

Qualitative Compound Report

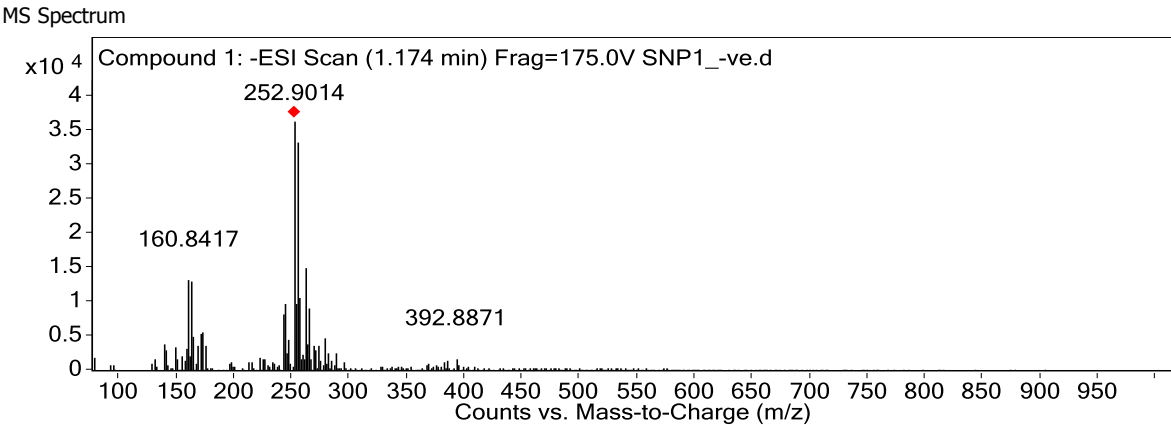
Data File	SNP1_-ve.d	Sample Name	SNP1
Sample Type	Sample	Position	P1-B8
Instrument Name	QTOF	User Name	
Acq Method	metabolite_ESI_-VE_MSMS.m	Acquired Time	7/5/2025 4:45:22 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.3)

Compound Table

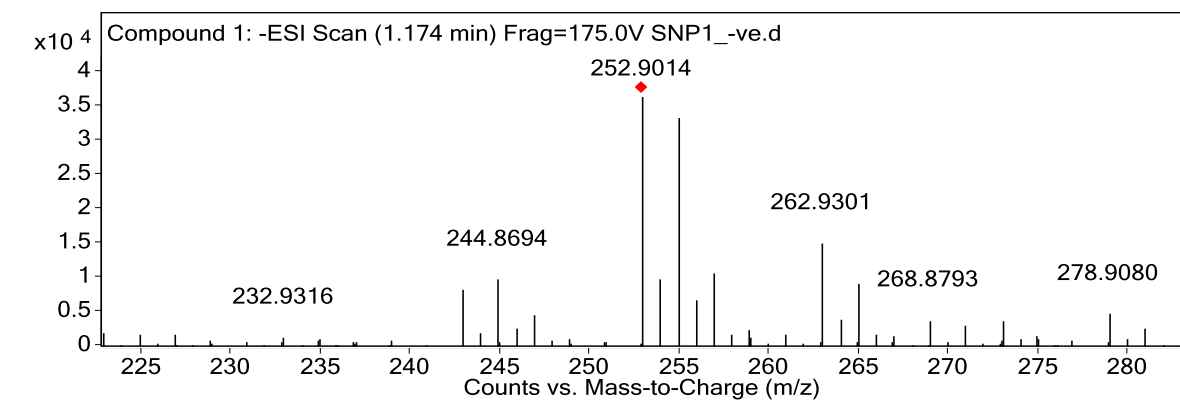
Compound Label	RT	Mass	Abund	Name	Formula	MFG Formula	DB Formula	DB Diff (ppm)	Hits (DB)
Compound 1	1.189		36414						
Compound 2	1.348								
Compound 3	1.388								
Cpd 4: Lespenefril; C27 H30 O14	8.32	578.1634	27109	Lespenefril	C27 H30 O14	C27 H30 O14	C27 H30 O14	0.27	10
Cpd 5: Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]; C28 H32 O16	9.014	624.1688		Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	C28 H32 O16	C28 H32 O16	C28 H32 O16	0.45	10
Cpd 6: 5'-Butyrylphosphoinosine; C14 H28 O9 P	9.334	418.0903	39638	5'-Butyrylphosphoinosine	C14 H19 N4 O9 P	C14 H19 N4 O9 P	C14 H19 N4 O9 P	-3.09	10
Cpd 7: 4',8-Dimethylgossypetin 3-glucoside; C23 H24 O13	9.389	508.1216		4',8-Dimethylgossypetin 3-glucoside	C23 H24 O13	C23 H24 O13	C23 H24 O13	0.12	10
Cpd 8: Lyoniresinol 9'-sulfate; C22 H28 O11 S	9.815	500.1354	51760	Lyoniresinol 9'-sulfate	C22 H28 O11 S	C22 H28 O11 S	C22 H28 O11 S	-0.42	4
Cpd 9: Aklanonic acid; C21 H16 O8	9.85	396.0844	27824	Aklanonic acid	C21 H16 O8	C21 H16 O8	C21 H16 O8	0.21	8
Cpd 10: Apimaysin; C27 H28 O13	10.204	560.1542		Apimaysin	C27 H28 O13	C27 H28 O13	C27 H28 O13	-2.2	4
Cpd 11: Aklanonic acid; C21 H16 O8	10.22	396.0855		Aklanonic acid	C21 H16 O8	C21 H16 O8	C21 H16 O8	-2.44	7
Compound 12	10.267								
Compound 13	10.306								
Cpd 14: Piceatannol 4'-galloylglucoside; C27 H26 O13	10.45	558.1367		Piceatannol 4'-galloylglucoside	C27 H26 O13	C27 H26 O13	C27 H26 O13	1.07	5
Cpd 15: Apimaysin; C27 H28 O13	10.561	560.1544		Apimaysin	C27 H28 O13	C27 H28 O13	C27 H28 O13	-2.59	4
Cpd 16: Aklanonic acid; C21 H16 O8	10.563	396.0852		Aklanonic acid	C21 H16 O8	C21 H16 O8	C21 H16 O8	-1.63	7
Compound 17	10.612								
Compound 18	10.659								
Cpd 19: Apimaysin; C27 H28 O13	10.952	560.1541	279569	Apimaysin	C27 H28 O13	C27 H28 O13	C27 H28 O13	-1.91	4
Cpd 20: Piceatannol 4'-galloylglucoside; C27 H26 O13	11.09	558.1372		Piceatannol 4'-galloylglucoside	C27 H26 O13	C27 H26 O13	C27 H26 O13	0.27	5
Cpd 21: Apimaysin; C27 H28 O13	11.224	560.1537	107478	Apimaysin	C27 H28 O13	C27 H28 O13	C27 H28 O13	-1.2	4
Cpd 22: Aklanonic acid; C21 H16 O8	11.316	396.0848	55785	Aklanonic acid	C21 H16 O8	C21 H16 O8	C21 H16 O8	-0.8	7
Cpd 23: Gyrocyenin; C17 H12 O5	12.923	296.0686	51908	Gyrocyenin	C17 H12 O5	C17 H12 O5	C17 H12 O5	-0.53	10
Cpd 24: Gyrocyenin; C17 H12 O5	13.298	296.0684	34460	Gyrocyenin	C17 H12 O5	C17 H12 O5	C17 H12 O5	0.32	10
Cpd 25: 2-Decarboxytetrangomycin; C20 H34 O7	13.685	366.0743	39843	2-Decarboxytetrangomycin	C20 H14 O7	C20 H14 O7	C20 H14 O7	-0.81	10
Cpd 26: Gravelliferone; C19 H22 O3	21.324	298.16	34267	Gravelliferone	C19 H22 O3	C19 H22 O3	C19 H22 O3	-10.49	8
Cpd 27: 5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone; C19 H22 O3	21.71	298.16		5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone	C19 H22 O3	C19 H22 O3	C19 H22 O3	-10.25	7
Cpd 28: G-418; C20 H40 N4 O10	24.712	496.2712		G-418	C20 H40 N4 O10	C20 H40 N4 O10	C20 H40 N4 O10	6.44	3
Cpd 29: G-418; C20 H40 N4 O10	25.08	496.2709		G-418	C20 H40 N4 O10	C20 H40 N4 O10	C20 H40 N4 O10	7.15	3
Compound 30	28.79		21346						

Compound Label	m/z	RT	Algorithm
Compound 1	252.9014	1.189	Auto MS/MS

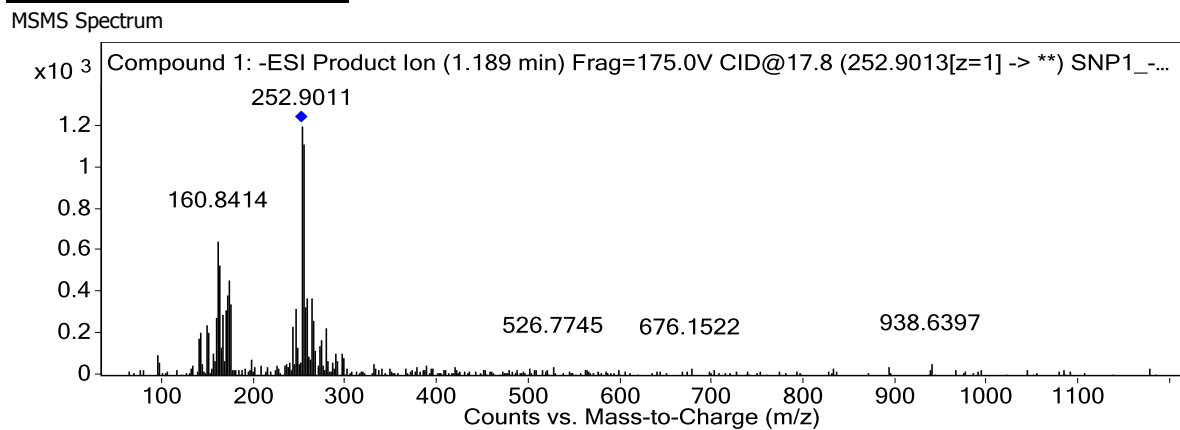


MS Zoomed Spectrum

Qualitative Compound Report

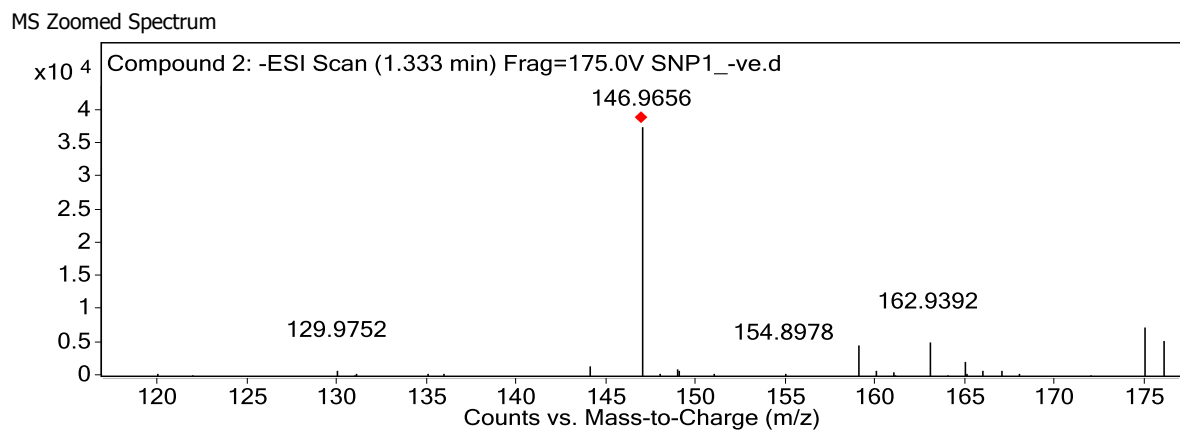
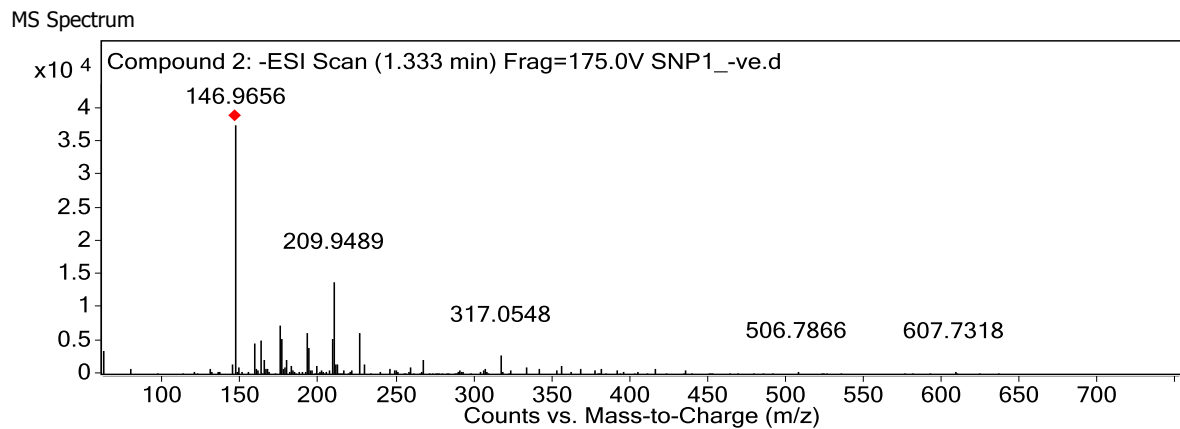


MS Spectrum Peak List		
m/z	z	Abund
160.8417	1	13201.43
162.8391	1	13046.76
244.8694	1	9723.99
252.9014	1	36413.64
253.9021	1	9776.88
254.8985	1	33195.13
255.8994	1	6714.06
256.8958	1	10571.03
257.8964	1	1671.77
262.9301	1	15057.36



MS/MS Spectrum Peak List		
m/z	z	Abund
160.8414	1	648.15
162.8392	1	532.47
170.8318		388.56
172.8306		456.49
174.956		346.95
252.9011	1	1201.84
253.9019	1	415.45
254.8984	1	1113.32
256.8953	1	373.63
262.9307	1	370.47

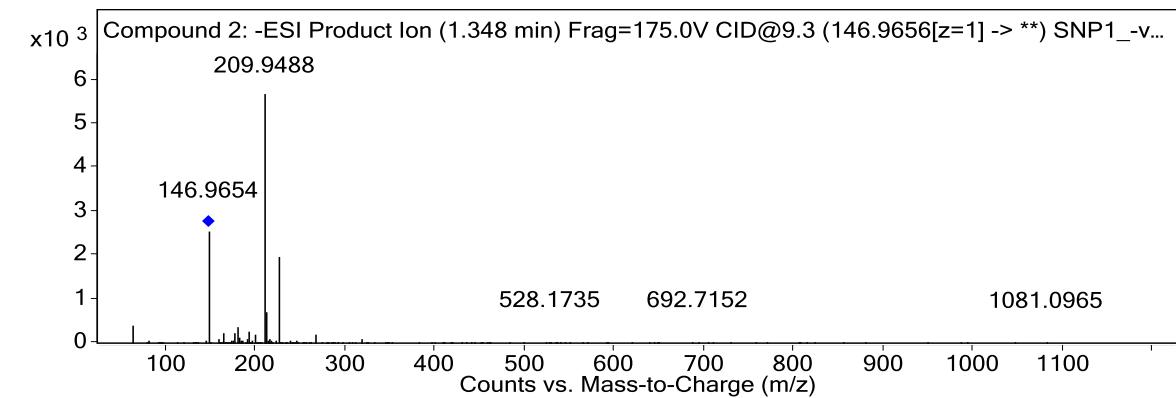
Compound Label	m/z	RT	Algorithm
Compound 2	146.9656	1.348	Auto MS/MS



MS Spectrum Peak List		
m/z	z	Abund
146.9656	1	37520.73
158.9783	1	4762.12
162.9392		5107.21
174.9559		7378.79
175.968	1	5363.18
191.9456		6305.7
192.9591	1	4094.24
208.9356		5328.73
209.9489	1	13809.8
225.9265		6203.56

MSMS Spectrum

Qualitative Compound Report

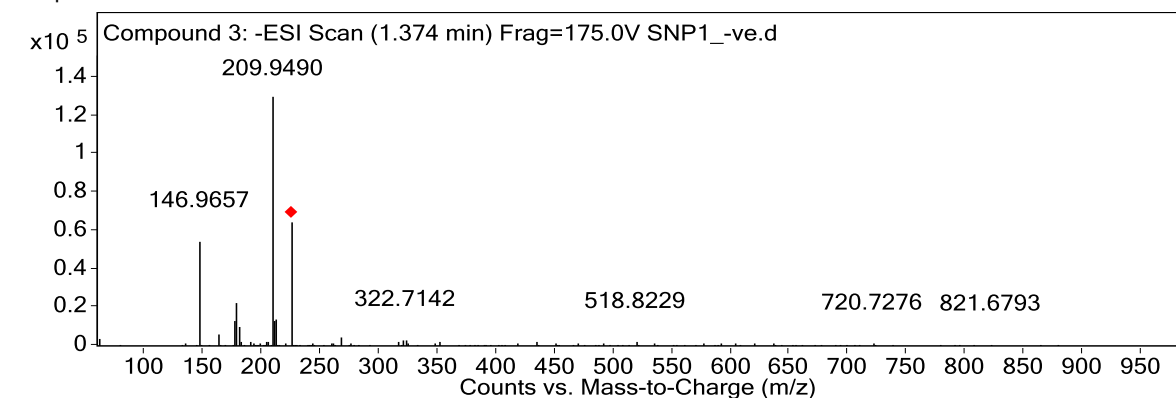


MS/MS Spectrum Peak List

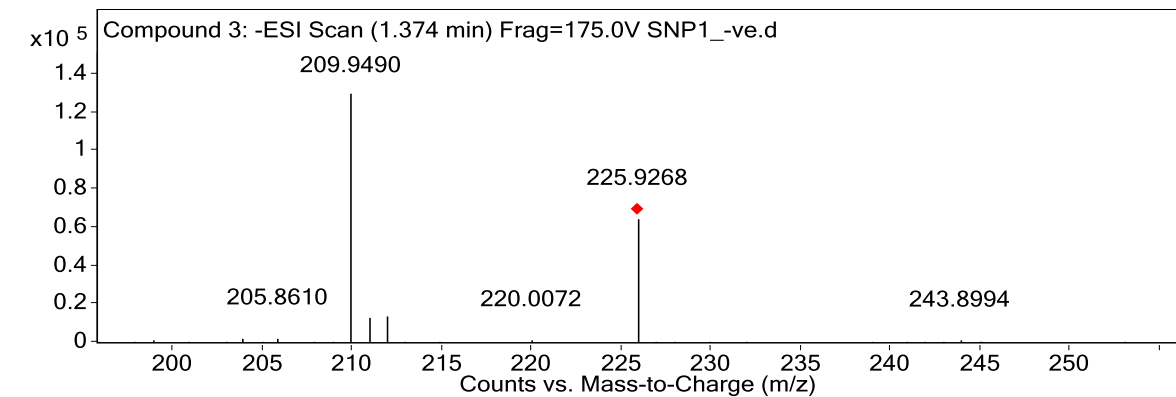
m/z	z	Abund
61.9875		418.17
146.9654	1	2552.03
162.9388		235.22
176.842		230.09
178.8419		370.15
192.9592		280
209.9488	1	5688.88
210.9481	1	726.9
211.9477	1	601.45
225.9265		1963.49

Compound Label	m/z	RT	Algorithm
Compound 3	225.9268	1.388	Auto MS/MS

MS Spectrum



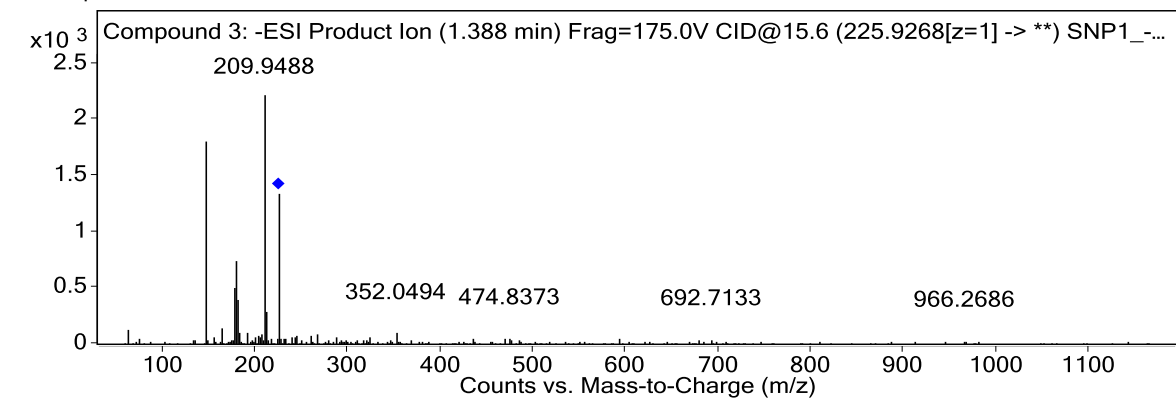
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
146.9657		54764.57
176.8429		13037.8
178.8419		22725.6
180.8398		9876.88
209.949	1	130057.52
210.9491	1	13261.03
211.9466	1	13999.02
225.9268	1	64795.61
226.9225	1	958.3
227.9298	1	1086.04

MSMS Spectrum



MS/MS Spectrum Peak List

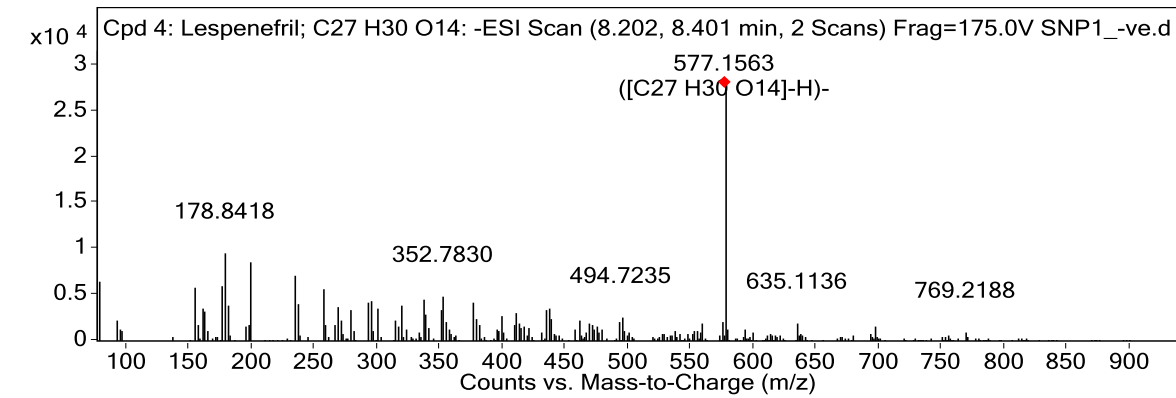
m/z	z	Abund
61.9874		127.5
146.9656		1807.73
162.9385		143.21
176.8432		504.2
178.8415		739.12
180.8395		393.44
209.9488	1	2218.99
210.9505	1	282.96
211.9468	1	291.78
225.9263		1335.13

Compound Label	Name	m/z	RT	Algorithm	Mass
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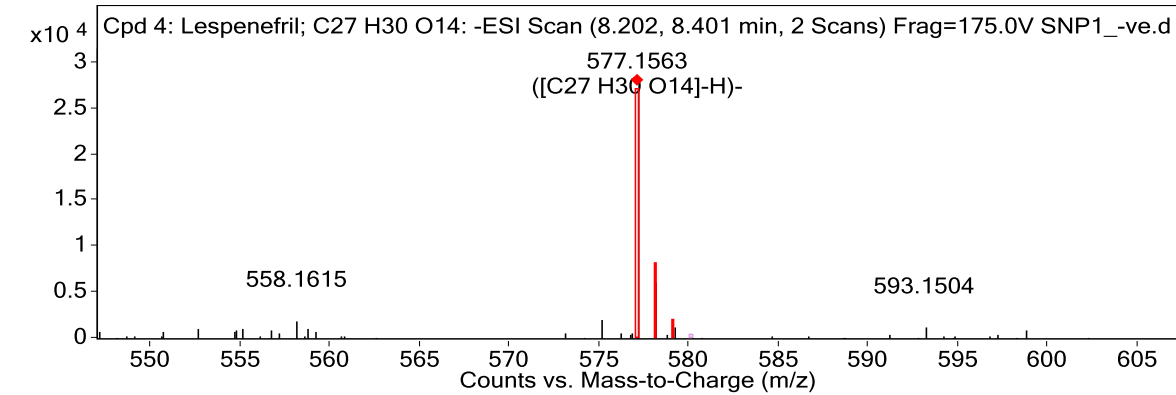
Qualitative Compound Report

Cpd 4: Lespenefril; C27 H30 O14	Lespenefril	577.1563	8.32	Auto MS/MS	578.1634
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MS Spectrum



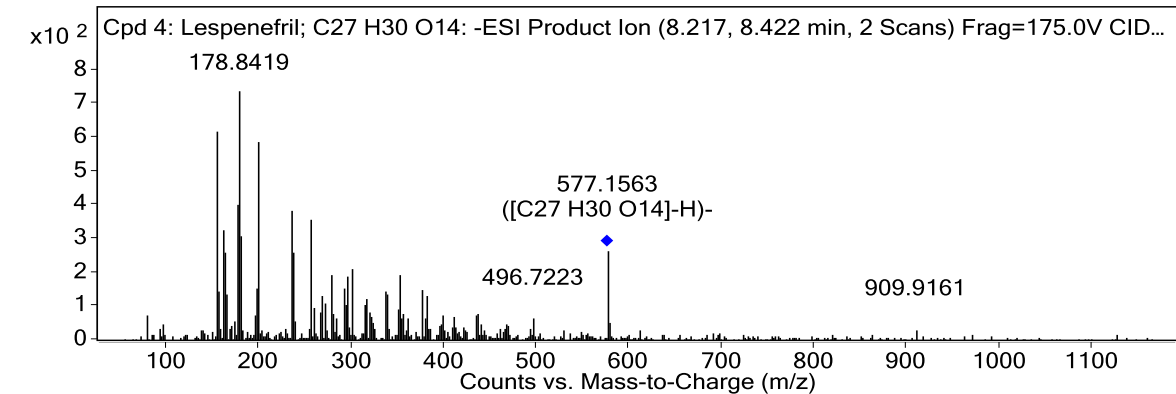
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.9581				6432.68		
154.9274				5907.32		
176.843				6017.35		
178.8418				9636.25		
198.9173				8515.63		
234.8687				7115.67		
256.8762				5683.25		
577.1563	577.1563	0.05	1	27108.91	C27 H30 O14	(M-H)-
578.1592	578.1597	0.84	1	6131.98	C27 H30 O14	(M-H)-
579.1609	579.1621	2.08	1	1374.99	C27 H30 O14	(M-H)-

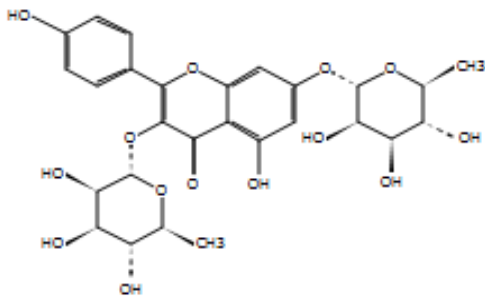
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
154.9276				616.01		
160.8414				324.67		
176.8423				399.78		
176.935				315.46		
178.8419				737.6		
180.8397				308.47		
198.9169				588.7		
234.8689				384.87		
256.8761				357.3		
577.1563	577.1563	-0.07	1	266.44	C27 H30 O14	(M-H)-

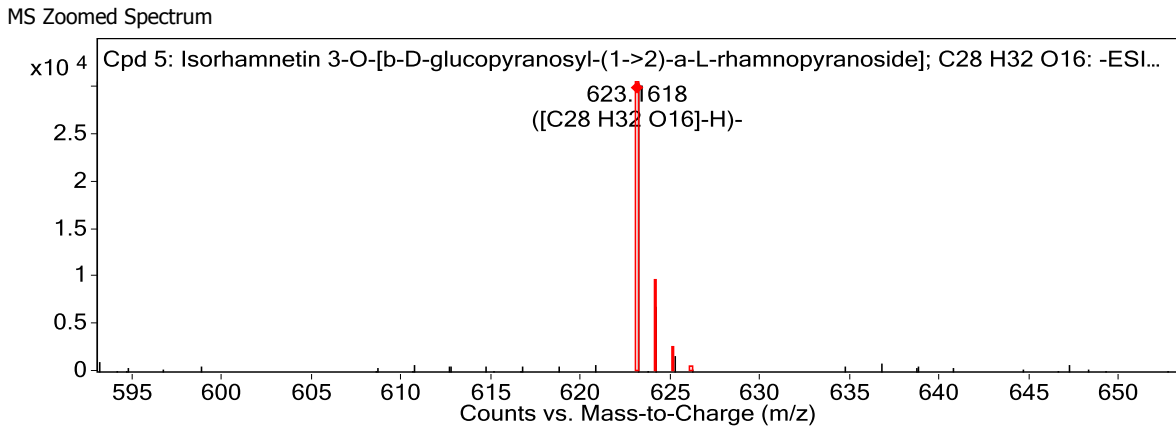
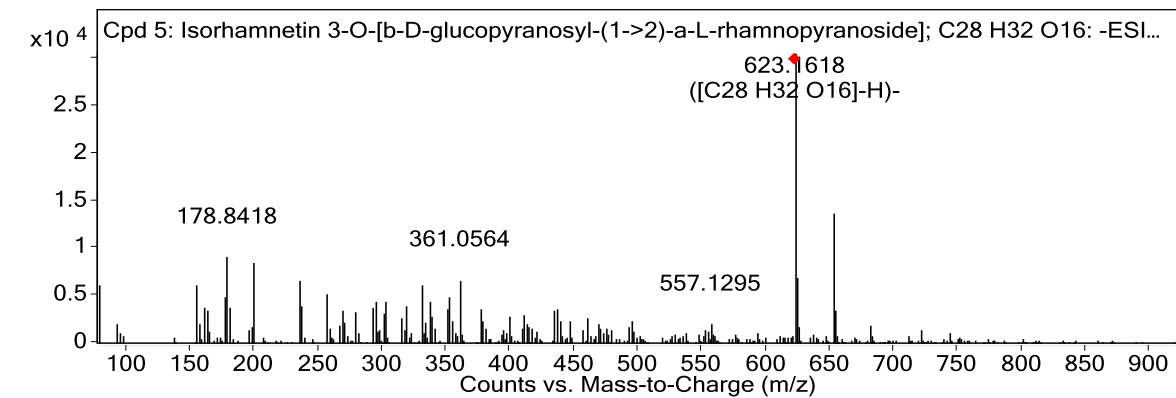
Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 5: Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]; C28	Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	623.1618	9.014	Auto MS/MS	624.1688

MS Spectrum

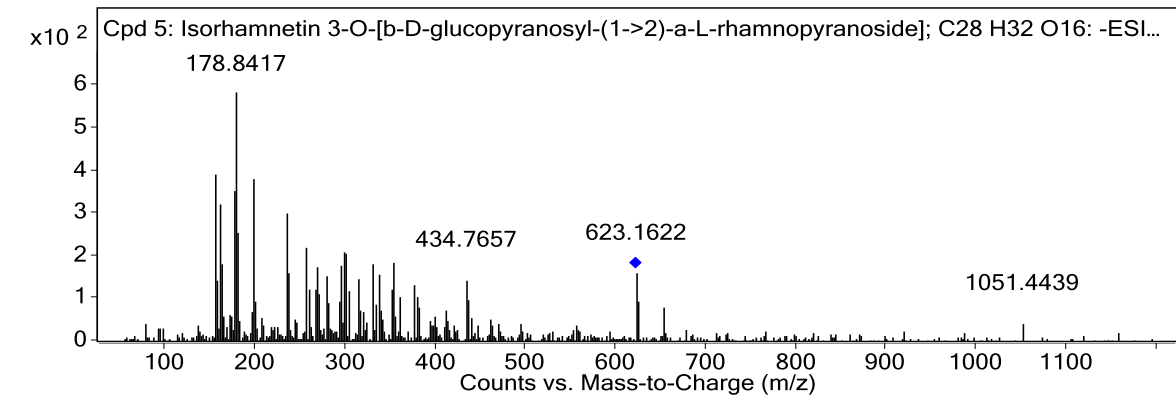
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
178.8418				9050.32		
198.9173				8432.24		
234.8686				6622.68		
331.046			1	6205.64		
361.0564			1	6639.88		
623.1618	623.1618	-0.09	1	30483.86	C28 H32 O16	(M-H)-
624.1639	624.1652	2	1	6925.66	C28 H32 O16	(M-H)-
625.1654	625.1675	3.39	1	1681.42	C28 H32 O16	(M-H)-
626.1686	626.1702	2.51	1	322.4	C28 H32 O16	(M-H)-
653.1722			1	13685.08		

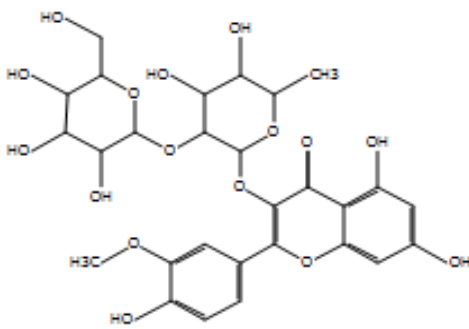
MSMS Spectrum



MS/MS Spectrum Peak List

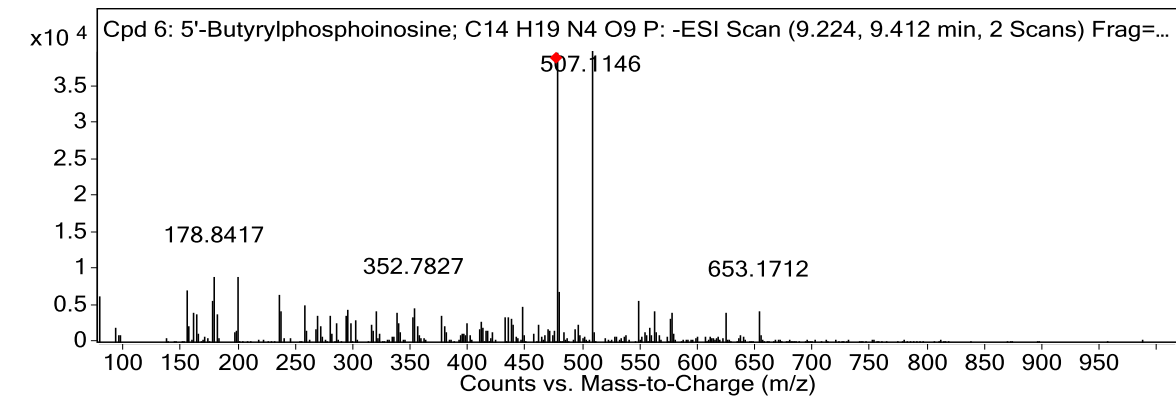
m/z	z	Abund
154.927		392.76
160.8413		323.13
176.8425		354.32
176.9352		267.47
178.8417		584.54
180.8378		254.1
198.9172		380.83
234.8683		301.22
256.8752		219.75
299.0191	1	209.86

Compound Structure



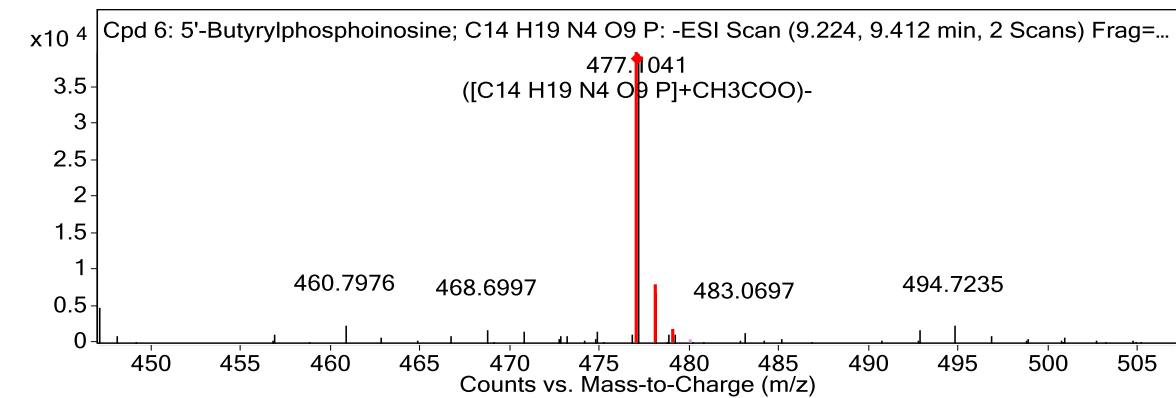
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 6: 5'-Butyrylphosphoinosine; C14 H19 N4 O9 P	5'-Butyrylphosphoinosine	477.1041	9.334	Auto MS/MS	418.0903

MS Spectrum



MS Zoomed Spectrum

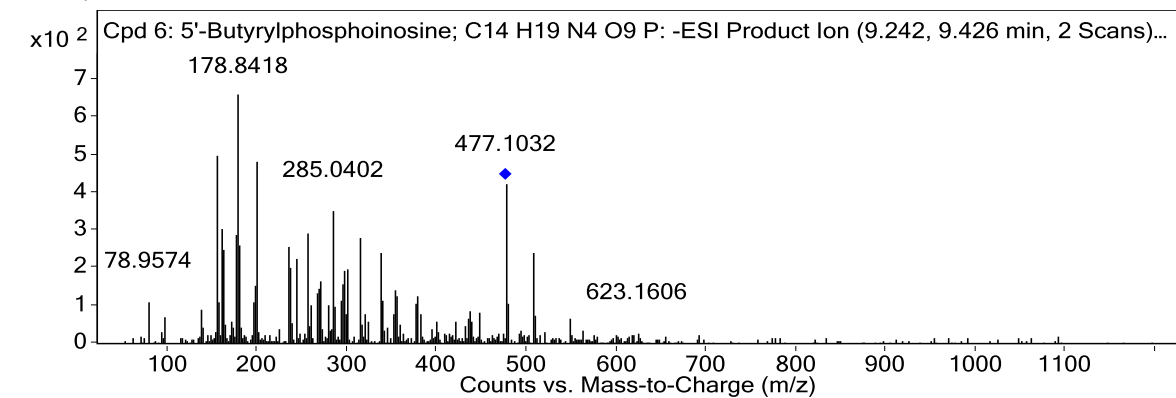
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.958				6378.09		
154.9274				7229.76		
178.8417				9041.7		
198.9171				8958.36		
234.8687				6637.35		
477.1041	477.1028	-2.72	1	39638.11	C14 H19 N4 O9 P	(M+CH3COO)-
478.107	478.1058	-2.67	1	6933.72	C14 H19 N4 O9 P	(M+CH3COO)-
479.1087	479.1078	-1.86	1	1286.95	C14 H19 N4 O9 P	(M+CH3COO)-
507.1146			1	42949.02		
508.1176			1	7593.71		

MSMS Spectrum

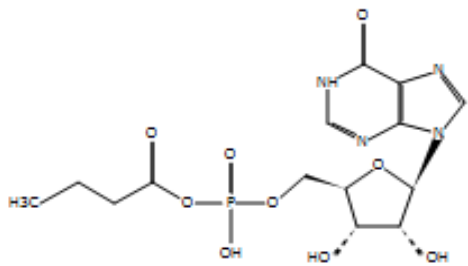


MS/MS Spectrum Peak List

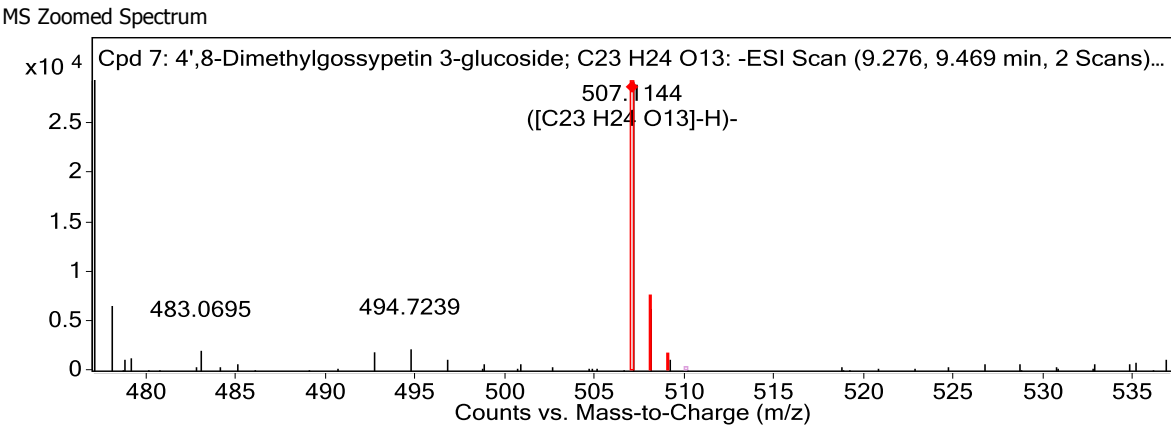
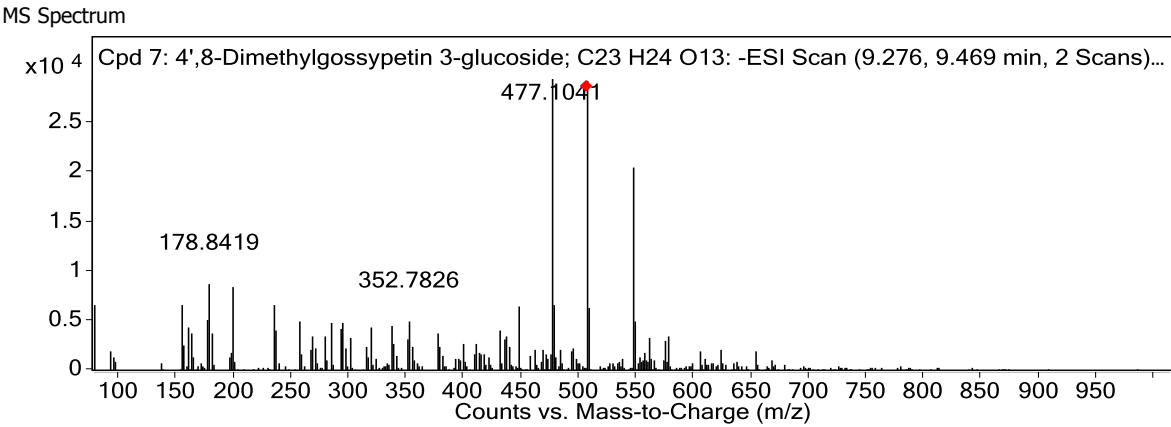
m/z	z	Abund
154.9271		497.53
160.8416	1	304.44
176.8439		289.88
178.8418		662.11
180.8404		261.52
198.9175		482.33
256.8766		292.14
285.0402	1	352.96
314.0422	1	280.47
477.1032	1	421.95

Qualitative Compound Report

Compound Structure

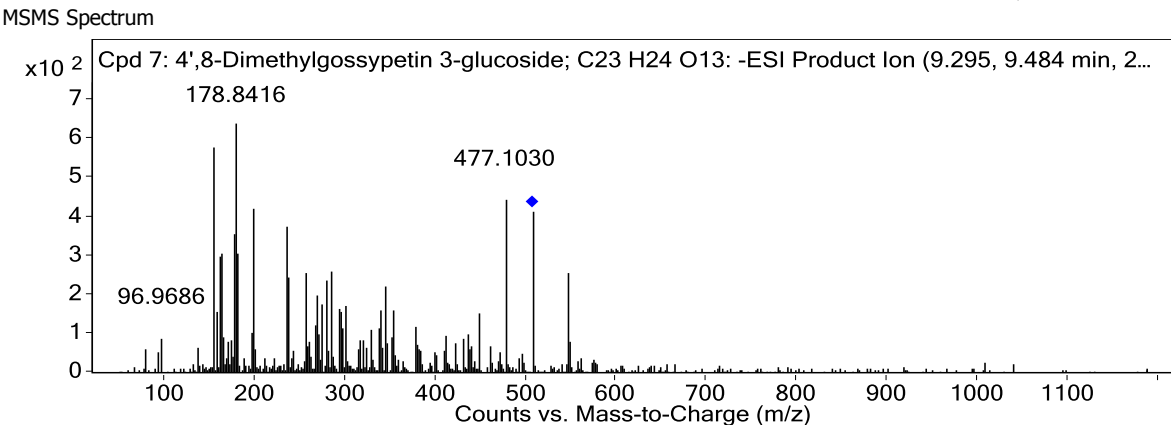


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 7: 4',8-Dimethylgossypetin 3-glucoside; C23 H24 O13	4',8-Dimethylgossypetin 3-glucoside	507.1144	9.389	Auto MS/MS	508.1216



MS Spectrum Peak List

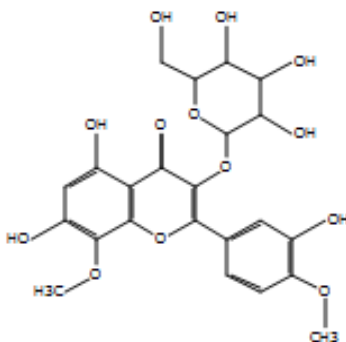
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.9581				6698.71		
154.9273				6663.96		
178.8419				8786.81		
198.9173				8472.44		
234.8687				6582.94		
477.1041			1	36247.38		
507.1144	507.1144	-0.07	1	29277.97	C23 H24 O13	(M-H)-
508.1174	508.1178	0.85	1	6289.43	C23 H24 O13	(M-H)-
509.1199	509.12	0.22	1	1253.75	C23 H24 O13	(M-H)-
547.146			1	20553.57		



MS/MS Spectrum Peak List

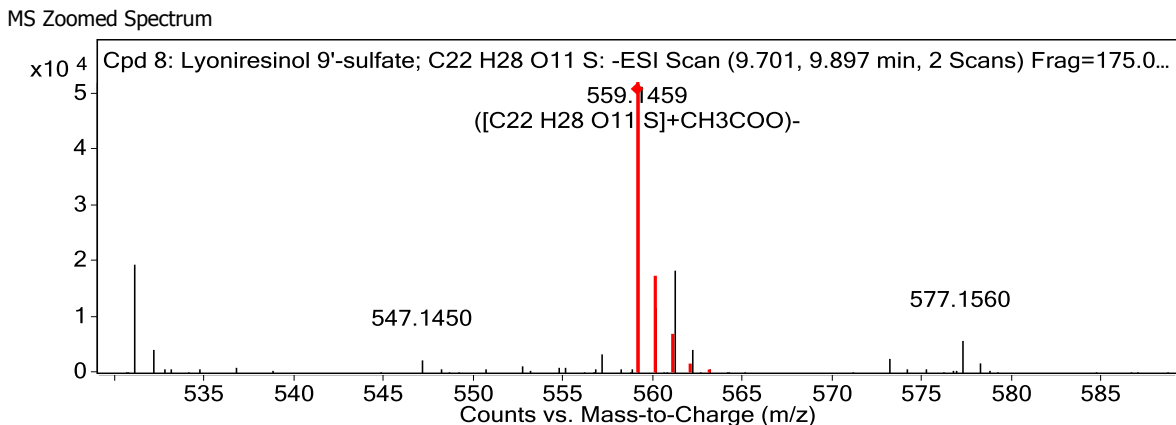
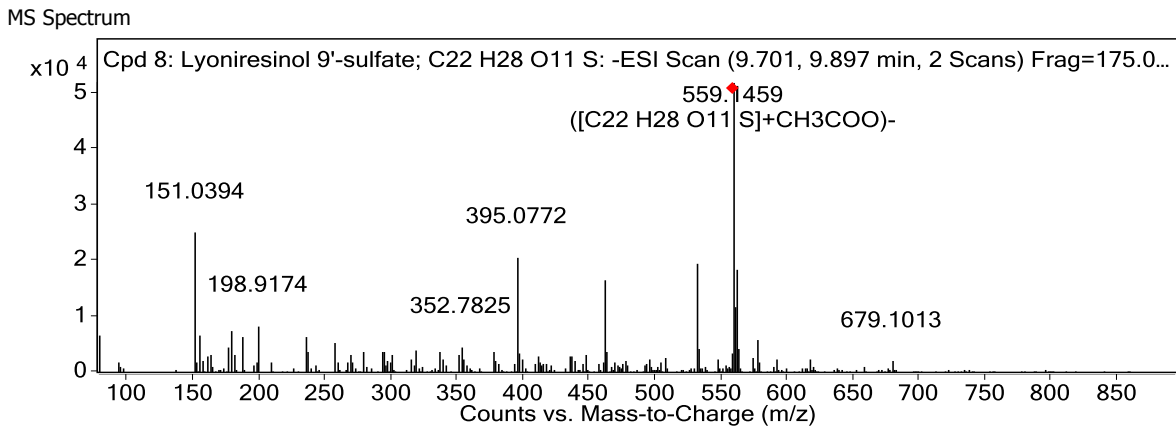
m/z	z	Abund
154.9277		577.37
160.8416		300.02
162.8391		306.95
176.8422		354.98
178.8416		640.7
180.8395		305.46
198.9169		422.97
234.8686		373.62
477.103	1	445.41
507.1124	1	411.87

Compound Structure



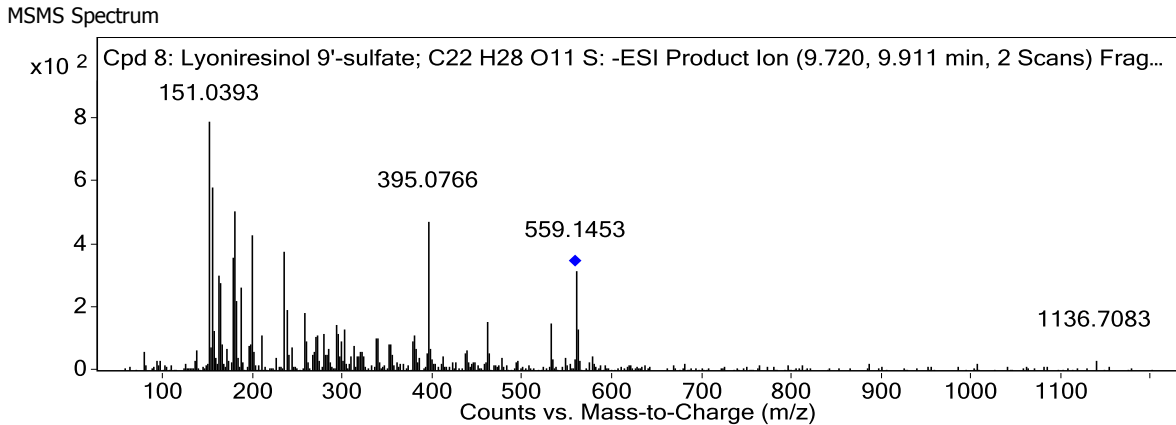
Qualitative Compound Report

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 8: Lyoniresinol 9'-sulfate; C22 H28 O11 S	Lyoniresinol 9'-sulfate	559.1459	9.815	Auto MS/MS	500.1354



MS Spectrum Peak List

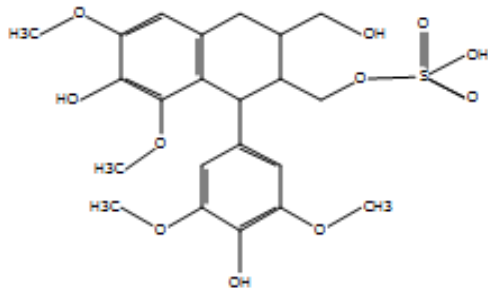
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
151.0394			1	25093.88		
198.9174				8382.55		
395.0772			1	20668.74		
461.1085			1	16544.78		
531.1142			1	19609.36		
559.1459	559.1491	5.72	1	51759.65	C22 H28 O11 S	(M+CH3COO)-
560.1488	560.1524	6.48	1	11625.45	C22 H28 O11 S	(M+CH3COO)-
561.16	561.1506	-16.76	1	18460.38	C22 H28 O11 S	(M+CH3COO)-
562.1634	562.1525	-19.47	1	4381.94	C22 H28 O11 S	(M+CH3COO)-
563.1591	563.1536	-9.77	1	927.31	C22 H28 O11 S	(M+CH3COO)-



MS/MS Spectrum Peak List

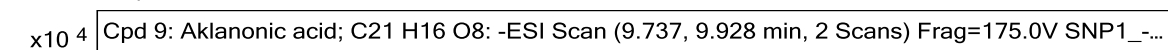
m/z	z	Abund
151.0393	1	792.93
154.9271		583.76
160.8414		304.42
162.8391		278
176.8424		361.27
178.842		505.95
198.9179		431.53
234.8688		380.06
395.0766	1	476.31
559.1453	1	317.98

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 9: Aklanonic acid; C21 H16 O8	Aklanonic acid	395.0772	9.85	Auto MS/MS	396.0844

MS Spectrum



<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	z	Abund	Formula	Ion
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MS/MS Spectrum

x10³ Cpd 9: Aklanonic acid; C21 H16 O8: -ESI Product Ion (9.756, 9.944 min, 2 Scans) Frag=175.0V Cl..



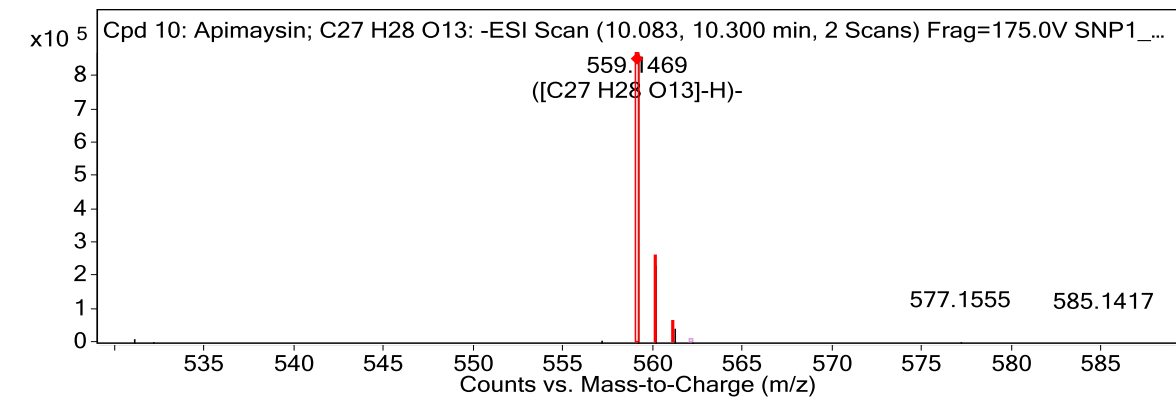
m/z	z	Abund
129.0333	1	100.00

Compound Structures

x10⁵ Cpd 10: Apimaysin; C27 H28 O13: -ESI Scan (10.083, 10.300 min, 2 Scans) Frag=175.0V SNP1_...



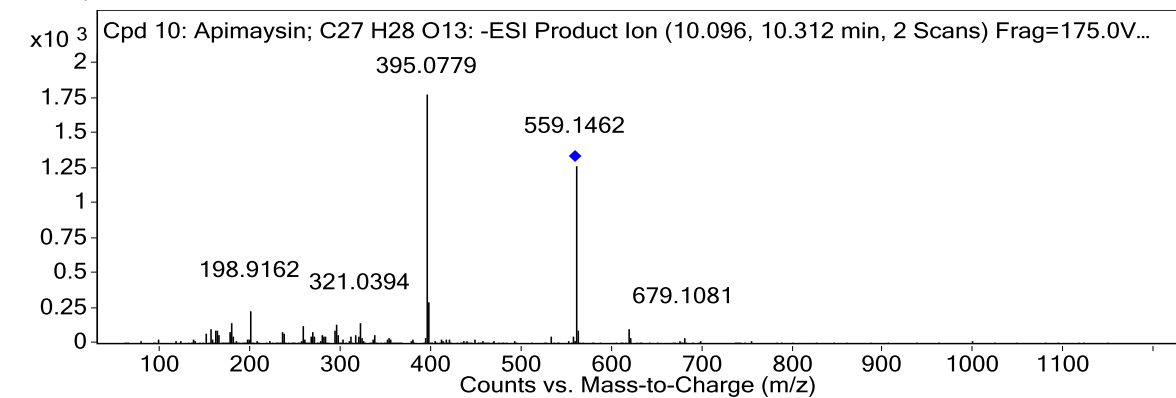
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
395.0783			1	340777.69		
396.0812			1	61481.43		
531.1142			1	12285.43		
559.1469	559.1457	-2.11	1	868347.13	C27 H28 O13	(M-H)-
560.1505	560.1491	-2.43	1	232920.08	C27 H28 O13	(M-H)-
561.1529	561.1515	-2.42	1	46007.11	C27 H28 O13	(M-H)-
617.1048			1	52996.53		
619.1028			1	15568.29		
657.1226			1	16435.69		
679.1045			1	25078.66		

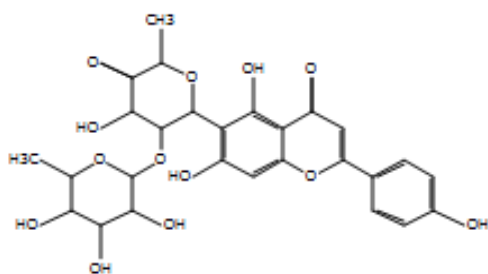
MSMS Spectrum



MS/MS Spectrum Peak List

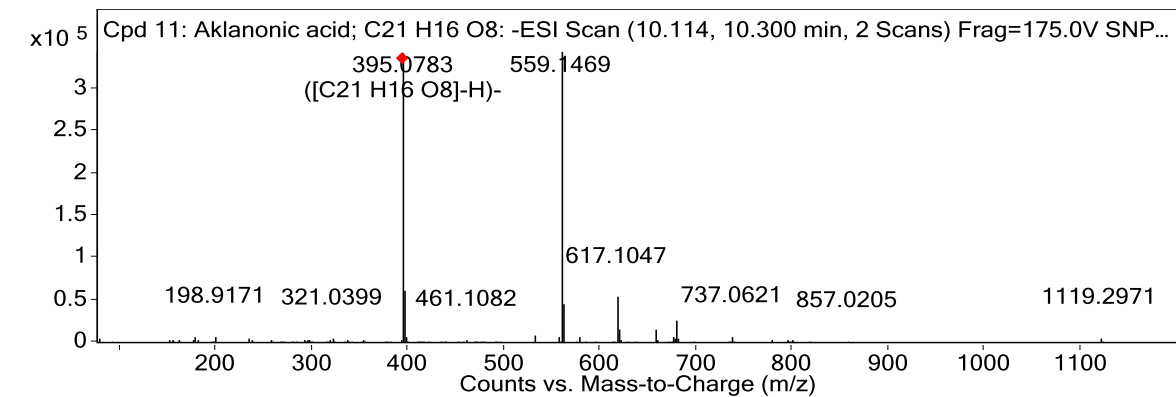
m/z	z	Abund
178.8411		152.33
198.9162		234.2
256.8779		126.18
295.0596	1	135.9
321.0394	1	146.04
395.0779	1	1782.87
396.0807	1	299.6
559.1462	1	1267.07
560.1491	1	301.24
617.1024		108.75

Compound Structure

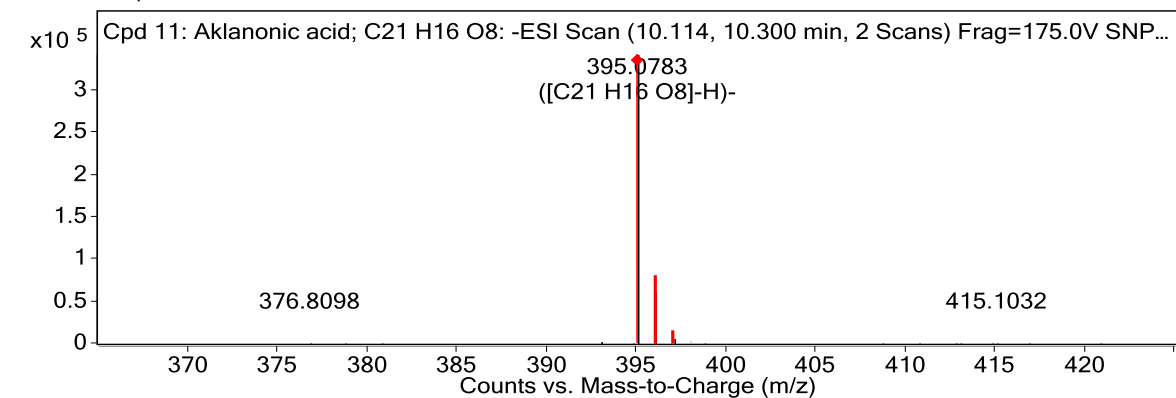


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 11: Aklanonic acid; C21 H16 O8	Aklanonic acid	395.0783	10.22	Auto MS/MS	396.0855

MS Spectrum



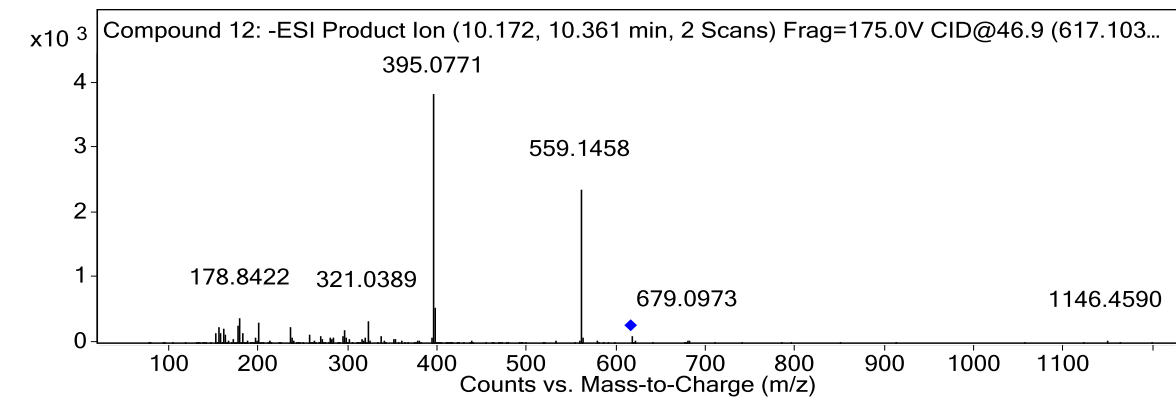
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
395.0783	395.0772	-2.72	1	341894.22	C21 H16 O8	(M-H)-

Qualitative Compound Report

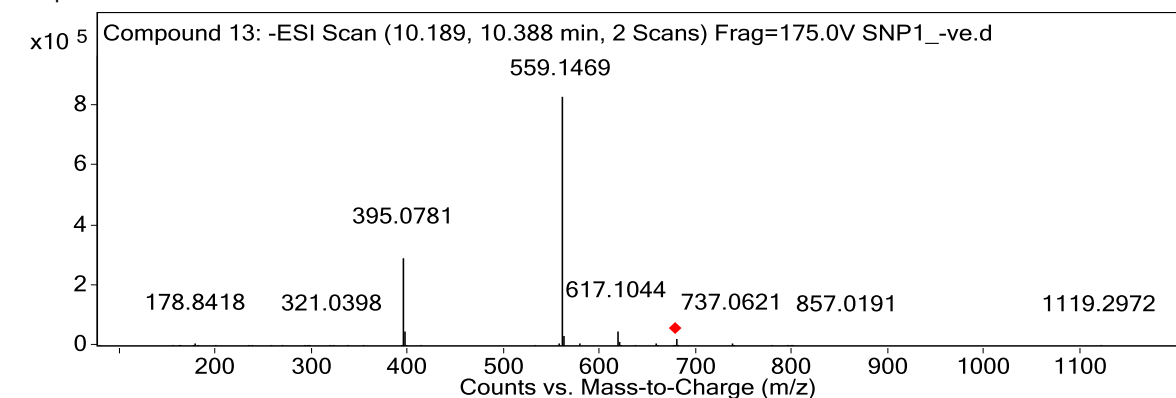


MS/MS Spectrum Peak List

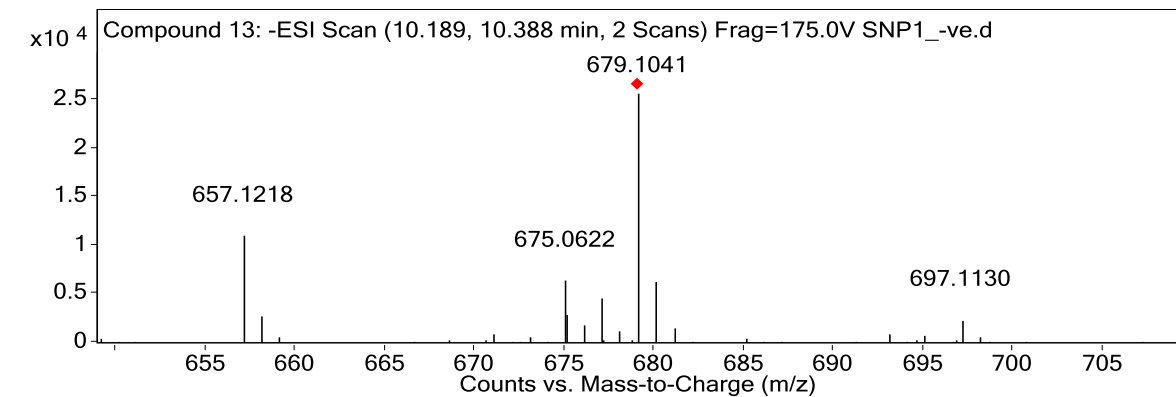
m/z	z	Abund
154.9272		257.63
176.8421		278.73
178.8422		381.76
198.9171		331.75
234.869		247.75
321.0389	1	342.19
395.0771	1	3839.86
396.0804	1	548.34
559.1458	1	2364.34
560.1487	1	627.8

Compound Label	m/z	RT	Algorithm
Compound 13	679.1041	10.306	Auto MS/MS

MS Spectrum



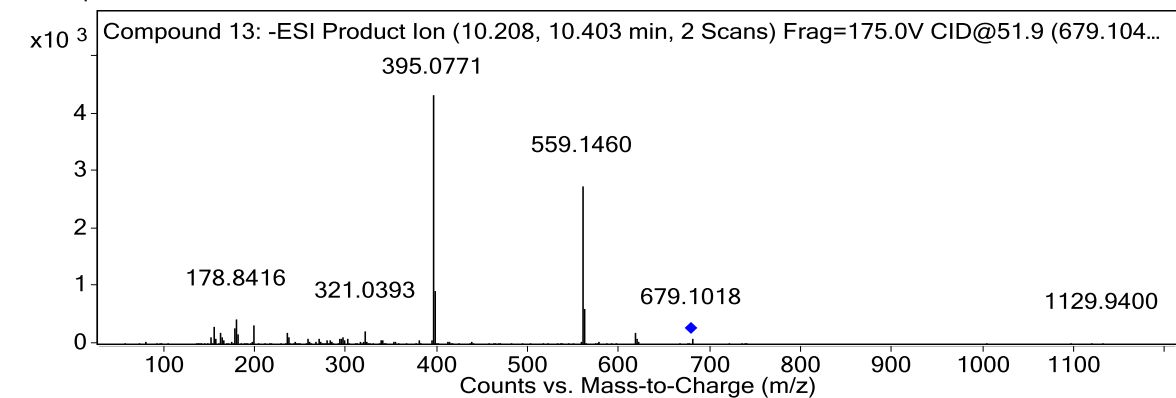
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
395.0781	1	295952.06
396.081	1	50292.59
559.1469	1	832046.44
560.1502	1	215017.09
561.1522	1	36698.19
617.1044	1	49404.09
619.1024	1	14434.94
679.1041	1	25715.53
680.107	1	6229.02
681.1093	1	1500.49

MSMS Spectrum



MS/MS Spectrum Peak List

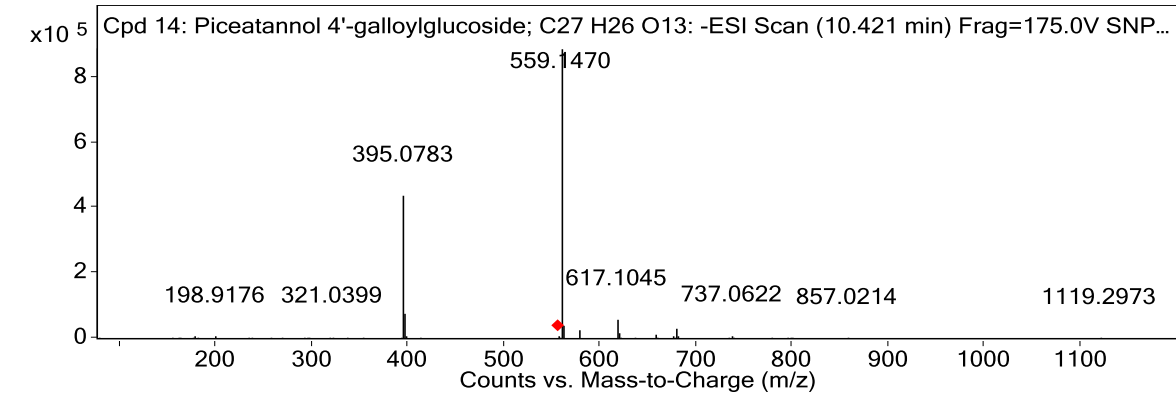
m/z	z	Abund
154.9268		317.86
176.8423		291.41
176.9354		231.48
178.8416		434.09
198.9174		336.5
321.0393	1	221.74
395.0771	1	4333.03
396.0801	1	943.26
559.146	1	2756.25
560.1484	1	619.4

Compound Label	Name	m/z	RT	Algorithm	Mass
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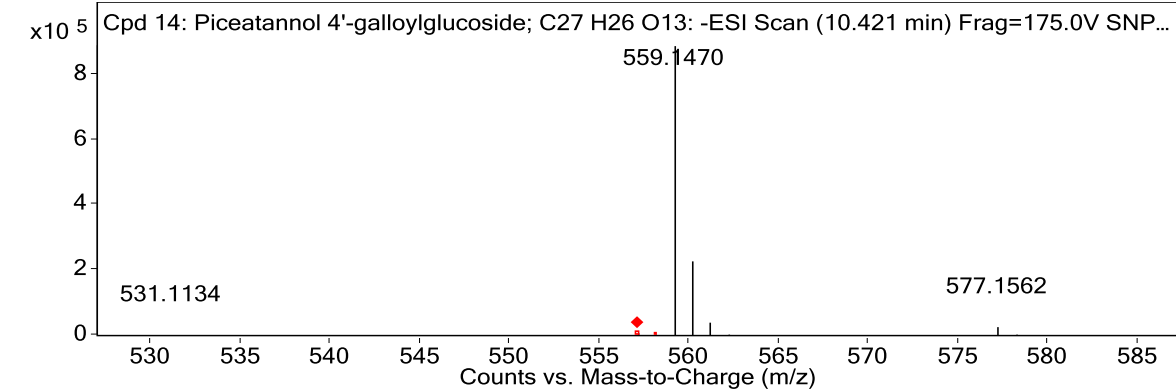
Qualitative Compound Report

Cpd 14: Piceatannol 4'-galloylglucoside; C27 H26 O13	Piceatannol 4'-galloylglucoside	557.1296	10.45	Auto MS/MS	558.1367
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MS Spectrum



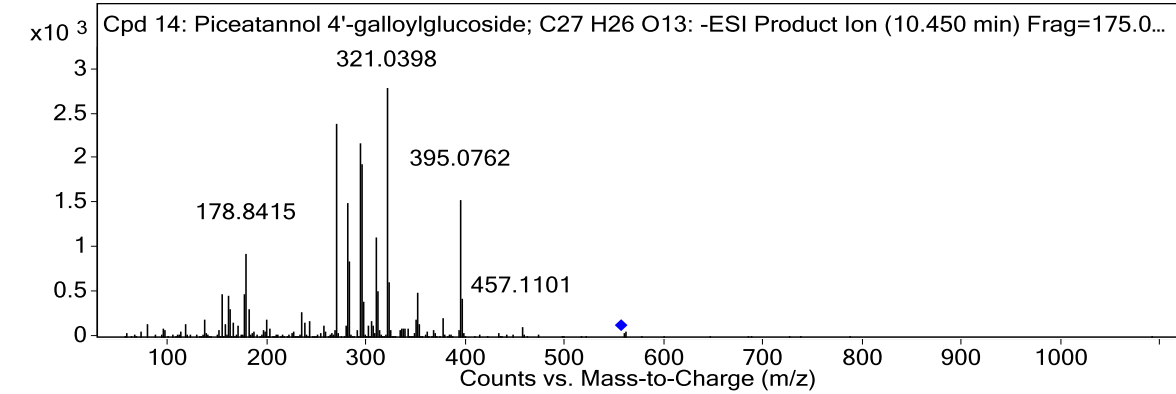
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
395.0783			1	438980.88		
396.0812			1	77593.6		
557.1296	557.1301	0.91	1	10375.45	C27 H26 O13	(M-H)-
558.1324	558.1335	1.87	1	2406.41	C27 H26 O13	(M-H)-
559.147			1	885313.25		
560.1503			1	228617.72		
561.1521			1	39844.87		
577.1562			1	25623.54		
617.1045			1	59762.24		
679.1045			1	32830.7		

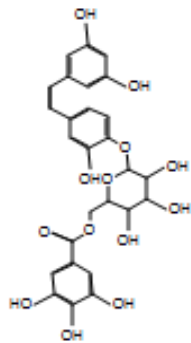
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
178.8415		943.61
269.0451	1	2395.7
281.0443		1505.1
282.0529		858.33
293.0449	1	2174.87
295.0606	1	1940.49
309.0406	1	1124.5
321.0398	1	2797.22
322.0442	1	612.12
395.0762	1	1545.31

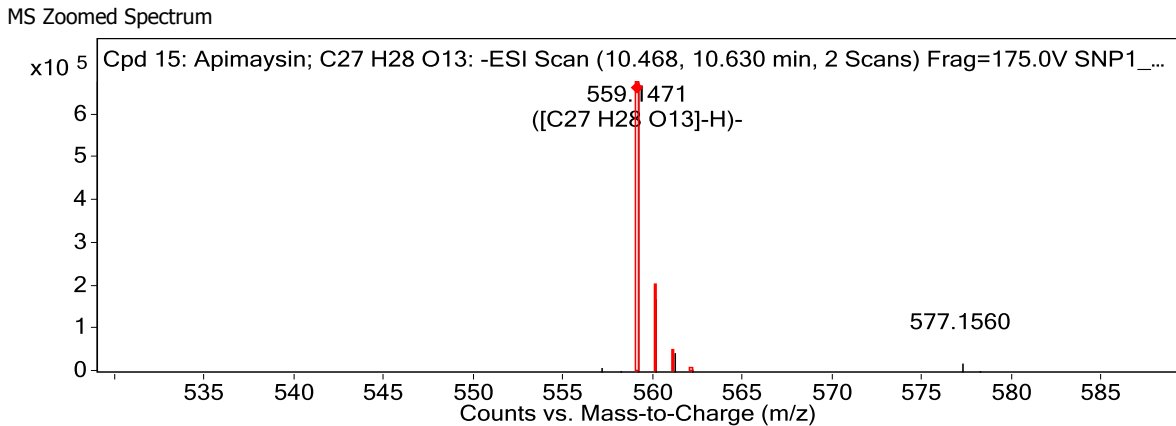
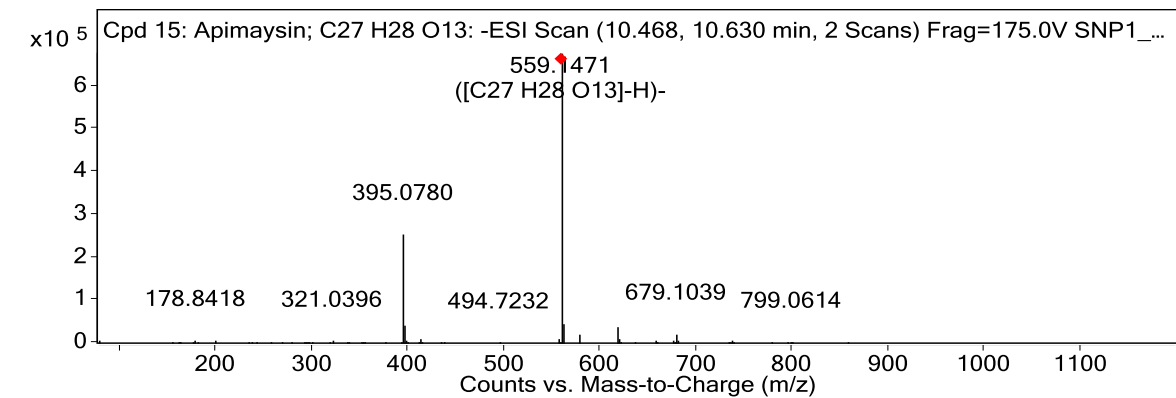
Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 15: Apimaysin; C27 H28 O13	Apimaysin	559.1471	10.561	Auto MS/MS	560.1544

MS Spectrum

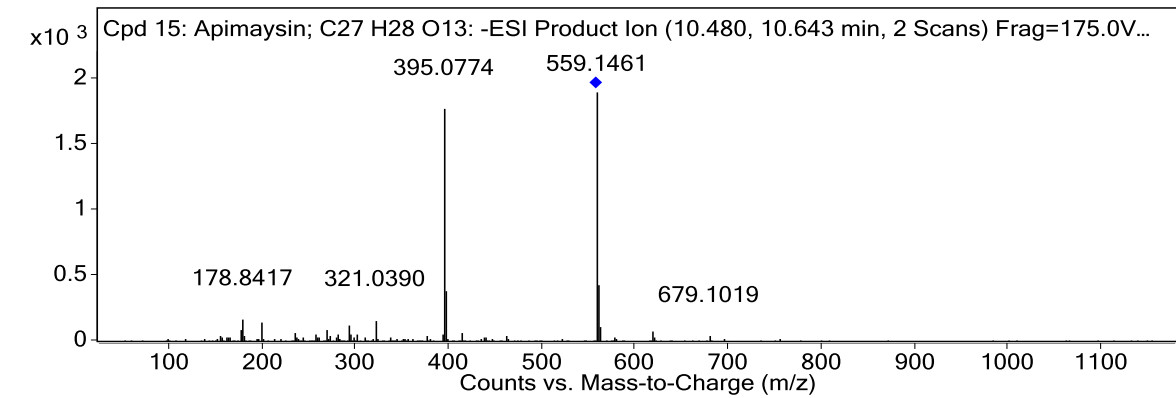
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
395.078			1	255703		
396.0808			1	43400.99		
559.1471	559.1457	-2.52	1	675948.31	C27 H28 O13	(M-H)-
560.15	560.1491	-1.54	1	171119.8	C27 H28 O13	(M-H)-
561.1558	561.1515	-7.51	1	44379.5	C27 H28 O13	(M-H)-
562.1596	562.1542	-9.54	1	7167.76	C27 H28 O13	(M-H)-
577.156			1	20891.07		
617.1041			1	38887.18		
619.103			1	11931.8		
679.1039			1	22498.03		

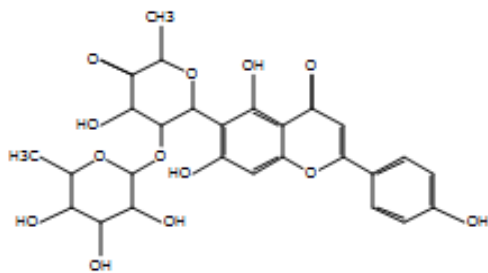
MSMS Spectrum



MS/MS Spectrum Peak List

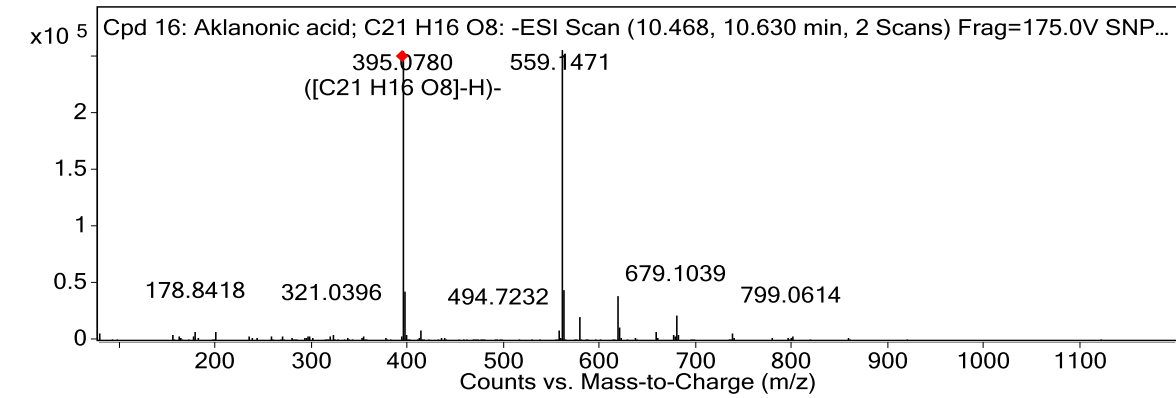
m/z	z	Abund
178.8417		170.1
198.9172		142.61
269.0465	1	93.85
293.0452		126.35
321.039	1	164.33
395.0774	1	1774.5
396.0811	1	383.1
559.1461	1	1898.7
560.1488	1	433.88
561.1543	1	109.32

Compound Structure

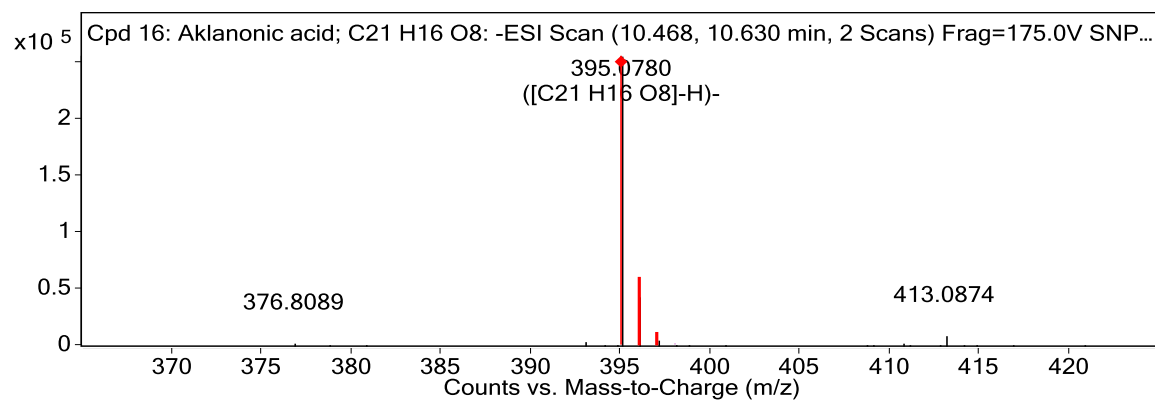


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 16: Aklanonic acid; C21 H16 O8	Aklanonic acid	395.078	10.563	Auto MS/MS	396.0852

MS Spectrum



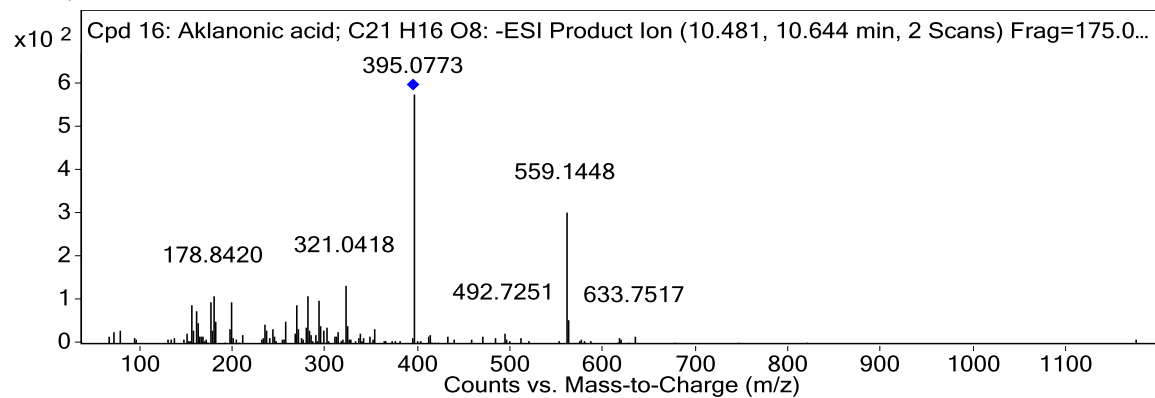
MS Zoomed Spectrum



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>z</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
395.078	395.0772	-1.96	1	255703	C21 H16 O8	(M-H)-
396.0808	396.0806	-0.42	1	43400.99	C21 H16 O8	(M-H)-
397.0822	397.083	2.21	1	5554.29	C21 H16 O8	(M-H)-
559.1471			1	675948.31		
560.15			1	171119.8		
561.1558			1	44379.5		
577.156			1	20891.07		
617.1041			1	38887.18		
619.103			1	11931.8		
679.1039			1	22498.03		

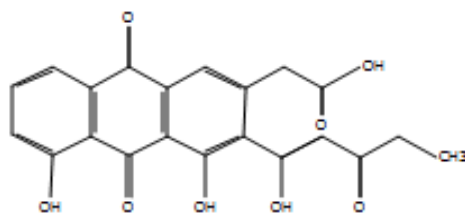
MSMS Spectrum



MS/MS Spectrum Peak List

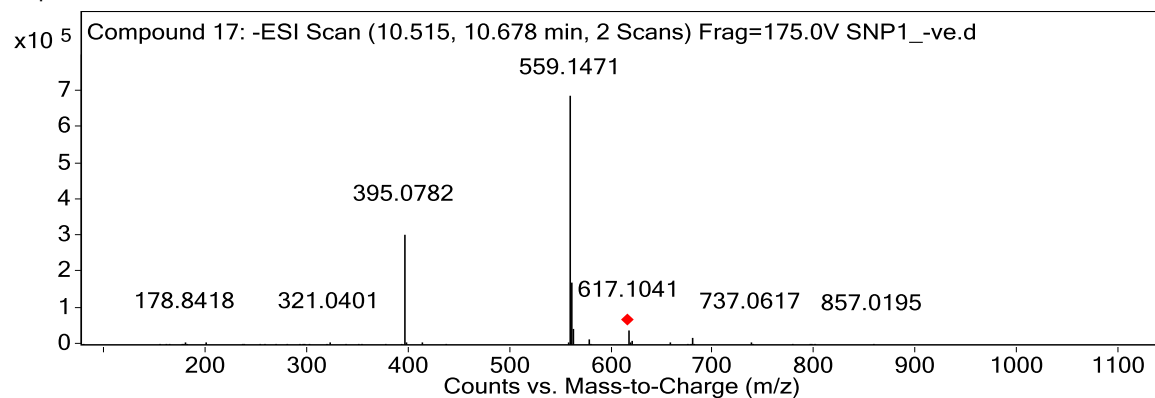
m/z	z	Abund
154.9266		89.72
176.8411		97.01
178.842		109.79
198.9166		95.55
281.0456	1	110.67
293.0479		101.46
321.0418	1	133.55
395.0773	1	578.41
396.0811	1	148.69
559.1448	1	303.21

Compound Structure

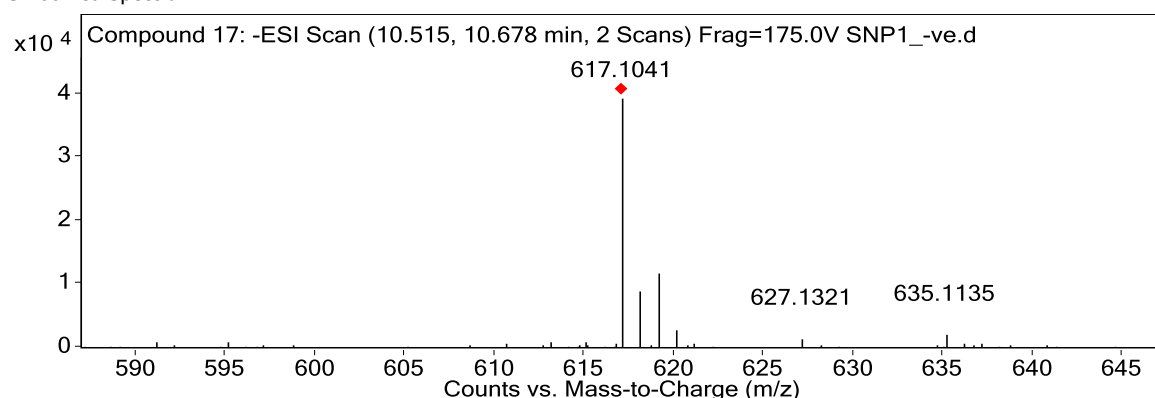


Compound Label	<i>m/z</i>	RT	Algorithm
Compound 17	617.1041	10.612	Auto MS/MS

MS Spectrum



MS Zoomed Spectrum



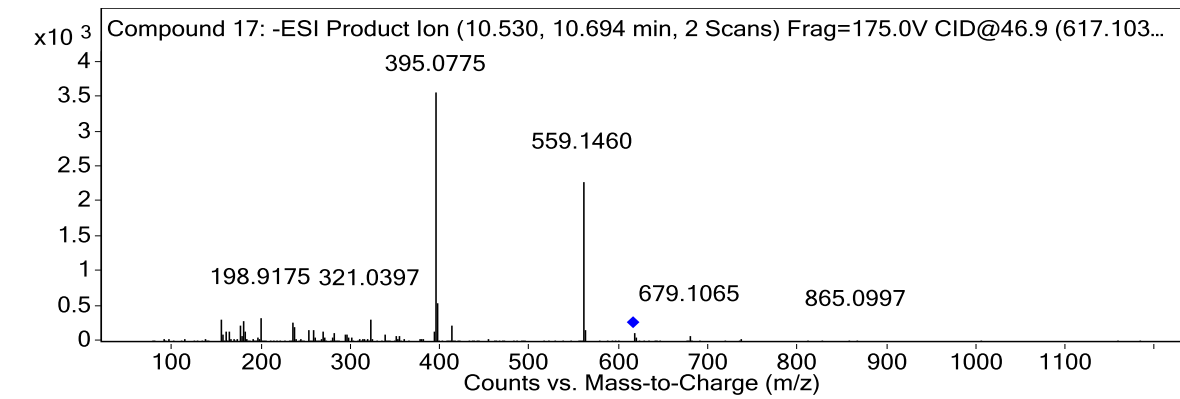
MS Spectrum Peak List

<i>m/z</i>	<i>z</i>	Abund
395.0782	1	304865
396.081	1	50005.93

Qualitative Compound Report

559.1471	1	688601.88
560.1502	1	174808.14
561.1558	1	43346.71
617.1041	1	39273.85
618.1066	1	8967.4
619.1032	1	11781.27
620.1053	1	2847.99
621.1109	1	749.52

MSMS Spectrum

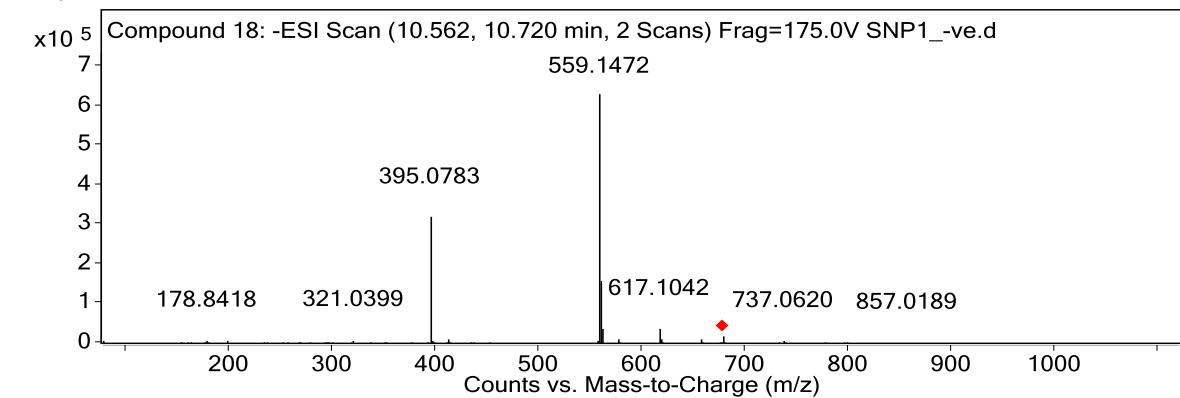


MS/MS Spectrum Peak List

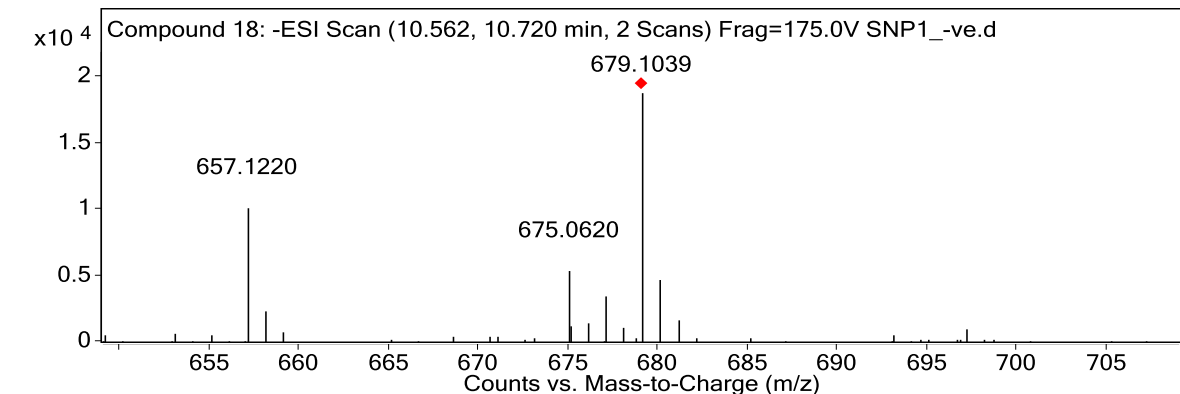
m/z	z	Abund
154.9277		316.37
178.8418		288.63
198.9175		338.16
234.8683		273.28
321.0397	1	322.26
395.0775	1	3571.04
396.0801	1	563.79
413.0859		236.77
559.146	1	2281.54
560.1497	1	583.79

Compound Label	m/z	RT	Algorithm
Compound 18	679.1039	10.659	Auto MS/MS

MS Spectrum



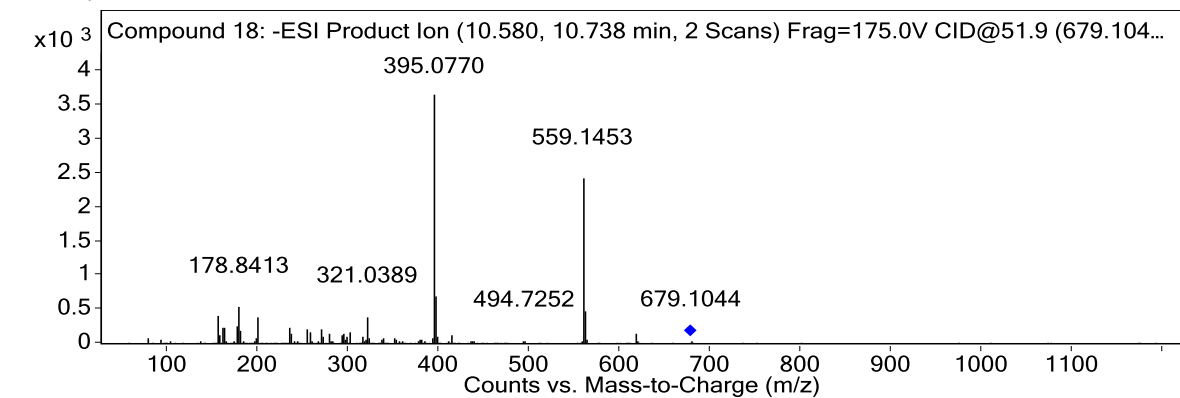
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
395.0783	1	318545.63
396.0811	1	55780.97
559.1472	1	628931
560.1501	1	159879.78
561.1559	1	36673.98
617.1042	1	36563.21
679.1039	1	18841.96
680.1065	1	4750.6
681.1123	1	1649.95
682.1179	1	320.99

MSMS Spectrum



MS/MS Spectrum Peak List

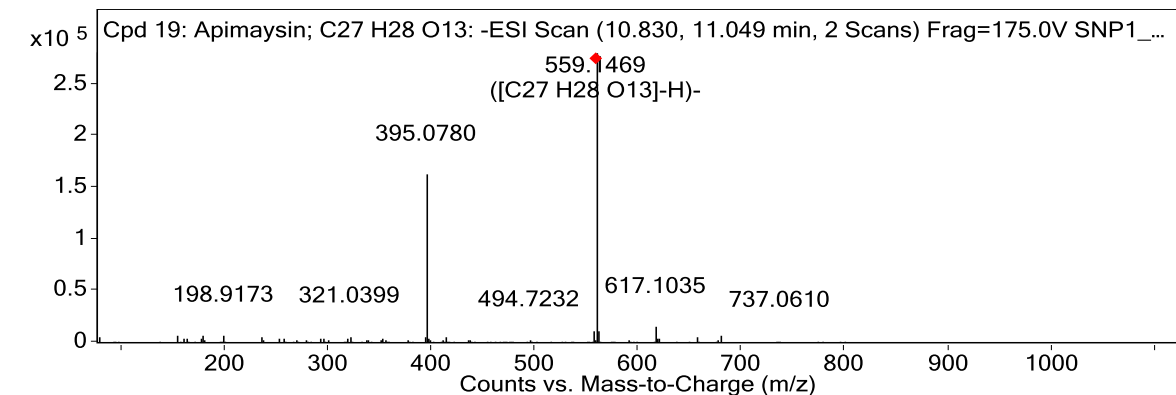
m/z	z	Abund
154.9277		413.82
176.8428		263.61
176.935		259.73
178.8413		544.92
198.9166		399.24
321.0389	1	402.78

Qualitative Compound Report

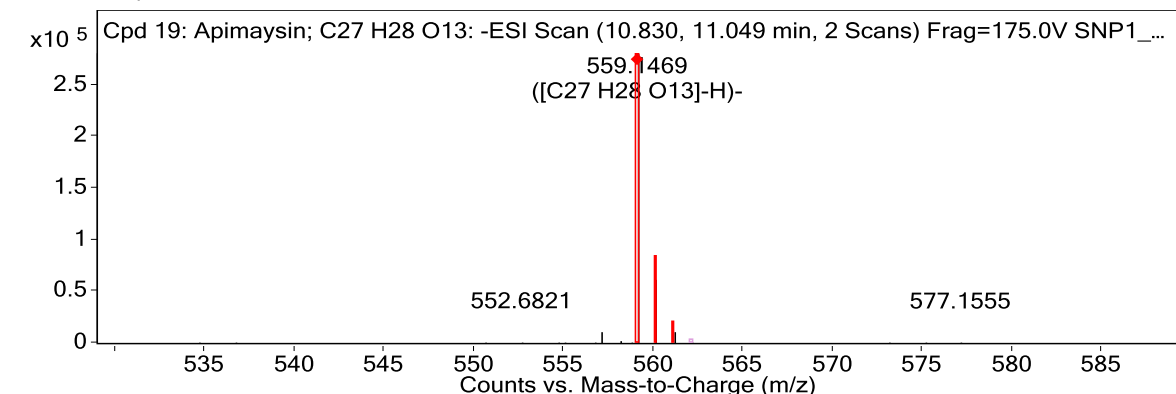
395.077	1	3662.7
396.0802	1	705.09
559.1453	1	2433.67
560.1481	1	486.25

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 19: Apimaysin; C27 H28 O13	Apimaysin	559.1469	10.952	Auto MS/MS	560.1541

MS Spectrum



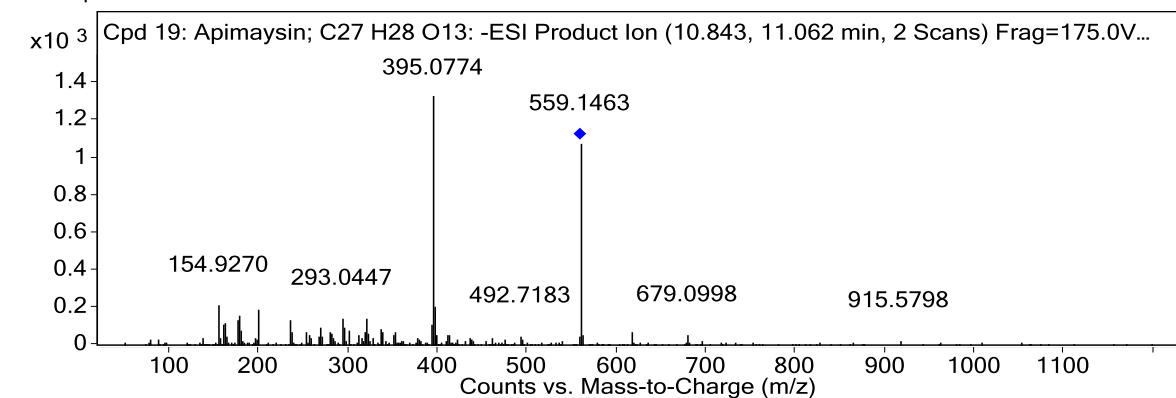
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
178.8418				6768.62		
198.9173				6919.62		
395.078			1	162796.63		
396.0808			1	26568.07		
557.1297			1	11011.74		
559.1469	559.1457	-2.19	1	279569.22	C27 H28 O13	(M-H)-
560.1495	560.1491	-0.65	1	62478.05	C27 H28 O13	(M-H)-
561.1532	561.1515	-3.01	1	12005.42	C27 H28 O13	(M-H)-
617.1035			1	15296.04		
679.1036			1	7139.02		

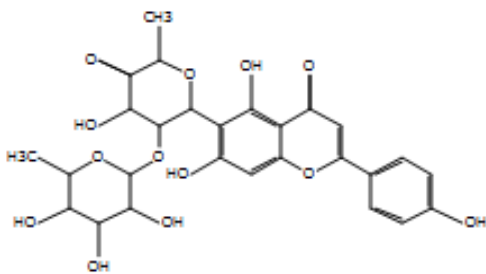
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
154.927		211.39
178.8423		156.26
198.9164		194.56
234.8687		136.67
293.0447		141.39
321.0394	1	139.75
395.0774	1	1332.47
396.0797	1	206.18
559.1463	1	1075.54
560.1477	1	244.96

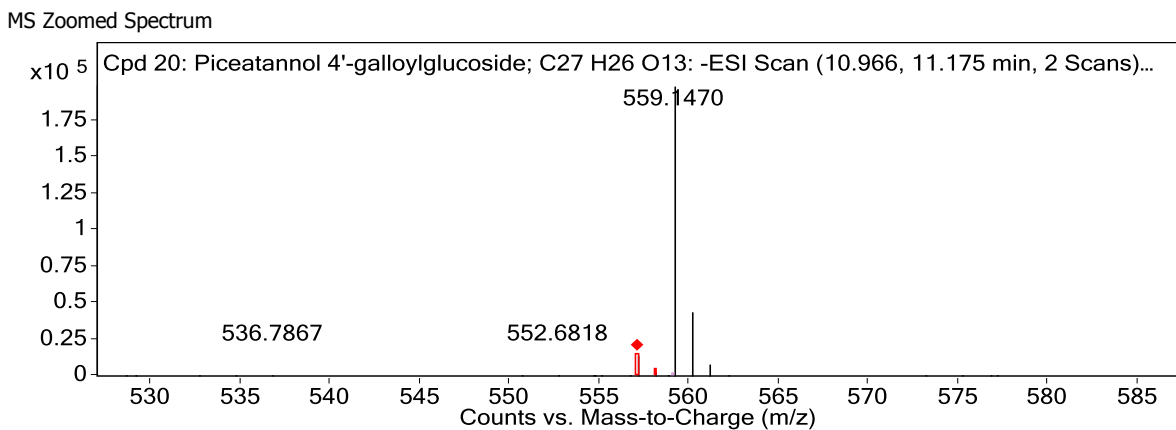
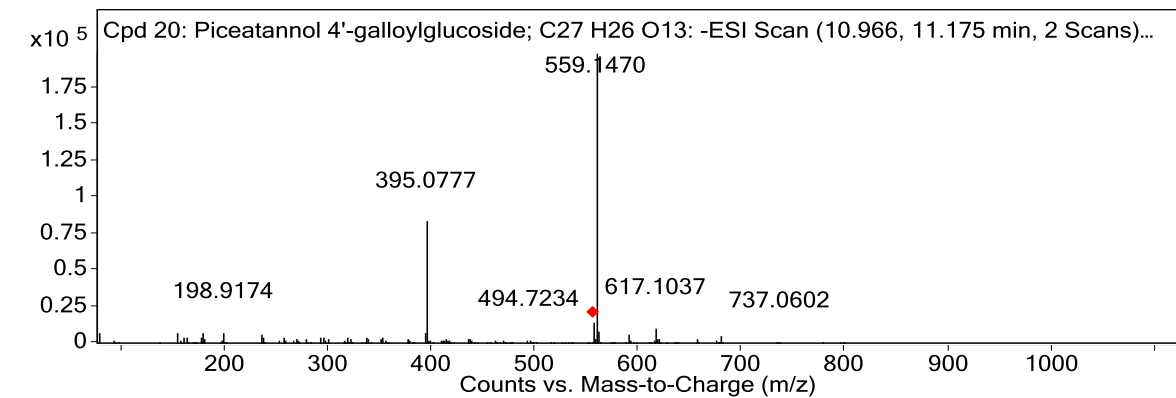
Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 20: Piceatannol 4'-galloylglucoside; C27 H26 O13	Piceatannol 4'-galloylglucoside	557.13	11.09	Auto MS/MS	558.1372

MS Spectrum

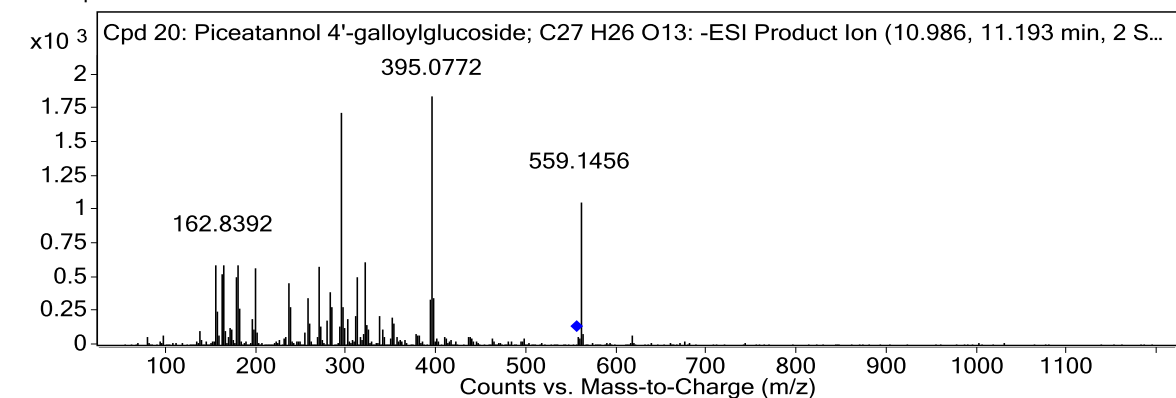
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
198.9174				7662.6		
393.0613			1	7299.61		
395.0777			1	83525.94		
396.0807			1	13545.58		
557.13	557.1301	0.1	1	14059.63	C27 H26 O13	(M-H)-
558.1329	558.1335	0.92	1	3457.26	C27 H26 O13	(M-H)-
559.147			1	198391.86		
560.1496			1	44325.95		
561.1524			1	7850.62		
617.1037			1	10389.64		

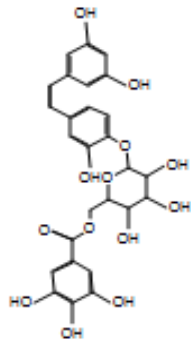
MSMS Spectrum



MS/MS Spectrum Peak List

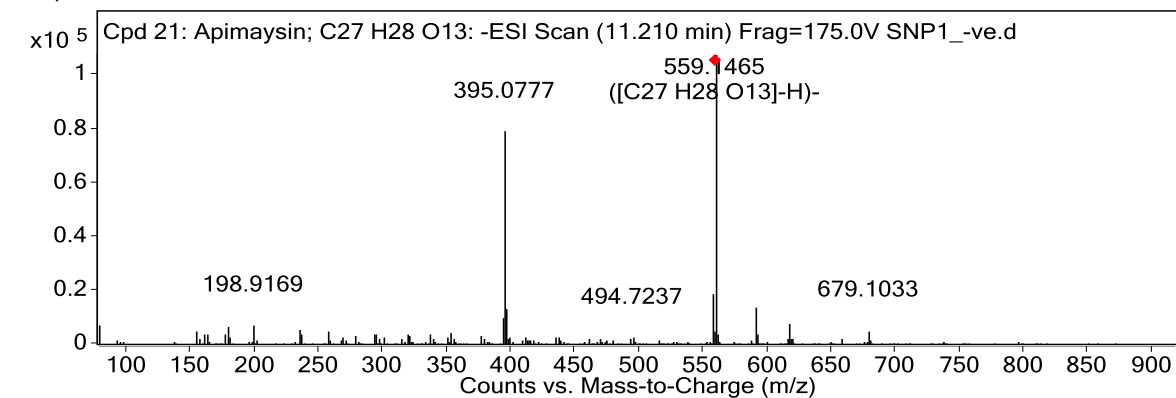
m/z	z	Abund
154.9271		593.29
160.8416		523.6
162.8392		593.35
178.8418		590.08
198.9167		572.13
269.0449	1	586.37
293.0447	1	1713.89
321.0396	1	621.01
395.0772	1	1842.46
559.1456	1	1059.16

Compound Structure



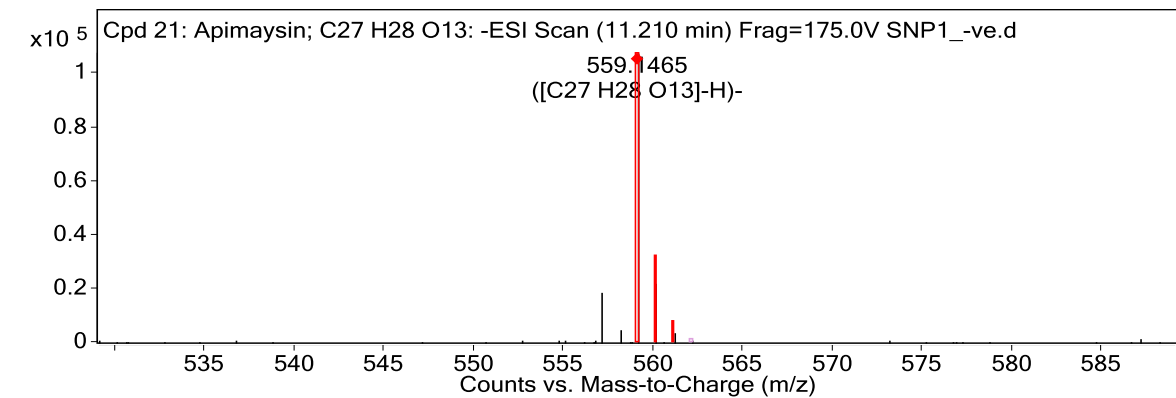
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 21: Apimaysin; C27 H28 O13	Apimaysin	559.1465	11.224	Auto MS/MS	560.1537

MS Spectrum



MS Zoomed Spectrum

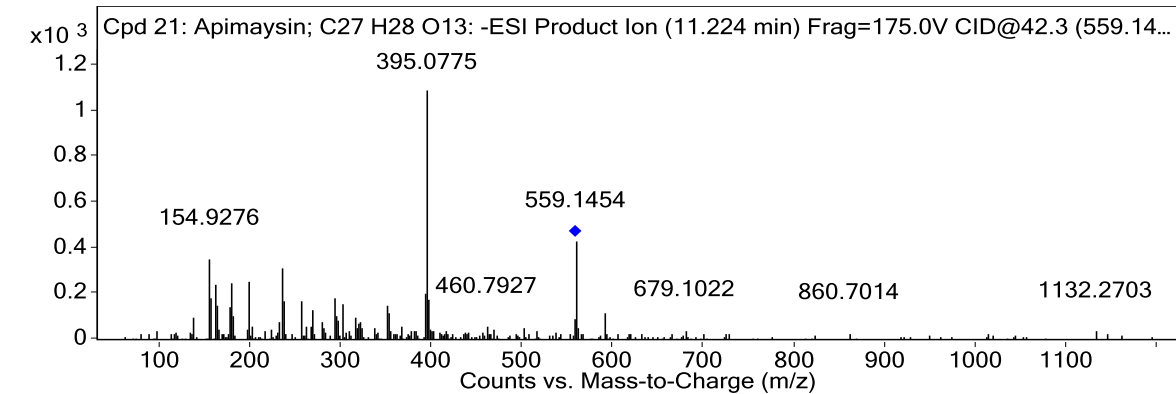
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
198.9169				7090.99		
393.0612			1	10162.96		
395.0777			1	79182.66		
396.0808			1	13469.68		
557.1299			1	18752.83		
559.1465	559.1457	-1.43	1	107478.27	C27 H28 O13	(M-H)-
560.149	560.1491	0.19	1	22358.12	C27 H28 O13	(M-H)-
561.1524	561.1515	-1.46	1	4135.88	C27 H28 O13	(M-H)-
591.1714			1	13854.22		
617.1027			1	7963.21		

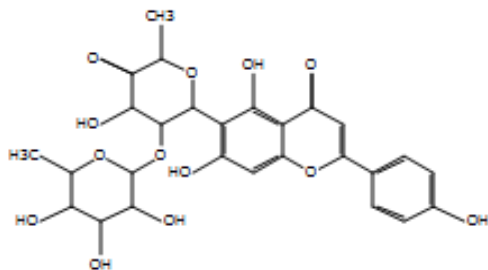
MS/MS Spectrum



MS/MS Spectrum Peak List

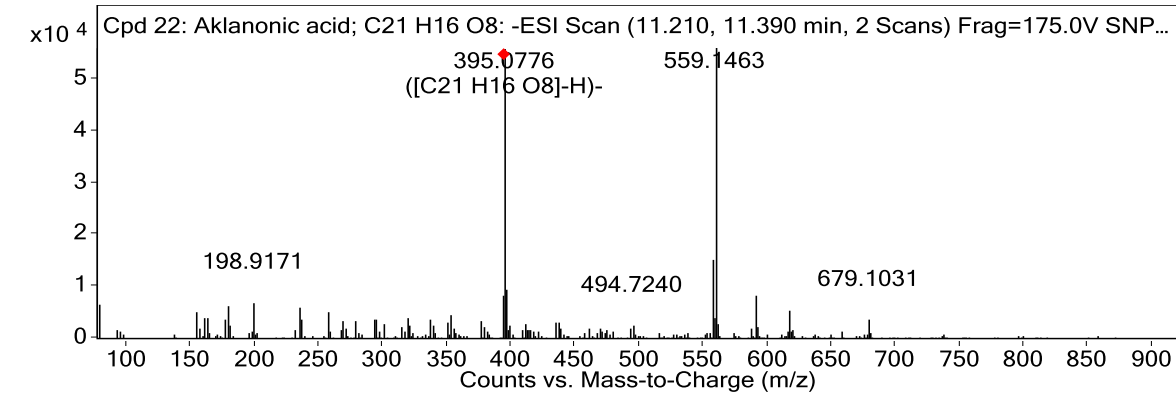
m/z	z	Abund
154.9276		354.52
156.9244		181.29
160.8416		239.26
178.8425		246.79
198.9167		252.46
234.8689		312.86
293.0453		179.6
393.0609	1	199.36
395.0775	1	1090.41
559.1454	1	431.03

Compound Structure

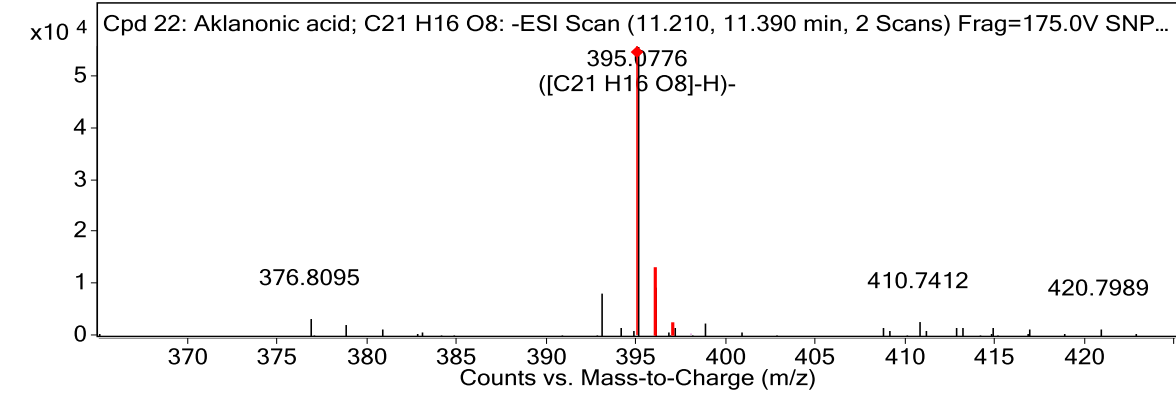


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 22: Aklanonic acid; C21 H16 O8	Aklanonic acid	395.0776	11.316	Auto MS/MS	396.0848

MS Spectrum



MS Zoomed Spectrum



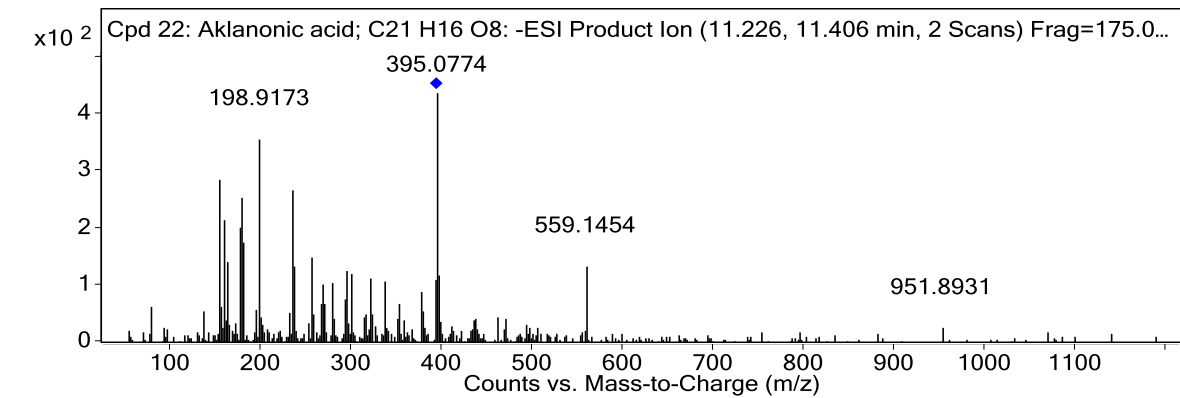
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.958				6671.48		

Qualitative Compound Report

198.9171				6940.83		
393.061			1	8291.26		
395.0776	395.0772	-0.85	1	55785.16	C21 H16 O8	(M-H)-
396.0807	396.0806	-0.14	1	9553.97	C21 H16 O8	(M-H)-
397.0842	397.083	-2.9	1	1789.59	C21 H16 O8	(M-H)-
557.1298			1	15304.56		
559.1463			1	66599.84		
560.1489			1	13849.06		
591.1713			1	8367.3		

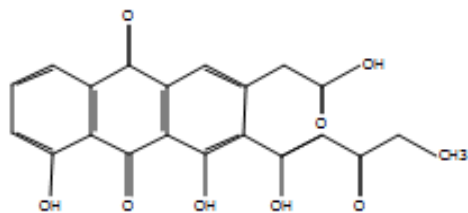
MSMS Spectrum



MS/MS Spectrum Peak List

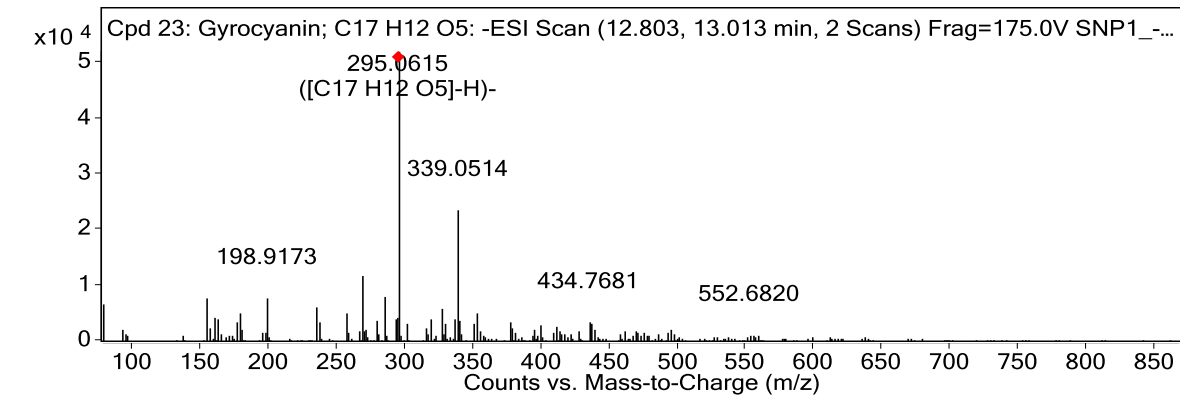
m/z	z	Abund
154.9274		285.88
160.8419		215.88
162.838		141.45
176.8431		201.27
178.842		254.14
180.8394		175.43
198.9173		357.18
234.8688		266.59
256.878		147.88
395.0774	1	437.84

Compound Structure

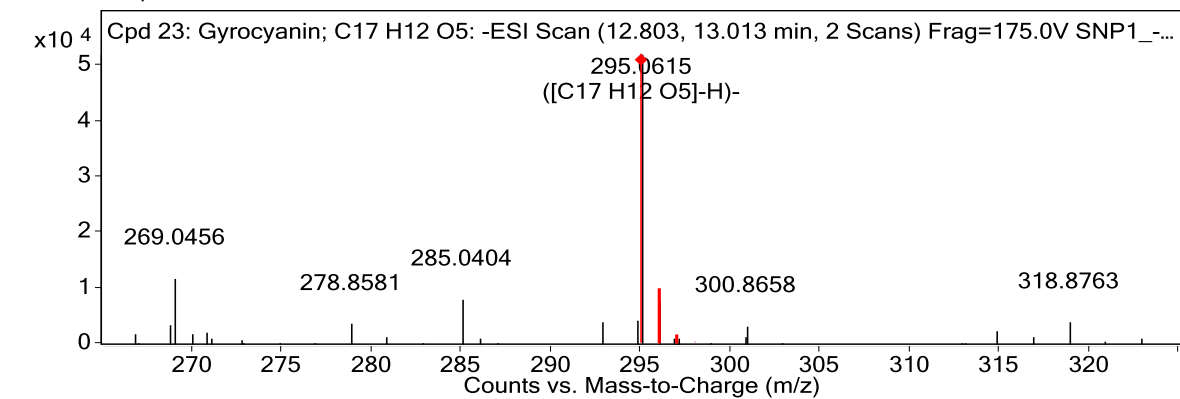


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 23: Gyrocyanin; C17 H12 O5	Gyrocyanin	295.0615	12.923	Auto MS/MS	296.0686

MS Spectrum



MS Zoomed Spectrum

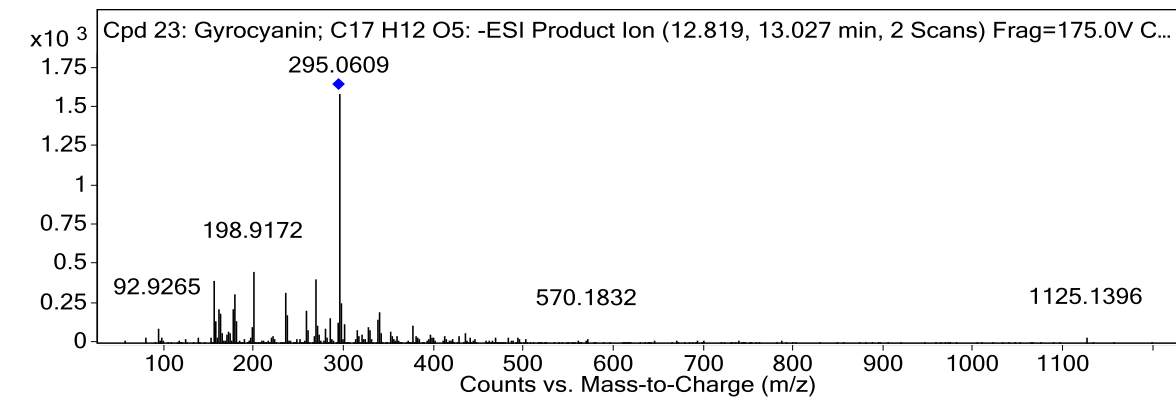


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.958				6634.91		
154.9274				7736.76		
198.9173				7782.7		
234.8687				6148.98		
269.0456			1	11824.08		
285.0404			1	8041.6		
295.0615	295.0612	-0.98	1	51908	C17 H12 O5	(M-H)-
296.0639	296.0646	2.23	1	7873.26	C17 H12 O5	(M-H)-
297.0662	297.067	2.7	1	942.36	C17 H12 O5	(M-H)-
339.0514			1	23617.6		

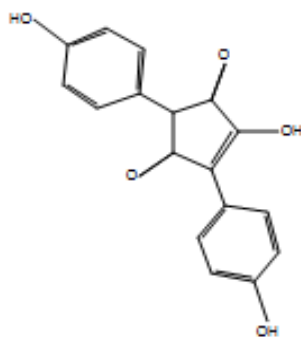
MSMS Spectrum

Qualitative Compound Report

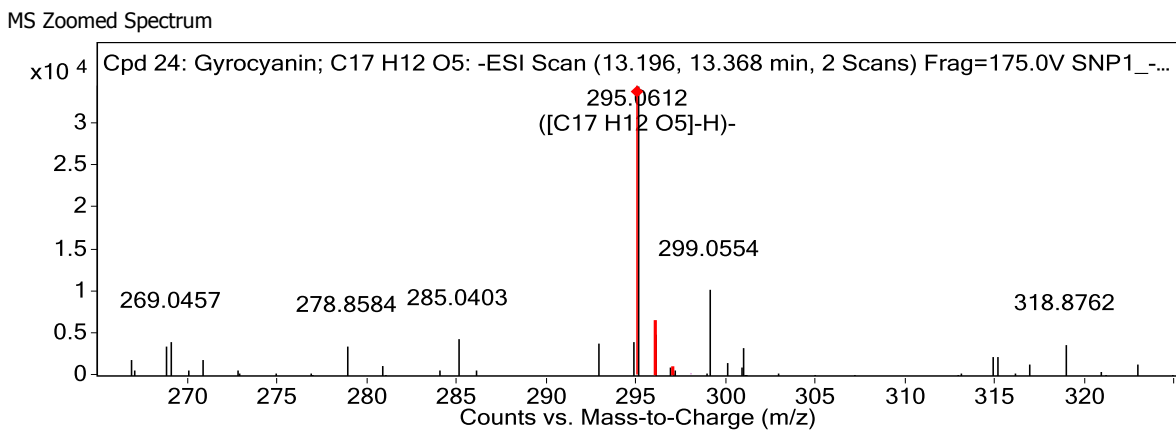
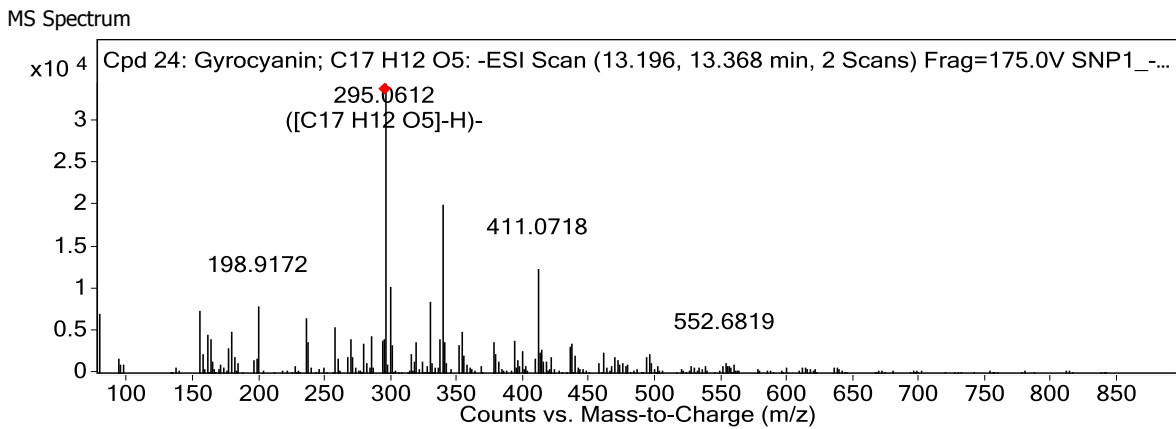


MS/MS Spectrum Peak List		
m/z	z	Abund
154.9275		396.55
160.8418		218.27
176.8429		223.2
178.842		309.25
198.9172		455.6
234.8685		326.42
256.8764		209.7
269.0452	1	404.68
295.0609	1	1588.76
296.0635	1	257.93

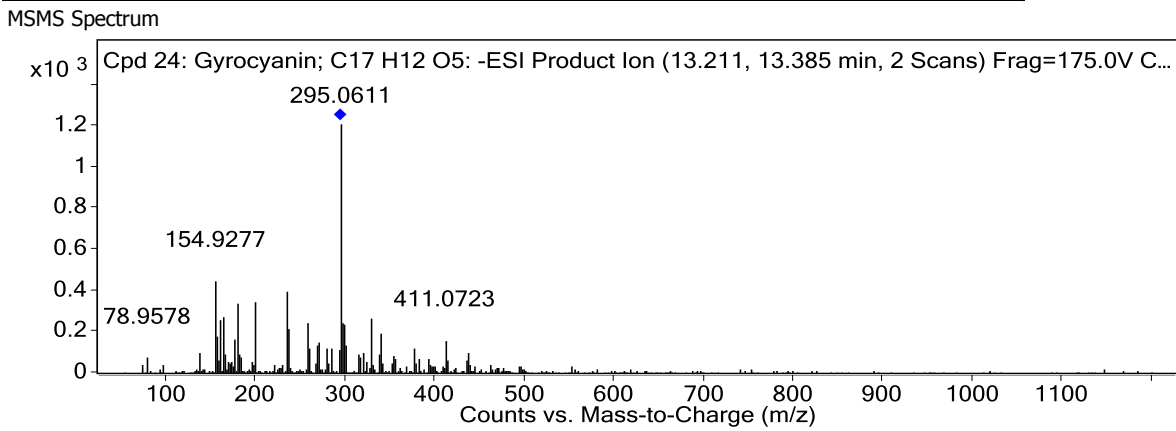
Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 24: Gyrocyanin; C17 H12 O5	Gyrocyanin	295.0612	13.298	Auto MS/MS	296.0684



m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.958				7180.62		
154.9274				7470.69		
198.9172				8010.69		
295.0612	295.0612	-0.03	1	34459.63	C17 H12 O5	(M-H)-
296.0638	296.0646	2.7	1	4981.14	C17 H12 O5	(M-H)-
297.066	297.067	3.2	1	622	C17 H12 O5	(M-H)-
299.0554			1	10262.17		
329.0667			1	8518.87		
339.051			1	20047.79		
411.0718			1	12517.27		

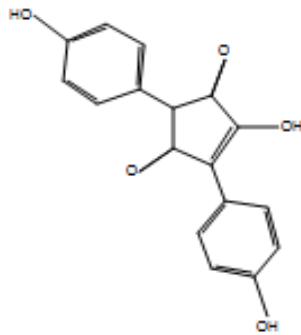


MS/MS Spectrum Peak List		
m/z	z	Abund
154.9277		450.41

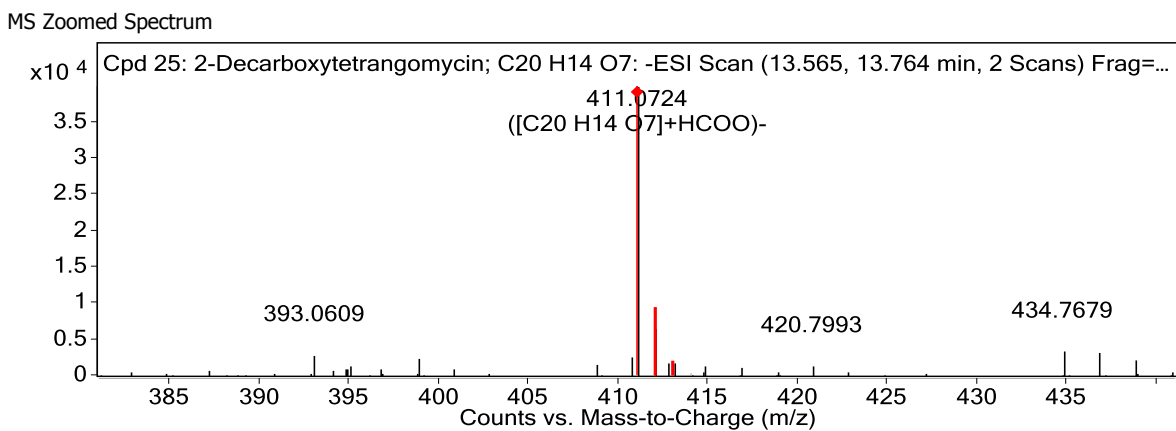
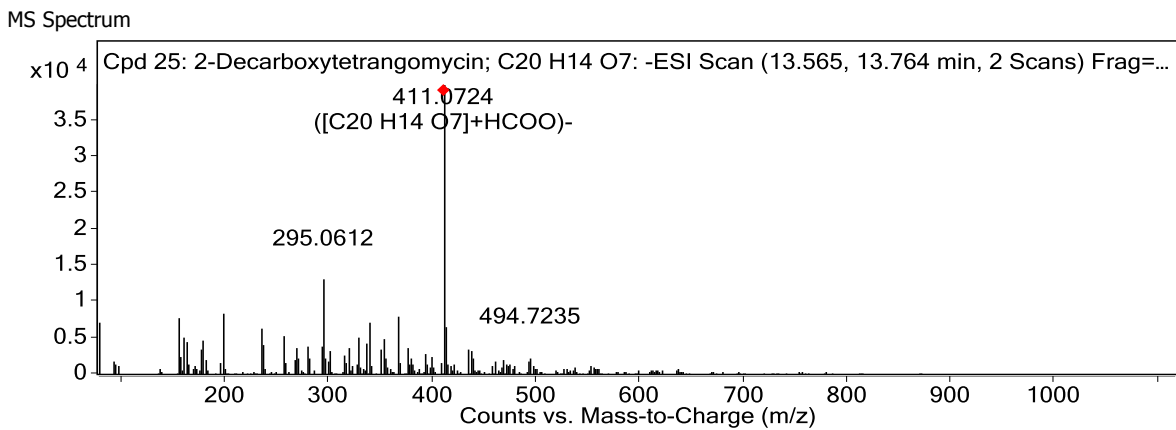
Qualitative Compound Report

160.8417		264.01
162.8394		277.26
178.8421		338.19
198.9177		347.79
234.8686		396.91
256.8773		248.53
295.0611	1	1210.5
296.0634	1	248.09
329.0668	1	271.26

Compound Structure

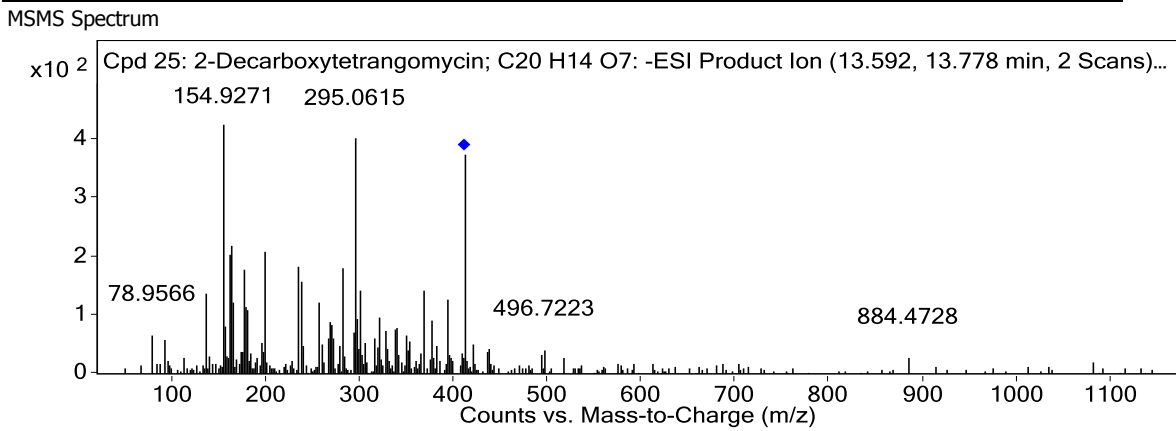


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 25: 2-Decarboxytetrangomycin; C20 H14 O7	2-Decarboxytetrangomycin	411.0724	13.685	Auto MS/MS	366.0743



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.958				7119.43		
154.9272				7846.16		
198.9173				8432.03		
234.8687				6350.15		
295.0612			1	13113.85		
339.0511			1	7278.2		
367.0821			1	8100.93		
411.0724	411.0722	-0.53	1	39842.57	C20 H14 O7	(M+HCOO)-
412.0751	412.0755	1.09	1	6602.61	C20 H14 O7	(M+HCOO)-
413.0821	413.0779	-10.19	1	1915.2	C20 H14 O7	(M+HCOO)-

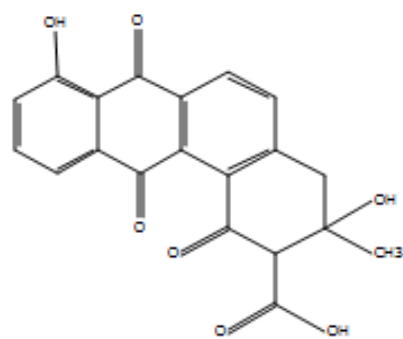


MS/MS Spectrum Peak List

m/z	z	Abund
154.9271		426.53
160.8416		202.83
162.8388		219.79
176.936		177.72
198.9161		208.53
234.8691		182.72
236.8636		158.19
281.0457	1	179.83
295.0615	1	402.39
411.0725	1	375.37

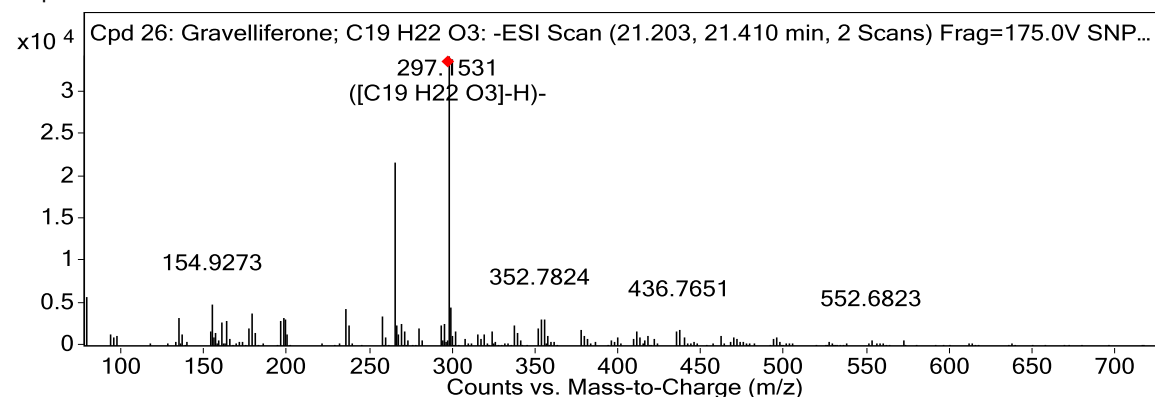
Compound Structure

Qualitative Compound Report

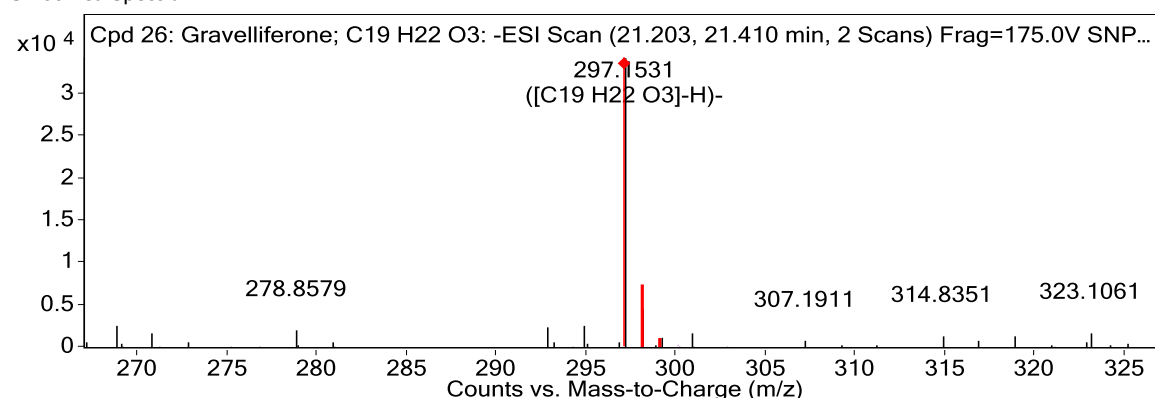


Compound Label	Name	<i>m/z</i>	RT	Algorithm	Mass
Cpd 26: Gravelliferone; C19 H22 O3	Gravelliferone	297.1531	21.324	Auto MS/MS	298.16

MS Spectrum



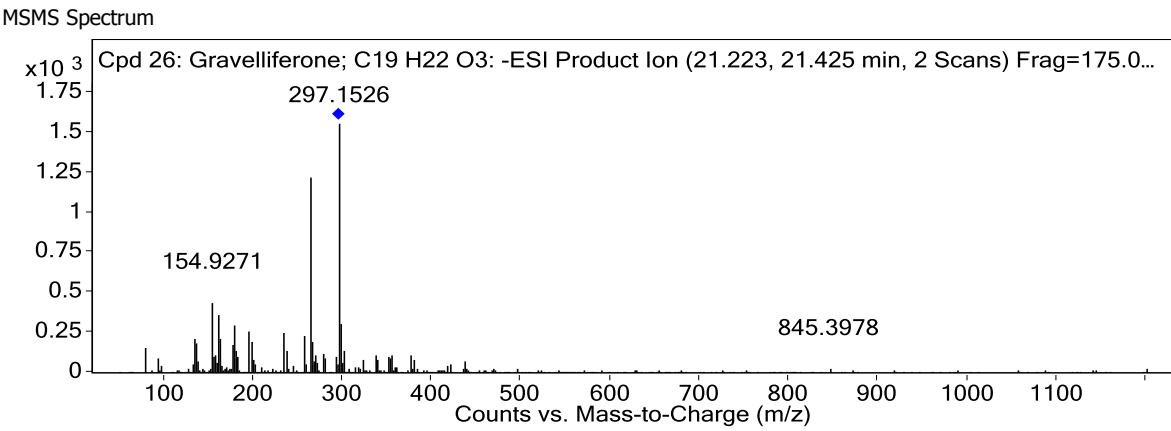
MS Zoomed Spectrum



MS Spectrum Peak List

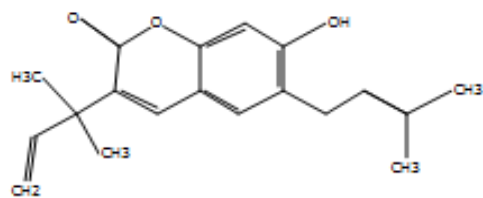
MS Spectrum Peak List						
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.9581				5765.73		
134.894				3443.57		
154.9273				4952.32		
178.8416				3853.12		
234.8688				4393.21		
256.8762				3521.7		
265.1478			1	21643.64		
297.1531	297.1496	-11.55	1	34267.07	C19 H22 O3	(M-H)-
298.156	298.153	-9.89	1	4599.31	C19 H22 O3	(M-H)-
299.1508	299.1558	16.78	1	1174.57	C19 H22 O3	(M-H)-

Qualitative Compound Report

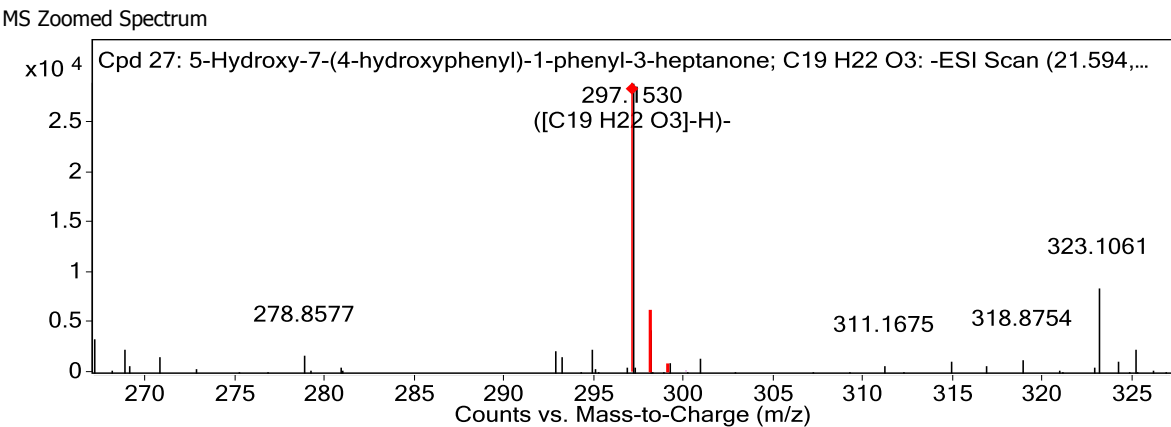
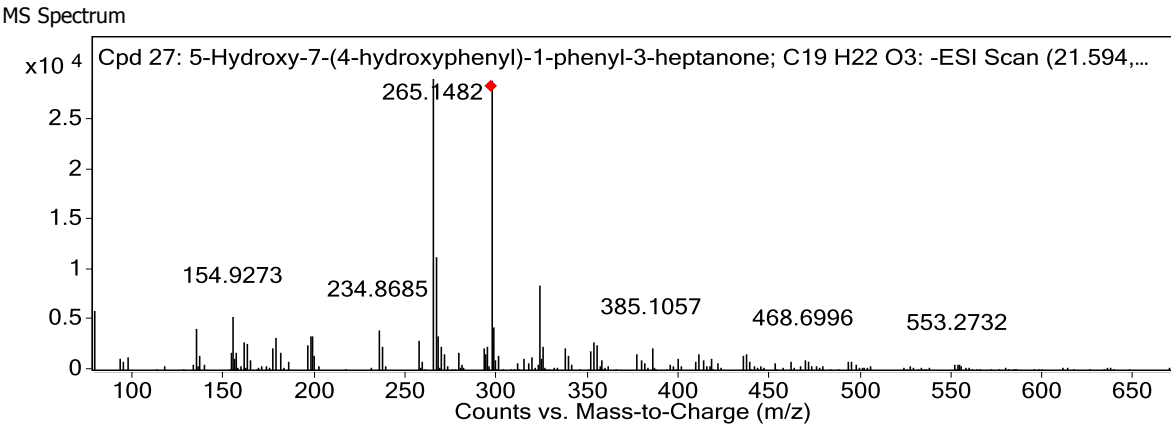


MS/MS Spectrum Peak List						
m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
153.8679				215.97		
154.9271				438.64		
160.8415				364.01		
178.8418				302.44		
195.8096				258.64		
234.8687				252.17		
256.8754				236.61		
265.1476			1	1220.35		
297.1526			1	1556.07		
298.156	298.153	-10.14	1	302.89	C19 H22 O3	(M-H)-

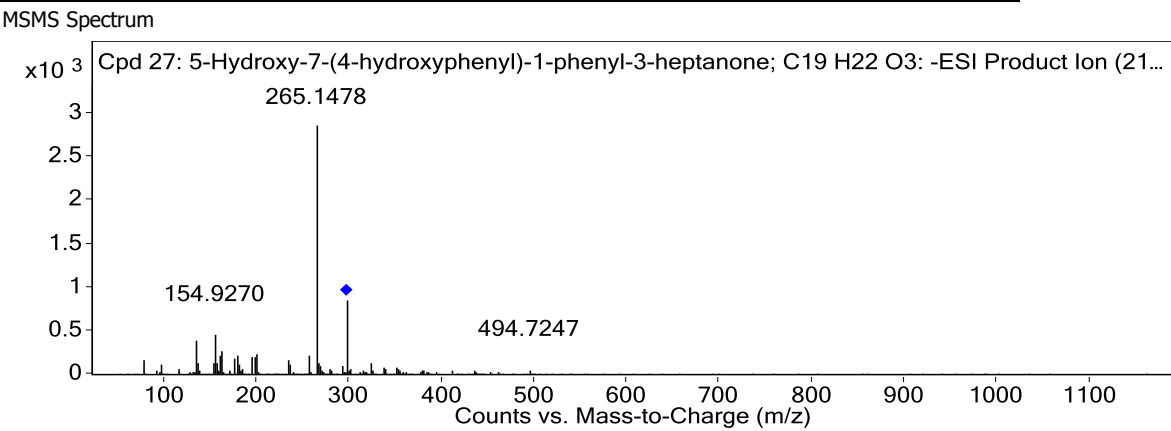
Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 27: 5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone; C19 H22 O3	5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-3-heptanone	297.153	21.71	Auto MS/MS	298.16



MS Spectrum Peak List						
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
78.9581				5887.35		
134.8939			1	4203.03		
154.9273				5350.71		
234.8685				3979.58		
265.1482			1	121109.63		
266.151			1	11314.38		
297.153	297.1496	-11.47	1	28906.51	C19 H22 O3	(M-H)-
298.1558	298.153	-9.47	1	4259.91	C19 H22 O3	(M-H)-
299.1507	299.1558	16.99	1	1084.96	C19 H22 O3	(M-H)-
323.1061			1	8535.11		

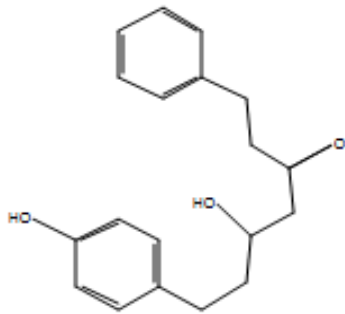


Qualitative Compound Report

MS/MS Spectrum Peak List

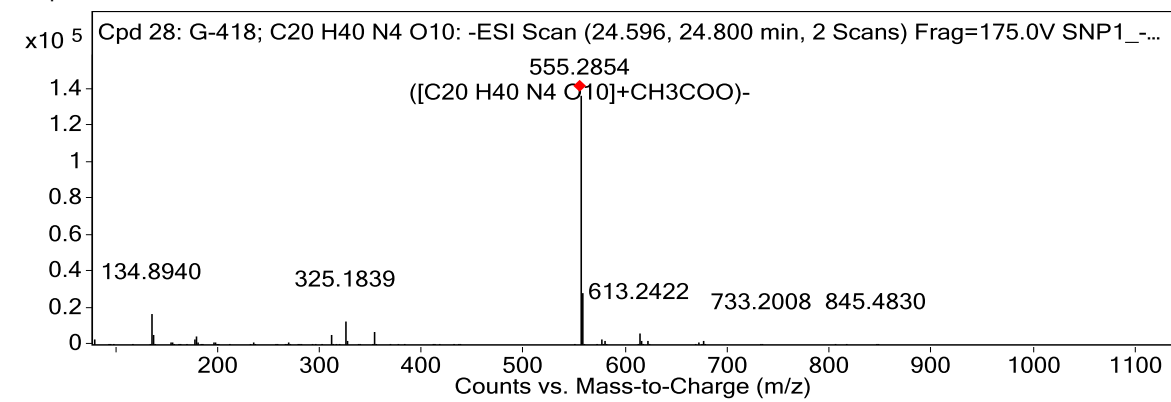
m/z	z	Abund
134.8935	1	391.61
154.927		456.13
160.8417		225.69
162.8392		282.24
178.8415		228.58
199.8048		240.5
256.8764		228.23
265.1478	1	2867.35
266.1517	1	265.61
297.1523	1	854.42

Compound Structure

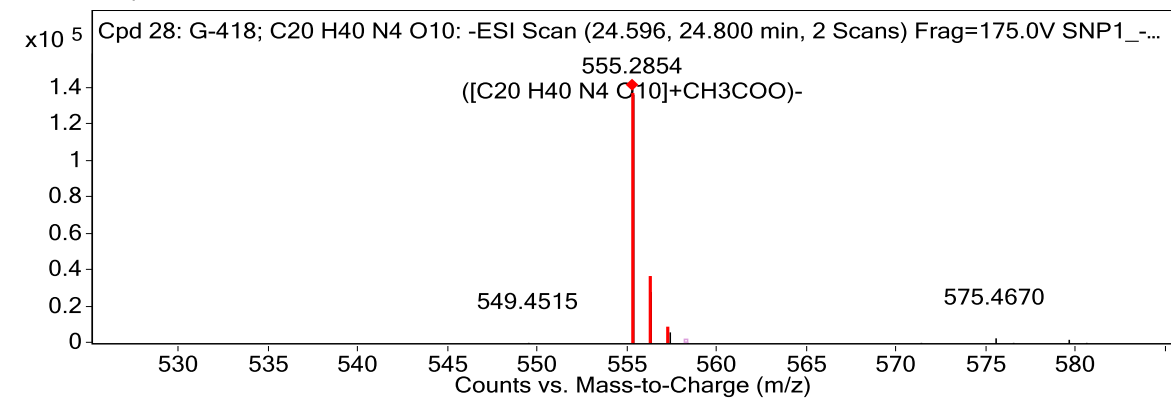


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 28: G-418; C20 H40 N4 O10	G-418	555.2854	24.712	Auto MS/MS	496.2712

MS Spectrum



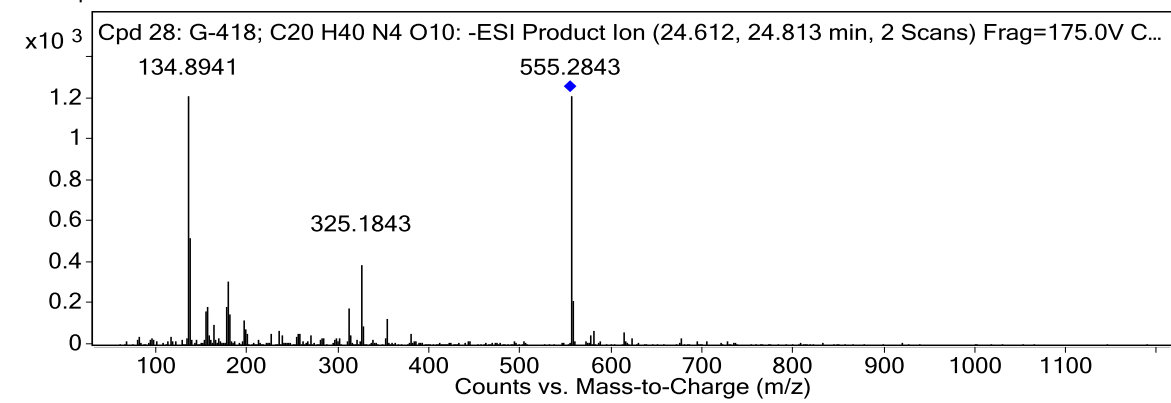
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
134.894			1	17469.9		
136.8913			1	5878.62		
178.8418				5032.89		
311.1686			1	5381.77		
325.1839			1	13422.86		
353.2001			1	7005.21		
555.2854	555.2883	5.21	1	136546.95	C20 H40 N4 O10	(M+CH3COO)-
556.2878	556.2914	6.5	1	28540.48	C20 H40 N4 O10	(M+CH3COO)-
557.2862	557.2936	13.37	1	6933.55	C20 H40 N4 O10	(M+CH3COO)-
613.2422			1	6557.17		

MSMS Spectrum

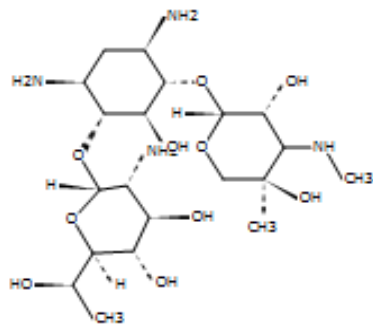


MS/MS Spectrum Peak List

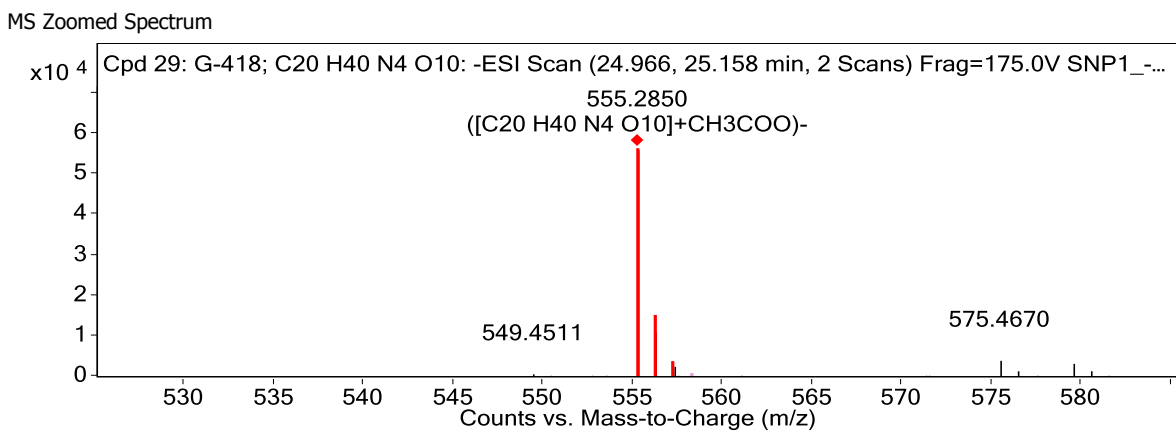
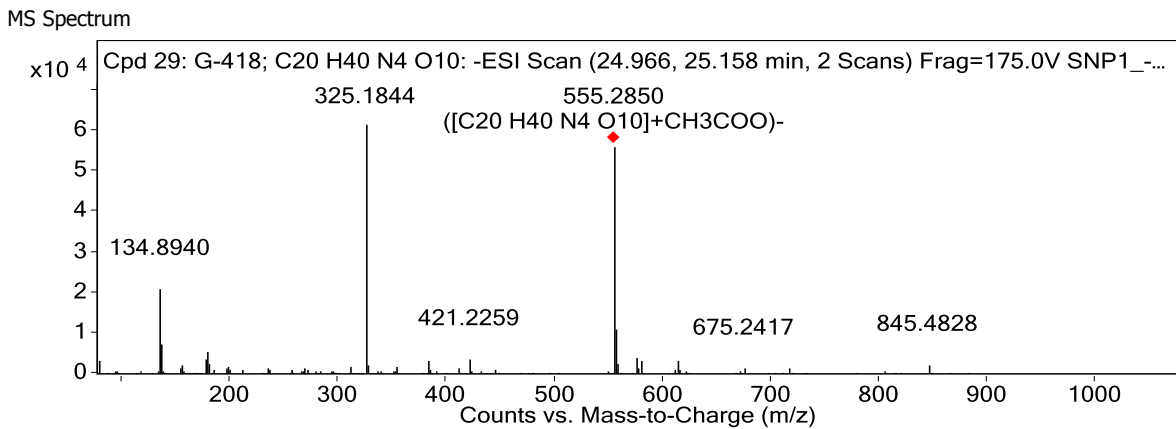
m/z	z	Abund
134.8941	1	1213.17
136.891	1	526.69
153.8673		170.68
154.9267		191.13
176.8424		190.97
178.841		311.27
311.1679	1	179.37
325.1843	1	390.81
555.2843	1	1215.59
556.285	1	219.12

Compound Structure

Qualitative Compound Report

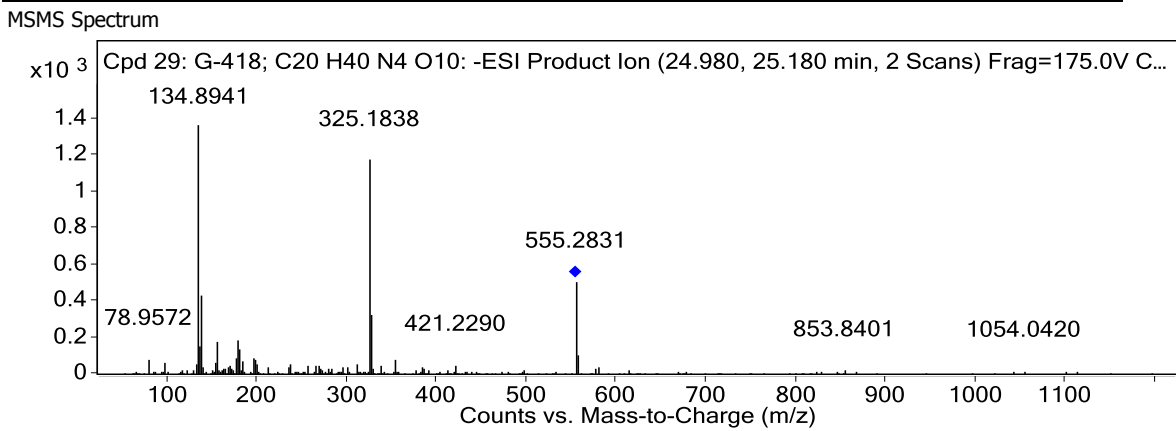


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 29: G-418; C20 H40 N4 O10	G-418	555.285	25.08	Auto MS/MS	496.2709



MS Spectrum Peak List

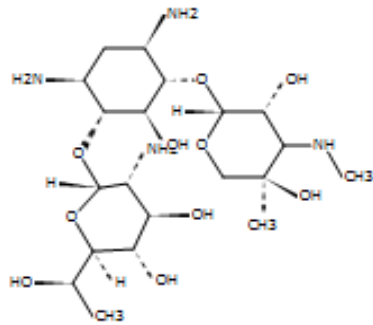
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
134.894			1	21033.94		
136.8912			1	7368.65		
178.8418				5531.29		
325.1844			1	61556.28		
326.1871			1	9951.68		
421.2259			1	3651.71		
555.285	555.2883	5.9	1	56103.2	C20 H40 N4 O10	(M+CH3COO)-
556.2874	556.2914	7.14	1	10955.16	C20 H40 N4 O10	(M+CH3COO)-
557.2858	557.2936	13.96	1	2754.09	C20 H40 N4 O10	(M+CH3COO)-
575.467			1	3996.85		



MS/MS Spectrum Peak List

m/z	z	Abund
134.8941	1	1368.4
135.8941	1	154.42
136.891	1	429.69
154.9268		182.43
178.8418		185.64
180.8404		135.05
325.1838	1	1177.41
326.1866	1	329.94
555.2831	1	509.56
556.2867	1	106.08

Compound Structure

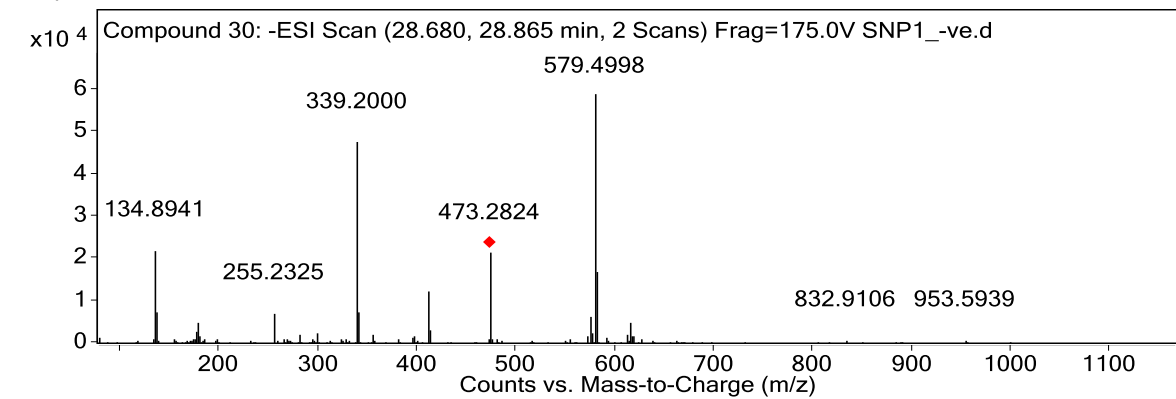


Compound Label	m/z	RT	Algorithm
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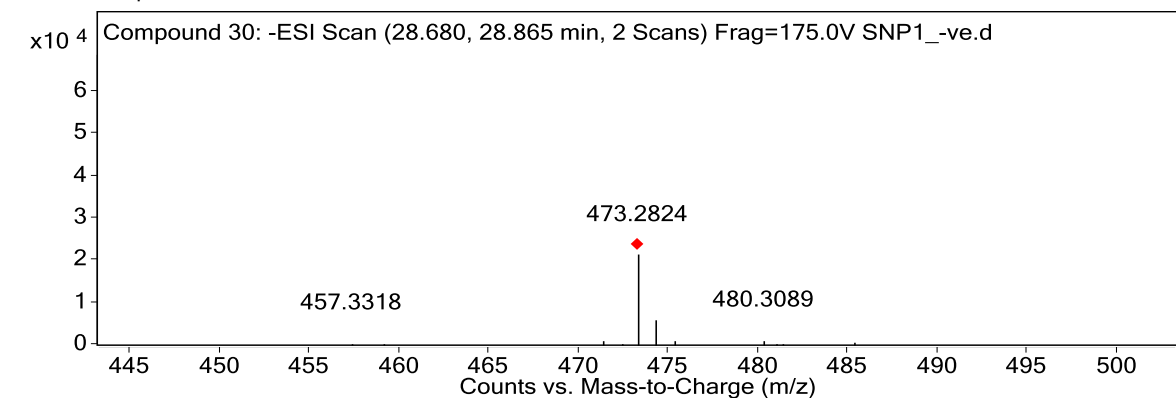
Qualitative Compound Report

Compound 30	473.2824	28.79	Auto MS/MS
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MS Spectrum



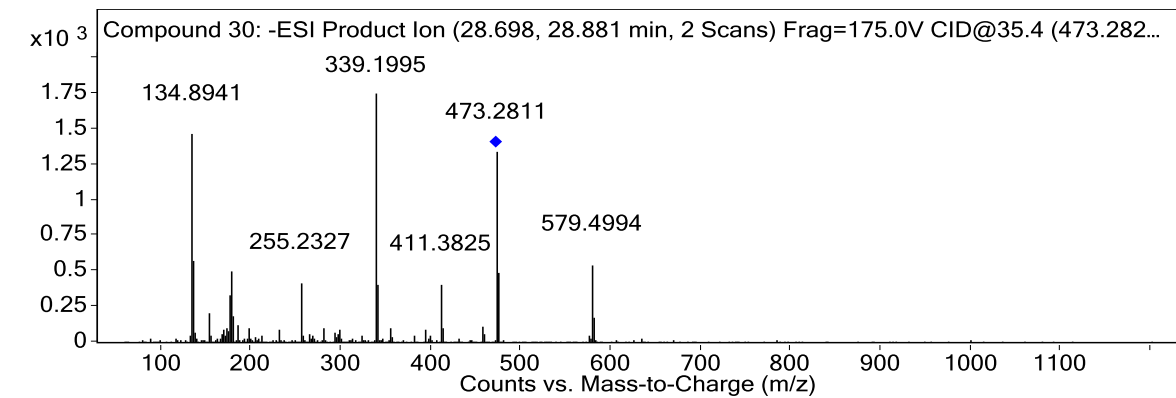
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
134.8941	1	22023.82
136.8911	1	7423.43
339.2	1	47632.8
340.2029	1	7358.88
411.3836	1	12253.13
473.2824	1	21345.84
474.2858	1	5871.1
475.2881	1	950.06
579.4998	1	58974.12
580.5023	1	17104.64

MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
134.8941	1	1466.28
136.8913	1	575.22
178.8421		499.74
255.2327	1	420.72
339.1995	1	1751
340.2023	1	405.26
411.3825	1	409.81
473.2811	1	1336.54
474.2856	1	496.21
579.4994	1	549.76

--- End Of Report ---