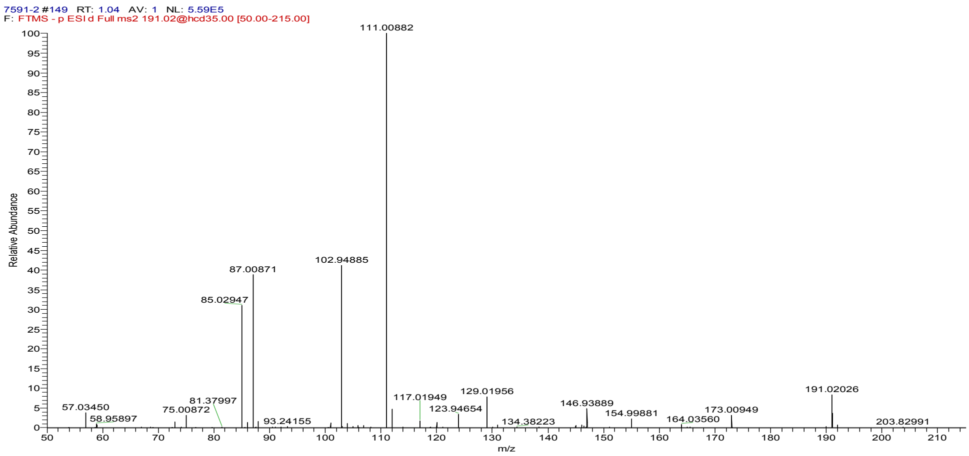
S84 Isomer of D-Galactaric acid, 1,5-lactone (t_R=1.04 min)

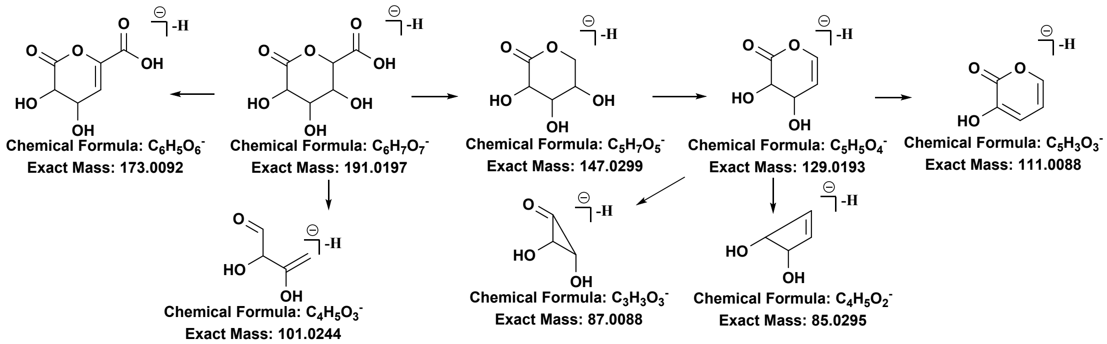
MS[1](−):

191.01969

MS[2](−):

173.00949(4),129.01956(8),117.01949(2),111.00882(100),87.00871(42),85.02947(34)


7591-2 #149 RT: 1.04 AV: 1 NL: 5.59E5
F: FTMS - p ESI d Full ms2 191.02@hcd35.00 [50.00-215.00]
Relative Abundance
m/z
111.00882
102.94885
87.00871
85.02947
81.37997
75.00872
57.03450
58.95897
93.24155
117.01949
123.94654
129.01956
134.38223
146.93889
154.99881
164.03560
173.00949
191.02026
203.82991


Chemical Formula: $C_6H_5O_6^-$
Exact Mass: 173.0092
Chemical Formula: $C_6H_7O_7^-$
Exact Mass: 191.0197
Chemical Formula: $C_5H_7O_5^-$
Exact Mass: 147.0299
Chemical Formula: $C_5H_5O_4^-$
Exact Mass: 129.0193
Chemical Formula: $C_5H_3O_3^-$
Exact Mass: 111.0088
Chemical Formula: $C_4H_5O_3^-$
Exact Mass: 101.0244
Chemical Formula: $C_3H_3O_3^-$
Exact Mass: 87.0088
Chemical Formula: $C_4H_5O_2^-$
Exact Mass: 85.0295

S85

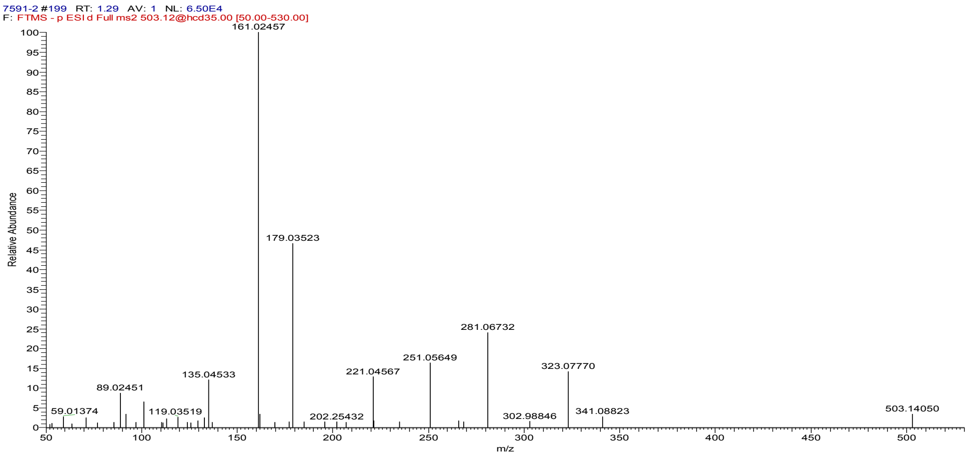
1-caffeyllaminaribiose (t_R=1.29 min)[74]

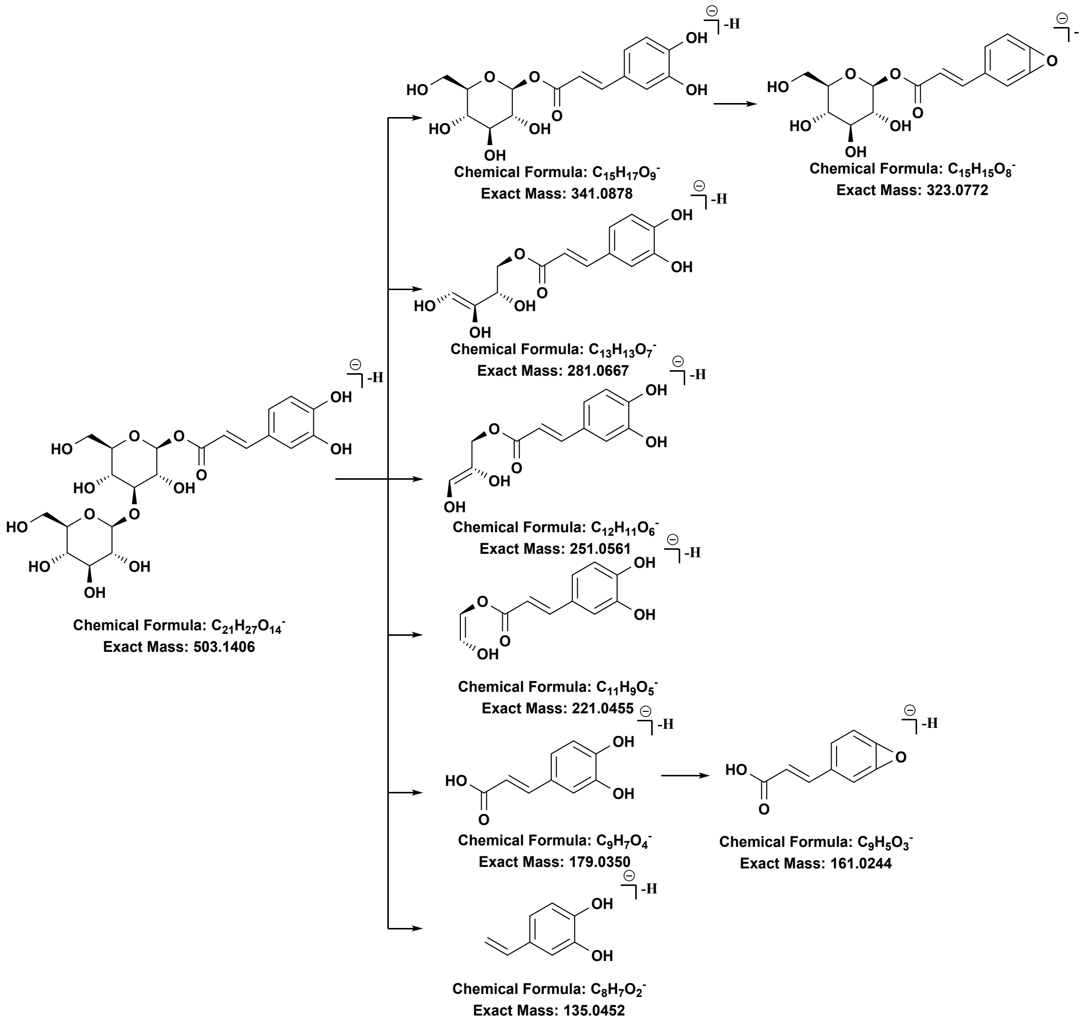
MS[1](−):

503.14106

MS[2](−):

341.08823(2),323.07770(13),281.06732(20),251.05649(10),223.97(2),221.04567(14),179.03532(44),161.02457(100),135.04533(12)





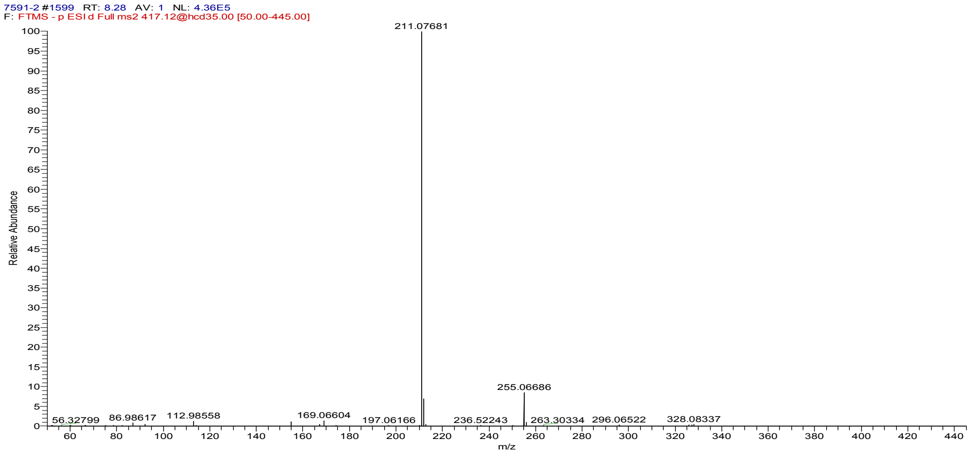
Gaylussacin (t_R=8.29 min)[75]

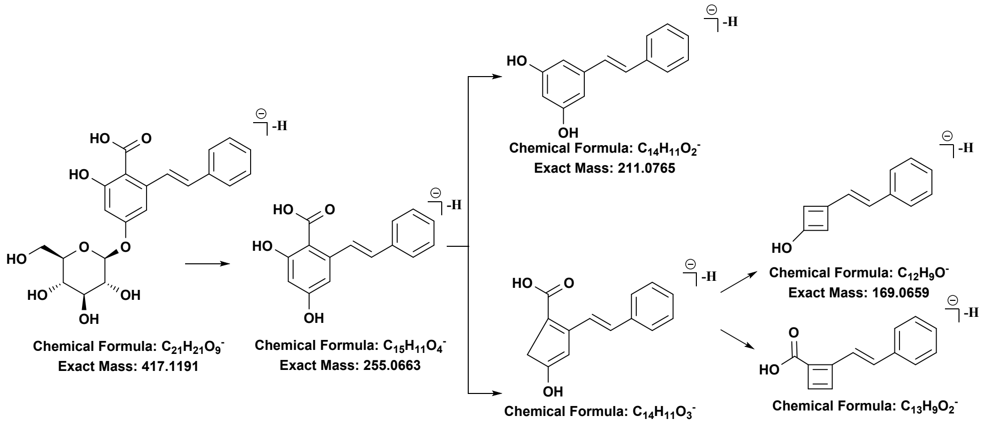
MS[1](−):

417.11947

MS[2](−):

255.06686(10),211.07681(100),197.06166(0.2),169.06604(5),112.98558(2)



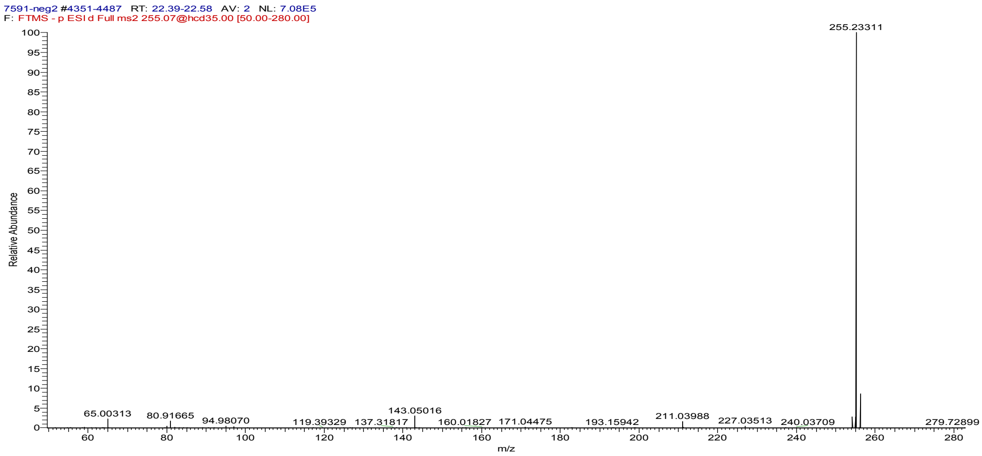


S87

Isomer of Hexadecanoic acid (t_R=22.48 min)[76]

MS^1(−):255.23276

MS^2(−):255.23302(100),237.22174(0.2),211.20708(0.2)



S88

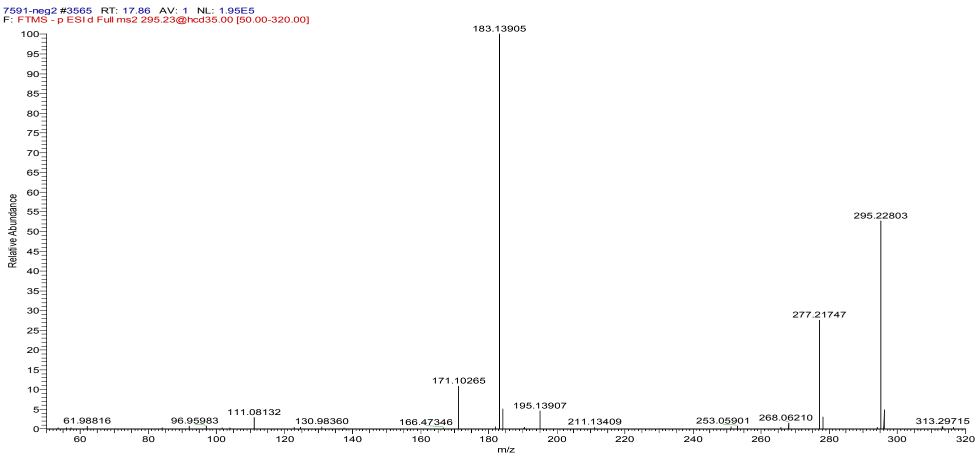
Isomer of 10-Hydroxyoctadecadienoic acid (t_R=17.94 min)

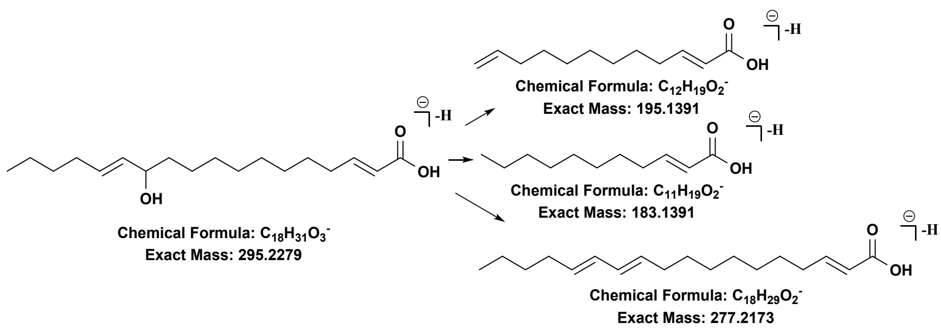
MS^1(−):

295.22773

MS^2(−):

277.21747(25),211.13409(1),195.13907(2),183.13905(100)





S89

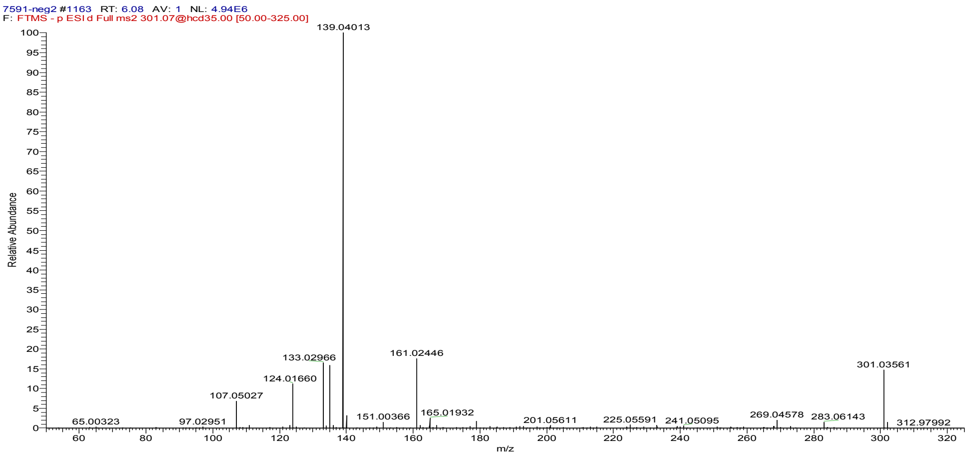
Isomer of 3-Hydroxy-4-*O*-glucosylbenzyl alcohol (t_R=6.12 min)

MS[1](−):

301.03561

MS[2](−):

161.02446(23),139.04013(100),135.04533(22),133.00966(16),124.01660(11),107.05027(10)



S90

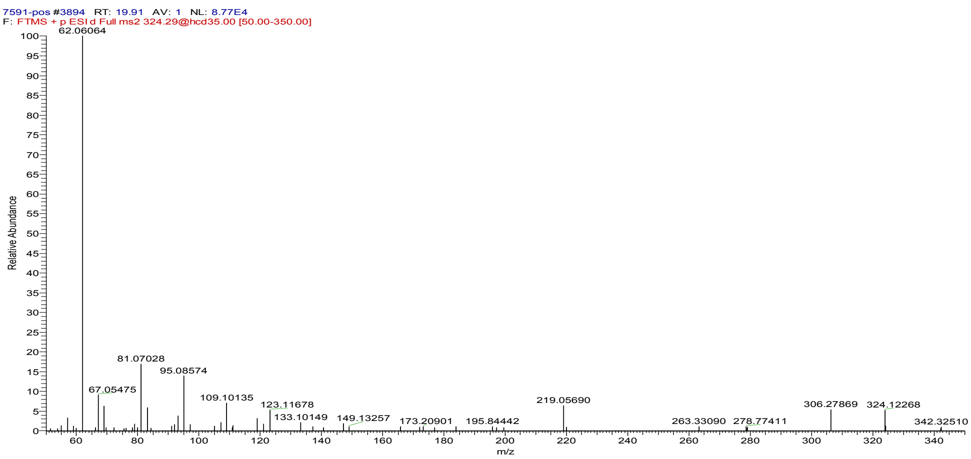
Isomer of Linoleoyl Ethanolamide (LEA) (t_R=19.97 min)

MS[1](−):

324.12268 (positive)

MS[2](−):

306.27869(6),219.05690(6),147.11668(2),123.11678(5),109.10135(7),95.08574(14),81.07028(17),62.06064(100)



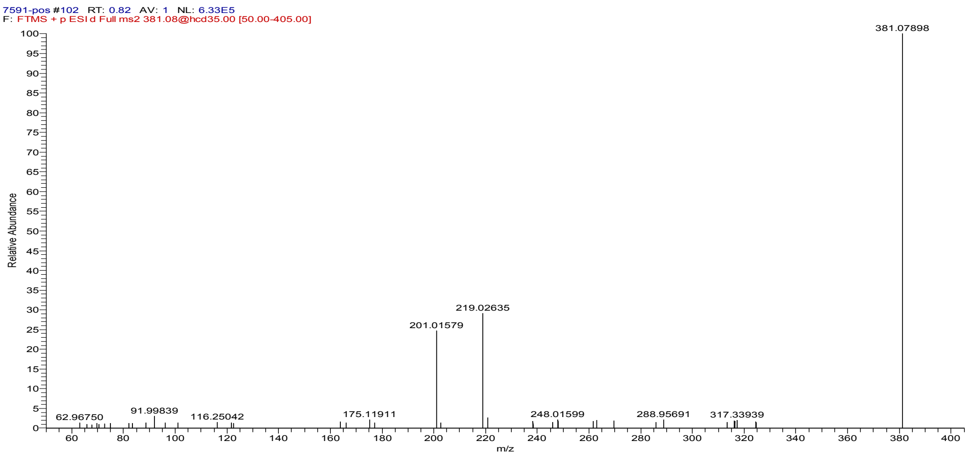
Isomer of 5-*O*-β-D-glucopyranosyl-6-hydroxyangelicin (t_R=0.87 min)[77]

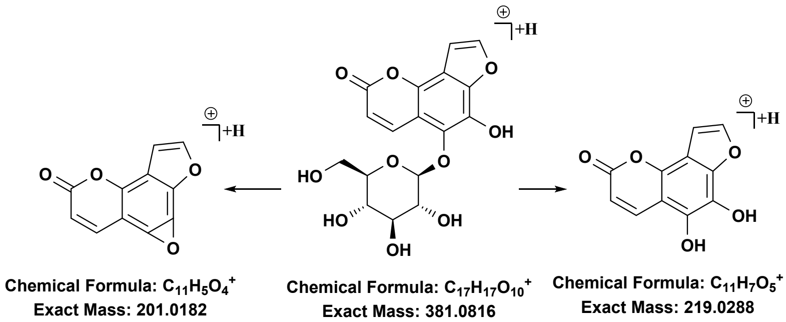
MS[1](+):

381.07891

MS[2](+):

381.08(100),219.02664(30),201.01584(25)





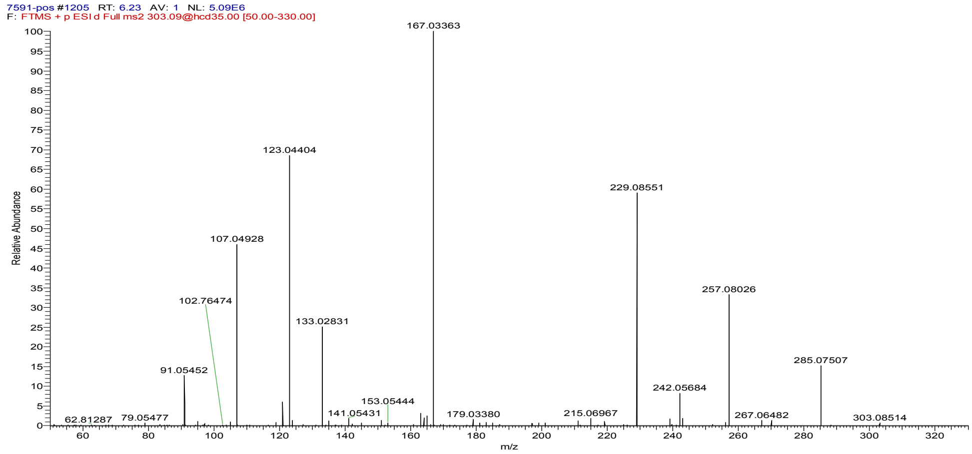
3,4-Dihydroxy-7-*O*-caffeoylbenzyl alcohol OR isomer (t_R=6.17 min)[78]

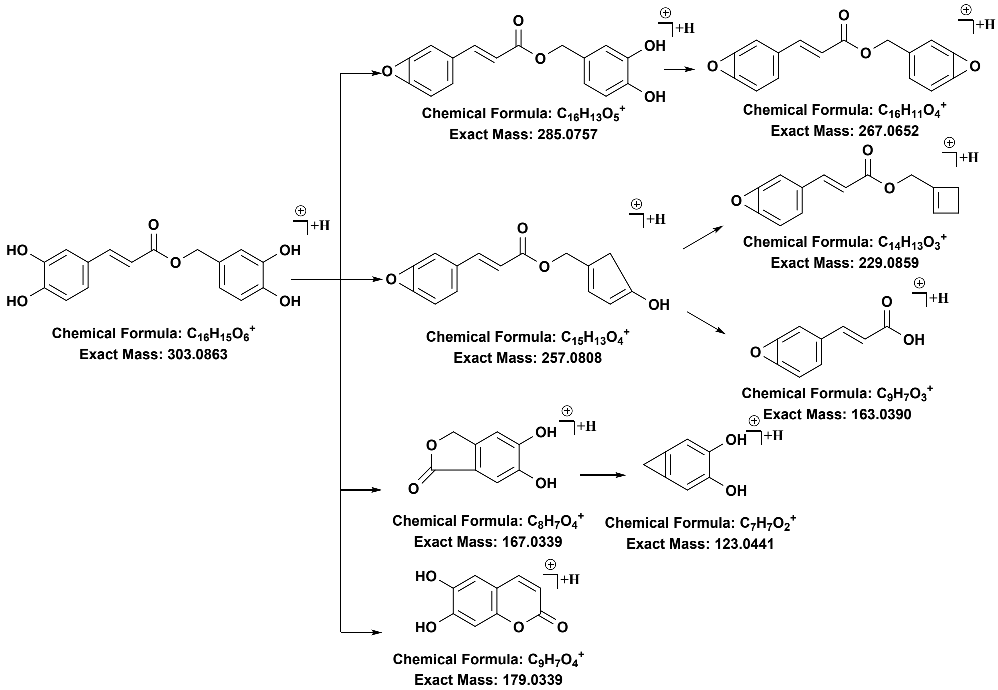
MS[1](+):

303.08598

MS[2](+):

285.07507(15),267.06482(1),257.08026(32),242.05684(8),229.08551(57),179.03380(2),167.03363(100),163.03865(3),133.02831(24),123.04404(69),107.04928(44)





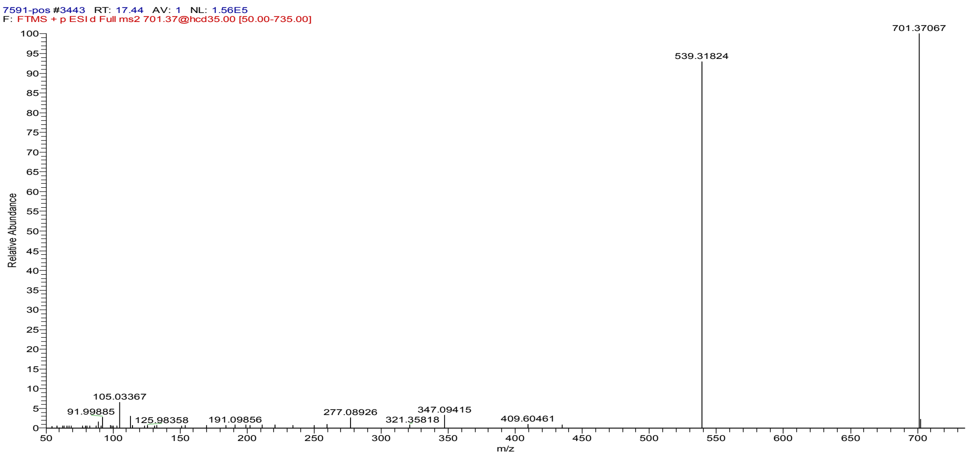
Unknown (t_R=17.44 min)

MS[1](+):

701.37151

MS[2](+):

701.37067(100),539.31824(96),191.09856(1),105.03367(7)



S94

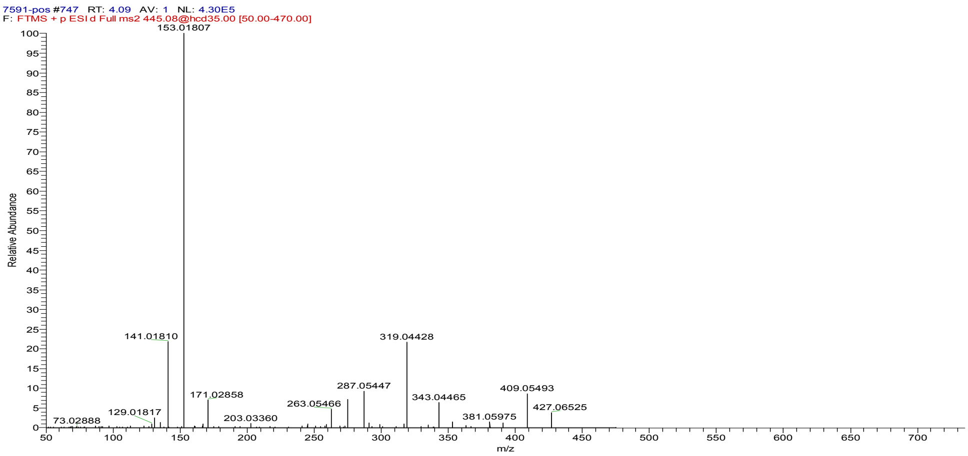
Benzoic acid, 3,4,5-trihydroxy-,1,1'-(2-methoxy-1,4-phenylene) ester OR isomer (t_R=4.17 min)

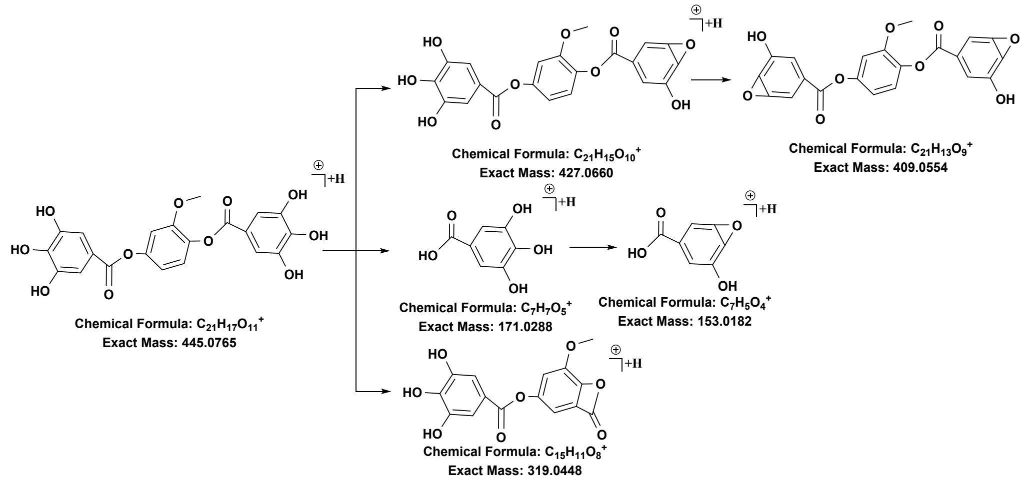
$MS^1(+)$:

445.07617

$MS^2(+)$:

427.06525(4),409.05493(9),381.05975(1),343.04465(6),319.04428(23),287.05(10),275.05447(7),263.05466(5),153.01807(100),141.01810(22)





S95

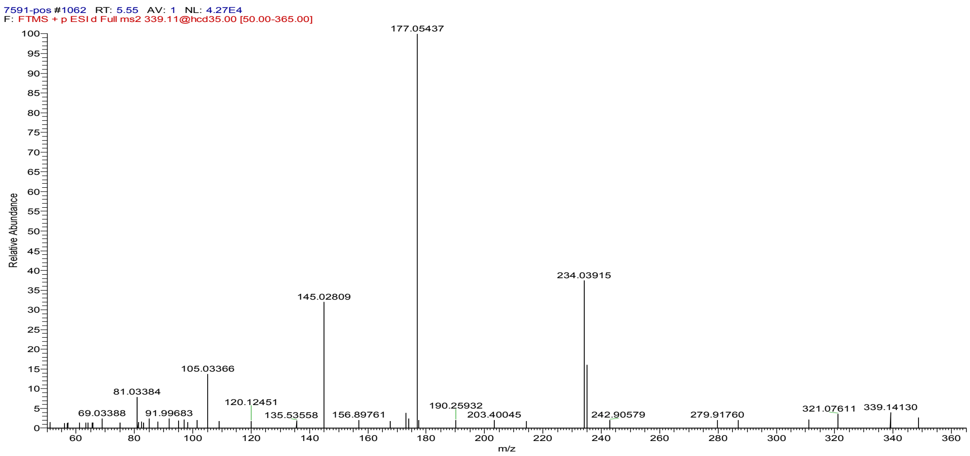
Unknown (t_R=5.67 min)

MS[1](+):

339.10696

MS[2](+):

321.07611(3),234.03915(37),177.05437(100),145.02809(31),105.03366(13)



S96

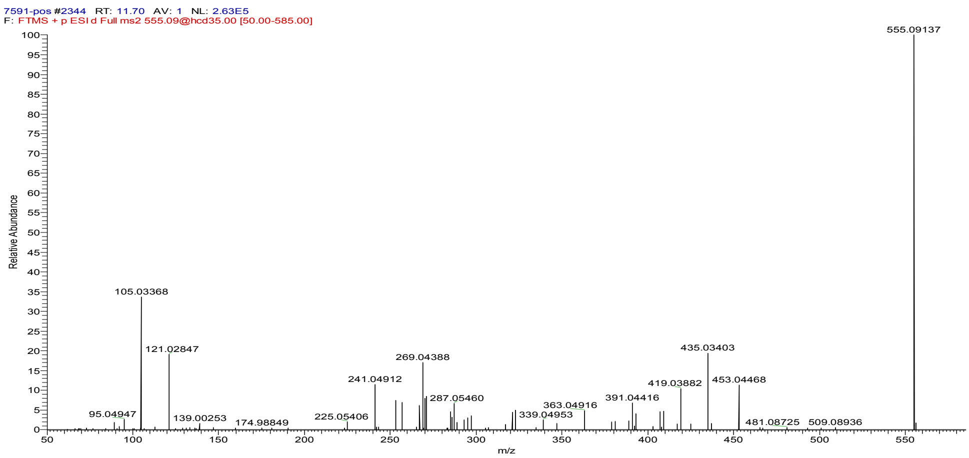
Isomer of hegoflavone A (t_R=11.70 min)

MS[1](+):

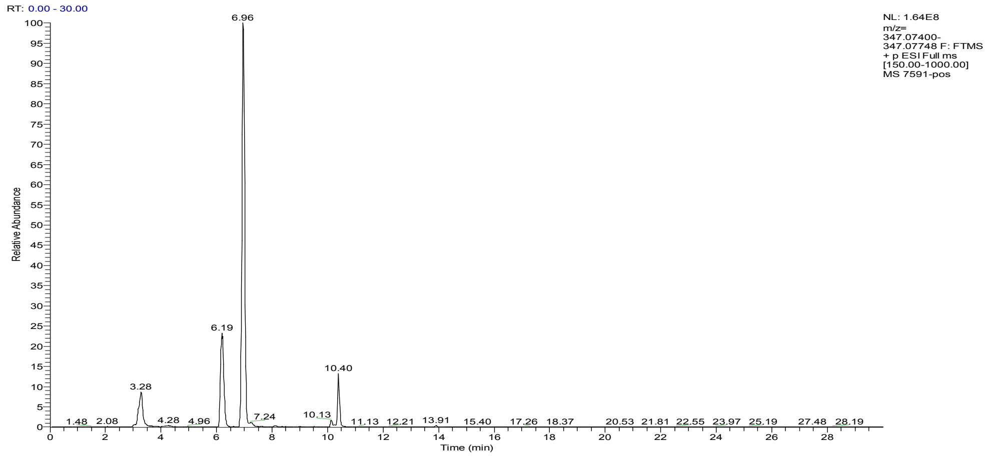
555.09167

MS[2](+):

453.04468(11),435.03403(20),419.03882(10),269.03884(18),241.04912(12),121.02847(19),105.03368(34)



S57, S97



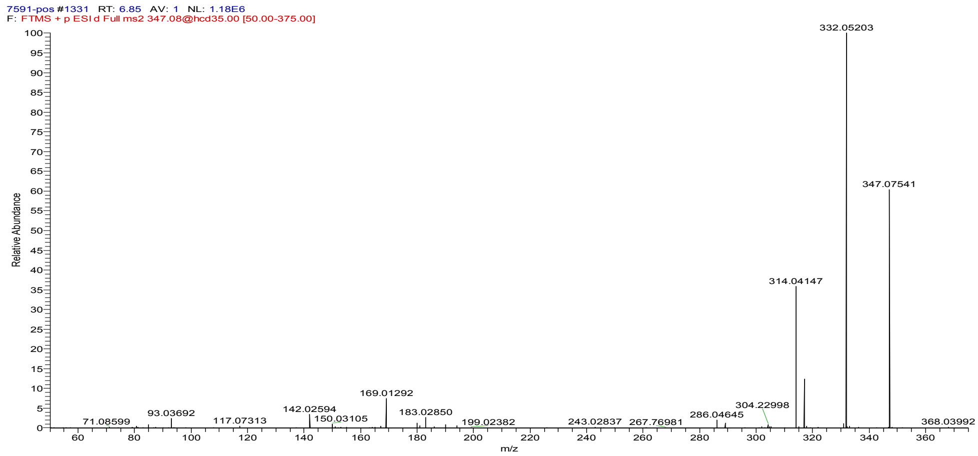
S57 Viscidulin III (t_R=6.95 min)[61]

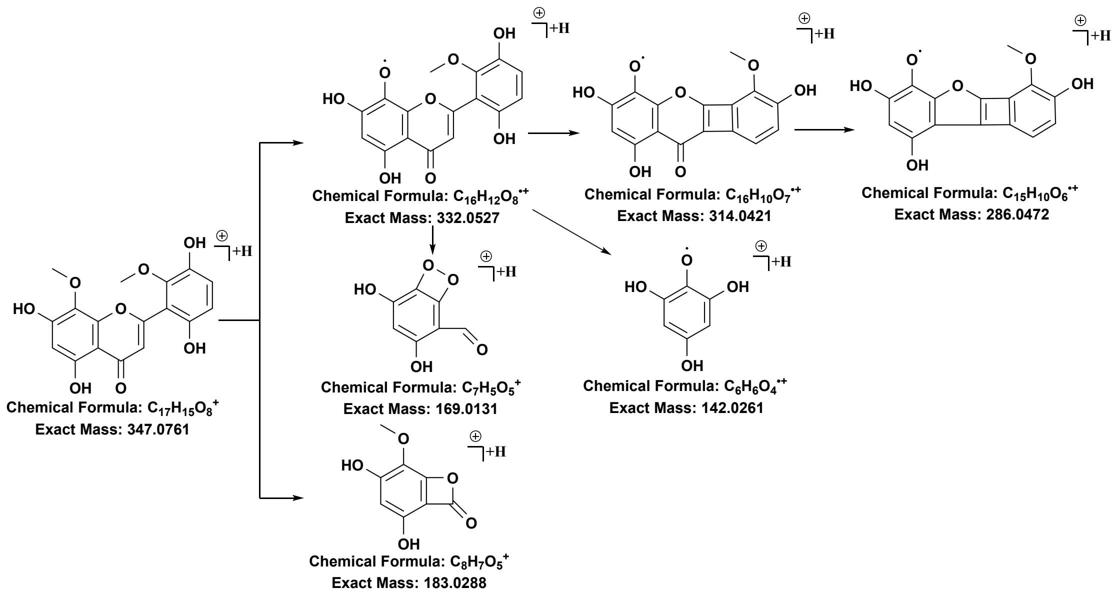
MS[1](+):

347.07574

MS[2](+):

347.07541(63),332.05203(100),314.04147(35),286.04645(2),183.02850(3),169.01292(7),142.02594(3)





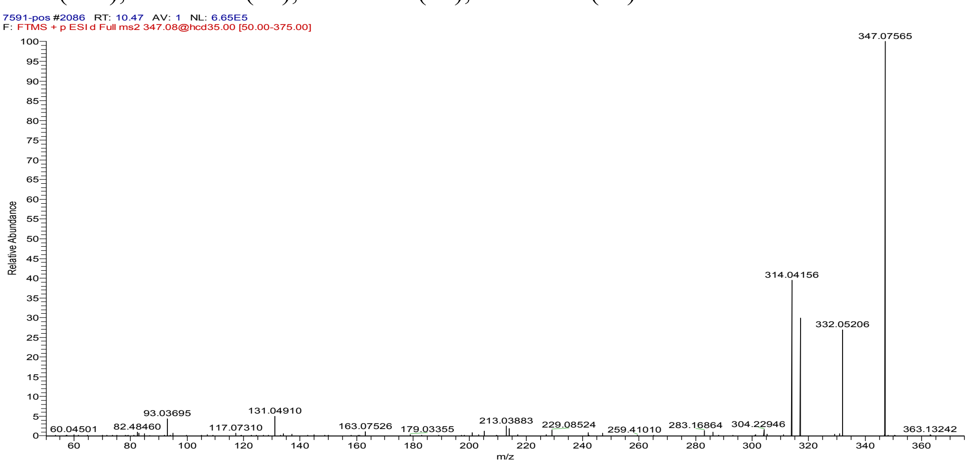
S97 Isomer of S57 (Tetrahydroxy-dimethoxyflavone) (t_R=10.39 min)

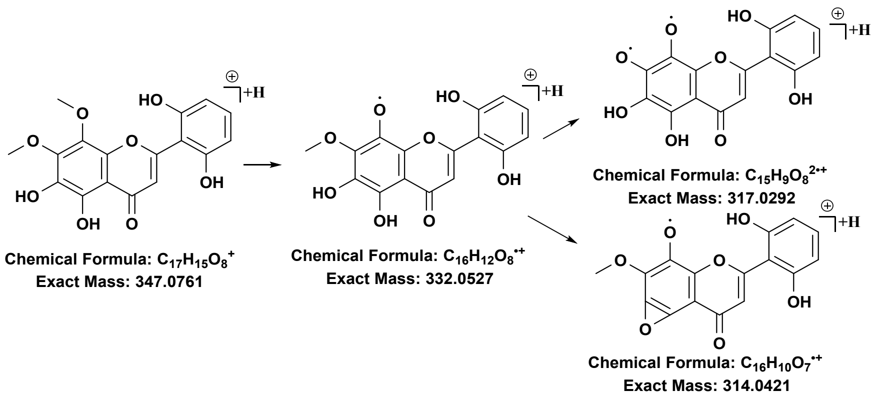
MS^1(+):

347.07572

MS^2(+):

347.07565(100),332.05206(26),317.02866(28),314.04156(37)





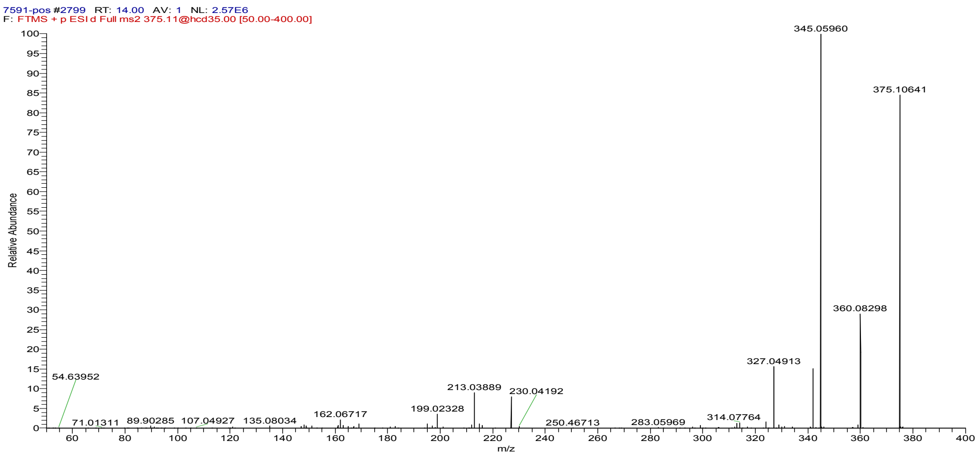
5,6'-Dihydroxy-6,7,8,2'-tetramethoxyflavone (t_R=14.00 min)[61]

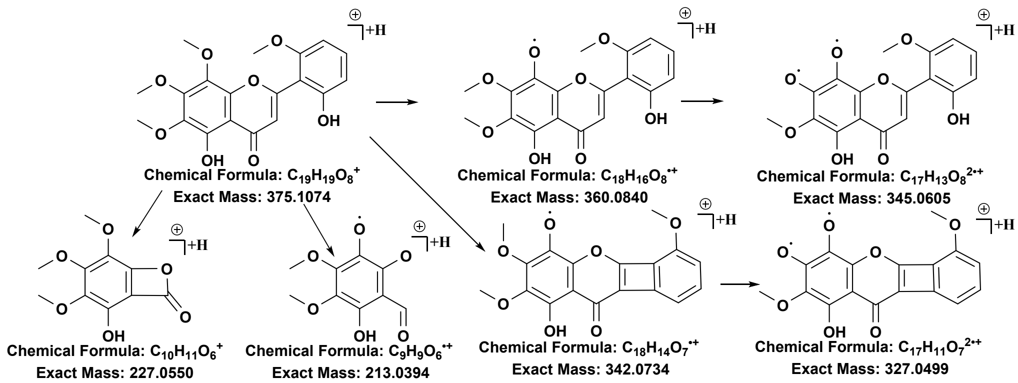
$MS^1(+)$:

375.10704

$MS^2(+)$:

360.08298(30),345.05960(100),342.07272(15),327.04913(16),227.05446(8),213.03889(9)





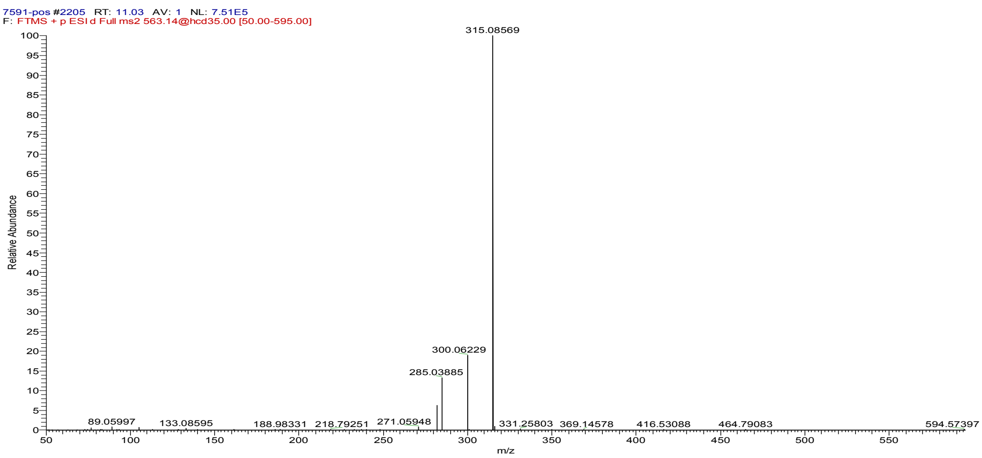
Dihydroxy-dimethoxyflavone *O*-6''-malonylglucoside (t_R=11.14 min)[79]

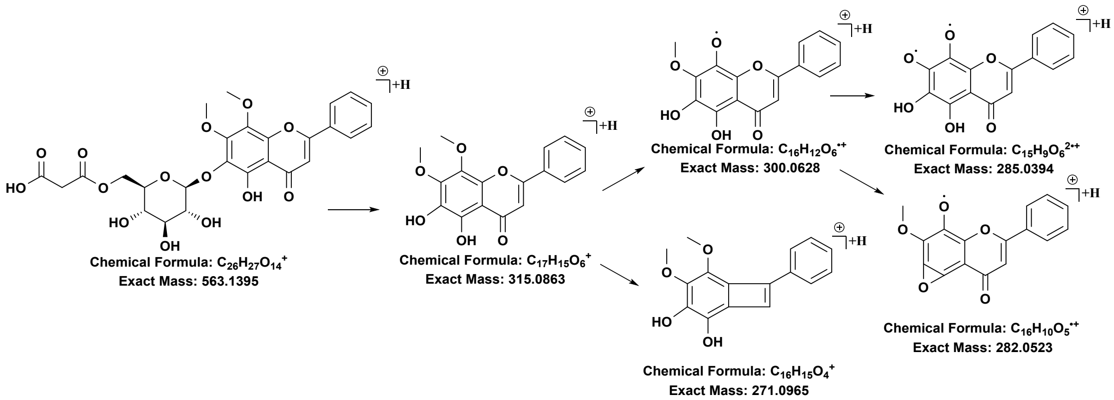
MS^1(+):

563.13929

MS^2(+):

315.08569(100),300.06229(19),285.03885(13),282.05182(7)





S100

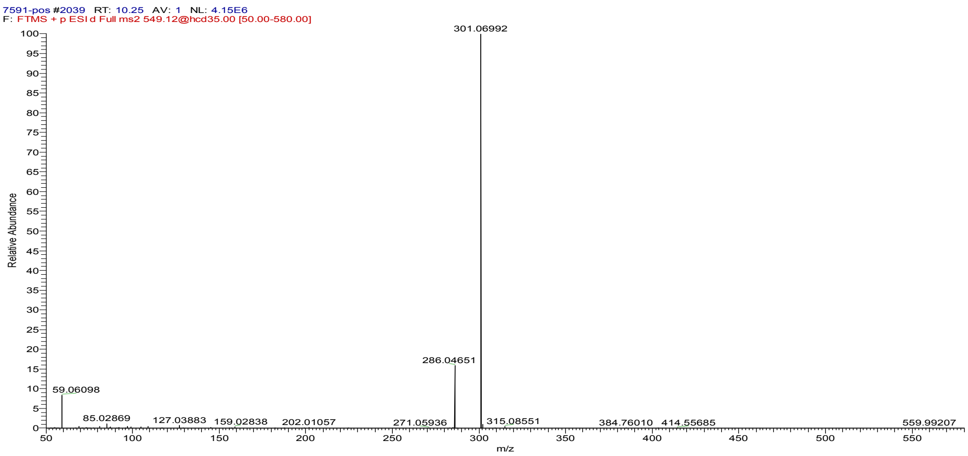
Trihydroxy-methoxyflavone *O*-6''-malonylglucoside (t_R=10.35 min)

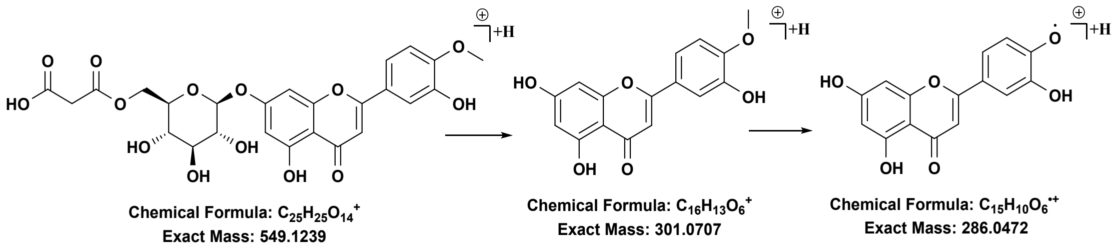
MS[1](+):

549.12346 (positive)

MS[2](+):

301.06992(100),286.04651(16)



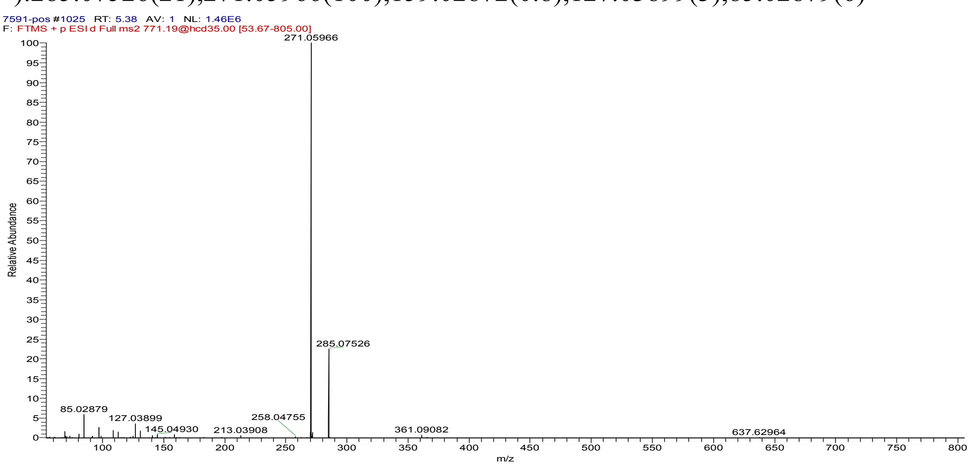


S102

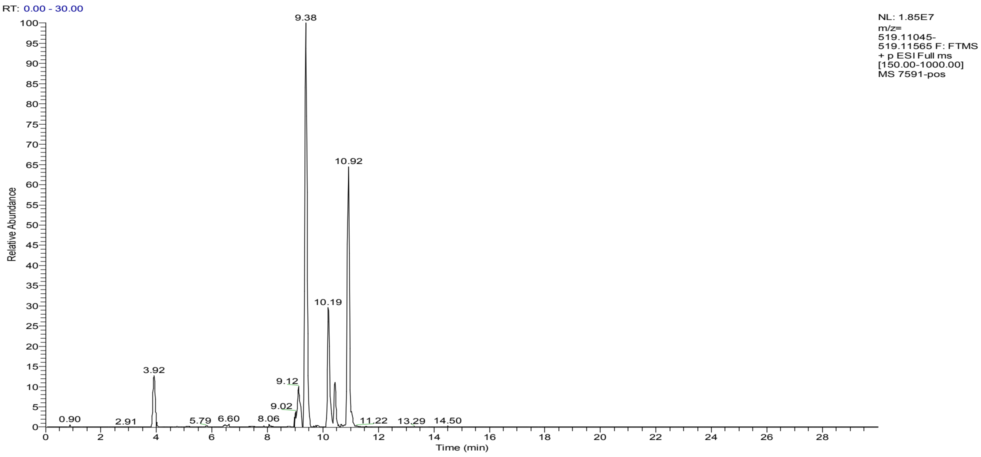
Baicalein 7-*O*-β-D-glucuronide-(1→3)[β-D-glucoside-(1→6)]-β-D-glucoside[80] (t_R 5.51)

MS[1](+):771.19748

MS[2](+):285.07526(21),271.05966(100),159.02872(0.8),127.03899(3),85.02879(6)



S103, and S106



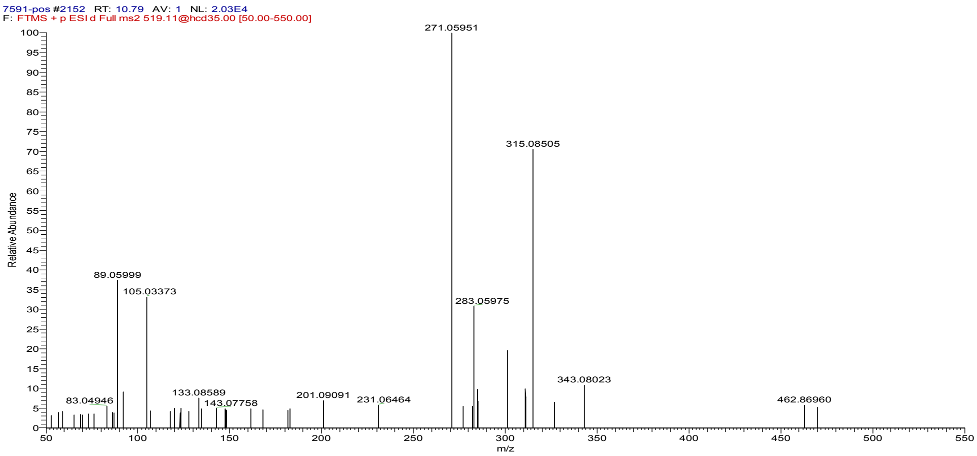
S103 Trihydroxyflavone *O*-(6''-malonylglucoside) (Isomer of apigenin 7-(6''-malonylglucoside)) (t_R=10.93 min)

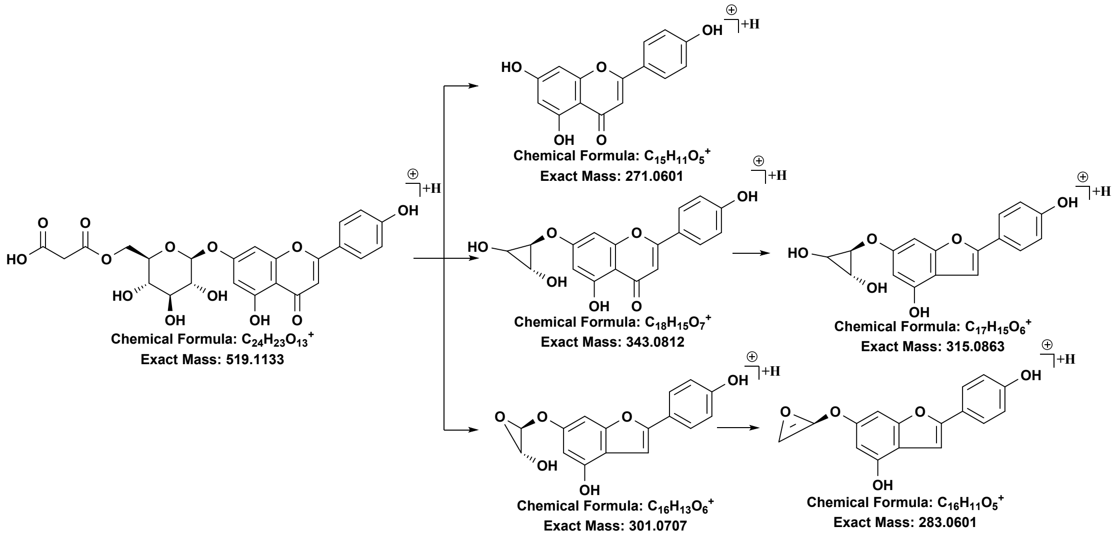
$MS^1(+)$:

519.11305

$MS^2(+)$:

343.08023(10),315.08505(69),311.05420(10),301.07013(20),283.05975(29),271.05951(100),231.06464(5),201.09091(7)





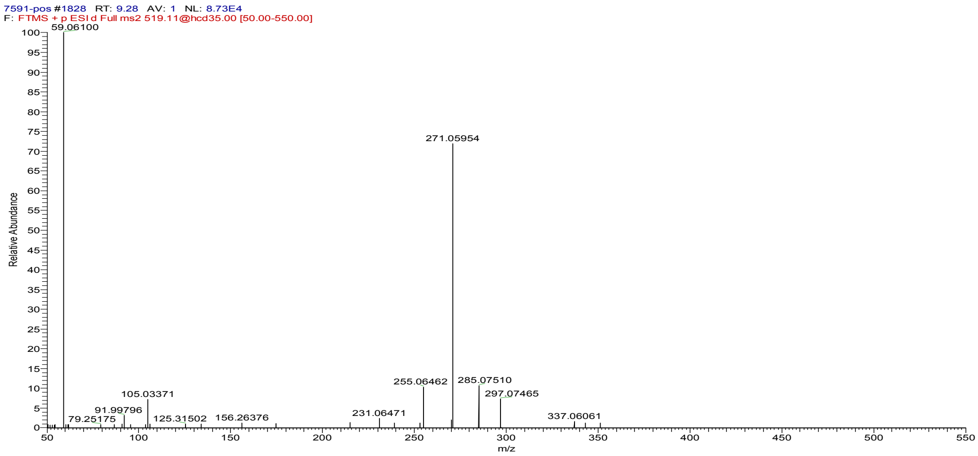
S106 Isomer of S103 (Trihydroxyflavone *O*-(6''-malonylglucoside)) (t_R=9.38 min)

MS[1](+):

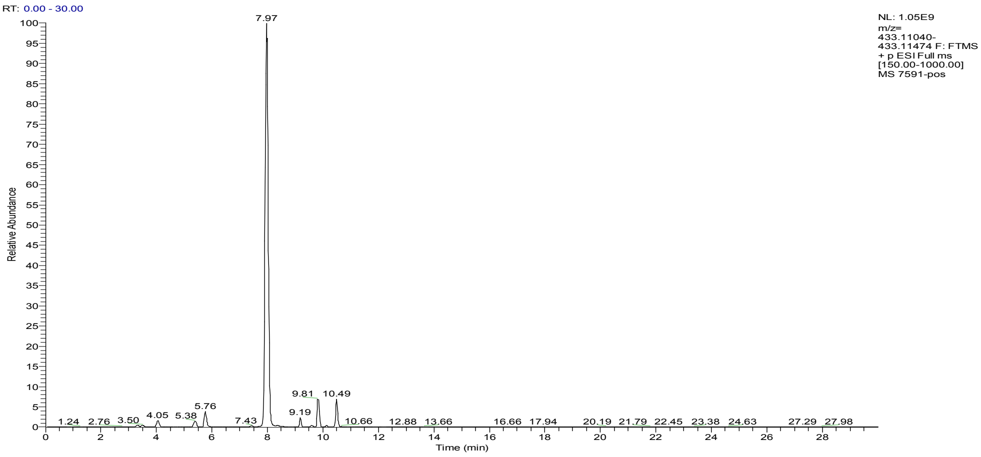
519.1129

MS[2](+):

337.06061(2),297.07465(7),285.07510(10),271.05954(73),255.06462(10),239.06934(1),231.06471(2),215.07065(1),174.55710(1),156.26376(1),105.03371(7),59.06100(100)



S104, and S108



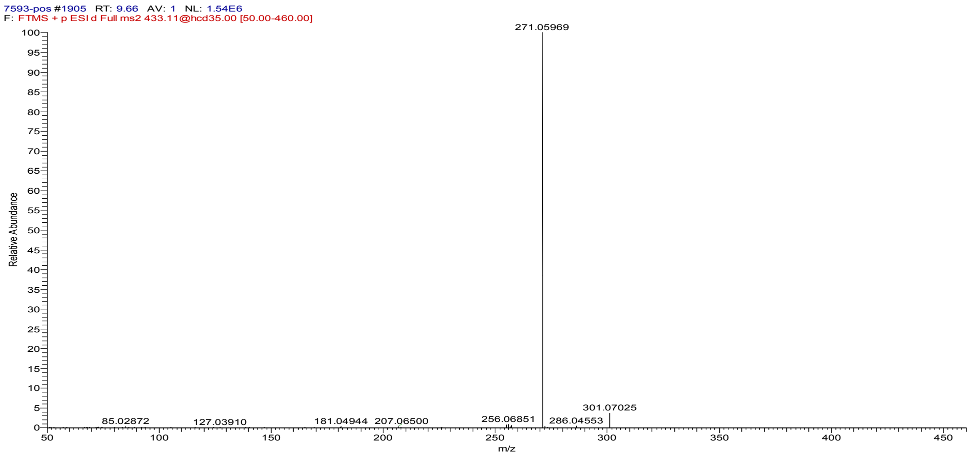
S104 Isomer of Baicalein 7-*O*-glucoside (Trihydroxyflavone *O*-glucoside) (t_R=9.49 min)[61]

$MS^1(+)$:

433.11257

$MS^2(+)$:

271.05969(100)



S105

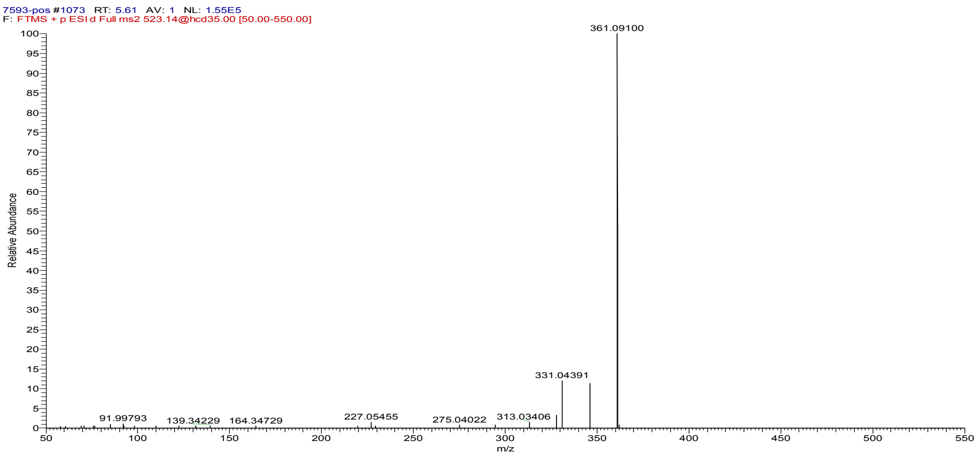
Trihydroxy-trimethoxyflavone-*O*-glucoside (t_R=5.72 min)[62]

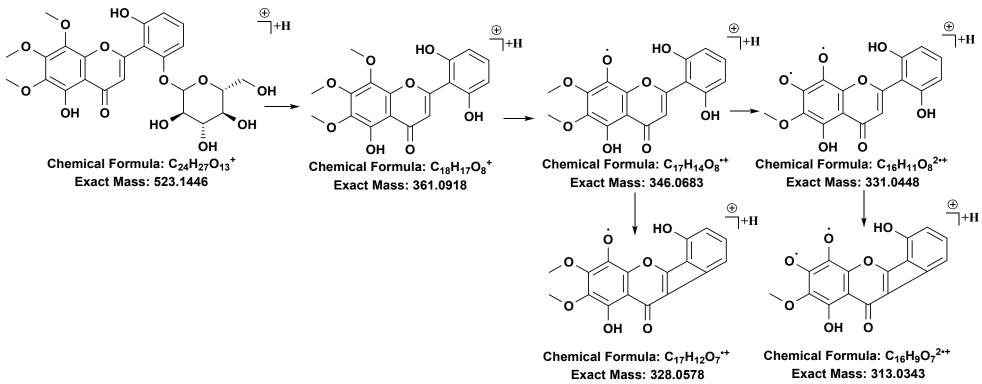
MS[1](+):

523.14417

MS[2](+):

361.09100(100),346.06732(8),331.04391(8),328.05756(3),313.03406(3)



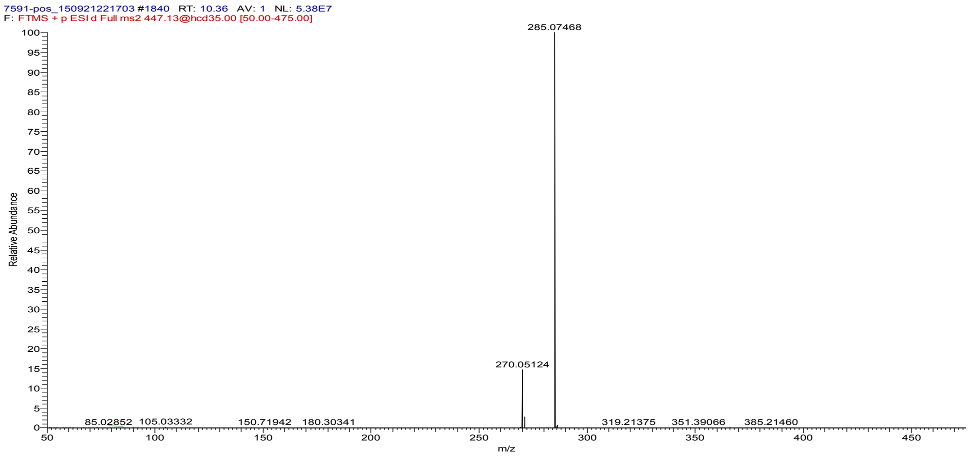


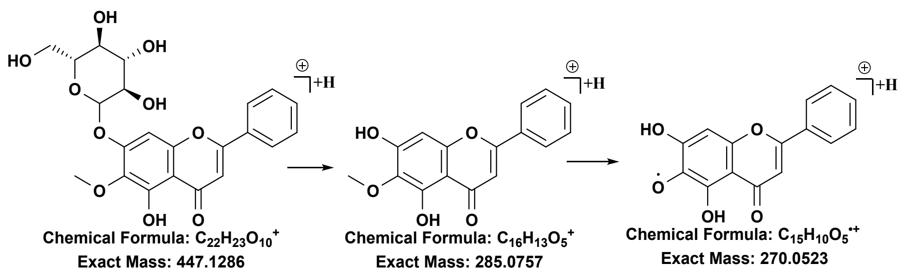
S107

Oroxylin A 7-*O*-glucoside (t_R=10.34 min)[61]

MS[1](+):447.12802

MS[2](+):285.07468(100),270.05124(15)



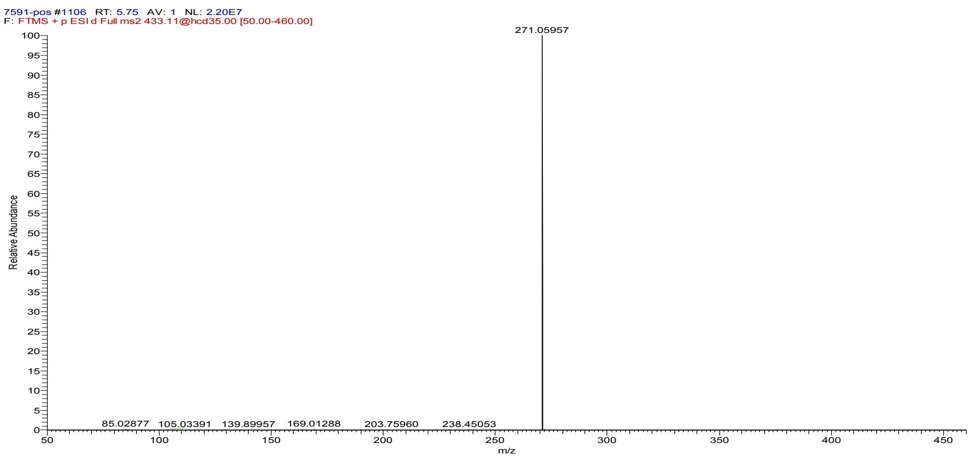


S108

Isomer of Baicalein 7-*O*-glucoside (Trihydroxyflavone *O*-glucoside) (t_R=9.49 min)[61] (tR 5.77)

MS[1](+):433.11249

MS[2](+):271.05957(100),169.01288(0.1)

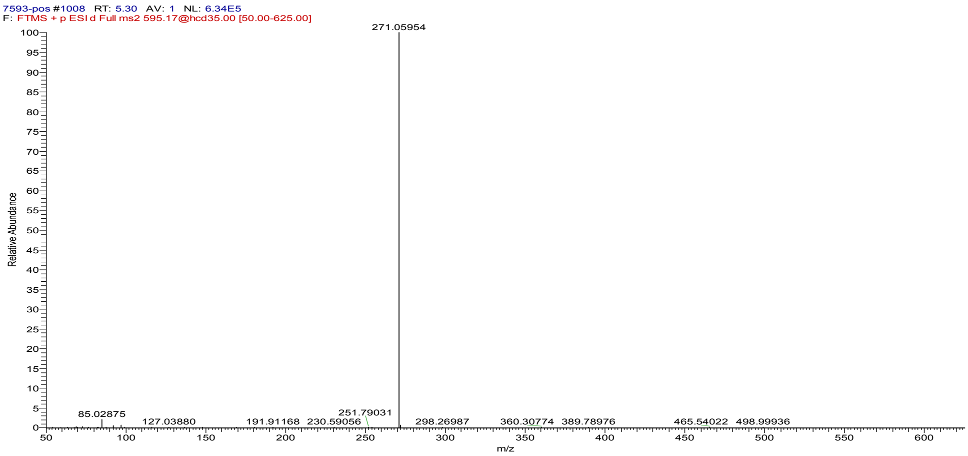


S109

Isomer of Apigenin 7-*O*-sophoroside (t_R=5.41 min)[81]

MS[1](+):595.16536

MS[2](+):271.05954(100),127.03880(1)

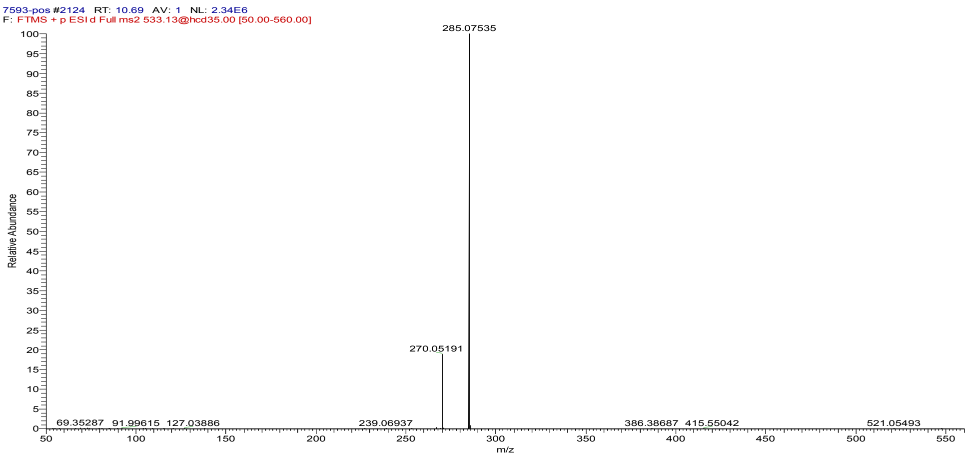


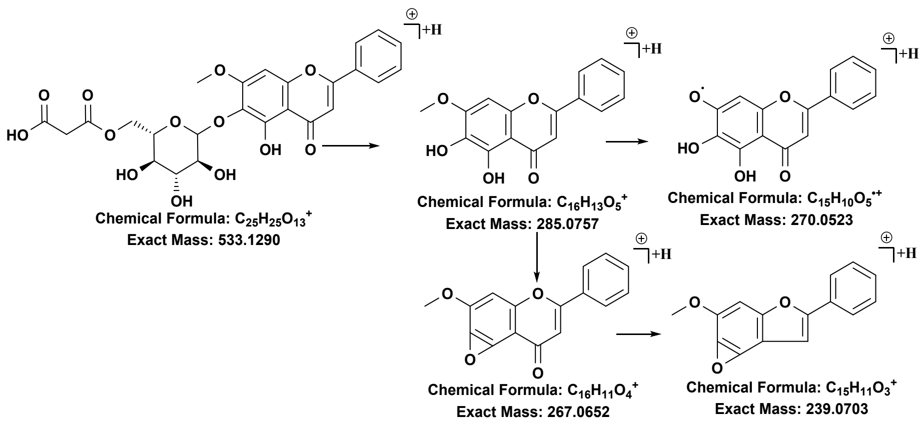
S110

Dihydroxy-methoxyflavone *O*-(6''-malonylglucoside) (t_R=10.63 min)

MS[1](+):533.12852

MS[2](+):285.07535(100),270.05191(18),267.06497(0.3),253.04749(0.1),239.06937(0.1)





S111

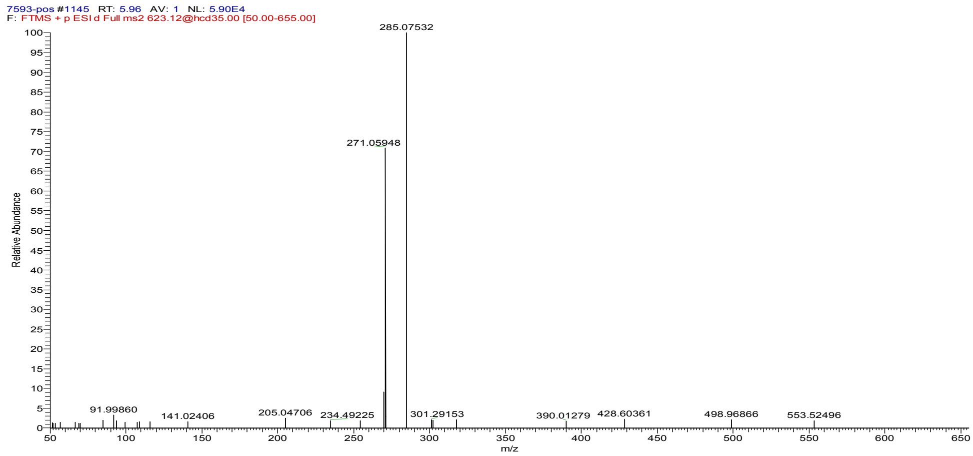
Isomer of Clerodendrin (t_R=5.97 min)[66]

MS[1](+):

623.12372

MS[2](+):

285.07532(100),271.05948(68),270.05182(15)



S112

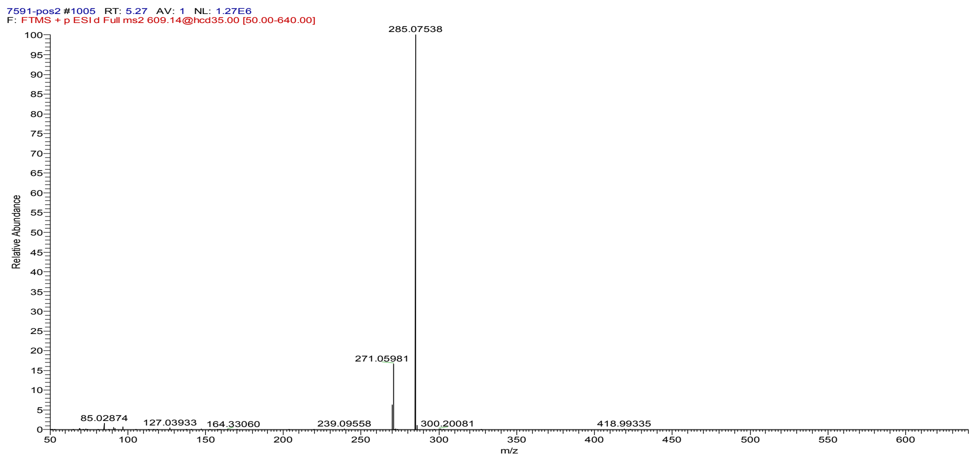
Isomer of Acacetin 7-*O*-β-sophoroside (t_R=5.36 min)

MS[1](+):

609.18105

MS[2](+):

285.07538(100),271.05981(15),270.05107(6)



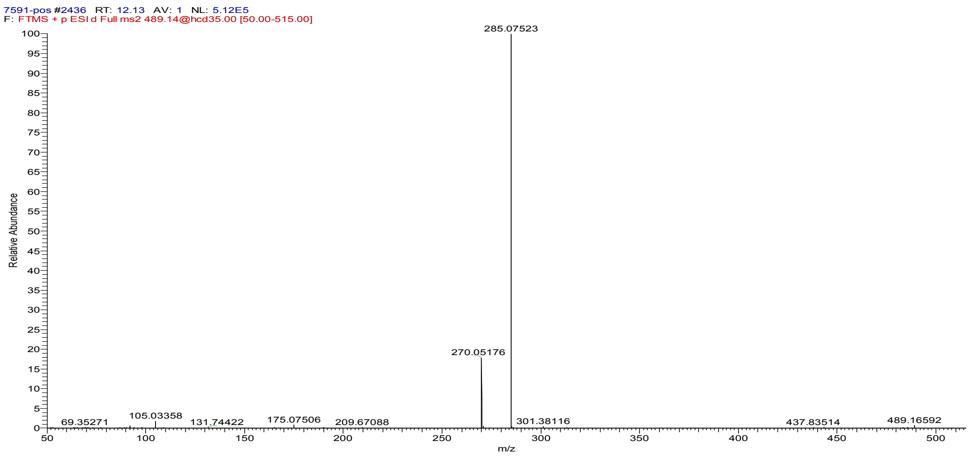
Dihydroxy-methoxyflavone *O*-glucuronide ethyl ester (t_R=12.13 min)[67]

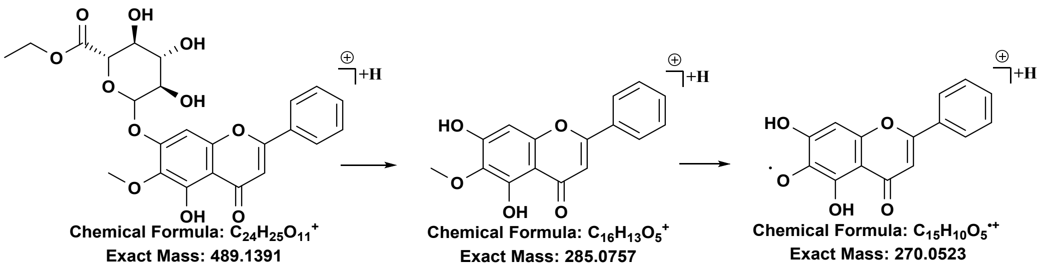
MS[1](+):

489.13876

MS[2](+):

285.07523(100),270.05176(18),175.07506(1),165.09137(0.2),105.03358(2)

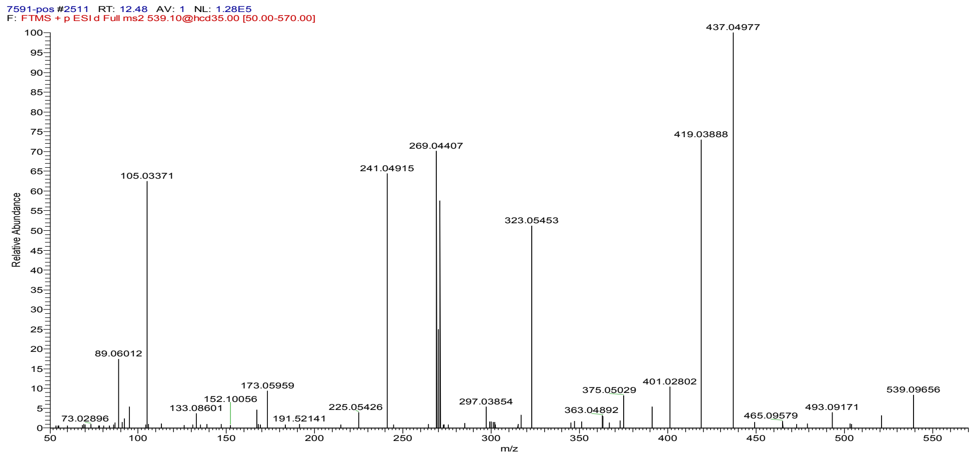


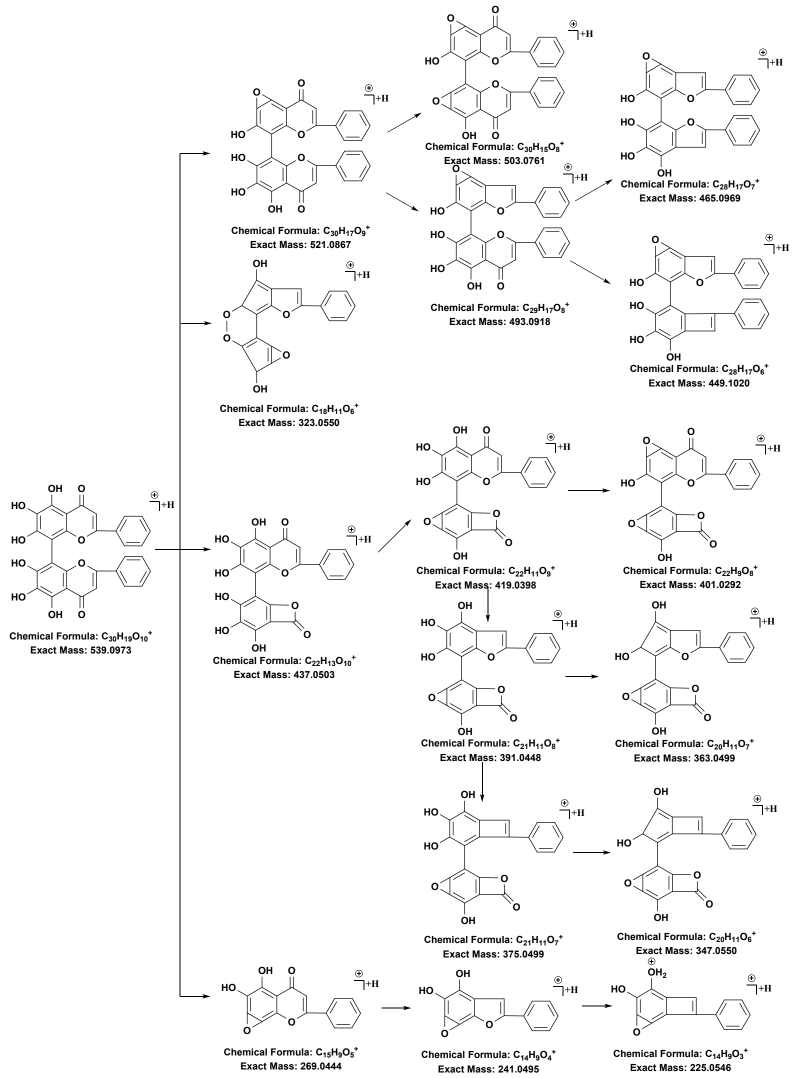


8,8'-Bibaicalein (t_R=12.57 min)[61]

MS^1(+):539.09695 (positive)

MS^2(+):521.08783(3),503.0761(1),493.09171(4),465.0969(2),449.1020(1),437.04977(100),419.03888(71),401.02802(10),391.04047(5),375.05029(8),363.0499(3),347.0550(2),323.05453(50),297.03854(6),271.05960(58),270.04407(24),269.04407(70),241.04915(62),225.05426(4)



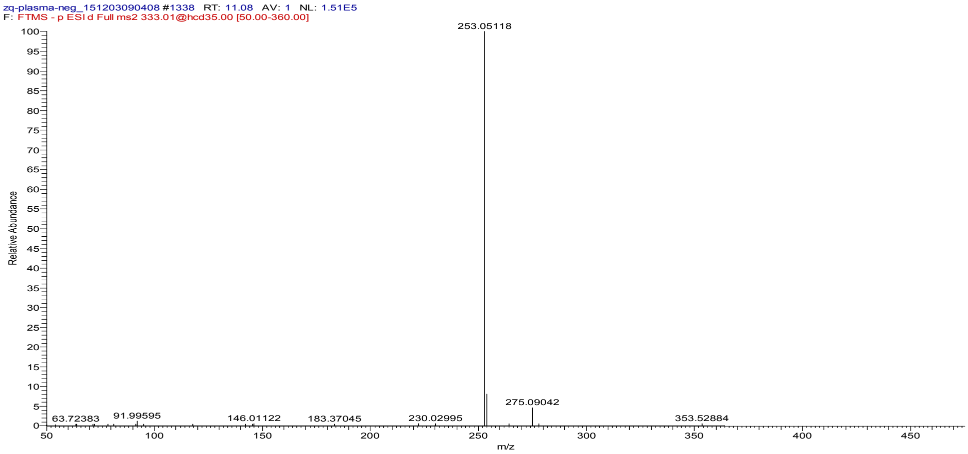


M1

Chrysin *O*-sulfate (t_R=11.1 min)

MS^1(−):333.00798

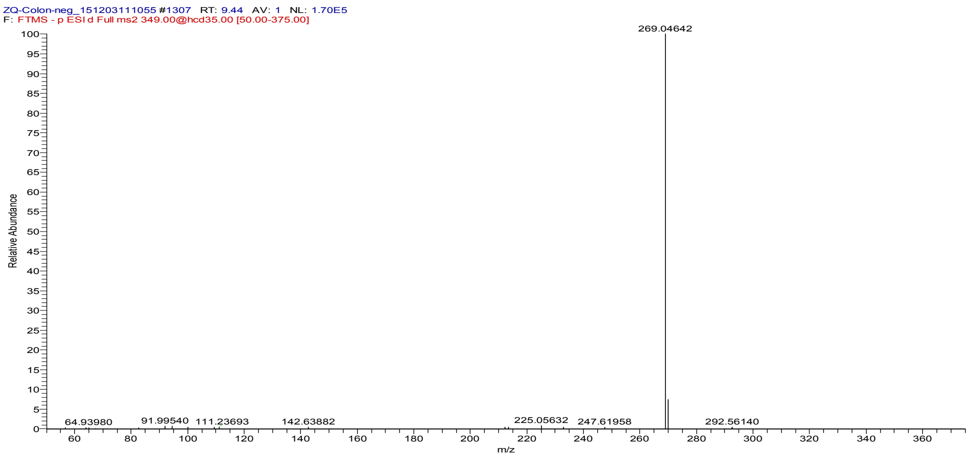
MS^2(−):253.05118(100)



M2 Apigenin *O*-sulfate (t_R=9.50 min)

MS^1(−):349.00297

MS^2(−):269.04642(100),225.05632(1)

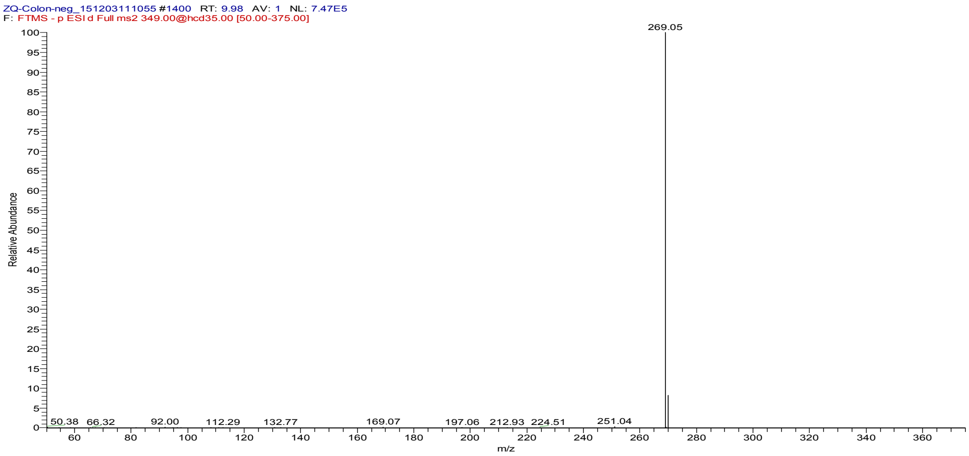


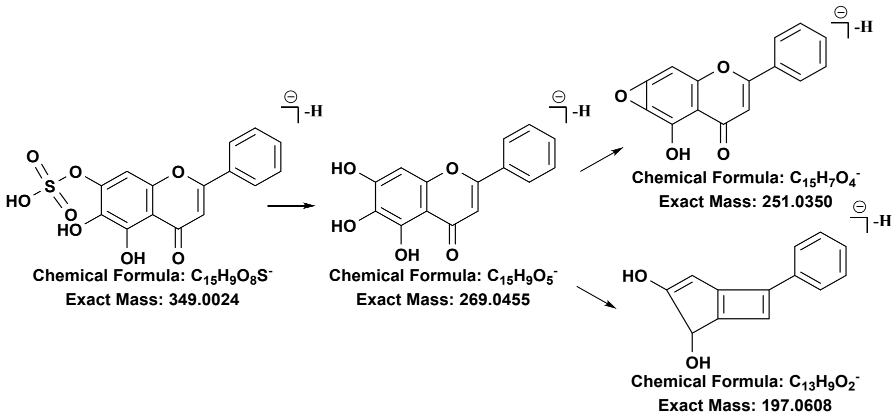
M3

Baicalein *O*-sulfate (t_R=10.06 min)

MS[1](−):349.00301

MS[2](−):269.04636(100),251.03532(0.3),197.06163(0.1)



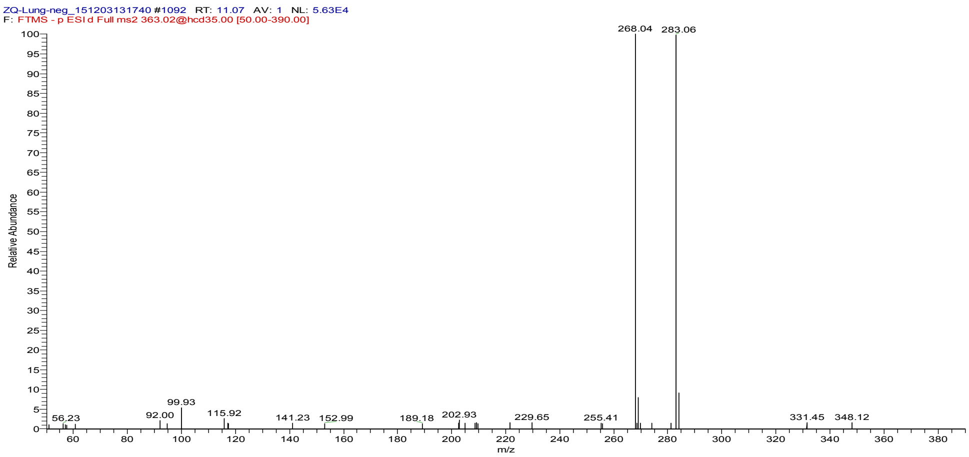


M4

Wogonin *O*-sulfate (t_R=11.10 min)

MS[1](−): 363.01881

MS[2](−):283.06204(96),268.03854(100)

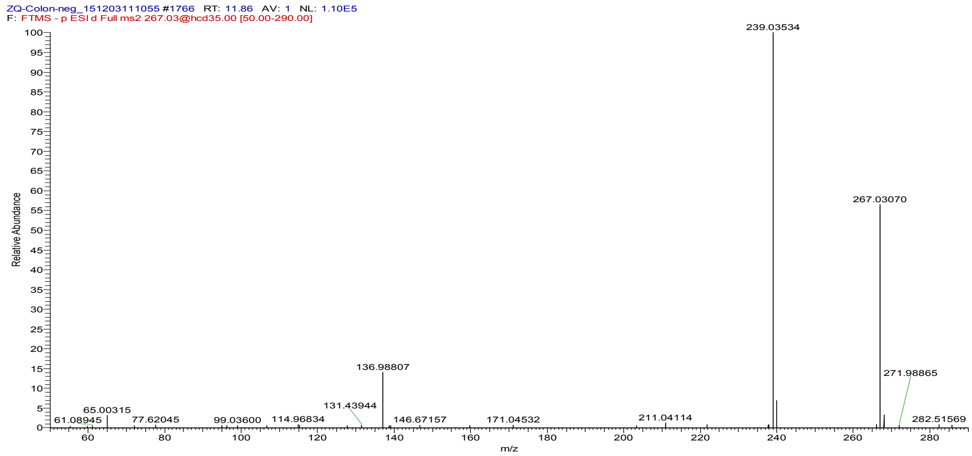


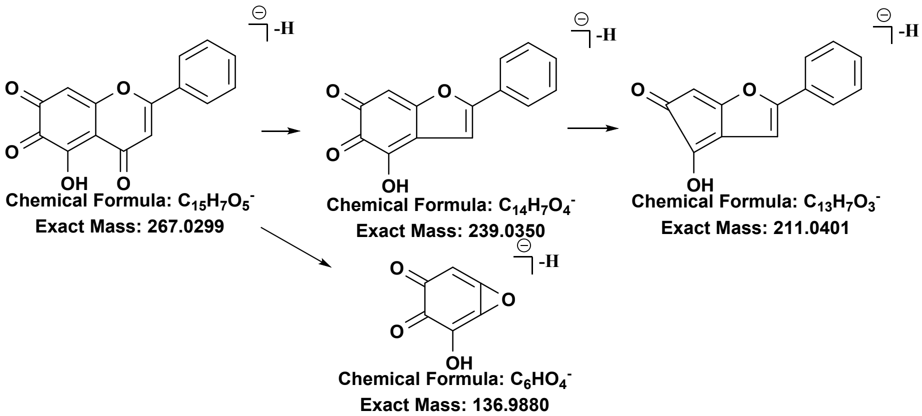
M5

6,7-Dehydrobaicalein (t_R=11.90 min)

MS[1](−): 267.03054

MS[2](−):239.03534(100),211.04114(1.14),136.98807(13.85)



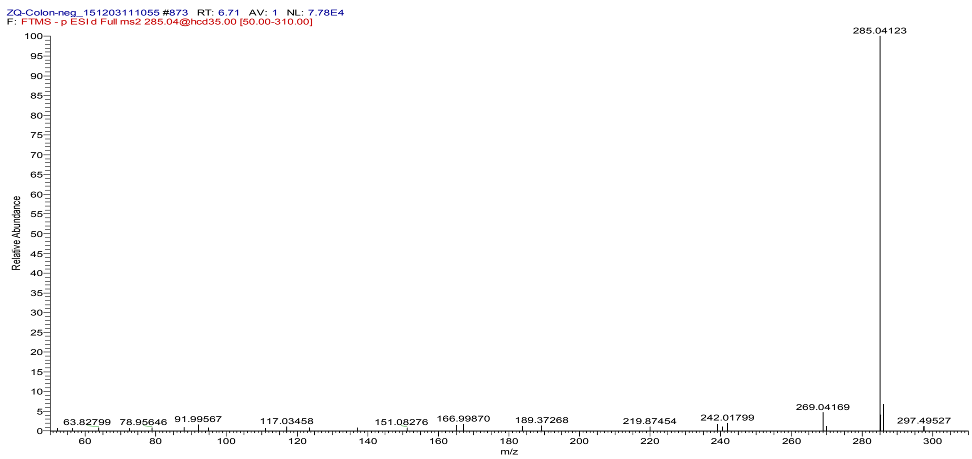


M6

Isomer of hydroxylation of baicalin (Tetrahydroxyflavone) (t_R=6.90 min)

MS[1](−):285.04126

MS[2](−):285.04123(100),151.08276(1)

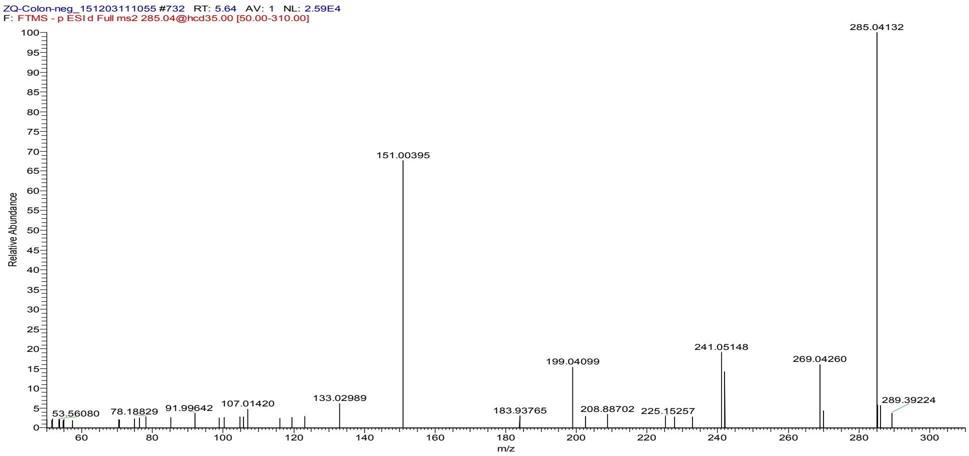


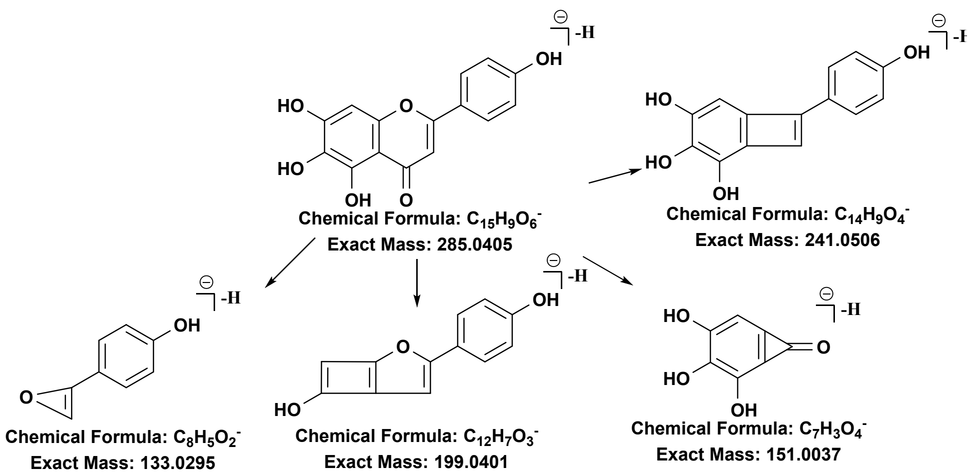
M7

Hydroxylation of baicalin (Tetrahydroxyflavone) (t_R=5.80 min)

MS[1](−):285.04125

MS[2](−):285.04132(100),241.05148(20),199.04099(15),151.00395(66),133.02989(6)





M8

Isomer of kanzakiflavone I (t_R=10.87 min)

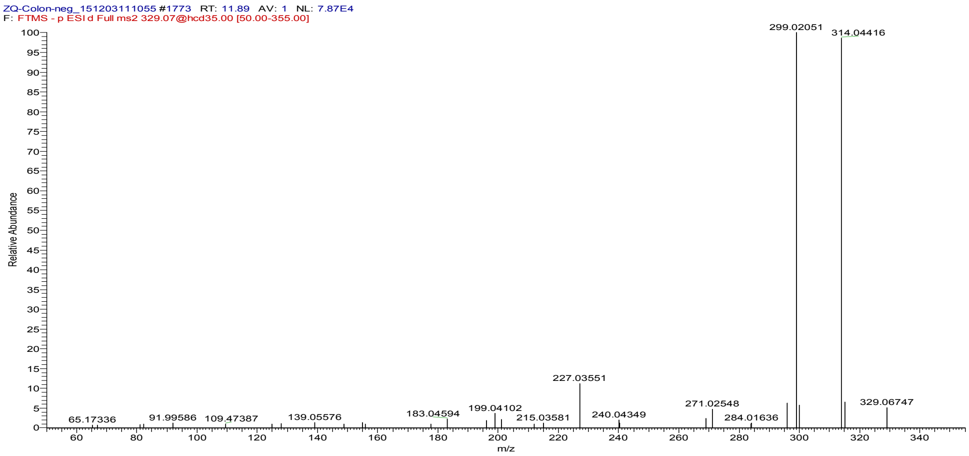
MS[1](−): 327.05179

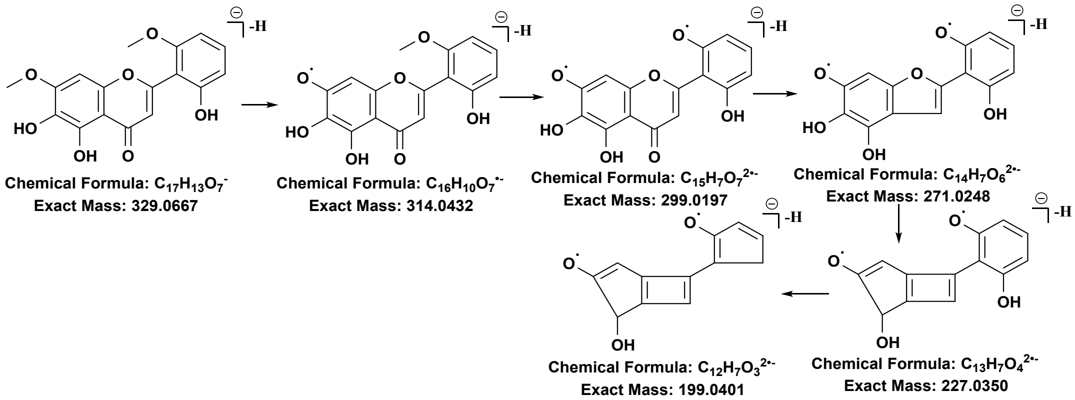
M9

Trihydroxy-dimethoxyflavone (t_R=11.80 min)

MS^1(−):329.06732

MS^2(−): 329.06747(5),314.04416(97),299.02051(100),271.02548(4),227.03551(11),199.04102(4)





M10

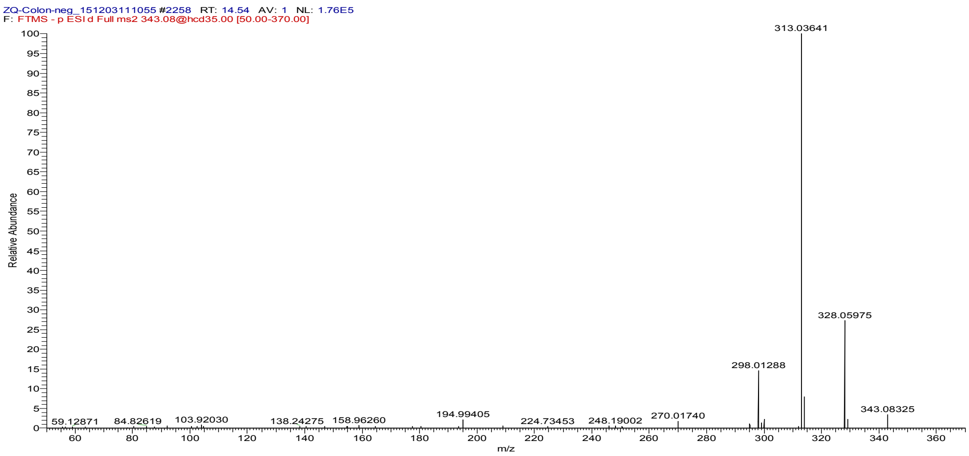
Dihydroxy-trimethoxyflavone (t_R=14.60 min)

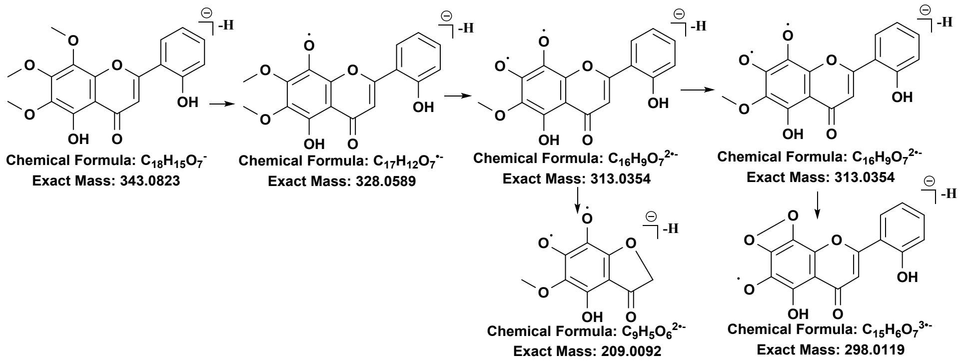
MS[1](−):

343.08295

MS[2](−):

328.05975(27),313.03641(100),298.01288(14),271.01740(2),209.00899(0.5),194.99405(2)



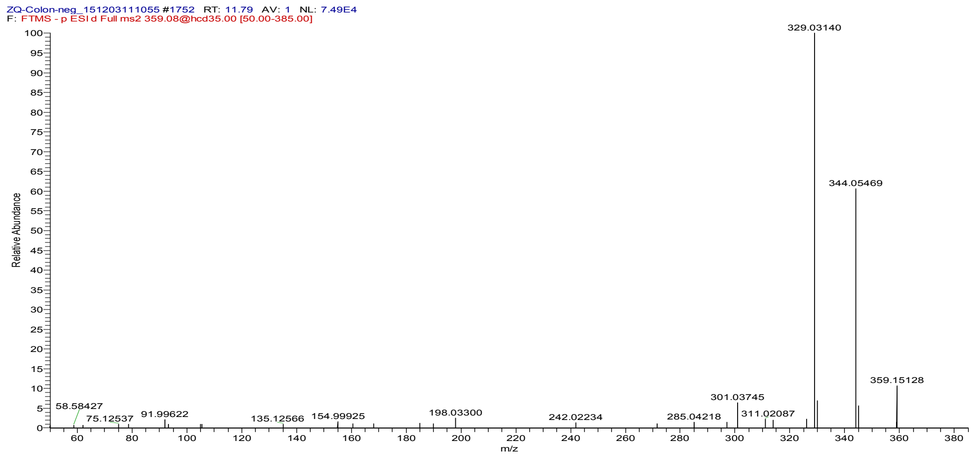


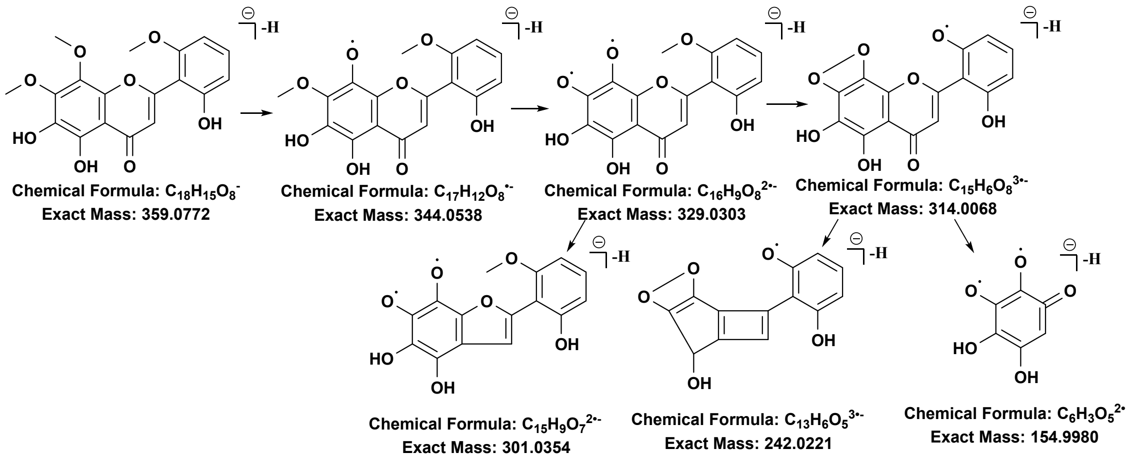
M11

Trihydroxy-trimethoxyflavone (t_R=11.80 min)

MS[1](−): 359.07789

MS[2](−):344.05469(60),329.03140(100),314.00830(2),311.02087(2),301.03745(6),297.00381(2),285.04218(1),242.02234(1),198.03300(3),154.99925(2)



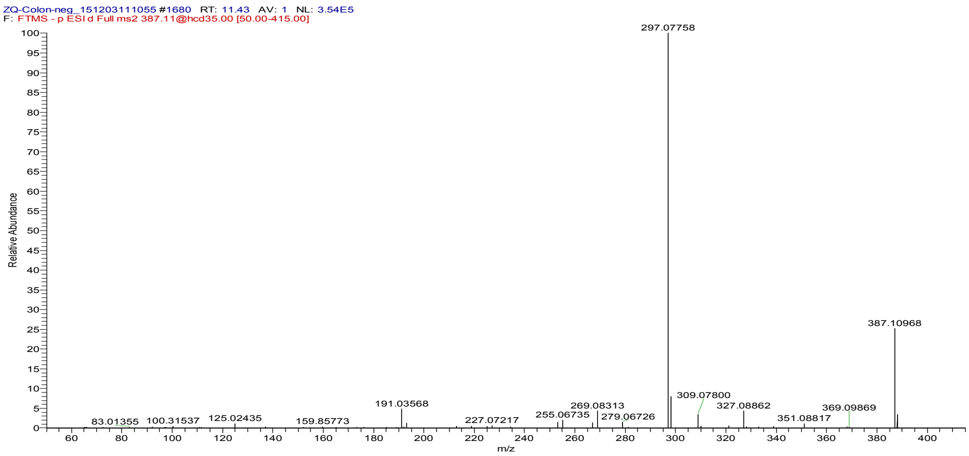


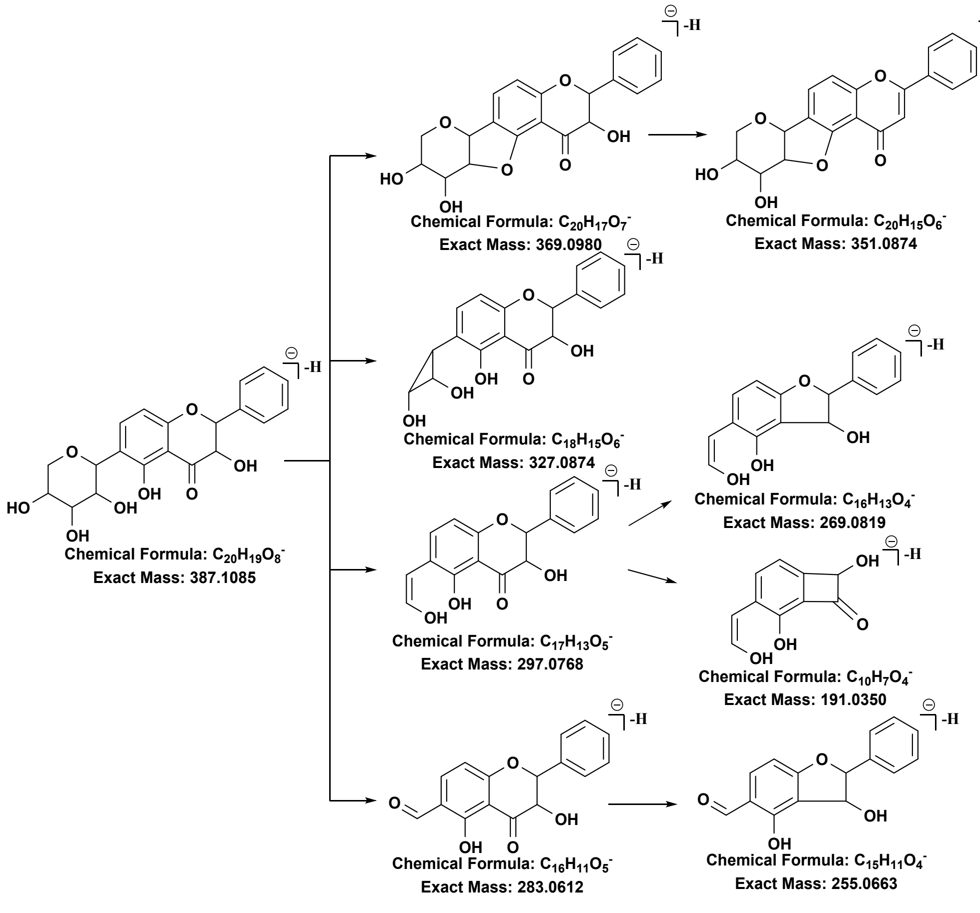
M12

2,5-Dihydroxyflavonone 6-*C*-arabinoside (t_R=11.40 min)

MS[1](−): 387.10951

MS[2](−):369.09869(0.4),351.08817(1),327.08862(4),309.08862(3),297.07758(100),269.08313(5),255.06735(2),191.03568(5)





M13

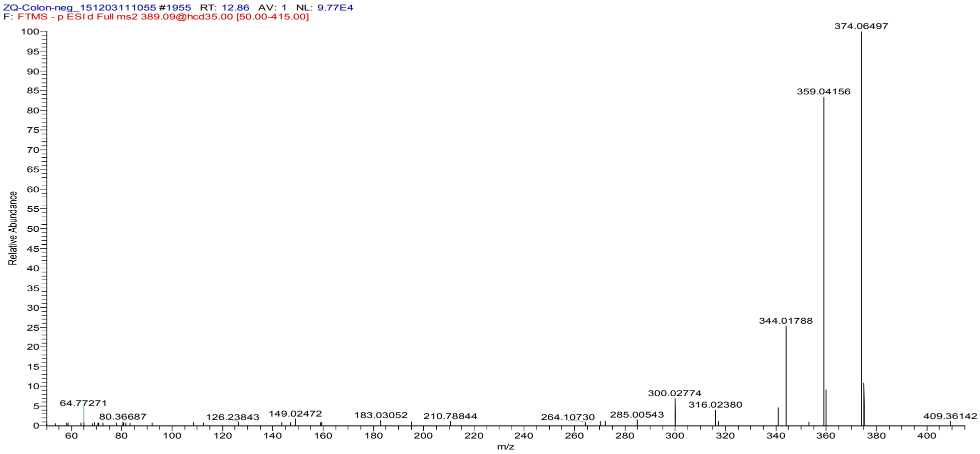
Trihydroxy-tetramethoxyflavone (t_R=12.9 min)

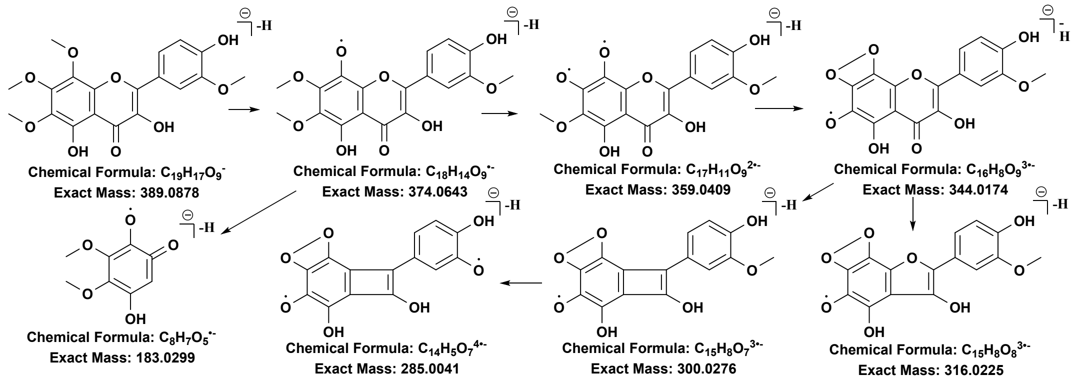
MS^1(−):

389.08871

MS^2(−):

374.06497(100),359.04156(84),344.01788(25),316.02380(4),300.02774(7),285.00543(1),183.030
52(1)





M14

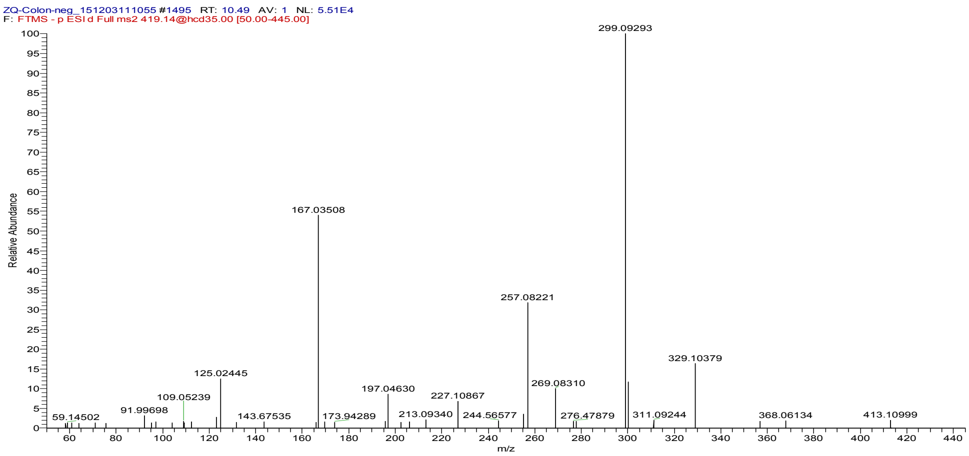
Phlorizin (t_R=10.50 min)

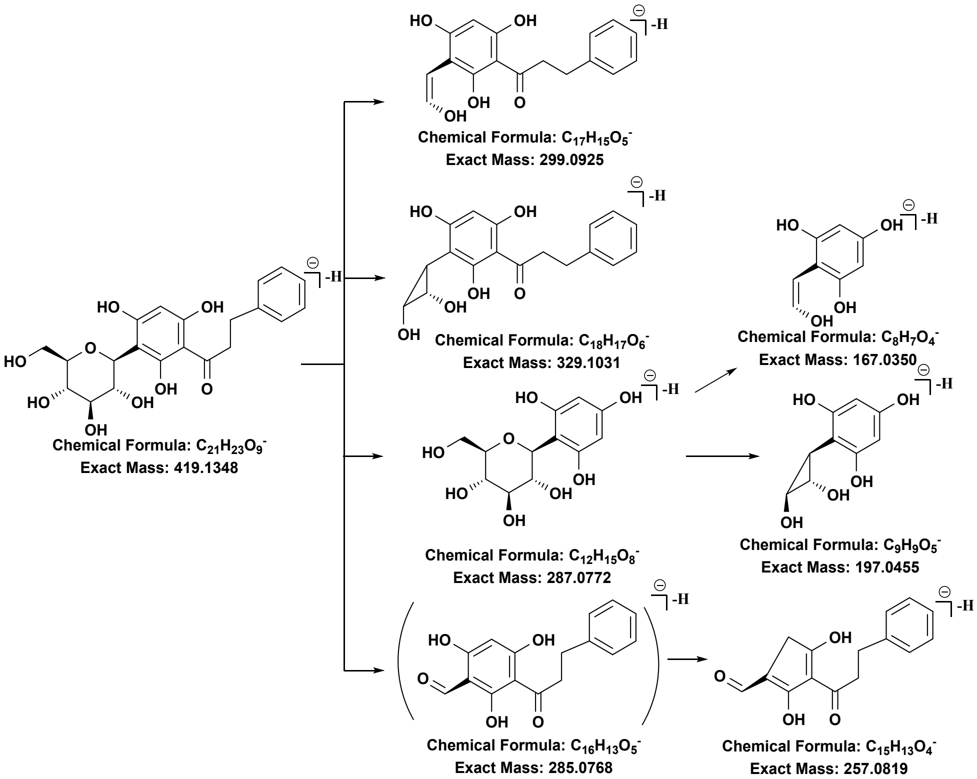
$MS^1(-)$:

419.13573

$MS^2(-)$:

329.10379(17),299.09293(100),257.08221(32),197.04630(9),195.77(2),167.03508(55)





M15

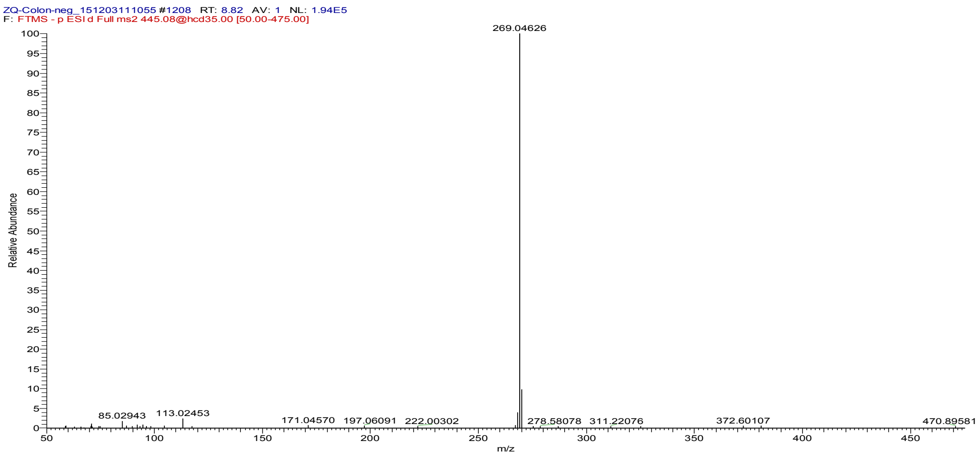
Trihydroxyflavone *O*-glucuronide (t_R=8.80 min)

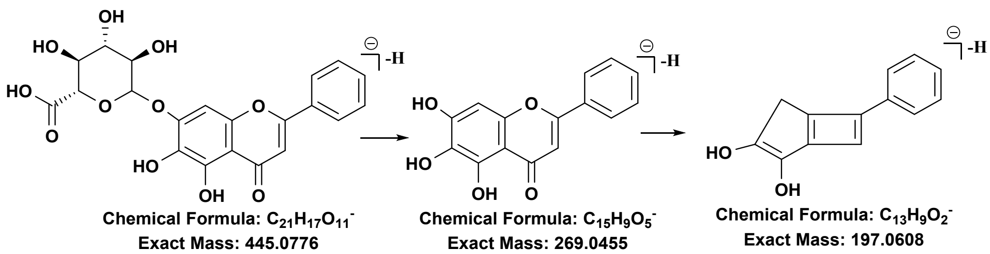
$MS^1(-)$:

445.07863

$MS^2(-)$:

269.04626(100),197.06091(0.6),171.04570(0.7),113.02453(2)





M16

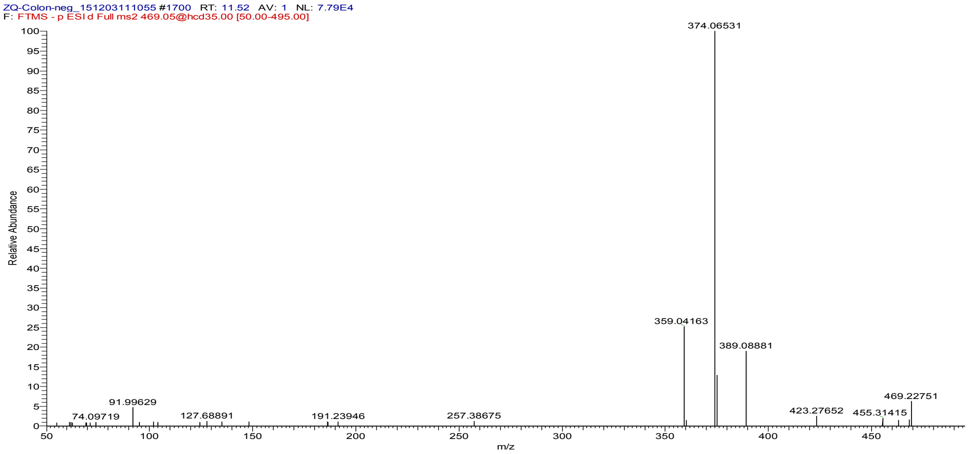
Trihydroxy-tetramethoxyflavone *O*-sulfate (t_R=11.50 min)

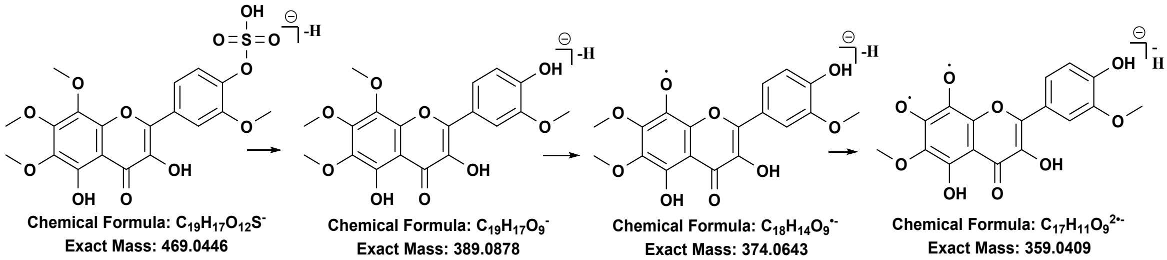
$MS^1(-)$:

469.04555

$MS^2(-)$:

389.08881(19),374.06531(100),359.04163(25)





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