Qualitative Compound Identification Report

Data File	20200723-dpf-1.d	**Sample Name**	Sample2
Sample Type	Sample	**Position**	P1-E5
Instrument Name	Instrument 1	**User Name**	
Acq Method	20200724.m	**Acquired Time**	7/28/2020 8:30:23 PM (UTC+08:00)
IRM Calibration Status	Success	**DA Method**	WZY+20191127.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition Time (Local)**	7/28/2020 8:30:23 PM (UTC+08:00)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.3 SP1)	**QTOF Driver Version**	8.00.00
QTOF Firmware Version	3.712	**Tune Mass Range Max.**	3200

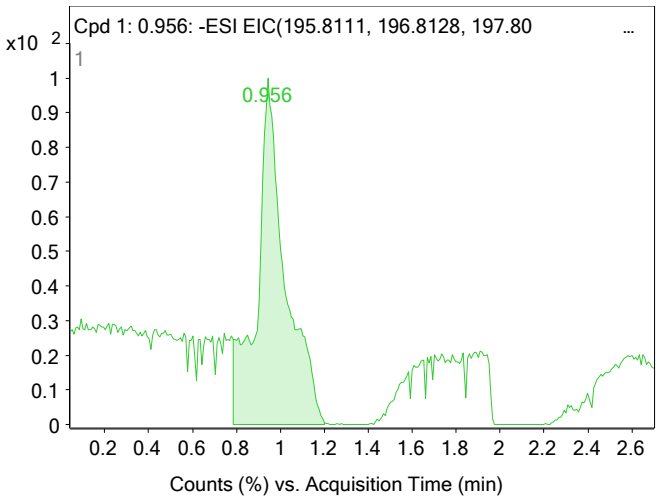
Compound Table

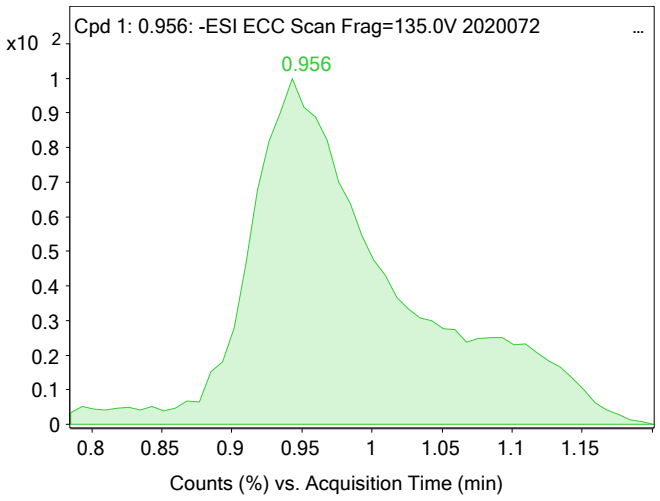
Compound Label	RT	Mass	Name	DB Formula	DB Diff (ppm)	Hits (DB)
Cpd 1: 0.956	0.956	196.8189				
Cpd 2: 1.096	1.096	186.0159				
Cpd 3: 1.187	1.187	226.0692				
Cpd 4: Gluconic acid; C6 H12 O7; 1.189	1.189	196.0586	Gluconic acid	C6 H12 O7	-1.55	1
Cpd 5: 1.193	1.193	166.0479				
Cpd 6: 1.199	1.199	328.1011				
Cpd 7: Cordycepic acid; C7 H12 O6; 1.206	1.206	192.0638	Cordycepic acid	C7 H12 O6	-2.14	3
Cpd 8: Inositol-b; C6 H12 O6; 1.207	1.207	180.0642	Inositol-b	C6 H12 O6	-4.38	10
Cpd 9: L-Galactoheptulose; C7 H14 O7; 1.209	1.209	210.0747	L-Galactoheptulose	C7 H14 O7	-3.73	4
Cpd 10: Purine; C5 H4 N4; 1.212	1.212	120.0433	Purine	C5 H4 N4	2.34	2
Cpd 11: beta-Hydroxy-alpha-methylene-gamma-butyllactone; C5 H6 O3; 1.221	1.221	114.0328	beta-Hydroxy-alpha-methylene-gamma-butyllactone	C5 H6 O3	-9.37	1
Cpd 12: Rhodojaponia IV; C24 H38 O8; 1.230	1.23	454.2557	Rhodojaponia IV	C24 H38 O8	2.19	4
Cpd 13: Manninotriose; C18 H32 O16; 1.231	1.231	504.1702	Manninotriose	C18 H32 O16	-2.25	9
Cpd 14: Ribose; C5 H10 O5; 1.236	1.236	150.054	Ribose	C5 H10 O5	-7.78	4
Cpd 15: Hexahydroxytaxadiene; C20 H32 O6; 1.245	1.245	368.219	Hexahydroxytaxadiene	C20 H32 O6	2.44	2
Cpd 16: 3,6-Anhydrogalactose; C6 H10 O5; 1.245	1.245	162.0537	3,6-Anhydrogalactose	C6 H10 O5	-5.55	2
Cpd 17: Andromedotoxin; C22 H36 O7; 1.249	1.249	412.2446	Andromedotoxin	C22 H36 O7	3.72	1
Cpd 18: Manninotriose; C18 H32 O16; 1.253	1.253	504.1706	Manninotriose	C18 H32 O16	-3.1	9
Cpd 19: Sarmentosin epoxide; C11 H17 N O8; 1.255	1.255	291.0964	Sarmentosin epoxide	C11 H17 N O8	-3.43	1
Cpd 20: 1.256	1.256	102.0329				
Cpd 21: 1.259	1.259	312.1068				
Cpd 22: 1.260	1.26	846.2861				
Cpd 23: Tuliposide B; C11 H18 O9; 1.263	1.263	294.0979	Tuliposide B	C11 H18 O9	-9.56	1
Cpd 24: 5-O-Methylembelin; C18 H28 O4; 1.265	1.265	308.1967	5-O-Methylembelin	C18 H28 O4	6.59	1
Cpd 25: 1.266	1.266	684.234				
Cpd 26: Cellobiose; C12 H22 O11; 1.268	1.268	342.1175	Cellobiose	C12 H22 O11	-3.76	10
Cpd 27: 1.270	1.27	593.2174				
Cpd 28: 1.283	1.283	978.3271				
Cpd 29: Allithiamine; C15 H22 N4 O2 S2; 1.290	1.29	354.1177	Allithiamine	C15 H22 N4 O2 S2	2.07	1
Cpd 30: Picrasinoside D; C28 H44 O11; 1.290	1.29	556.2866	Picrasinoside D	C28 H44 O11	3.16	1
Cpd 31: beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside; C17 H30 O15; 1.290	1.29	474.1613	beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside	C17 H30 O15	-5.92	1
Cpd 32: Fumaric acid; C4 H4 O4; 1.318	1.318	116.0121	Fumaric acid	C4 H4 O4	-10.02	1
Cpd 33: Malic acid; C4 H6 O5; 1.320	1.32	134.0222	Malic acid	C4 H6 O5	-5.01	1
Cpd 34: beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside; C17 H30 O15; 1.334	1.334	474.1586	beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside	C17 H30 O15	-0.22	3
Cpd 35: 1.337	1.337	423.1383				
Cpd 36: Cepharanoline; C36 H36 N2 O6; 1.346	1.346	592.2627	Cepharanoline	C36 H36 N2 O6	-9.05	3
Cpd 37: 1.349	1.349	619.2333				
Cpd 38: Carmichaeline; C22 H35 N O4; 1.355	1.355	377.2543	Carmichaeline	C22 H35 N O4	6.2	3
Cpd 39: gamma-Amino-alpha-methylene butyric acid; C5 H9 N O2; 1.369	1.369	115.0639	gamma-Amino-alpha-methylene butyric acid	C5 H9 N O2	-5.29	3
Cpd 40: 5alpha-Acetoxy-1 beta-benzoyl-8alpha-cinnamoyl-4alpha-hydroxy-dihydroagarofuran; C33 H38 O8; 1.420	1.42	562.2518	5alpha-Acetoxy-1 beta-benzoyl-8alpha-cinnamoyl-4alpha-hydroxy-dihydroagarofuran	C33 H38 O8	8.74	3
Cpd 41: Linustatin; C16 H27 N O11; 1.432	1.432	409.1579	Linustatin	C16 H27 N O11	1.13	1
Cpd 42: Heteratisine; C22 H33 N O5; 1.447	1.447	391.2323	Heteratisine	C22 H33 N O5	9.07	1
Cpd 43: Pyroglutamic acid; C5 H7 N O3; 1.454	1.454	129.0421	Pyroglutamic acid	C5 H7 N O3	3.74	1
Cpd 44: 8-epi-Grandifloric acid; C15 H22 O9; 1.710	1.71	346.1263	8-epi-Grandifloric acid	C15 H22 O9	0.16	4
Cpd 45: Loganic acid; C16 H24 O10; 1.711	1.711	376.137	Loganic acid	C16 H24 O10	-0.19	7
Cpd 46: Yopaaoside C; C17 H26 O12; 1.712	1.712	422.1424	Yopaaoside C	C17 H26 O12	-0.01	4
Cpd 47: 1.871	1.871	494.1268				
Cpd 48: 2.024	2.024	113.9929				
Cpd 49: 2.041	2.041	129.9666				
Cpd 50: 2.135	2.135	336.1644				
Cpd 51: L-Arginine; C6 H14 N4 O2; 2.145	2.145	174.1106	L-Arginine	C6 H14 N4 O2	6.32	1
Cpd 52: 6-O-Galloyl-glucose; C13 H16 O10; 2.163	2.163	332.0744	6-O-Galloyl-glucose	C13 H16 O10	-0.06	3

Cpd 53: Usambarensine; C29 H28 N4; 2.232	2.232	432.2294	Usambarensine	C29 H28 N4	4.61	1
Cpd 54: 2.240	2.24	494.1268				
Cpd 55: 2.417	2.417	397.1585				
Cpd 56: 6-O-Galloyl-glucose; C13 H16 O10; 2.486	2.486	332.0748	6-O-Galloyl-glucose	C13 H16 O10	-1.39	3
Cpd 57: Ipolamiide; C17 H26 O11; 2.753	2.753	406.1476	Ipolamiide	C17 H26 O11	-0.25	6
Cpd 58: 2.757	2.757	294.8861				
Cpd 59: Maltol; C6 H6 O3; 2.766	2.766	126.0313	Maltol	C6 H6 O3	3.28	6
Cpd 60: Gallic acid; C7 H6 O5; 2.769	2.769	170.0208	Gallic acid	C7 H6 O5	4.28	1
Cpd 61: 6-O-Galloyl-glucose; C13 H16 O10; 2.826	2.826	332.0743	6-O-Galloyl-glucose	C13 H16 O10	0.09	3
Cpd 62: Armillaripin; C24 H30 O6; 3.010	3.01	414.2017	Armillaripin	C24 H30 O6	6.21	3
Cpd 63: 3.154	3.154	464.1169				
Cpd 64: Loganin; C17 H26 O10; 4.577	4.577	390.1505	Loganin	C17 H26 O10	5.32	9
Cpd 65: 5.860	5.86	272.9249				
Cpd 66: 3-Methoxygallic acid; C8 H8 O5; 5.872	5.872	184.0368	3-Methoxygallic acid	C8 H8 O5	1.83	2
Cpd 67: Ampelopsisin; C23 H28 O12; 5.879	5.879	496.1584	Ampelopsisin	C23 H28 O12	-0.72	3
Cpd 68: Epicatechin; C15 H14 O6; 6.028	6.028	290.0786	Epicatechin	C15 H14 O6	1.42	9
Cpd 69: p-Hydroxybenzoic acid; C7 H6 O3; 6.064	6.064	138.0317	p-Hydroxybenzoic acid	C7 H6 O3	0.13	6
Cpd 70: Inumakilactone A glucoside; C24 H30 O13; 6.412	6.412	526.1679	Inumakilactone A glucoside	C24 H30 O13	1.34	1
Cpd 71: Cistanoside H; C21 H30 O14; 6.769	6.769	506.1636	Cistanoside H	C21 H30 O14	-0.1	1
Cpd 72: Albiflorin R1; C23 H28 O11; 7.988	7.988	480.1633	Albiflorin R1	C23 H28 O11	-0.28	3
Cpd 73: Inumakilactone A glucoside; C24 H30 O13; 7.988	7.988	526.1688	Inumakilactone A glucoside	C24 H30 O13	-0.37	1
Cpd 74: Melampyroside; C22 H26 O10; 7.988	7.988	450.1528	Melampyroside	C22 H26 O10	-0.44	4
Cpd 75: Secologanoside; C25 H32 O14; 8.918	8.918	556.1783	Secologanoside	C25 H32 O14	1.69	1
Cpd 76: Inumakilactone A glucoside; C24 H30 O13; 9.628	9.628	526.1684	Inumakilactone A glucoside	C24 H30 O13	0.44	1
Cpd 77: 9.763	9.763	633.1773				
Cpd 78: Magnolignan H; C35 H34 O6; 9.763	9.763	550.2471	Magnolignan H	C35 H34 O6	-21.08	1
Cpd 79: 3,5,4'-Trihydroxystilene-4'-glucoside; C20 H22 O8; 10.040	10.04	390.1317	3,5,4'-Trihydroxystilene-4'-glucoside	C20 H22 O8	-0.46	10
Cpd 80: 10.041	10.041	941.1187				
Cpd 81: N-Methyl lycodine; C17 H24 N2; 10.176	10.176	256.1942	N-Methyl lycodine	C17 H24 N2	-1.01	1
Cpd 82: 10.589	10.589	616.1795				
Cpd 83: Benzoyl-oxypaeoniflorin; C30 H32 O13; 12.487	12.487	600.1838	Benzoyl-oxypaeoniflorin	C30 H32 O13	0.85	1
Cpd 84: Benzoyl-oxypaeoniflorin; C30 H32 O13; 12.984	12.984	600.1845	Benzoyl-oxypaeoniflorin	C30 H32 O13	-0.39	1
Cpd 85: 7-O-Methylaloeresin A; C29 H30 O11; 14.996	14.996	554.1786	7-O-Methylaloeresin A	C29 H30 O11	0.43	3
Cpd 86: Zizybeoside II; C25 H38 O16; 14.996	14.996	594.2189	Zizybeoside II	C25 H38 O16	-4.84	1
Cpd 87: Benzoylpaeoniflorin; C30 H32 O12; 14.997	14.997	584.1896	Benzoylpaeoniflorin	C30 H32 O12	-0.37	1
Cpd 88: 19.458	19.458	398.2342				
Cpd 89: 20.485	20.485	326.1919				
Cpd 90: 20.761	20.761	326.192				
Cpd 91: 21.761	21.761	340.2076				
Cpd 92: Hydroxymangiferonic acid; C29 H44 O4; 24.056	24.056	456.324	Hydroxymangiferonic acid	C29 H44 O4	-0.08	4
Cpd 93: Queretaroic acid; C30 H48 O4; 25.172	25.172	472.3515	Queretaroic acid	C30 H48 O4	7.86	10
Cpd 94: 25.494	25.494	312.2073				
Cpd 95: 26.718	26.718	340.2399				
Cpd 96: 3-Epioleanolic acid; C30 H48 O3; 27.626	27.626	456.3604	3-Epioleanolic acid	C30 H48 O3	-0.03	10
Cpd 97: Chlorogenin; C27 H44 O4; 28.796	28.796	432.324	Chlorogenin	C27 H44 O4	-0.18	10
Cpd 98: 32.498	32.498	113.9929				

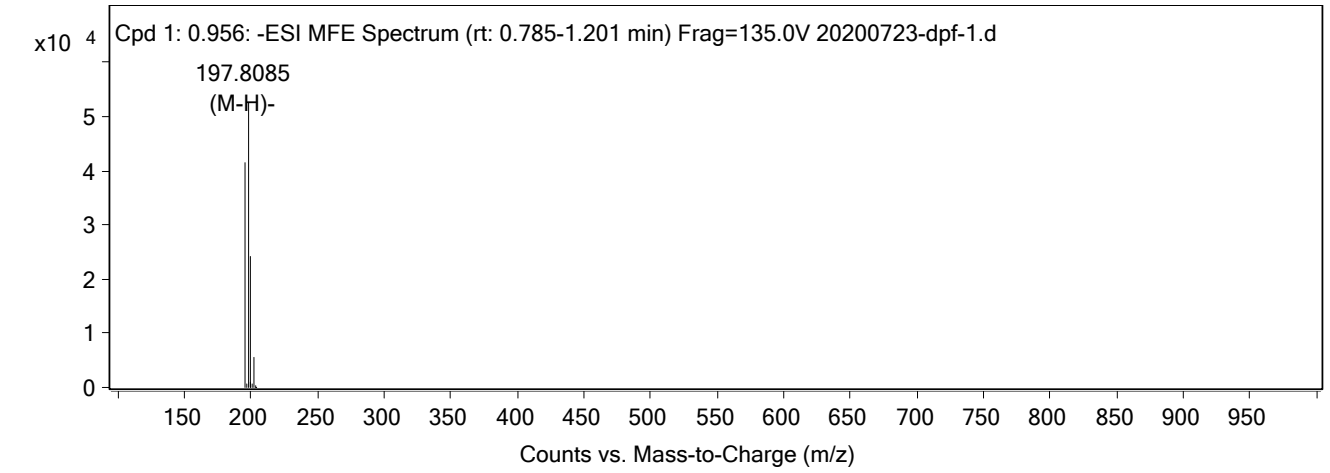
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.956	195.8116	0.956	Find by Molecular Feature	196.8189

Compound Chromatograms

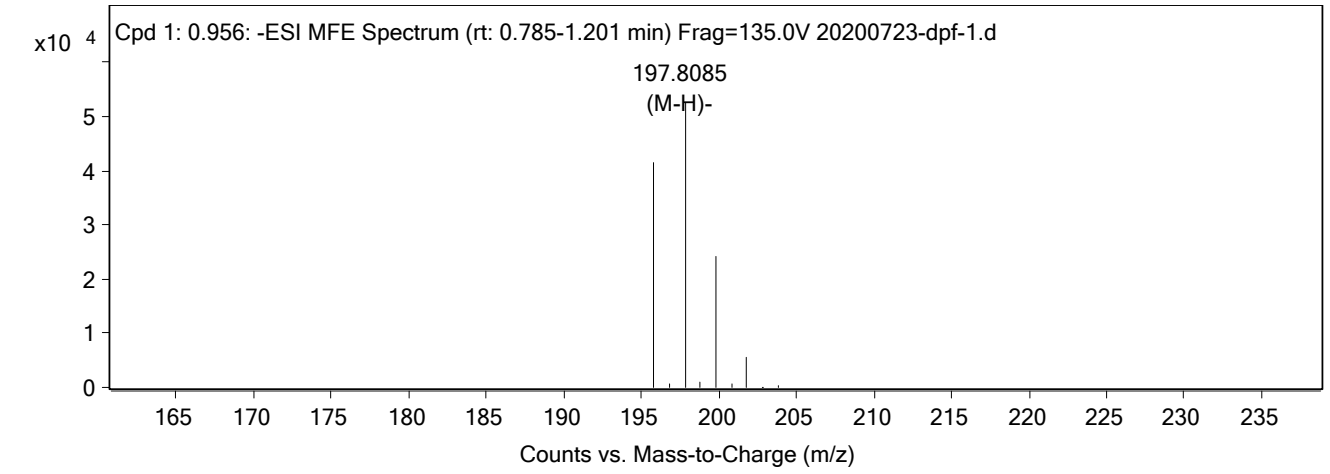




MFE MS Spectrum



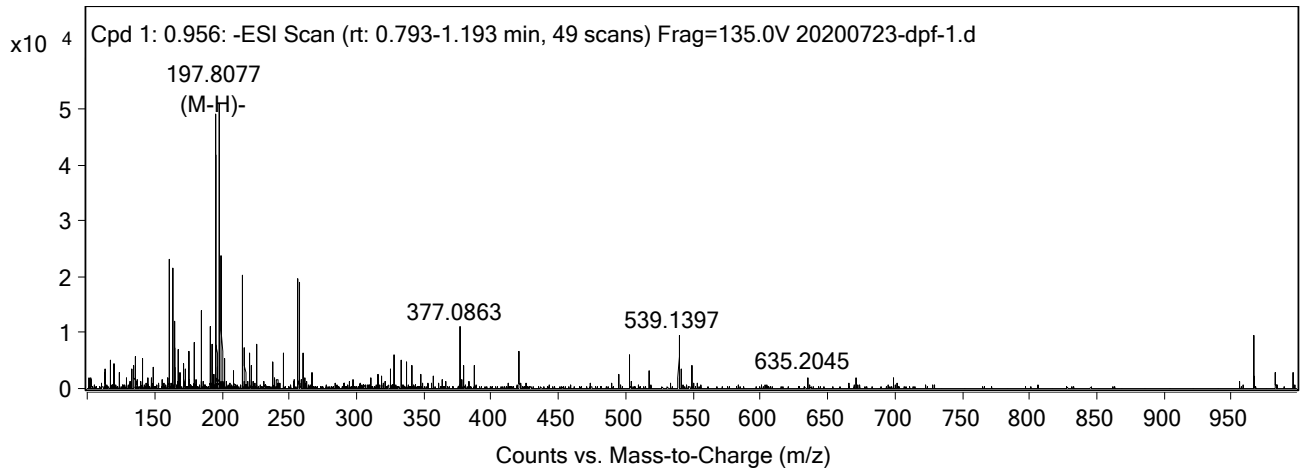
MFE MS Zoomed Spectrum



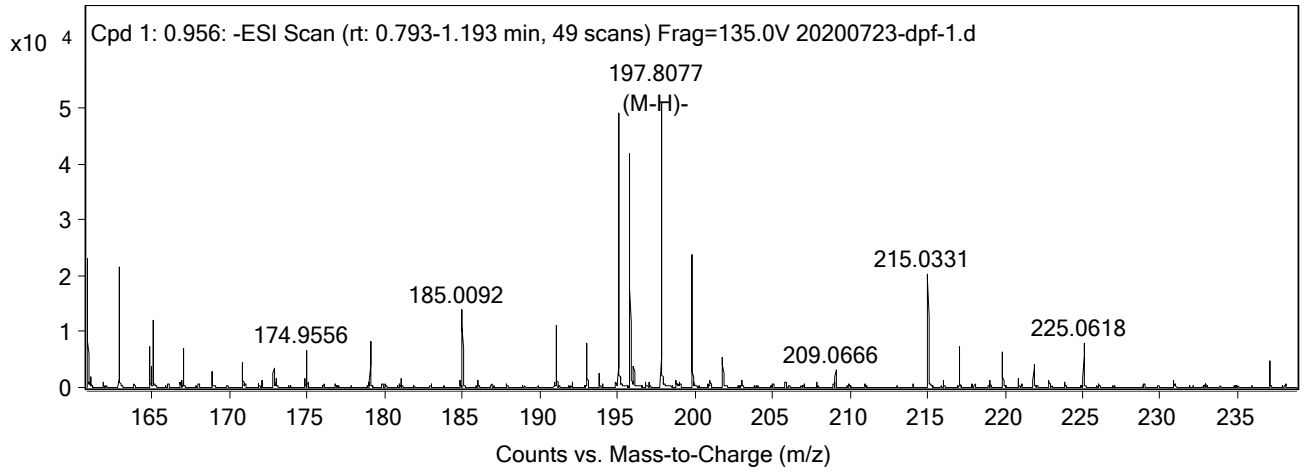
MS Spectrum Peak List

m/z	z	Abund	Ion
195.8116	-1	41493.06	(M-H)-
196.8129	-1	832.64	(M-H)-
197.8085	-1	52634.87	(M-H)-
198.8097	-1	1022.34	(M-H)-
199.8056	-1	24208.88	(M-H)-
200.8065	-1	621.71	(M-H)-
201.8024	-1	5412.53	(M-H)-
202.8102	-1	119.56	(M-H)-
203.8008	-1	364.69	(M-H)-

MS Spectrum

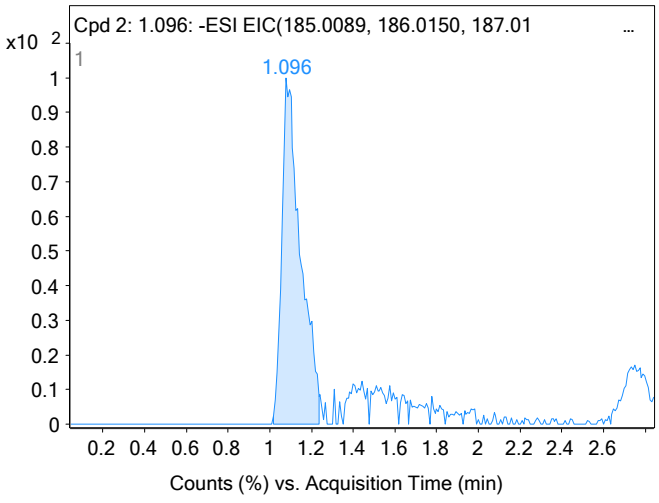


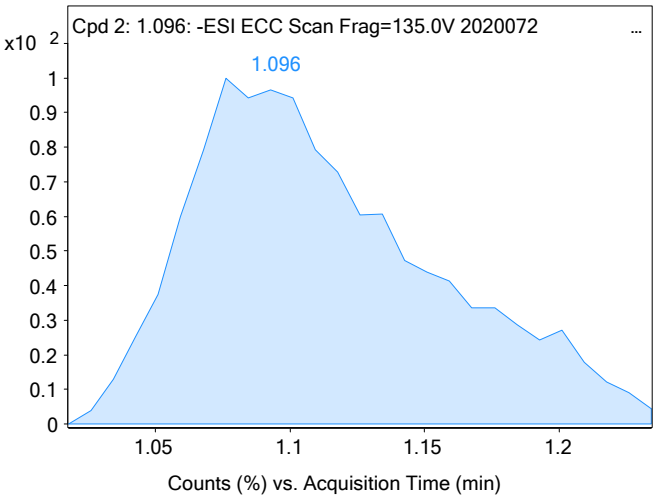
MS Zoomed Spectrum



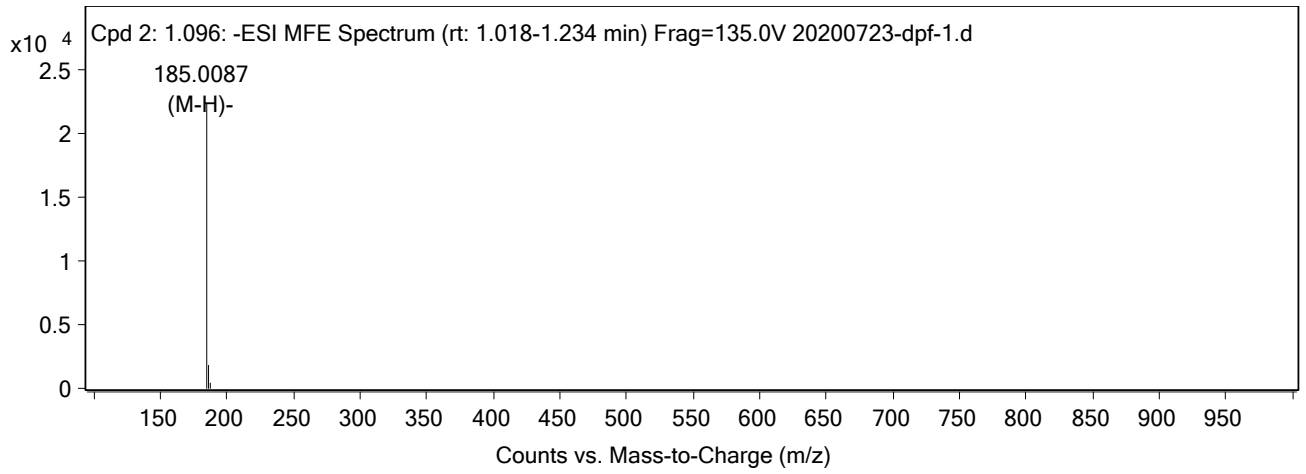
Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: 1.096	185.0087	1.096	Find by Molecular Feature	186.0159

Compound Chromatograms

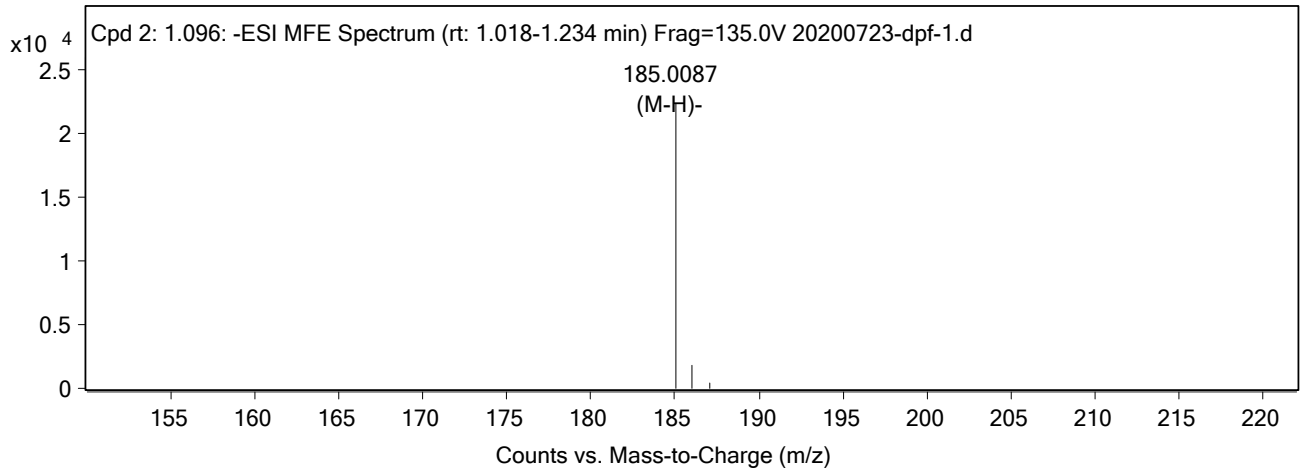




MFE MS Spectrum



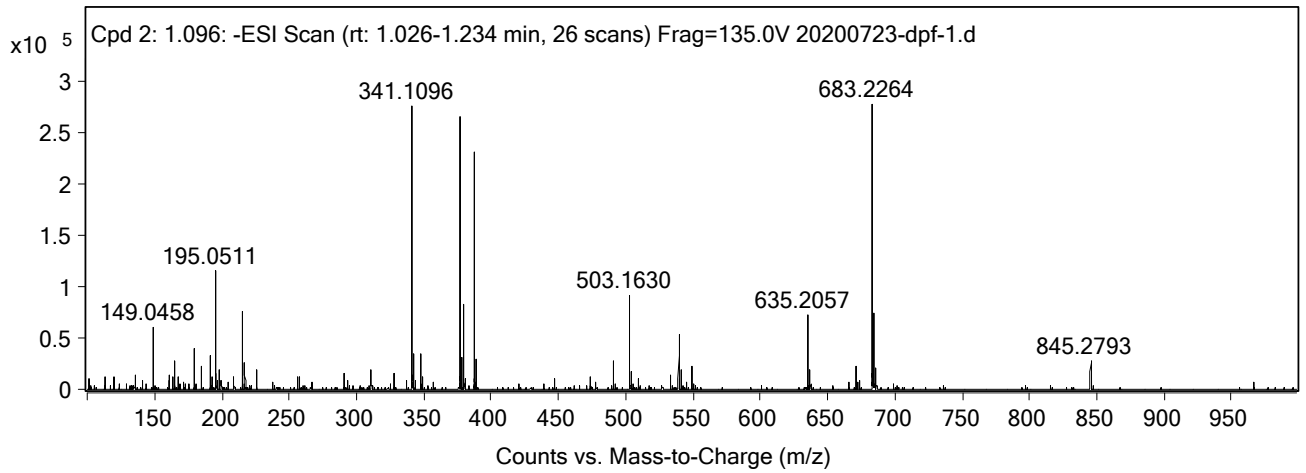
MFE MS Zoomed Spectrum



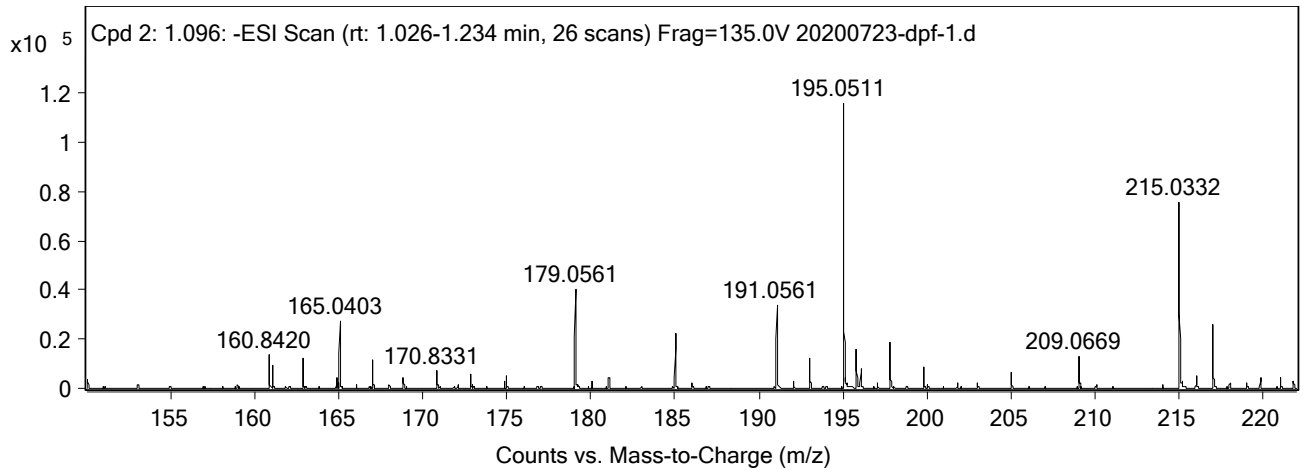
MS Spectrum Peak List

m/z	z	Abund	Ion
185.0087	-1	22494.6	(M-H)-
186.0124	-1	1883.01	(M-H)-
187.0177	-1	422.06	(M-H)-

MS Spectrum

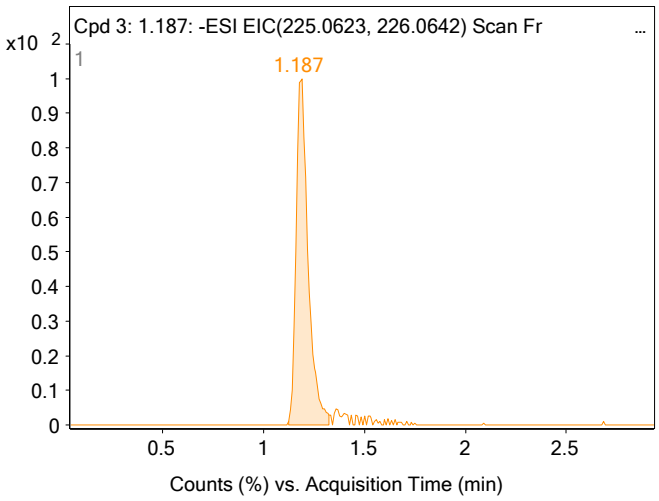


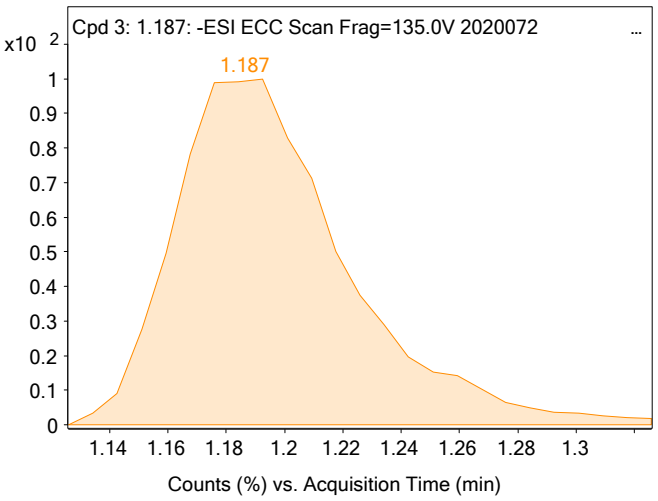
MS Zoomed Spectrum



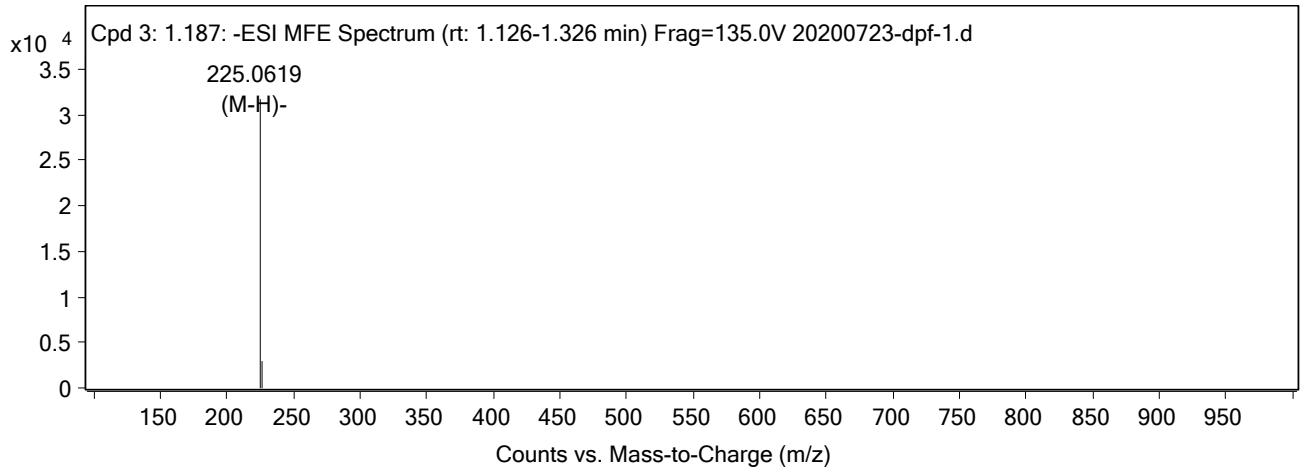
Compound Label	m/z	RT	Algorithm	Mass
Cpd 3: 1.187	225.0619	1.187	Find by Molecular Feature	226.0692

Compound Chromatograms

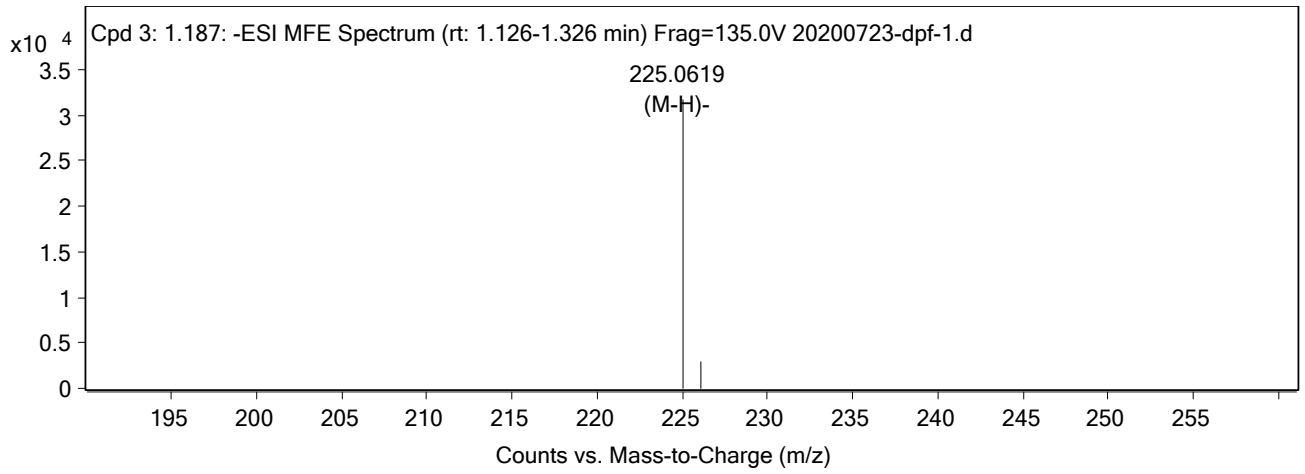




MFE MS Spectrum



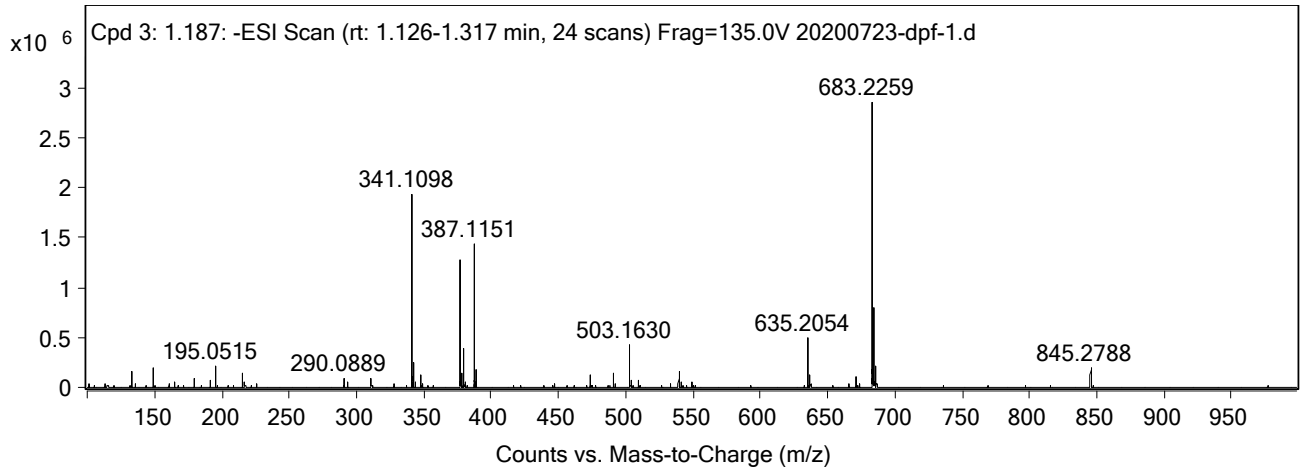
MFE MS Zoomed Spectrum



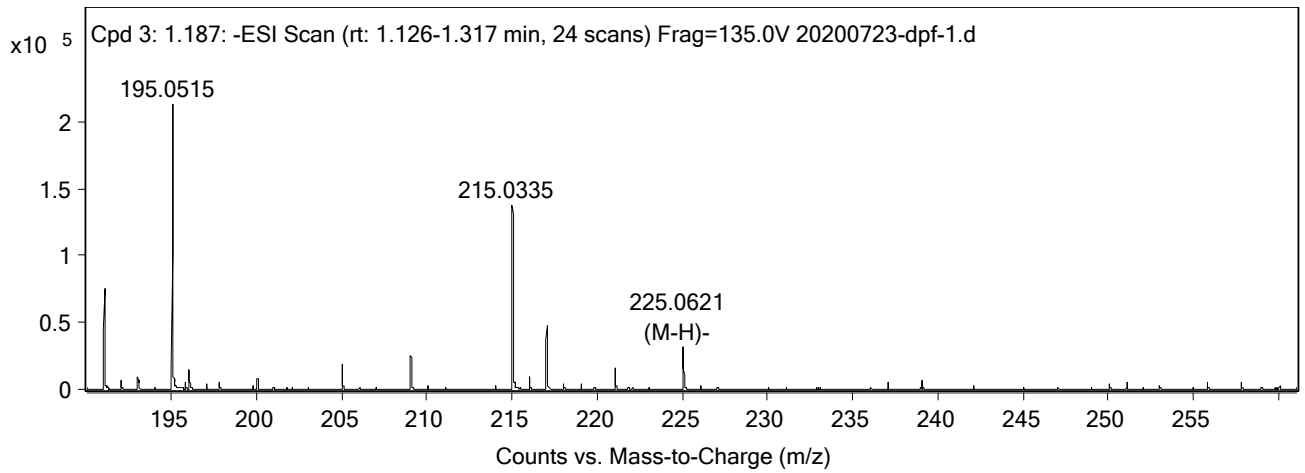
MS Spectrum Peak List

m/z	z	Abund	Ion
225.0619	-1	31715.89	(M-H)-
226.0648	-1	2852.55	(M-H)-

MS Spectrum

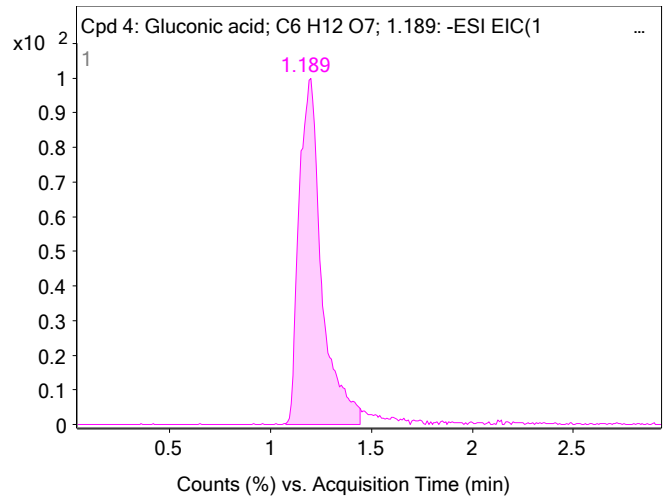


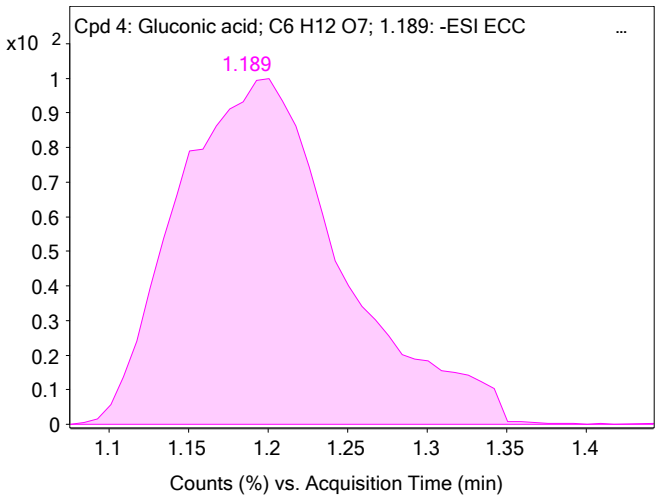
MS Zoomed Spectrum



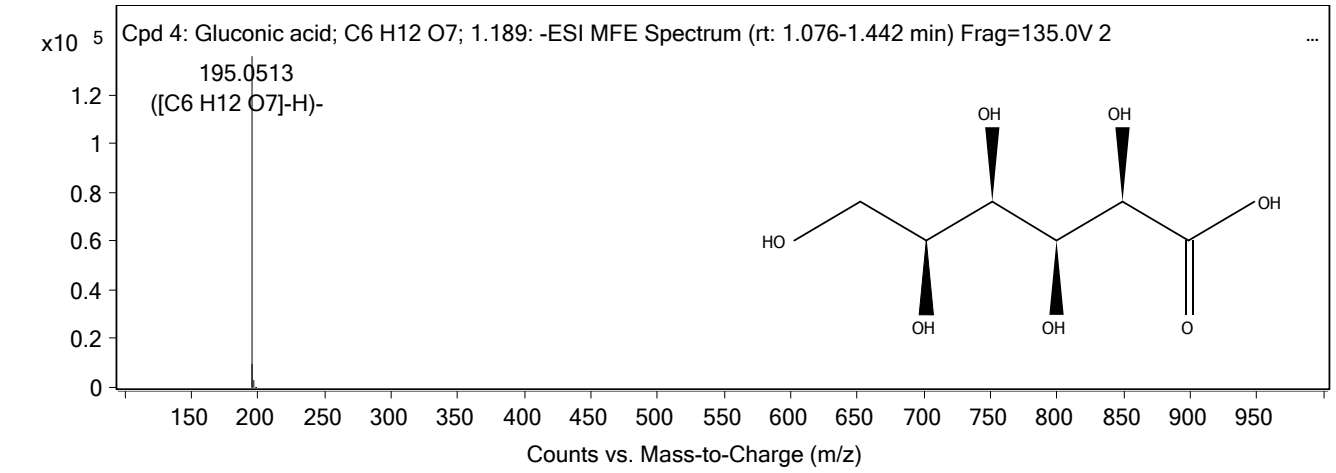
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 4: Gluconic acid; C6 H12 O7; 1.189	**Gluconic acid**	195.0513	1.189	Find by Molecular Feature	196.0586

Compound Chromatograms

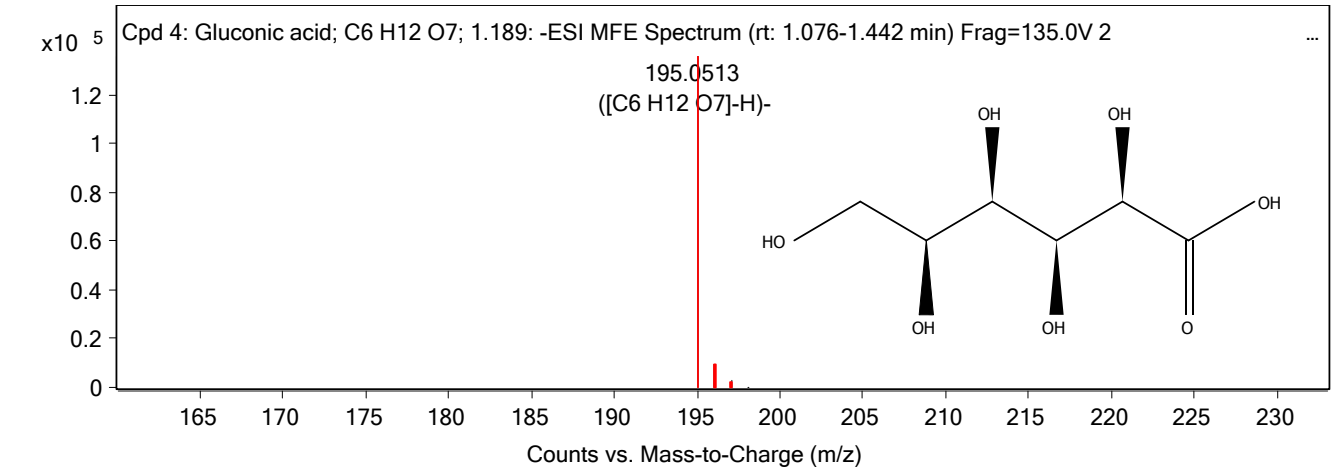




MFE MS Spectrum



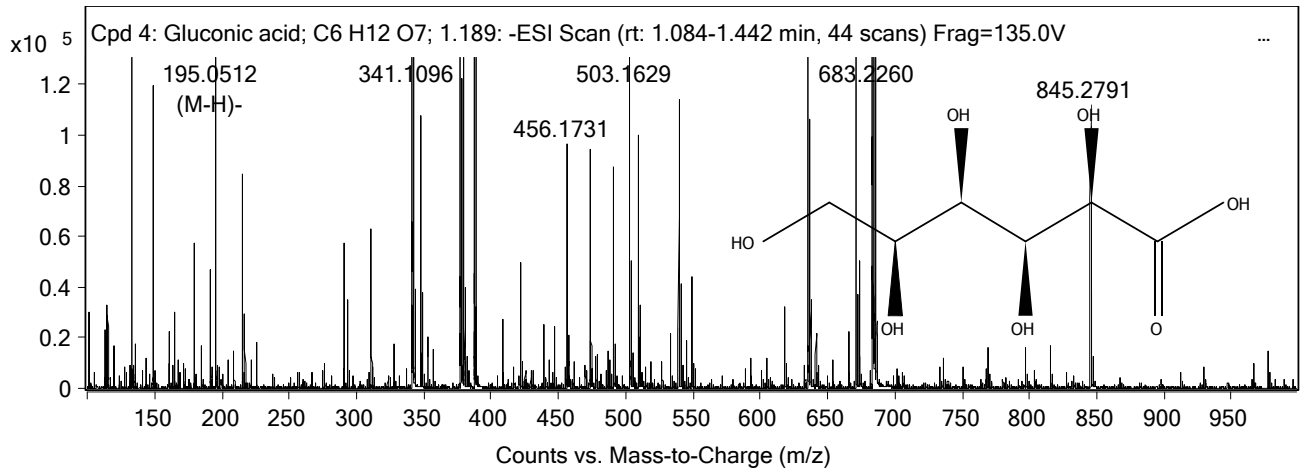
MFE MS Zoomed Spectrum



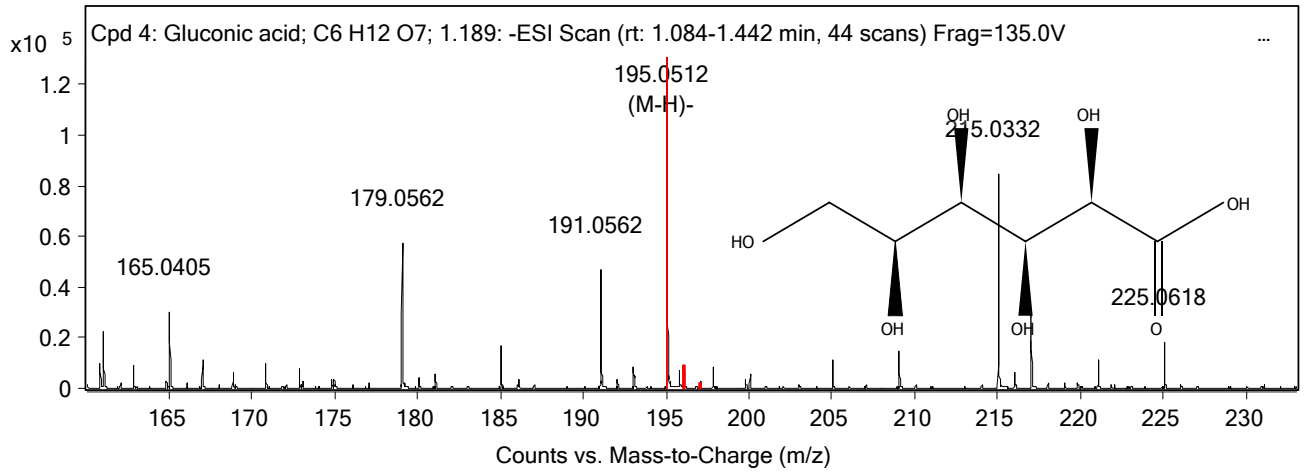
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
195.0513	-1	135801.16	C6 H12 O7	(M-H)-
196.0547	-1	9272.98	C6 H12 O7	(M-H)-
197.0565	-1	2599.3	C6 H12 O7	(M-H)-
198.05	-1	92.91	C6 H12 O7	(M-H)-

MS Spectrum



MS Zoomed Spectrum

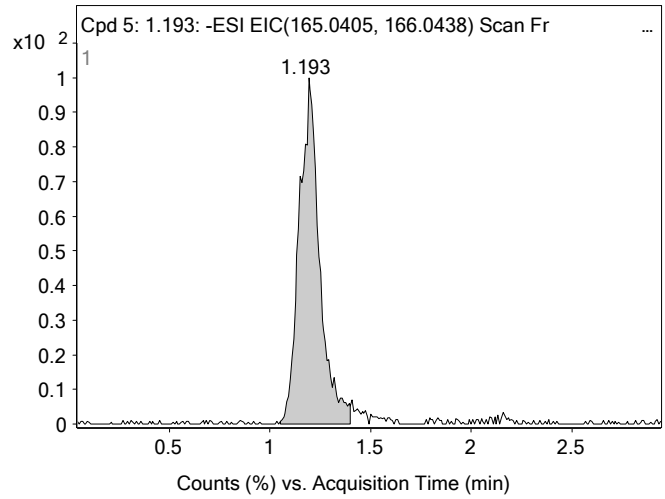


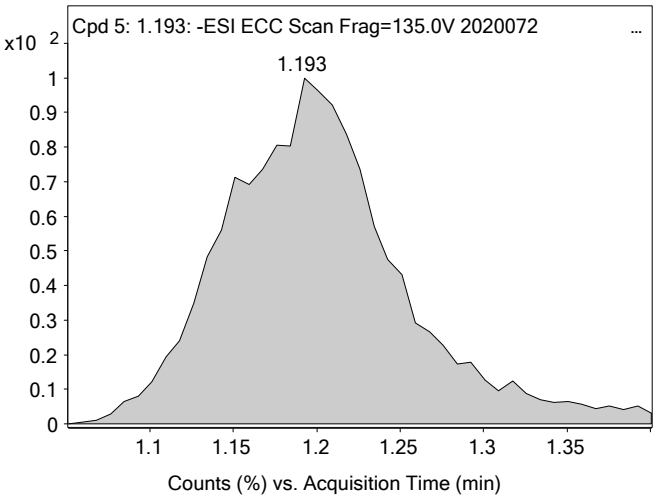
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Gluconic acid	1.189	C6 H12 O7		99.5	196.0586	-0.3	(M-H)-

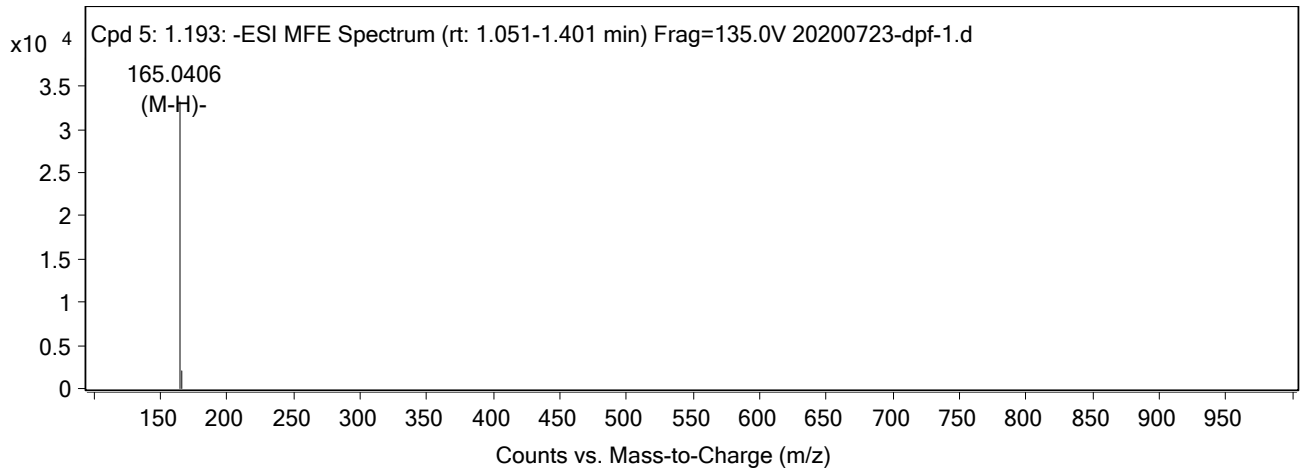
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: 1.193	165.0406	1.193	Find by Molecular Feature	166.0479

Compound Chromatograms

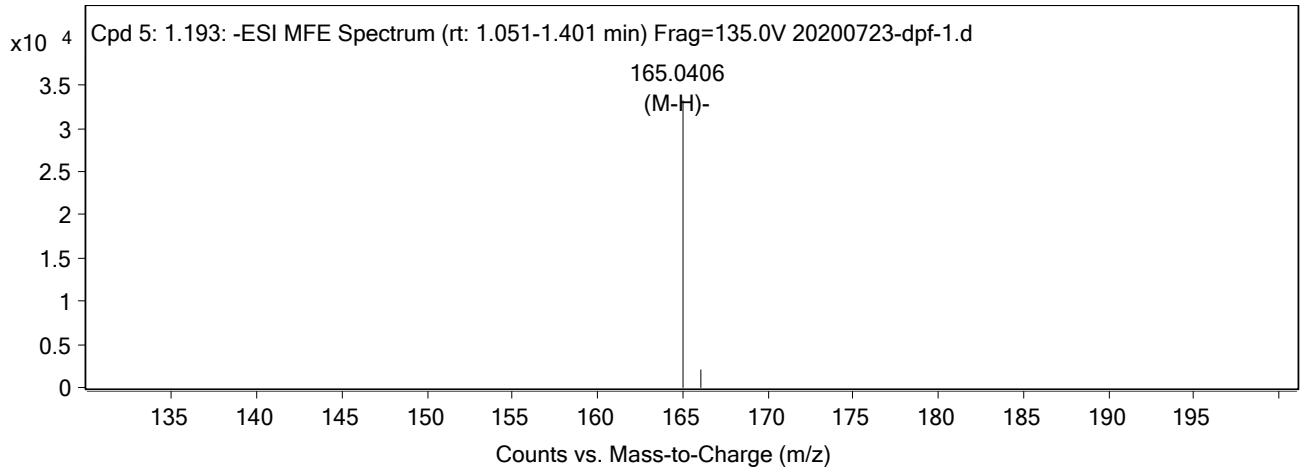




MFE MS Spectrum



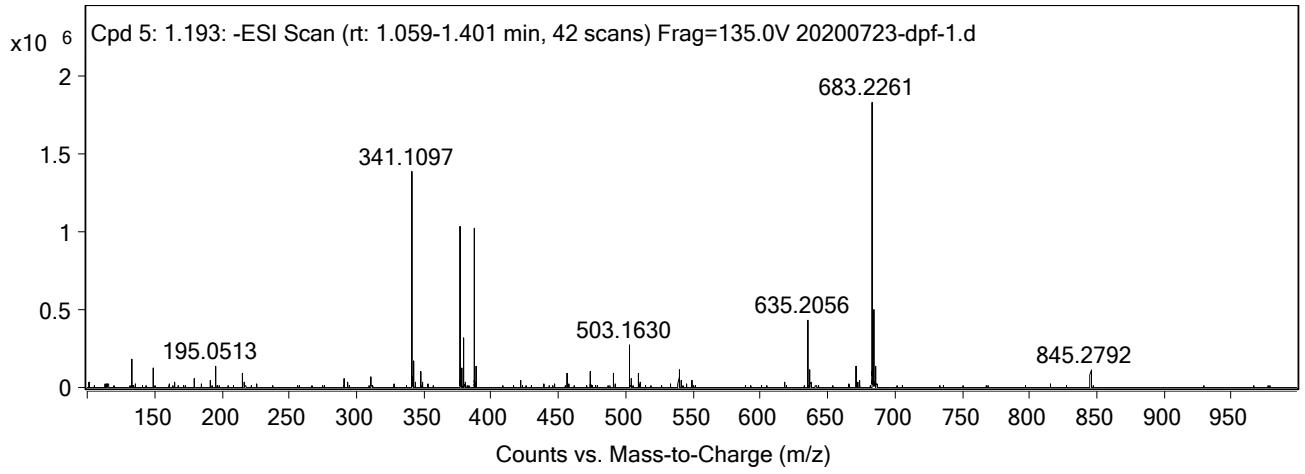
MFE MS Zoomed Spectrum



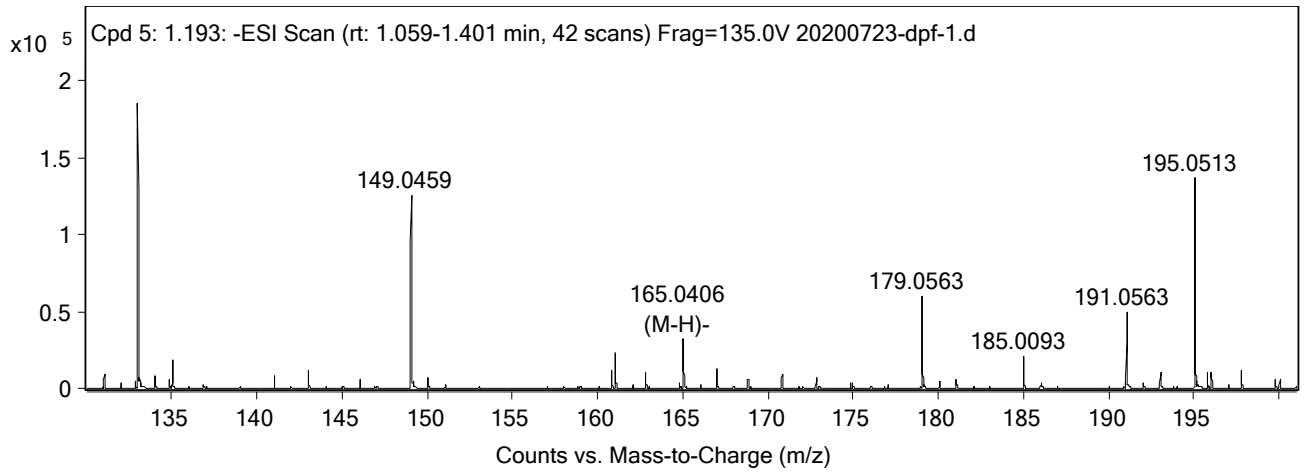
MS Spectrum Peak List

m/z	z	Abund	Ion
165.0406	-1	33287.06	(M-H)-
166.0443	-1	2063.05	(M-H)-

MS Spectrum

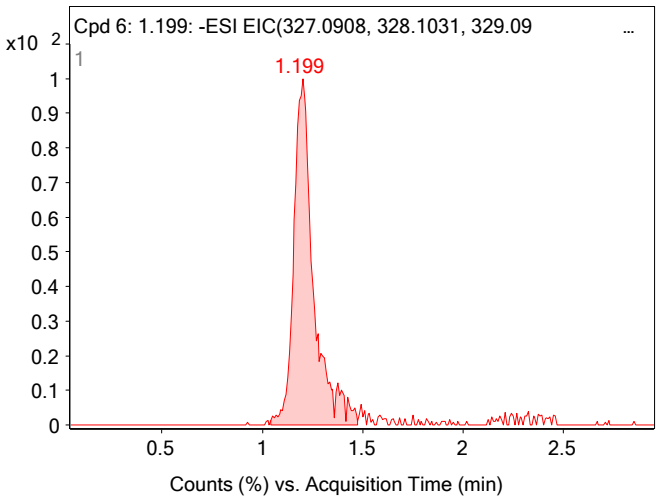


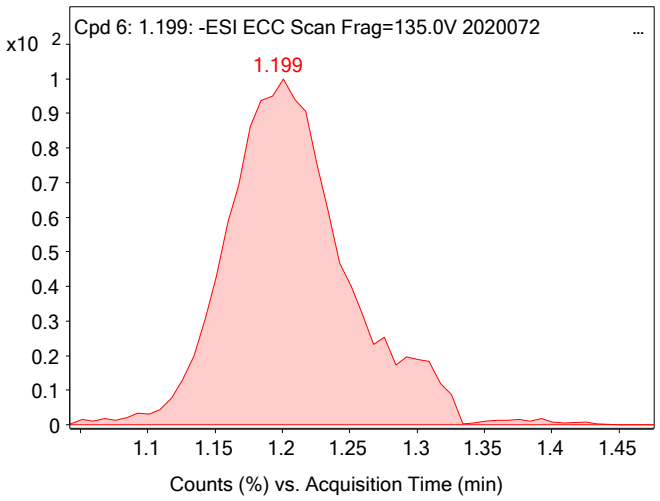
MS Zoomed Spectrum



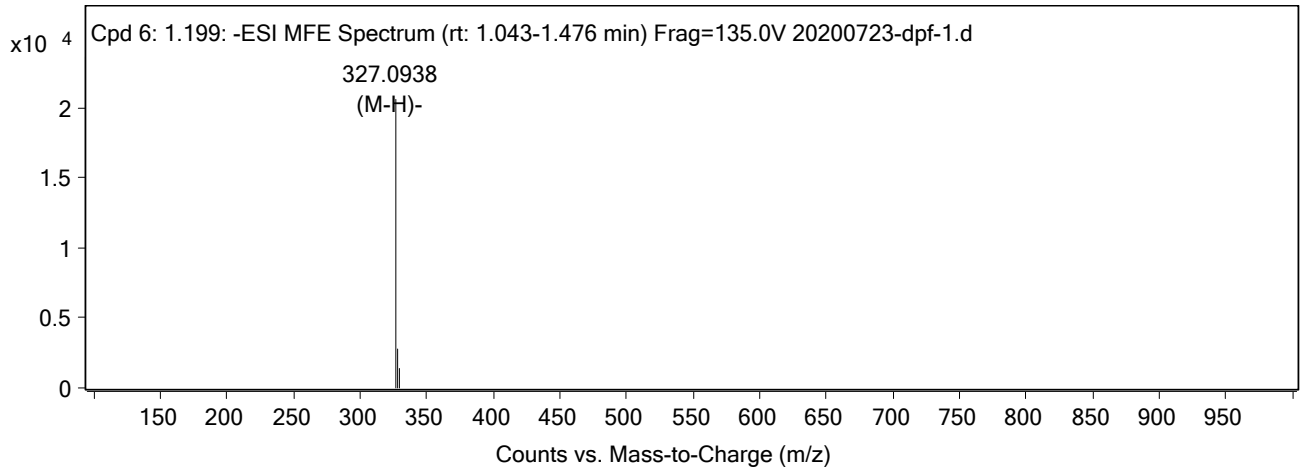
Compound Label	m/z	RT	Algorithm	Mass
Cpd 6: 1.199	327.0938	1.199	Find by Molecular Feature	328.1011

Compound Chromatograms

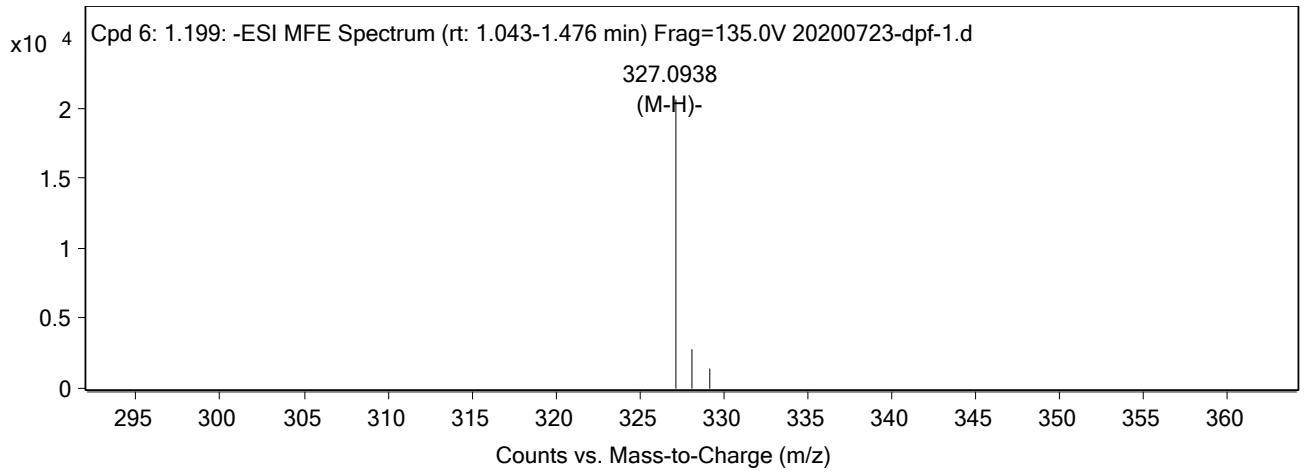




MFE MS Spectrum



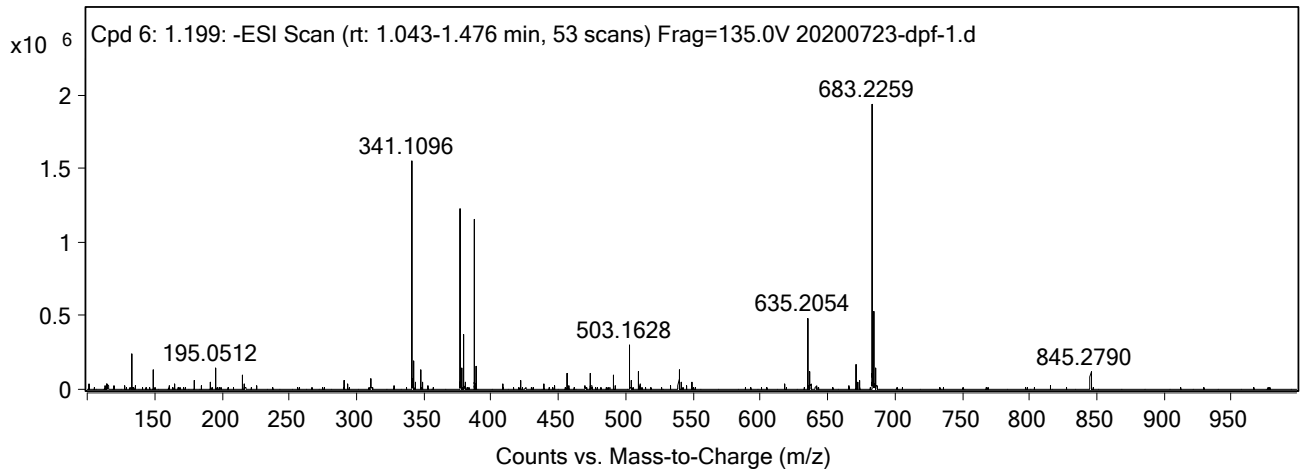
MFE MS Zoomed Spectrum



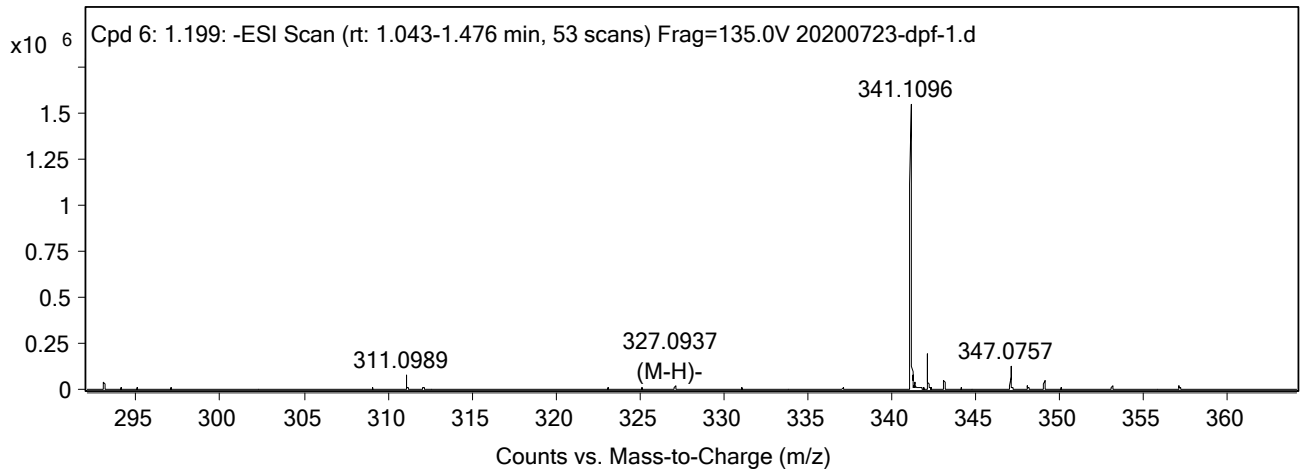
MS Spectrum Peak List

m/z	z	Abund	Ion
327.0938	-1	20536.24	(M-H)-
328.0976	-1	2775.23	(M-H)-
329.0993	-1	1415.09	(M-H)-

MS Spectrum

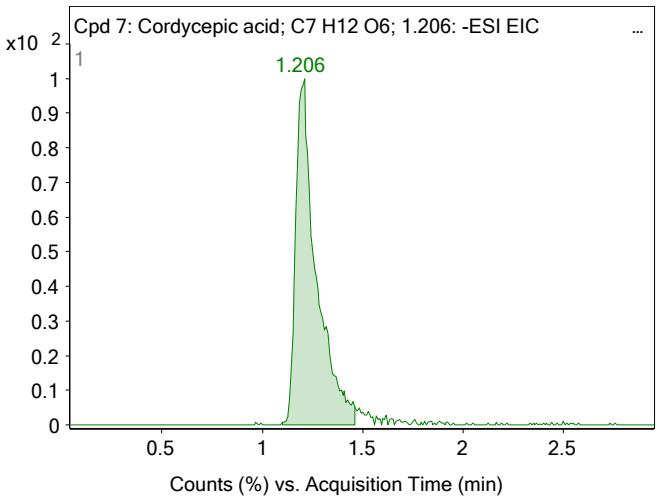


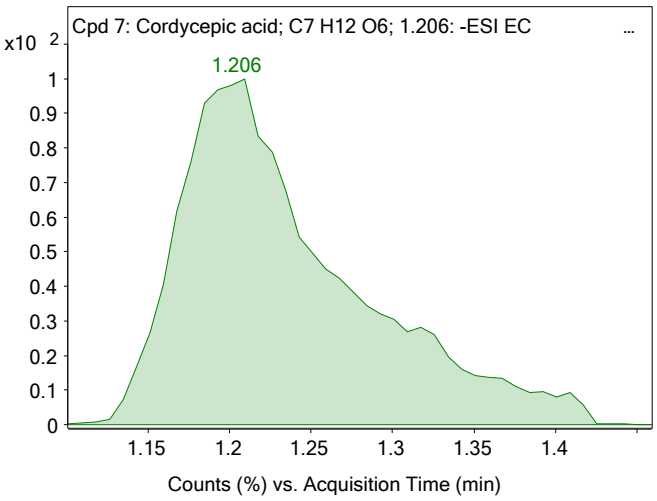
MS Zoomed Spectrum



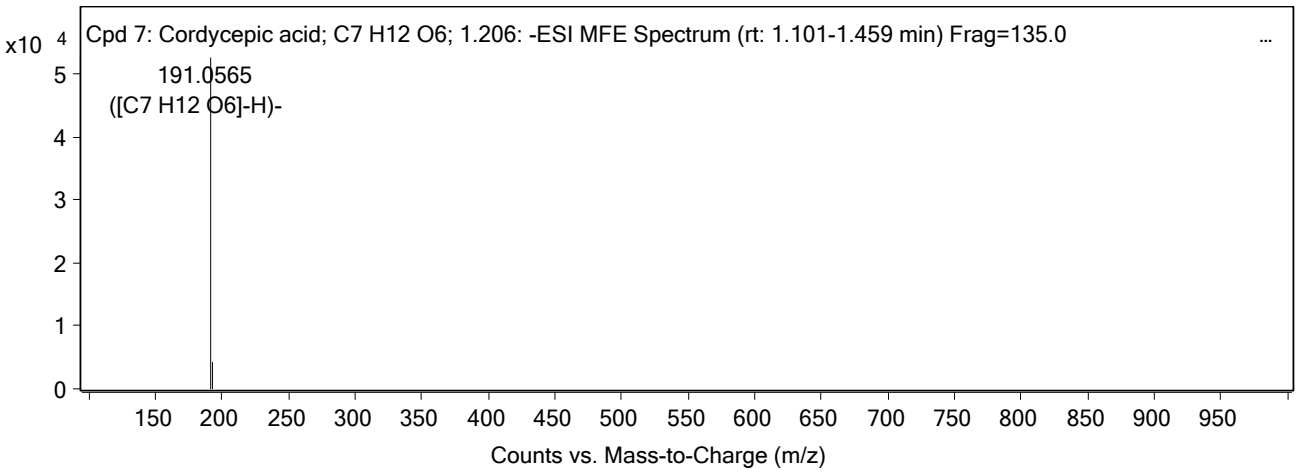
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 7: Cordycepic acid; C7 H12 O6; 1.206	**Cordycepic acid**	191.0565	1.206	Find by Molecular Feature	192.0638

Compound Chromatograms

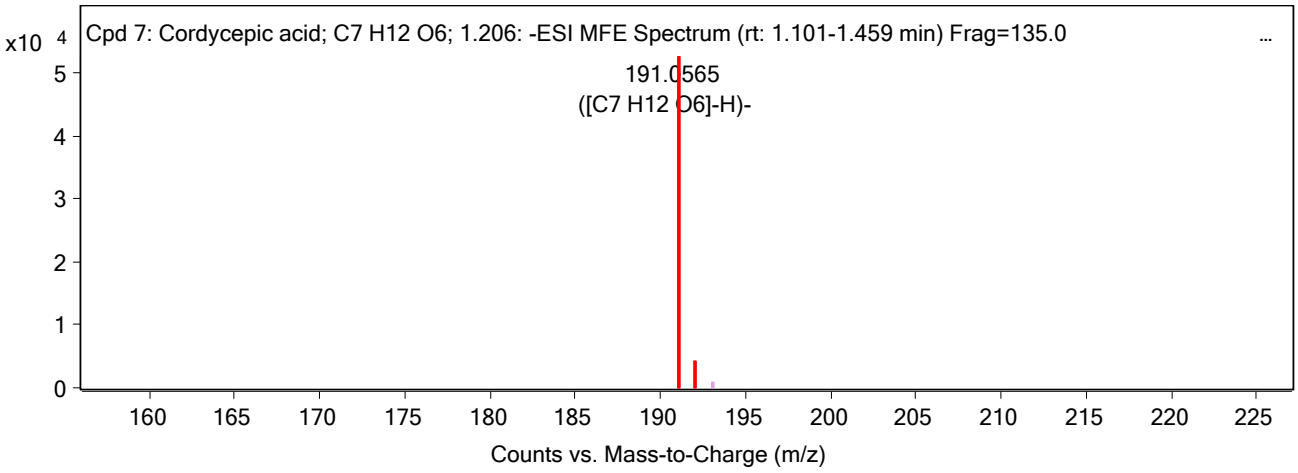




MFE MS Spectrum



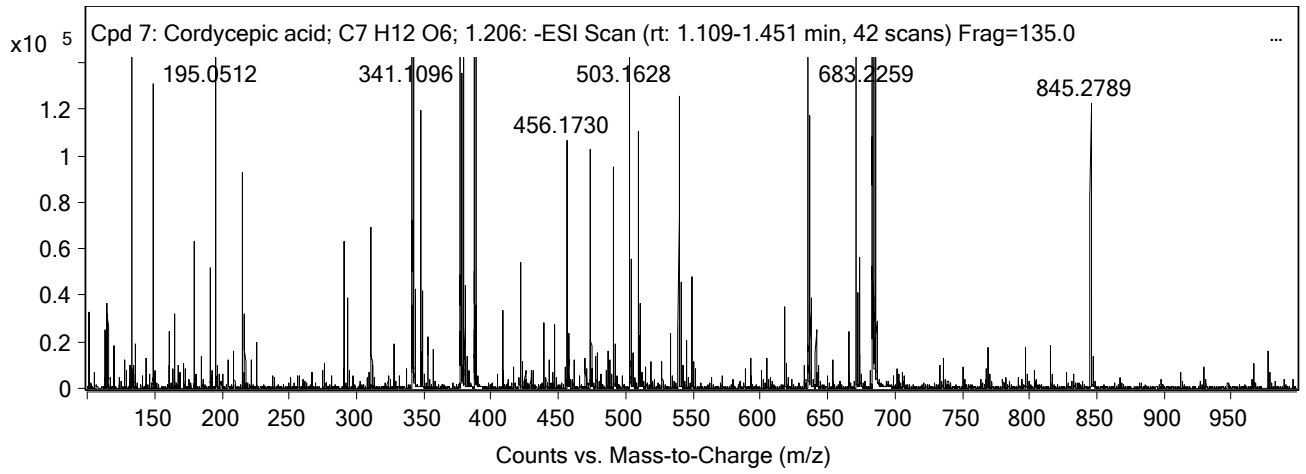
MFE MS Zoomed Spectrum



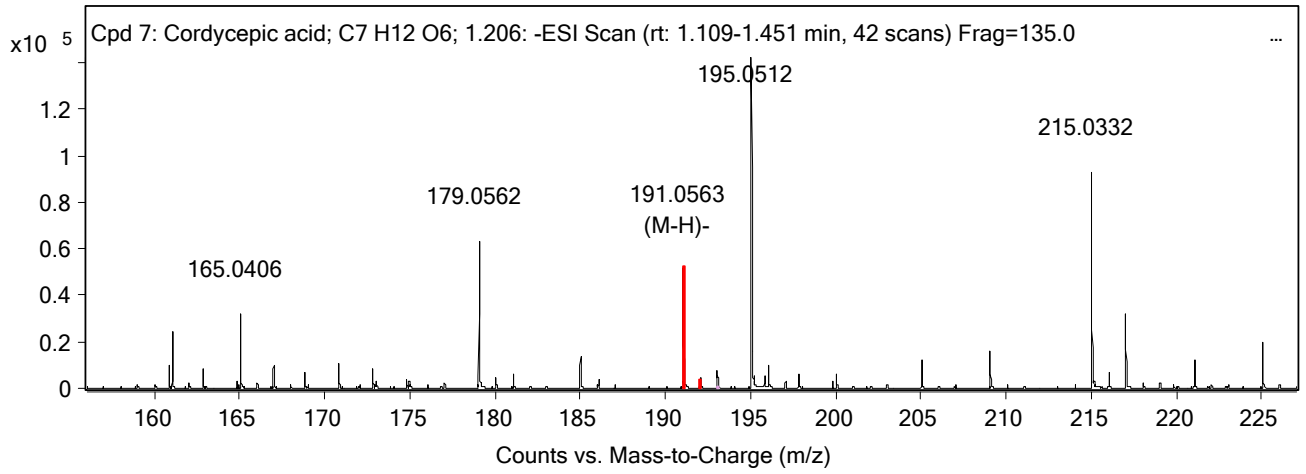
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
191.0565	-1	52519.27	C7 H12 O6	(M-H)-
192.0598	-1	4206.72	C7 H12 O6	(M-H)-

MS Spectrum



MS Zoomed Spectrum

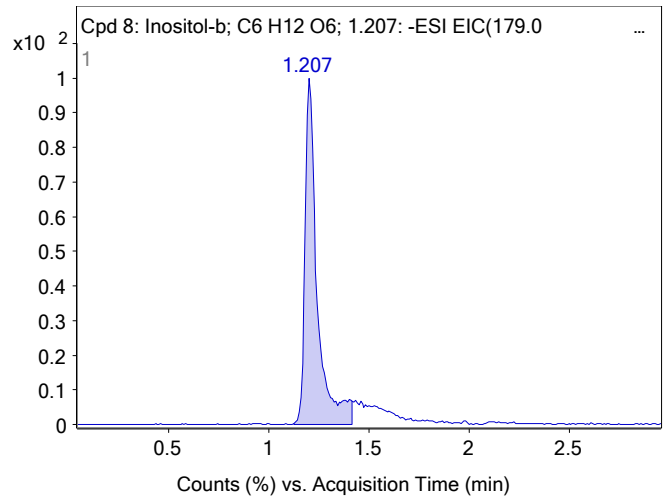


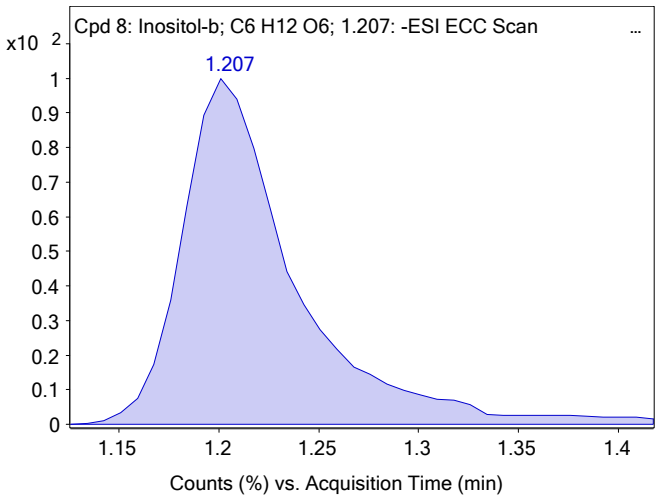
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Cordycepic acid	1.206	C7 H12 O6		86.25	192.0638	-0.41	(M-H)-
	D-Galacturonic acid	1.206	C7 H12 O6		86.25	192.0638	-0.41	(M-H)-
	Quinic acid	1.206	C7 H12 O6		86.25	192.0638	-0.41	(M-H)-

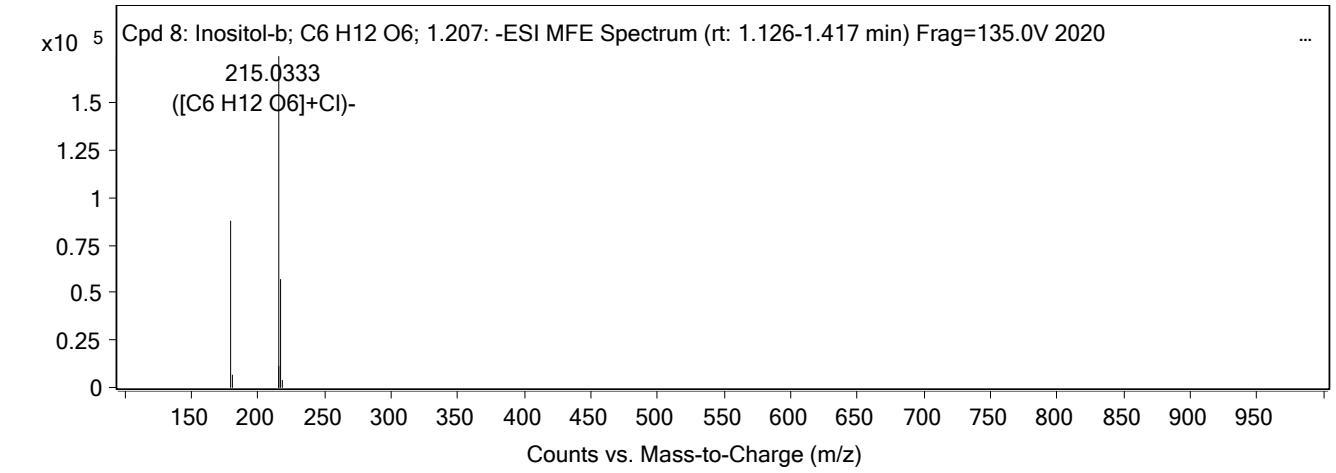
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 8: Inositol-b; C6 H12 O6; 1.207	**Inositol-b**	215.0333	1.207	Find by Molecular Feature	180.0642

Compound Chromatograms

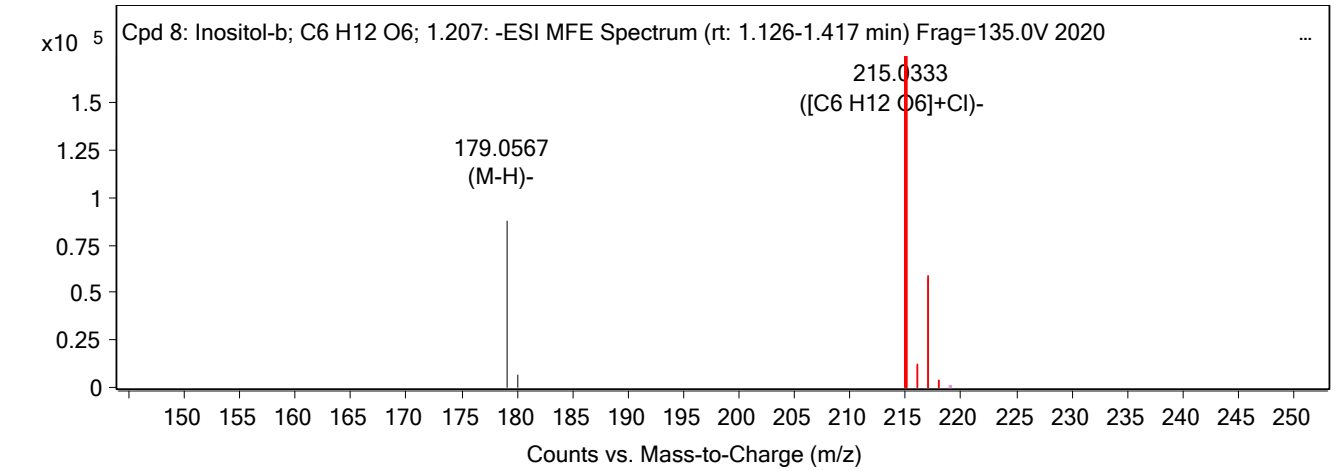




MFE MS Spectrum



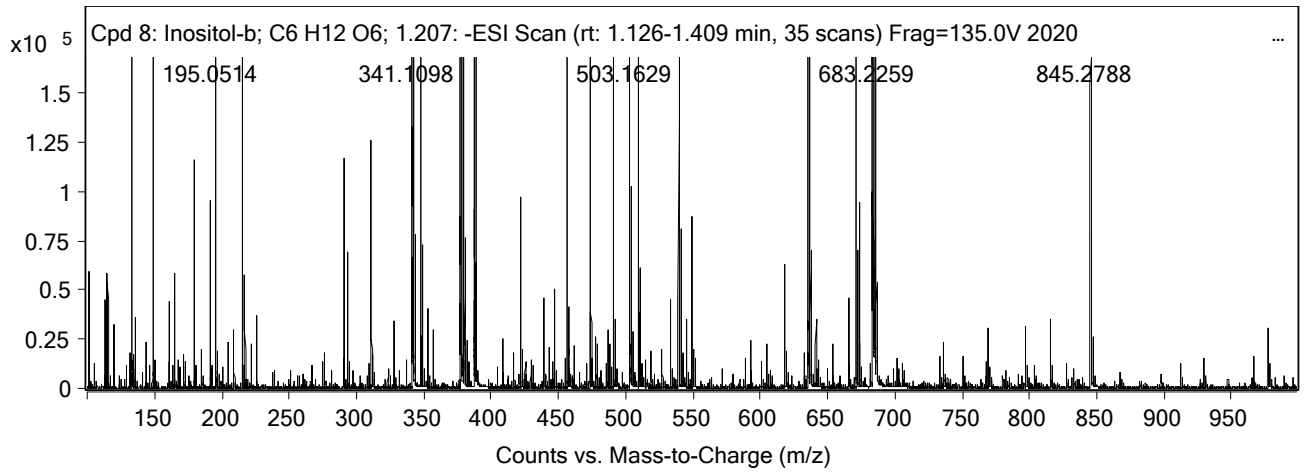
MFE MS Zoomed Spectrum



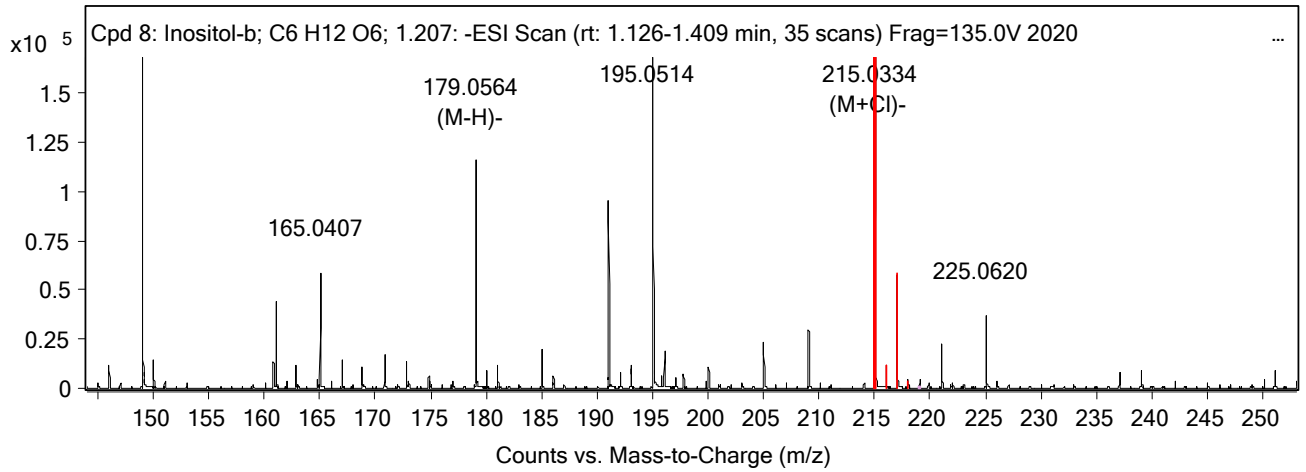
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
179.0567	-1	87694.13		(M-H)-
180.0603	-1	6386.16		(M-H)-
215.0333	-1	174745.88	C6 H12 O6	(M+Cl)-
216.037	-1	11648.64	C6 H12 O6	(M+Cl)-
217.0316	-1	57360.36	C6 H12 O6	(M+Cl)-
218.0354	-1	4104.84	C6 H12 O6	(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

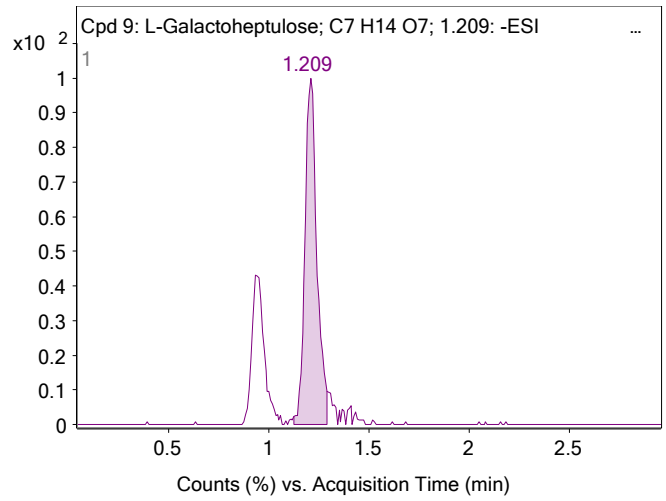


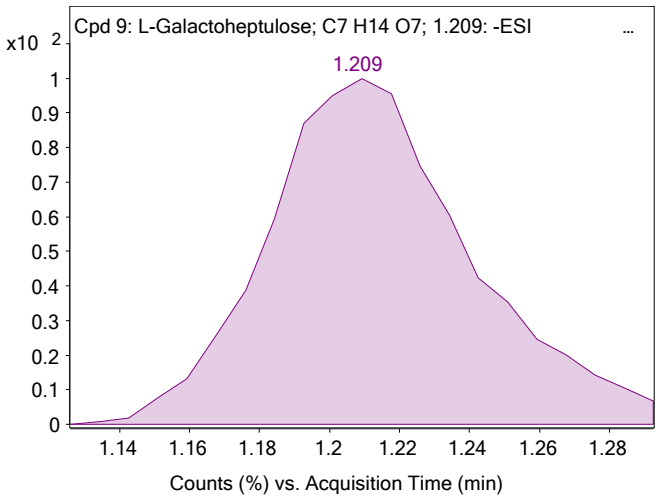
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Inositol-b	1.207	C6 H12 O6		96.05	180.0642	-0.79	(M+Cl)-
	Inositol c	1.207	C6 H12 O6		96.05	180.0642	-0.79	(M+Cl)-
	Fructose	1.207	C6 H12 O6		96.05	180.0642	-0.79	(M+Cl)-
	Inositol	1.207	C6 H12 O6		96.05	180.0642	-0.79	(M+Cl)-
	Mannose	1.207	C6 H12 O6		96.05	180.0642	-0.79	(M+Cl)-
	Cocositol	1.207	C6 H12 O6		96.05	180.0642	-0.79	(M+Cl)-
	Sorbose	1.207	C6 H12 O6		96.05	180.0642	-0.79	(M+Cl)-
	Mannose-b	1.207	C6 H12 O6		96.05	180.0642	-0.79	(M+Cl)-
	Theophylline	1.207	C7 H8 N4 O2		95.26	180.0643	0.45	(M+Cl)-
	Theobromine	1.207	C7 H8 N4 O2		95.26	180.0643	0.45	(M+Cl)-

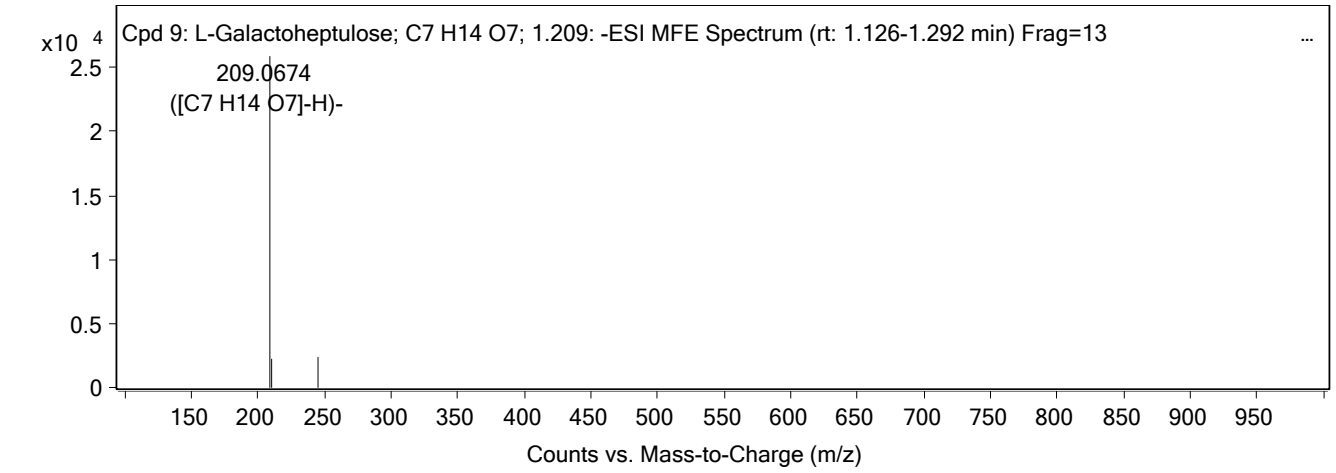
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 9: L-Galactoheptulose; C7 H14 O7; 1.209	**L-Galactoheptulose**	209.0674	1.209	Find by Molecular Feature	210.0747

Compound Chromatograms

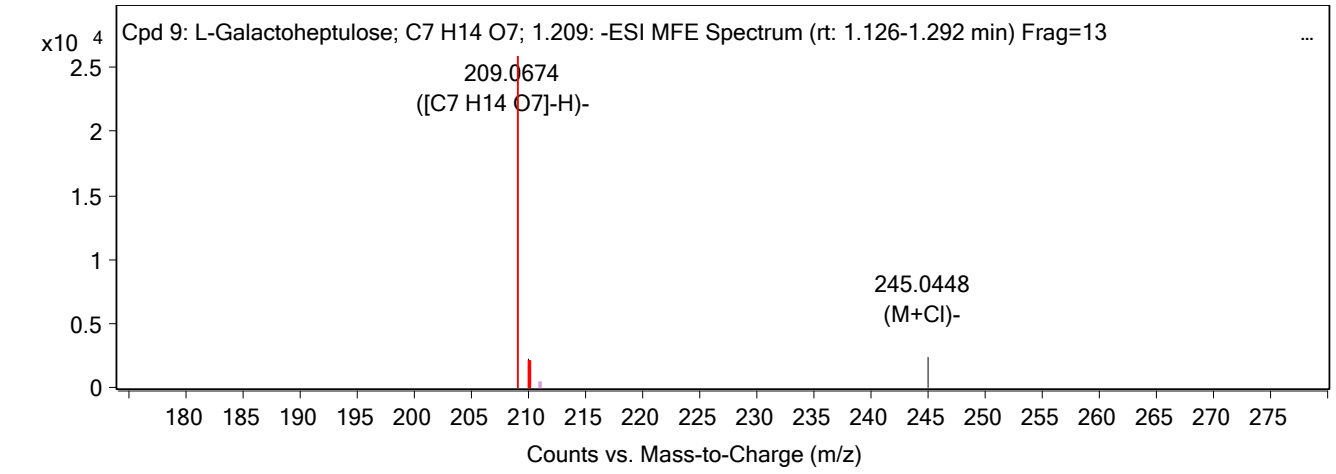




MFE MS Spectrum



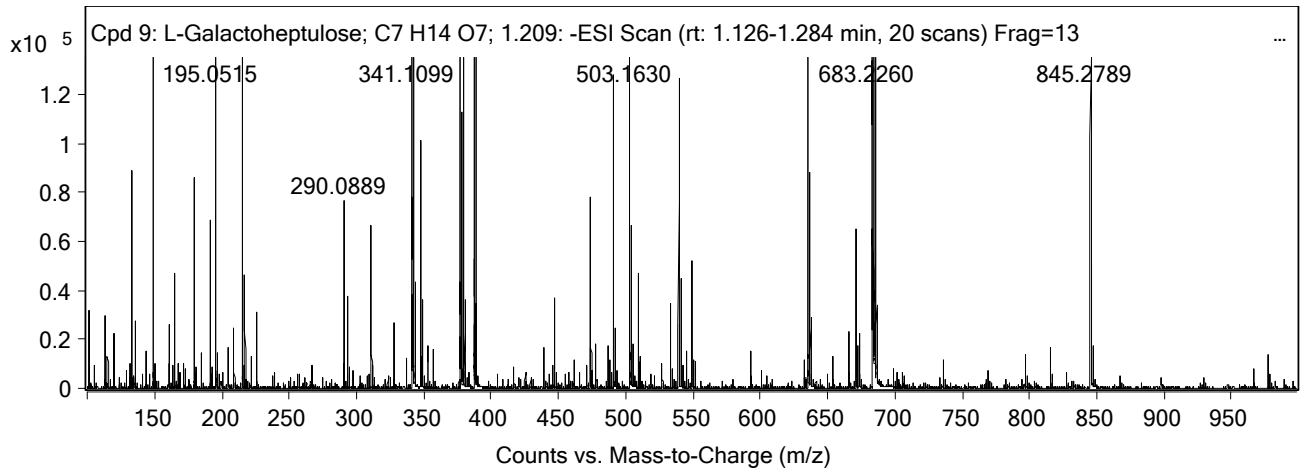
MFE MS Zoomed Spectrum



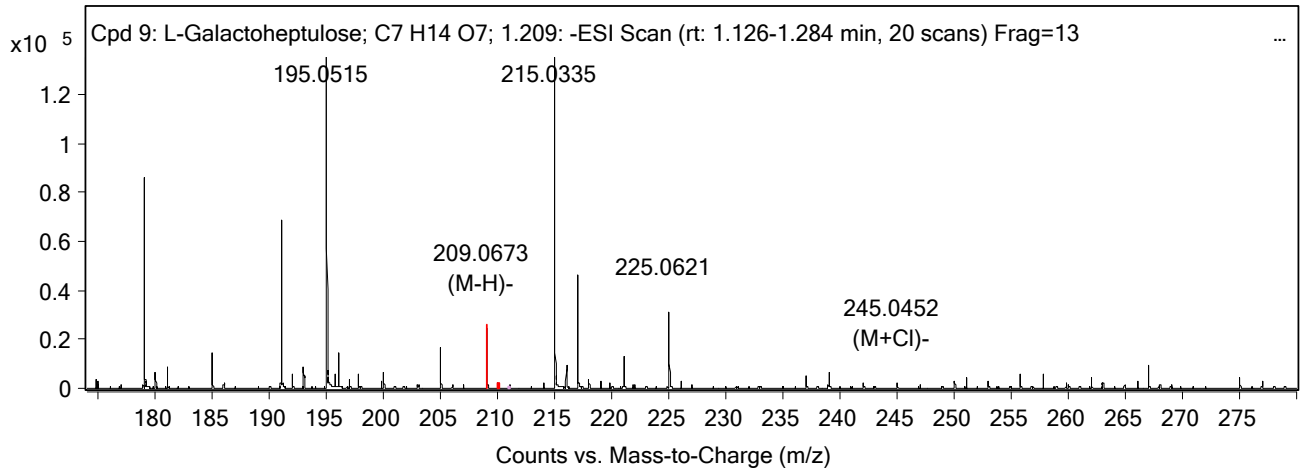
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
209.0674	-1	25866.3	C7 H14 O7	(M-H)-
210.0713	-1	2195	C7 H14 O7	(M-H)-
245.0448	-1	2296.72		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

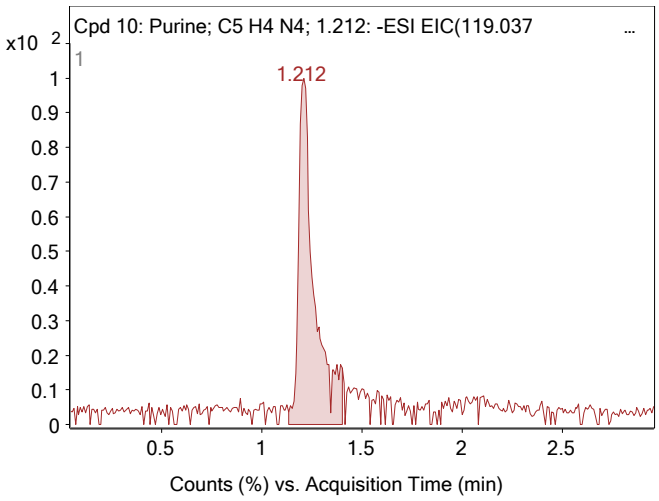


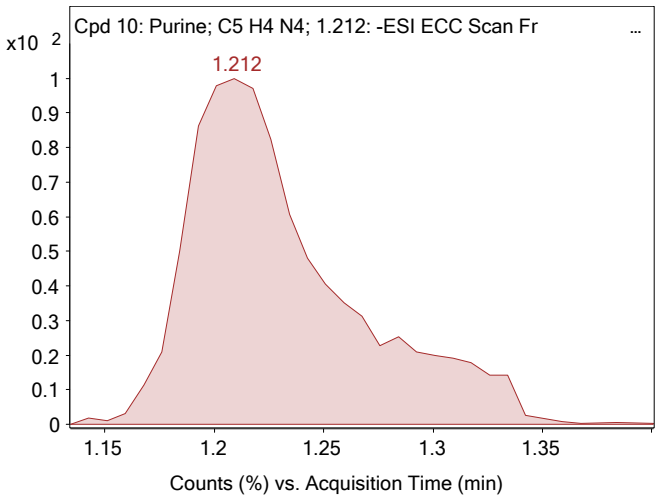
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	L-Galactoheptulose	1.209	C7 H14 O7		83.59	210.0747	-0.78	(M-H)-
	D-Mannoheptulose	1.209	C7 H14 O7		83.59	210.0747	-0.78	(M-H)-
	Coriose	1.209	C7 H14 O7		83.59	210.0747	-0.78	(M-H)-
	Vachellin	1.209	C8 H10 N4 O3		83.04	210.0748	0.48	(M-H)-

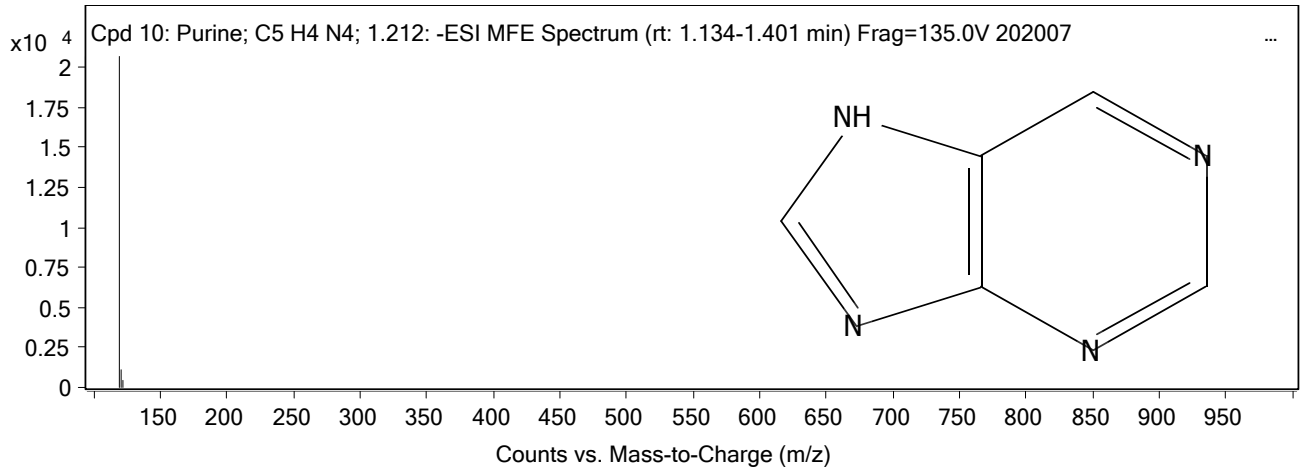
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 10: Purine; C5 H4 N4; 1.212	**Purine**	119.036	1.212	Find by Molecular Feature	120.0433

Compound Chromatograms

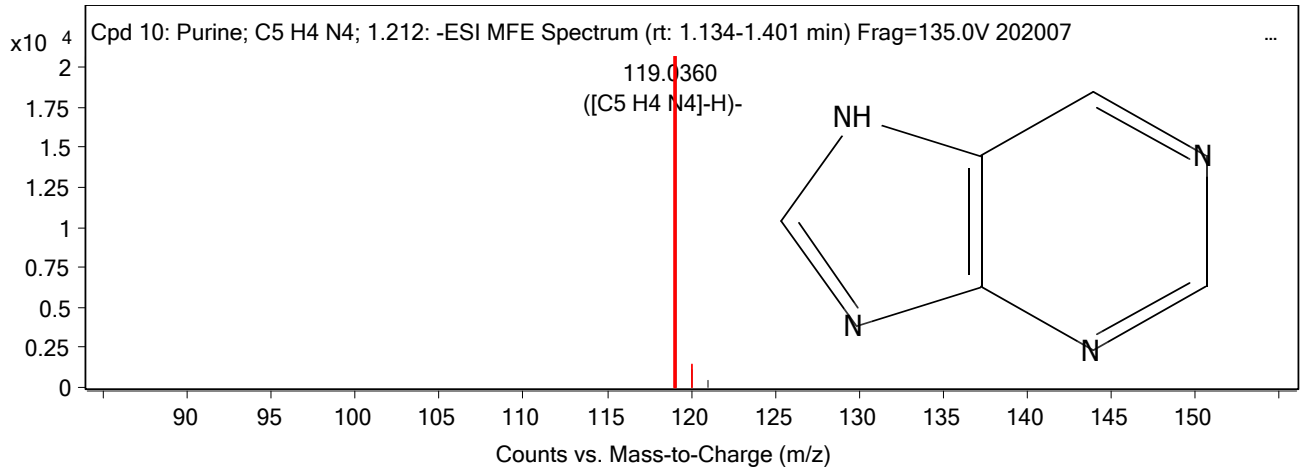




MFE MS Spectrum



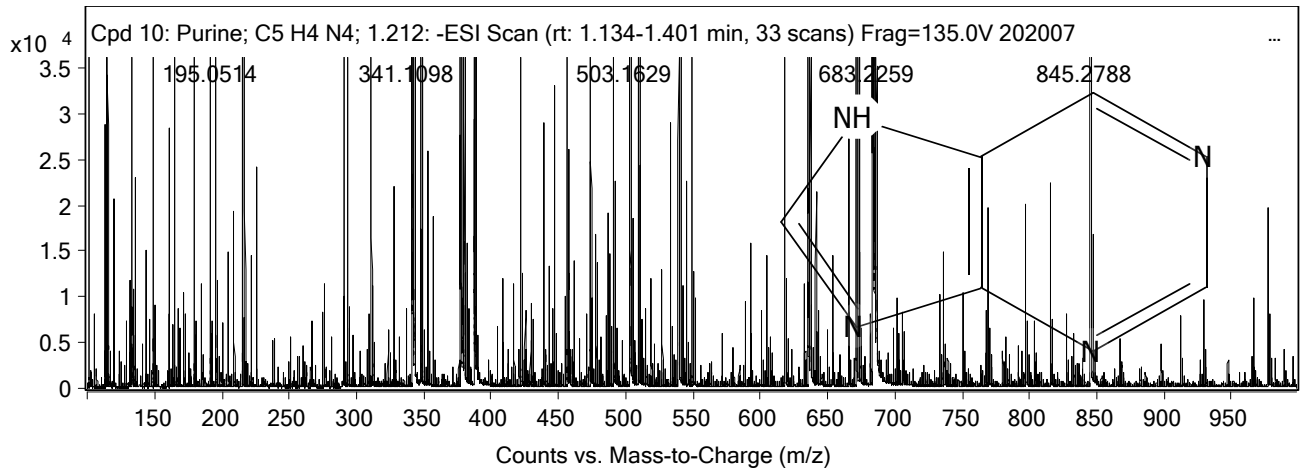
MFE MS Zoomed Spectrum



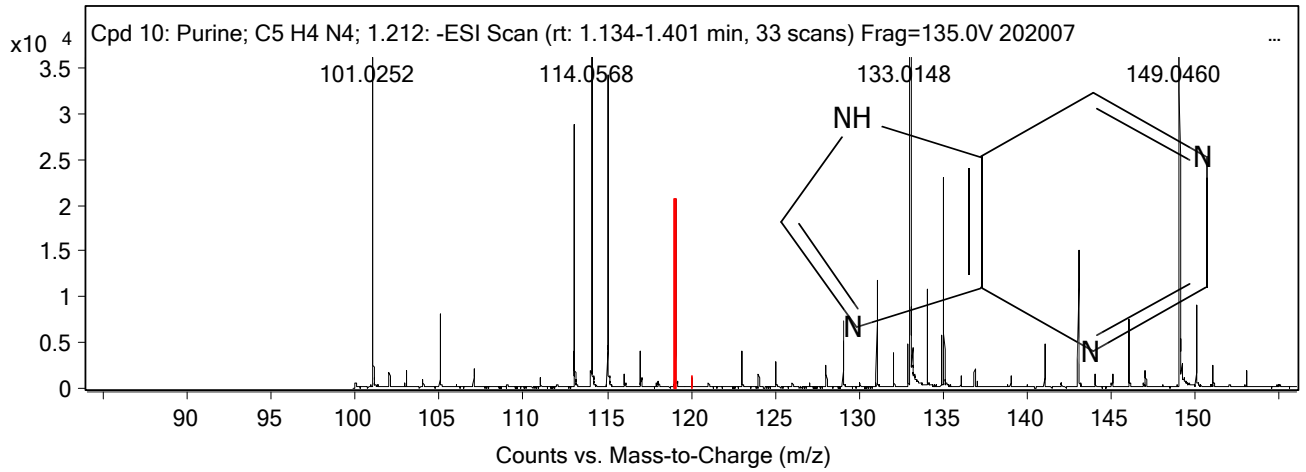
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
119.036	-1	20698.75	C5 H4 N4	(M-H)-
120.0395	-1	1060.34	C5 H4 N4	(M-H)-
121.0376	-1	438.12	C5 H4 N4	(M-H)-

MS Spectrum



MS Zoomed Spectrum

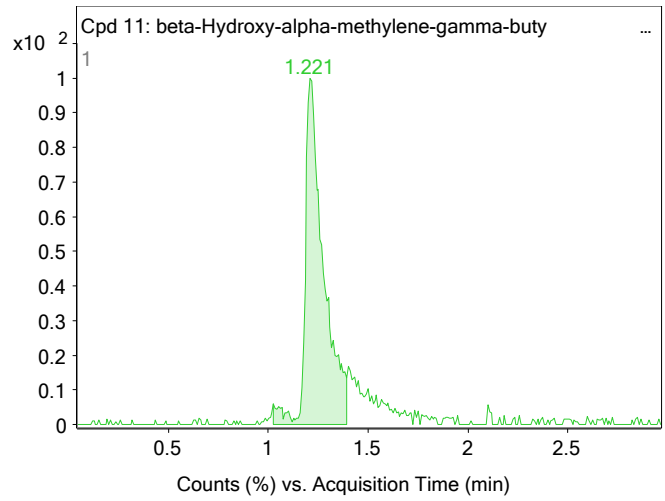


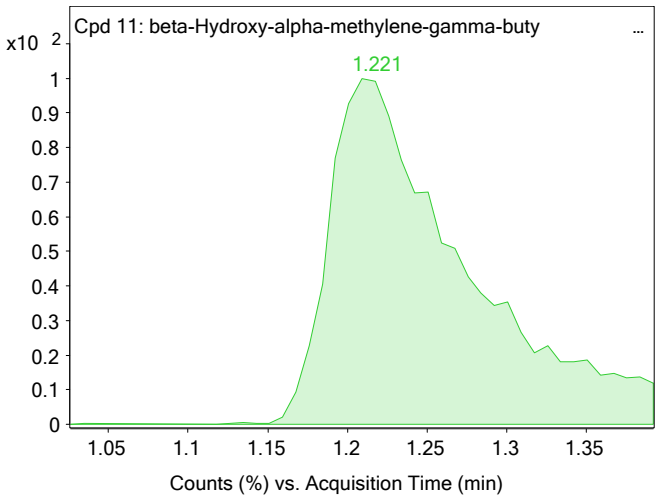
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Purine	1.212	C5 H4 N4		94.95	120.0433	0.28	(M-H)-
	Methyl allyl tetrasulfide	1.212	C4 H8 O4		92.82	120.0432	-0.98	(M-H)-

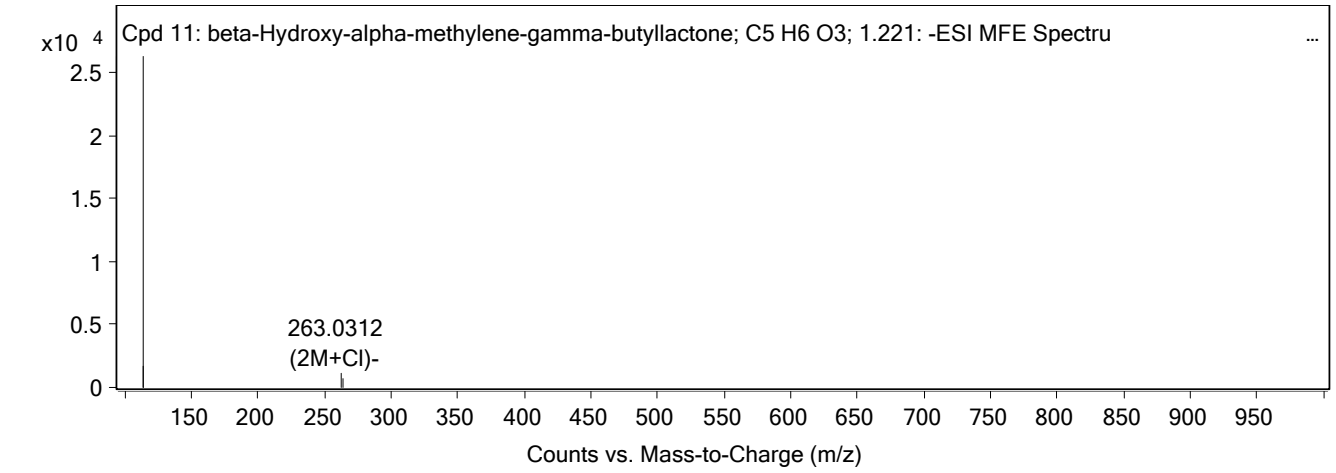
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 11: beta-Hydroxy-alpha-methylene-gamma-butyllactone; C5 H6 O3; 1.221	**beta-Hydroxy-alpha-methylene-gamma-butyllactone**	113.0255	1.221	Find by Molecular Feature	114.0328

Compound Chromatograms

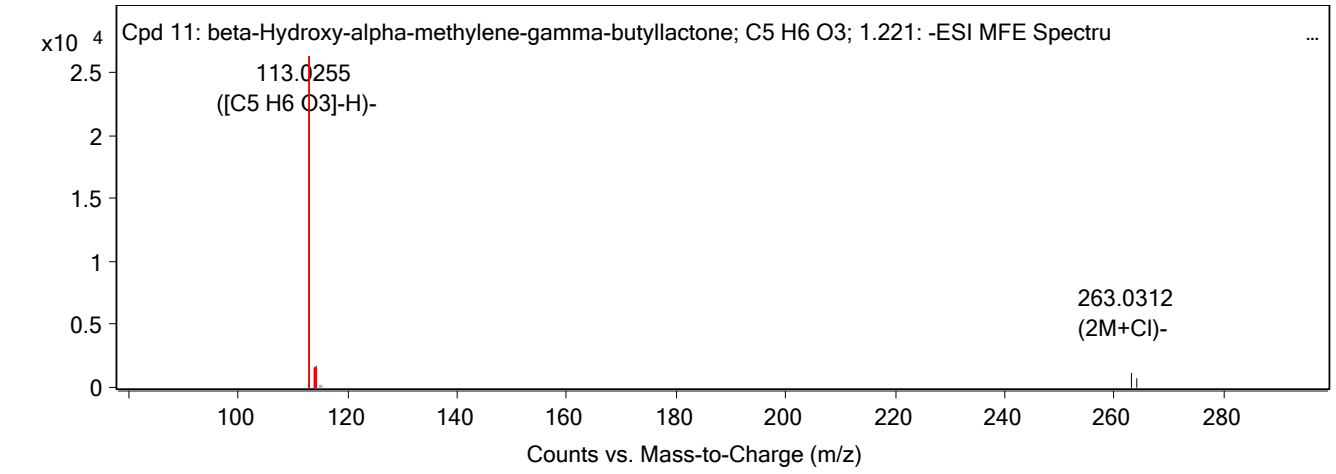




MFE MS Spectrum



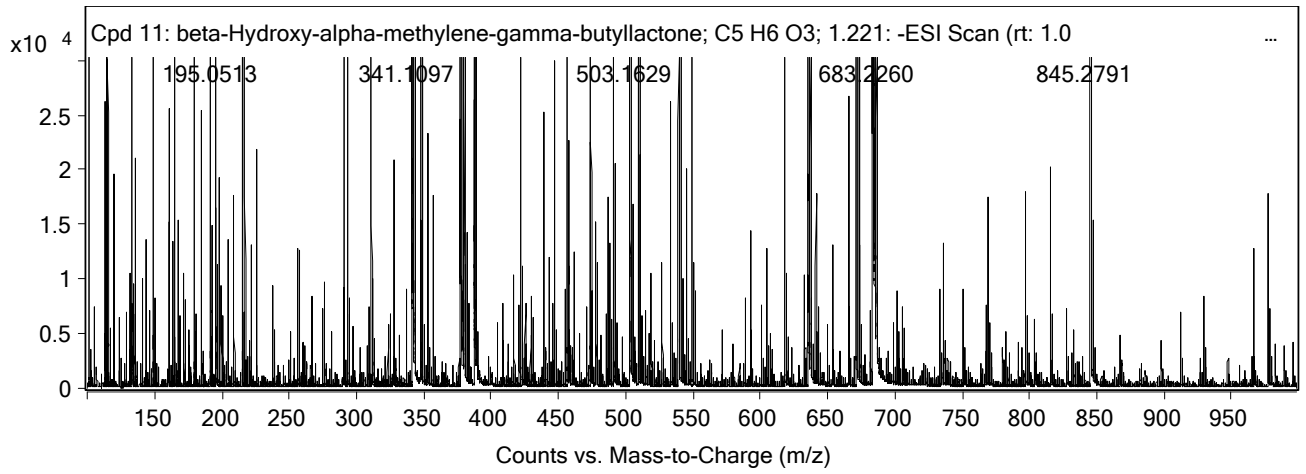
MFE MS Zoomed Spectrum



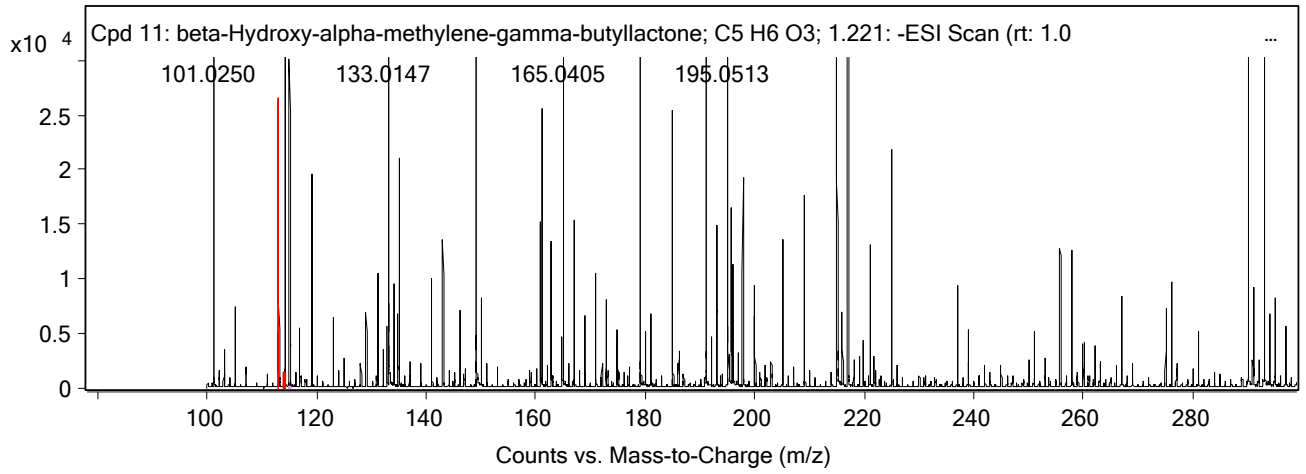
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
113.0255	-1	26284.62	C5 H6 O3	(M-H)-
114.0284	-1	1759.93	C5 H6 O3	(M-H)-
263.0312	-1	1114.12		(2M+Cl)-
264.0332	-1	662.57		(2M+Cl)-

MS Spectrum



MS Zoomed Spectrum

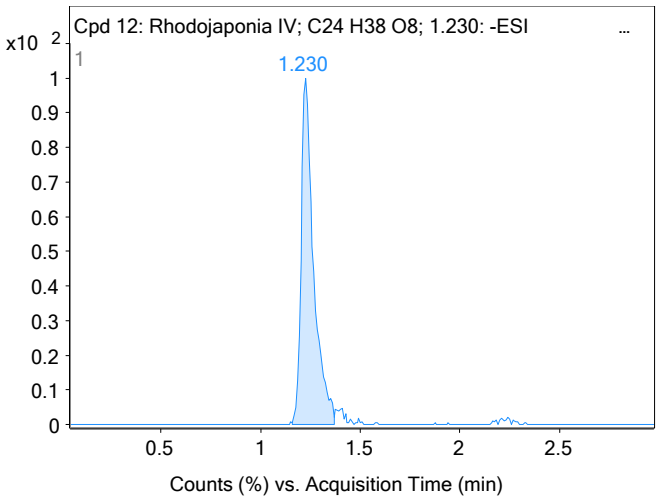


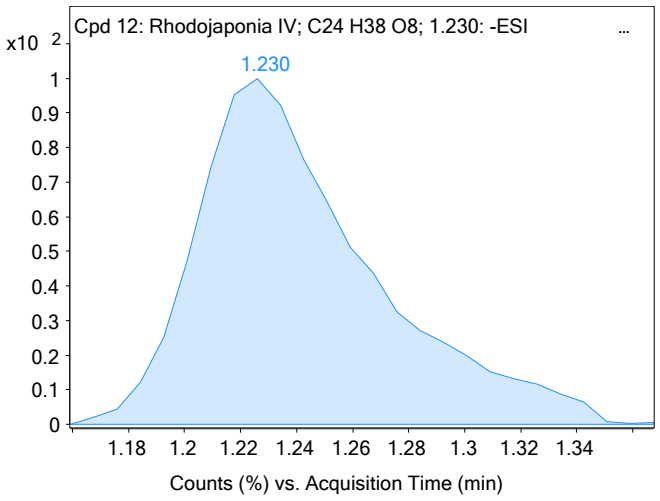
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	beta-Hydroxy-alpha-methylene-gamma-butyllactone	1.221	C5 H6 O3		79.81	114.0328	-1.07	(M-H)-

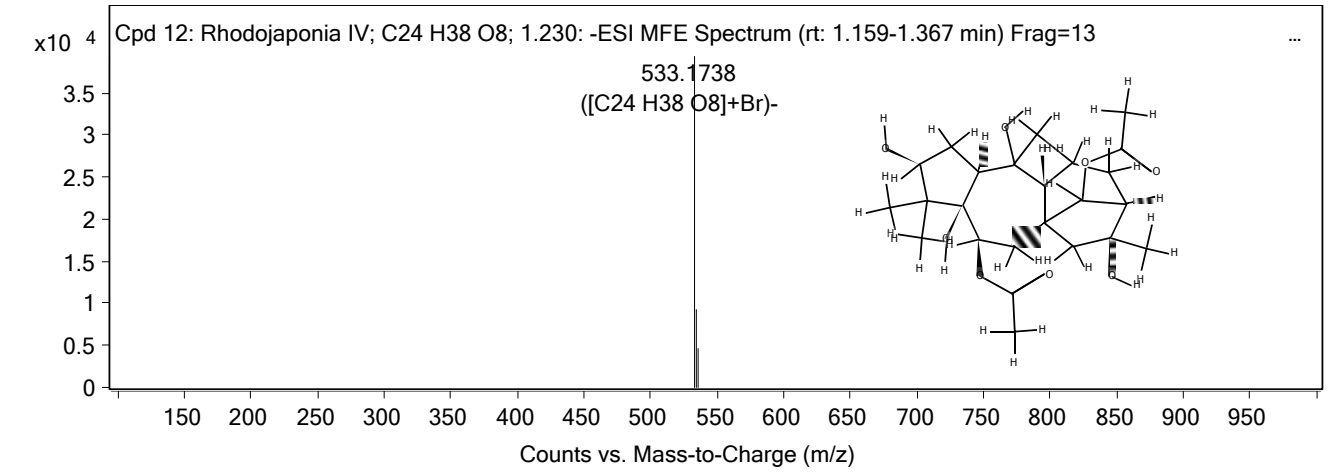
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 12: Rhodojaponia IV; C24 H38 O8; 1.230	**Rhodojaponia IV**	533.1738	1.23	Find by Molecular Feature	454.2557

Compound Chromatograms

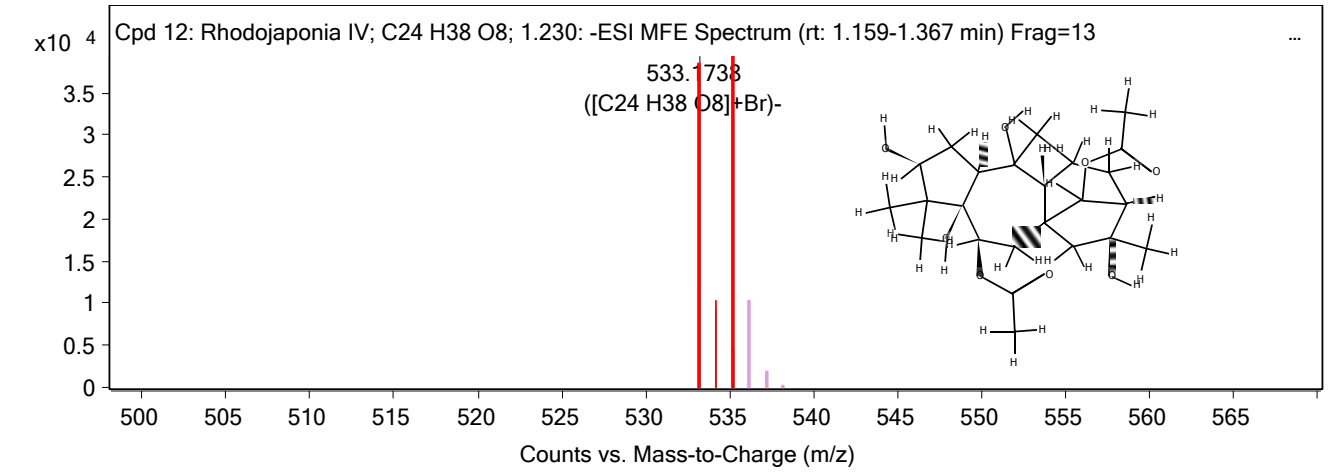




MFE MS Spectrum



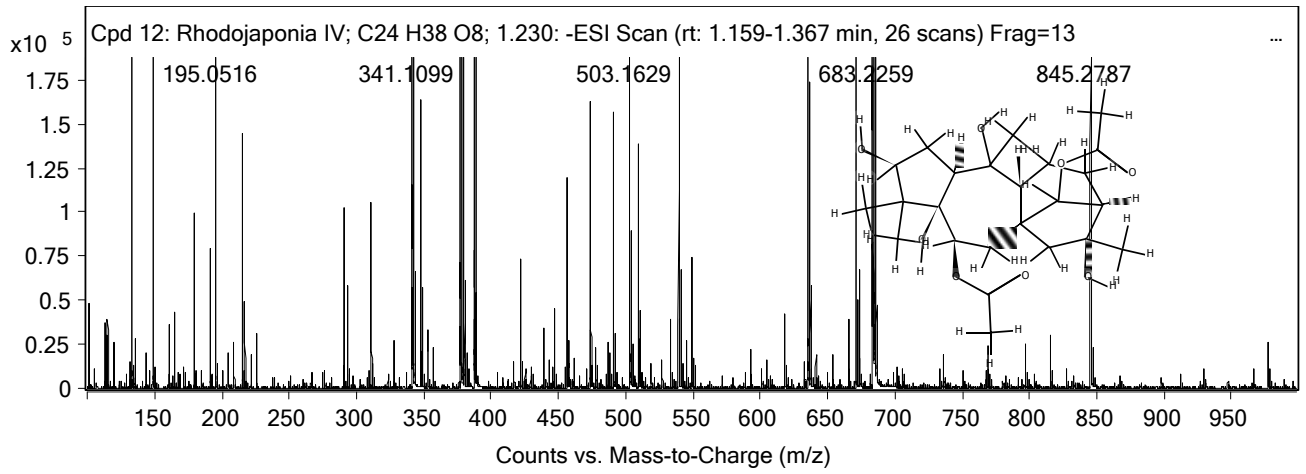
MFE MS Zoomed Spectrum



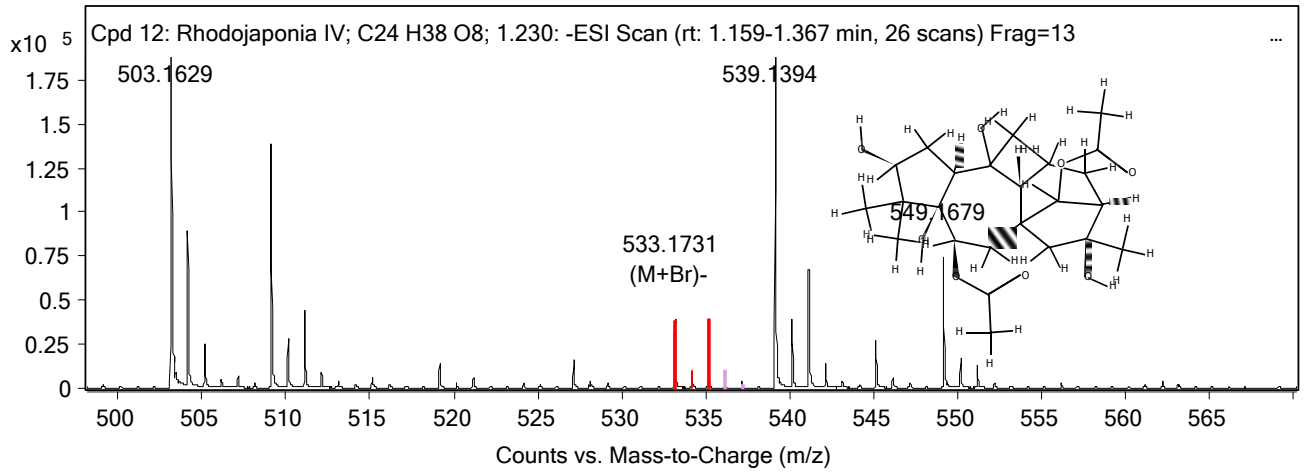
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
533.1738	-1	39335.39	C24 H38 O8	(M+Br)-
534.177	-1	9202.7	C24 H38 O8	(M+Br)-
535.1812	-1	4722.05	C24 H38 O8	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

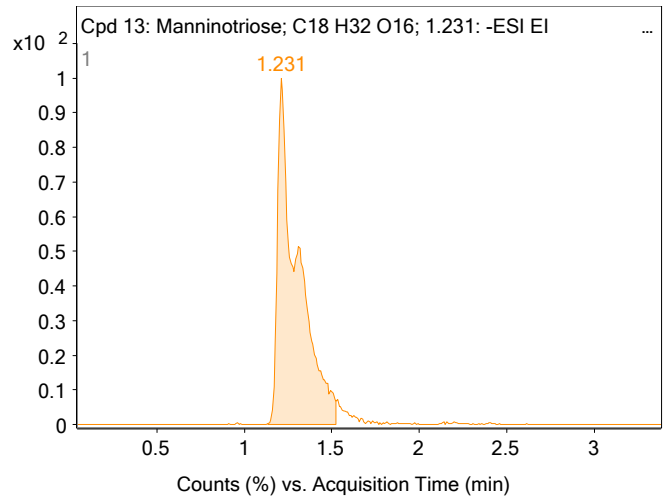


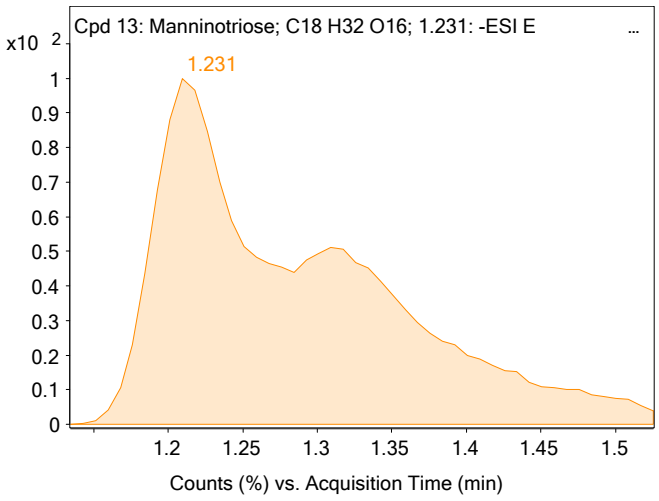
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Rhodojaponia IV	1.23	C24 H38 O8		60.11	454.2557	0.99	(M+Br)-
	Strictosamide	1.23	C26 H30 N2 O8		32.15	498.2052	-4.97	(M+Cl)-
	Vincosamide	1.23	C26 H30 N2 O8		32.15	498.2052	-4.97	(M+Cl)-
	Vincoside lactam	1.23	C26 H30 N2 O8		32.15	498.2052	-4.97	(M+Cl)-

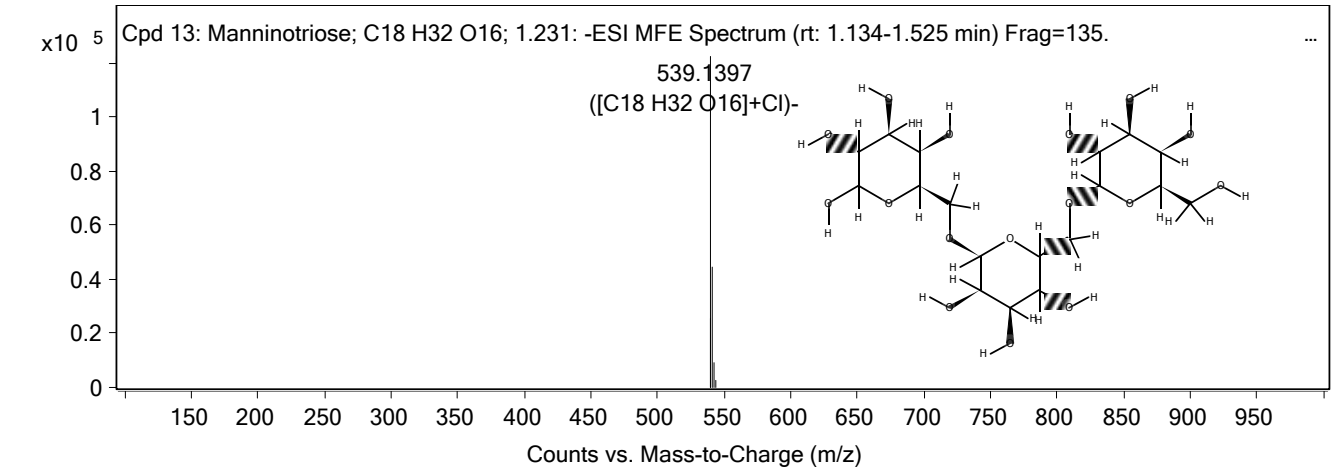
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 13: Manninotriose; C18 H32 O16; 1.231	**Manninotriose**	539.1397	1.231	Find by Molecular Feature	504.1702

Compound Chromatograms

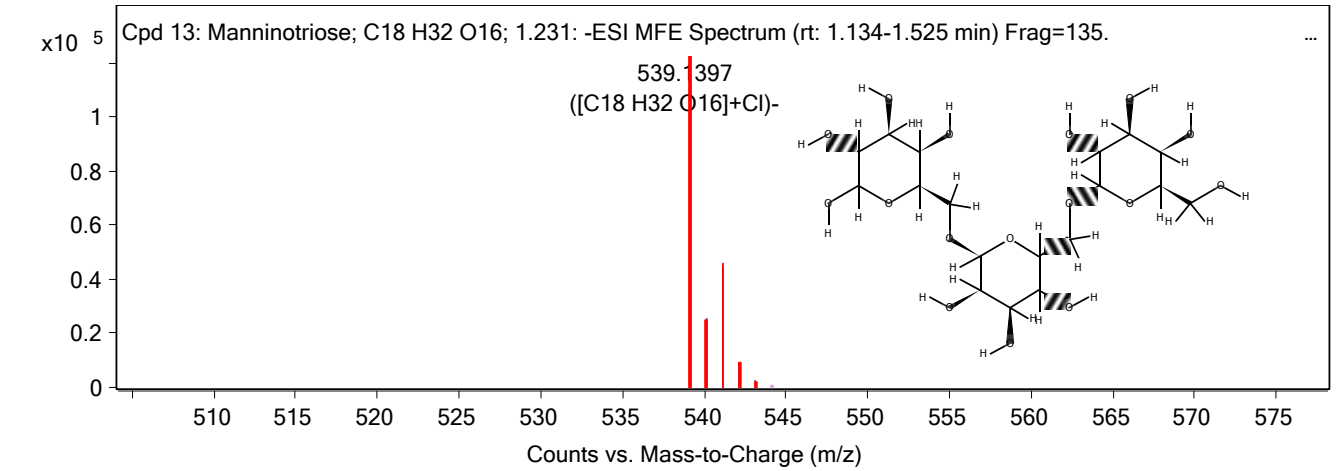




MFE MS Spectrum



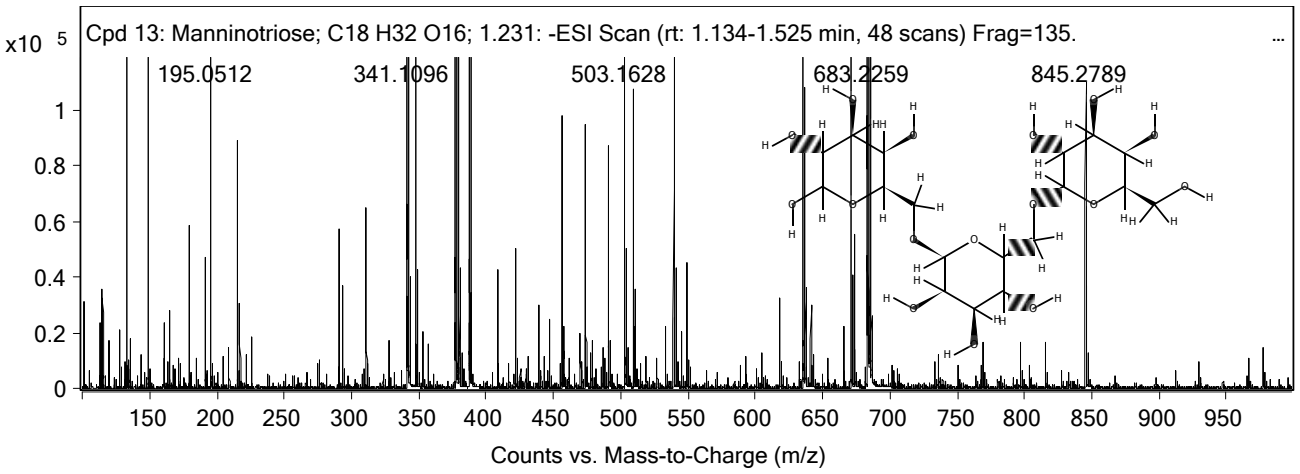
MFE MS Zoomed Spectrum



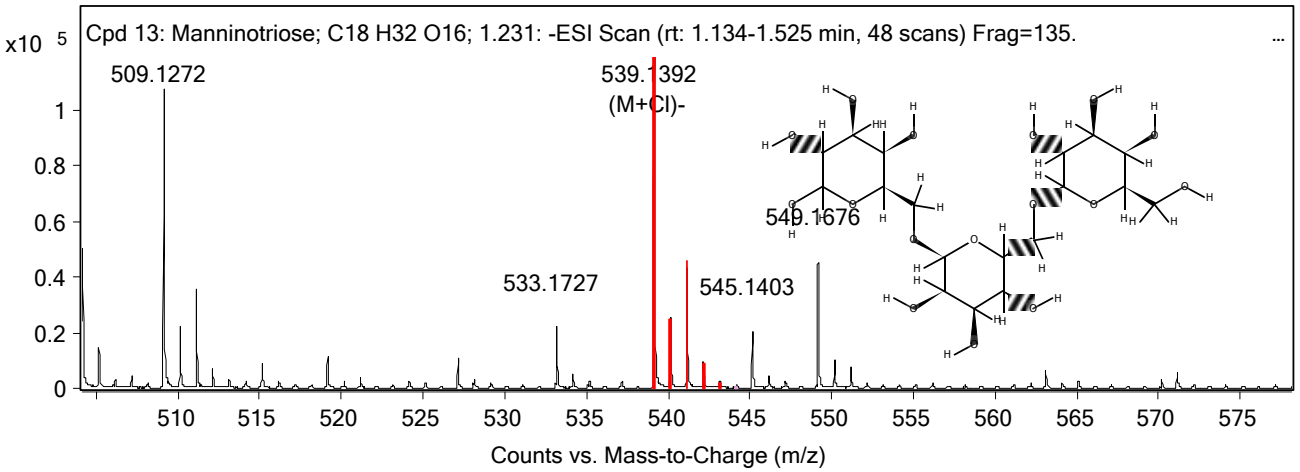
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
539.1397	-1	122397.07	C18 H32 O16	(M+Cl)-
540.1426	-1	25687.75	C18 H32 O16	(M+Cl)-
541.1377	-1	44547.48	C18 H32 O16	(M+Cl)-
542.1405	-1	9349.36	C18 H32 O16	(M+Cl)-
543.144	-1	2779.13	C18 H32 O16	(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

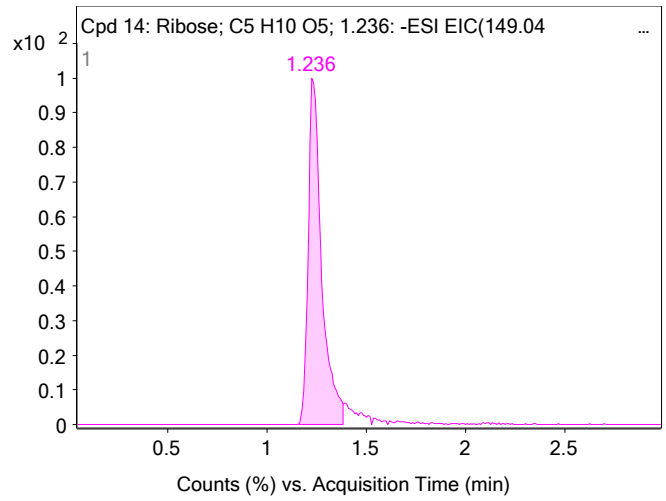


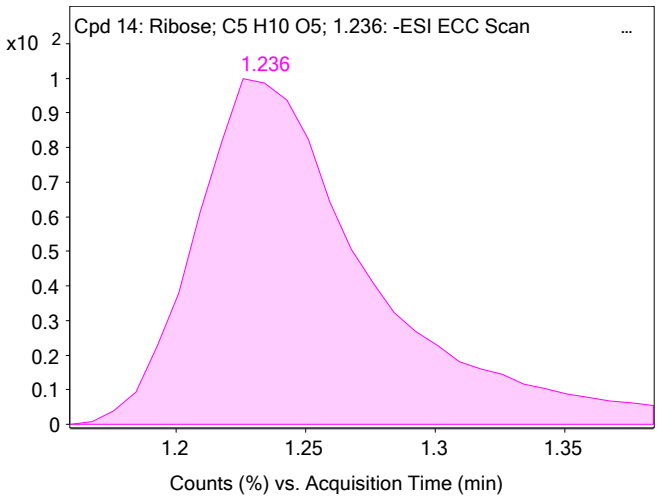
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Manninotriose	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-
	Neokestose	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-
	Gentianose	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-
	1-Kestose	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-
	Panose	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-
	Planteose	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-
	Raffinose	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-
	Panose B	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-
	Panose C	1.231	C18 H32 O16		96.95	504.1702	-1.13	(M+Cl)-

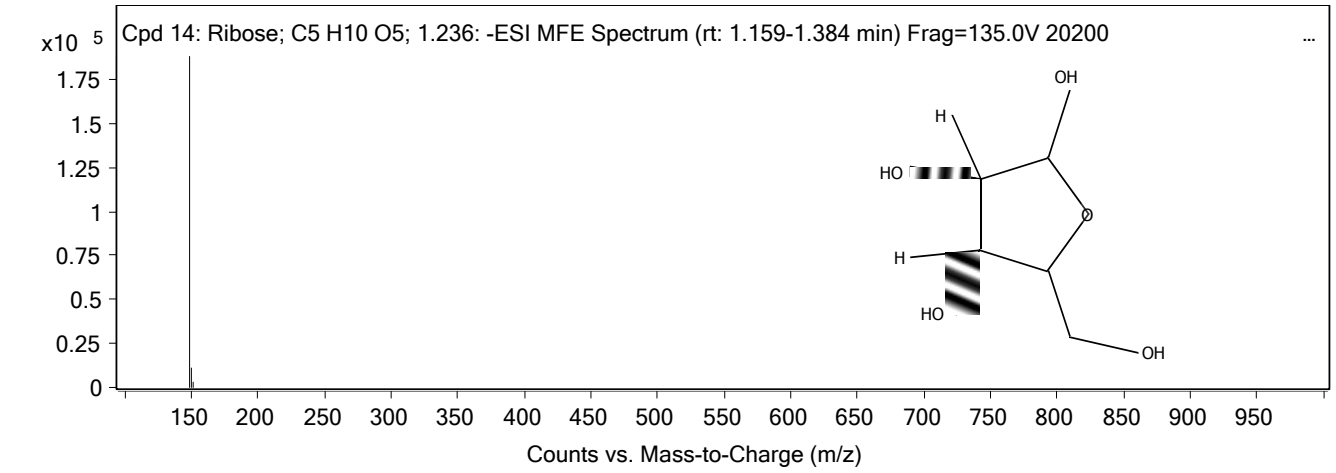
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 14: Ribose; C5 H10 O5; 1.236	**Ribose**	149.0467	1.236	Find by Molecular Feature	150.054

Compound Chromatograms

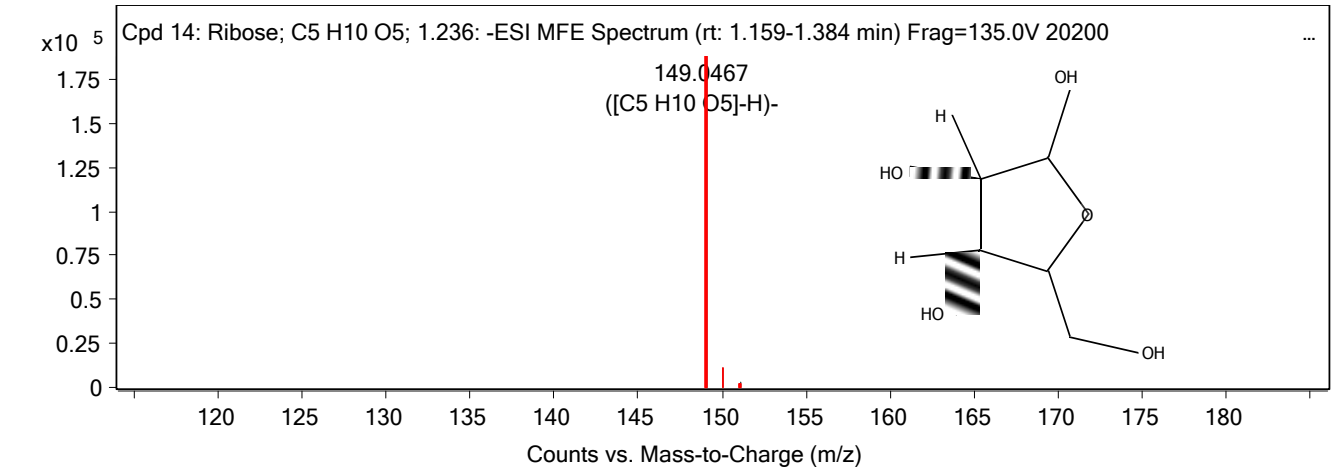




MFE MS Spectrum



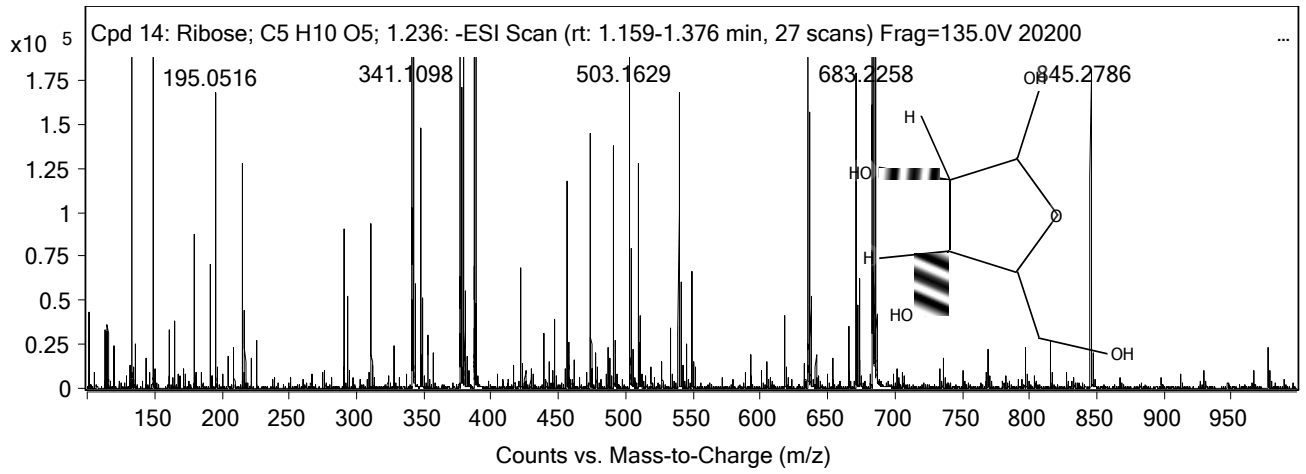
MFE MS Zoomed Spectrum



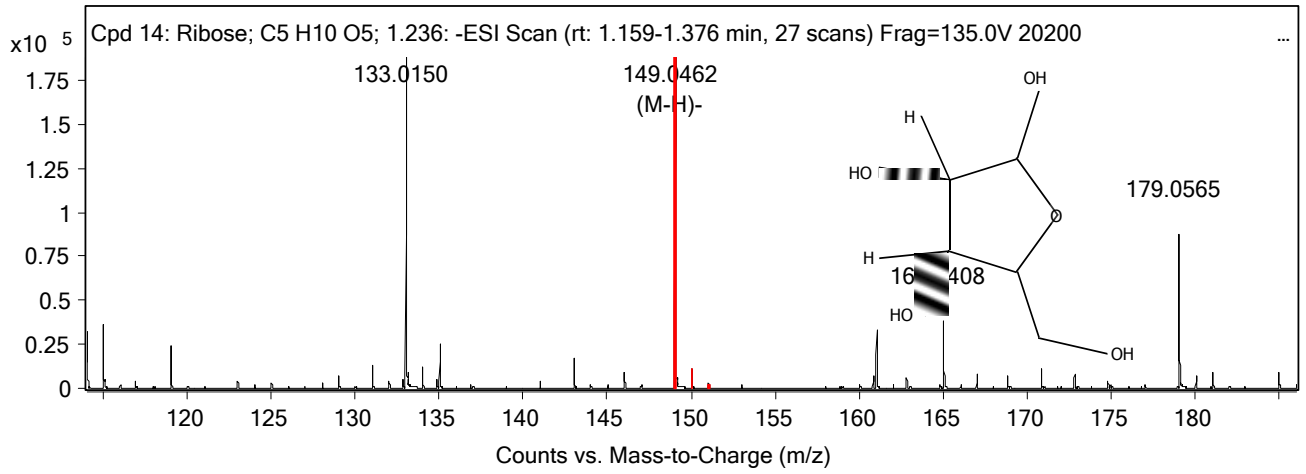
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
149.0467	-1	188253.77	C5 H10 O5	(M-H)-
150.0498	-1	10959.99	C5 H10 O5	(M-H)-
151.0546	-1	2807.13	C5 H10 O5	(M-H)-

MS Spectrum



MS Zoomed Spectrum

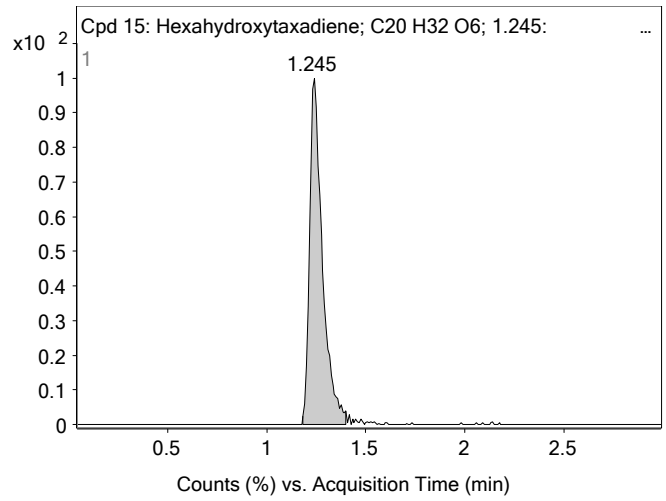


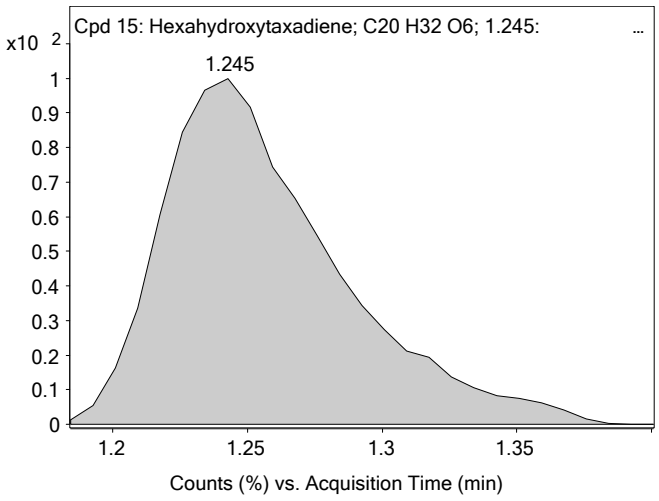
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Ribose	1.236	C5 H10 O5		92.2	150.054	-1.17	(M-H)-
	Xylose	1.236	C5 H10 O5		92.2	150.054	-1.17	(M-H)-
	Apiose	1.236	C5 H10 O5		92.2	150.054	-1.17	(M-H)-
	Dipropyl disulfide	1.236	C6 H14 S2		80.33	150.0541	-0.46	(M-H)-

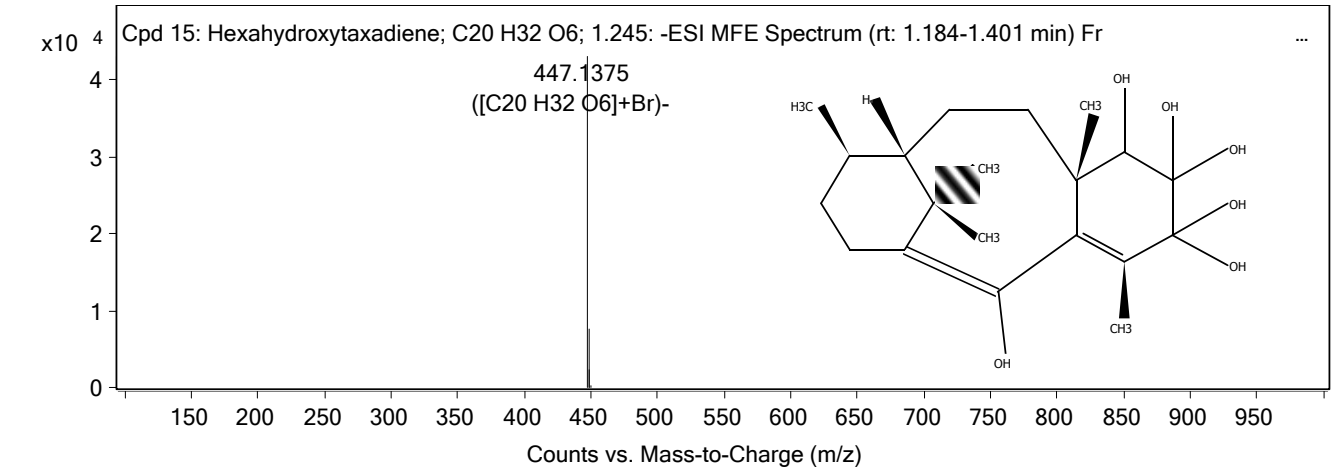
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 15: Hexahydroxytaxadiene; C20 H32 O6; 1.245	**Hexahydroxytaxadiene**	447.1375	1.245	Find by Molecular Feature	368.219

Compound Chromatograms

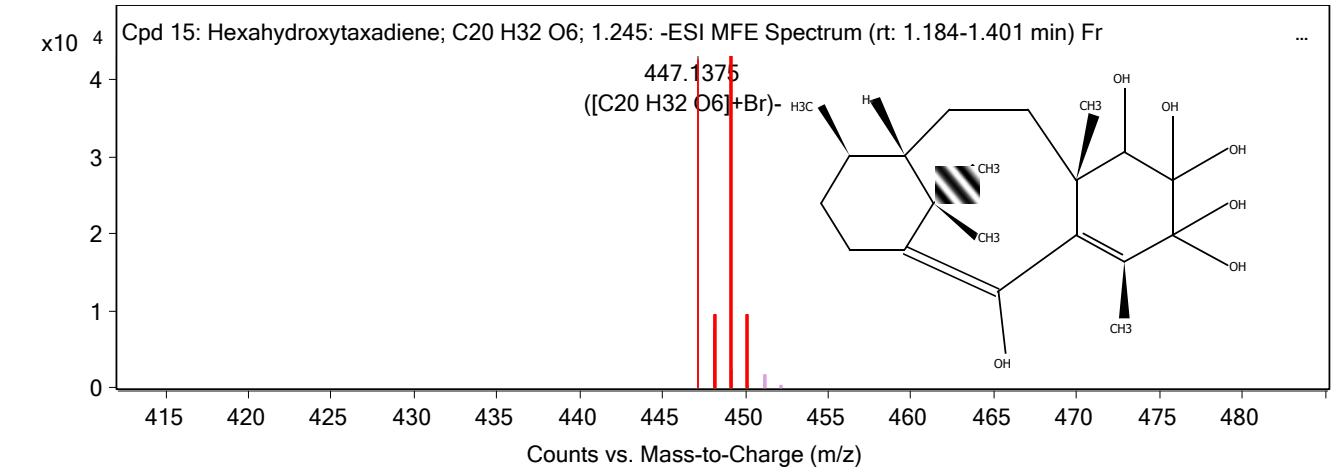




MFE MS Spectrum



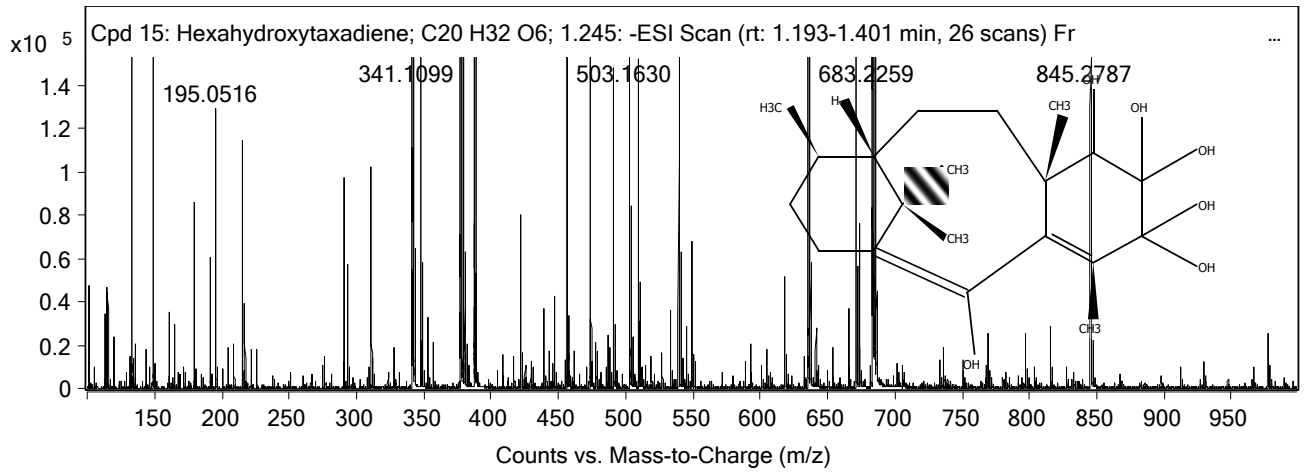
MFE MS Zoomed Spectrum



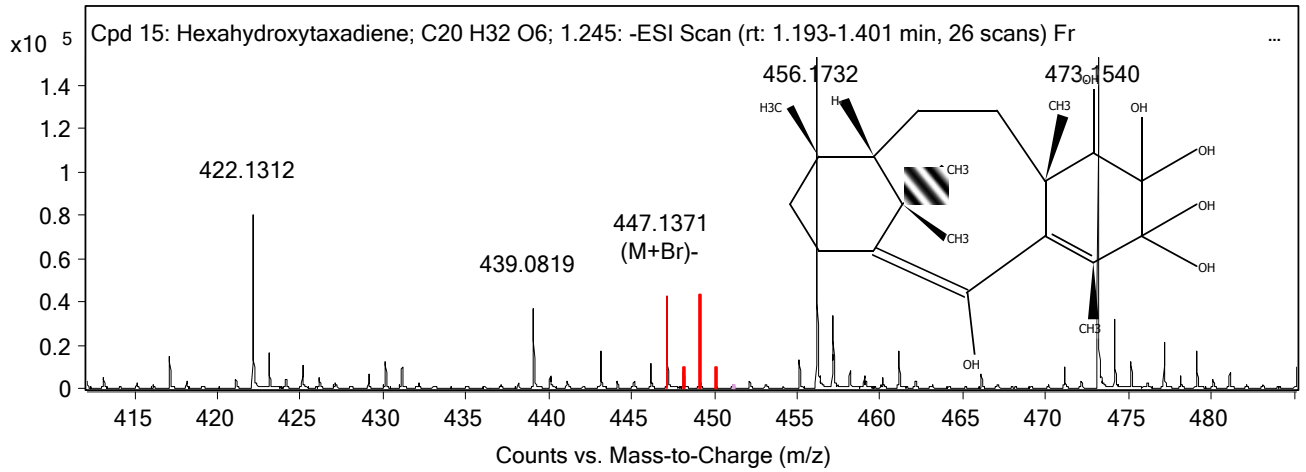
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
447.1375	-1	43055.69	C20 H32 O6	(M+Br)-
448.1415	-1	7661.08	C20 H32 O6	(M+Br)-
449.1427	-1	2264.4	C20 H32 O6	(M+Br)-
450.1487	-1	134.58	C20 H32 O6	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

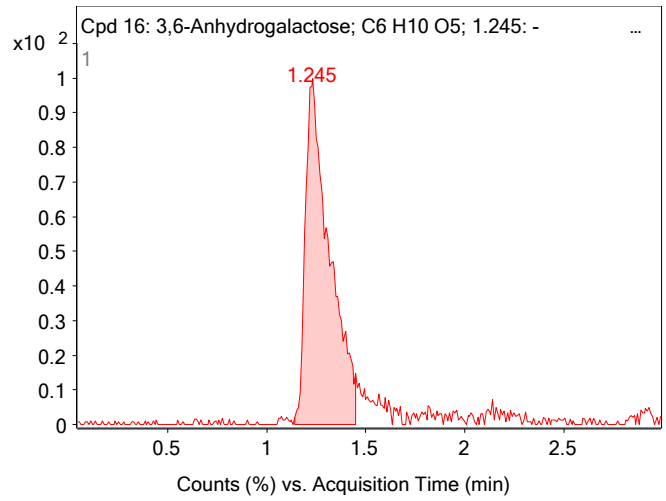


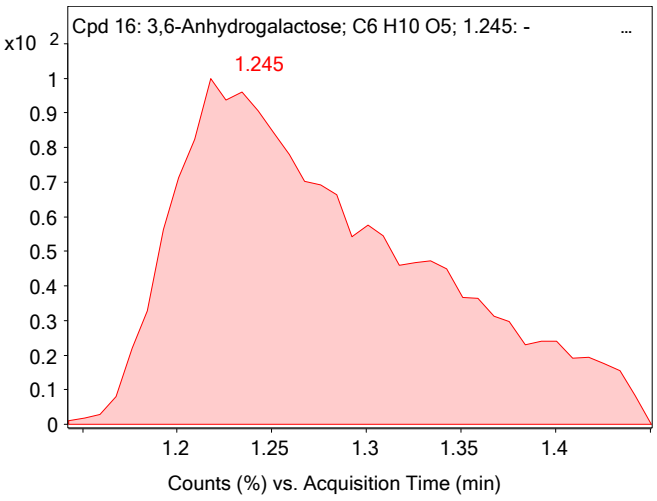
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Hexahydroxytaxadiene	1.245	C20 H32 O6		64.53	368.219	0.9	(M+Br)-
	Lyoniol B	1.245	C20 H32 O6		64.53	368.219	0.9	(M+Br)-

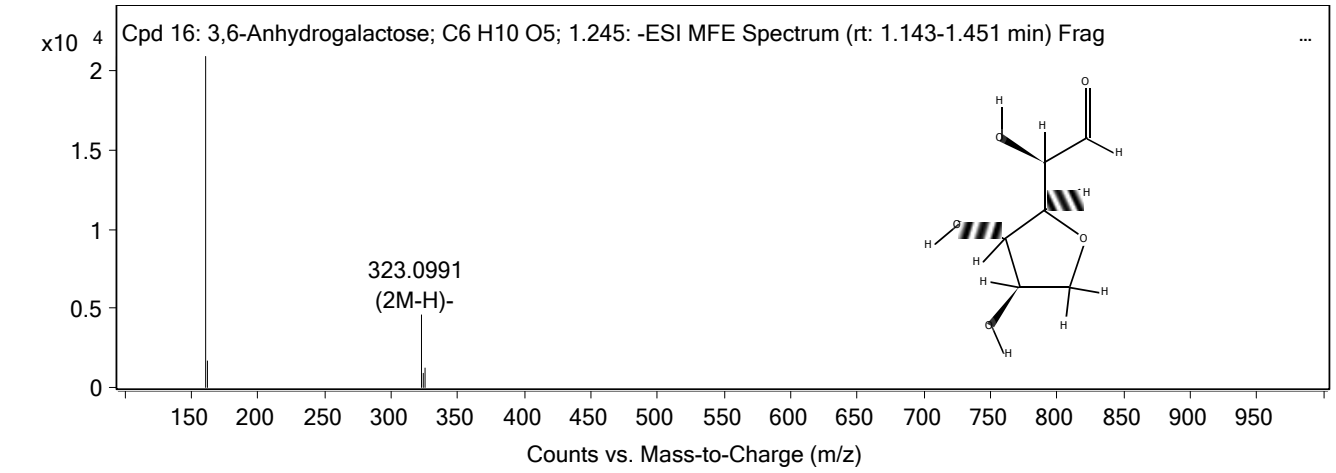
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 16: 3,6-Anhydrogalactose; C6 H10 O5; 1.245	**3,6-Anhydrogalactose**	161.0465	1.245	Find by Molecular Feature	162.0537

Compound Chromatograms

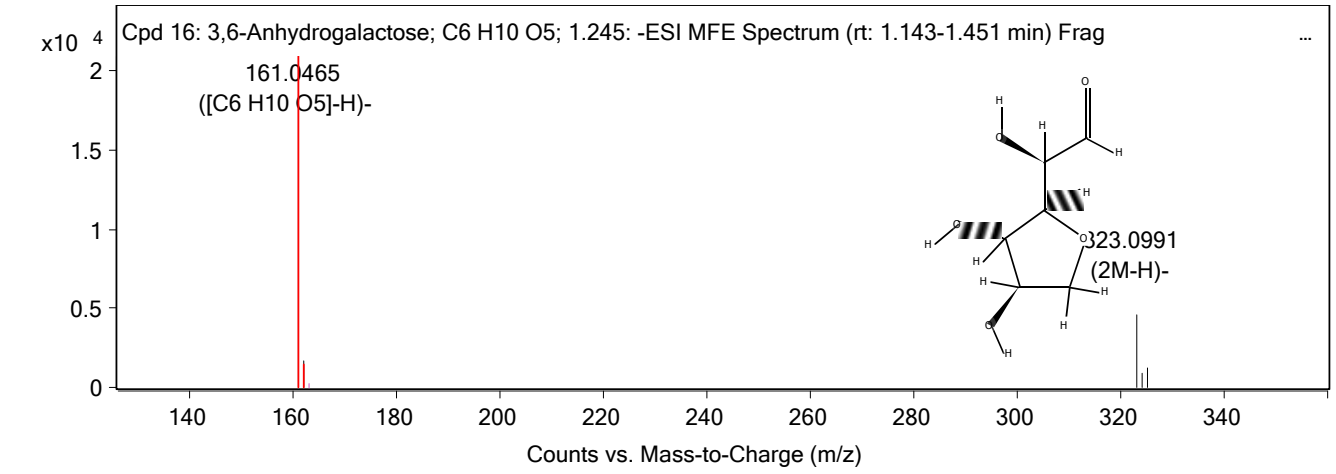




MFE MS Spectrum



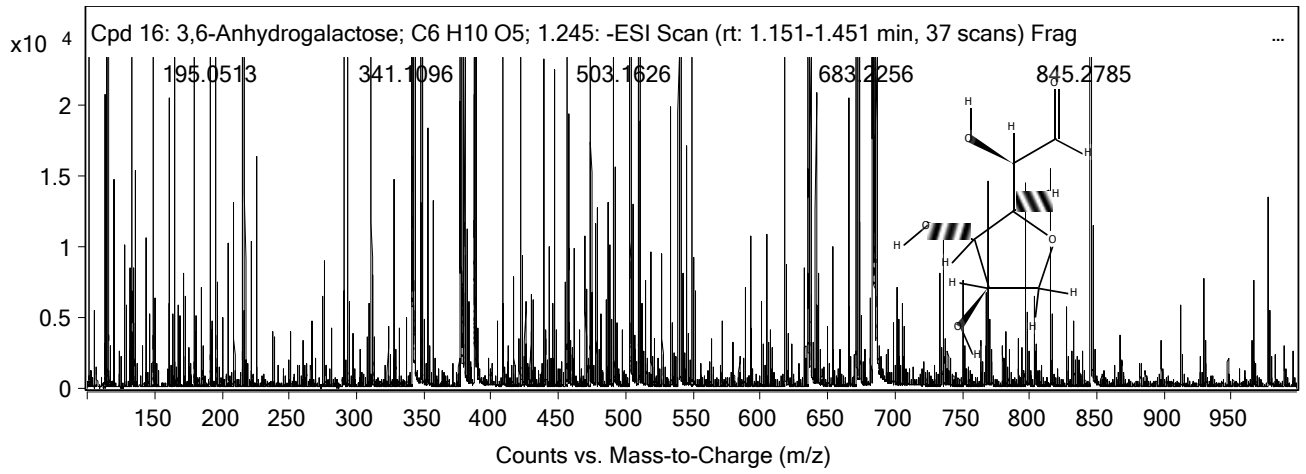
MFE MS Zoomed Spectrum



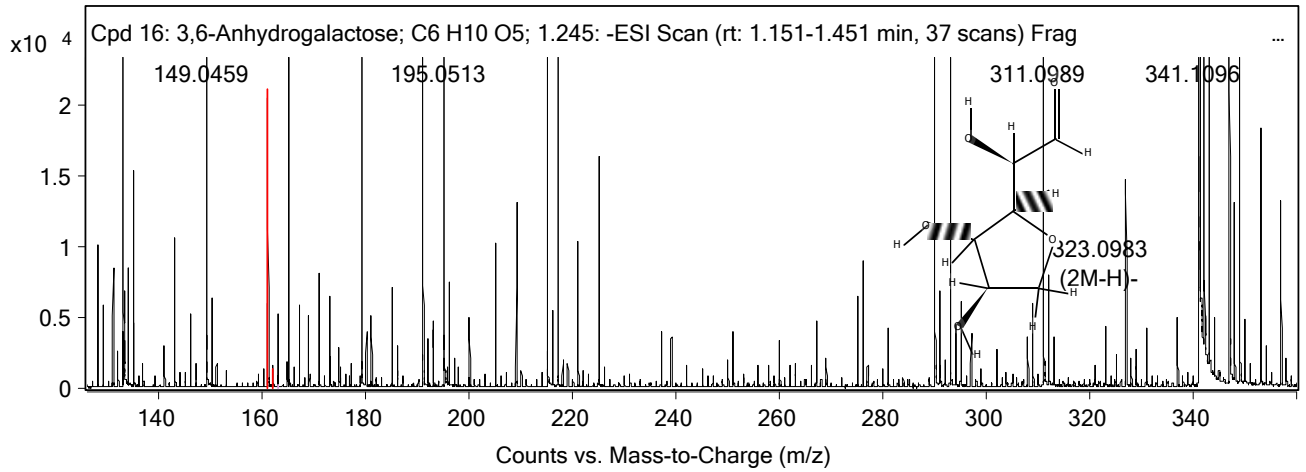
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
161.0465	-1	20924.79	C6 H10 O5	(M-H)-
162.0497	-1	1636.5	C6 H10 O5	(M-H)-
323.0991	-1	4605.02		(2M-H)-
324.1031	-1	886.01		(2M-H)-
325.0896	-1	1194.68		(2M-H)-

MS Spectrum



MS Zoomed Spectrum

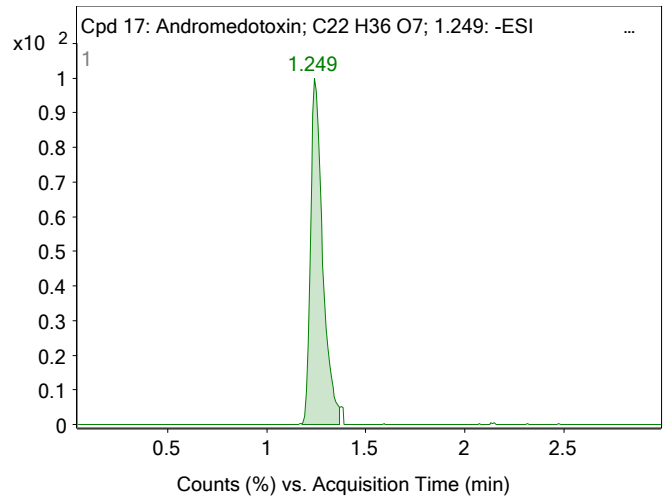


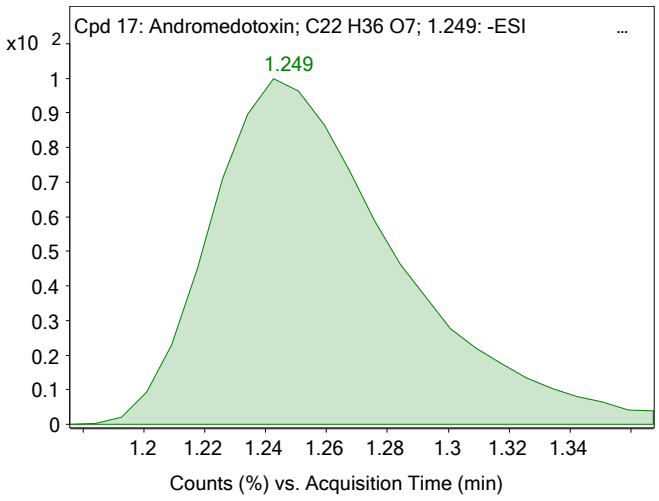
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	3,6-Anhydrogalactose	1.245	C6 H10 O5		82.59	162.0537	-0.9	(M-H)-
	Danshensu	1.245	C6 H10 O5		82.59	162.0537	-0.9	(M-H)-

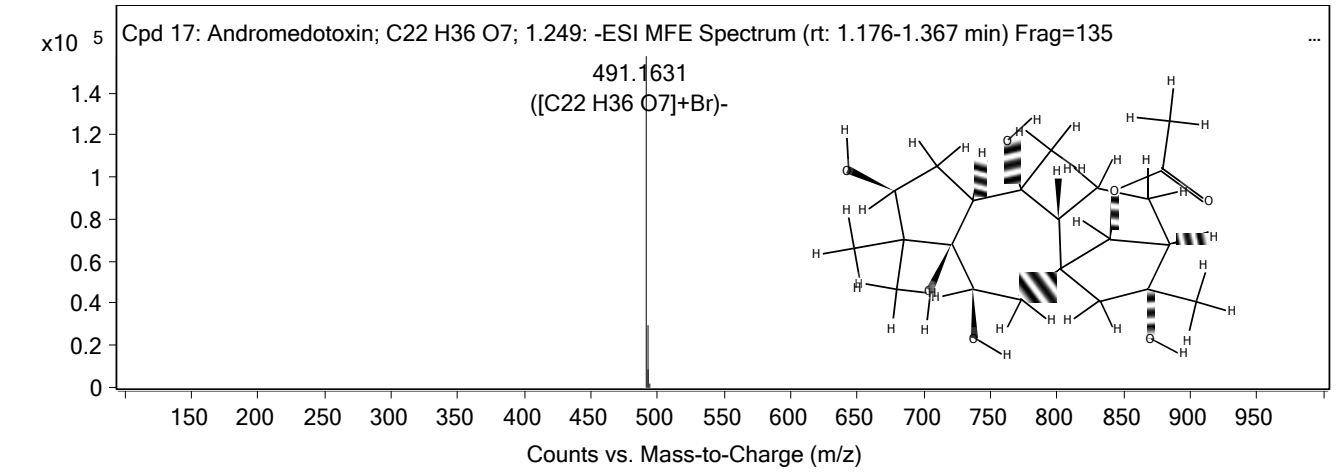
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 17: Andromedotoxin; C22 H36 O7; 1.249	**Andromedotoxin**	491.1631	1.249	Find by Molecular Feature	412.2446

Compound Chromatograms

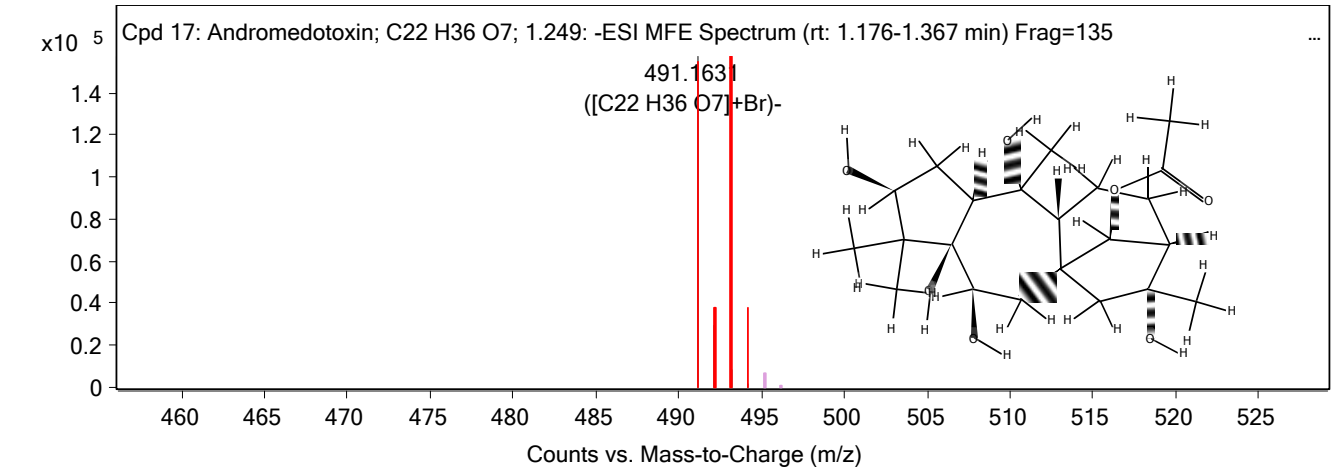




MFE MS Spectrum



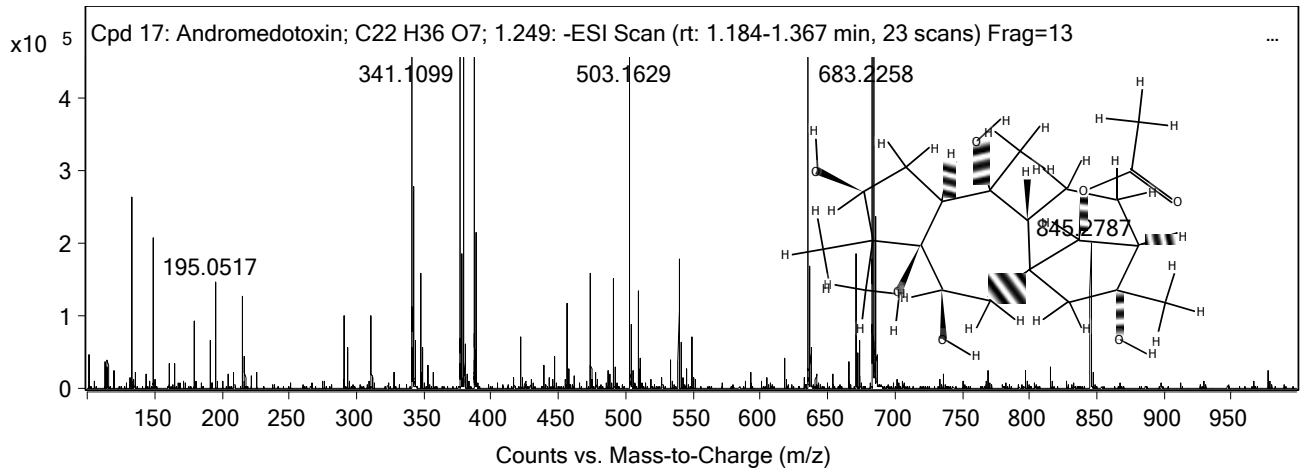
MFE MS Zoomed Spectrum



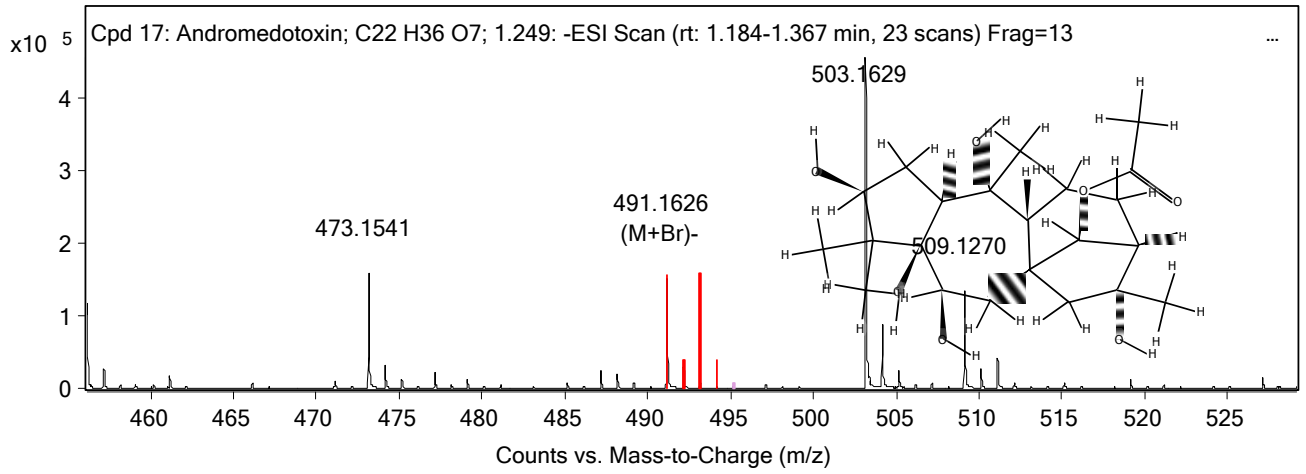
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
491.1631	-1	157443.14	C22 H36 O7	(M+Br)-
492.1667	-1	29627.92	C22 H36 O7	(M+Br)-
493.1677	-1	8345.93	C22 H36 O7	(M+Br)-
494.1714	-1	1448.58	C22 H36 O7	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

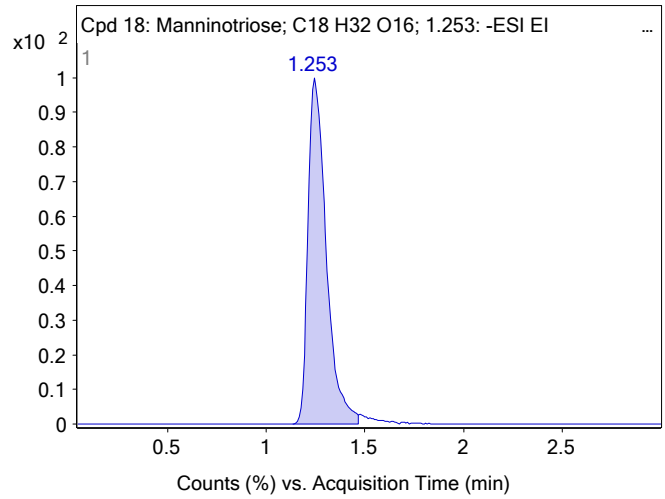


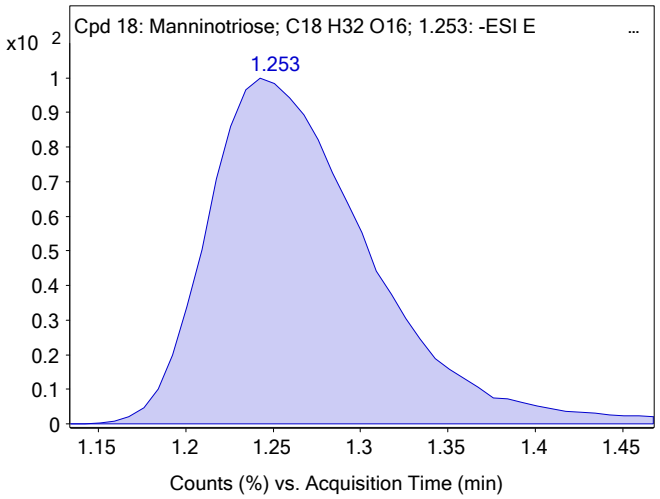
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Andromedotoxin	1.249	C22 H36 O7		62.34	412.2446	1.54	(M+Br)-

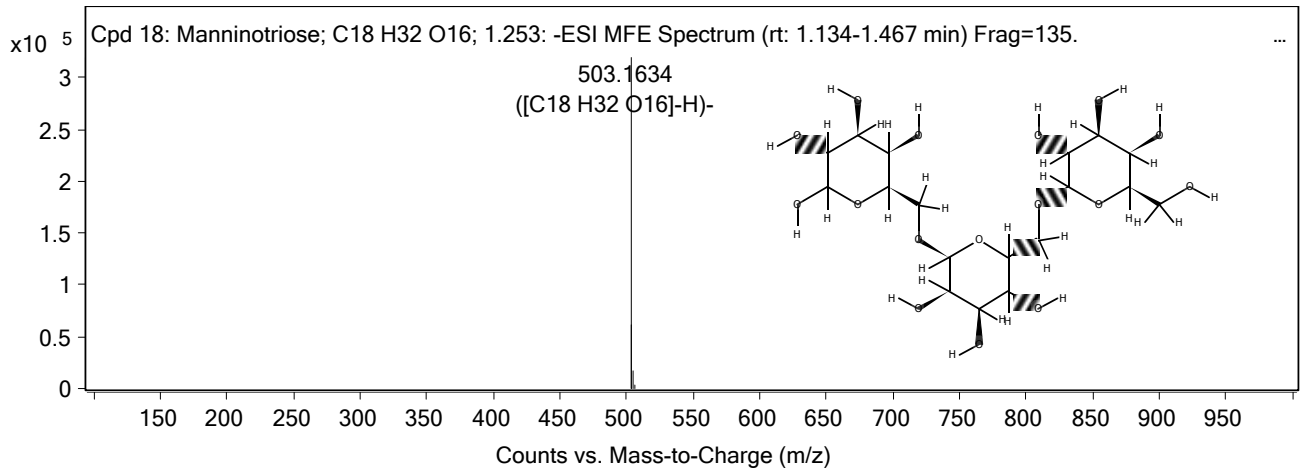
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 18: Manninotriose; C18 H32 O16; 1.253	**Manninotriose**	503.1634	1.253	Find by Molecular Feature	504.1706

Compound Chromatograms

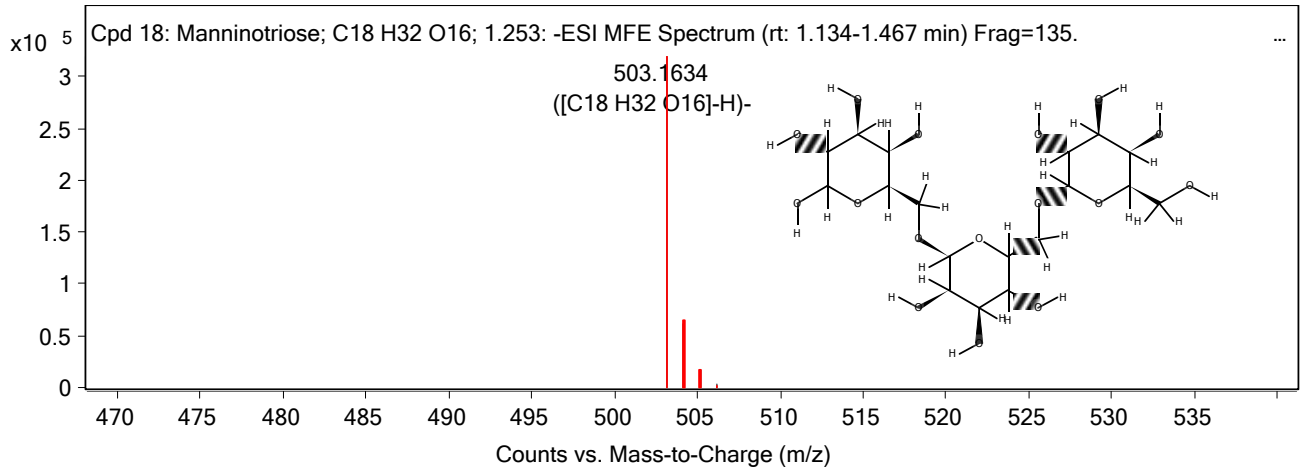




MFE MS Spectrum



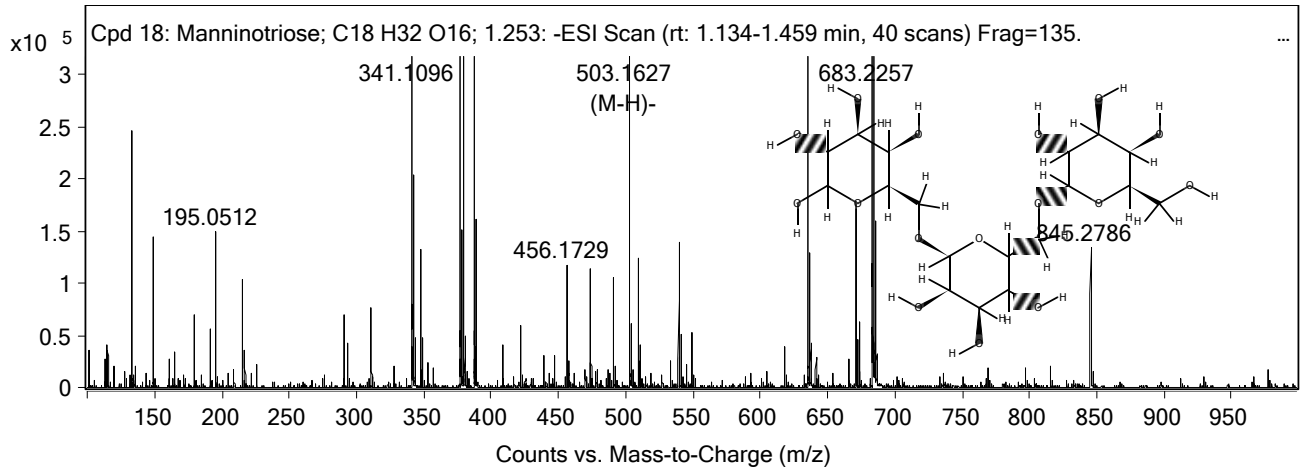
MFE MS Zoomed Spectrum



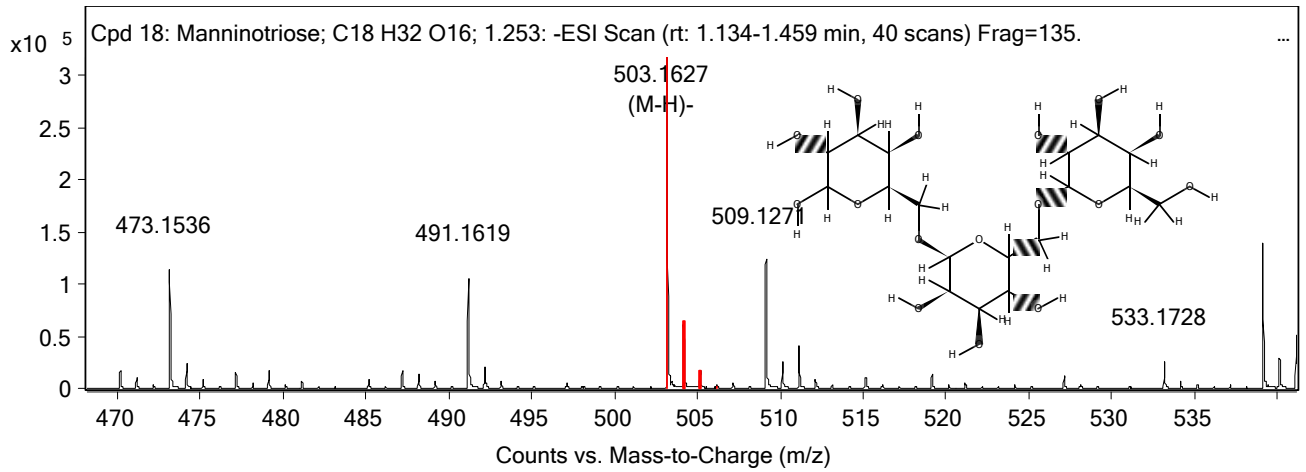
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
503.1634	-1	319432.97	C18 H32 O16	(M-H)-
504.1665	-1	61513.01	C18 H32 O16	(M-H)-
505.168	-1	16838.37	C18 H32 O16	(M-H)-
506.1685	-1	3006.99	C18 H32 O16	(M-H)-

MS Spectrum



MS Zoomed Spectrum

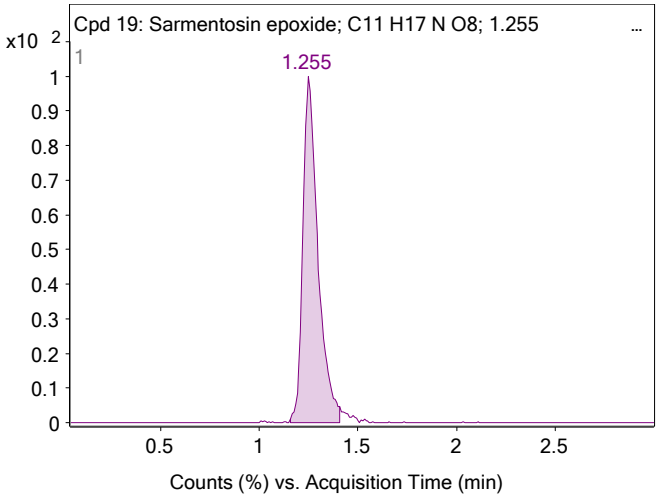


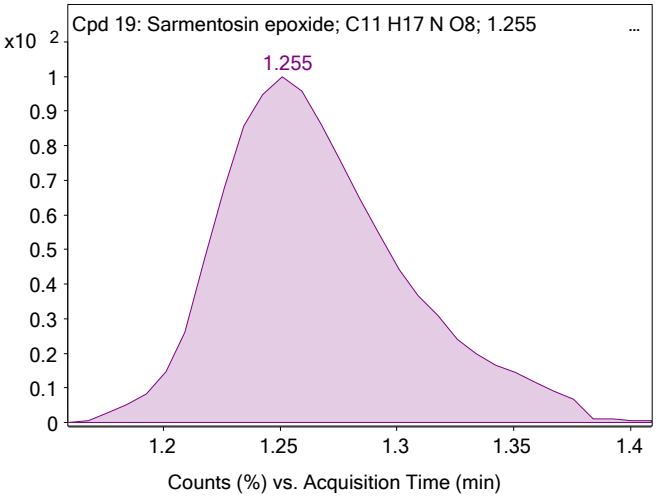
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Manninotriose	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-
	Neokestose	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-
	Gentianose	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-
	1-Kestose	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-
	Panose	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-
	Planteose	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-
	Raffinose	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-
	Panose B	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-
	Panose C	1.253	C18 H32 O16		94.79	504.1706	-1.56	(M-H)-

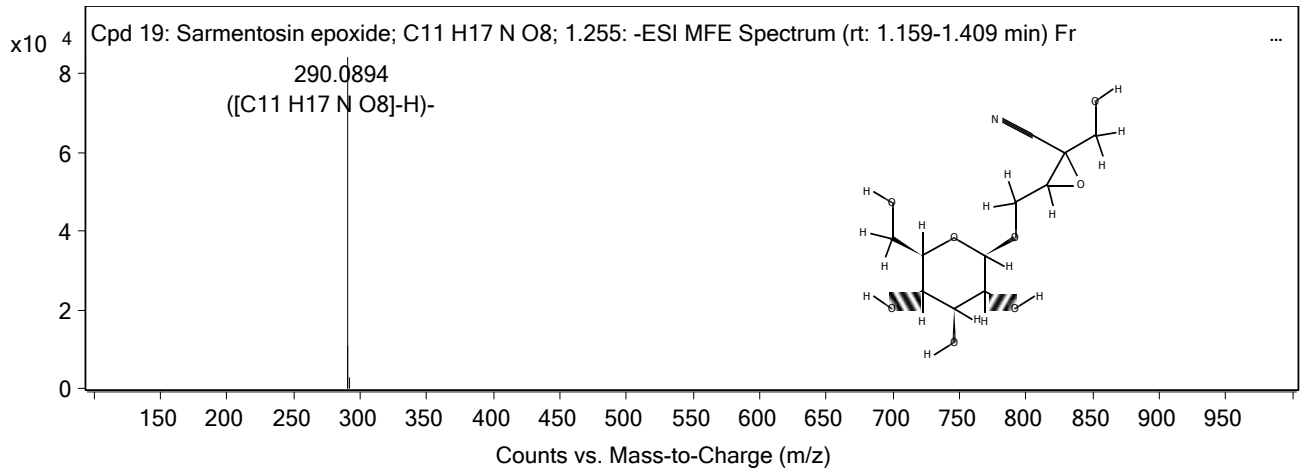
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 19: Sarmentosin epoxide; C11 H17 N O8; 1.255	**Sarmentosin epoxide**	290.0894	1.255	Find by Molecular Feature	291.0964

Compound Chromatograms

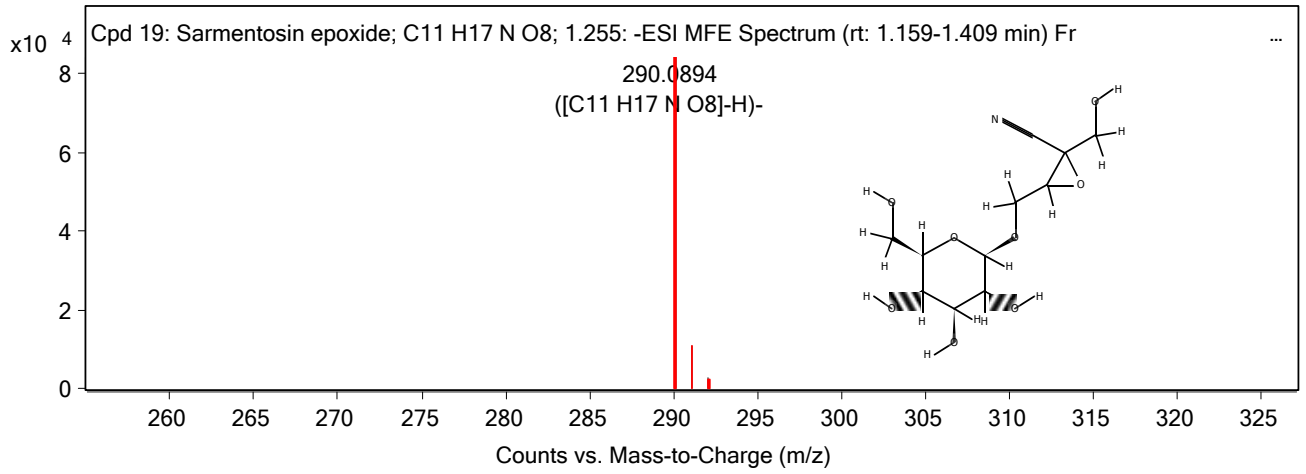




MFE MS Spectrum



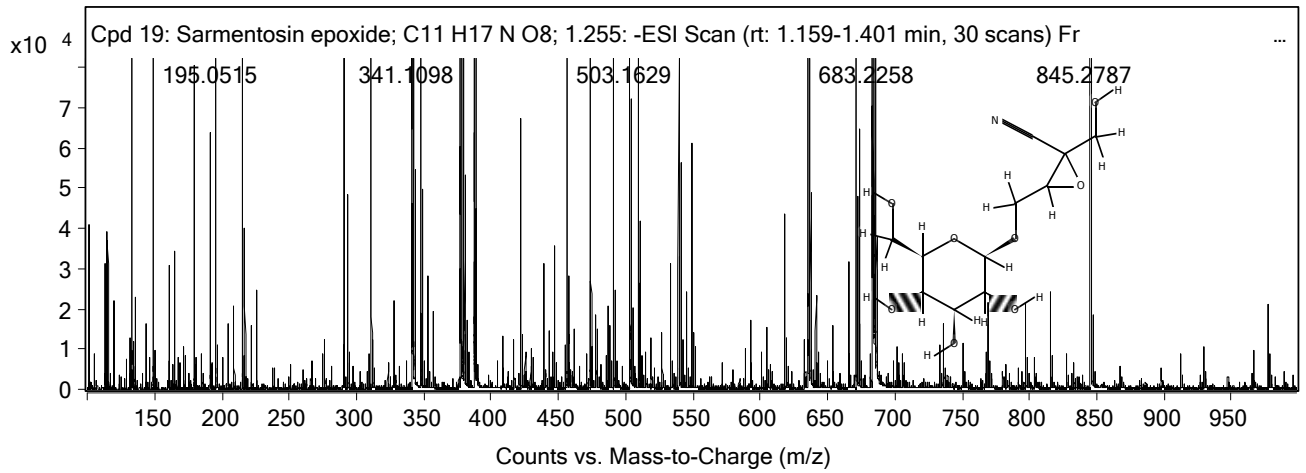
MFE MS Zoomed Spectrum



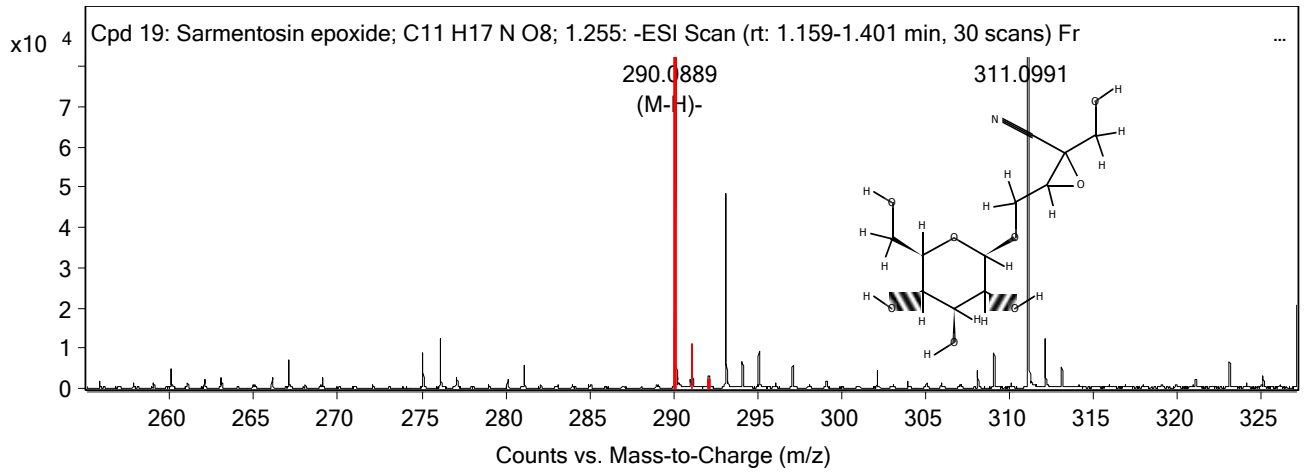
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
290.0894	-1	84180.89	C11 H17 N O8	(M-H)-
291.0923	-1	10856.52	C11 H17 N O8	(M-H)-
292.0859	-1	2868.91	C11 H17 N O8	(M-H)-

MS Spectrum



MS Zoomed Spectrum

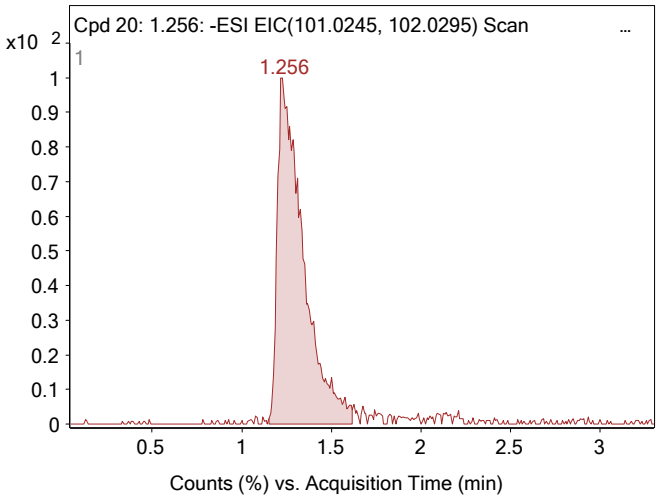


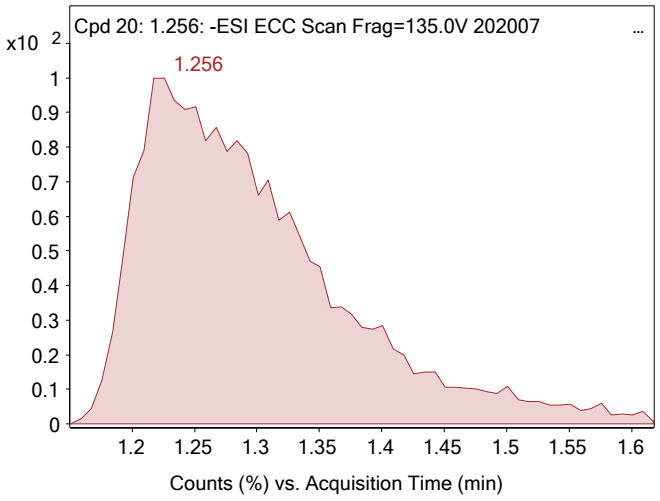
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Sarmentosin epoxide	1.255	C11 H17 N O8		91.71	291.0964	-1	(M-H)-

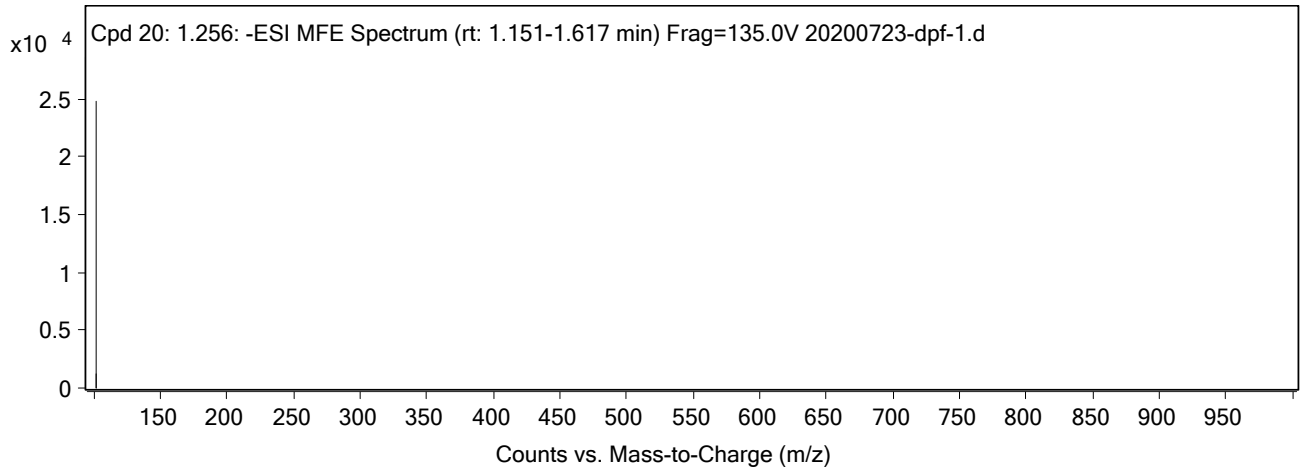
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 20: 1.256	101.0256	1.256	Find by Molecular Feature	102.0329

Compound Chromatograms

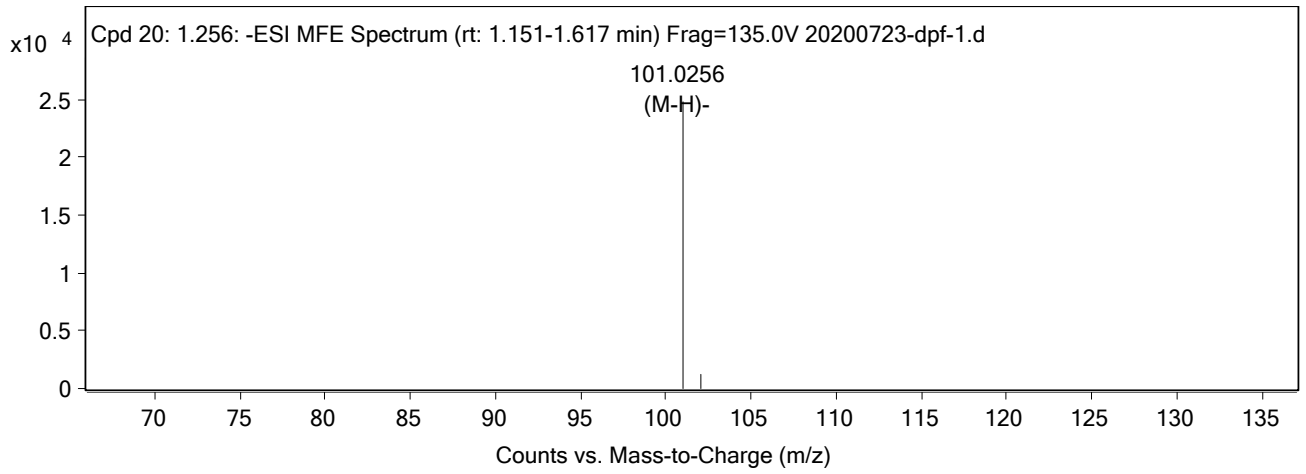




MFE MS Spectrum



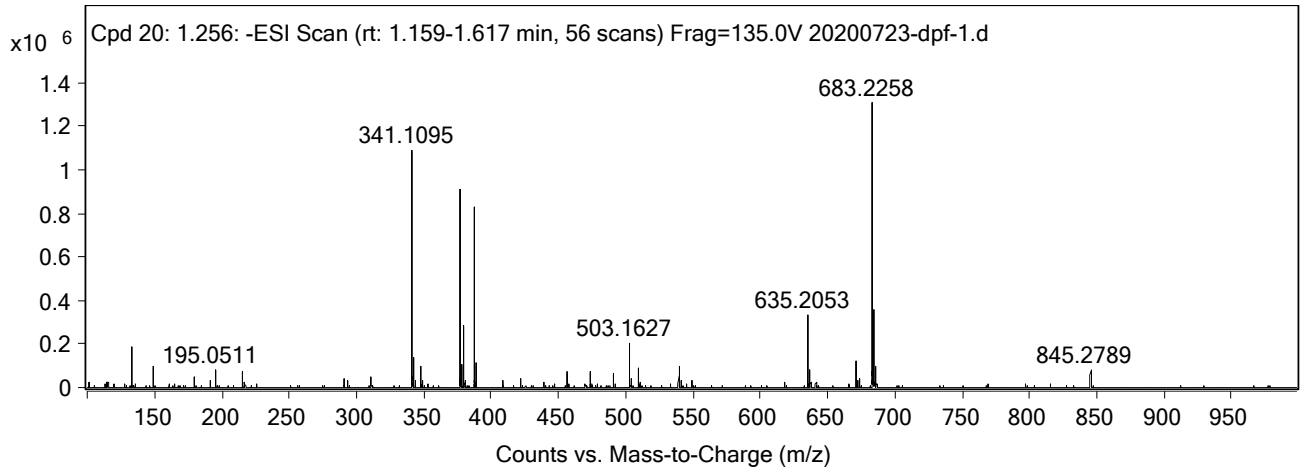
MFE MS Zoomed Spectrum



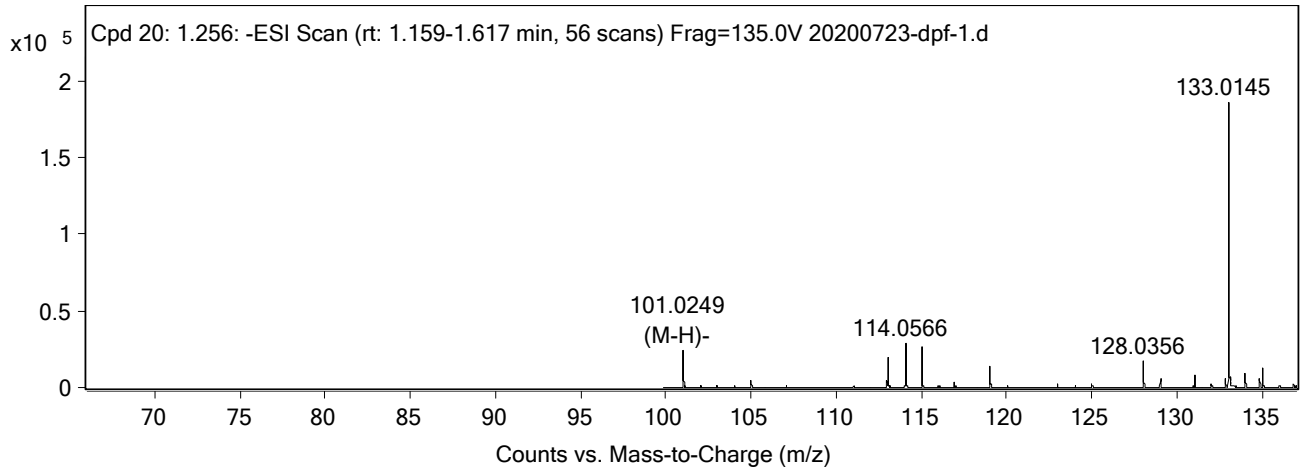
MS Spectrum Peak List

m/z	z	Abund	Ion
101.0256	-1	24838.19	(M-H)-
102.03	-1	1245.34	(M-H)-

MS Spectrum

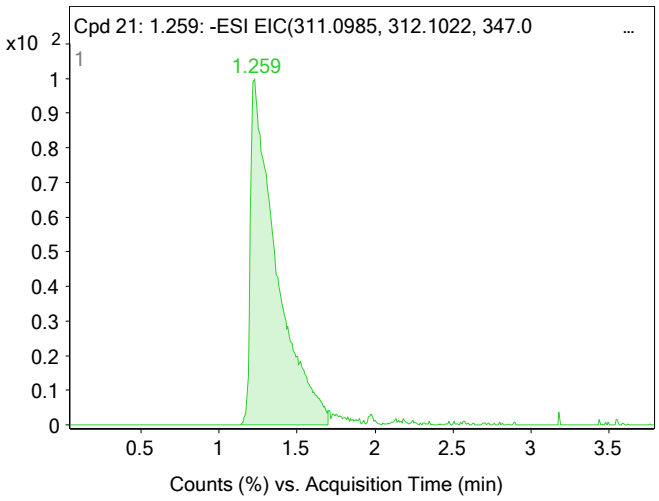


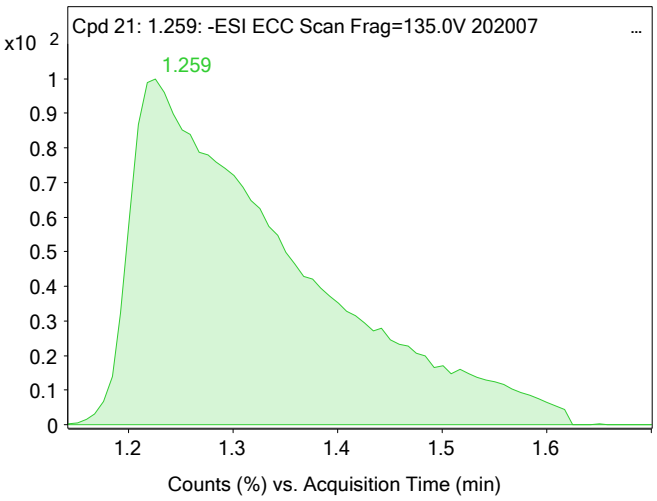
MS Zoomed Spectrum



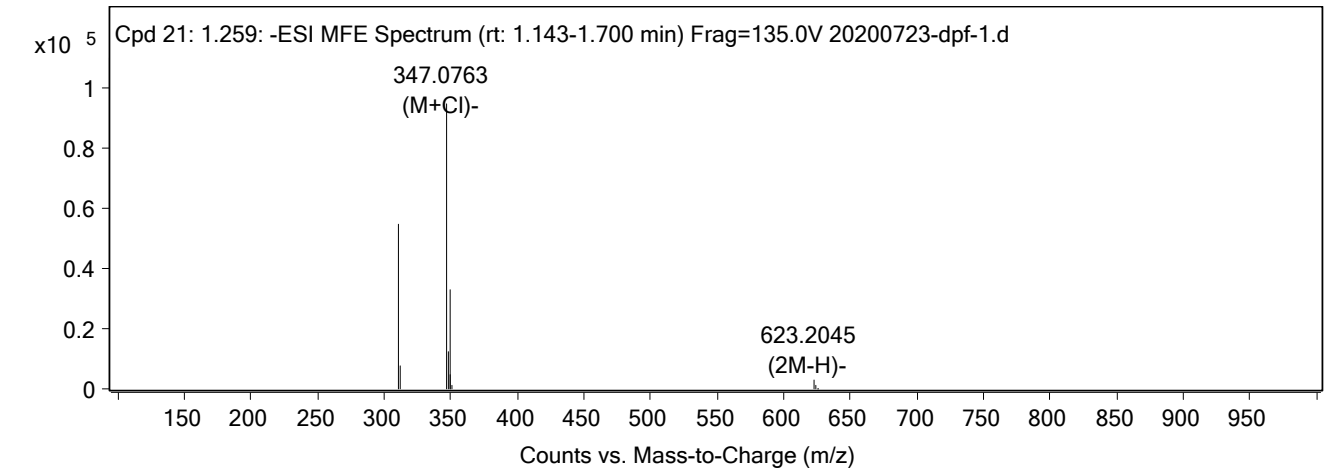
Compound Label	m/z	RT	Algorithm	Mass
Cpd 21: 1.259	347.0763	1.259	Find by Molecular Feature	312.1068

Compound Chromatograms

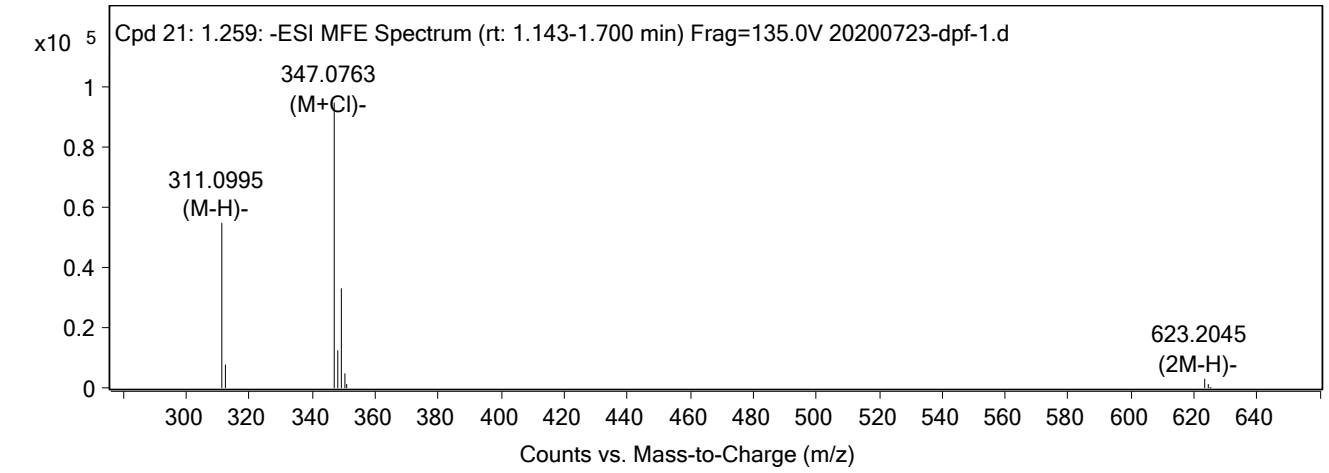




MFE MS Spectrum



MFE MS Zoomed Spectrum

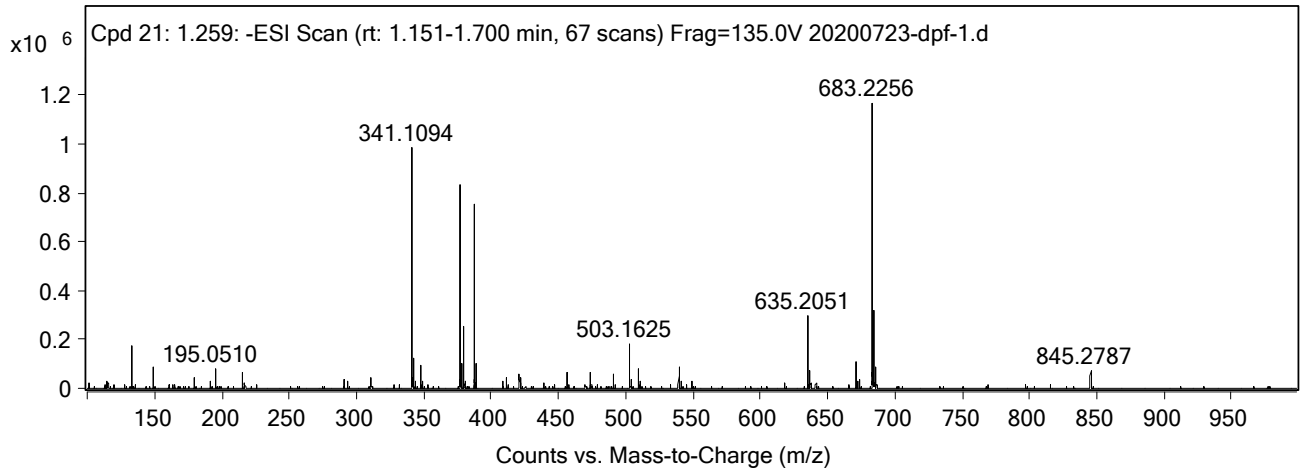


MS Spectrum Peak List

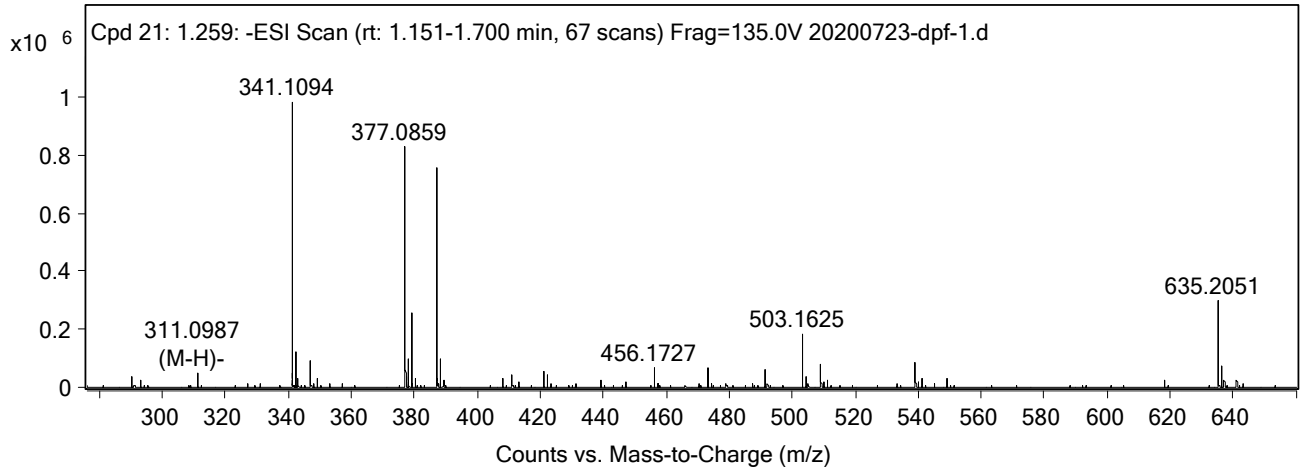
m/z	z	Abund	Ion
311.0995	-1	54360.32	(M-H)-
312.1027	-1	7387.63	(M-H)-
347.0763	-1	94596.51	(M+Cl)-
348.0795	-1	12090.9	(M+Cl)-
349.0742	-1	32800.4	(M+Cl)-
350.0776	-1	4515.81	(M+Cl)-

351.0794	-1	1408.68	(M+Cl)-
623.2045	-1	2940.09	(2M-H)-
624.2055	-1	988.9	(2M-H)-
625.1896	-1	138.7	(2M-H)-

MS Spectrum

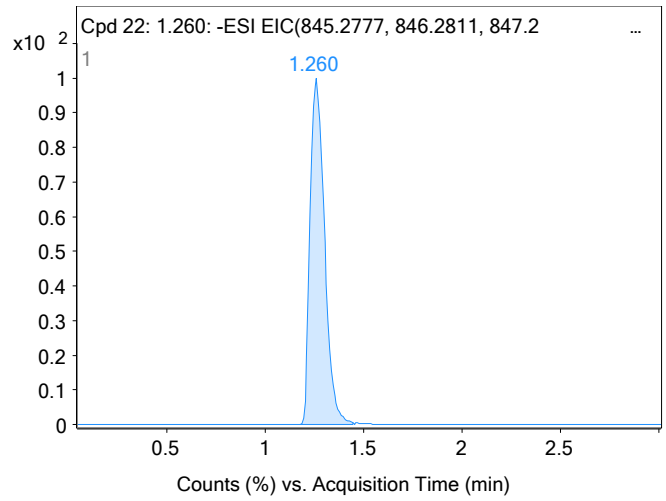


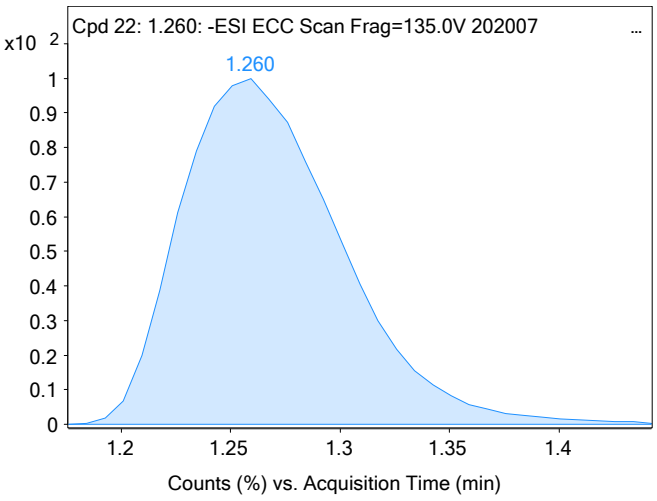
MS Zoomed Spectrum



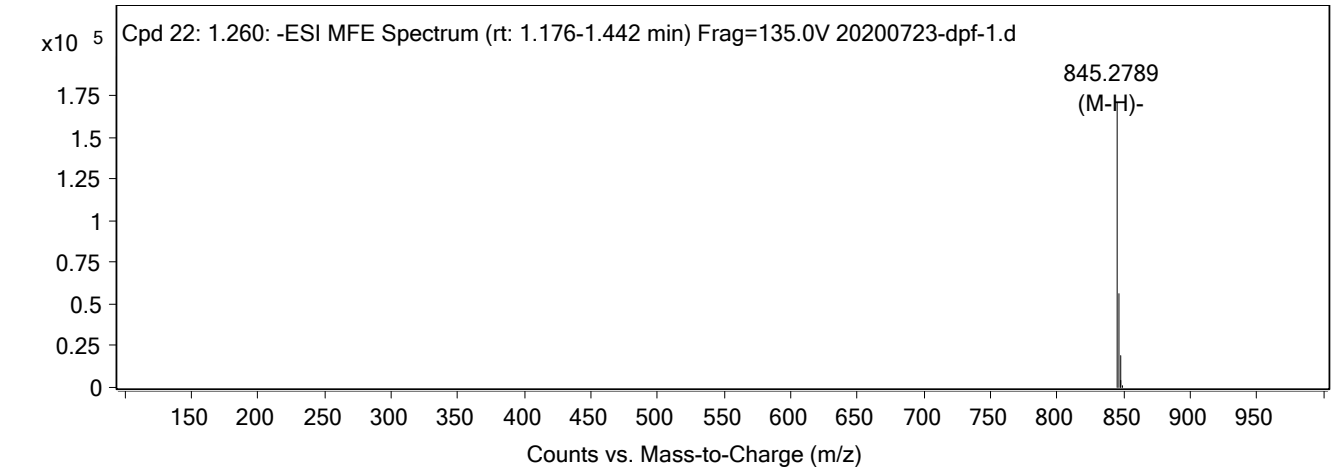
Compound Label	m/z	RT	Algorithm	Mass
Cpd 22: 1.260	845.2789	1.26	Find by Molecular Feature	846.2861

Compound Chromatograms

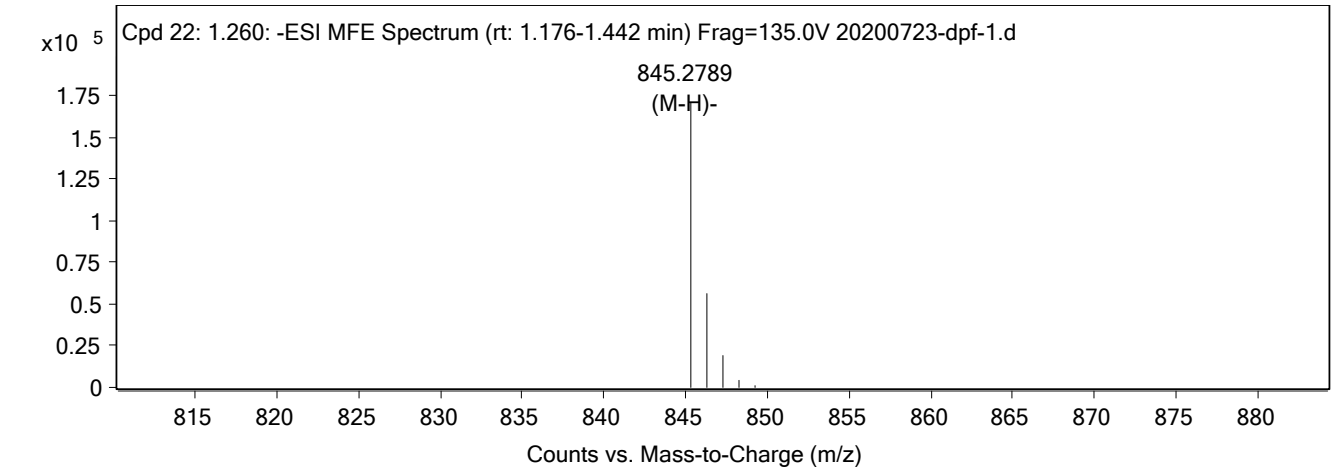




MFE MS Spectrum



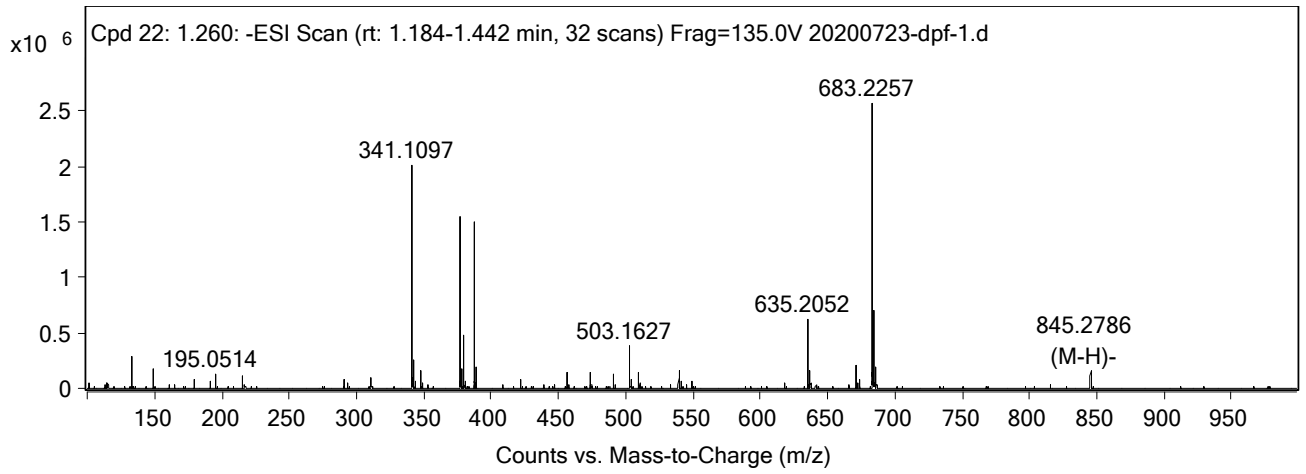
MFE MS Zoomed Spectrum



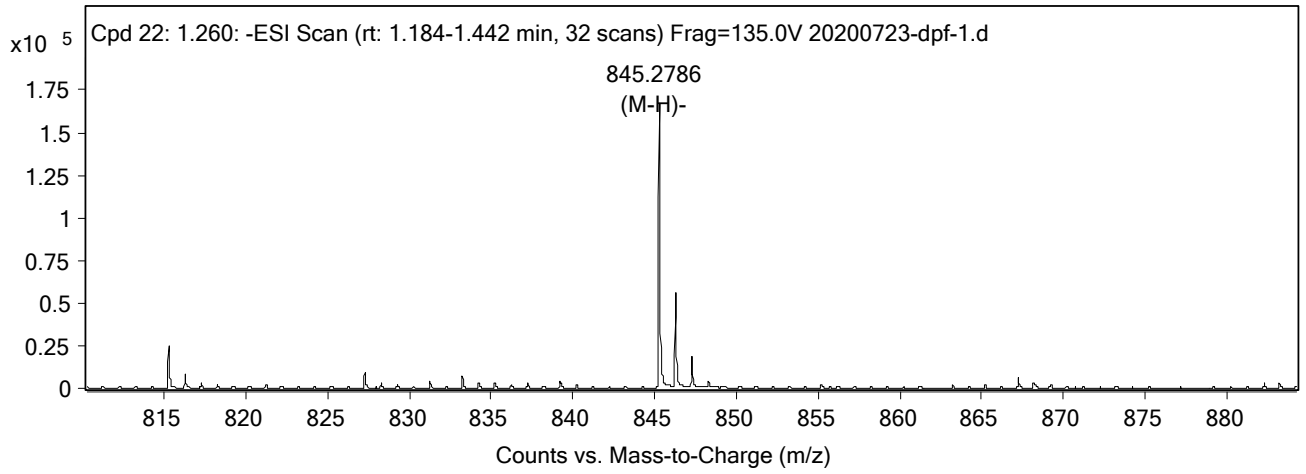
MS Spectrum Peak List

m/z	z	Abund	Ion
845.2789	-1	171371.09	(M-H)-
846.2817	-1	56796.21	(M-H)-
847.2838	-1	18795.05	(M-H)-
848.2861	-1	4115.38	(M-H)-
849.2869	-1	994.58	(M-H)-

MS Spectrum

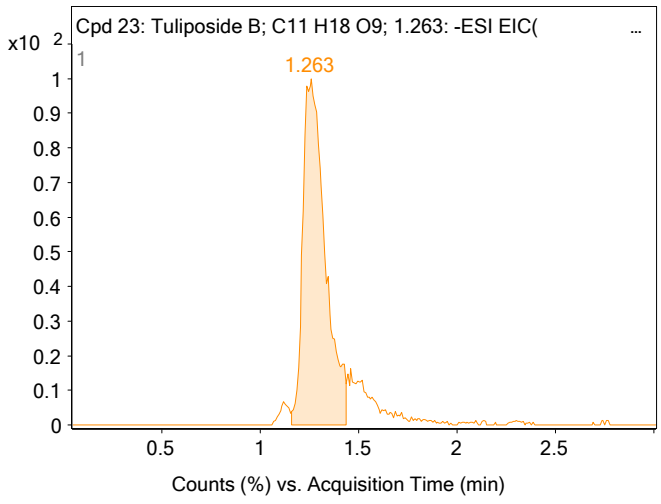


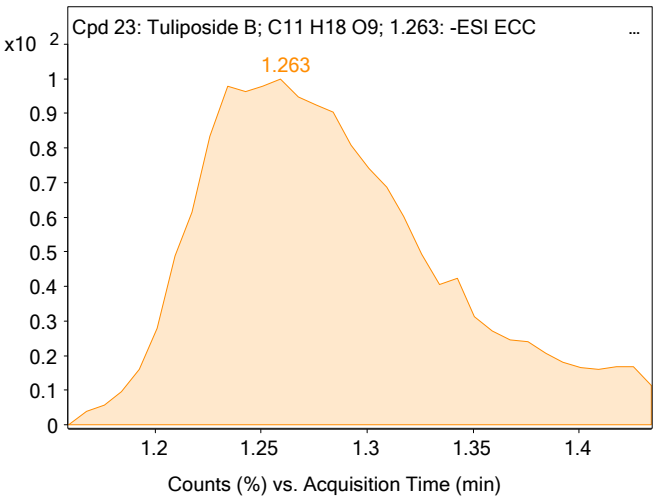
MS Zoomed Spectrum



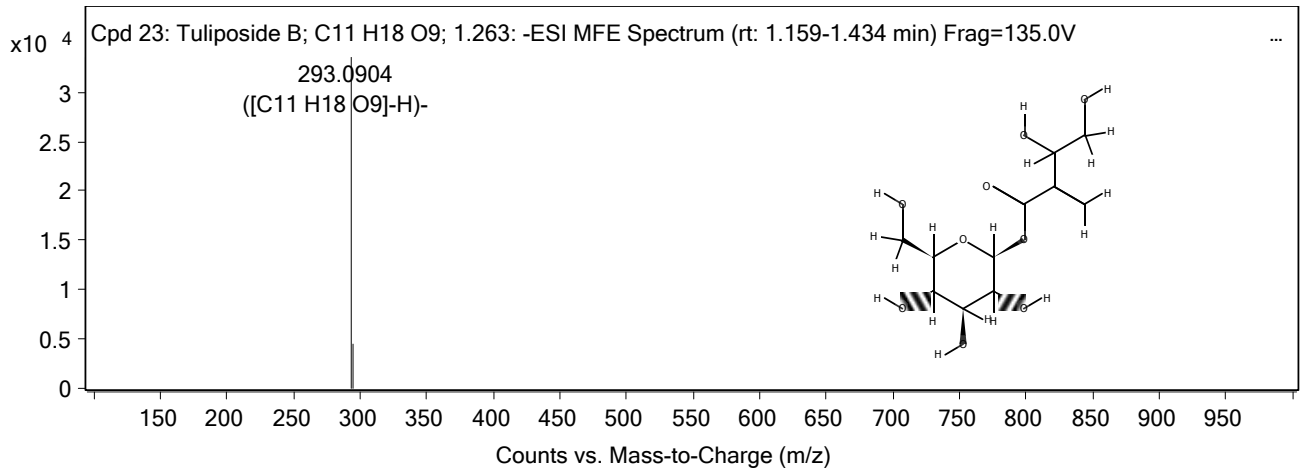
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 23: Tuliposide B; C11 H18 O9; 1.263	**Tuliposide B**	293.0904	1.263	Find by Molecular Feature	294.0979

Compound Chromatograms

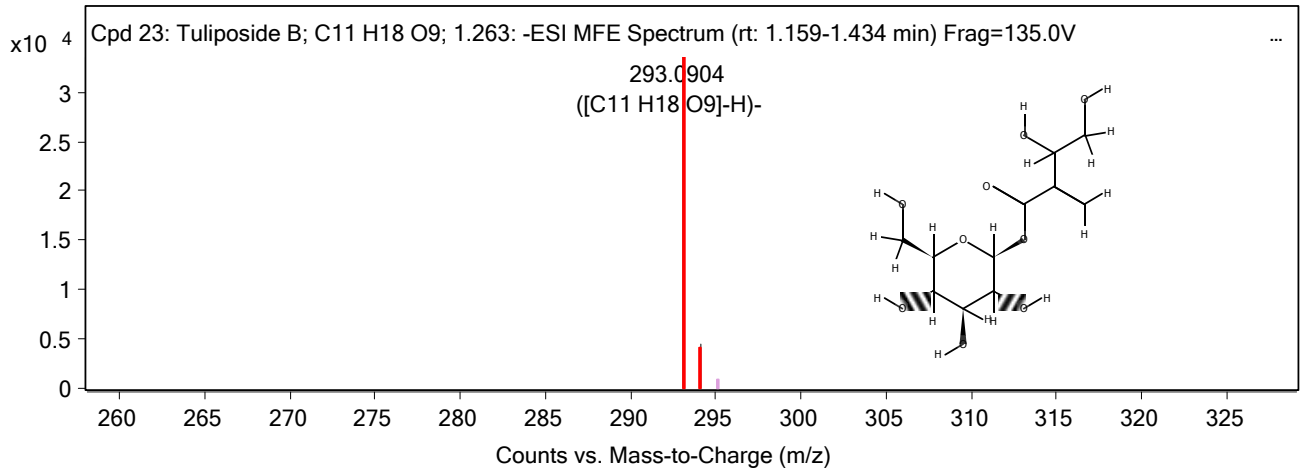




MFE MS Spectrum



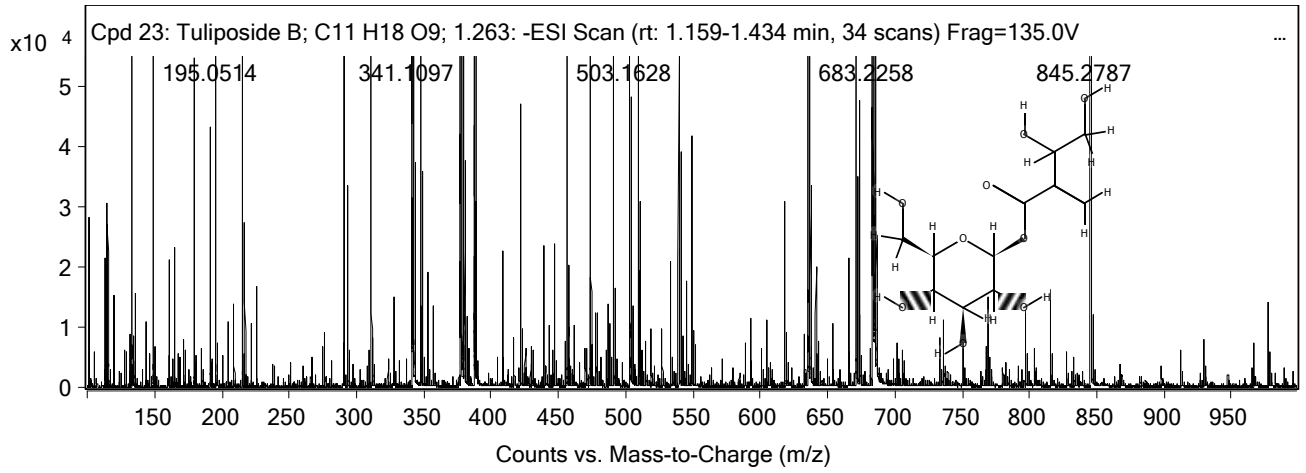
MFE MS Zoomed Spectrum



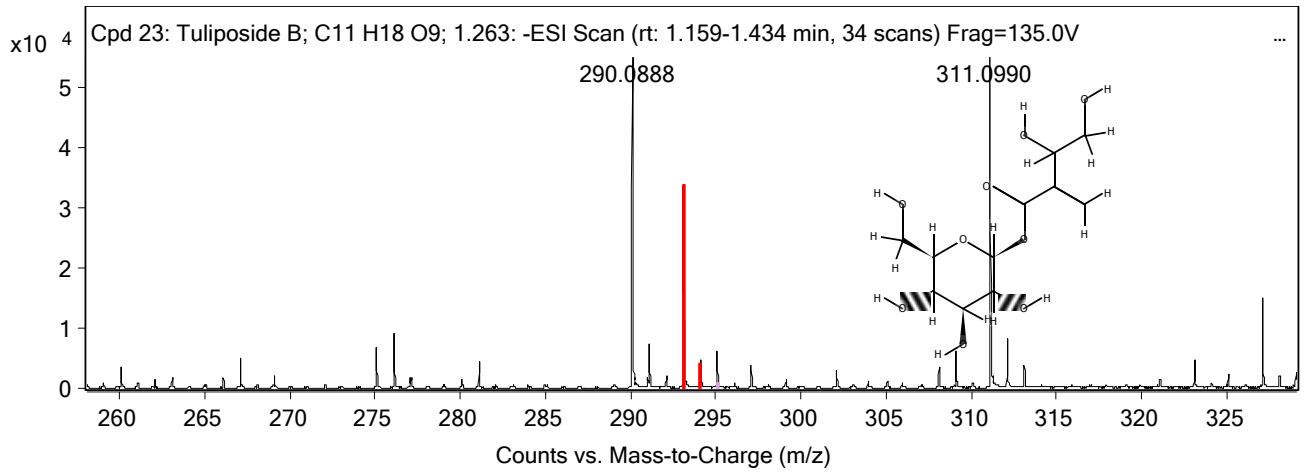
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
293.0904	-1	33534.71	C11 H18 O9	(M-H)-
294.0956	-1	4475.3	C11 H18 O9	(M-H)-

MS Spectrum



MS Zoomed Spectrum

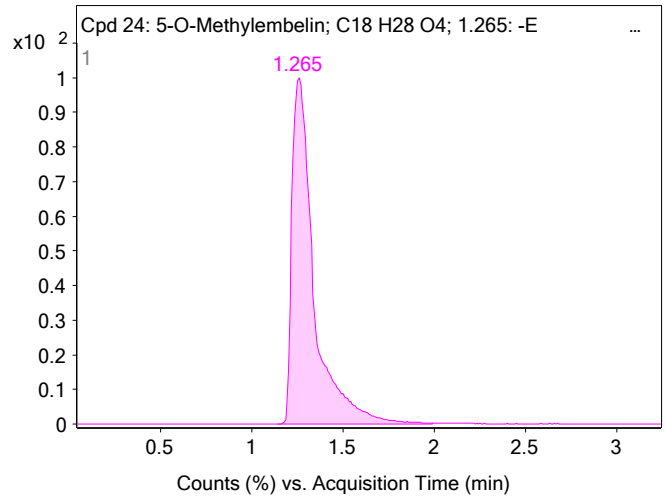


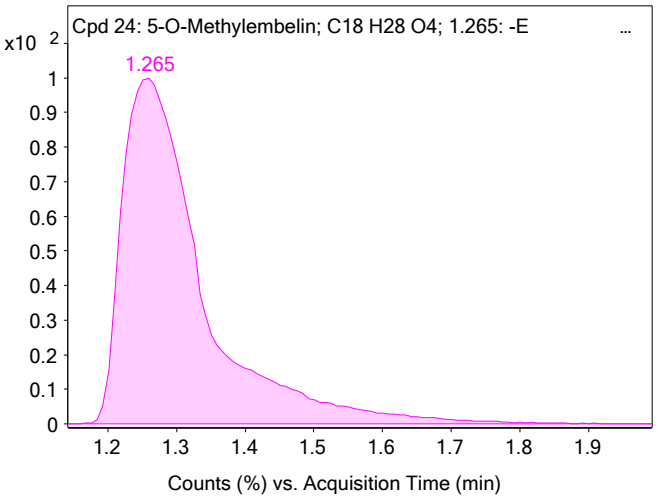
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Tuliposide B	1.263	C11 H18 O9		60.17	294.0979	-2.81	(M-H)-

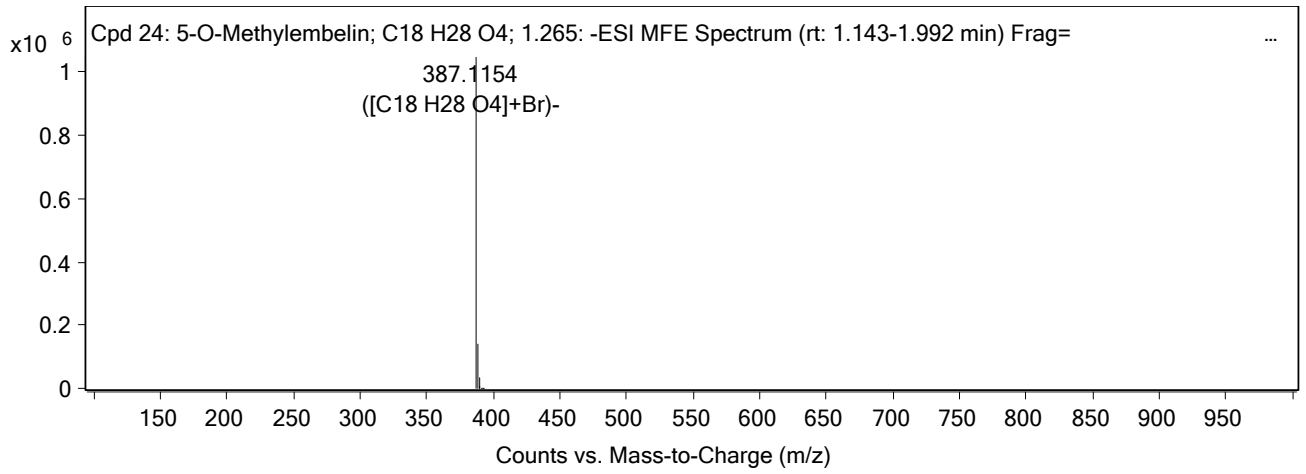
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 24: 5-O-Methylembelin; C18 H28 O4; 1.265	**5-O-Methylembelin**	387.1154	1.265	Find by Molecular Feature	308.1967

Compound Chromatograms

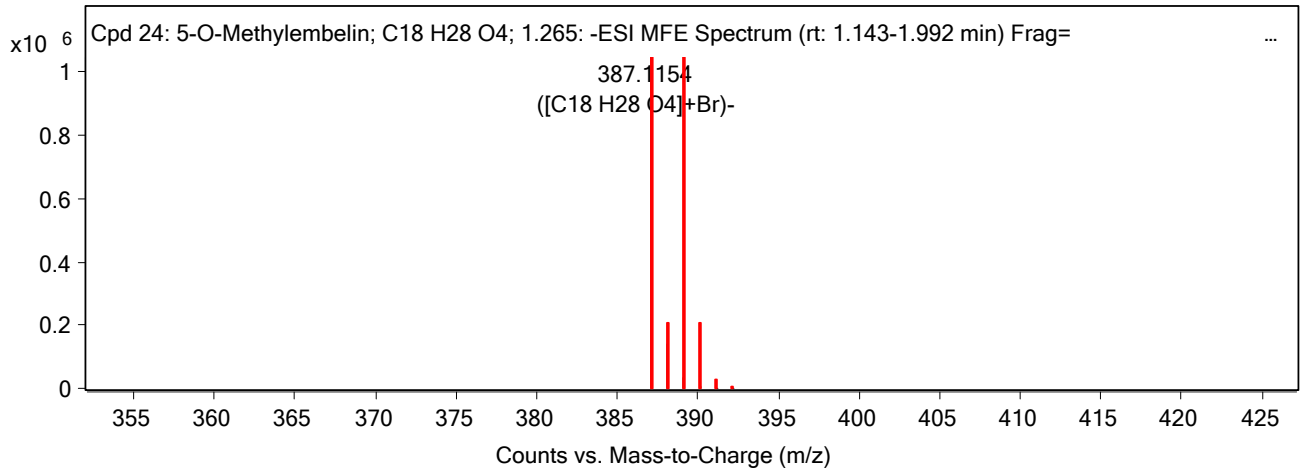




MFE MS Spectrum



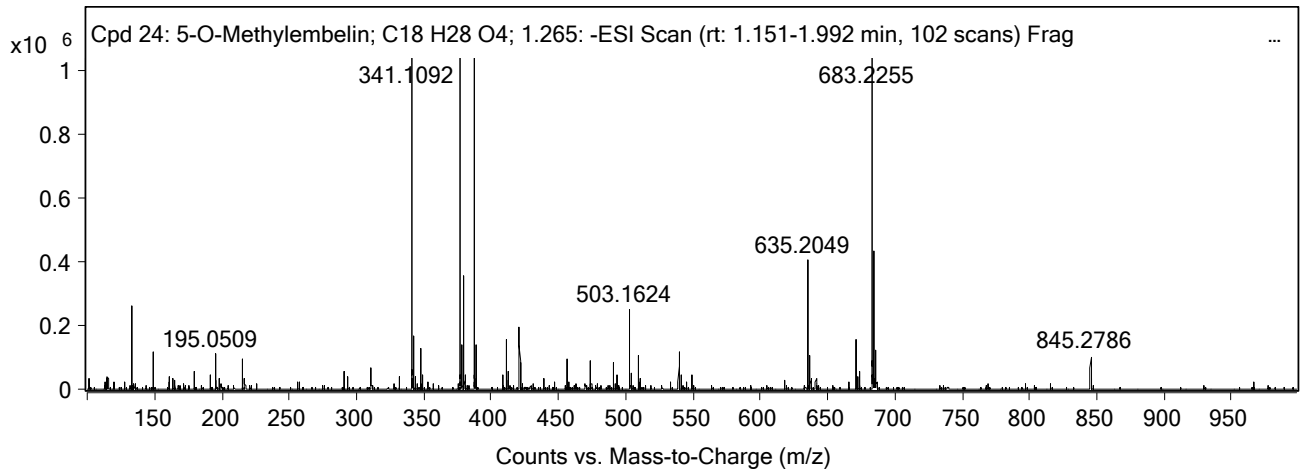
MFE MS Zoomed Spectrum



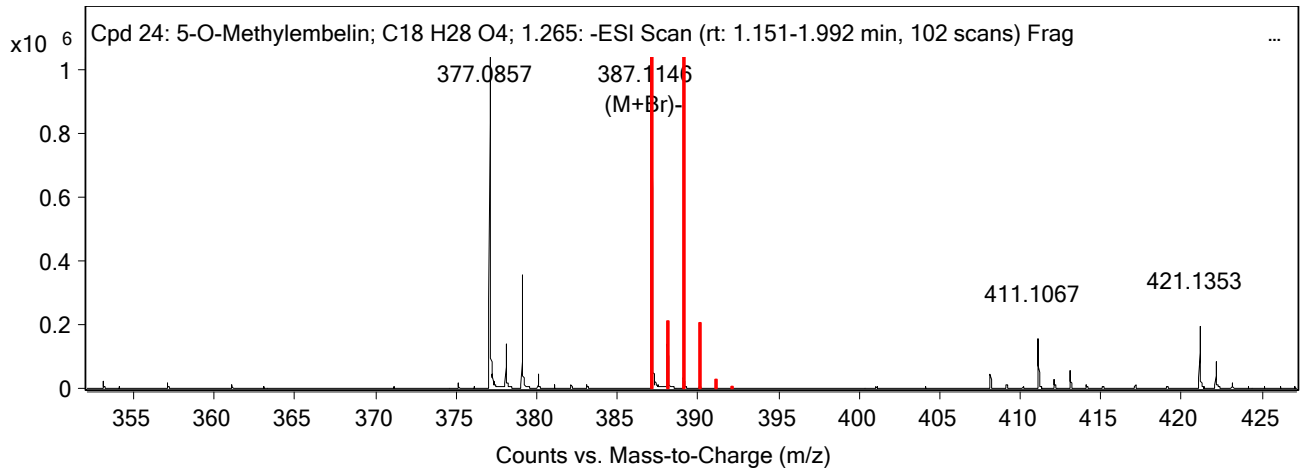
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
387.1154	-1	1047478.81	C18 H28 O4	(M+Br)-
388.119	-1	139595.56	C18 H28 O4	(M+Br)-
389.1208	-1	33803.17	C18 H28 O4	(M+Br)-
390.1232	-1	3864.83	C18 H28 O4	(M+Br)-
391.1254	-1	754.53	C18 H28 O4	(M+Br)-
392.1403	-1	34.09	C18 H28 O4	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

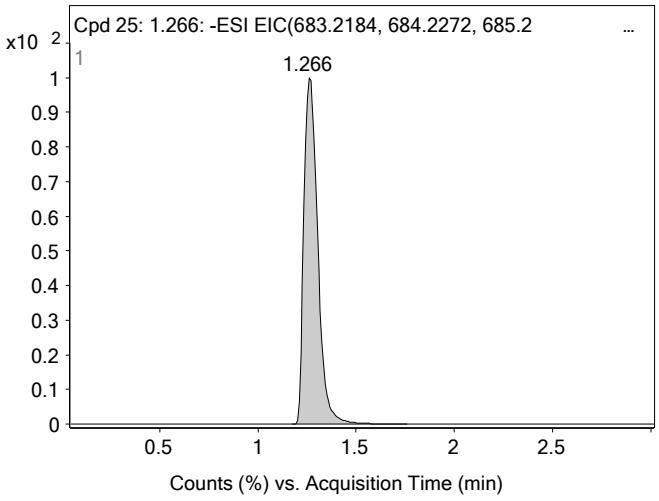


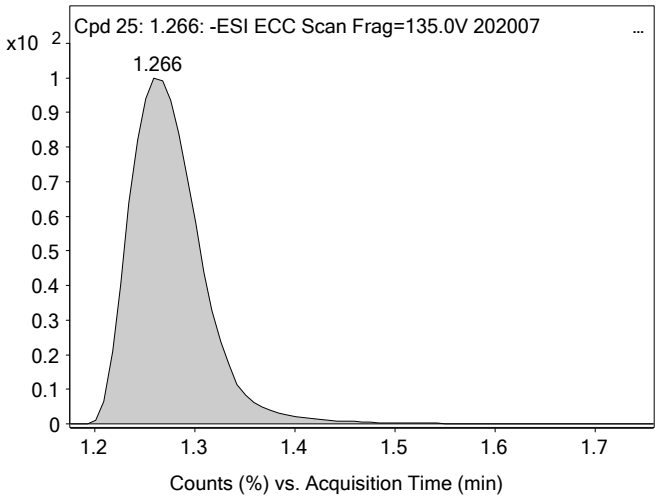
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	5-O-Methylembelin	1.265	C18 H28 O4		56.75	308.1967	2.03	(M+Br)-

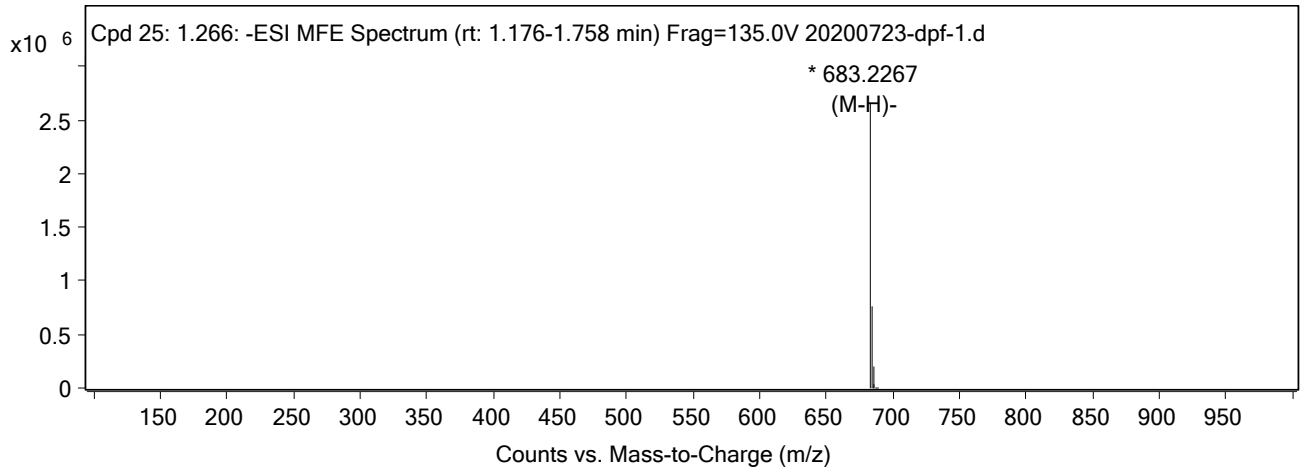
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 25: 1.266	683.2267	1.266	Find by Molecular Feature	684.234

Compound Chromatograms

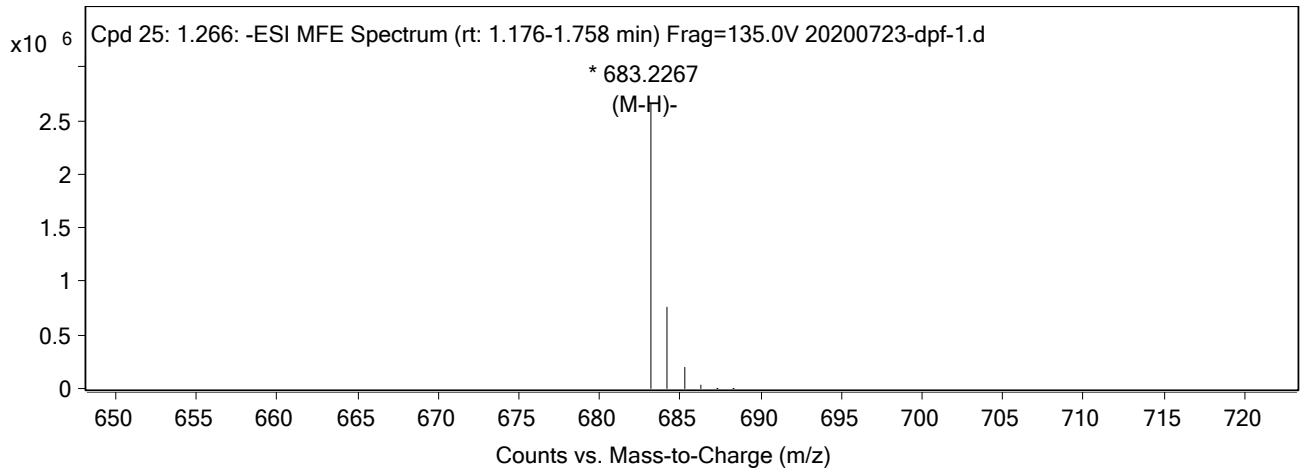




MFE MS Spectrum



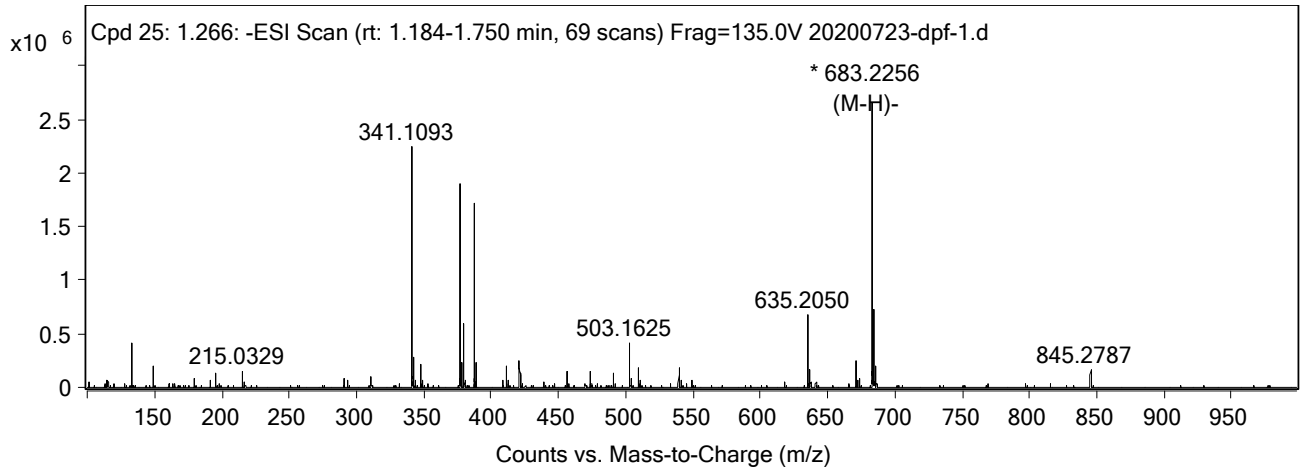
MFE MS Zoomed Spectrum



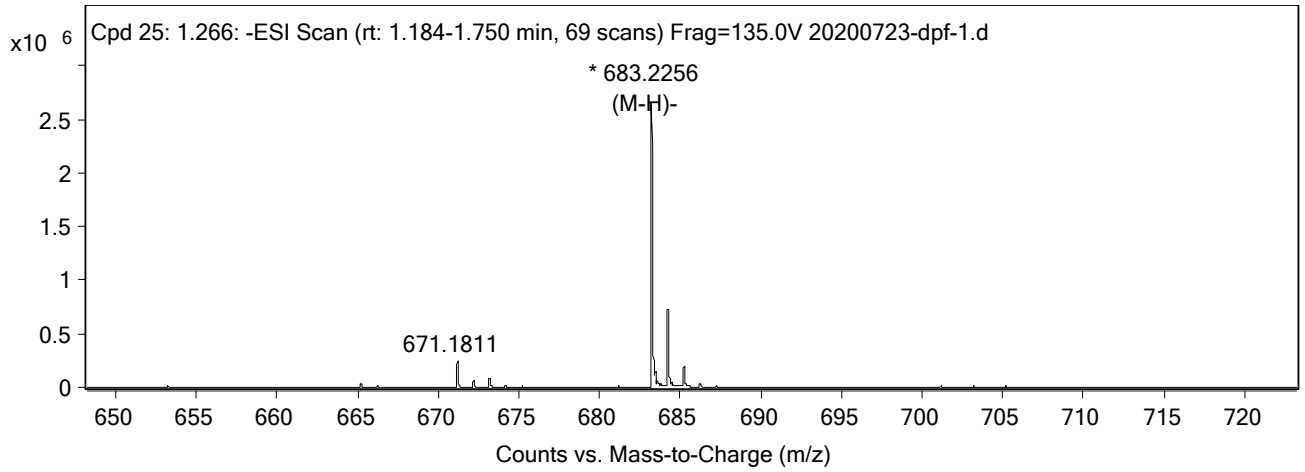
MS Spectrum Peak List

m/z	z	Abund	Ion
683.2267	-1	2660398.25	(M-H)-
684.2291	-1	752209.26	(M-H)-
685.2317	-1	201043.42	(M-H)-
686.2338	-1	34770.5	(M-H)-
687.2354	-1	6116.78	(M-H)-
688.2382	-1	950.24	(M-H)-

MS Spectrum



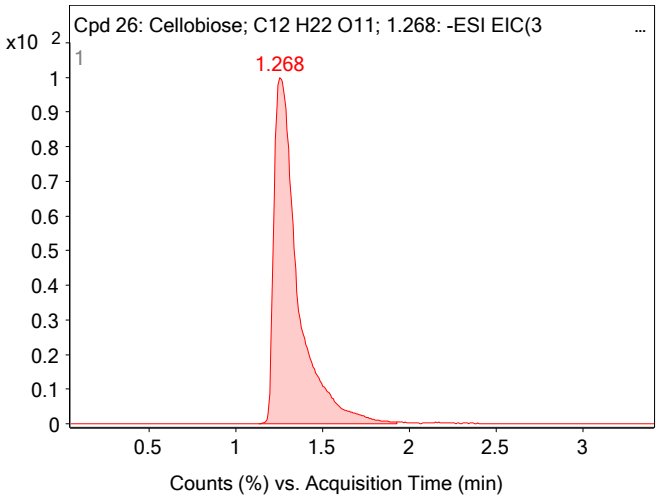
MS Zoomed Spectrum

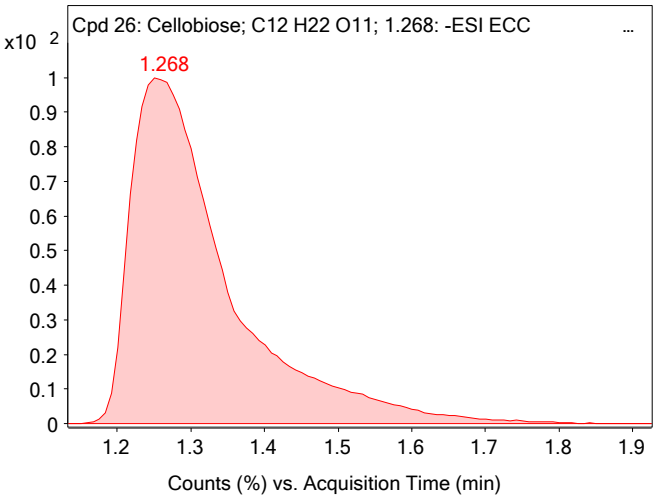


Qualitative Compound Identification Report

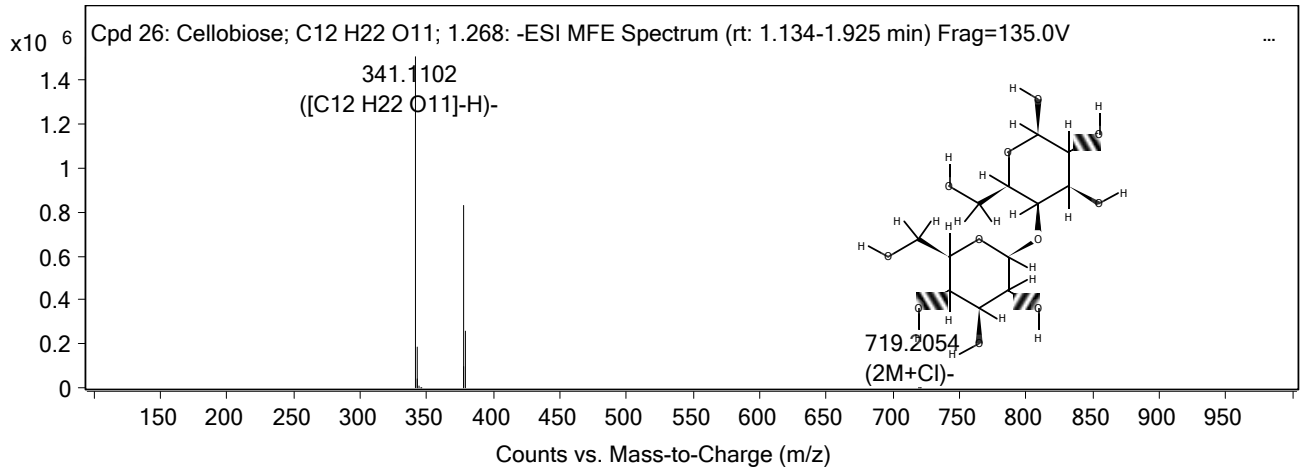
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 26: Cellobiose; C12 H22 O11; 1.268	**Cellobiose**	341.1102	1.268	Find by Molecular Feature	342.1175

Compound Chromatograms

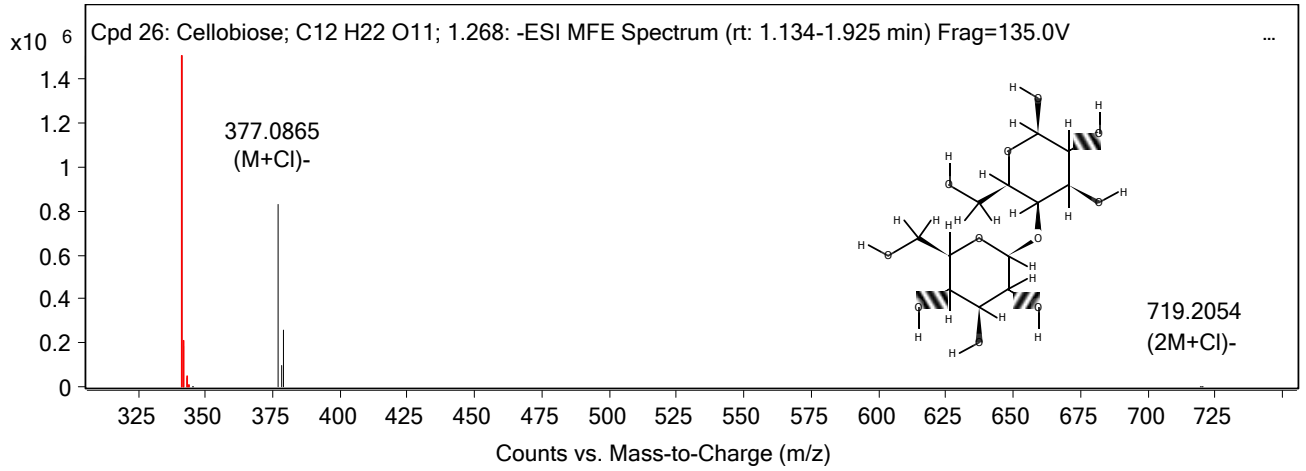




MFE MS Spectrum



MFE MS Zoomed Spectrum

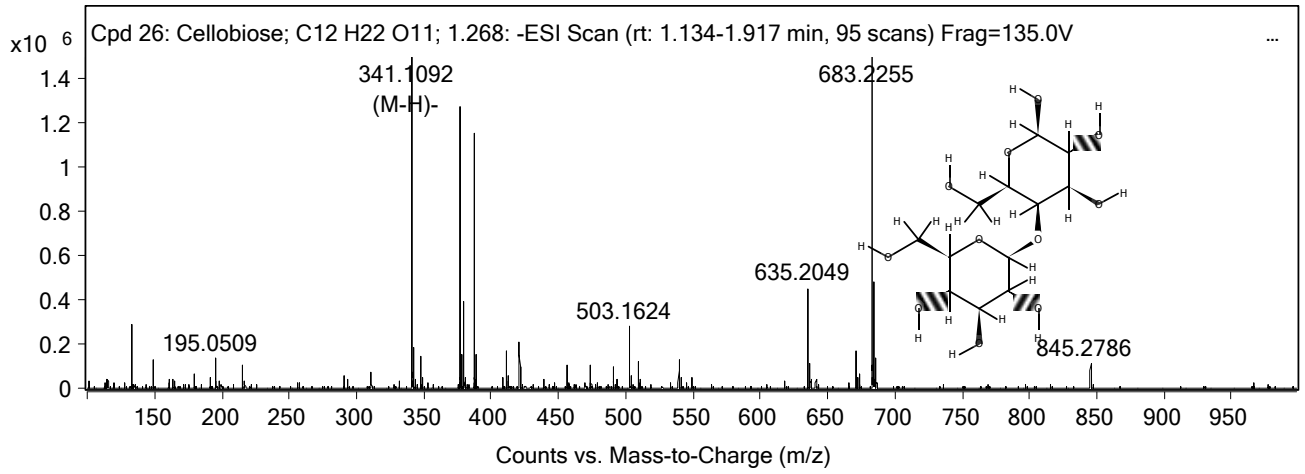


MS Spectrum Peak List

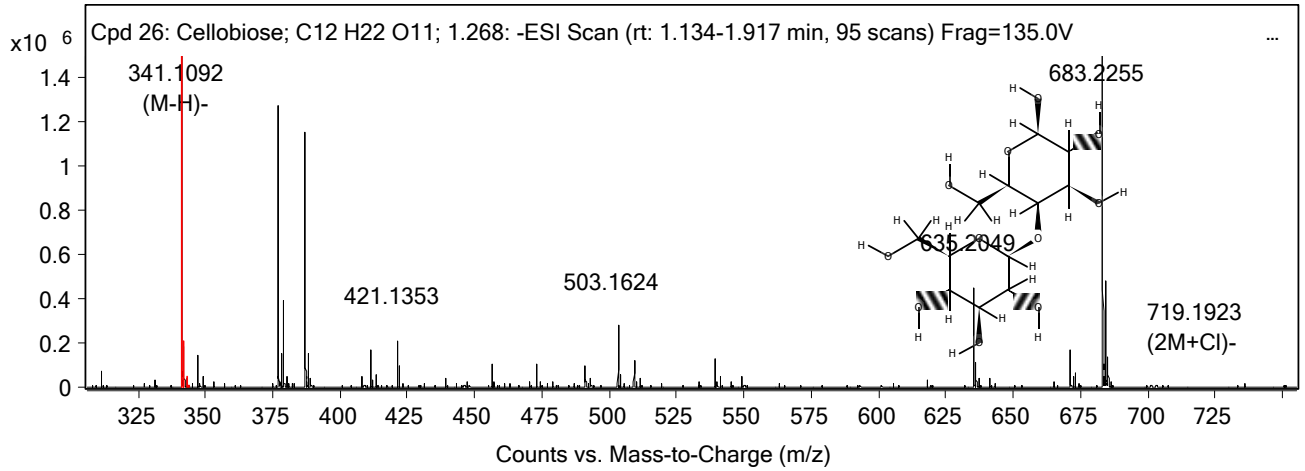
m/z	z	Abund	Formula	Ion
341.1102	-1	1506070.13	C12 H22 O11	(M-H)-
342.1138	-1	189223.94	C12 H22 O11	(M-H)-
343.1157	-1	43081.8	C12 H22 O11	(M-H)-

344.1186	-1	5171.35	C12 H22 O11	(M-H)-
345.1175	-1	751.12	C12 H22 O11	(M-H)-
377.0865	-1	827632.44		(M+Cl)-
378.0902	-1	99331.62		(M+Cl)-
379.0848	-1	256775.89		(M+Cl)-
719.2054	-1	912.44		(2M+Cl)-
720.2076	-1	415.37		(2M+Cl)-

MS Spectrum



MS Zoomed Spectrum

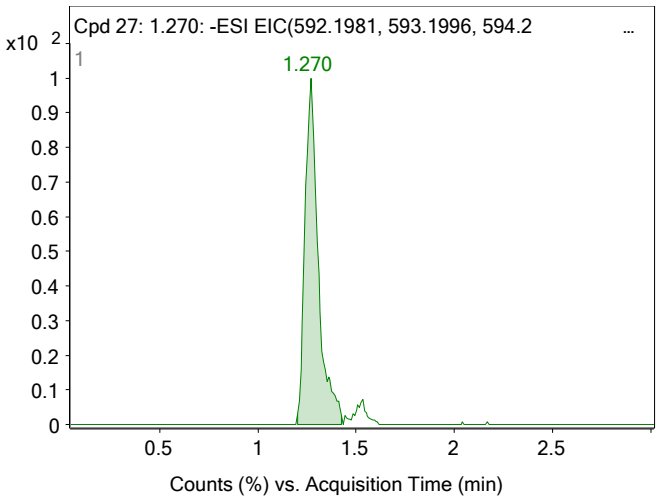


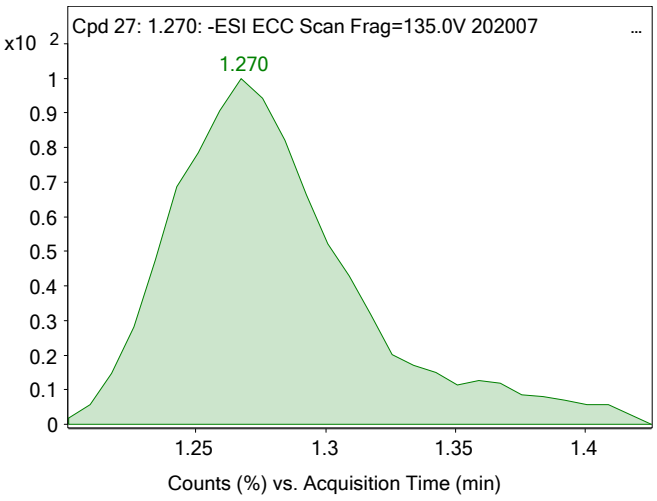
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Cellobiose	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Gentiobiose	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Maltose-b	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Lactose	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Maltose	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Timobiose	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Turanose	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Trehalose (beta:beta)	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Isomaltose	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-
	Sophorose	1.268	C12 H22 O11		94.73	342.1175	-1.29	(M-H)-

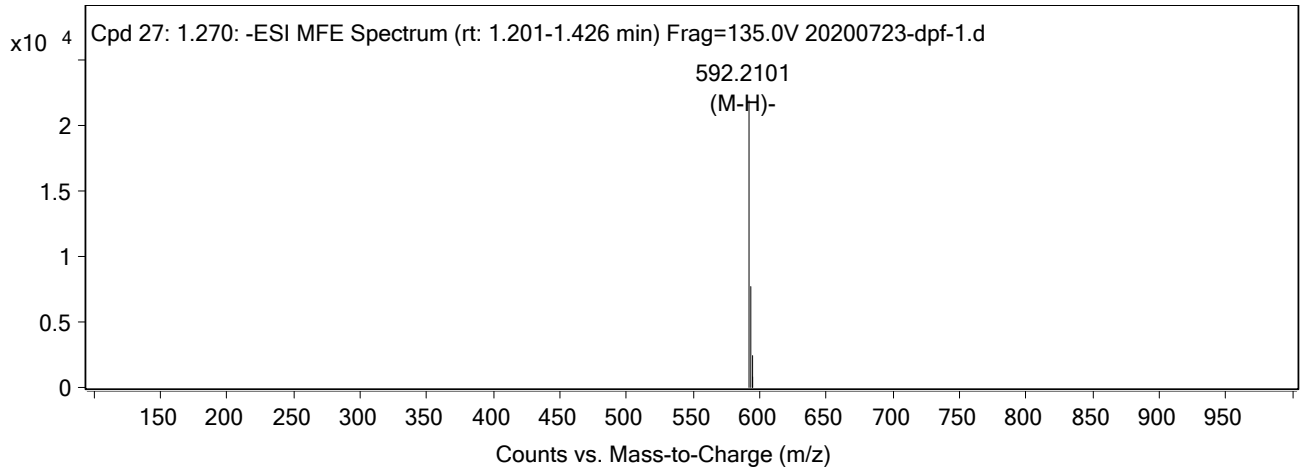
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 27: 1.270	592.2101	1.27	Find by Molecular Feature	593.2174

Compound Chromatograms

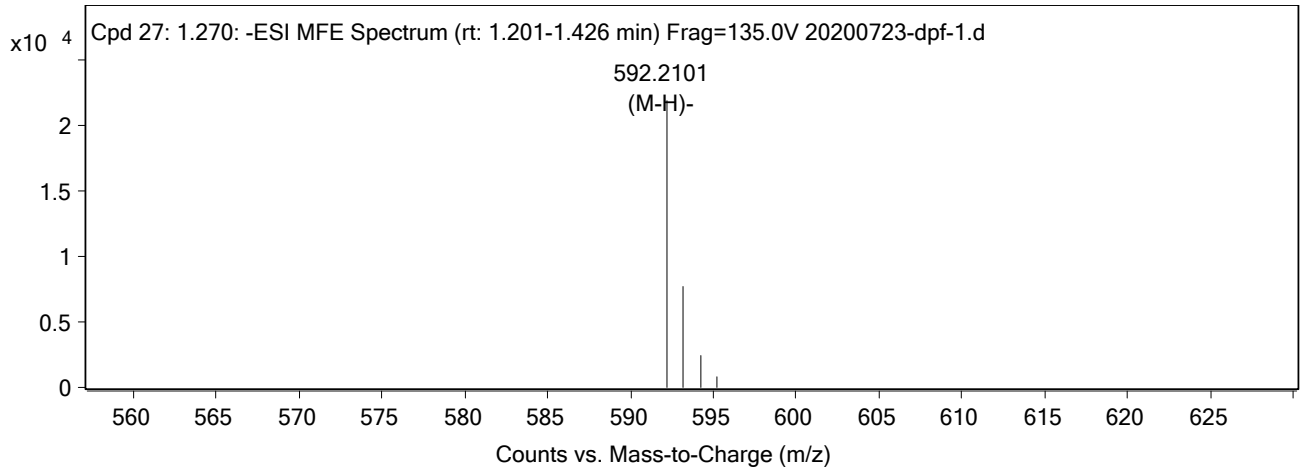




MFE MS Spectrum



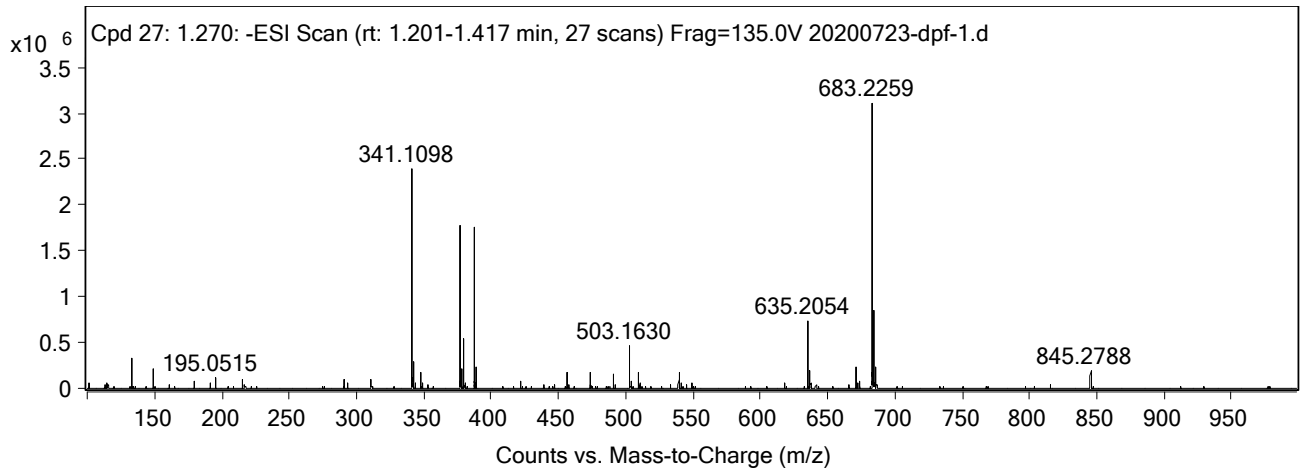
MFE MS Zoomed Spectrum



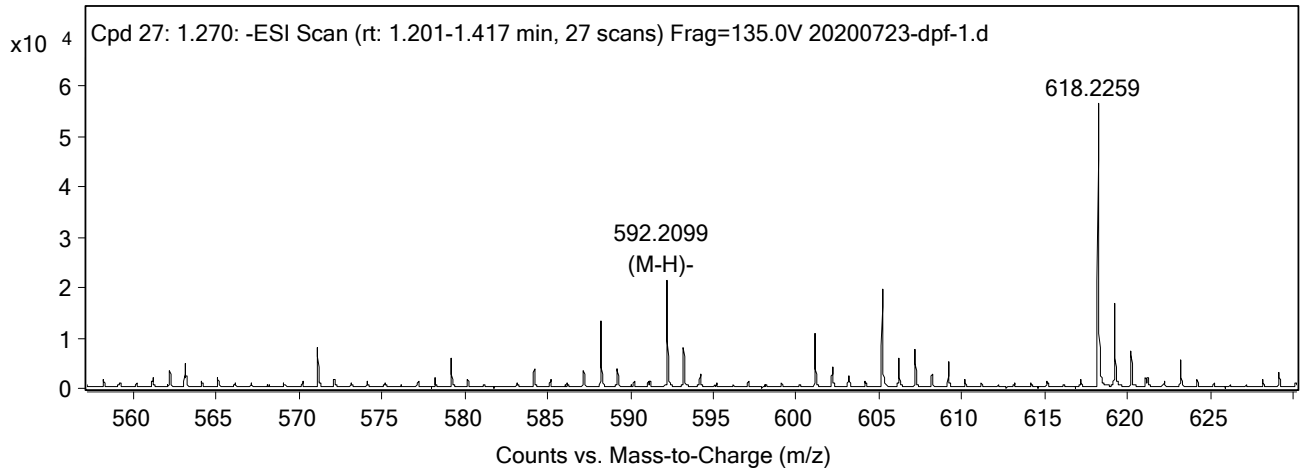
MS Spectrum Peak List

m/z	z	Abund	Ion
592.2101	-1	21904.41	(M-H)-
593.2099	-1	7677.69	(M-H)-
594.2109	-1	2474.19	(M-H)-
595.2081	-1	820.48	(M-H)-

MS Spectrum

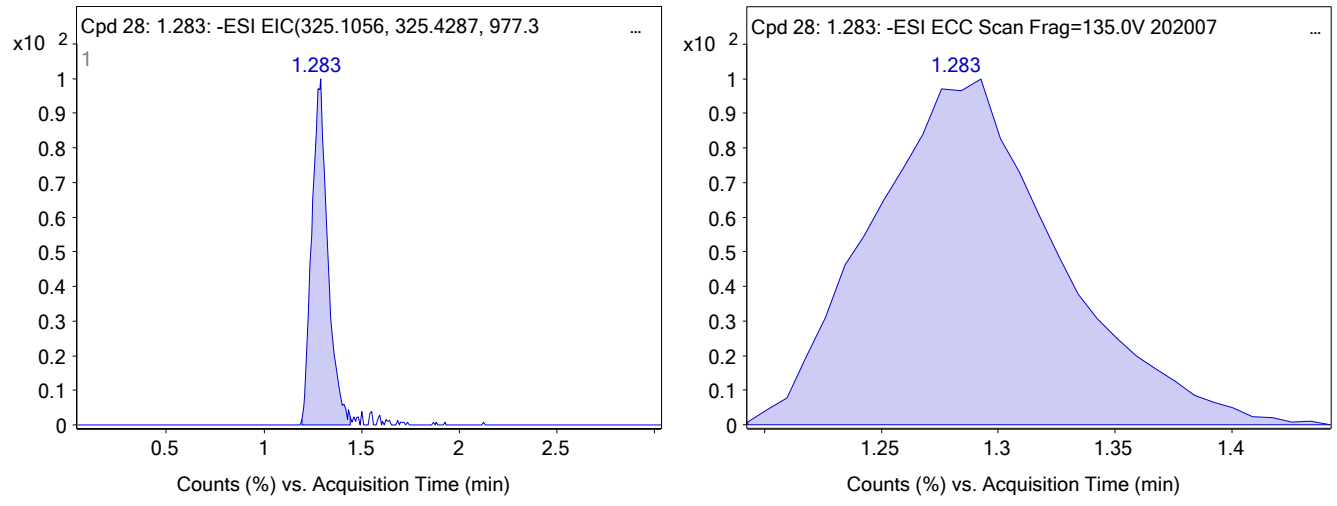


MS Zoomed Spectrum

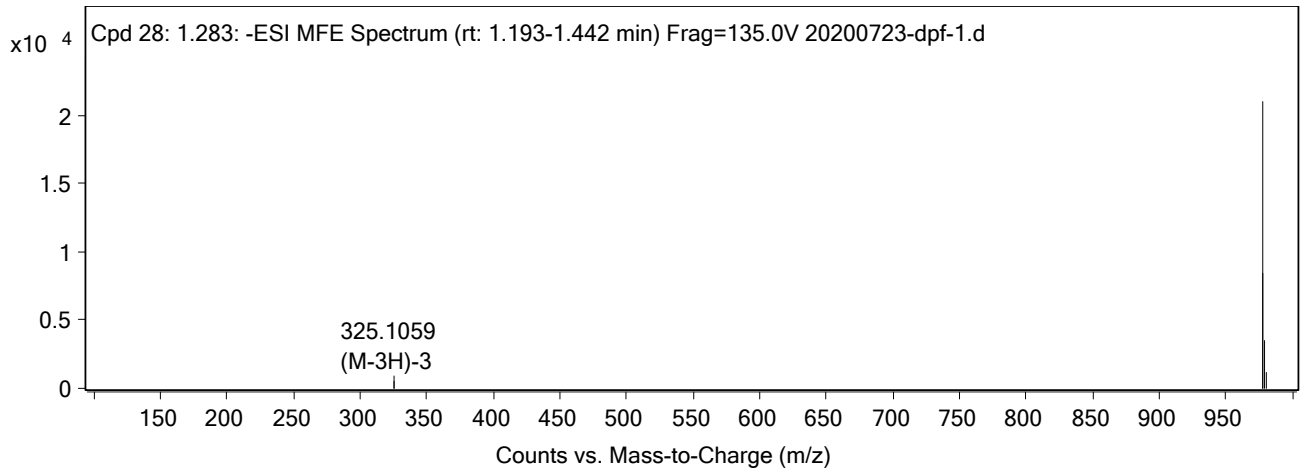


Compound Label	m/z	RT	Algorithm	Mass
Cpd 28: 1.283	977.3197	1.283	Find by Molecular Feature	978.3271

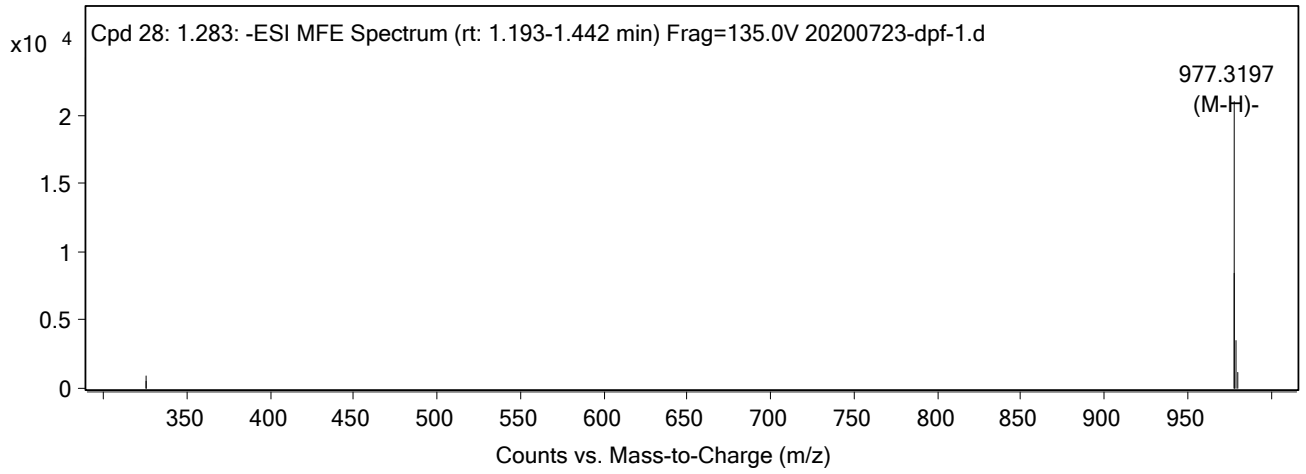
Compound Chromatograms



MFE MS Spectrum



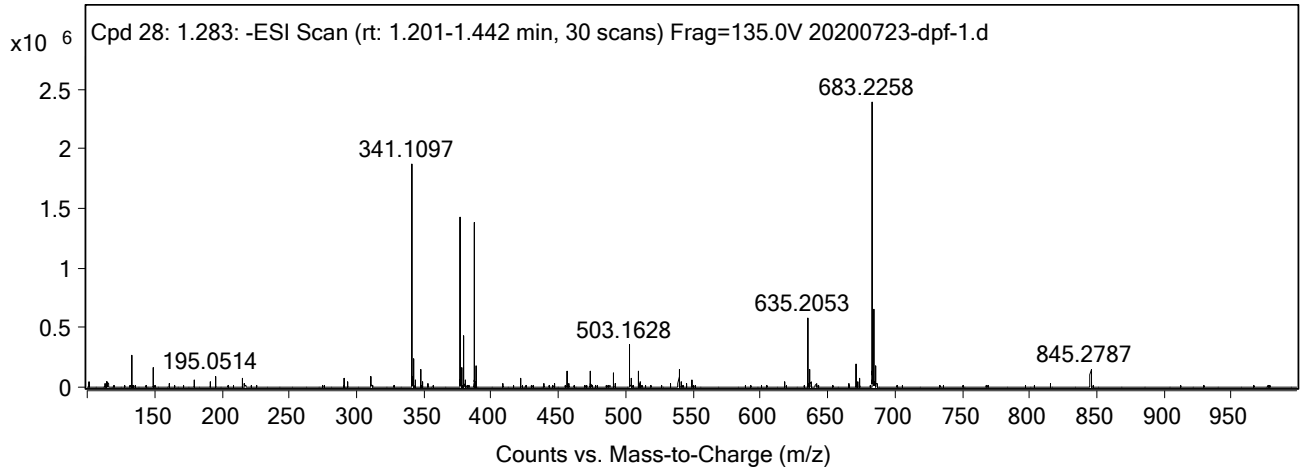
MFE MS Zoomed Spectrum



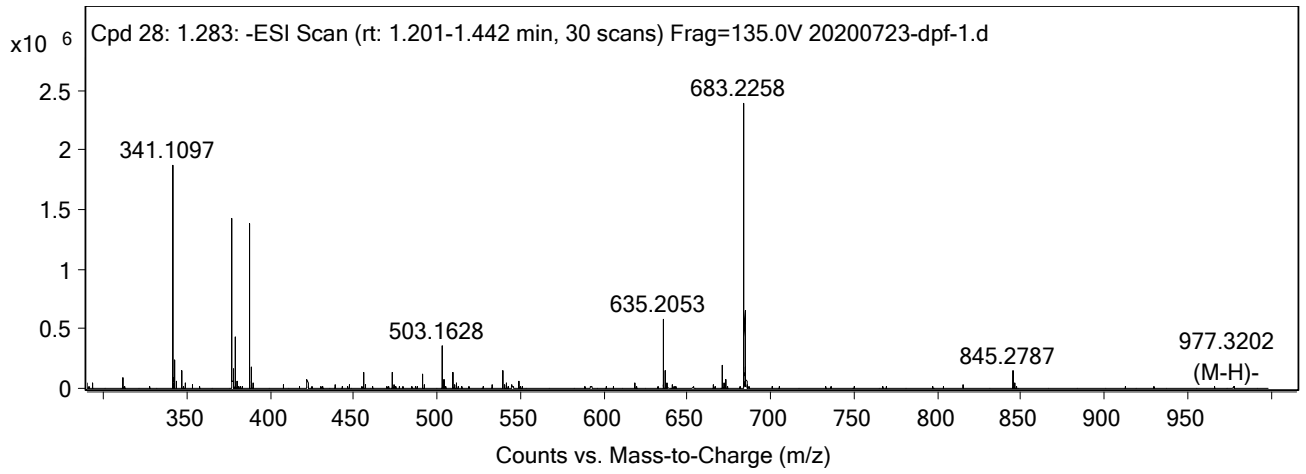
MS Spectrum Peak List

m/z	z	Abund	Ion
325.1059	-3	875.78	(M-3H)-3
325.4333	-3	473.07	(M-3H)-3
977.3197	-1	20975.89	(M-H)-
978.3233	-1	8467.81	(M-H)-
979.3267	-1	3456.42	(M-H)-
980.3285	-1	1177.07	(M-H)-

MS Spectrum

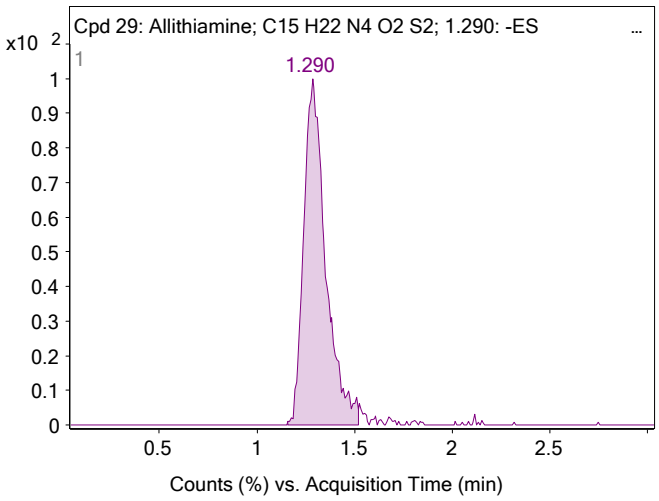


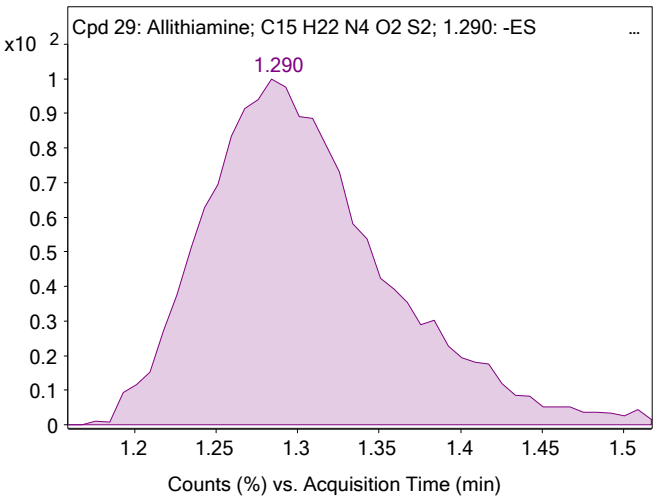
MS Zoomed Spectrum



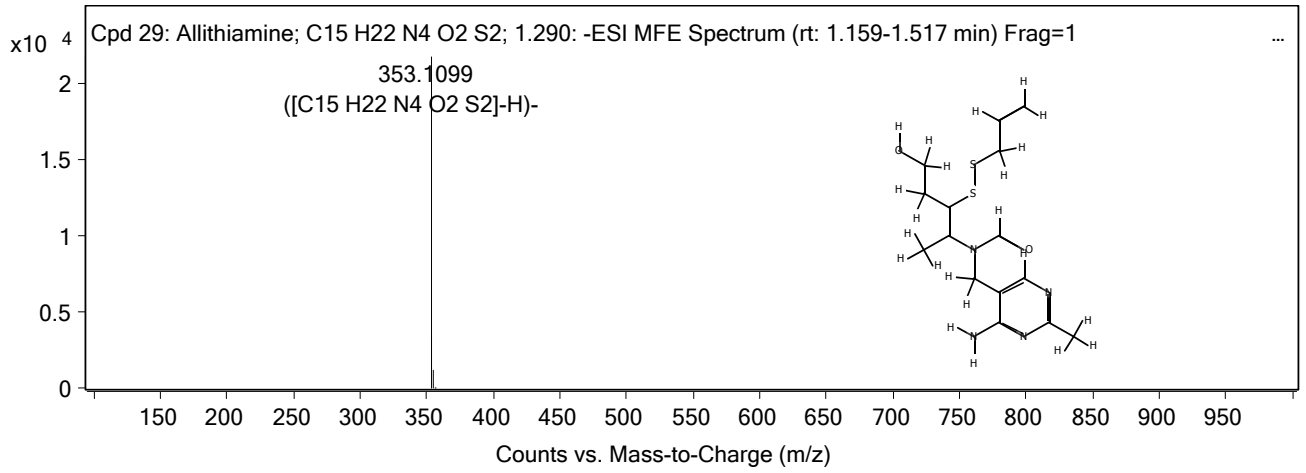
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 29: Allithiamine; C15 H22 N4 O2 S2; 1.290	**Allithiamine**	353.1099	1.29	Find by Molecular Feature	354.1177

Compound Chromatograms

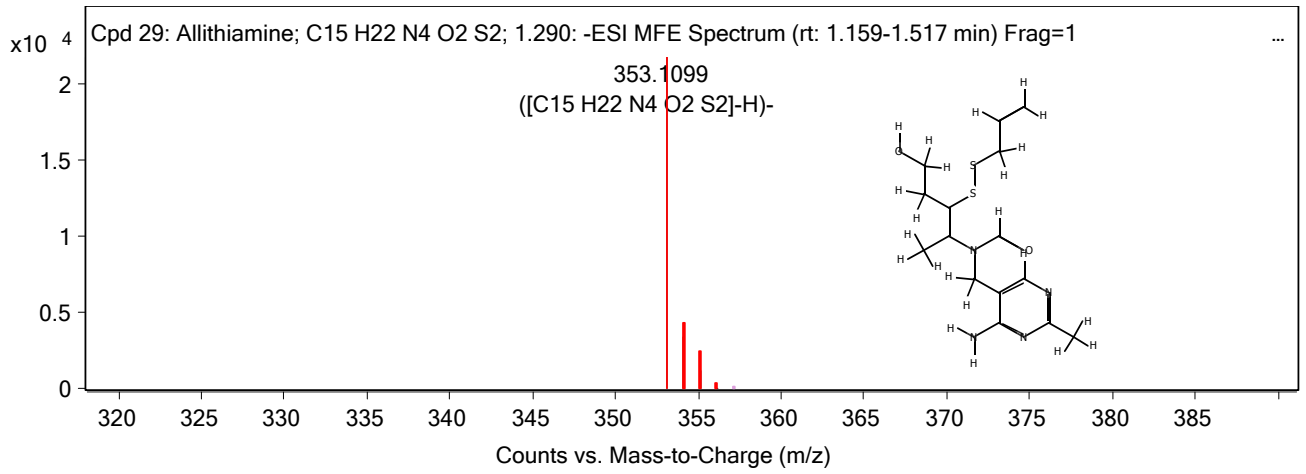




MFE MS Spectrum



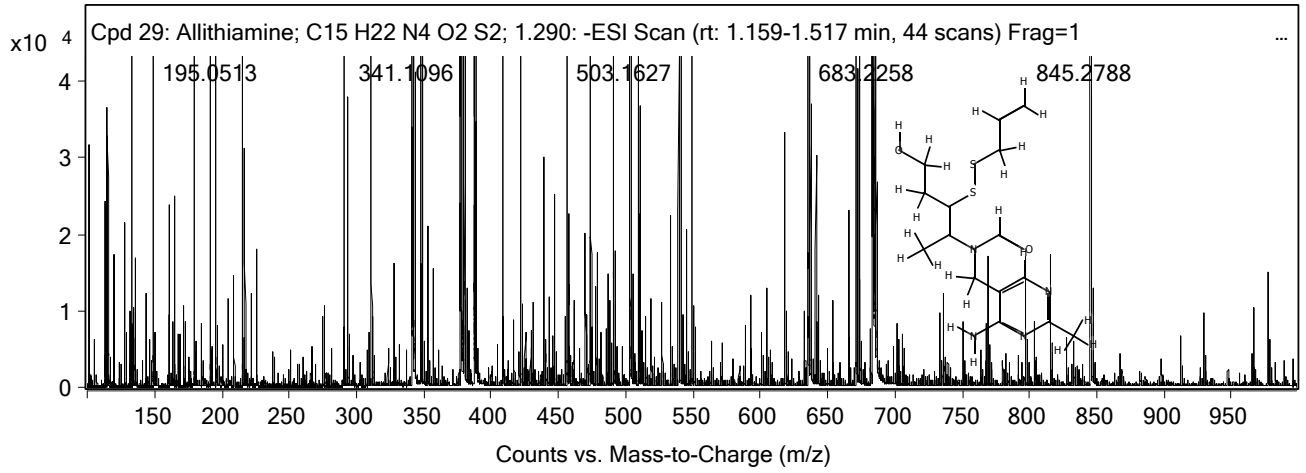
MFE MS Zoomed Spectrum



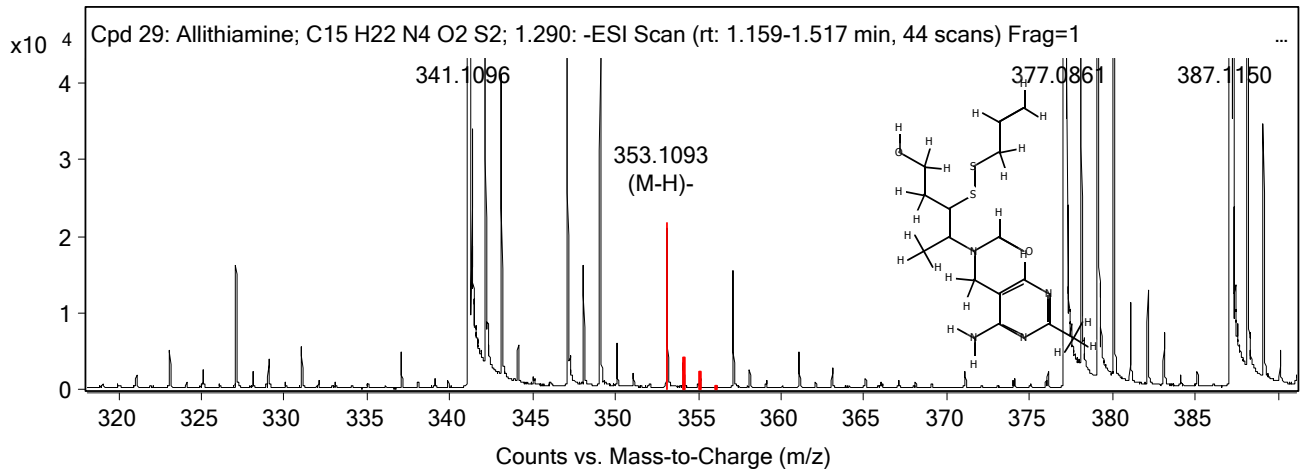
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
353.1099	-1	21686.57	C15 H22 N4 O2 S2	(M-H)-
354.1134	-1	3357.6	C15 H22 N4 O2 S2	(M-H)-
355.1155	-1	1208.98	C15 H22 N4 O2 S2	(M-H)-
356.1238	-1	61.97	C15 H22 N4 O2 S2	(M-H)-

MS Spectrum



MS Zoomed Spectrum



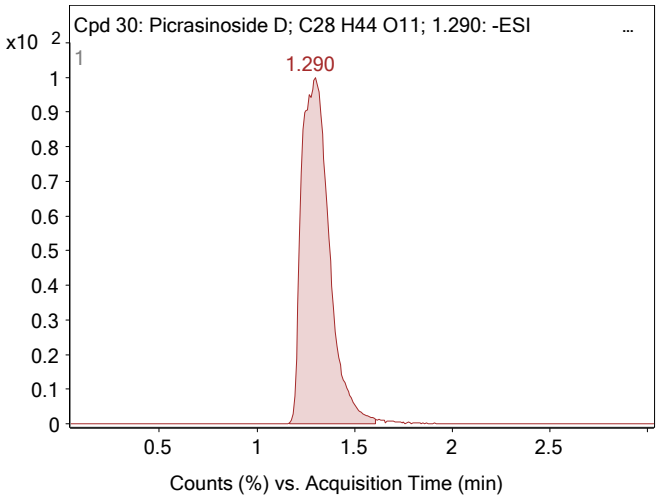
Identification Hit Table

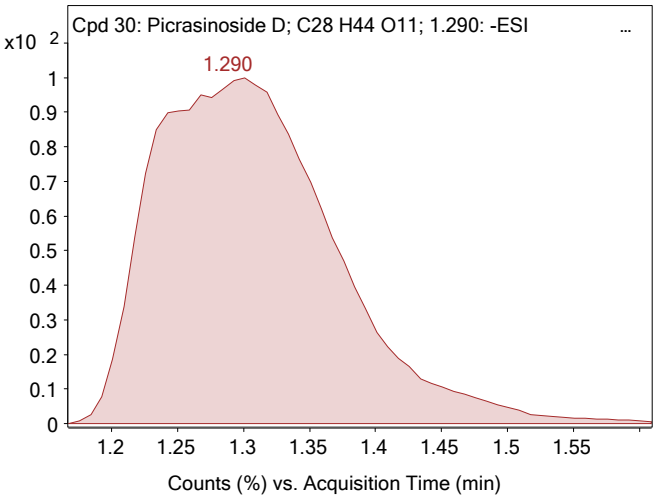
Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Allithiamine	1.29	C15 H22 N4 O2 S2		82.47	354.1177	0.73	(M-H)-

Qualitative Compound Identification Report

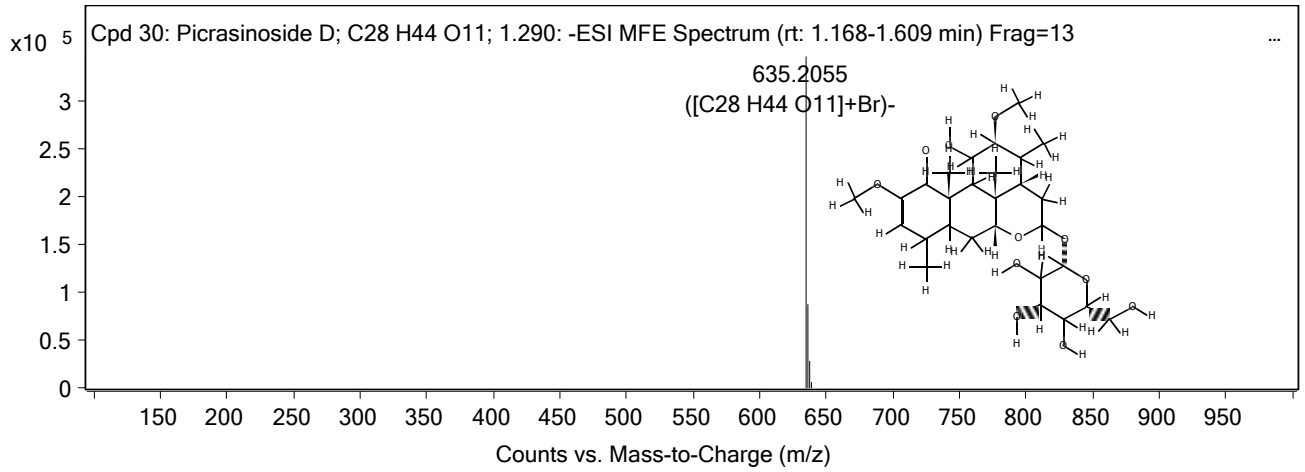
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 30: Picrasinoside D; C28 H44 O11; 1.290	**Picrasinoside D**	635.2055	1.29	Find by Molecular Feature	556.2866

Compound Chromatograms

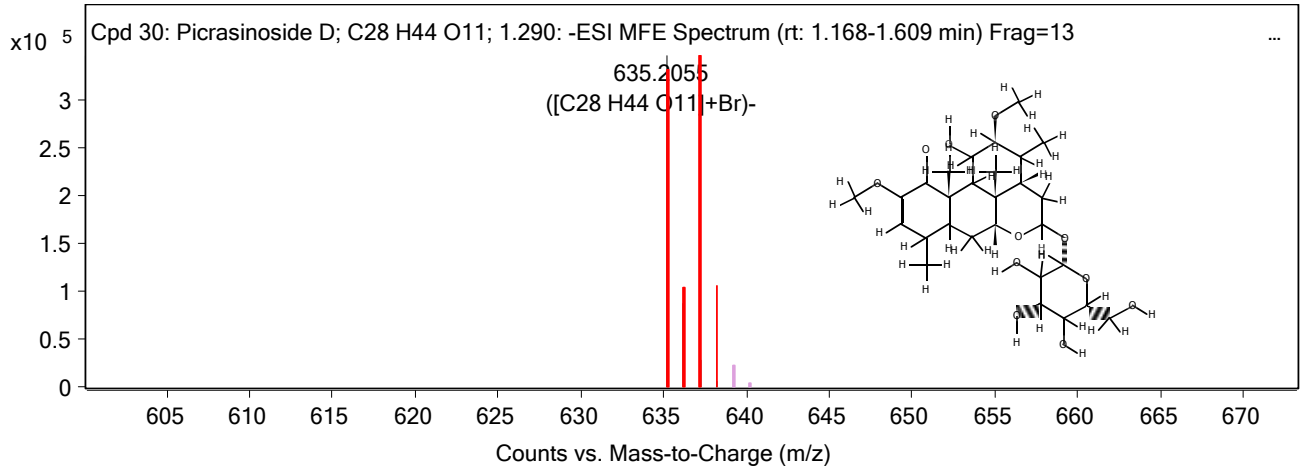




MFE MS Spectrum



MFE MS Zoomed Spectrum

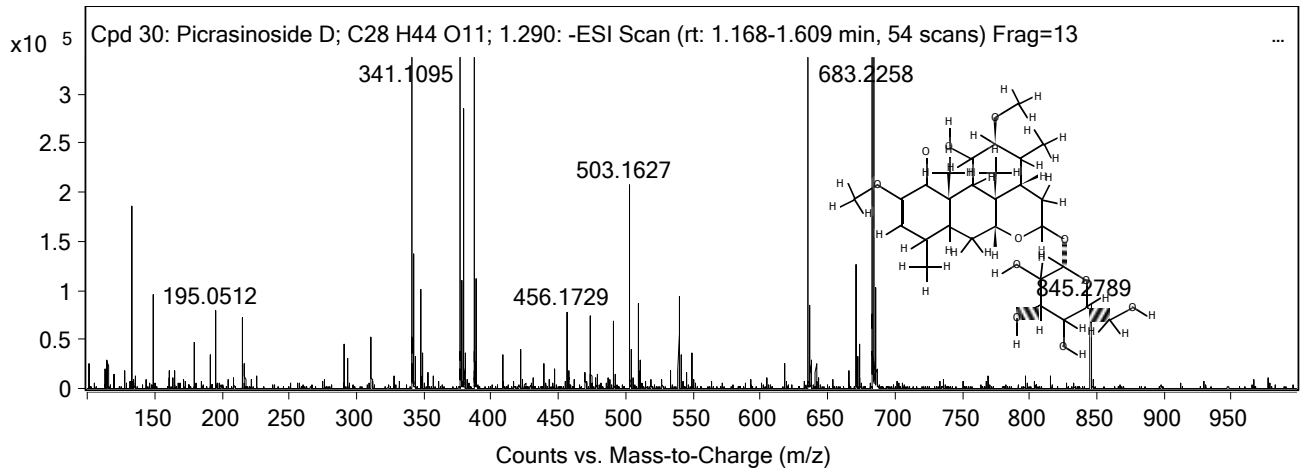


MS Spectrum Peak List

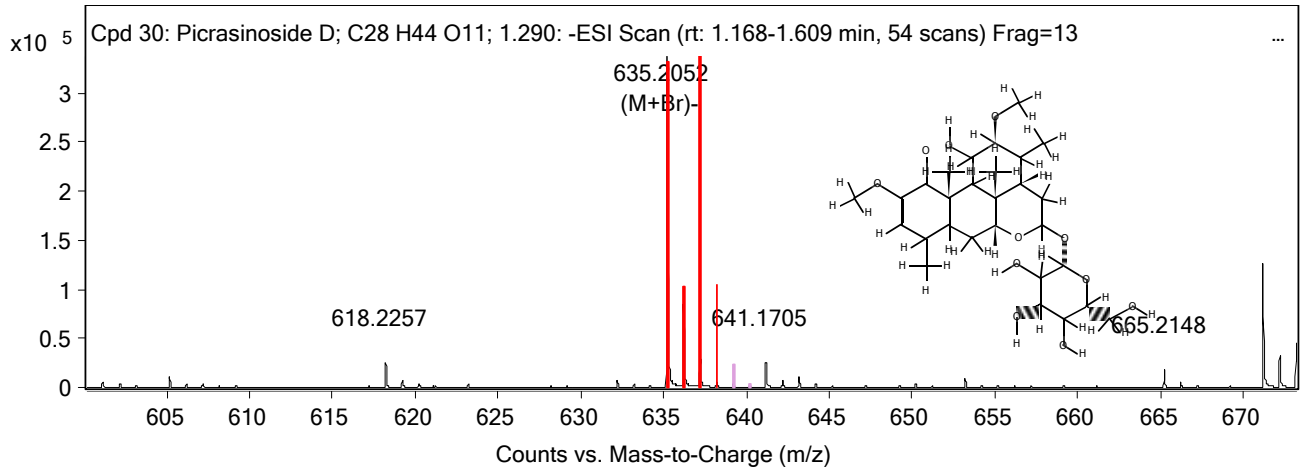
m/z	z	Abund	Formula	Ion
635.2055	-1	345583.16	C28 H44 O11	(M+Br)-
636.2084	-1	86767.72	C28 H44 O11	(M+Br)-
637.2057	-1	28255.14	C28 H44 O11	(M+Br)-

638.2067	-1	5264.22	C28 H44 O11	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

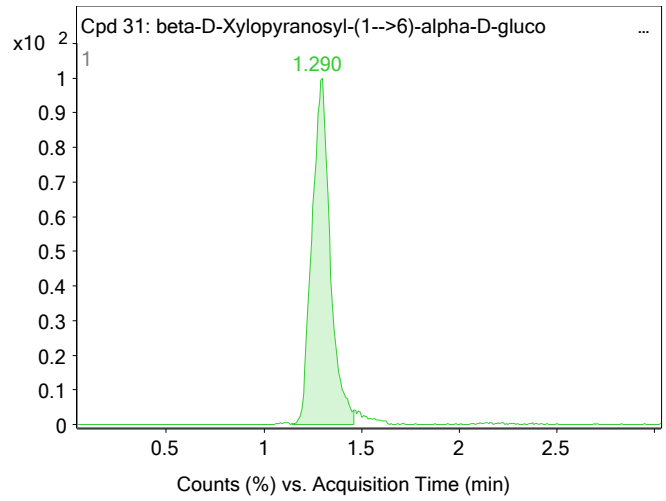


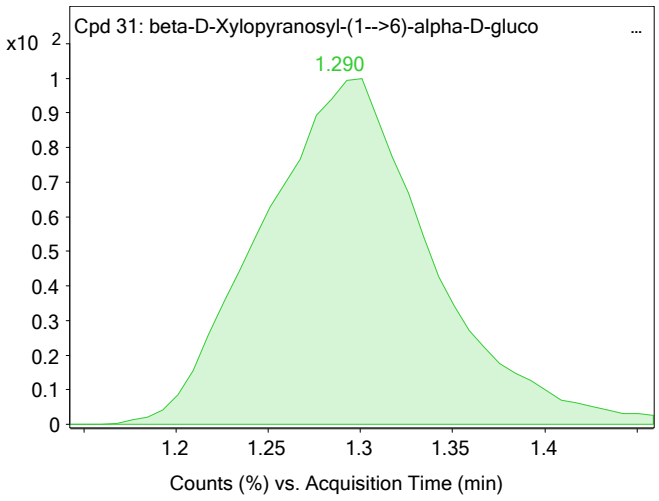
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Picrasinoside D	1.29	C28 H44 O11		65.38	556.2866	1.76	(M+Br)-

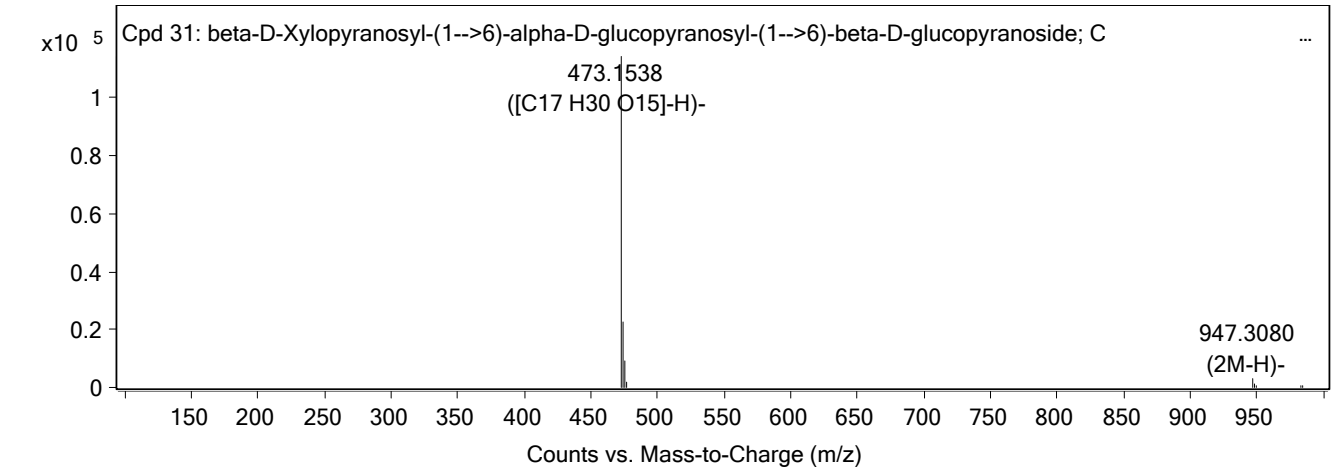
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 31: beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside; C17 H30 O15; 1.290	**beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside**	473.1538	1.29	Find by Molecular Feature	474.1613

Compound Chromatograms

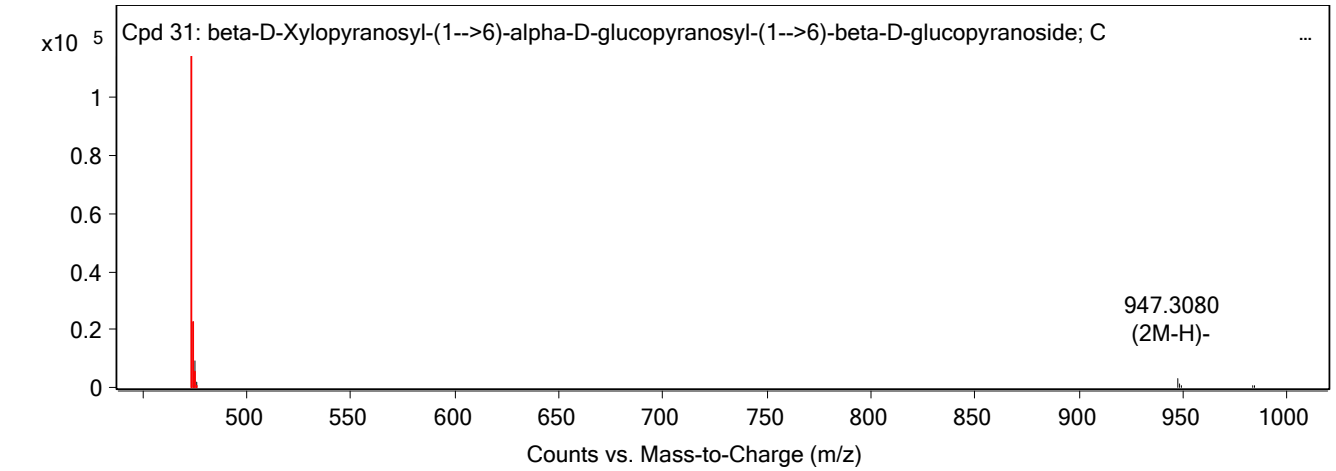




MFE MS Spectrum



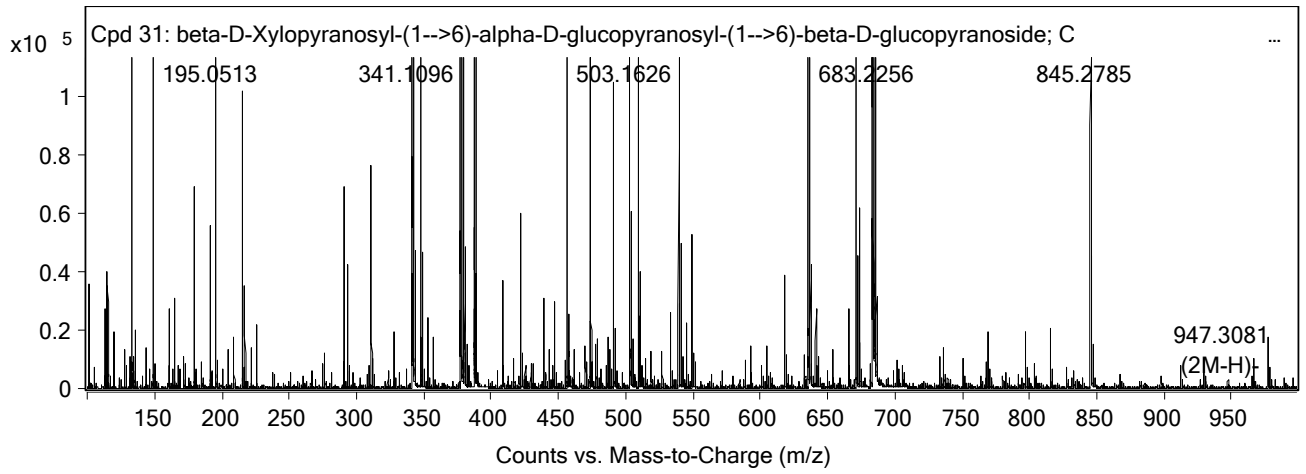
MFE MS Zoomed Spectrum



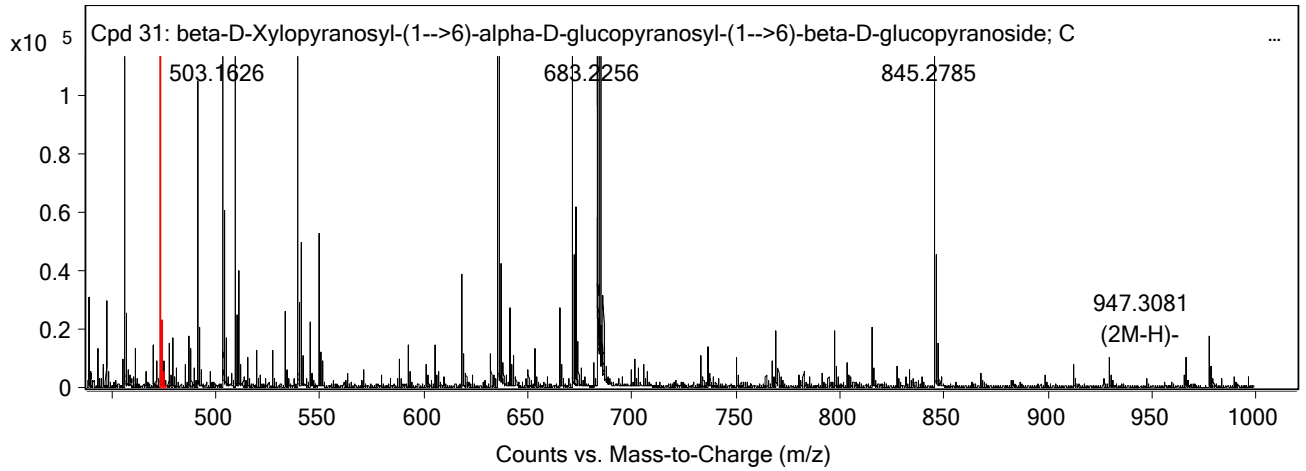
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
473.1538	-1	114351.59	C17 H30 O15	(M-H)-
474.1578	-1	22786.39	C17 H30 O15	(M-H)-
475.1609	-1	8938.55	C17 H30 O15	(M-H)-
476.162	-1	1877.74	C17 H30 O15	(M-H)-
947.308	-1	3001.82		(2M-H)-
948.3113	-1	1424.26		(2M-H)-
949.3091	-1	731.32		(2M-H)-
983.3005	-1	500.68		(2M+Cl)-
984.2915	-1	449.02		(2M+Cl)-

MS Spectrum



MS Zoomed Spectrum

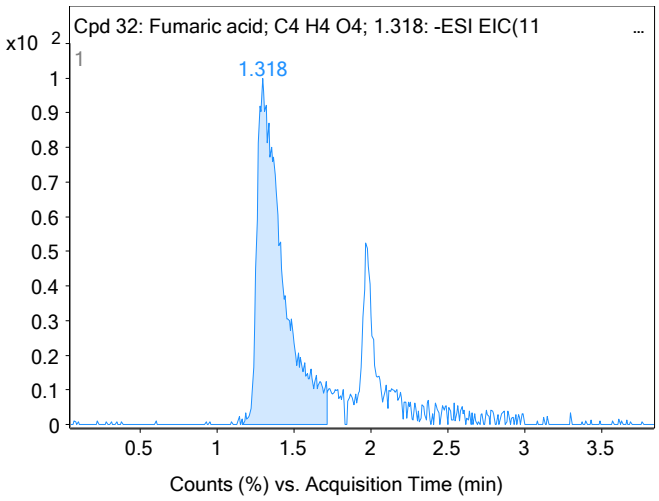


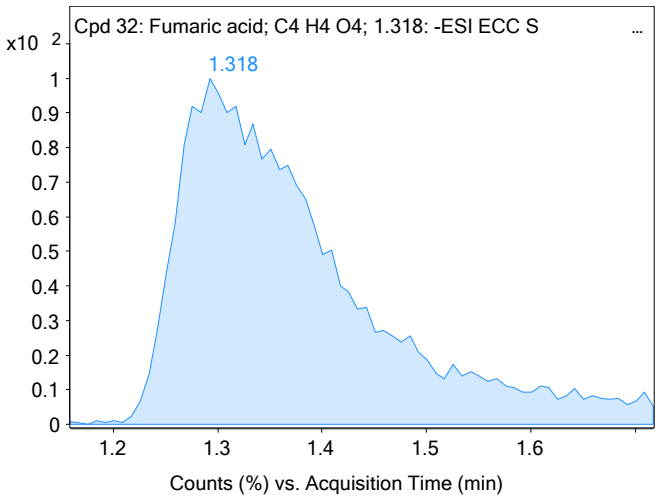
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside	1.29	C17 H30 O15		81.83	474.1613	-2.81	(M-H)-

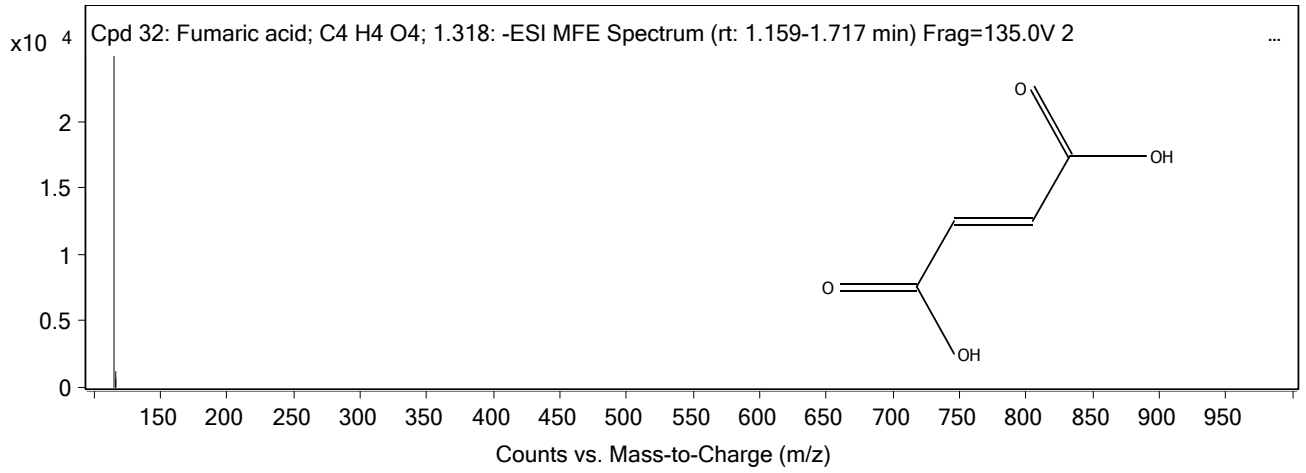
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 32: Fumaric acid; C4 H4 O4; 1.318	**Fumaric acid**	115.0046	1.318	Find by Molecular Feature	116.0121

Compound Chromatograms

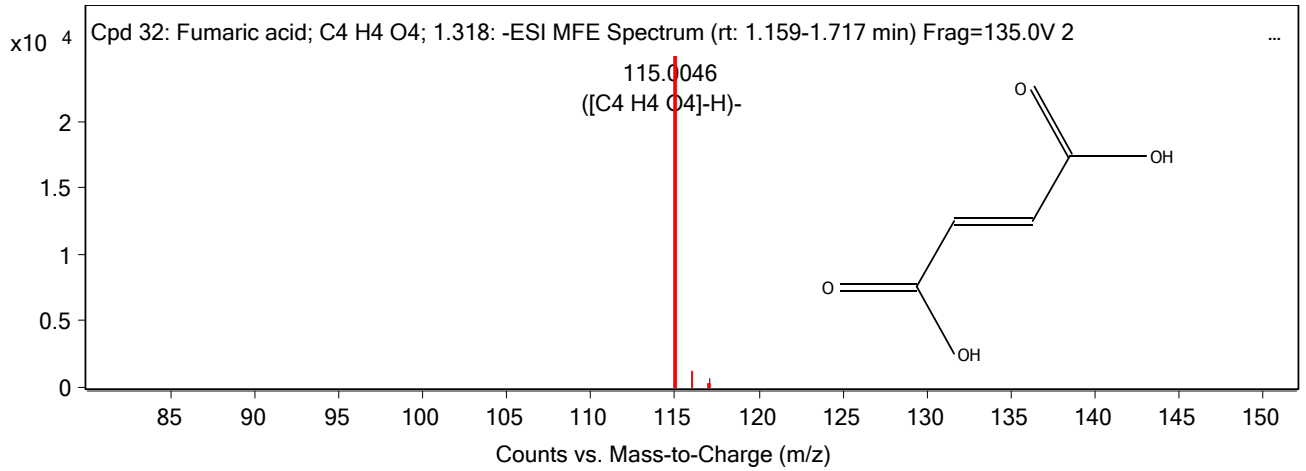




MFE MS Spectrum



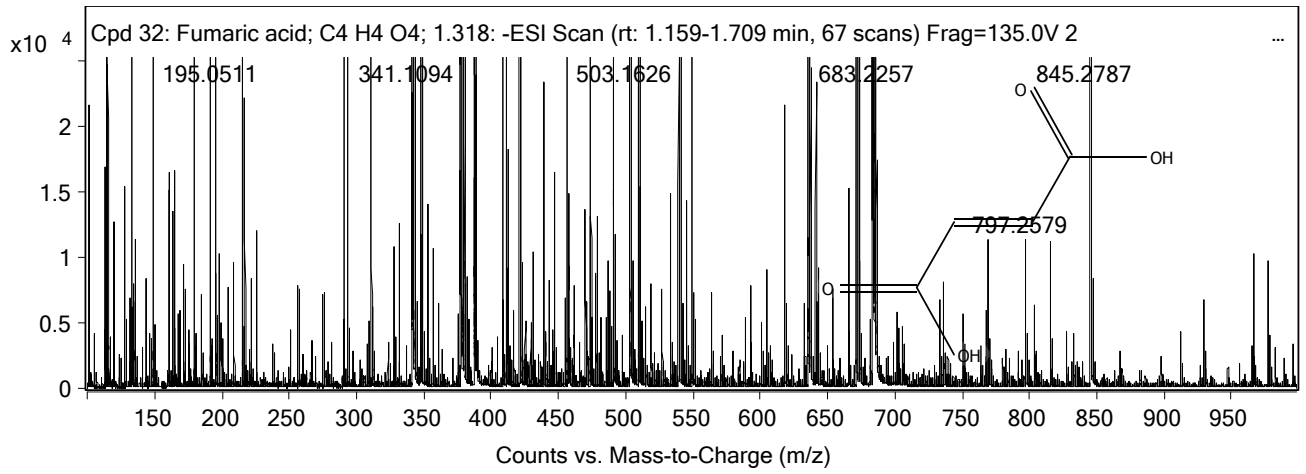
MFE MS Zoomed Spectrum



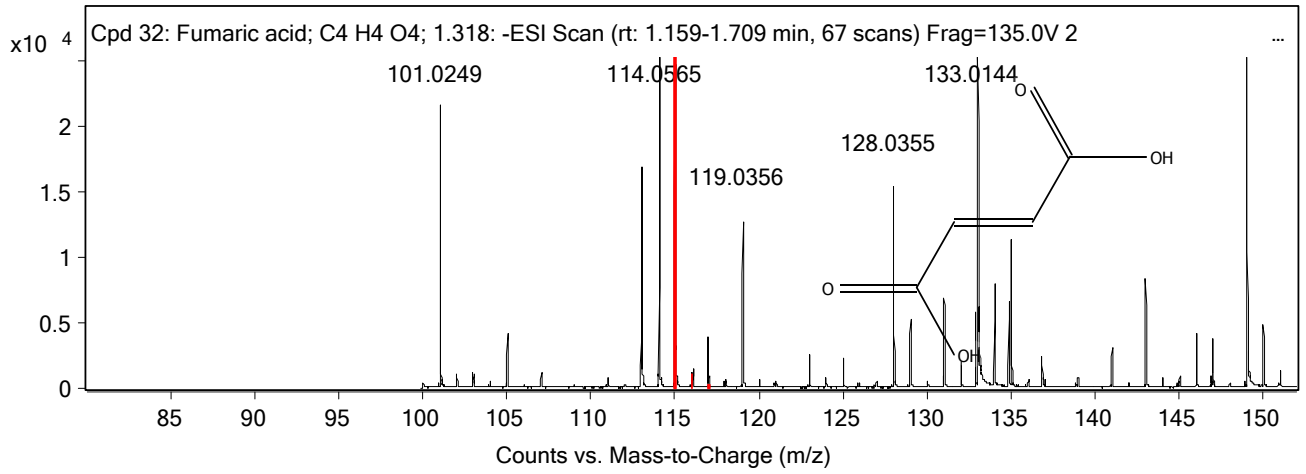
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
115.0046	-1	24906.61	C4 H4 O4	(M-H)-
116.0084	-1	1192.62	C4 H4 O4	(M-H)-
117.0181	-1	656.49	C4 H4 O4	(M-H)-

MS Spectrum



MS Zoomed Spectrum

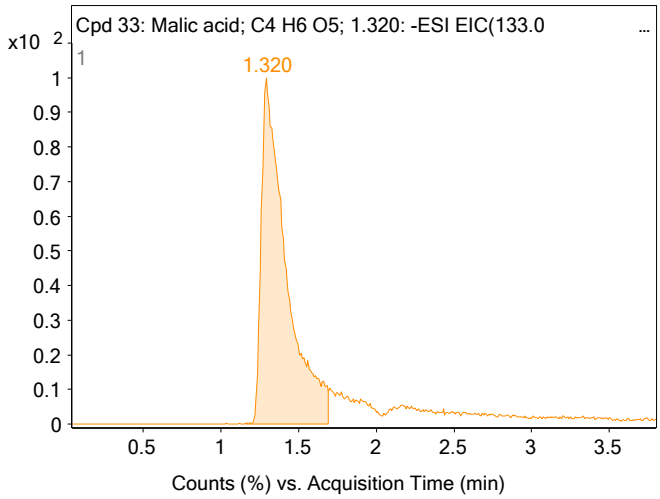


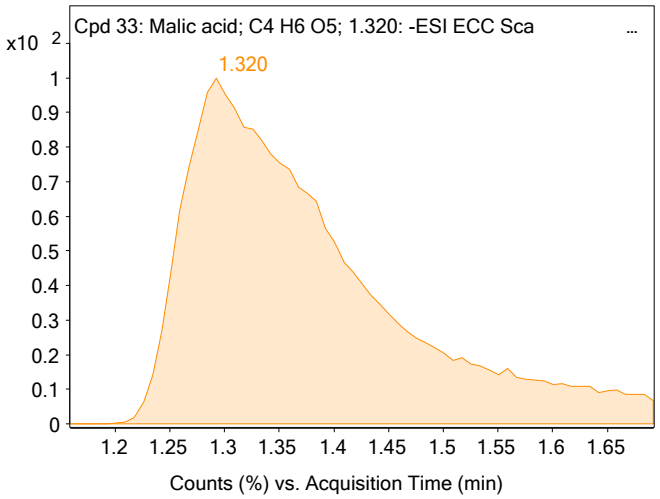
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Fumaric acid	1.318	C4 H4 O4		85.31	116.0121	-1.16	(M-H)-

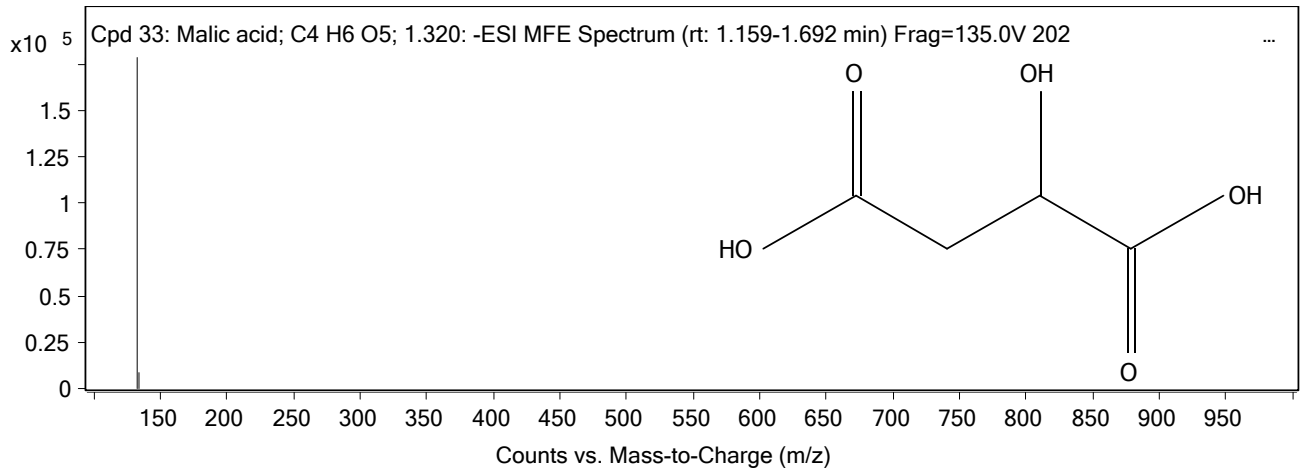
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 33: Malic acid; C4 H6 O5; 1.320	**Malic acid**	133.0149	1.32	Find by Molecular Feature	134.0222

Compound Chromatograms

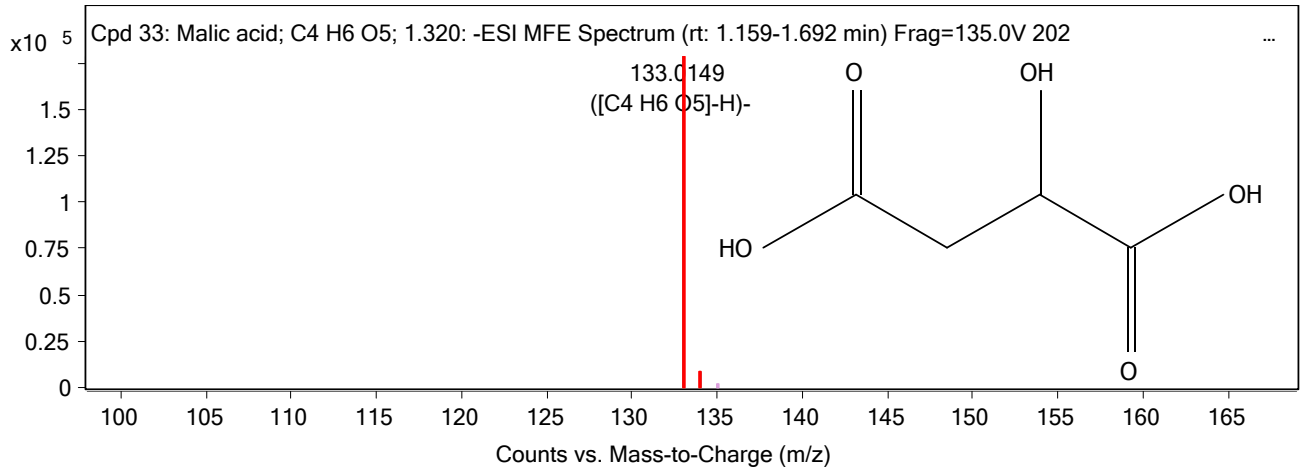




MFE MS Spectrum



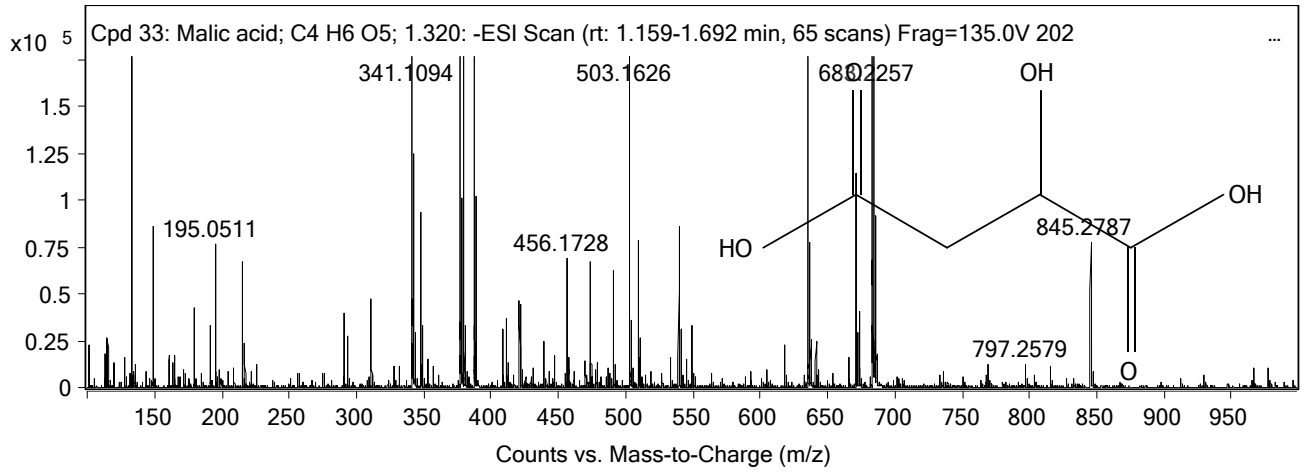
MFE MS Zoomed Spectrum



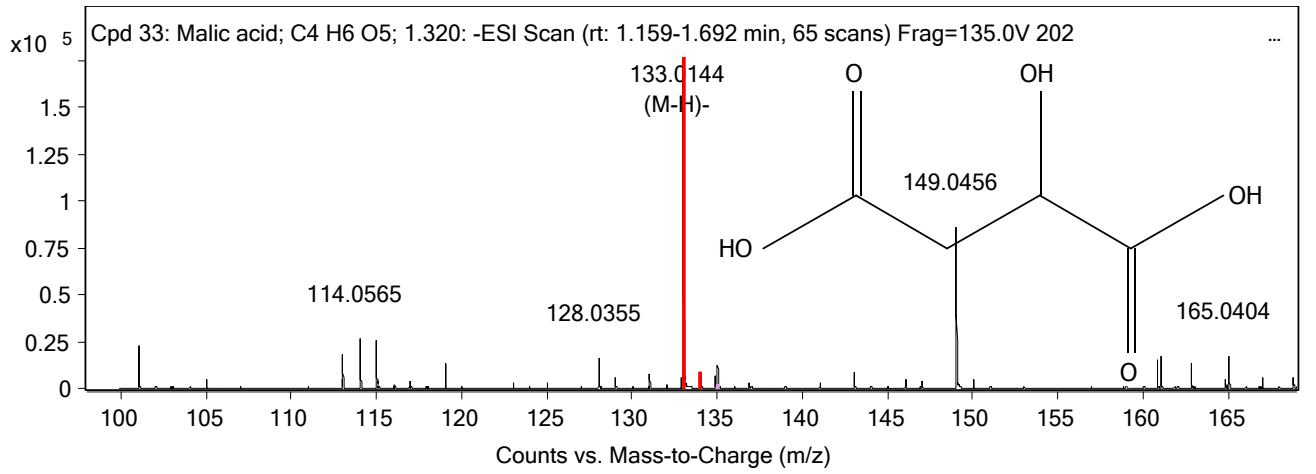
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
133.0149	-1	178615.72	C4 H6 O5	(M-H)-
134.0183	-1	8213.65	C4 H6 O5	(M-H)-

MS Spectrum



MS Zoomed Spectrum

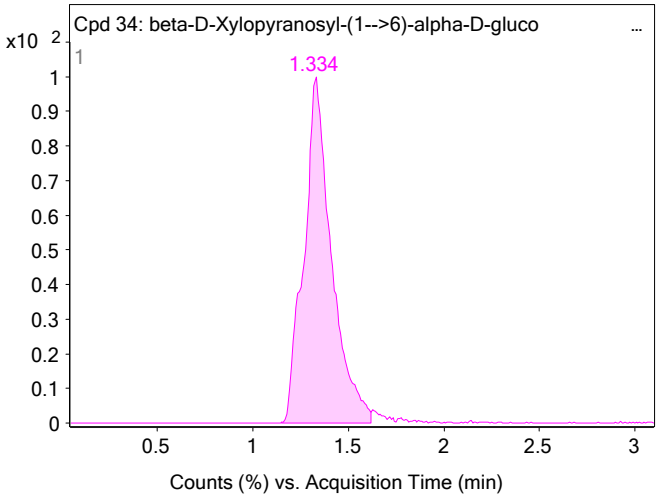


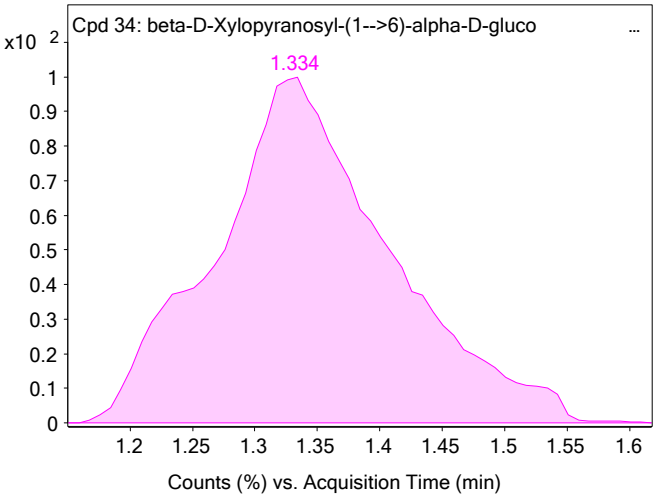
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Malic acid	1.32	C4 H6 O5		84.78	134.0222	-0.67	(M-H)-

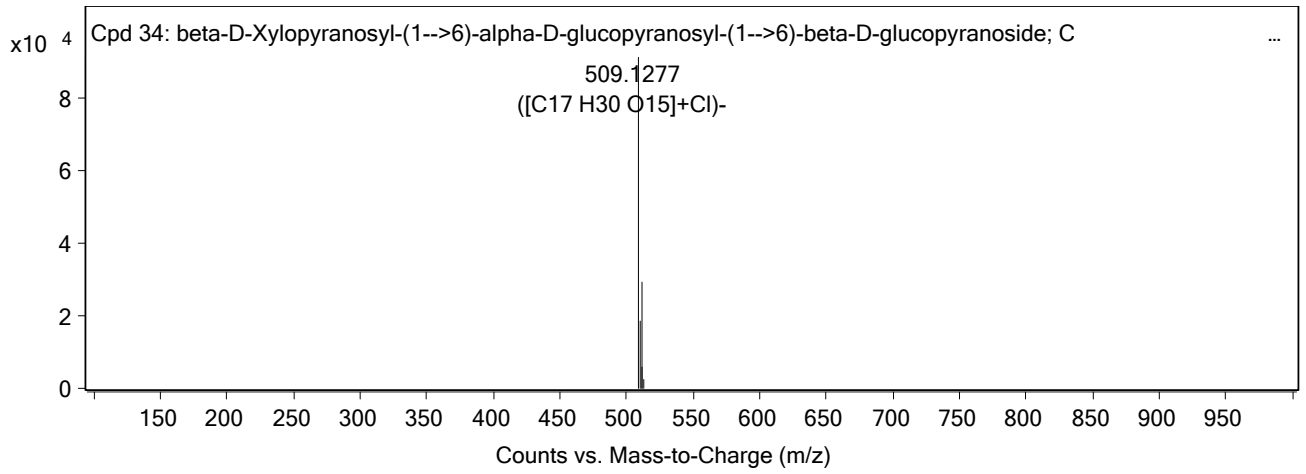
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 34: beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside; C17 H30 O15; 1.334	**beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside**	509.1277	1.334	Find by Molecular Feature	474.1586

Compound Chromatograms

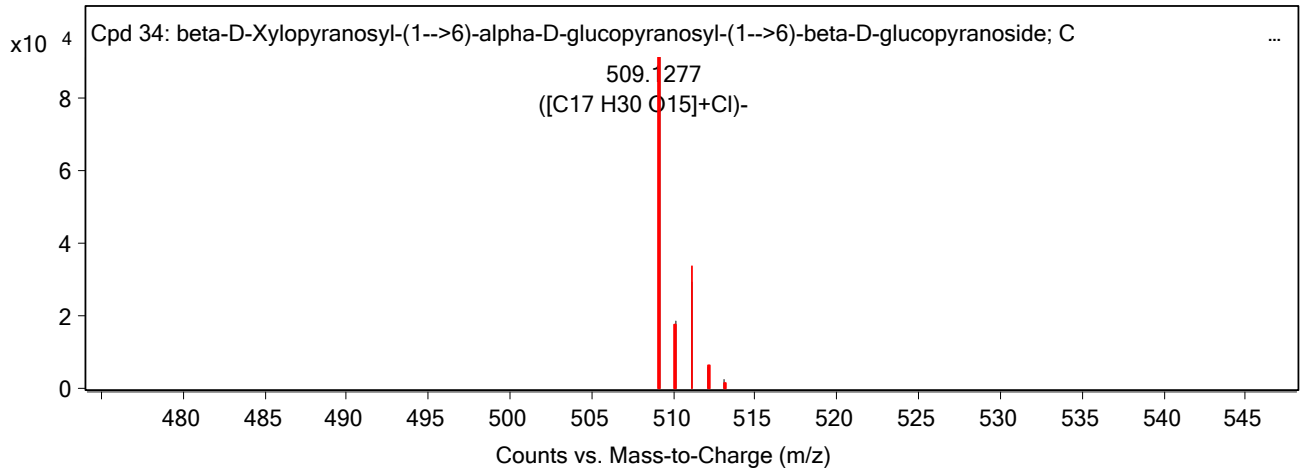




MFE MS Spectrum



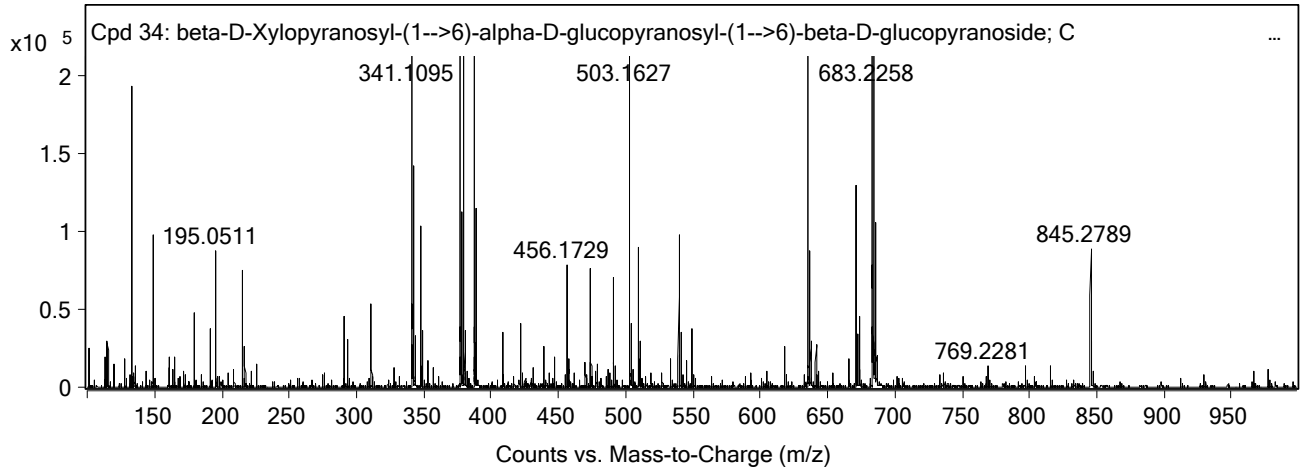
MFE MS Zoomed Spectrum



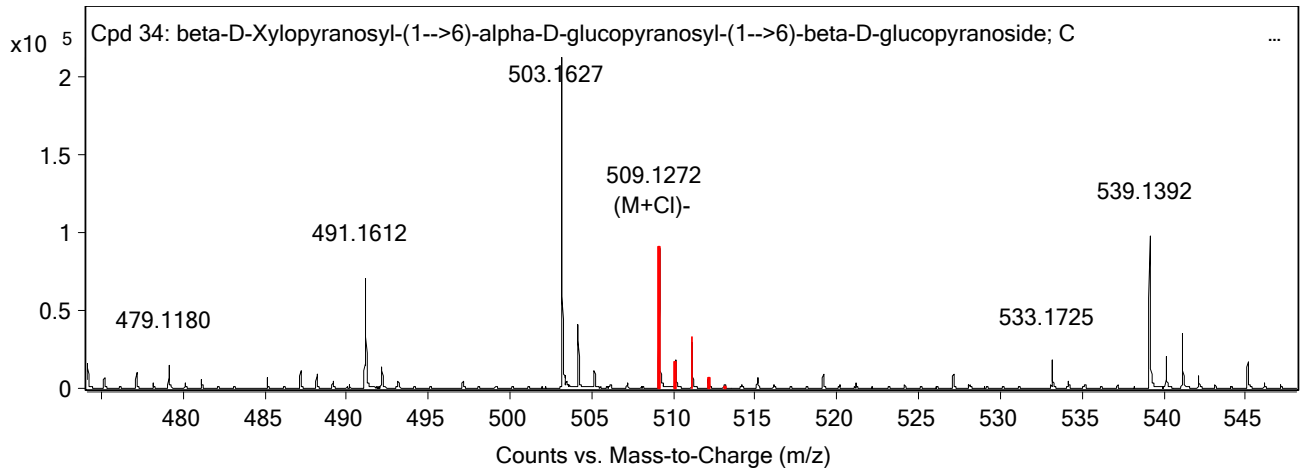
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
509.1277	-1	91052.8	C17 H30 O15	(M+Cl)-
510.1312	-1	18673.15	C17 H30 O15	(M+Cl)-
511.1269	-1	29452.51	C17 H30 O15	(M+Cl)-
512.1303	-1	5798.7	C17 H30 O15	(M+Cl)-
513.13	-1	2240.69	C17 H30 O15	(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

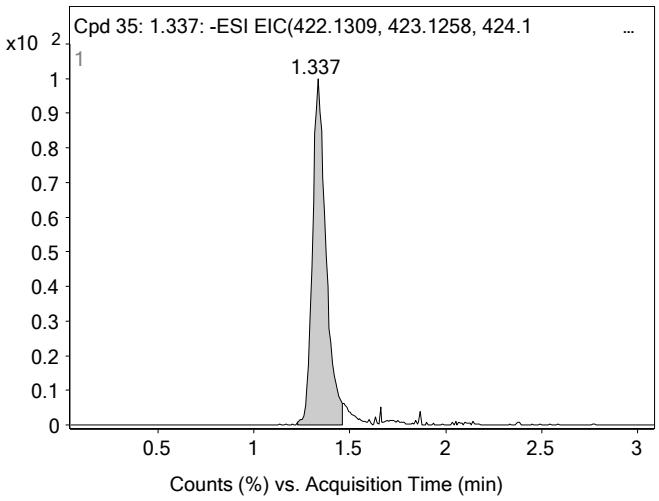


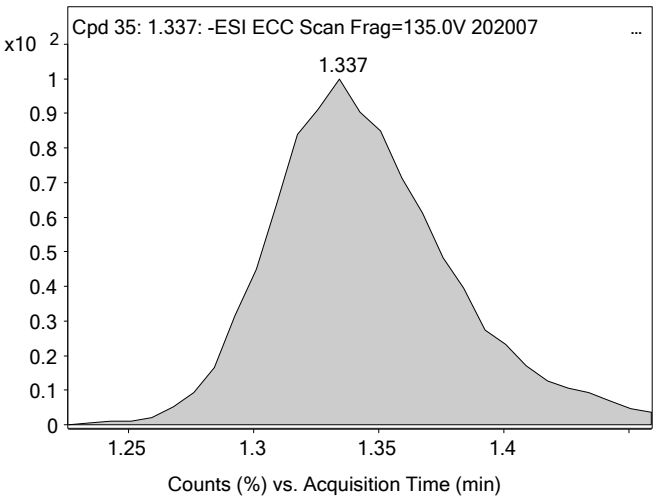
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	beta-D-Xylopyranosyl-(1-->6)-alpha-D-glucopyranosyl-(1-->6)-beta-D-glucopyranoside	1.334	C17 H30 O15		96.33	474.1586	-0.11	(M+Cl)-
	Aloeemodin bianthrone	1.334	C30 H22 O8		57.64	510.1332	-1.74	(M-H)-
	Palmidin A	1.334	C30 H22 O8		57.64	510.1332	-1.74	(M-H)-

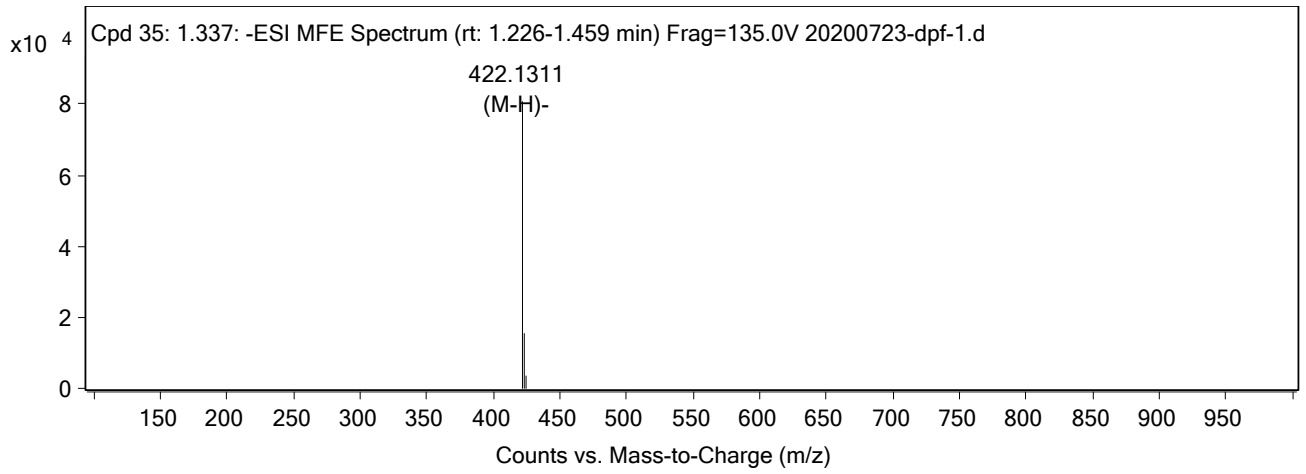
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 35: 1.337	422.1311	1.337	Find by Molecular Feature	423.1383

Compound Chromatograms

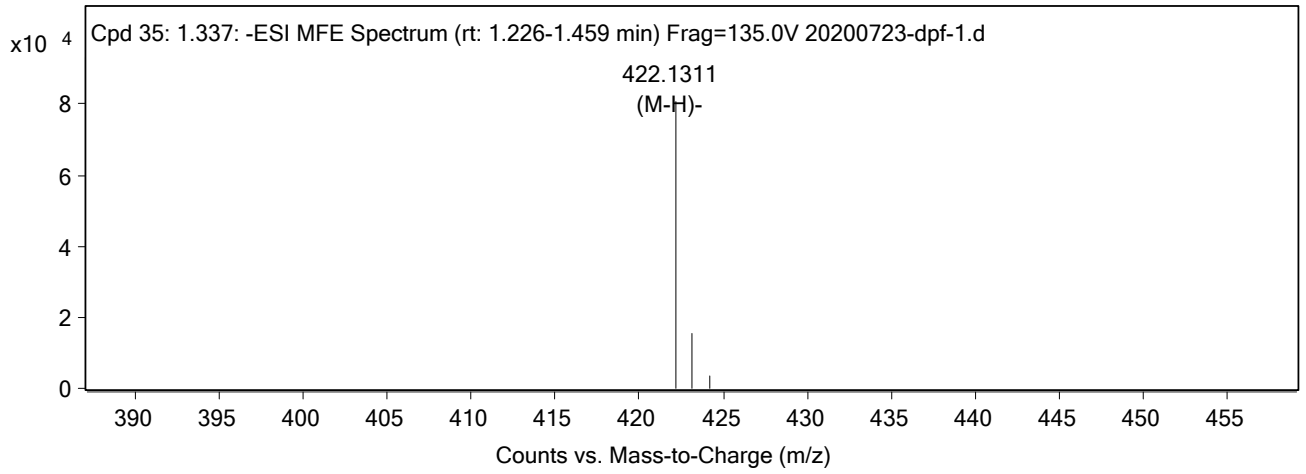




MFE MS Spectrum



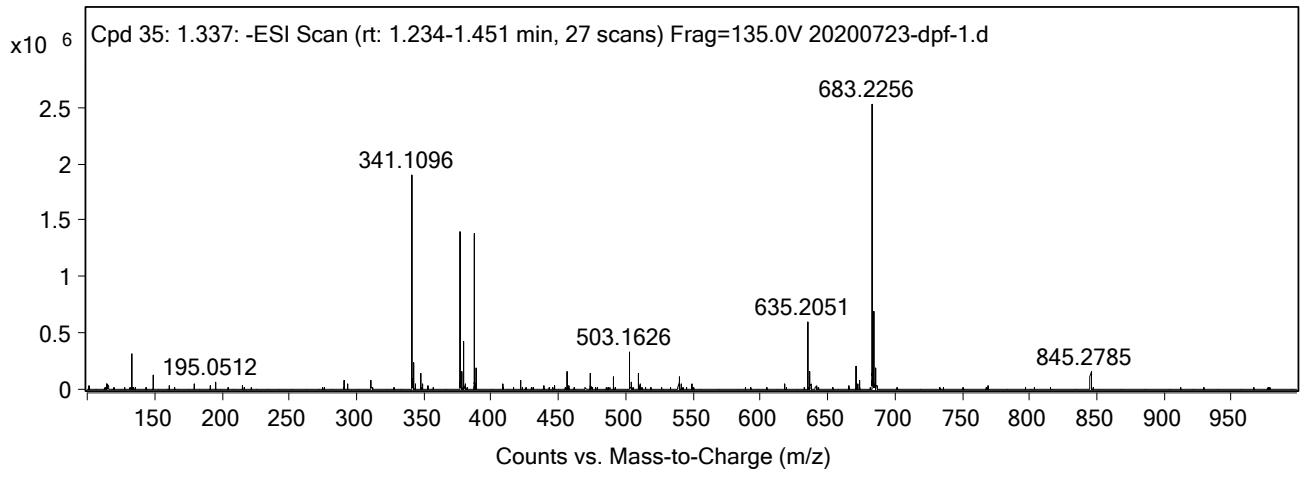
MFE MS Zoomed Spectrum



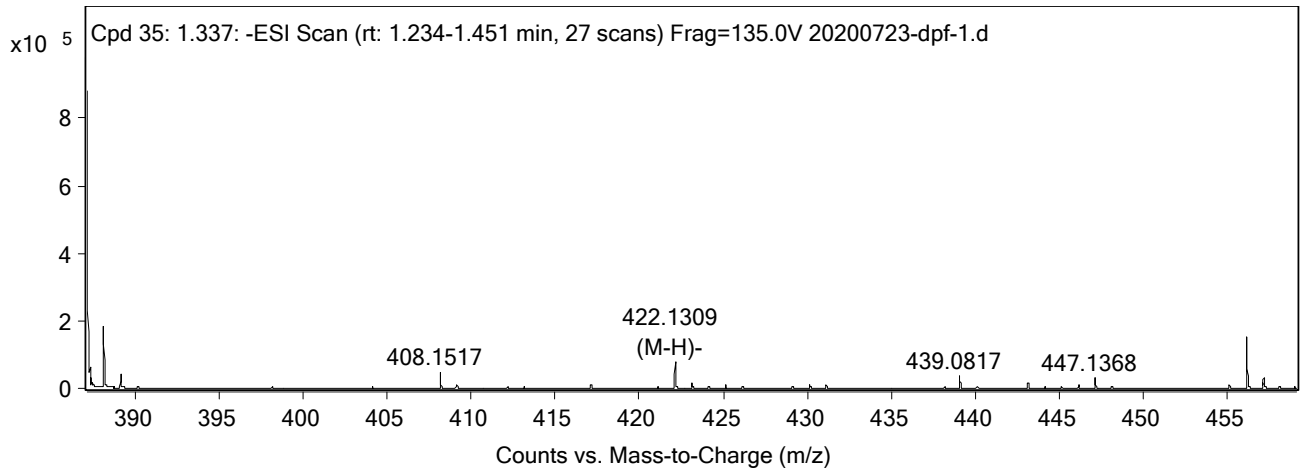
MS Spectrum Peak List

m/z	z	Abund	Ion
422.1311	-1	80796.69	(M-H)-
423.1337	-1	15608.47	(M-H)-
424.1366	-1	3742.84	(M-H)-

MS Spectrum

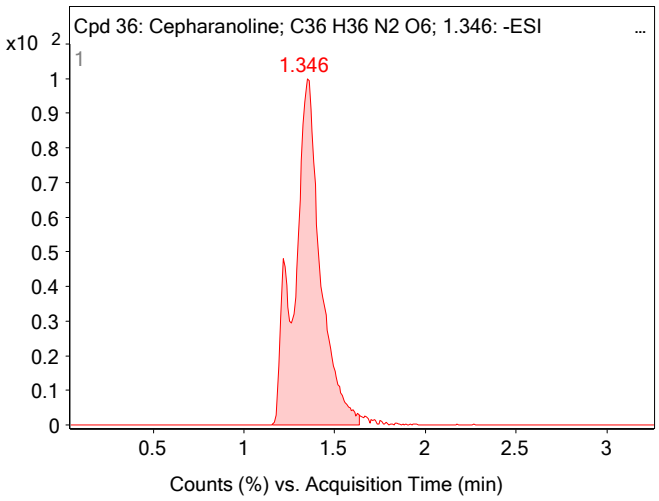


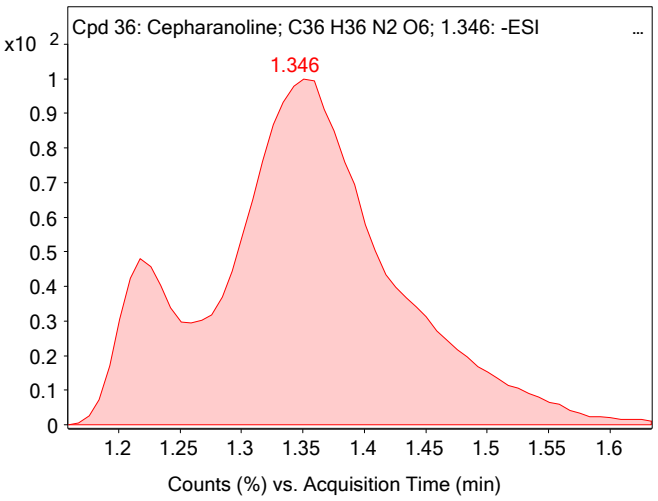
MS Zoomed Spectrum



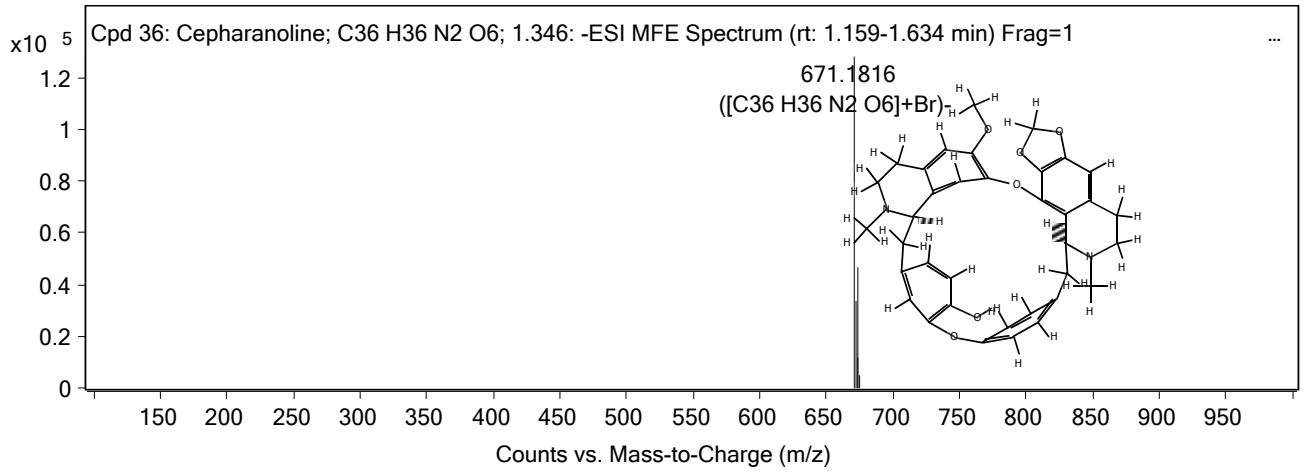
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 36: Cepharanoline; C36 H36 N2 O6; 1.346	**Cepharanoline**	671.1816	1.346	Find by Molecular Feature	592.2627

Compound Chromatograms

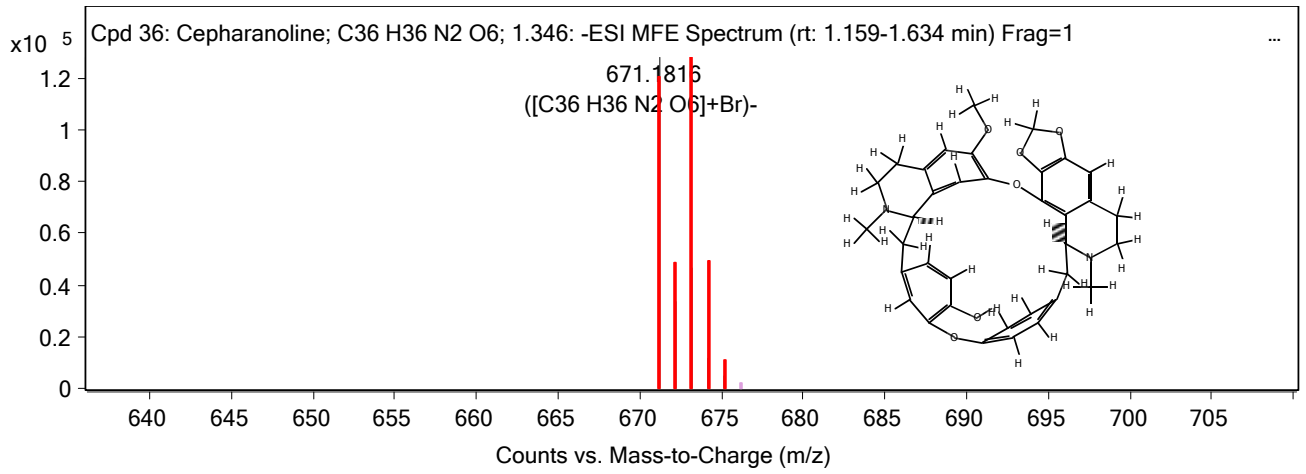




MFE MS Spectrum



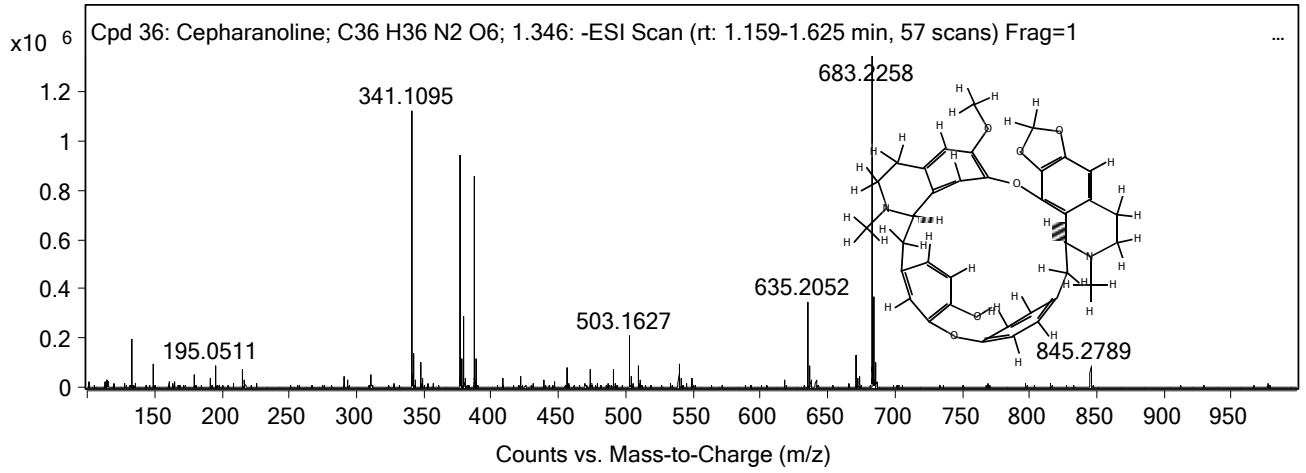
MFE MS Zoomed Spectrum



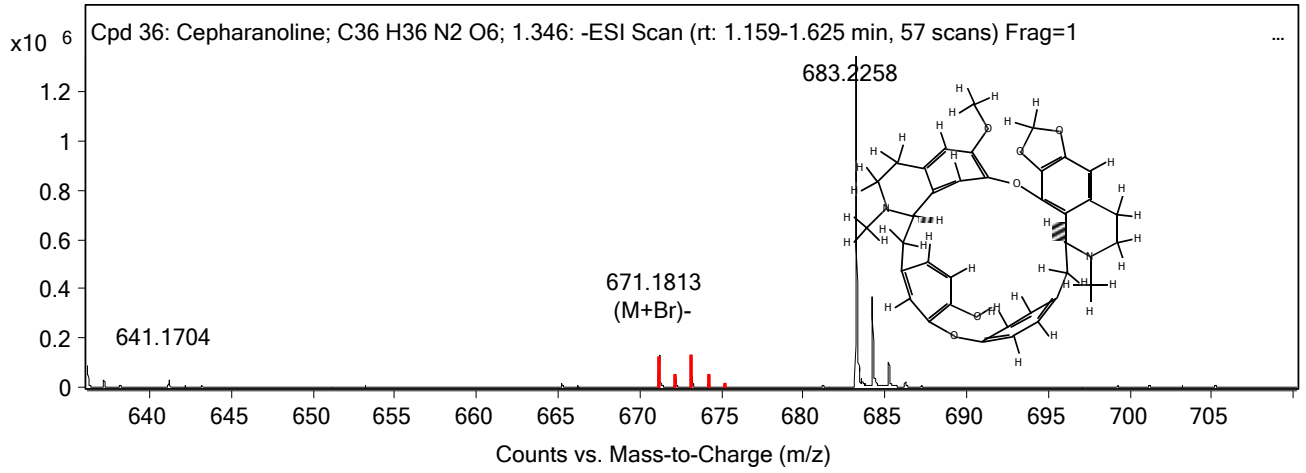
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
671.1816	-1	128095.13	C36 H36 N2 O6	(M+Br)-
672.1846	-1	33293.48	C36 H36 N2 O6	(M+Br)-
673.1804	-1	46382.24	C36 H36 N2 O6	(M+Br)-
674.1825	-1	11824.64	C36 H36 N2 O6	(M+Br)-
675.1881	-1	5013.82	C36 H36 N2 O6	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

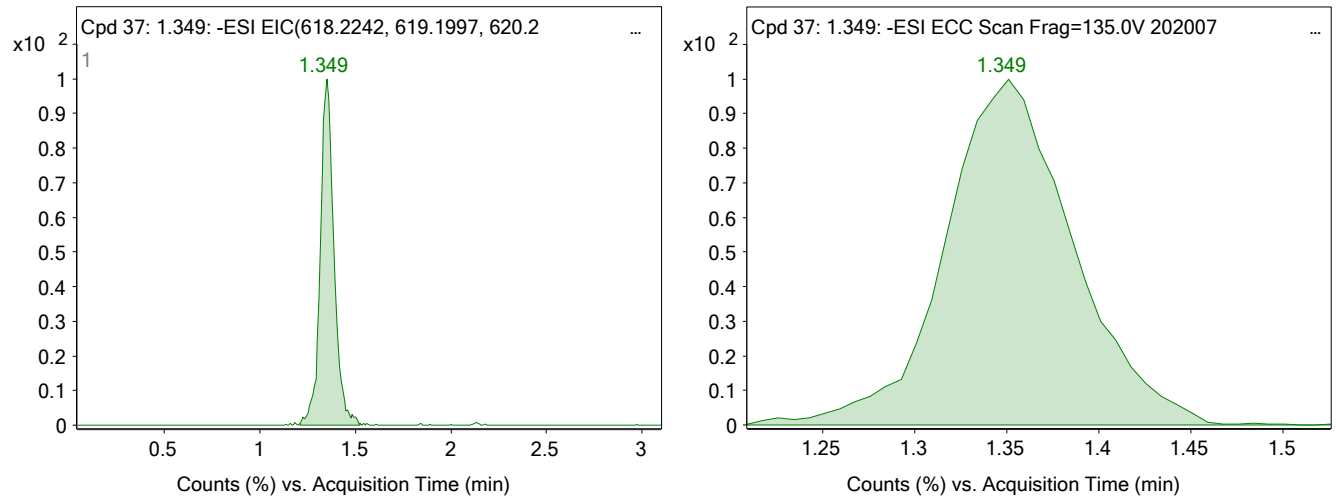


Identification Hit Table

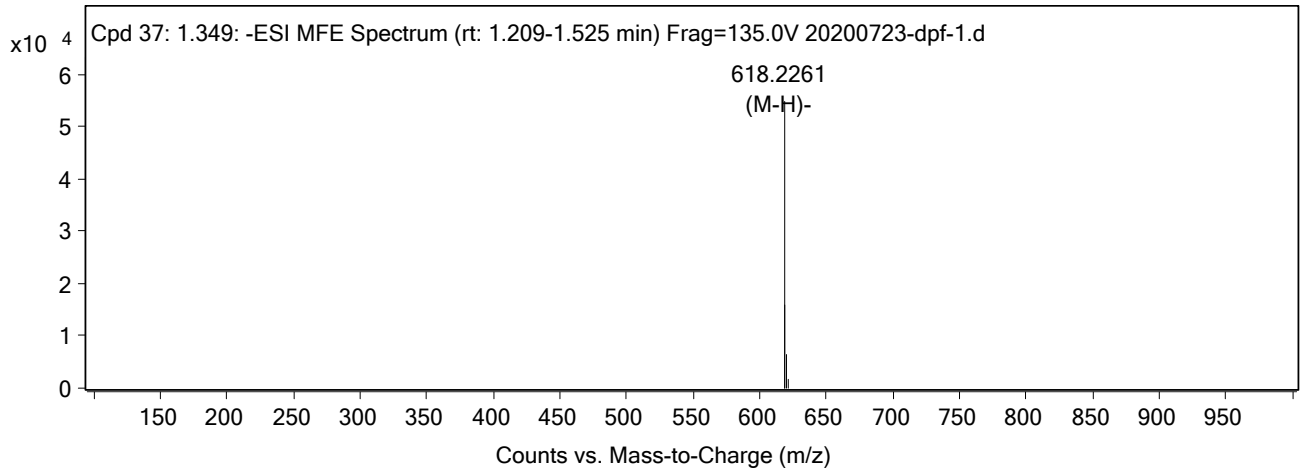
Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Cepharanoline	1.346	C36 H36 N2 O6		40.99	592.2627	-5.36	(M+Br)-
	Hypoepistephanine	1.346	C36 H36 N2 O6		40.99	592.2627	-5.36	(M+Br)-
	Isotrilobine-N-2-oxide	1.346	C36 H36 N2 O6		40.99	592.2627	-5.36	(M+Br)-

Compound Label	m/z	RT	Algorithm	Mass
Cpd 37: 1.349	618.2261	1.349	Find by Molecular Feature	619.2333

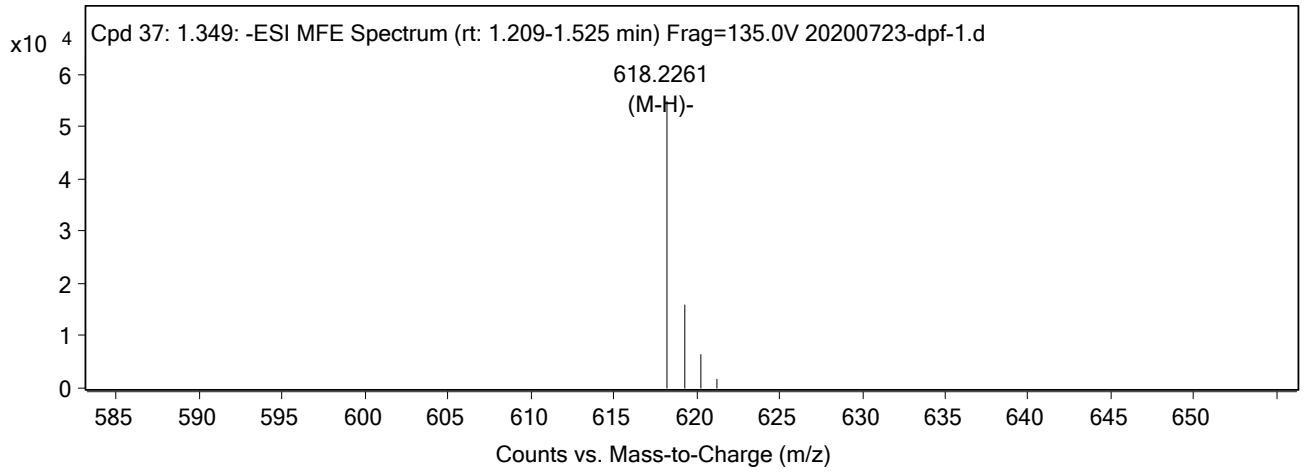
Compound Chromatograms



MFE MS Spectrum



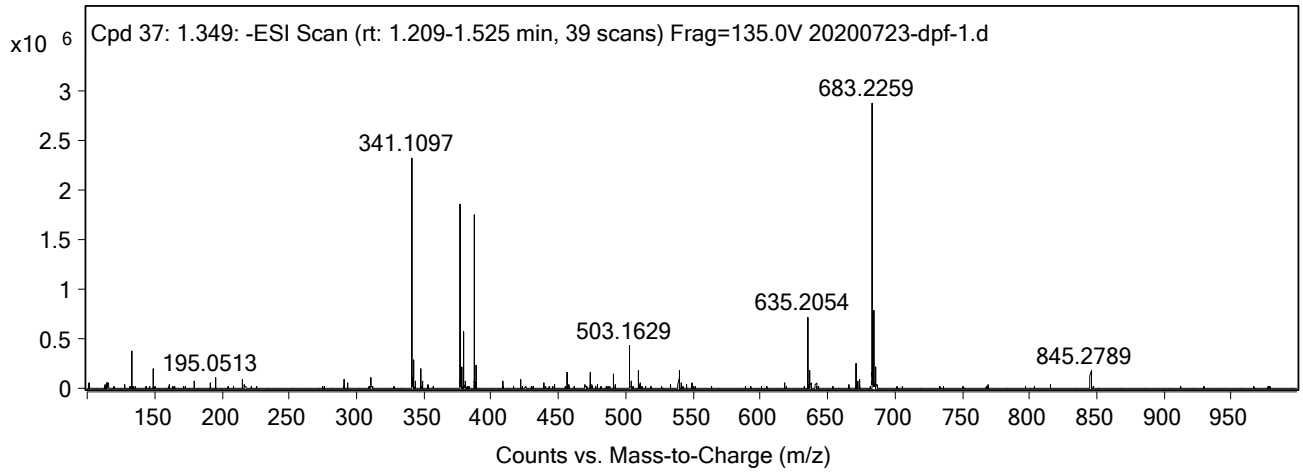
MFE MS Zoomed Spectrum



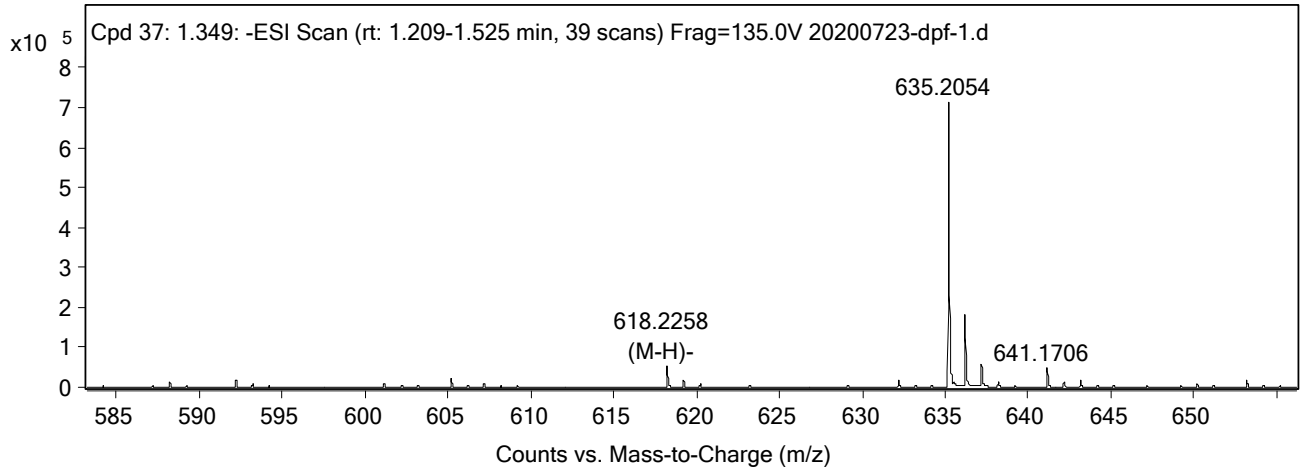
MS Spectrum Peak List

m/z	z	Abund	Ion
618.2261	-1	54764.18	(M-H)-
619.2289	-1	15848.28	(M-H)-
620.2199	-1	6413.26	(M-H)-
621.2124	-1	1630.55	(M-H)-

MS Spectrum

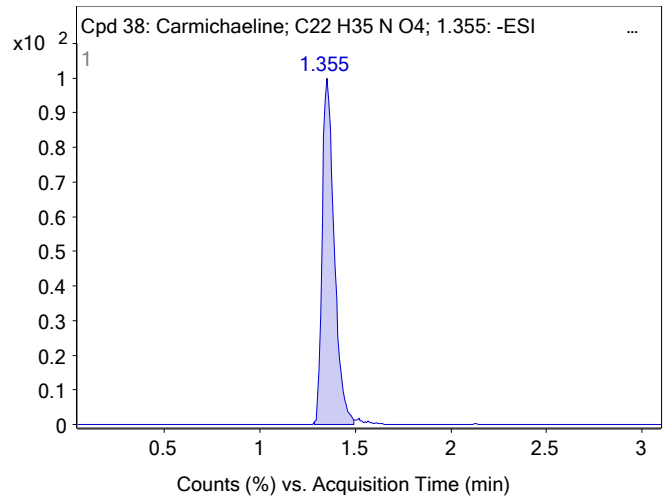


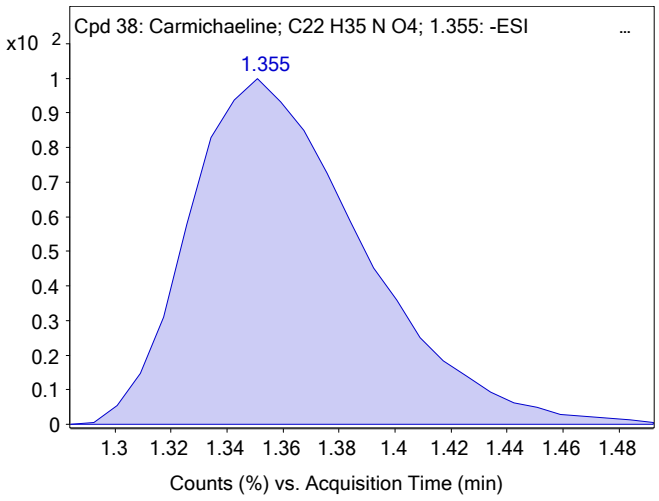
MS Zoomed Spectrum



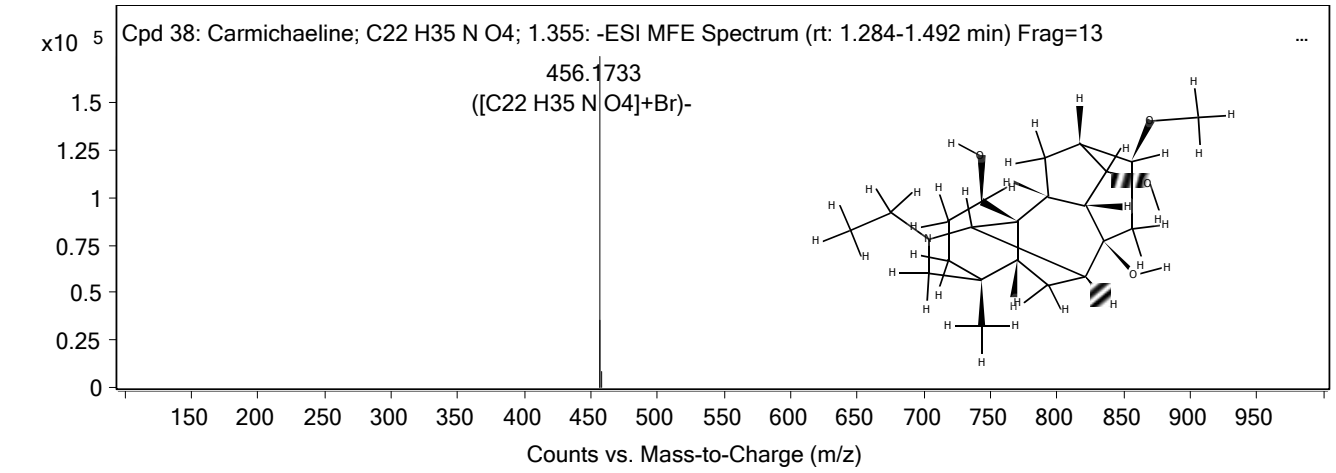
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 38: Carmichaeline; C22 H35 N O4; 1.355	**Carmichaeline**	456.1733	1.355	Find by Molecular Feature	377.2543

Compound Chromatograms

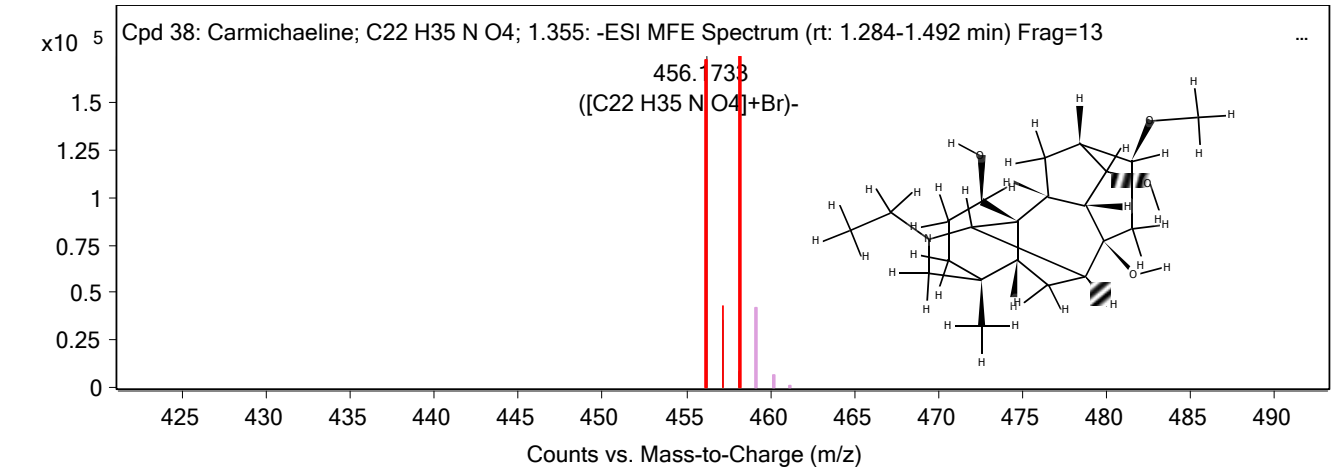




MFE MS Spectrum



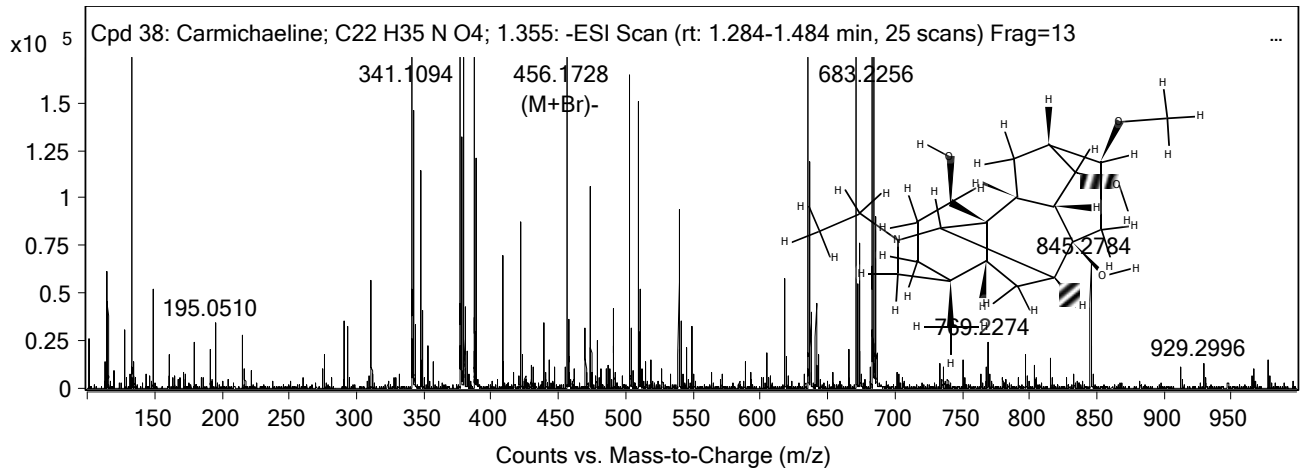
MFE MS Zoomed Spectrum



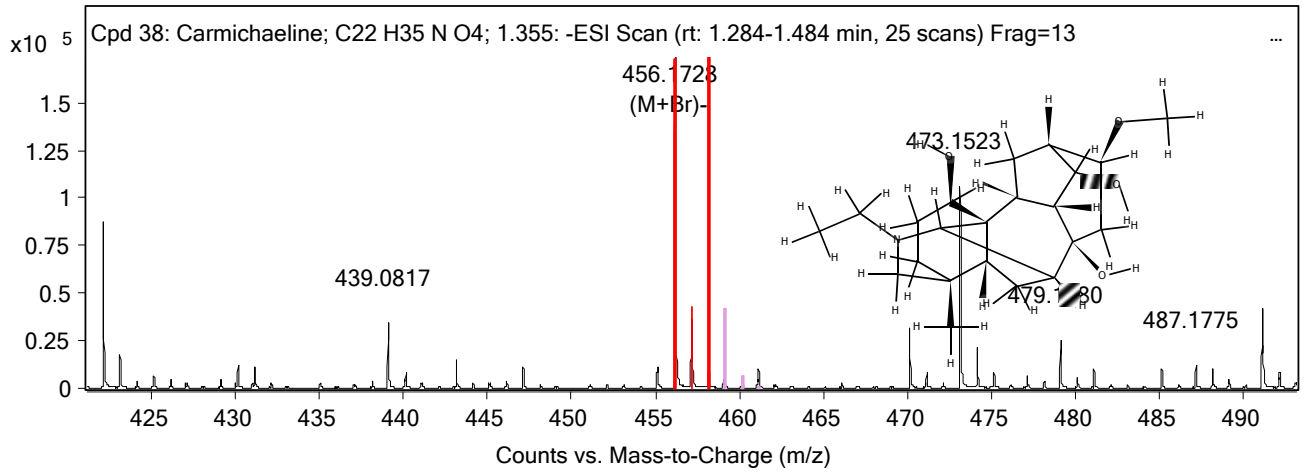
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
456.1733	-1	174363.56	C22 H35 N O4	(M+Br)-
457.1745	-1	35832.33	C22 H35 N O4	(M+Br)-
458.1765	-1	8403.23	C22 H35 N O4	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

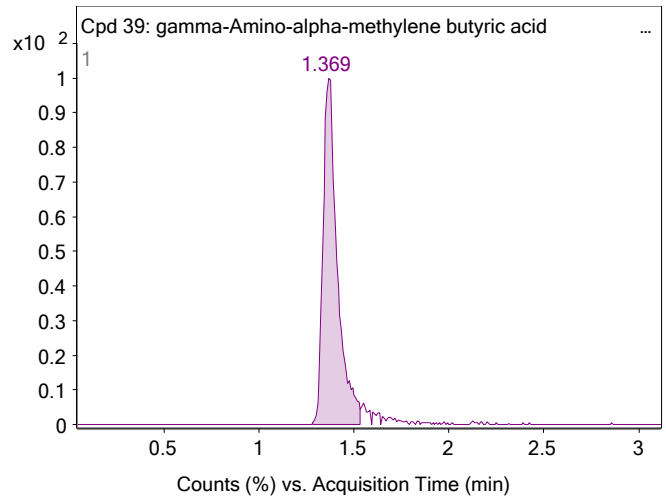


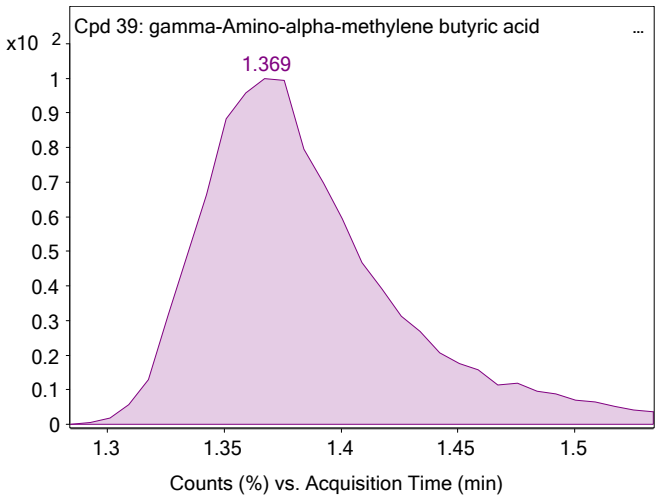
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Carmichaeline	1.355	C22 H35 N O4		52.84	377.2543	2.34	(M+Br)-
	Genicunine A	1.355	C22 H35 N O4		52.84	377.2543	2.34	(M+Br)-
	Karacoline	1.355	C22 H35 N O4		52.84	377.2543	2.34	(M+Br)-

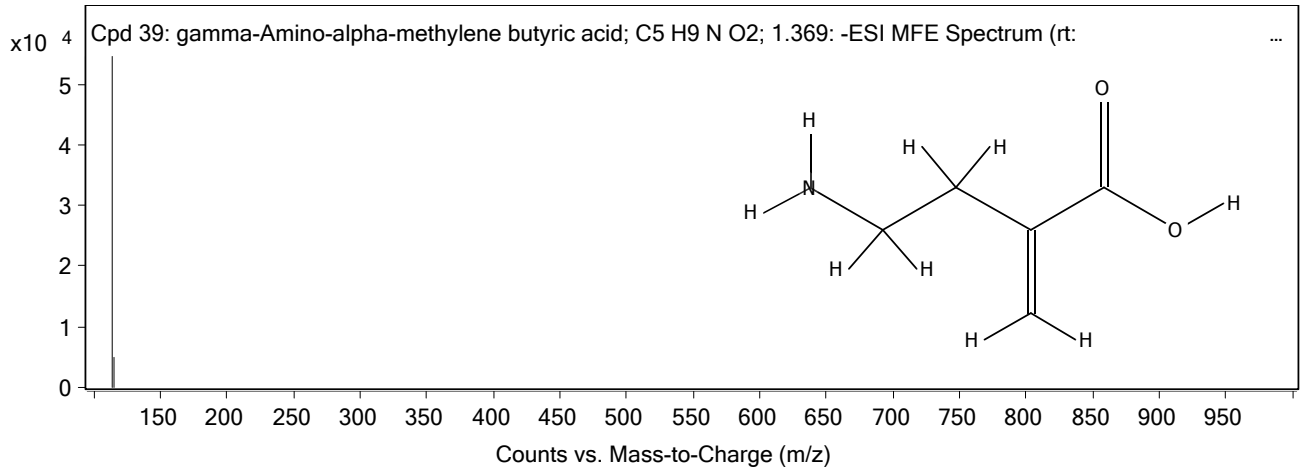
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 39: gamma-Amino-alpha-methylene butyric acid; C5 H9 N O2; 1.369	**gamma-Amino-alpha-methylene butyric acid**	114.0569	1.369	Find by Molecular Feature	115.0639

Compound Chromatograms

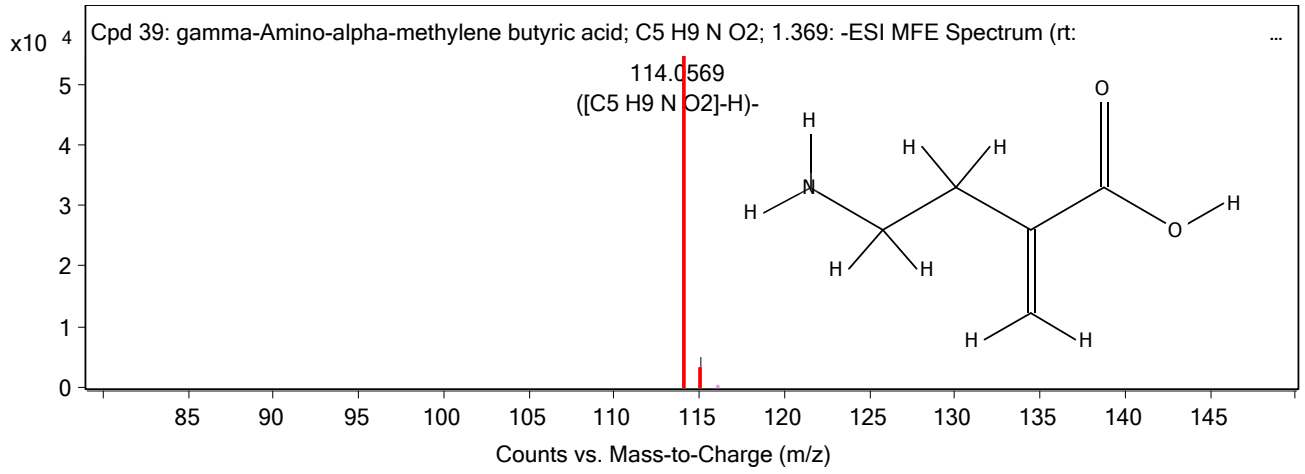




MFE MS Spectrum



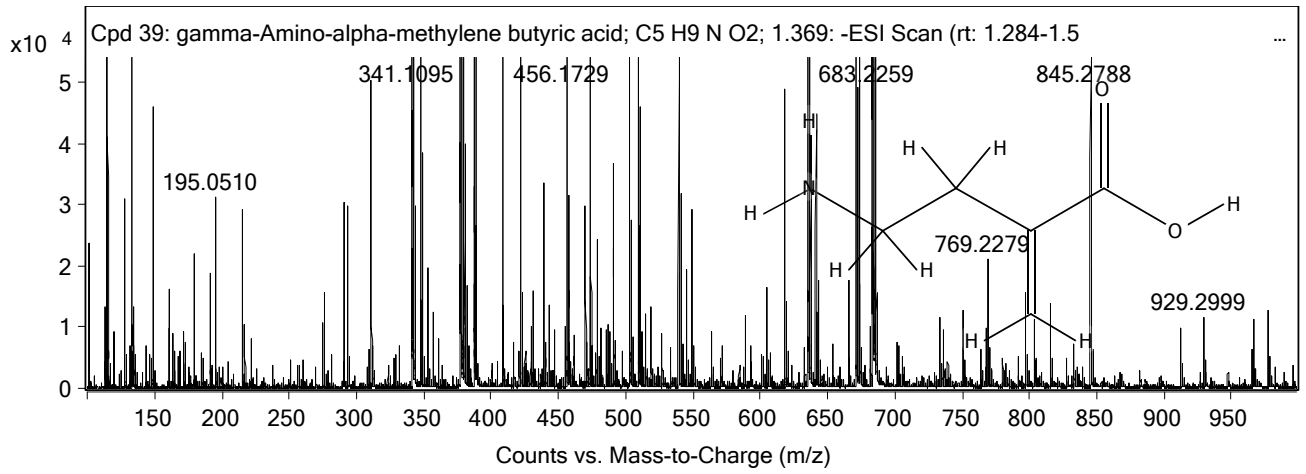
MFE MS Zoomed Spectrum



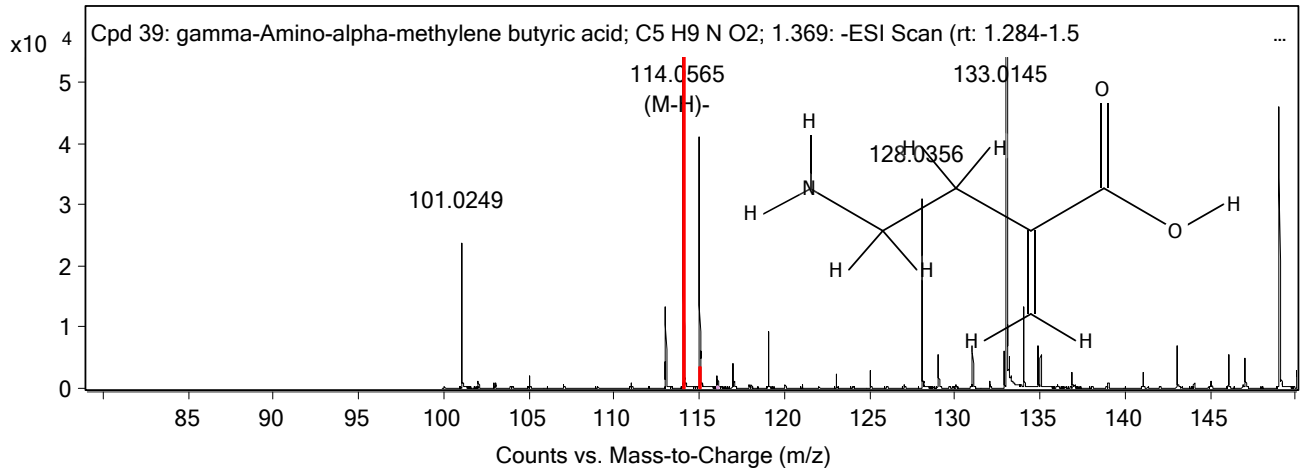
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
114.0569	-1	54529.22	C5 H9 N O2	(M-H)-
115.0574	-1	5058.11	C5 H9 N O2	(M-H)-

MS Spectrum



MS Zoomed Spectrum

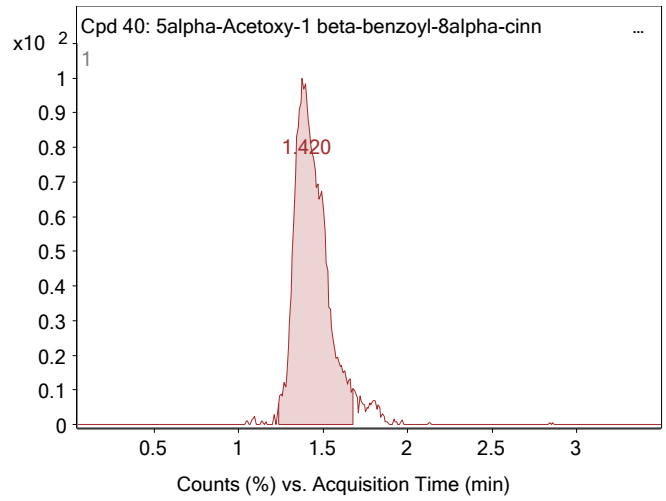


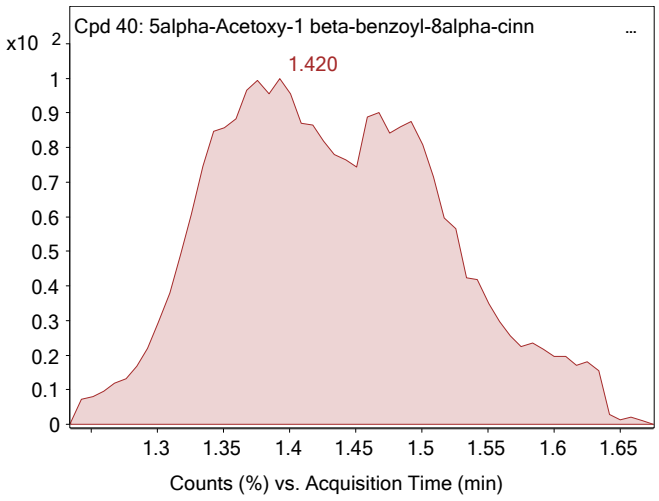
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	gamma-Amino-alpha-methylene butyric acid	1.369	C5 H9 N O2		74.02	115.0639	-0.61	(M-H)-
	Pyrrolidine carboxylic acd	1.369	C5 H9 N O2		74.02	115.0639	-0.61	(M-H)-
	Pterolactam	1.369	C5 H9 N O2		74.02	115.0639	-0.61	(M-H)-

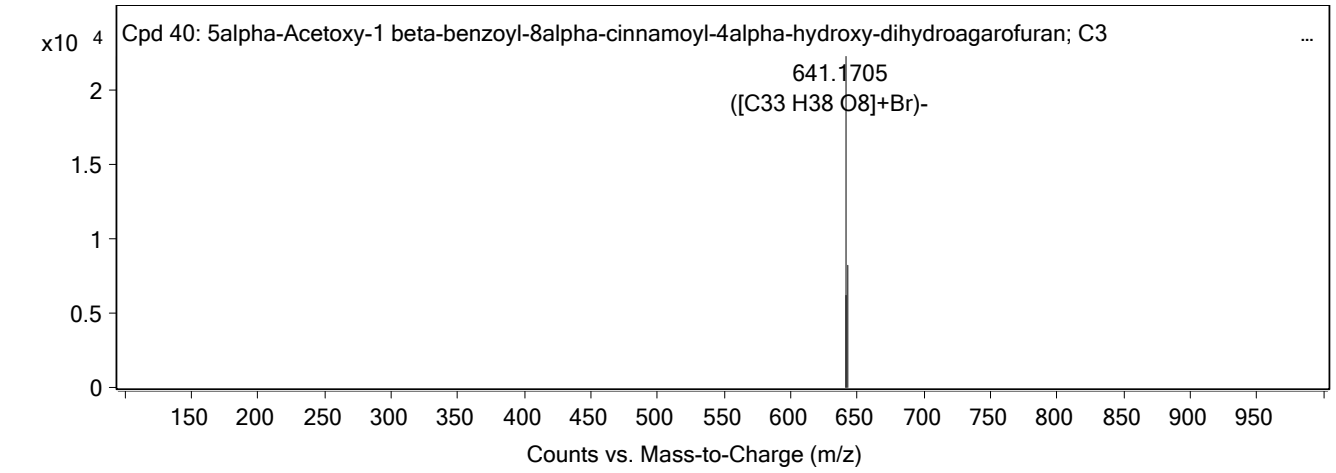
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 40: 5alpha-Acetoxy-1 beta-benzoyl-8alpha-cinnamoyl-4alpha-hydroxy-dihydroagarofuran; C33 H38 O8; 1.420	**5alpha-Acetoxy-1 beta-benzoyl-8alpha-cinnamoyl-4alpha-hydroxy-dihydroagarofuran**	641.1705	1.42	Find by Molecular Feature	562.2518

Compound Chromatograms

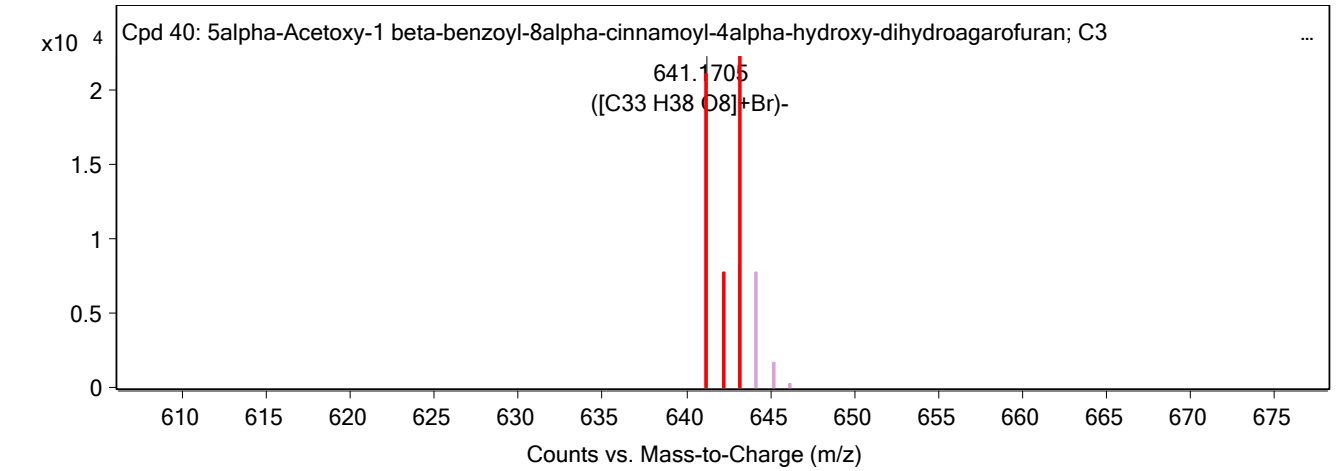




MFE MS Spectrum



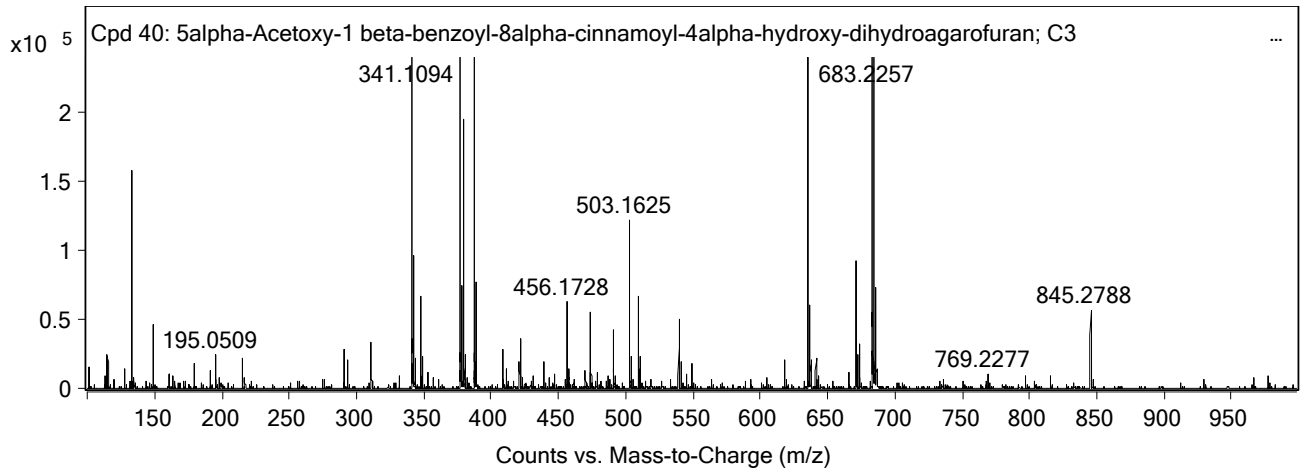
MFE MS Zoomed Spectrum



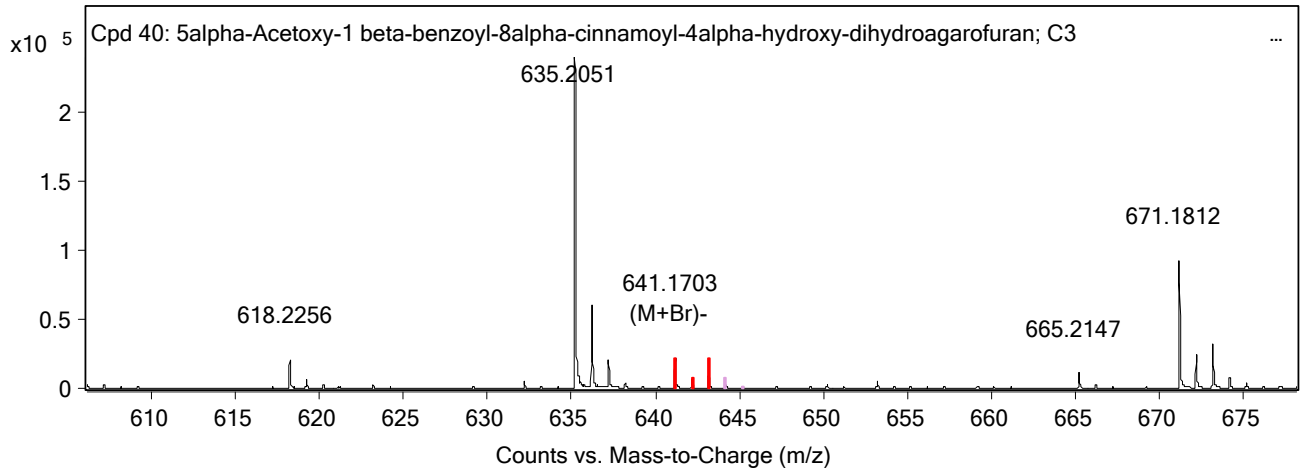
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
641.1705	-1	22307.51	C33 H38 O8	(M+Br)-
642.1738	-1	6214.8	C33 H38 O8	(M+Br)-
643.1696	-1	8255.18	C33 H38 O8	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

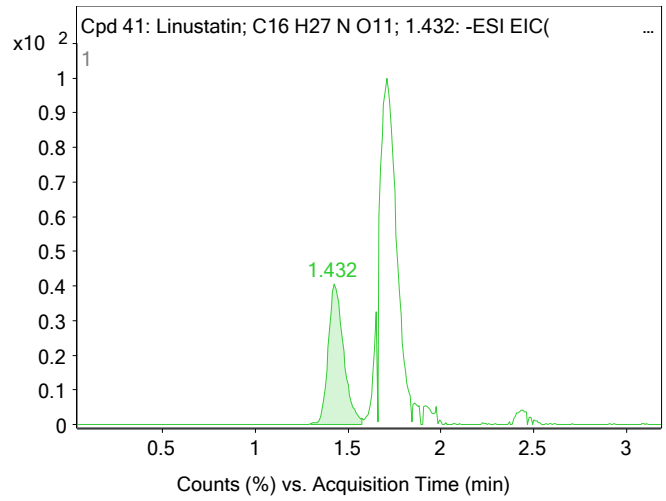


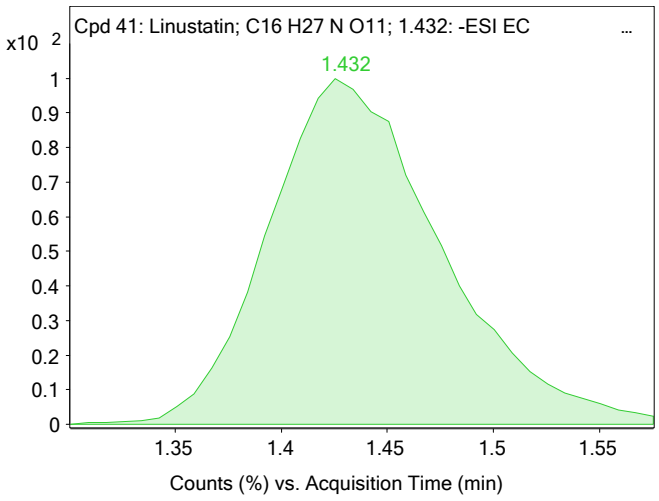
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	5alpha-Acetoxy-1 beta-benzoyl-8alpha-cinnamoyl-4alpha-hydroxy-dihydroagarofuran	1.42	C33 H38 O8		42.88	562.2518	4.91	(M+Br)-
	O-Methyldeoxopunjabine	1.42	C35 H34 N2 O5		42.28	562.2518	-5	(M+Br)-
	Trilobine	1.42	C35 H34 N2 O5		42.28	562.2518	-5	(M+Br)-

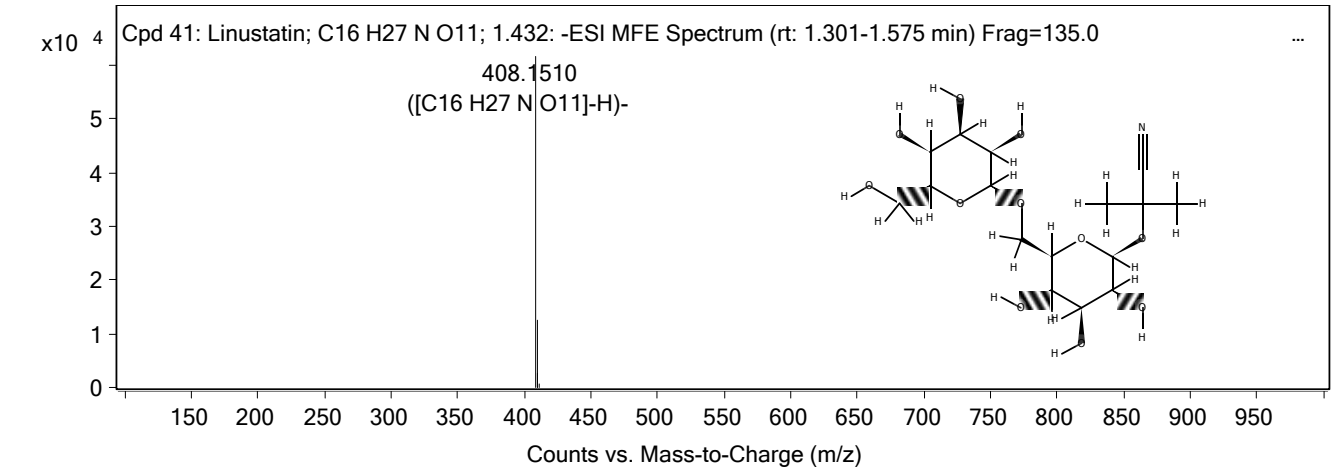
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 41: Linustatin; C16 H27 N O11; 1.432	**Linustatin**	408.151	1.432	Find by Molecular Feature	409.1579

Compound Chromatograms

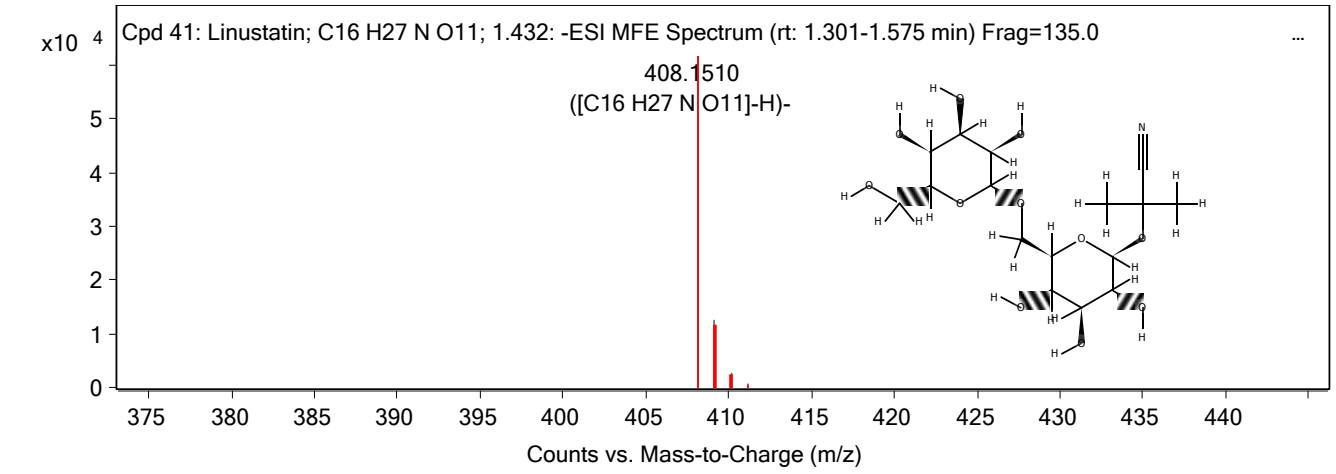




MFE MS Spectrum



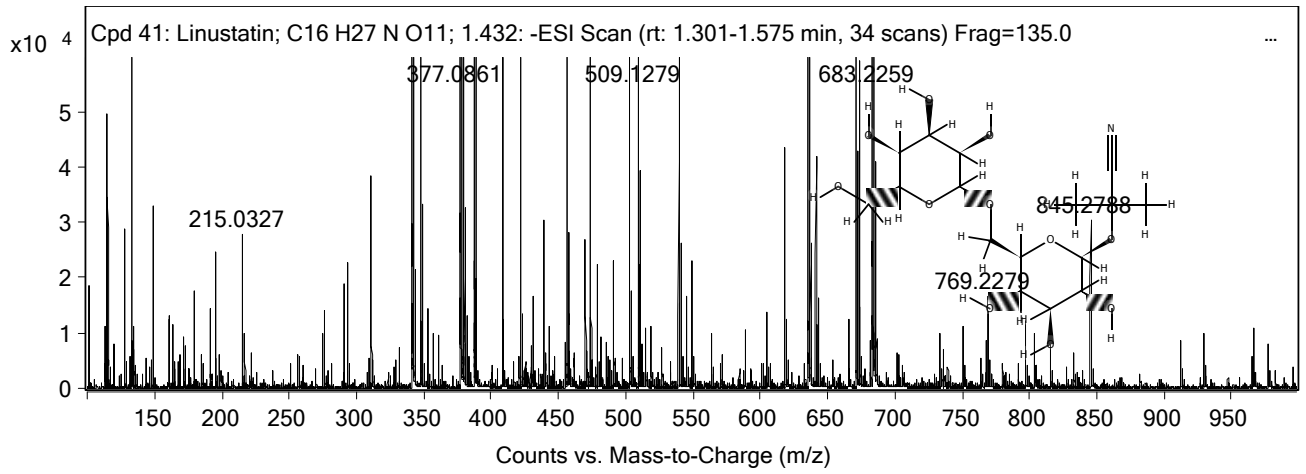
MFE MS Zoomed Spectrum



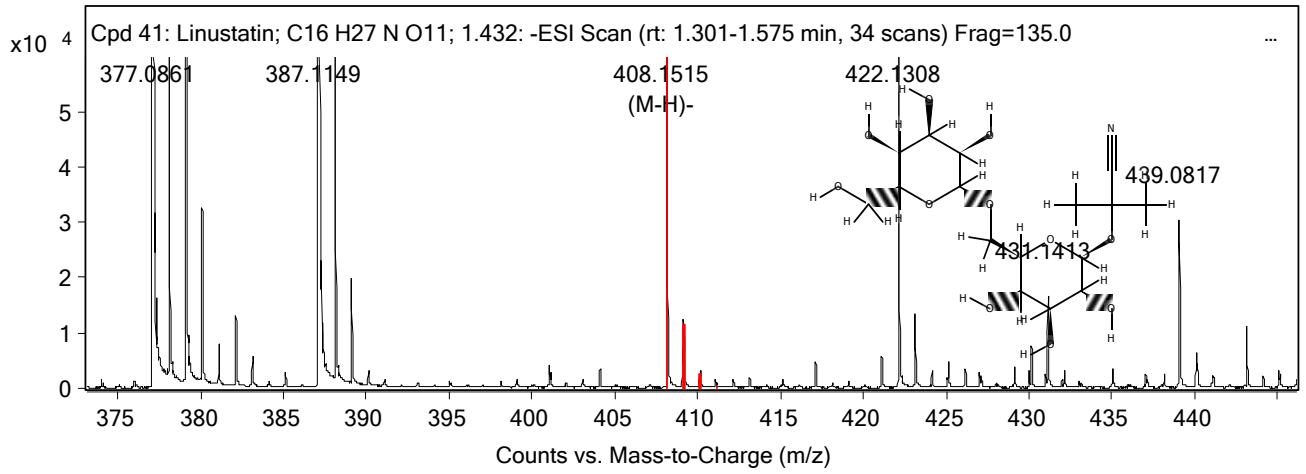
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
408.151	-1	61573.04	C16 H27 N O11	(M-H)-
409.1531	-1	12598.63	C16 H27 N O11	(M-H)-
410.1544	-1	2738.74	C16 H27 N O11	(M-H)-
411.1503	-1	528.07	C16 H27 N O11	(M-H)-

MS Spectrum



MS Zoomed Spectrum

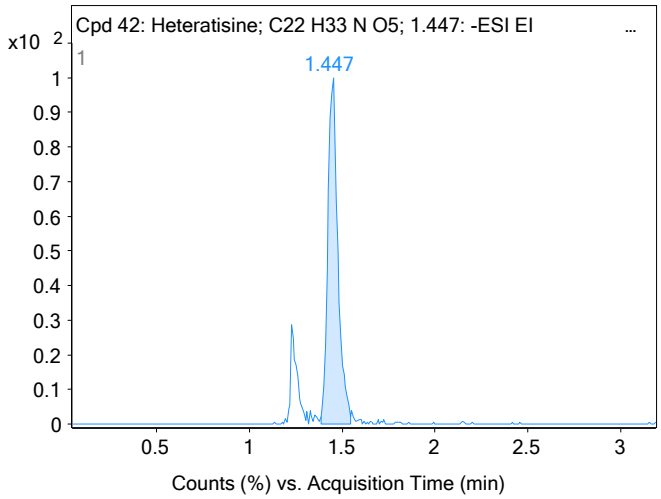


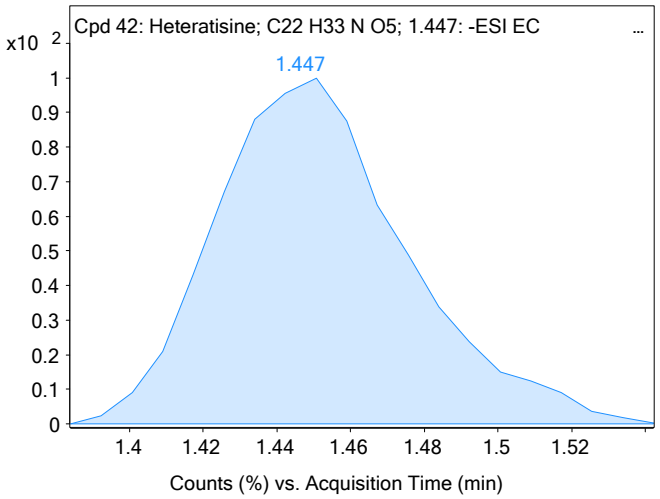
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Linustatin	1.432	C16 H27 N O11		96.87	409.1579	0.46	(M-H)-

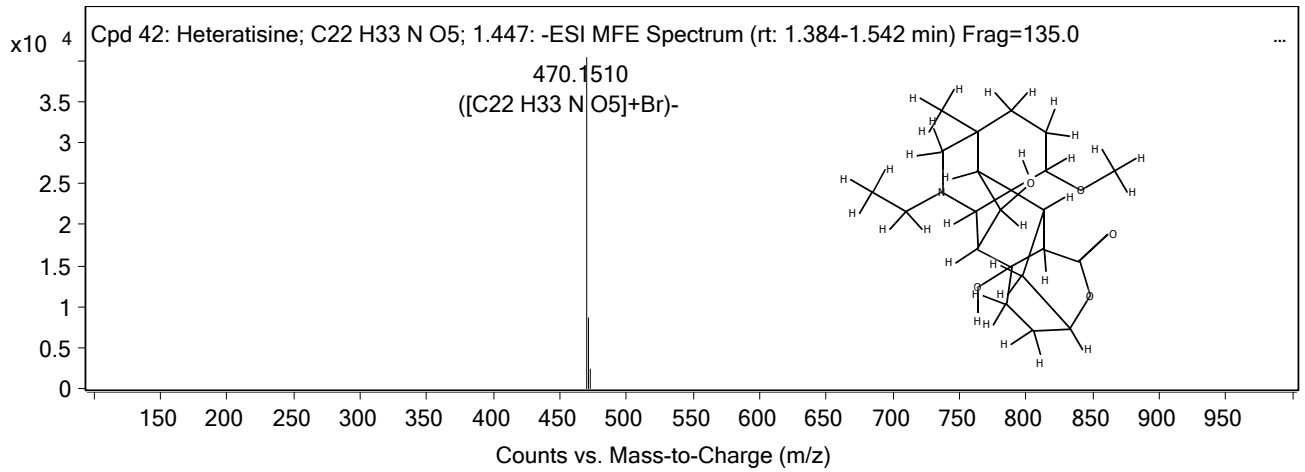
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 42: Heteratisine; C22 H33 N O5; 1.447	**Heteratisine**	470.151	1.447	Find by Molecular Feature	391.2323

Compound Chromatograms

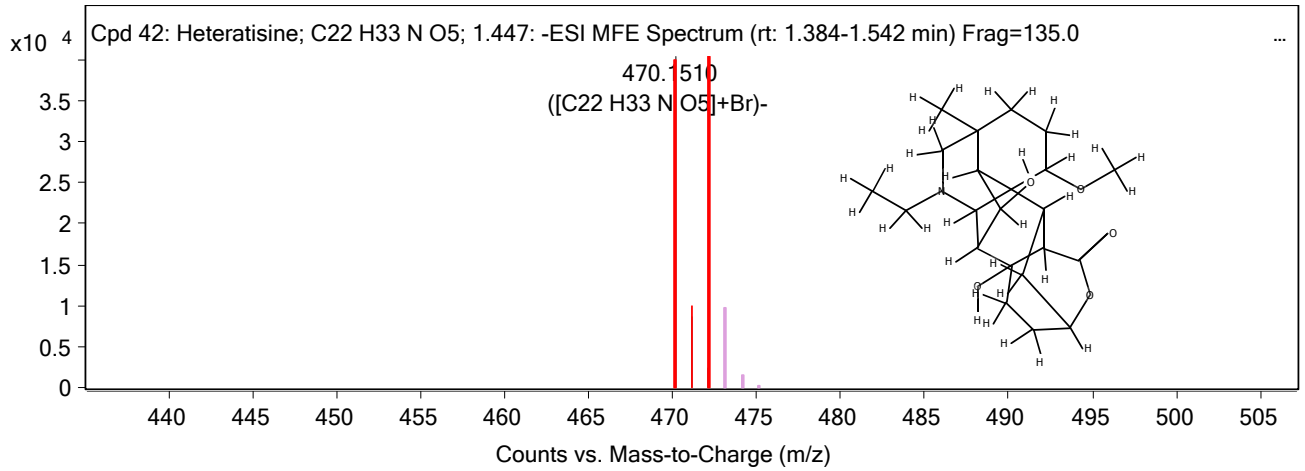




MFE MS Spectrum



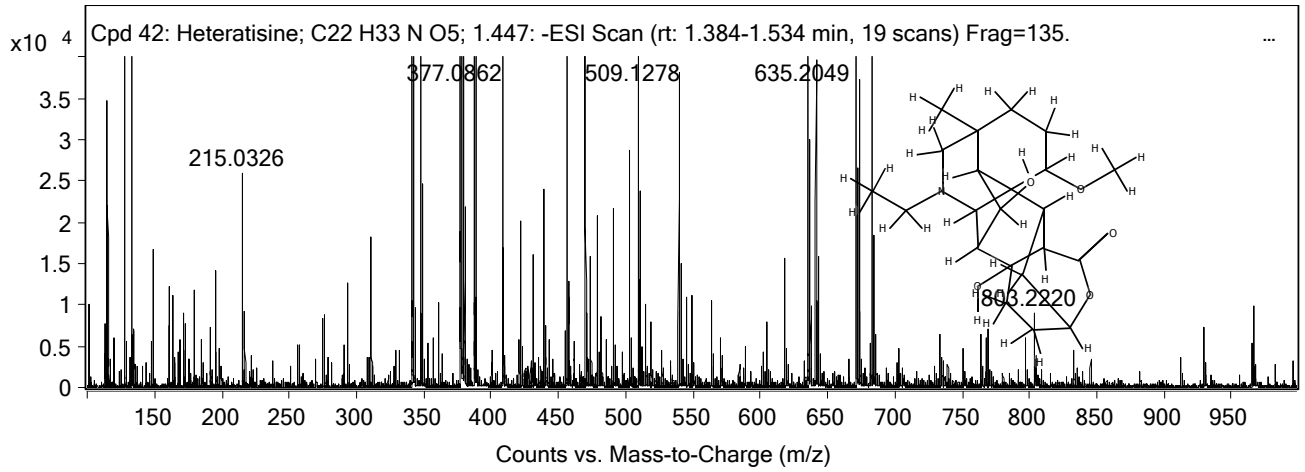
MFE MS Zoomed Spectrum



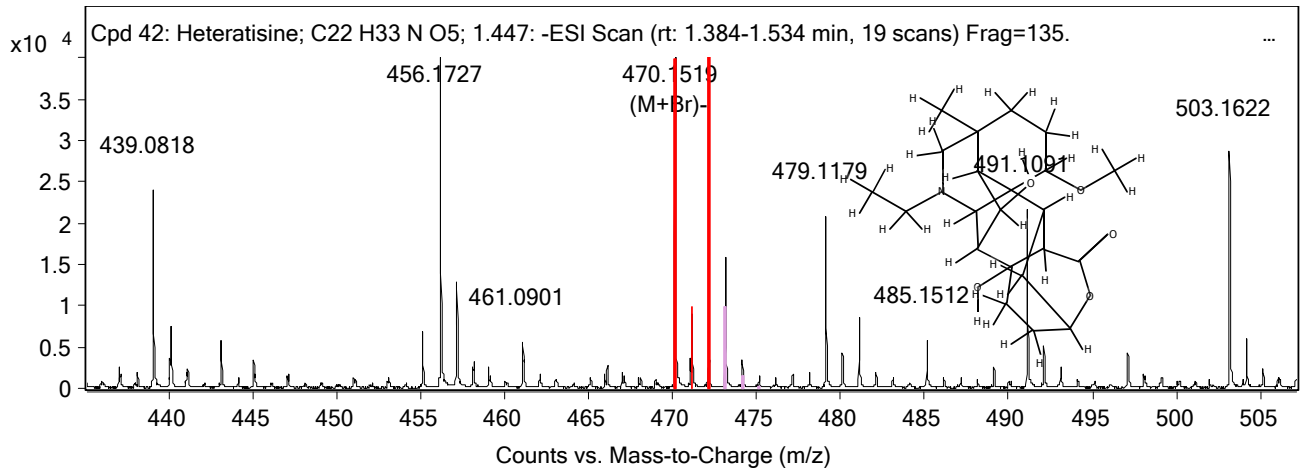
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
470.151	-1	40379.03	C22 H33 N O5	(M+Br)-
471.1537	-1	8707.79	C22 H33 N O5	(M+Br)-
472.1558	-1	2312.2	C22 H33 N O5	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

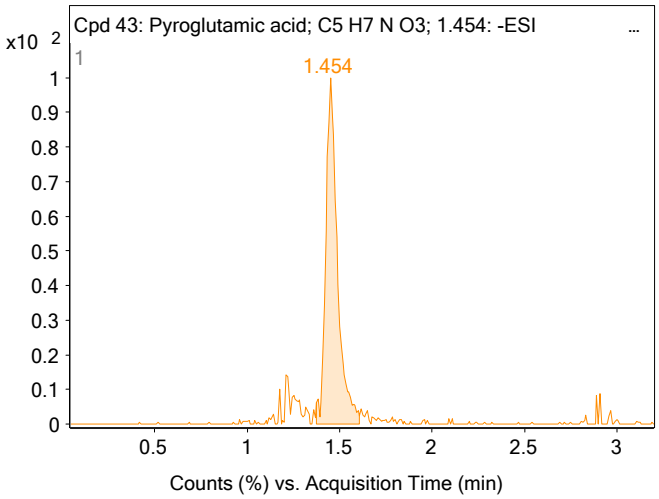


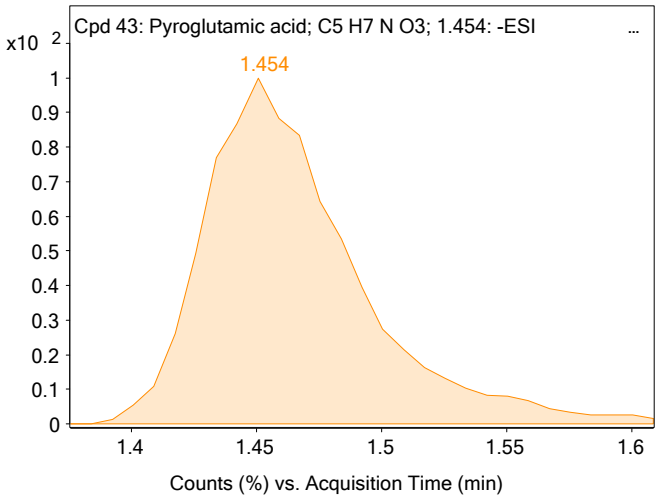
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Heteratisine	1.447	C22 H33 N O5		42.43	391.2323	3.55	(M+Br)-

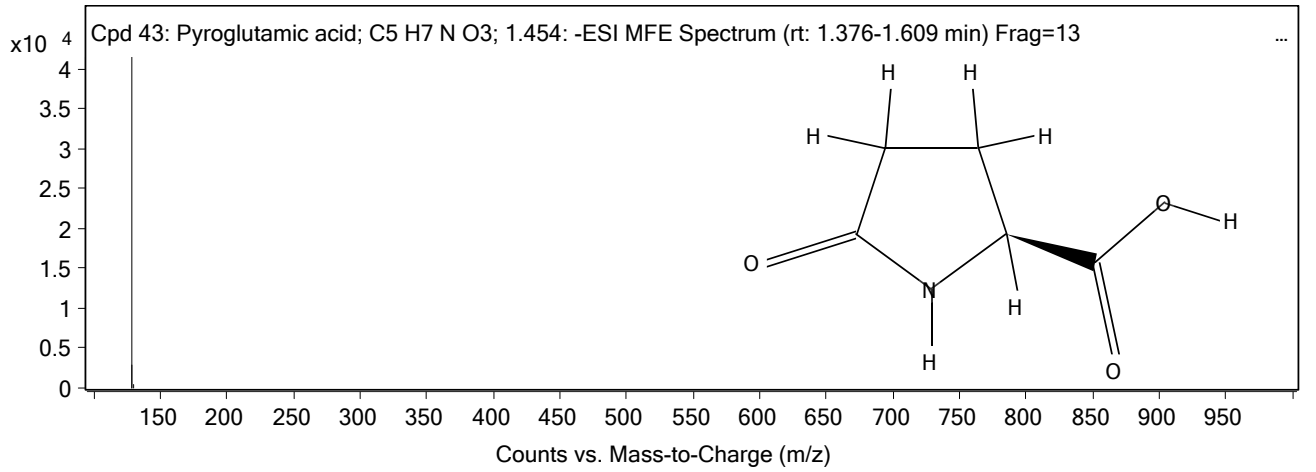
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 43: Pyroglutamic acid; C5 H7 N O3; 1.454	**Pyroglutamic acid**	128.0352	1.454	Find by Molecular Feature	129.0421

Compound Chromatograms

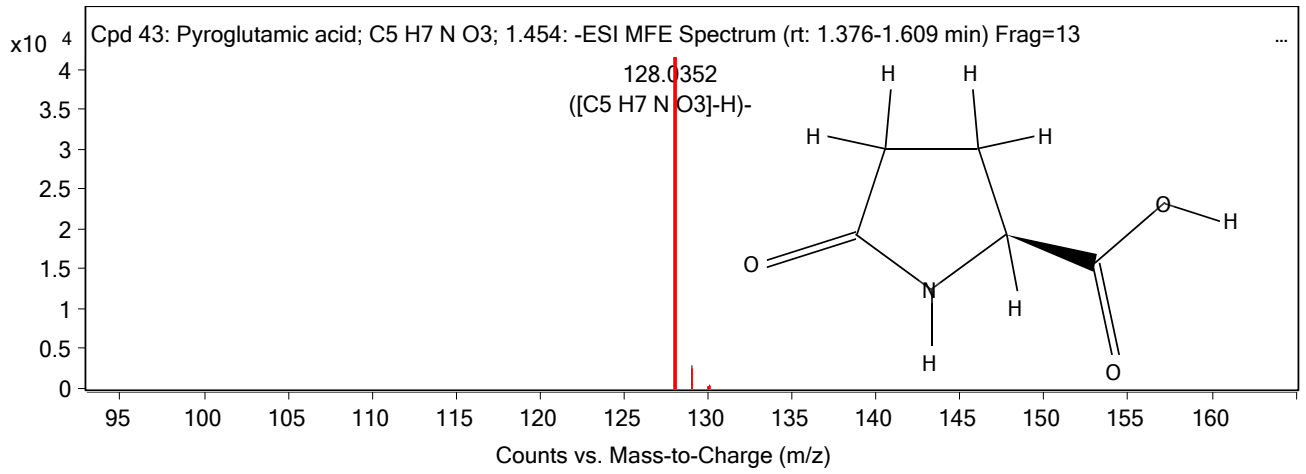




MFE MS Spectrum



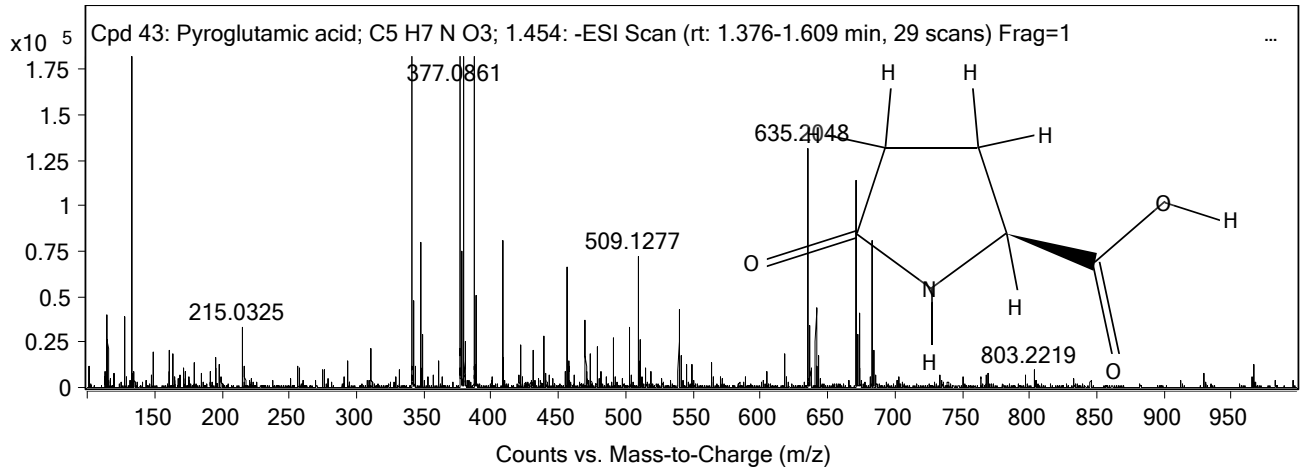
MFE MS Zoomed Spectrum



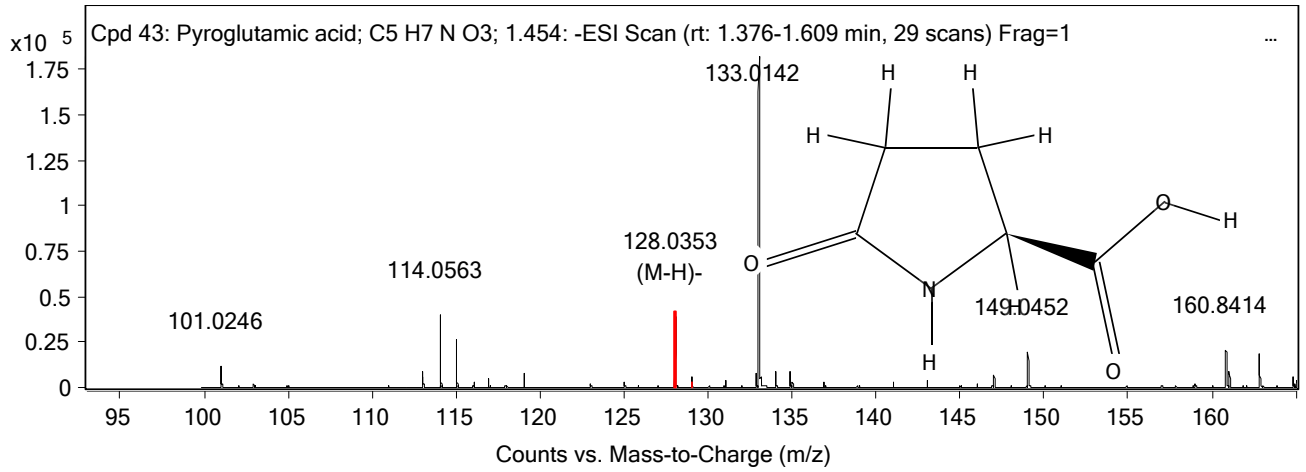
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
128.0352	-1	41476.82	C5 H7 N O3	(M-H)-
129.0318	-1	2897.02	C5 H7 N O3	(M-H)-
130.0413	-1	419.16	C5 H7 N O3	(M-H)-

MS Spectrum



MS Zoomed Spectrum



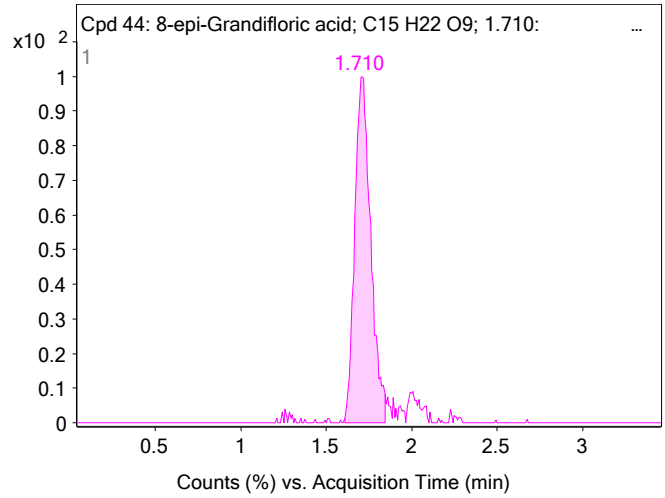
Identification Hit Table

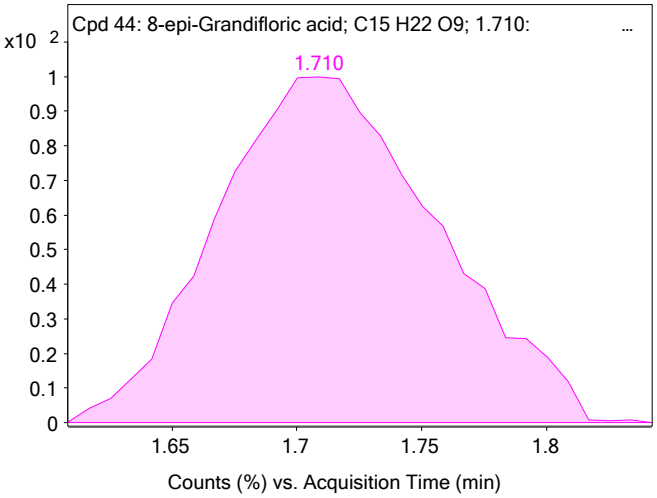
Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Pyroglutamic acid	1.454	C5 H7 N O3		88.59	129.0421	0.48	(M-H)-

Qualitative Compound Identification Report

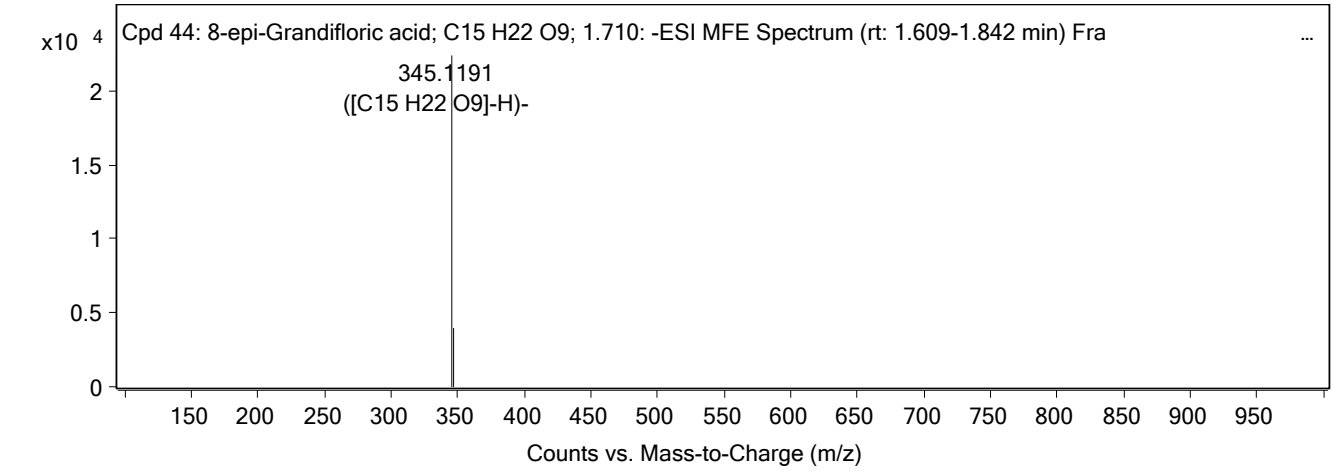
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 44: 8-epi-Grandifloric acid; C15 H22 O9; 1.710	**8-epi-Grandifloric acid**	345.1191	1.71	Find by Molecular Feature	346.1263

Compound Chromatograms

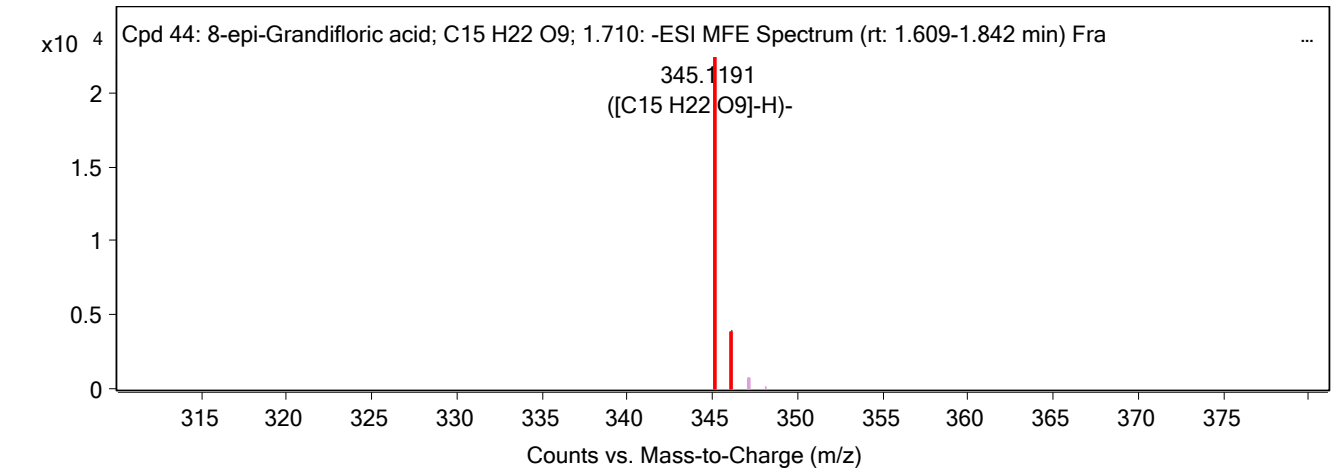




MFE MS Spectrum



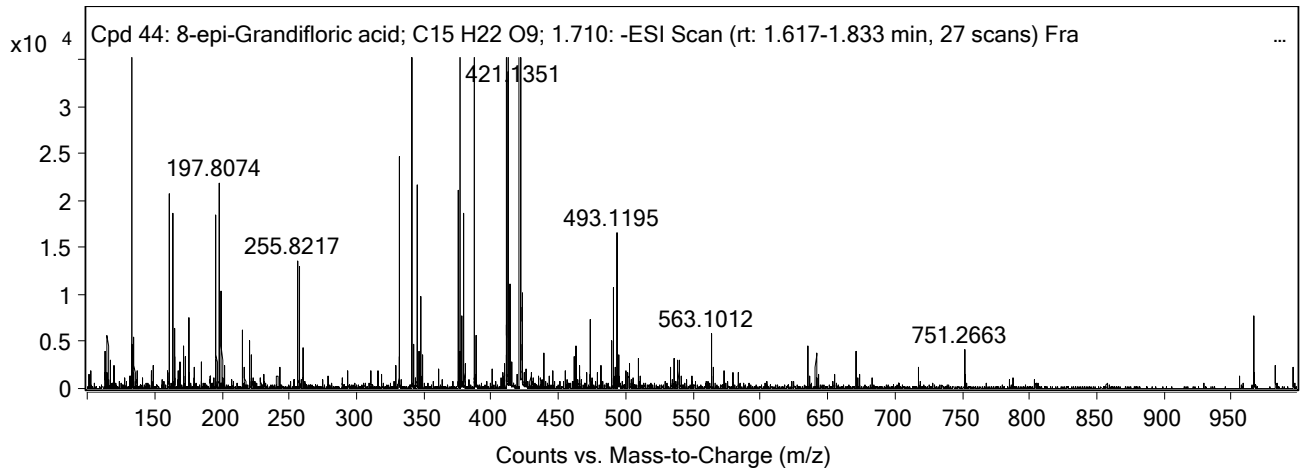
MFE MS Zoomed Spectrum



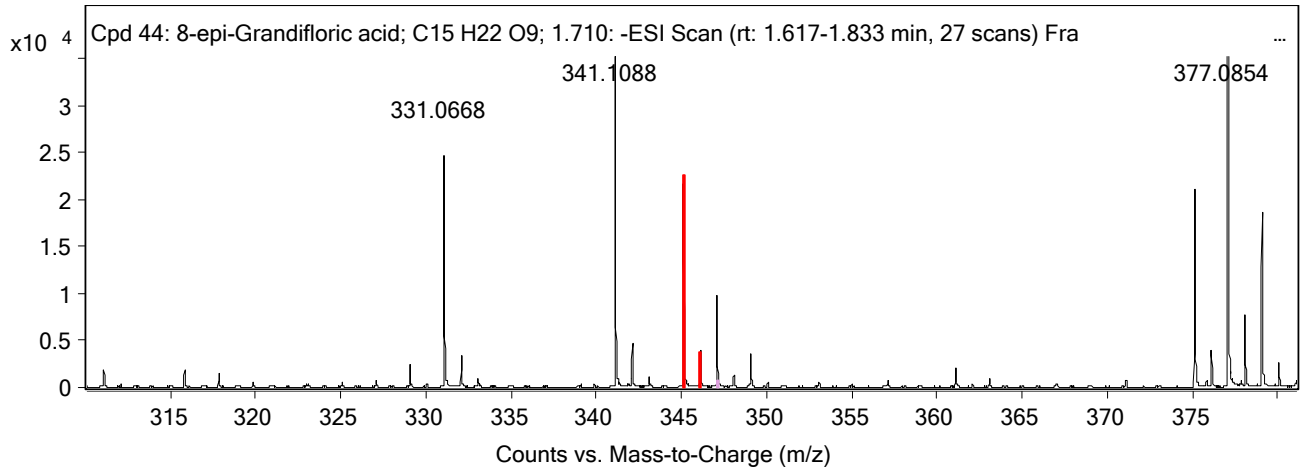
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
345.1191	-1	22350.85	C15 H22 O9	(M-H)-
346.1222	-1	3979.23	C15 H22 O9	(M-H)-

MS Spectrum



MS Zoomed Spectrum

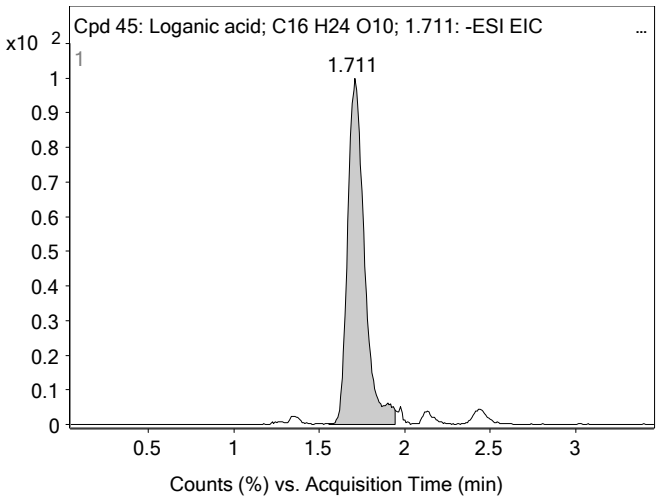


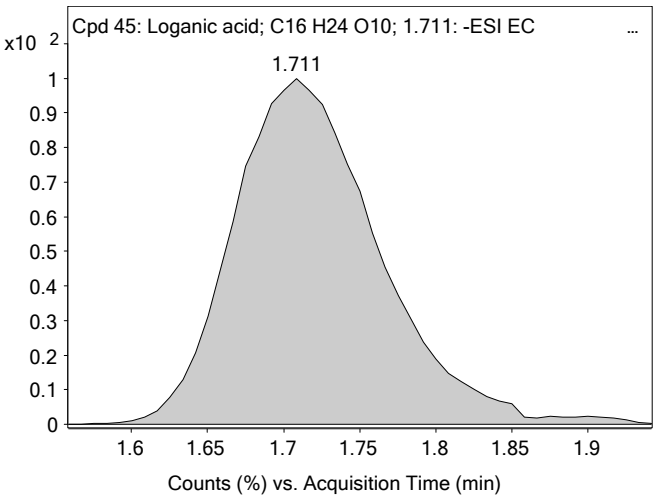
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	8-epi-Grandifloric acid	1.71	C15 H22 O9		84.05	346.1263	0.05	(M-H)-
	Aucubin	1.71	C15 H22 O9		84.05	346.1263	0.05	(M-H)-
	Pedicularis-lactone-1-O-beta-D-glucoside	1.71	C15 H22 O9		84.05	346.1263	0.05	(M-H)-
	Jioglutoside A	1.71	C15 H22 O9		84.05	346.1263	0.05	(M-H)-

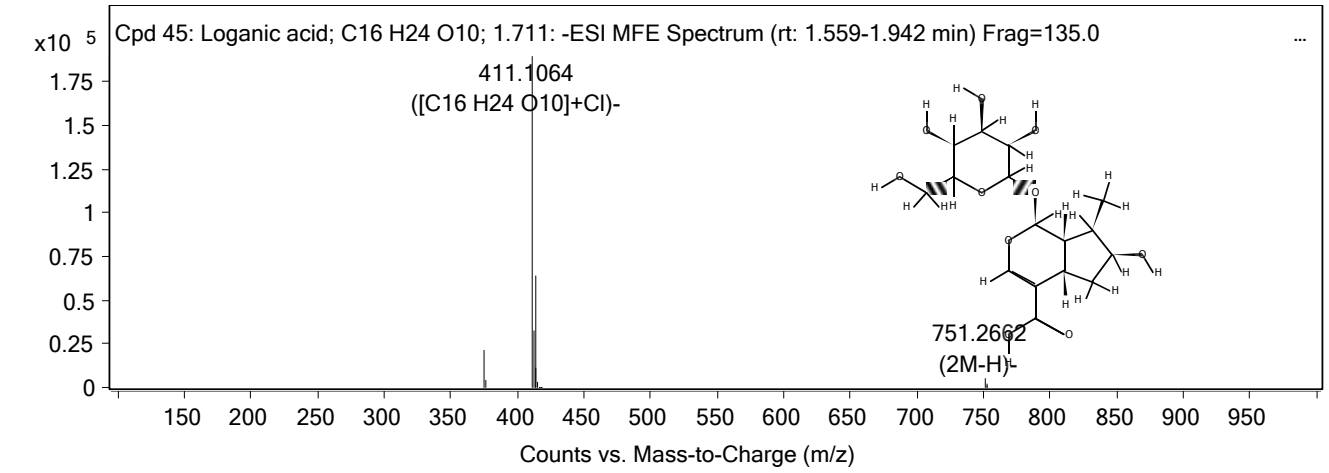
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 45: Loganic acid; C16 H24 O10; 1.711	**Loganic acid**	411.1064	1.711	Find by Molecular Feature	376.137

Compound Chromatograms

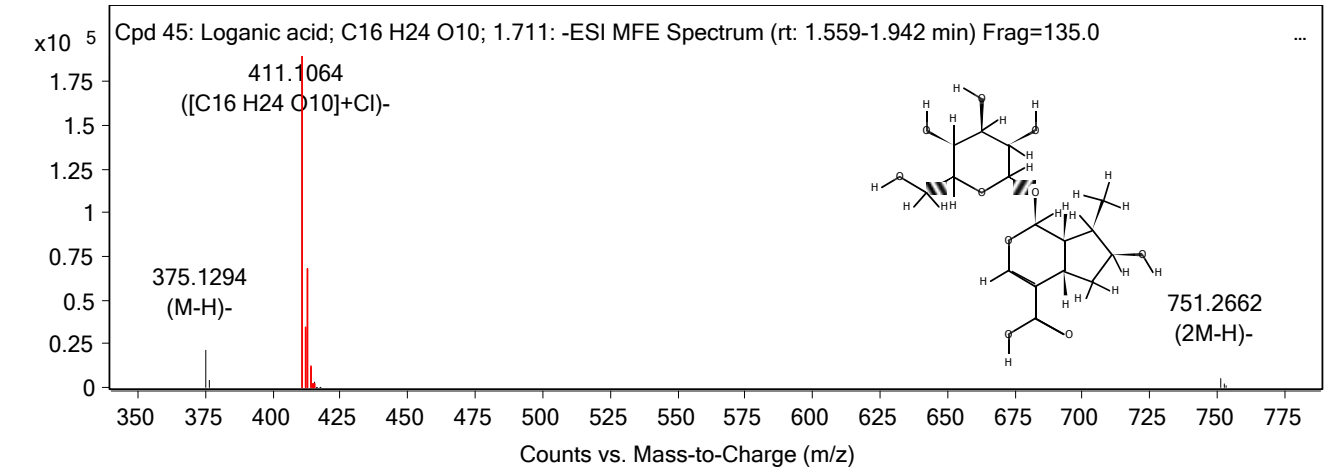




MFE MS Spectrum



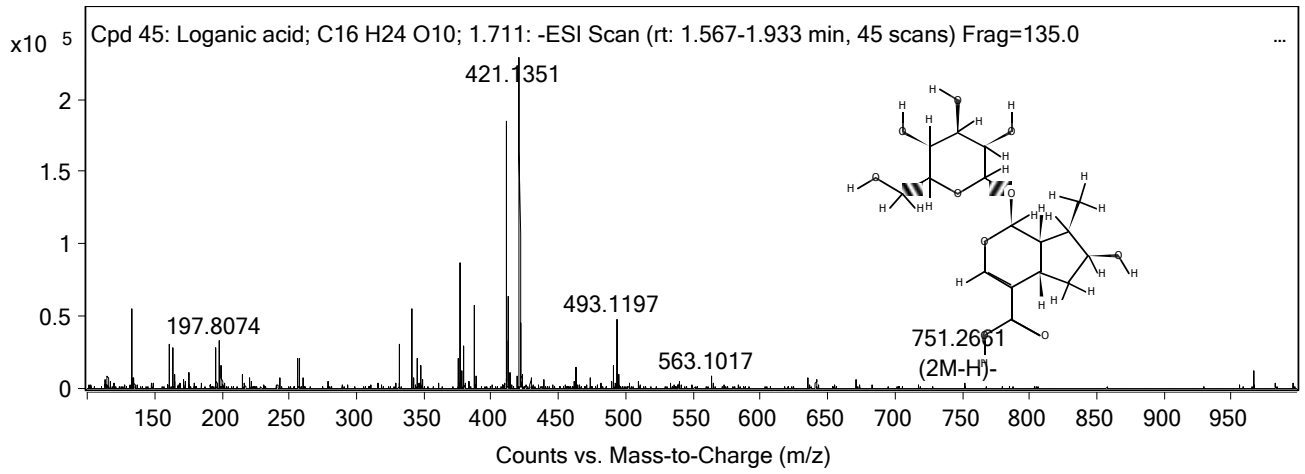
MFE MS Zoomed Spectrum



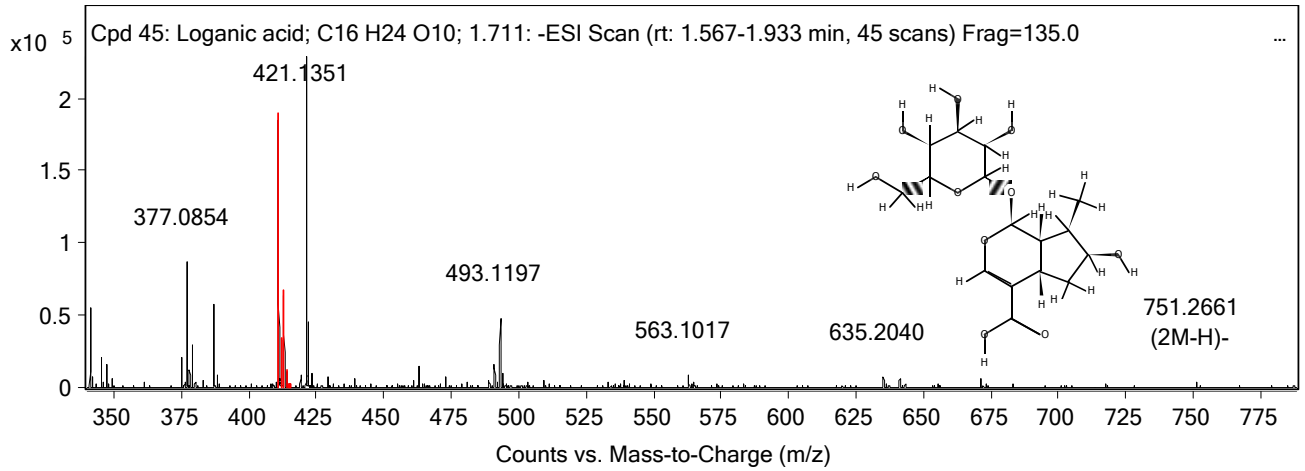
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
375.1294	-1	20839.43		(M-H)-
376.1327	-1	3901.89		(M-H)-
411.1064	-1	189497.22	C16 H24 O10	(M+Cl)-
412.1093	-1	32869.8	C16 H24 O10	(M+Cl)-
413.1043	-1	64184.61	C16 H24 O10	(M+Cl)-
414.1073	-1	10860.69	C16 H24 O10	(M+Cl)-
415.1162	-1	2800.23	C16 H24 O10	(M+Cl)-
751.2662	-1	5149.35		(2M-H)-
752.2682	-1	1880.22		(2M-H)-
753.2703	-1	692.21		(2M-H)-

MS Spectrum



MS Zoomed Spectrum

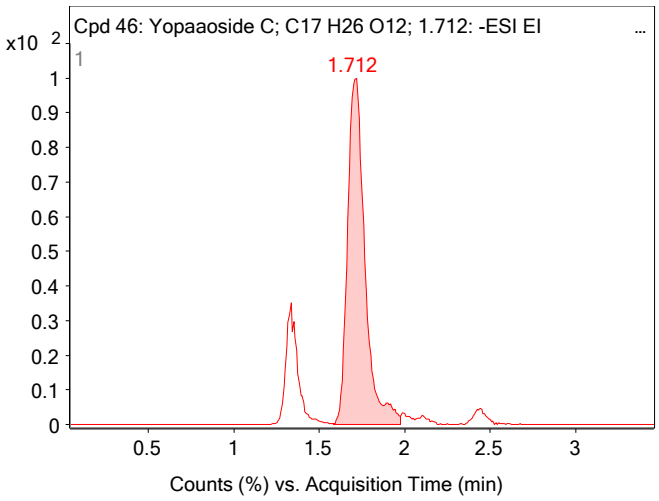


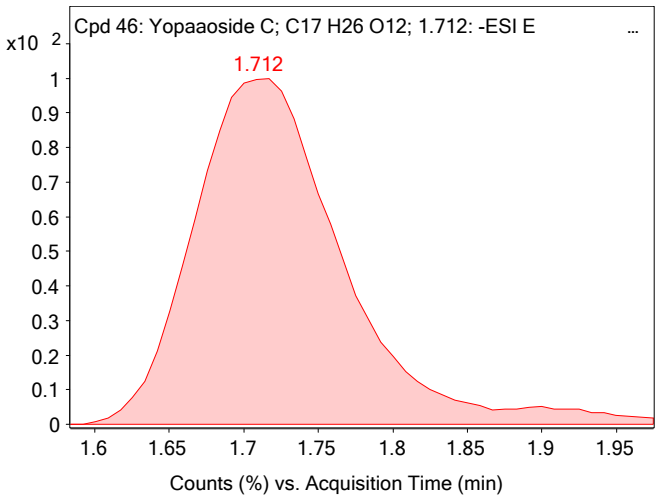
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Loganic acid	1.711	C16 H24 O10		99.35	376.137	-0.07	(M+Cl)-
	8-Hydroxy-10-hydrosweroside	1.711	C16 H24 O10		99.35	376.137	-0.07	(M+Cl)-
	8-Epiloganic acid	1.711	C16 H24 O10		99.35	376.137	-0.07	(M+Cl)-
	8-Diebenzoylpaeoniflorin	1.711	C16 H24 O10		99.35	376.137	-0.07	(M+Cl)-
	6-O-Methyl catalpol	1.711	C16 H24 O10		99.35	376.137	-0.07	(M+Cl)-
	Vitamin B2	1.711	C17 H20 N4 O6		94.99	376.1371	1.16	(M+Cl)-
	Riboflavin	1.711	C17 H20 N4 O6		94.99	376.1371	1.16	(M+Cl)-

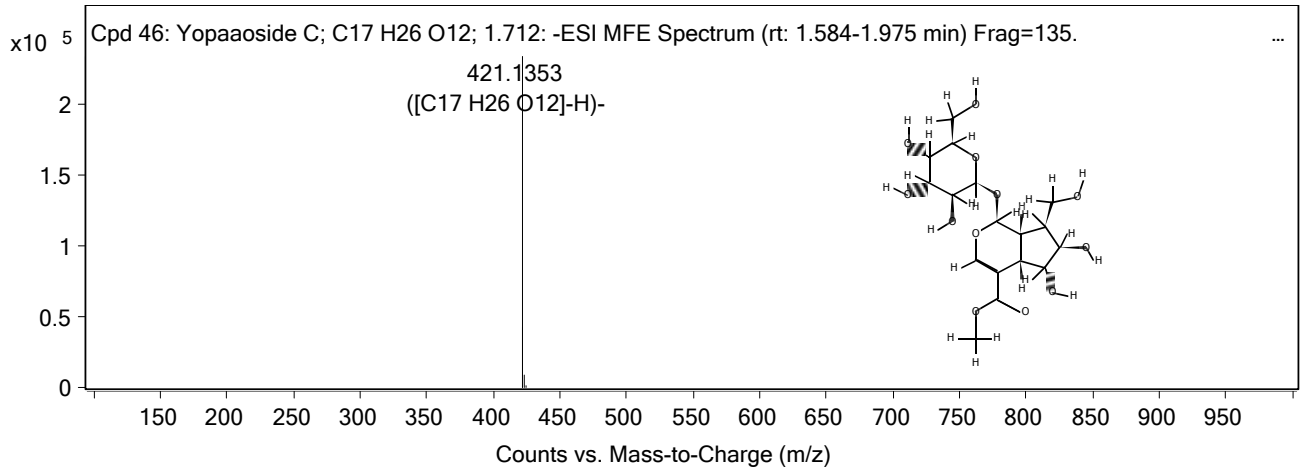
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 46: Yopaaoside C; C17 H26 O12; 1.712	**Yopaaoside C**	421.1353	1.712	Find by Molecular Feature	422.1424

Compound Chromatograms

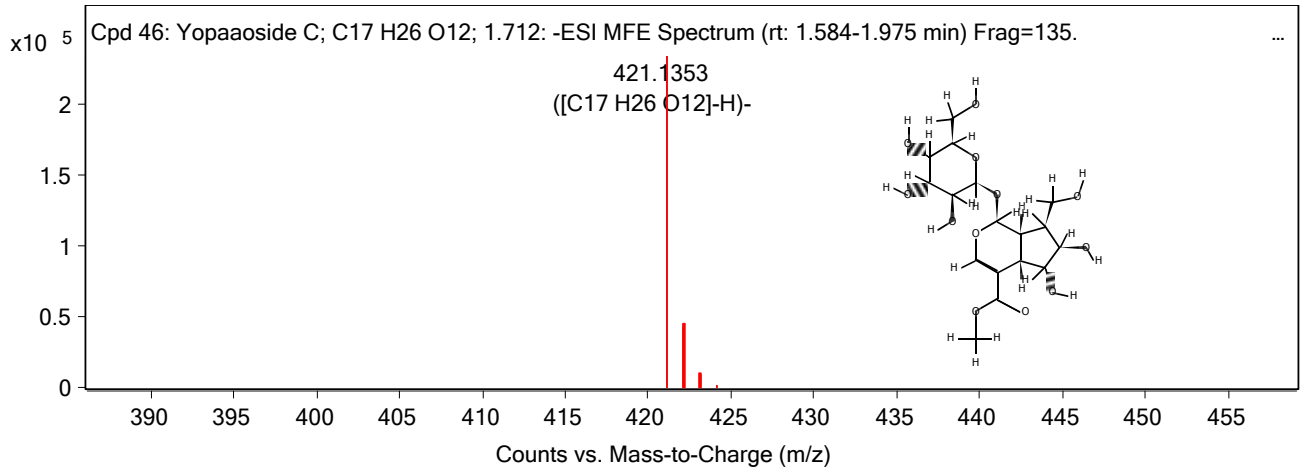




MFE MS Spectrum



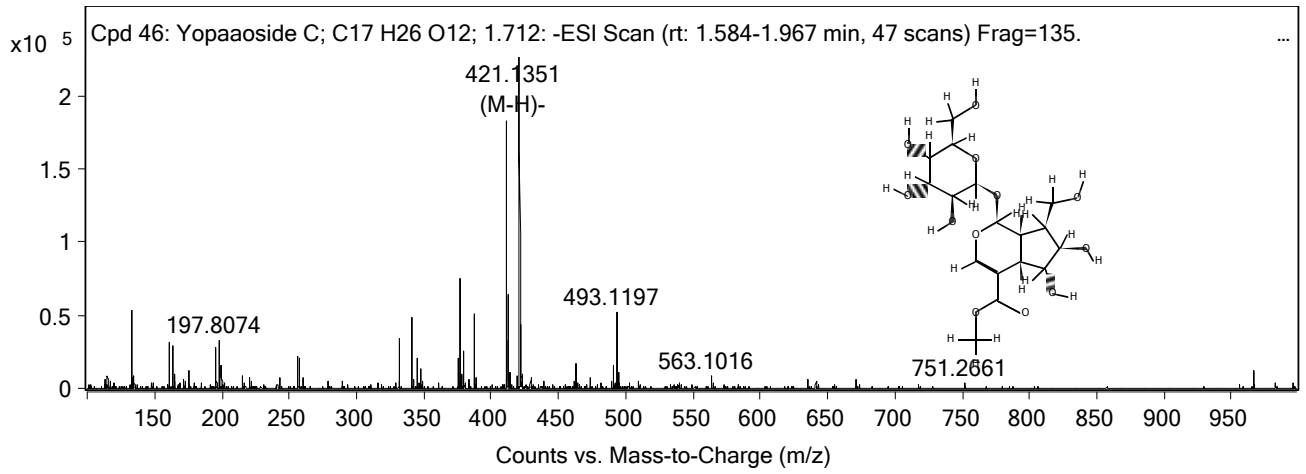
MFE MS Zoomed Spectrum



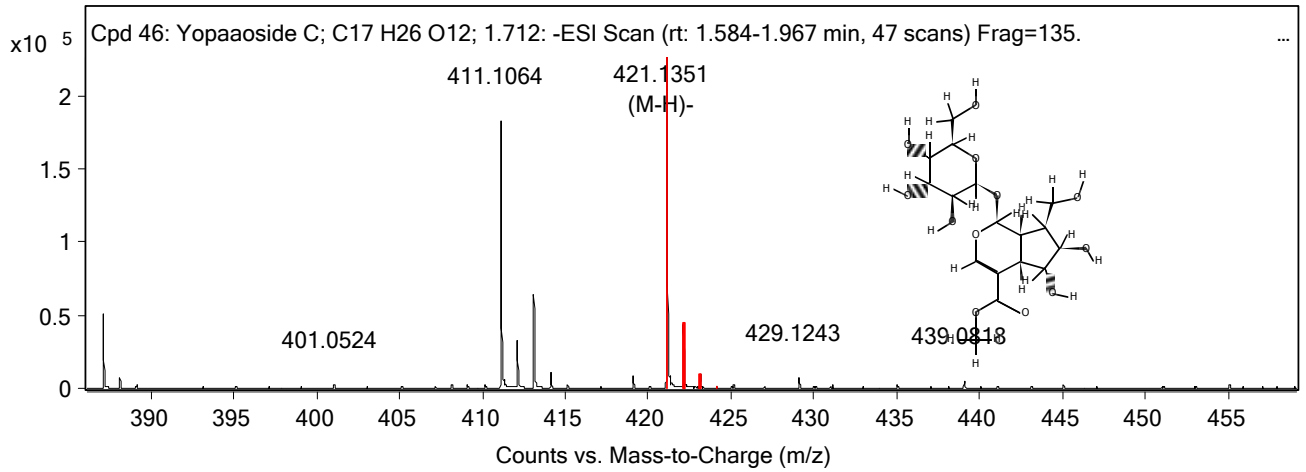
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
421.1353	-1	233688.47	C17 H26 O12	(M-H)-
422.1381	-1	43065.36	C17 H26 O12	(M-H)-
423.1404	-1	9432.05	C17 H26 O12	(M-H)-
424.1428	-1	1447.05	C17 H26 O12	(M-H)-

MS Spectrum



MS Zoomed Spectrum

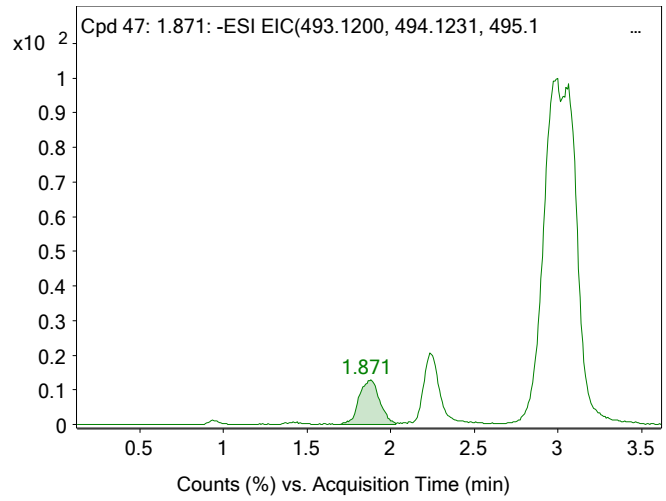


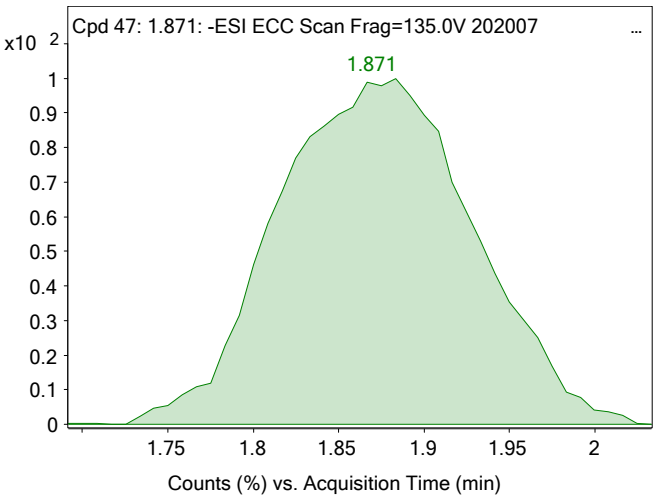
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Yopaaoside C	1.712	C17 H26 O12		99.51	422.1424	0	(M-H)-
	Lamiide	1.712	C17 H26 O12		99.51	422.1424	0	(M-H)-
	Guggulsterone M	1.712	C22 H30 O3		47.52	342.2165	2.95	(M+Br)-
	Anacardic acid D	1.712	C22 H30 O3		47.52	342.2165	2.95	(M+Br)-

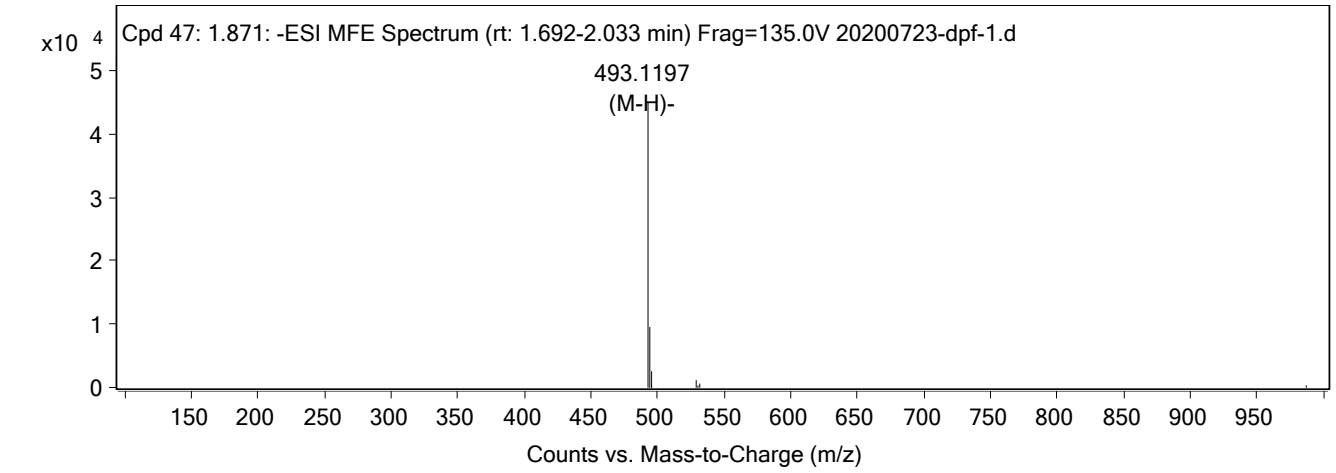
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 47: 1.871	493.1197	1.871	Find by Molecular Feature	494.1268

Compound Chromatograms

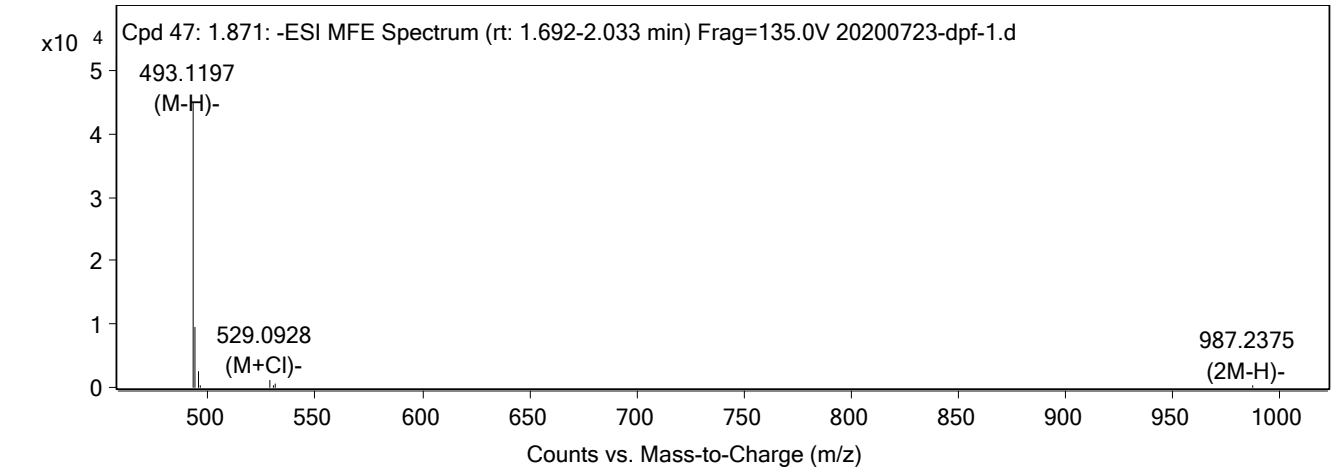




MFE MS Spectrum



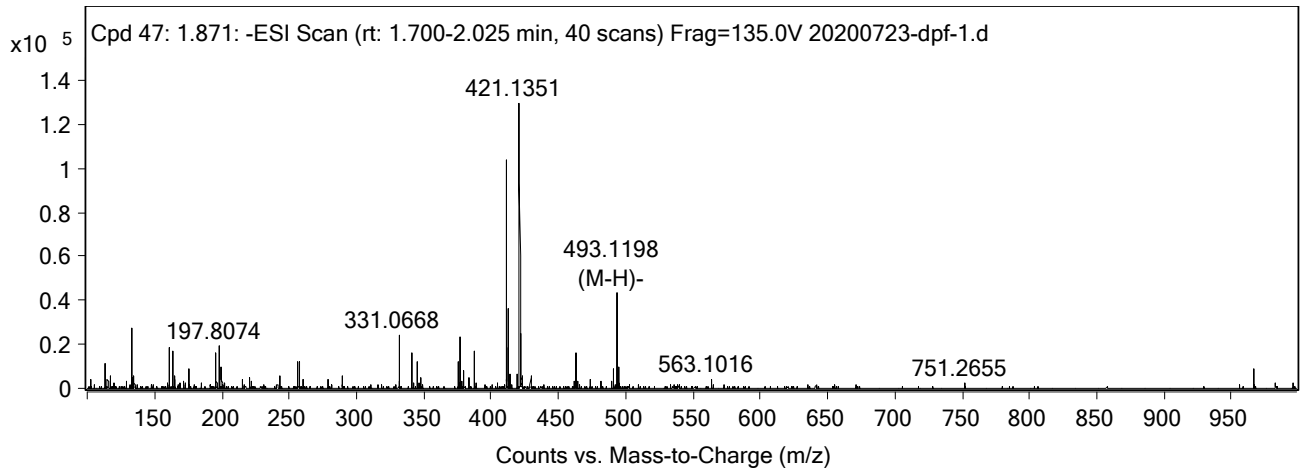
MFE MS Zoomed Spectrum



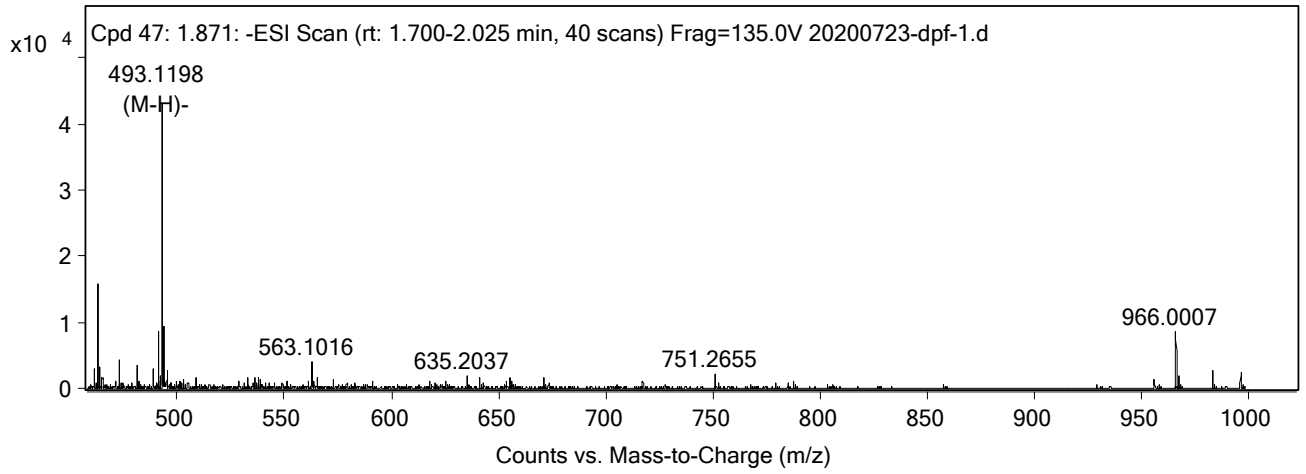
MS Spectrum Peak List

m/z	z	Abund	Ion
493.1197	-1	45061.54	(M-H)-
494.1228	-1	9558.9	(M-H)-
495.1236	-1	2574.95	(M-H)-
496.128	-1	415.18	(M-H)-
529.0928	-1	1215.7	(M+Cl)-
530.0971	-1	365.84	(M+Cl)-
531.0931	-1	537.86	(M+Cl)-
987.2375	-1	291.5	(2M-H)-

MS Spectrum

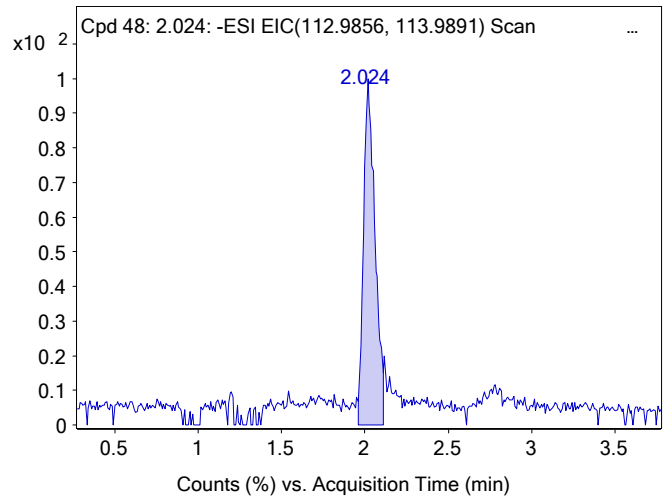


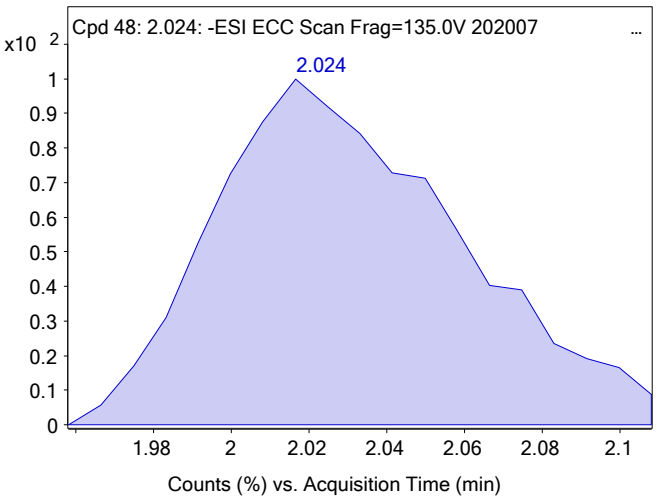
MS Zoomed Spectrum



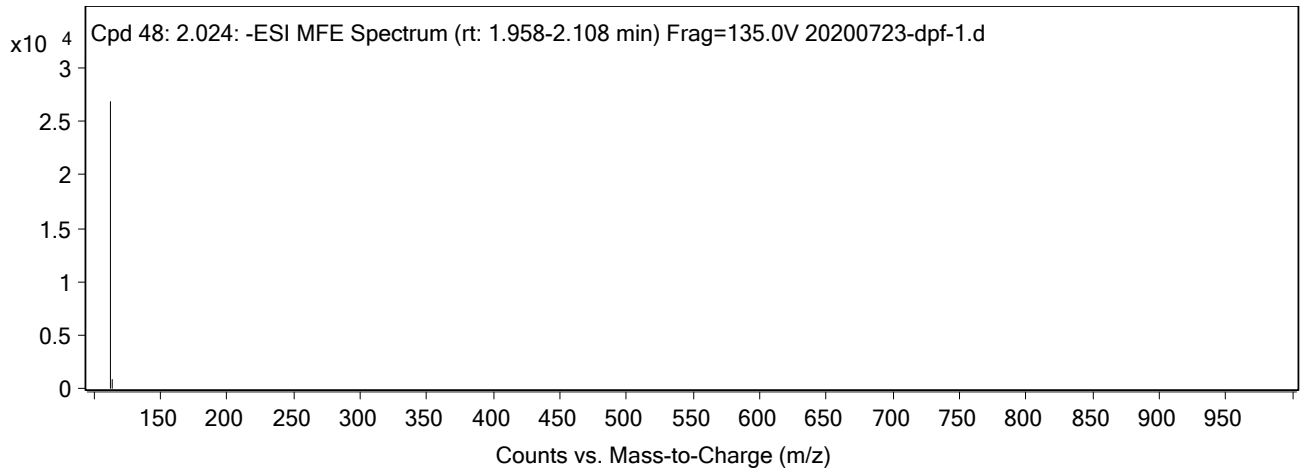
Compound Label	m/z	RT	Algorithm	Mass
Cpd 48: 2.024	112.9856	2.024	Find by Molecular Feature	113.9929

Compound Chromatograms

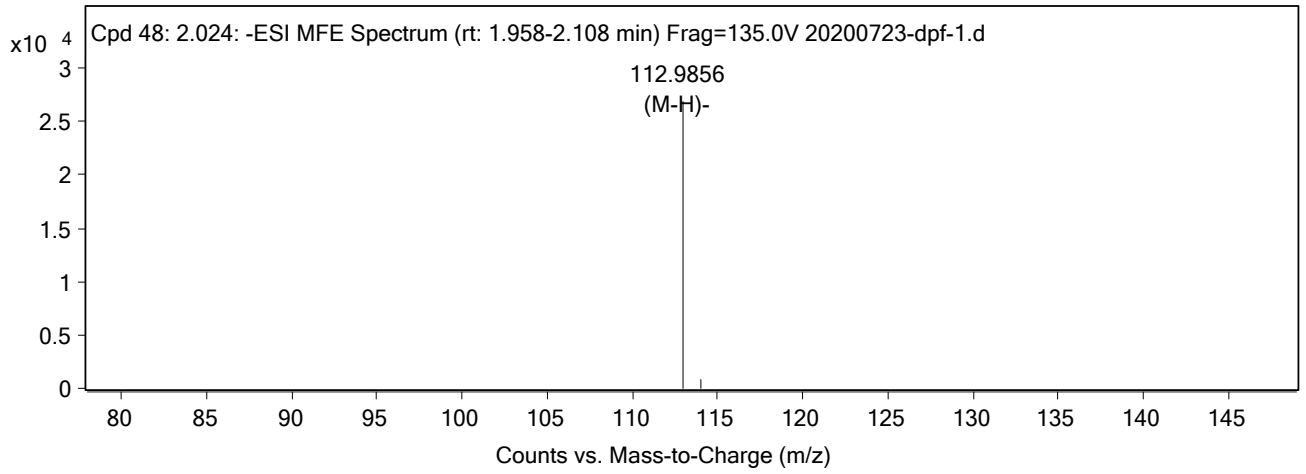




MFE MS Spectrum



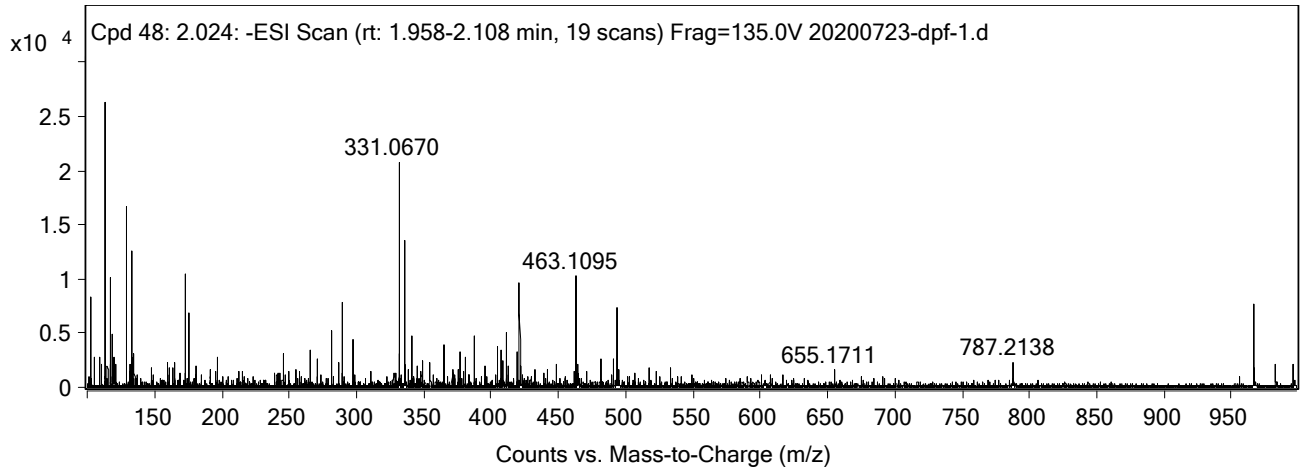
MFE MS Zoomed Spectrum



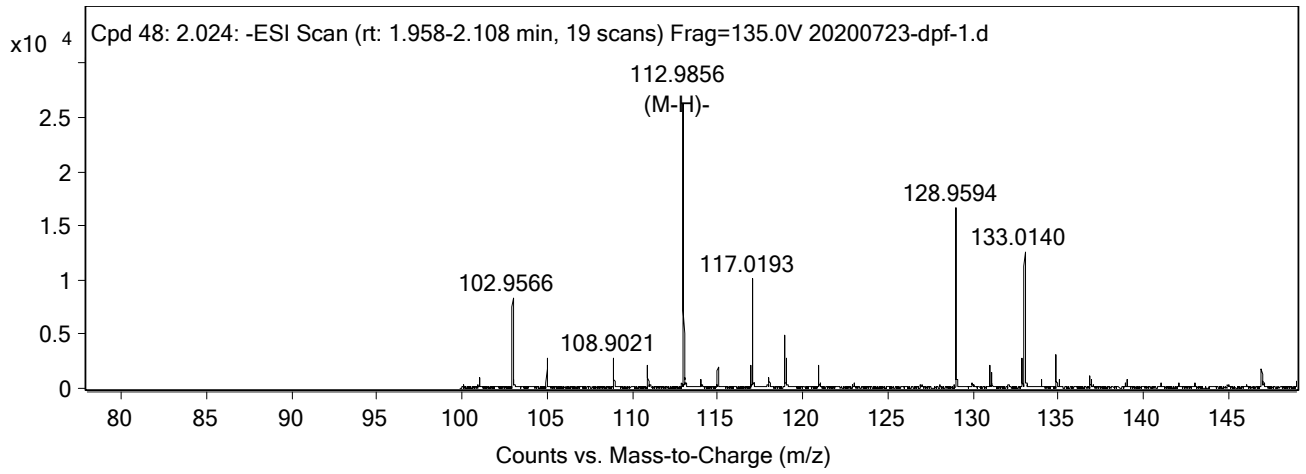
MS Spectrum Peak List

m/z	z	Abund	Ion
112.9856	-1	26835.29	(M-H)-
113.989	-1	878.12	(M-H)-

MS Spectrum

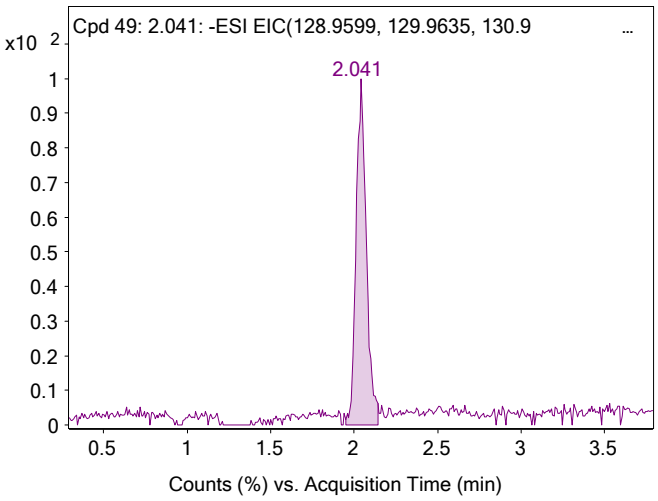


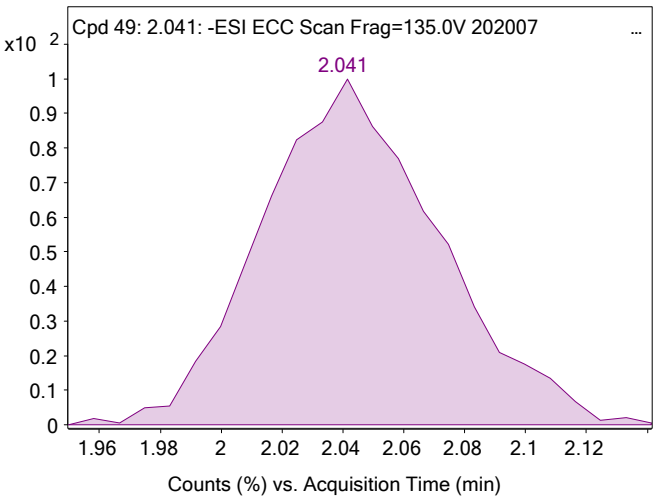
MS Zoomed Spectrum



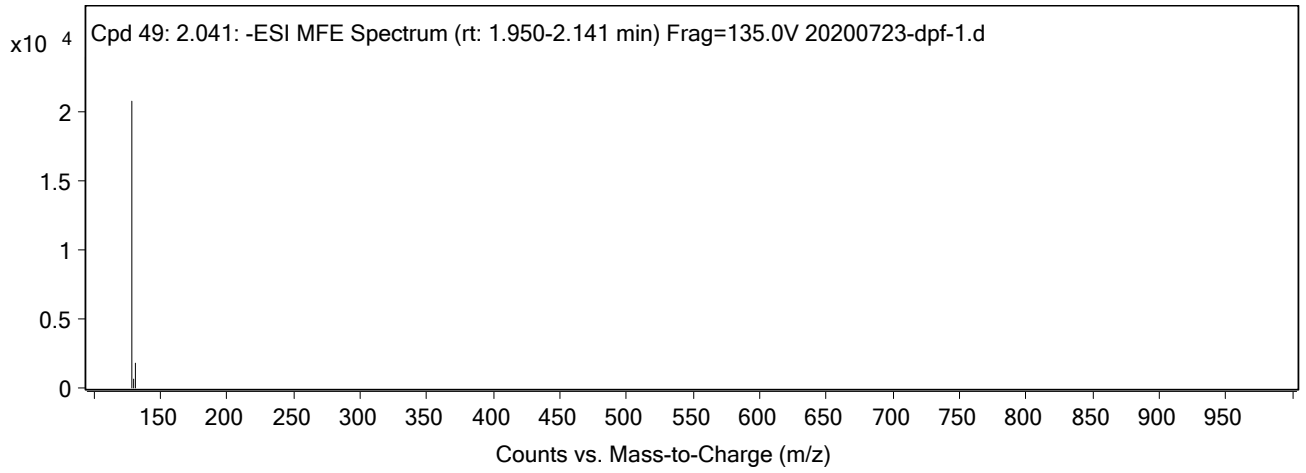
Compound Label	m/z	RT	Algorithm	Mass
Cpd 49: 2.041	128.9593	2.041	Find by Molecular Feature	129.9666

Compound Chromatograms

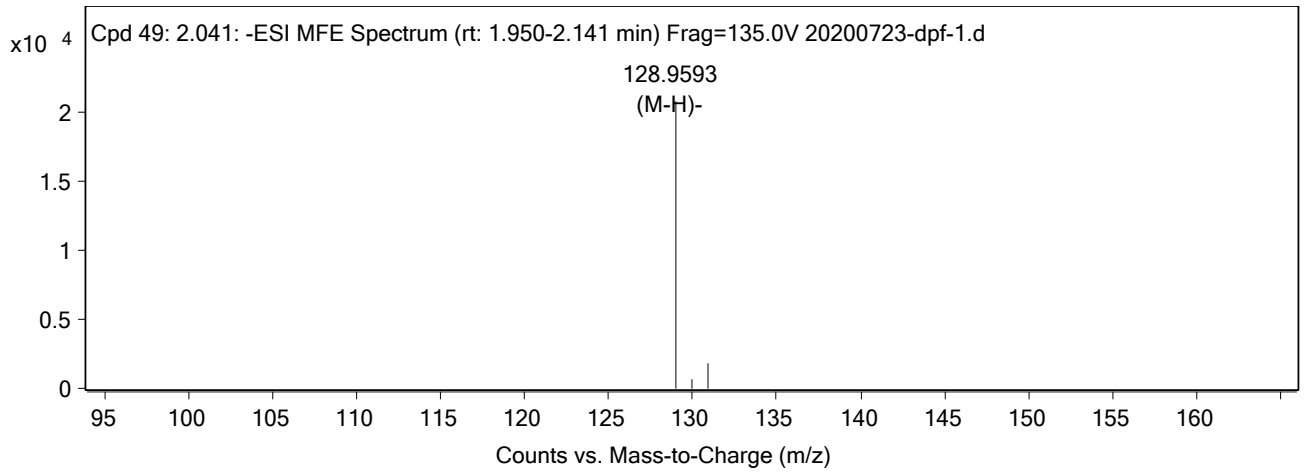




MFE MS Spectrum



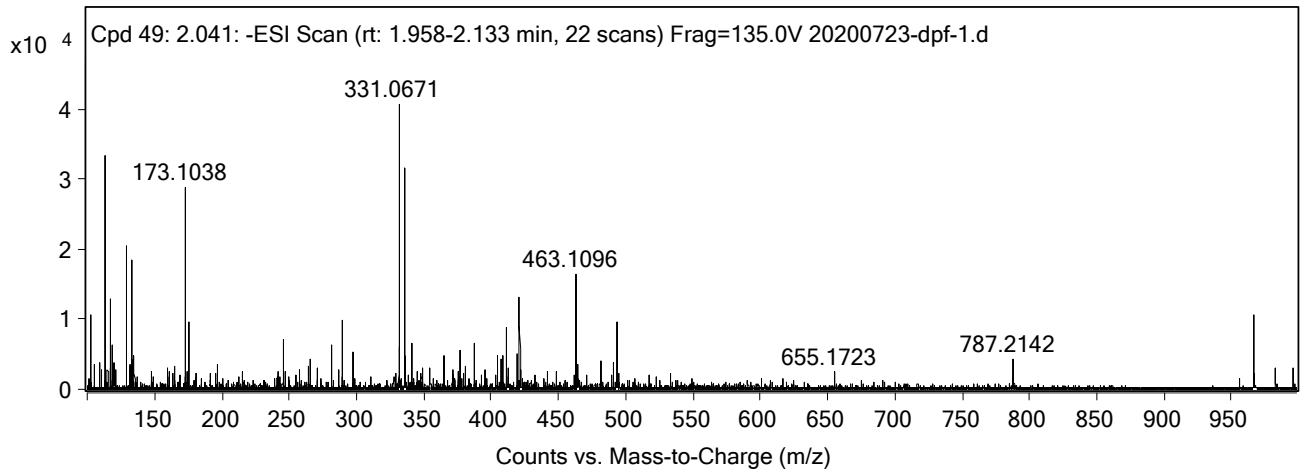
MFE MS Zoomed Spectrum



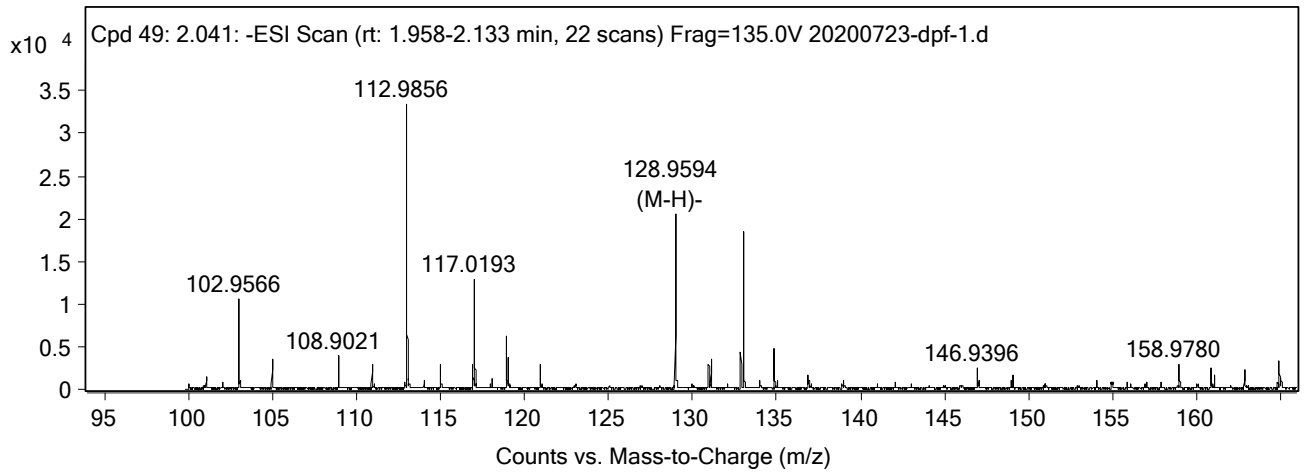
MS Spectrum Peak List

m/z	z	Abund	Ion
128.9593	-1	20745.53	(M-H)-
129.9629	-1	617.69	(M-H)-
130.9609	-1	1827.2	(M-H)-

MS Spectrum

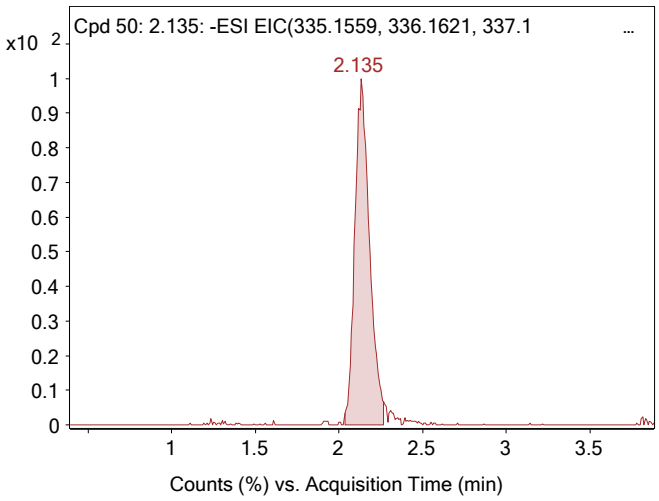


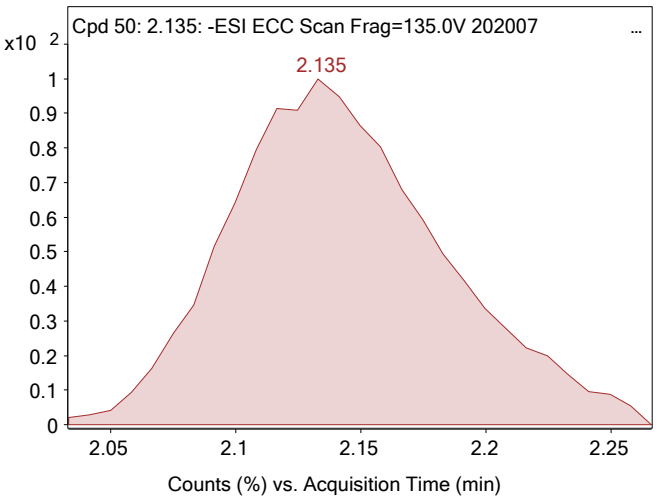
MS Zoomed Spectrum



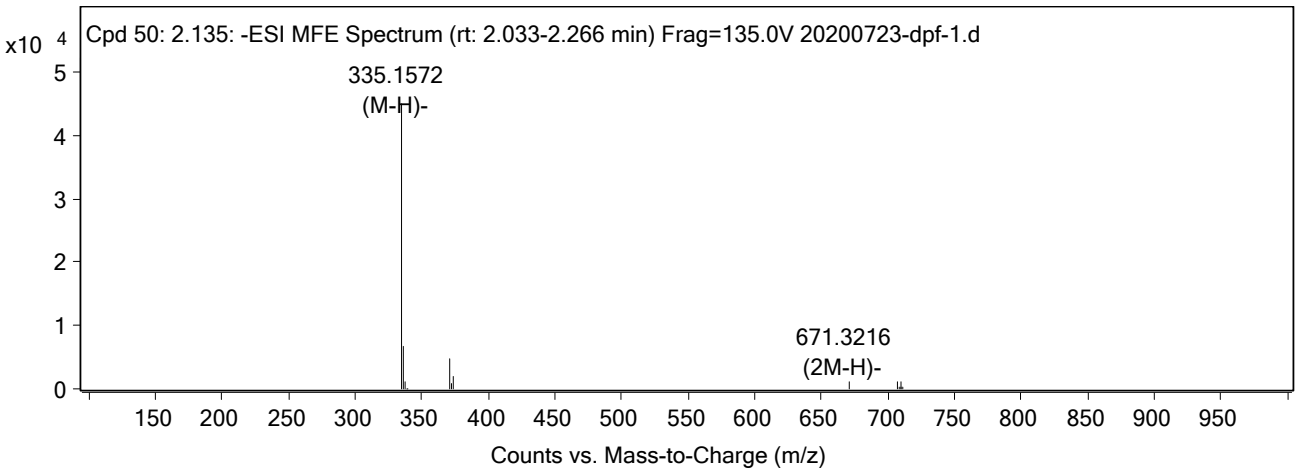
Compound Label	m/z	RT	Algorithm	Mass
Cpd 50: 2.135	335.1572	2.135	Find by Molecular Feature	336.1644

Compound Chromatograms

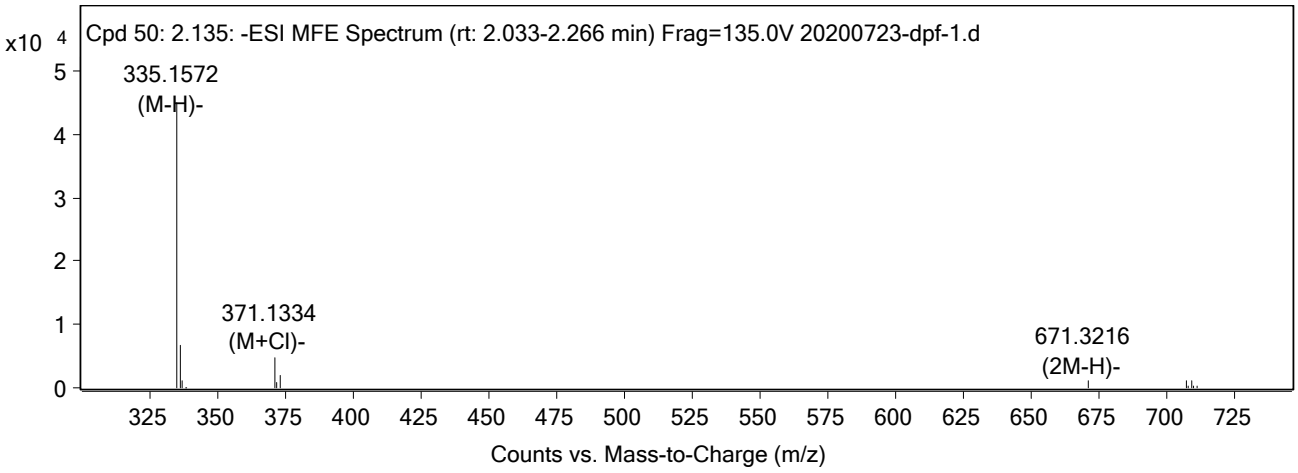




MFE MS Spectrum



MFE MS Zoomed Spectrum

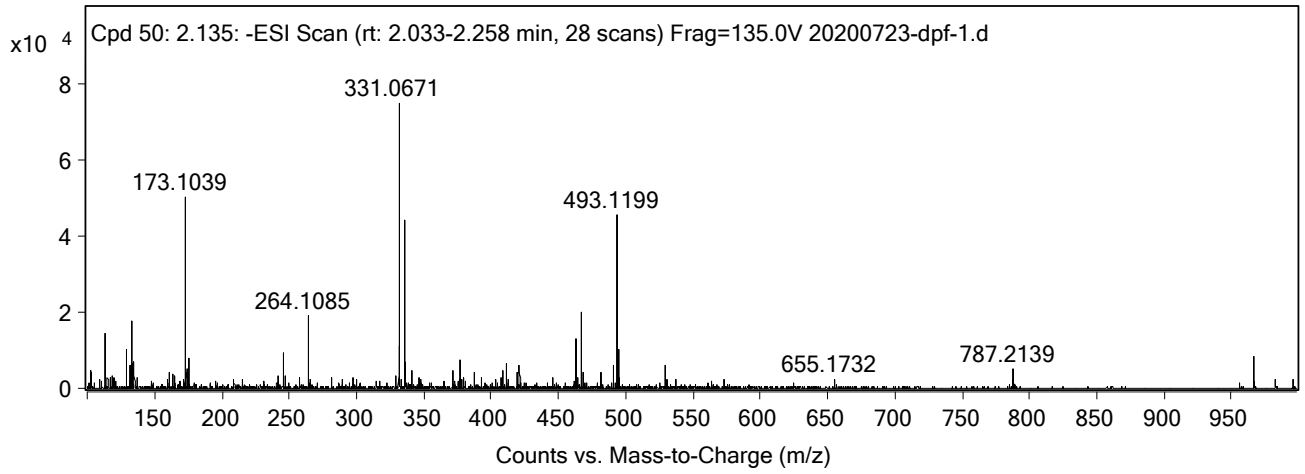


MS Spectrum Peak List

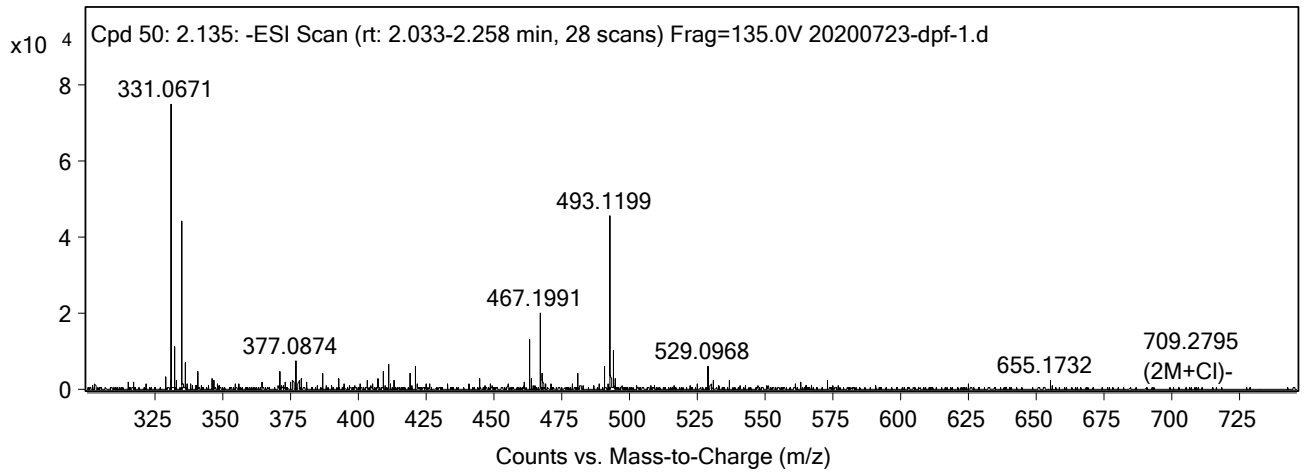
m/z	z	Abund	Ion
335.1572	-1	45069.3	(M-H)-
336.1599	-1	6834.7	(M-H)-
337.1619	-1	1231.24	(M-H)-
371.1334	-1	4904.95	(M+Cl)-
372.135	-1	852.9	(M+Cl)-
373.1298	-1	1845.64	(M+Cl)-

671.3216	-1	1063.19	(2M-H)-
707.2982	-1	1013.35	(2M+Cl)-
708.2986	-1	365.74	(2M+Cl)-
709.2828	-1	1025.11	(2M+Cl)-

MS Spectrum

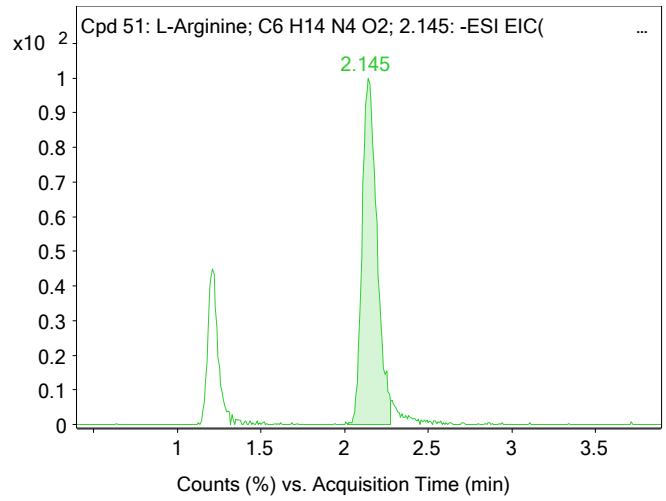


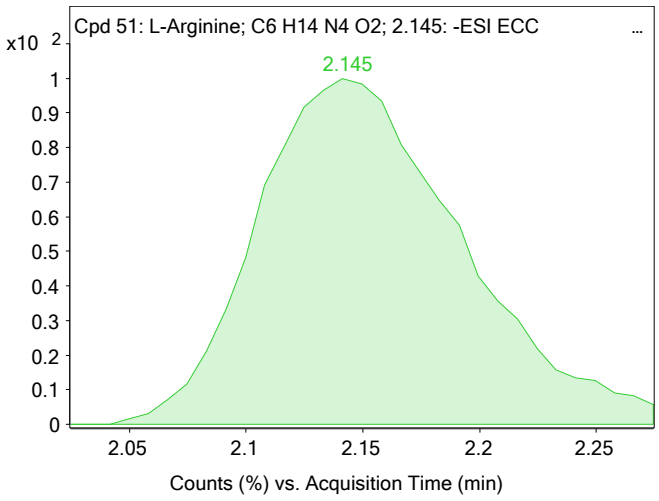
MS Zoomed Spectrum



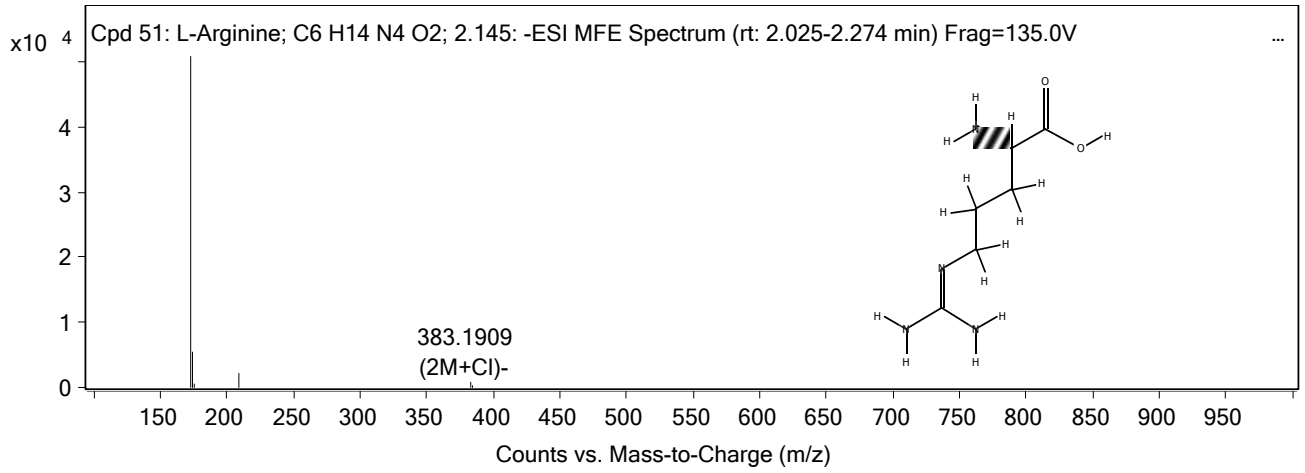
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 51: L-Arginine; C6 H14 N4 O2; 2.145	**L-Arginine**	173.1039	2.145	Find by Molecular Feature	174.1106

Compound Chromatograms

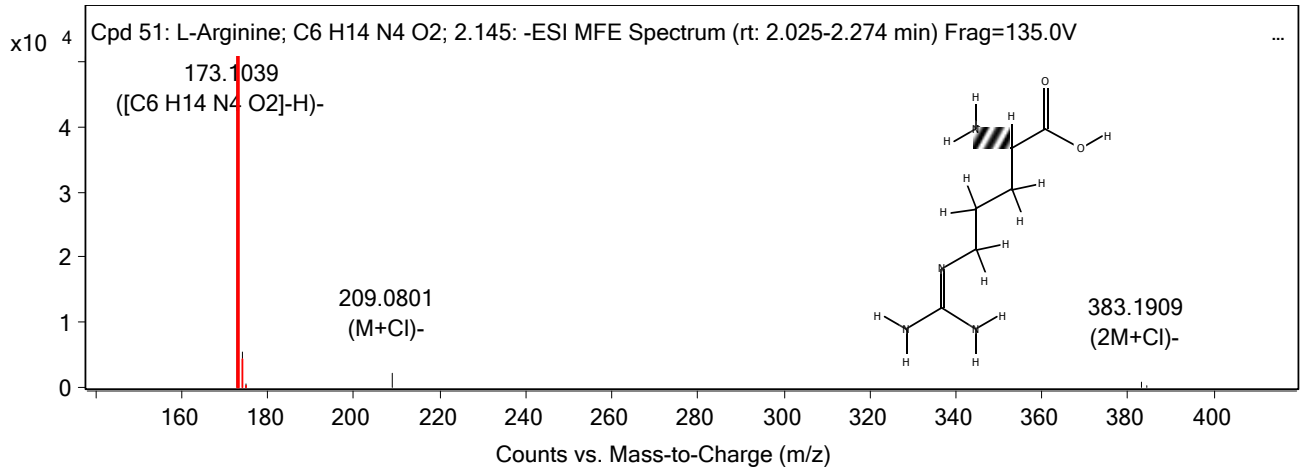




MFE MS Spectrum



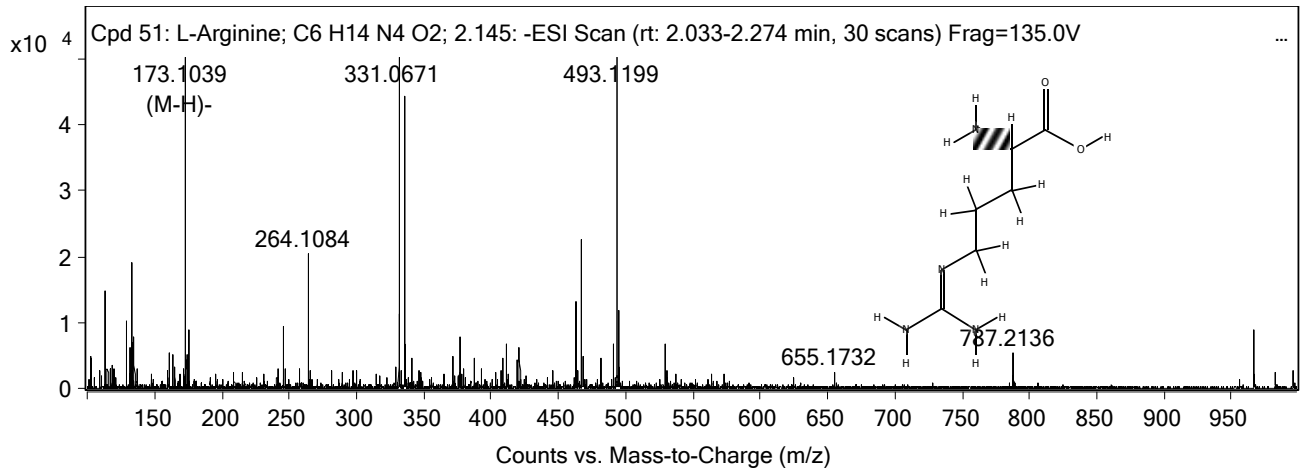
MFE MS Zoomed Spectrum



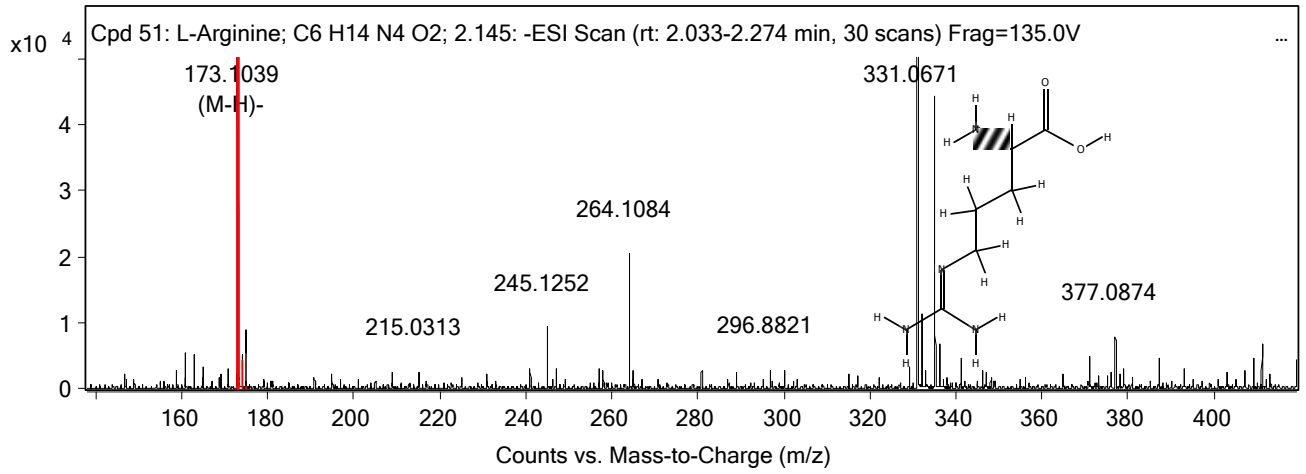
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
173.1039	-1	50817.18	C6 H14 N4 O2	(M-H)-
174.1009	-1	5419.67	C6 H14 N4 O2	(M-H)-
175.1038	-1	688.14	C6 H14 N4 O2	(M-H)-
209.0801	-1	2315.54		(M+Cl)-
383.1909	-1	890.7		(2M+Cl)-
384.1879	-1	343.37		(2M+Cl)-

MS Spectrum



MS Zoomed Spectrum

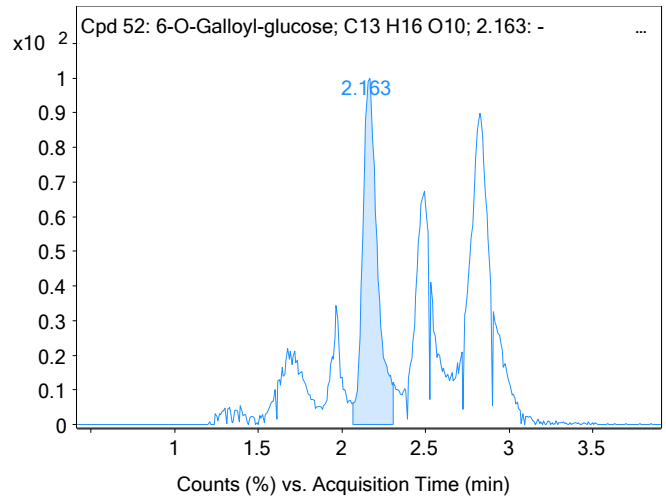


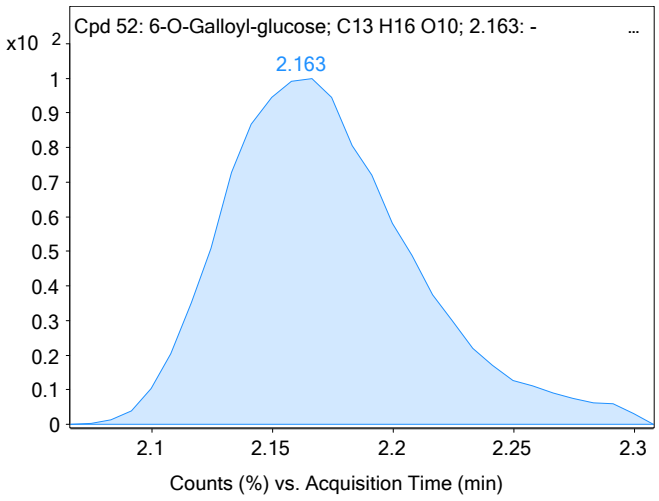
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	L-Arginine	2.145	C6 H14 N4 O2		81.94	174.1106	1.1	(M-H)-

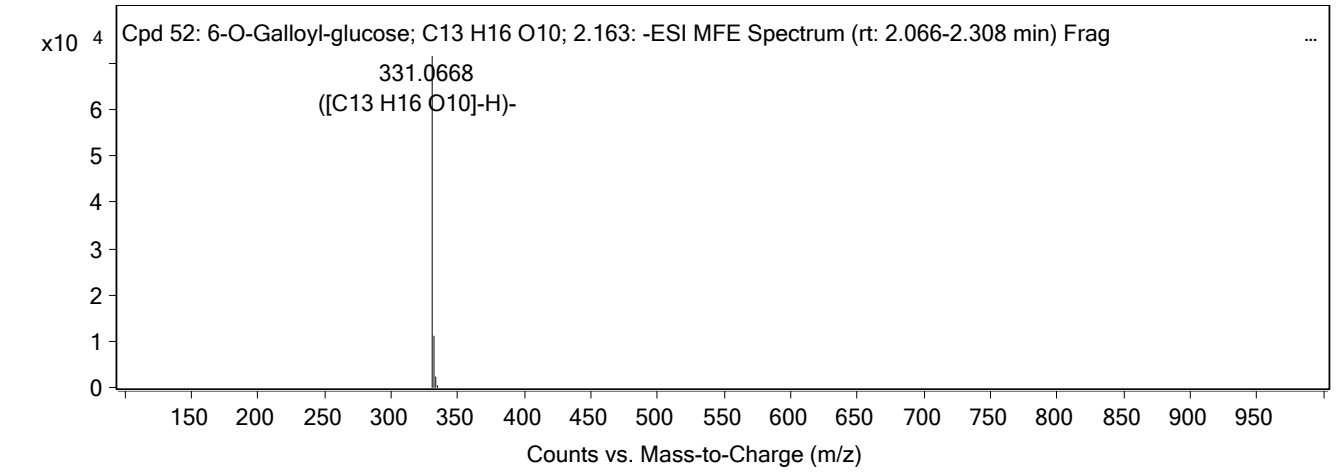
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 52: 6-O-Galloyl-glucose; C13 H16 O10; 2.163	**6-O-Galloyl-glucose**	331.0668	2.163	Find by Molecular Feature	332.0744

Compound Chromatograms

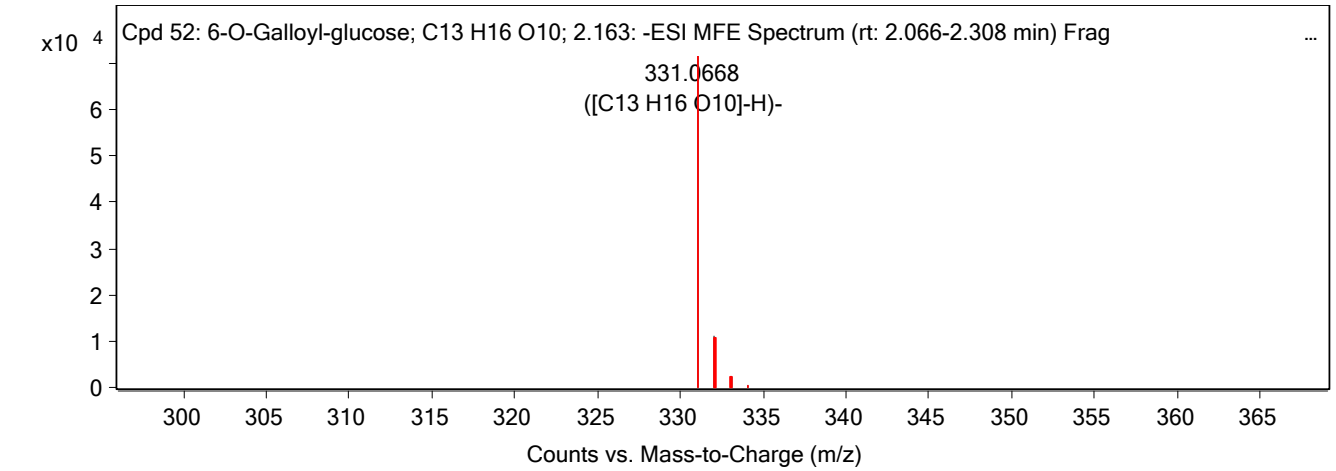




MFE MS Spectrum



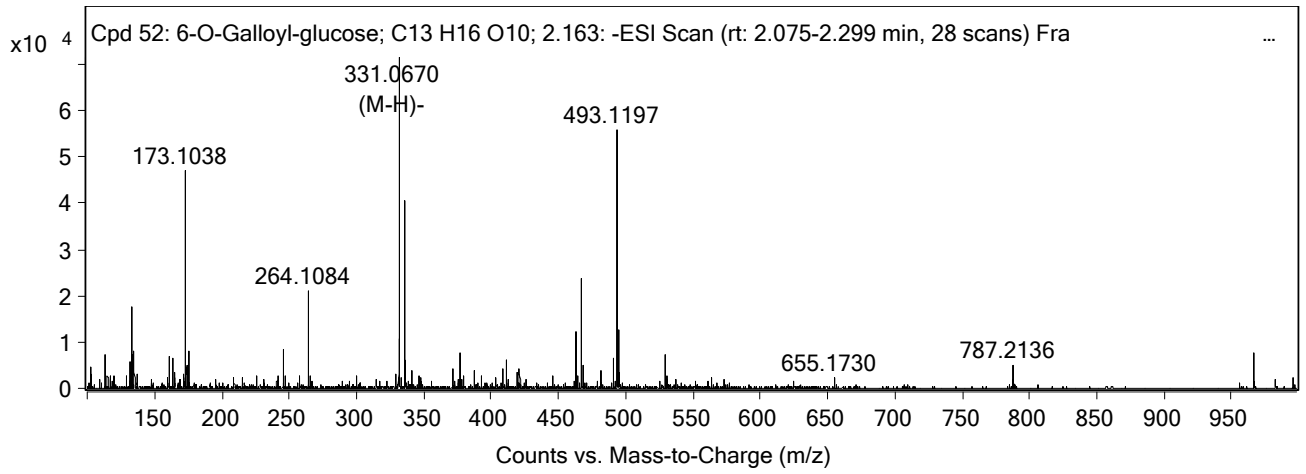
MFE MS Zoomed Spectrum



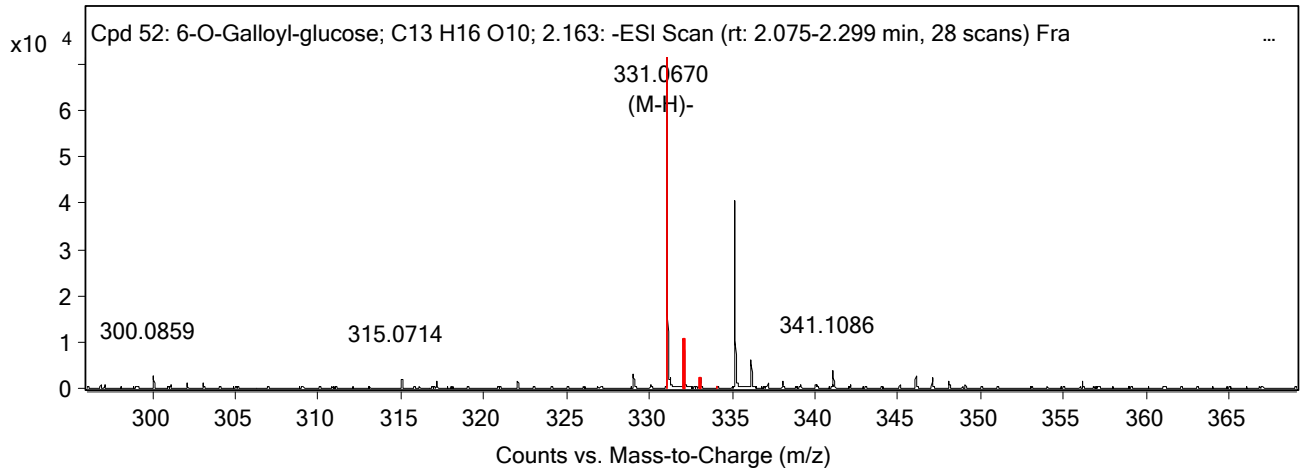
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
331.0668	-1	71522.23	C13 H16 O10	(M-H)-
332.0718	-1	11076.43	C13 H16 O10	(M-H)-
333.0736	-1	2324.73	C13 H16 O10	(M-H)-
334.0759	-1	481.87	C13 H16 O10	(M-H)-

MS Spectrum



MS Zoomed Spectrum

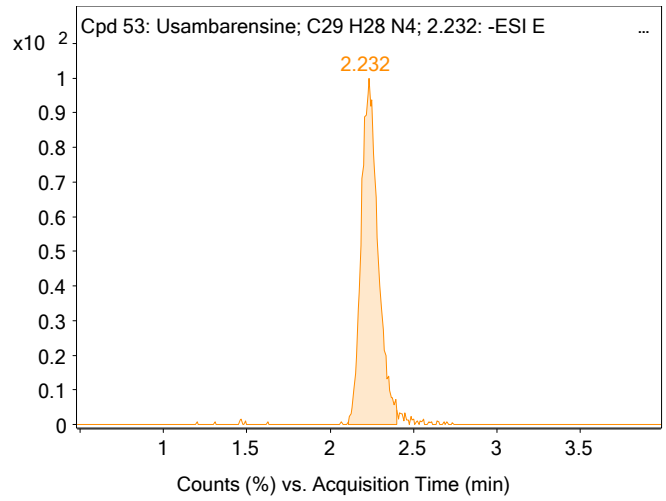


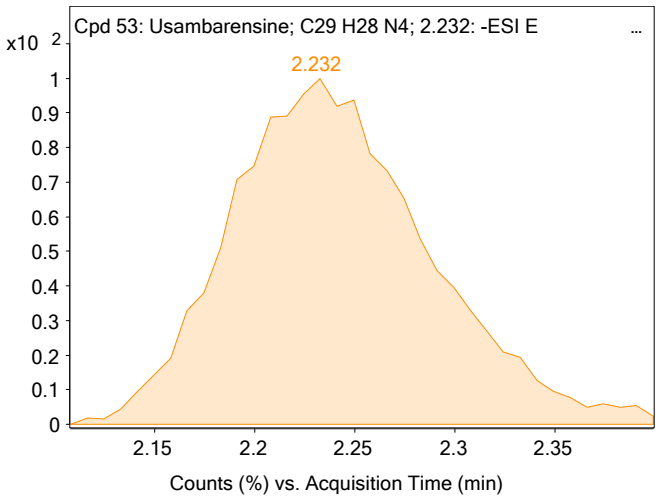
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	6-O-Galloyl-glucose	2.163	C13 H16 O10		96.98	332.0744	-0.02	(M-H)-
	1-Galloyl-glucose	2.163	C13 H16 O10		96.98	332.0744	-0.02	(M-H)-
	Gluco-syringic acid	2.163	C13 H16 O10		96.98	332.0744	-0.02	(M-H)-

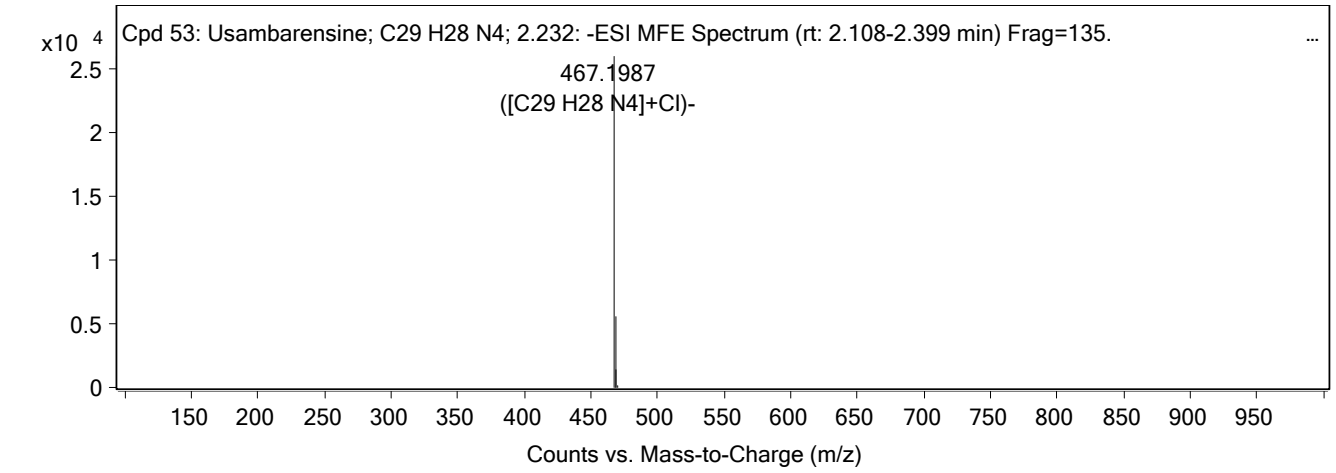
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 53: Usambarensine; C29 H28 N4; 2.232	**Usambarensine**	467.1987	2.232	Find by Molecular Feature	432.2294

Compound Chromatograms

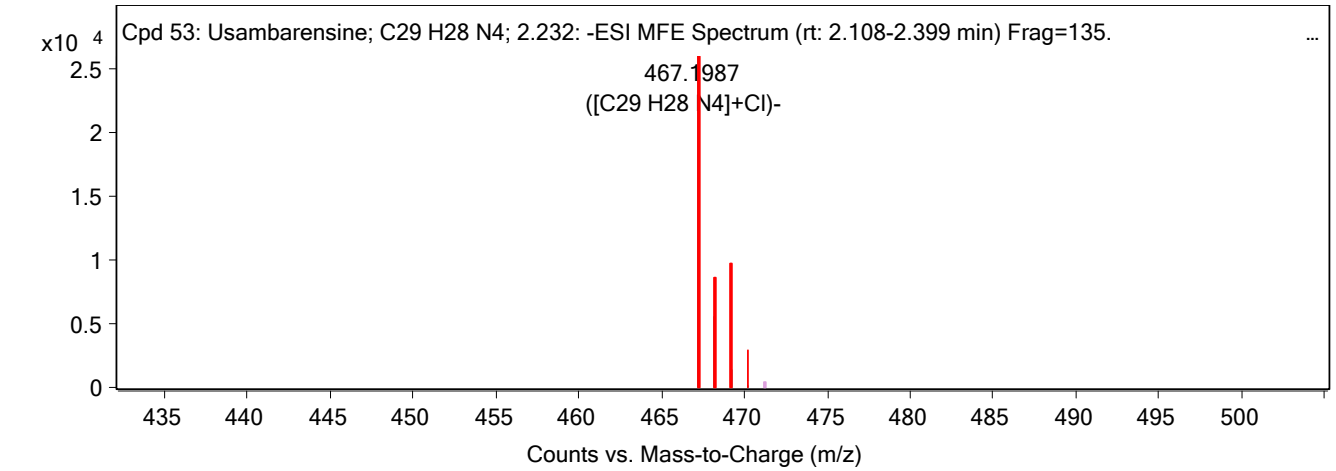




MFE MS Spectrum



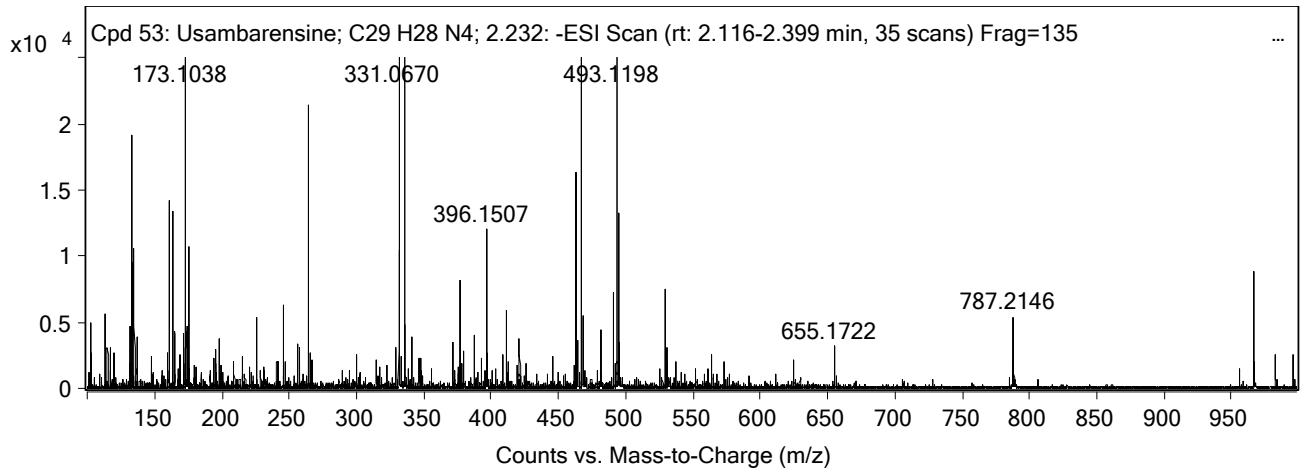
MFE MS Zoomed Spectrum



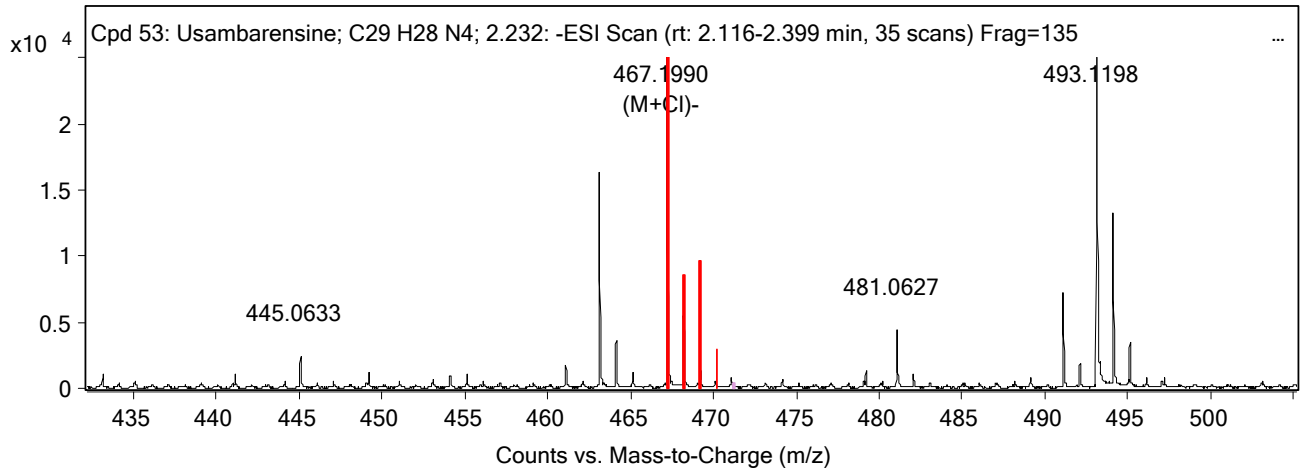
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
467.1987	-1	25903.17	C29 H28 N4	(M+Cl)-
468.201	-1	5547.67	C29 H28 N4	(M+Cl)-
469.2031	-1	1375.73	C29 H28 N4	(M+Cl)-
470.194	-1	89.66	C29 H28 N4	(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

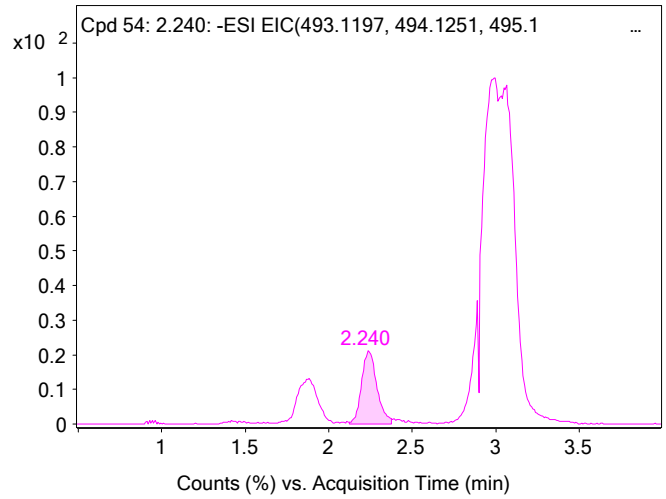


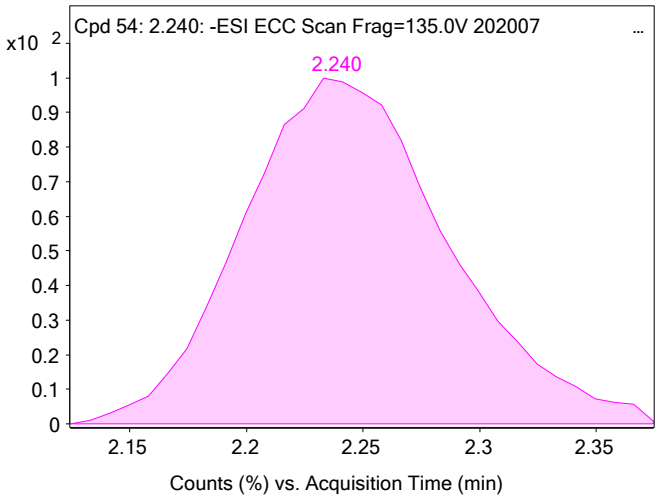
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Usambarensine	2.232	C29 H28 N4		58.79	432.2294	1.99	(M+Cl)-

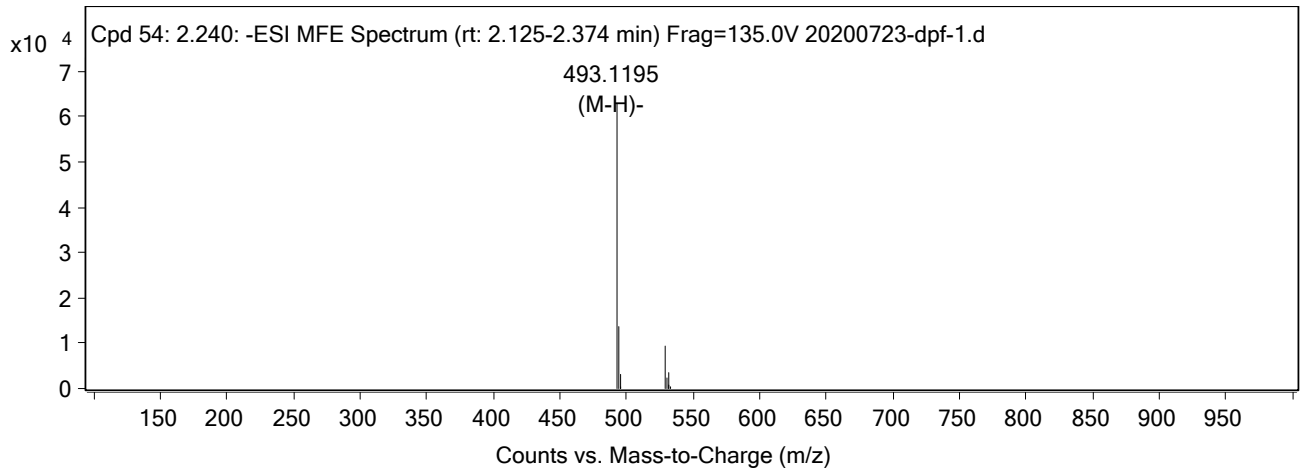
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 54: 2.240	493.1195	2.24	Find by Molecular Feature	494.1268

Compound Chromatograms

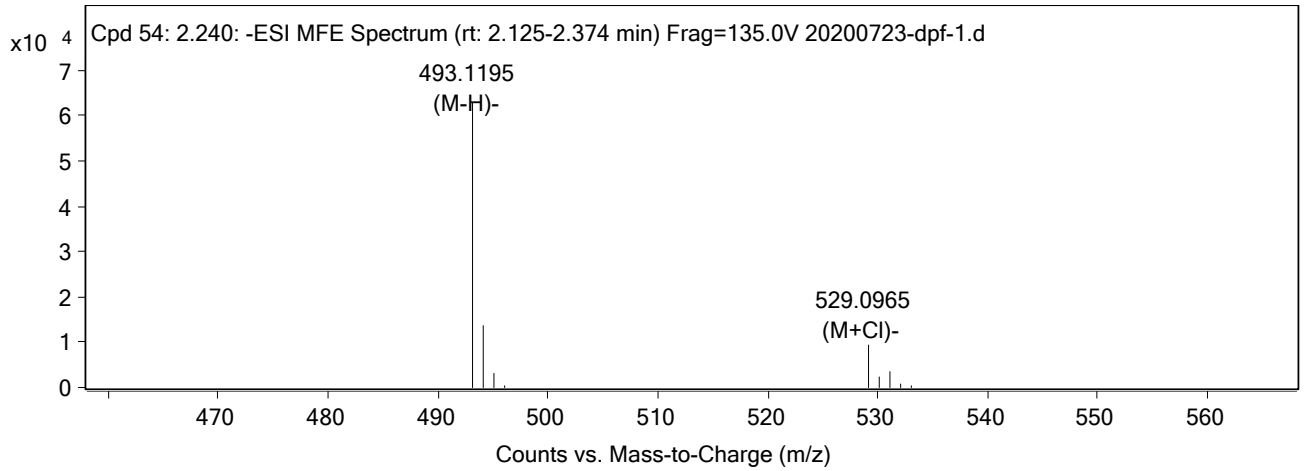




MFE MS Spectrum



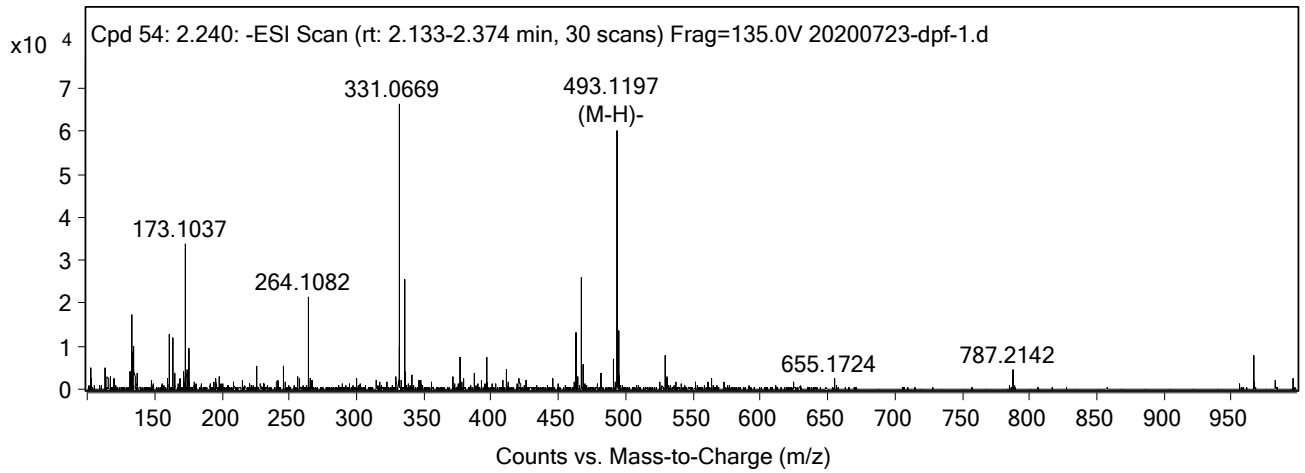
MFE MS Zoomed Spectrum



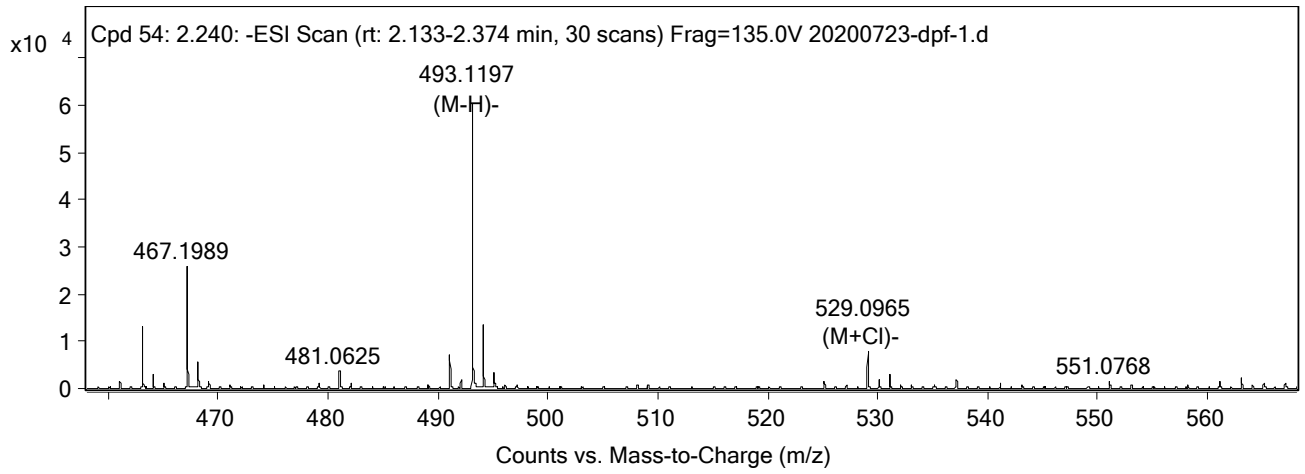
MS Spectrum Peak List

m/z	z	Abund	Ion
493.1195	-1	62952.97	(M-H)-
494.1231	-1	13768.95	(M-H)-
495.125	-1	3302.85	(M-H)-
496.1281	-1	493.77	(M-H)-
529.0965	-1	9265.99	(M+Cl)-
530.1006	-1	2267.83	(M+Cl)-
531.0952	-1	3444.65	(M+Cl)-
532.0983	-1	790.59	(M+Cl)-
533.0931	-1	337.39	(M+Cl)-

MS Spectrum

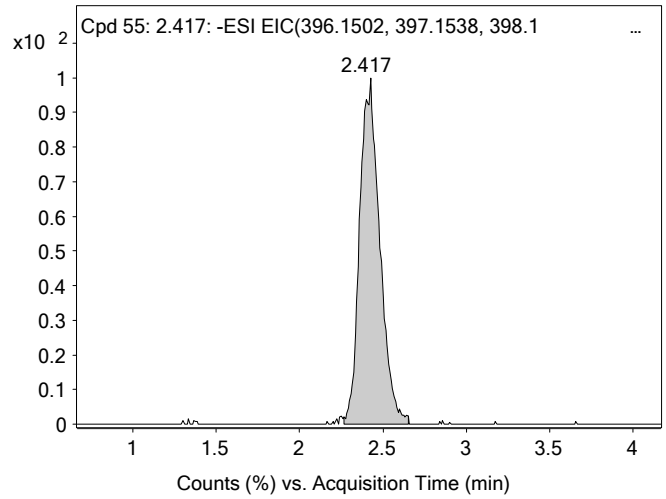


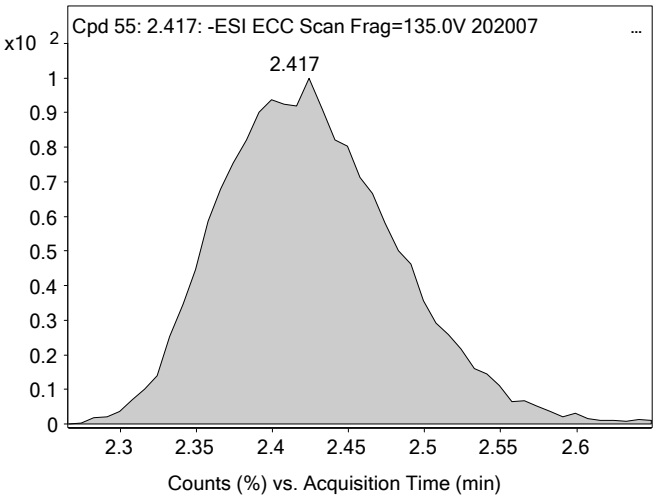
MS Zoomed Spectrum



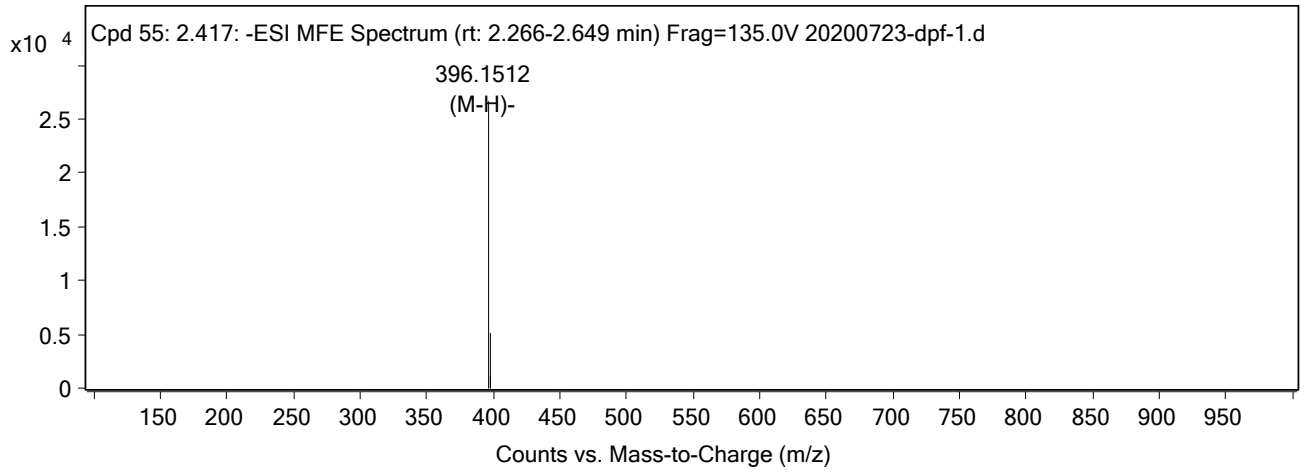
Compound Label	m/z	RT	Algorithm	Mass
Cpd 55: 2.417	396.1512	2.417	Find by Molecular Feature	397.1585

Compound Chromatograms

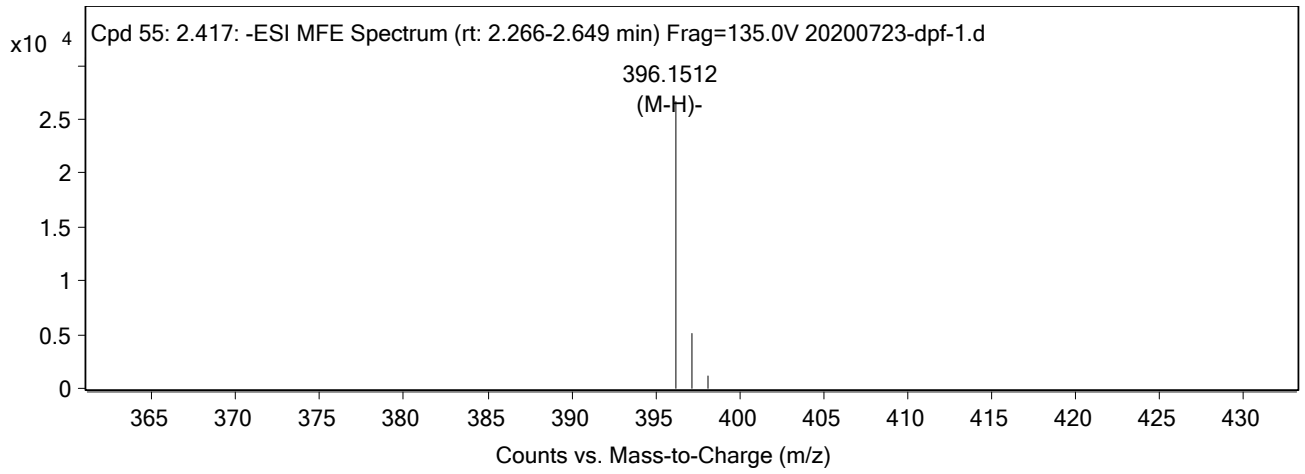




MFE MS Spectrum



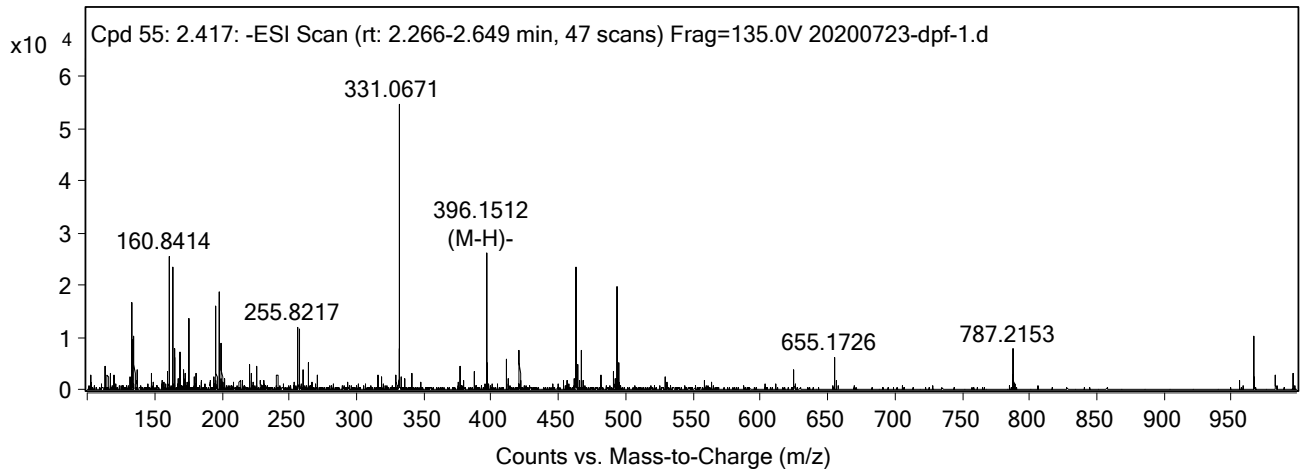
MFE MS Zoomed Spectrum



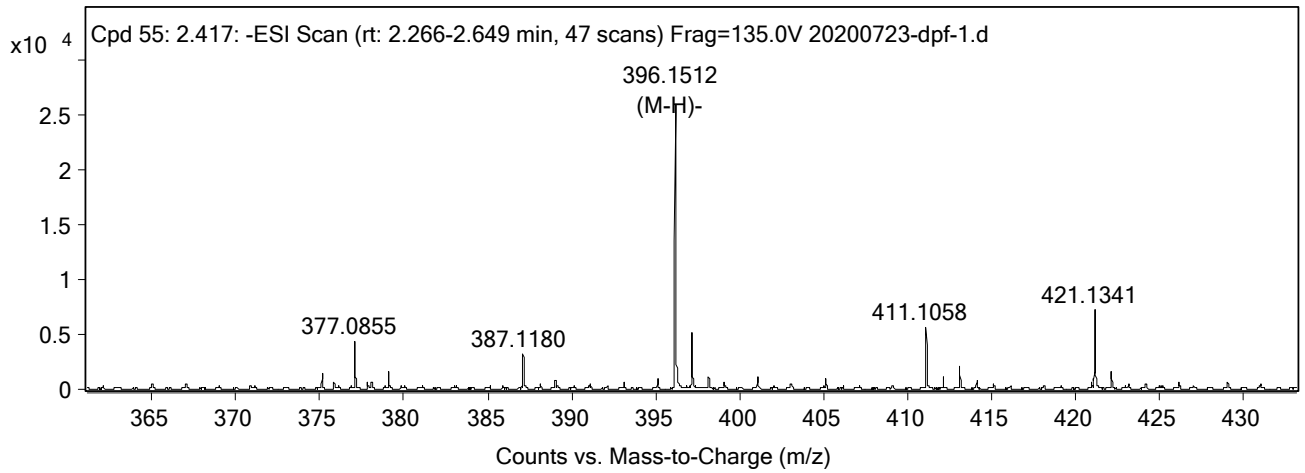
MS Spectrum Peak List

m/z	z	Abund	Ion
396.1512	-1	26679.69	(M-H)-
397.1537	-1	5105.82	(M-H)-
398.1556	-1	1126.4	(M-H)-

MS Spectrum

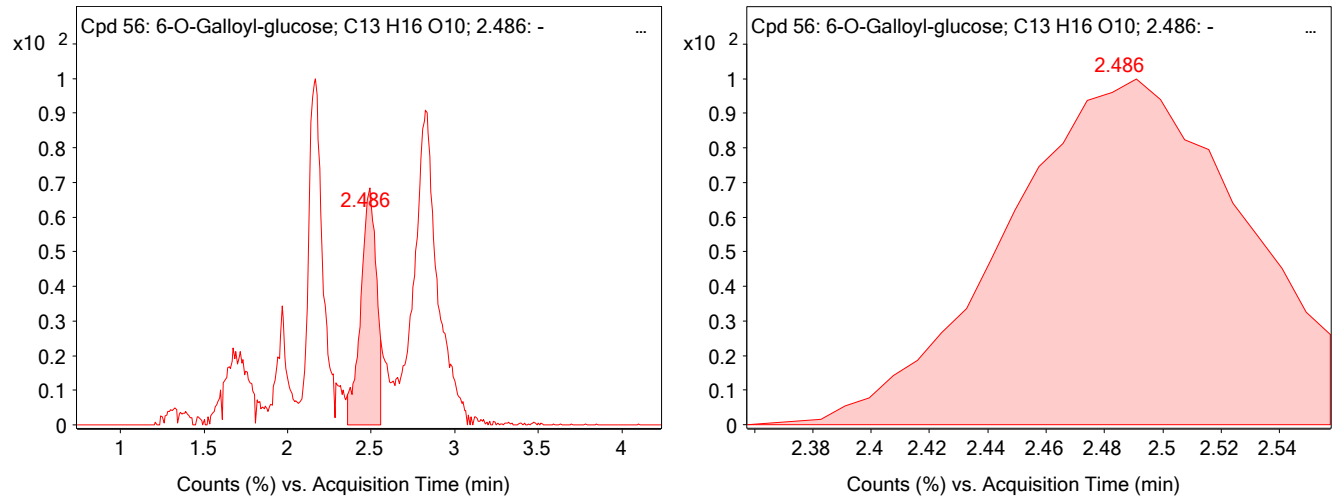


MS Zoomed Spectrum

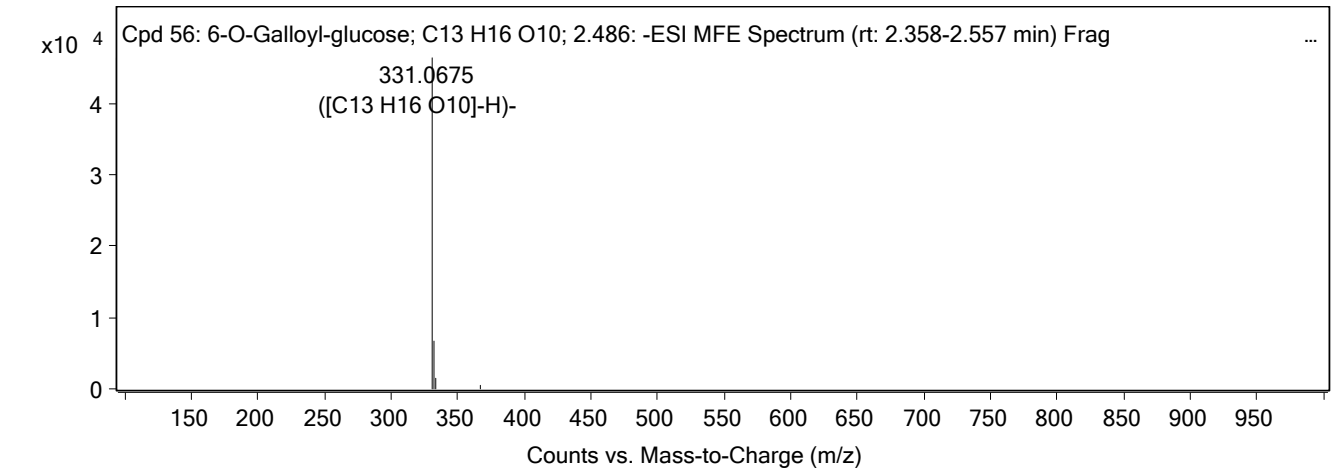


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 56: 6-O-Galloyl-glucose; C13 H16 O10; 2.486	**6-O-Galloyl-glucose**	331.0675	2.486	Find by Molecular Feature	332.0748

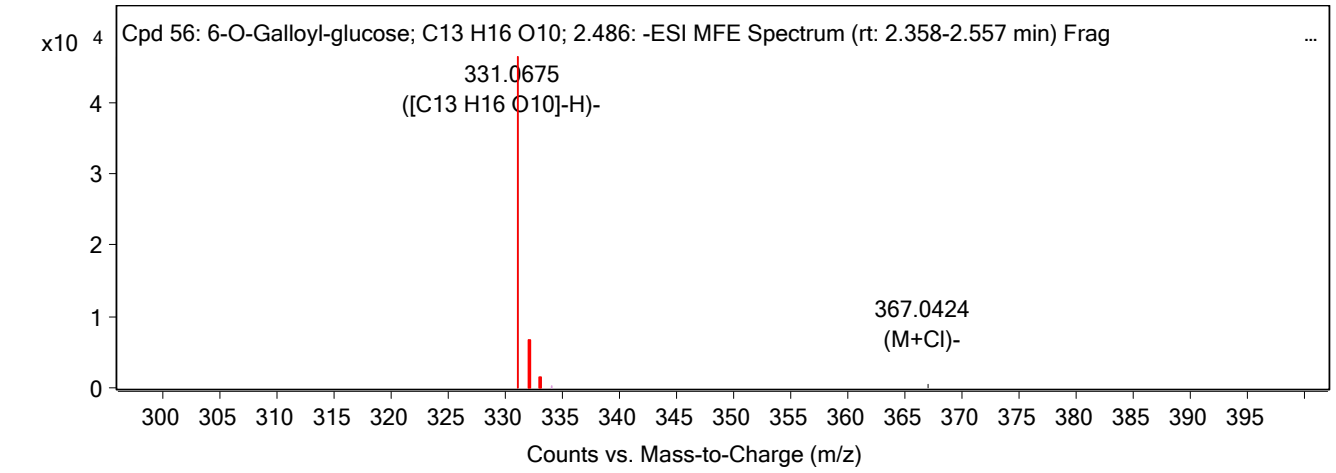
Compound Chromatograms



MFE MS Spectrum



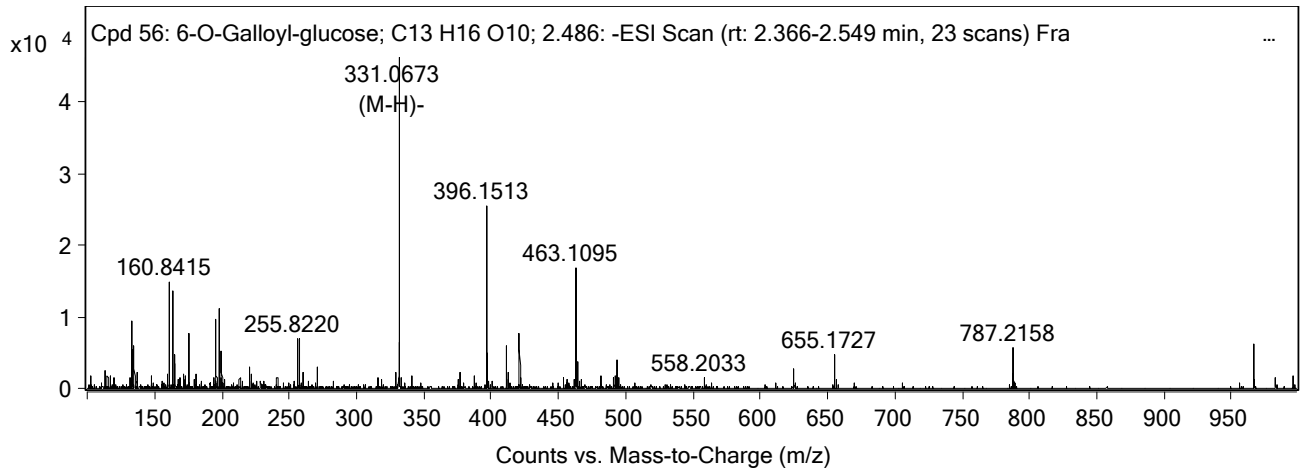
MFE MS Zoomed Spectrum



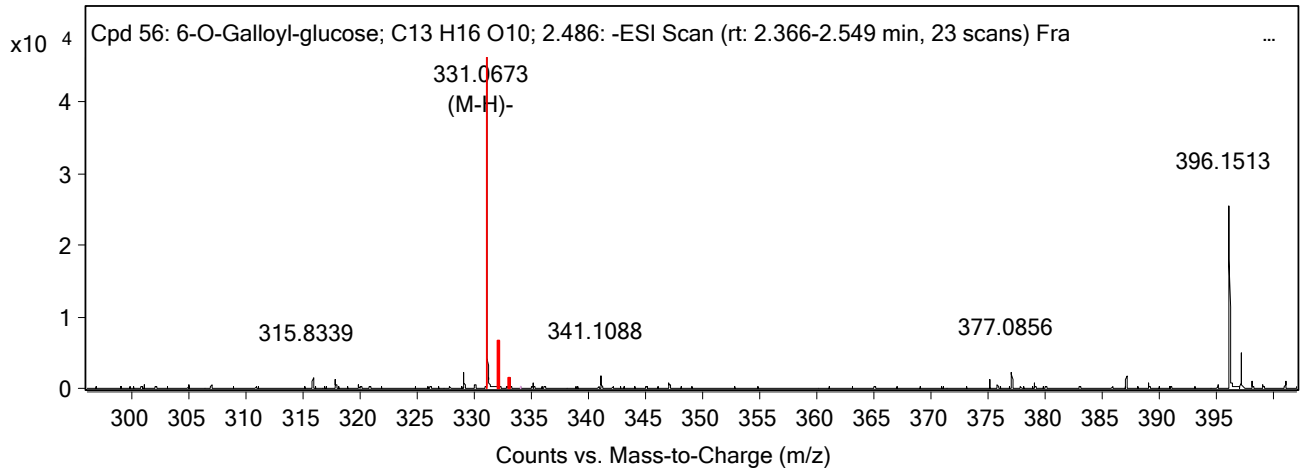
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
331.0675	-1	46317.59	C13 H16 O10	(M-H)-
332.0705	-1	6585.66	C13 H16 O10	(M-H)-
333.075	-1	1528.62	C13 H16 O10	(M-H)-
367.0424	-1	623.13		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

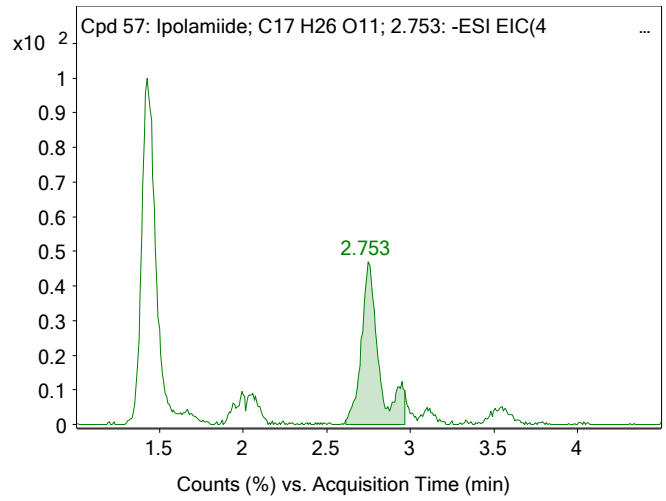


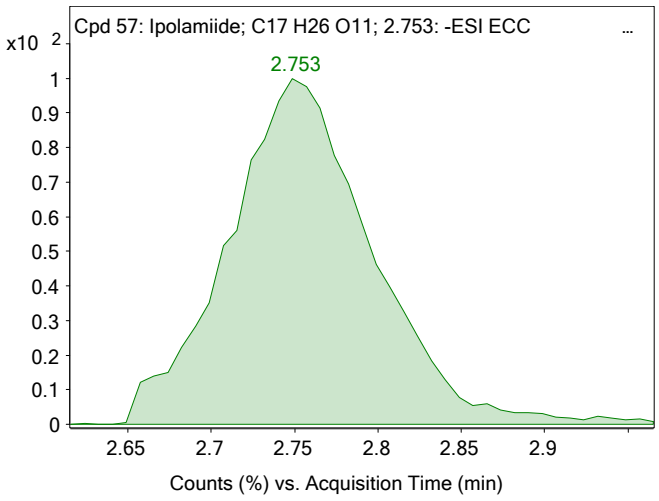
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	6-O-Galloyl-glucose	2.486	C13 H16 O10		98.65	332.0748	-0.46	(M-H)-
	1-Galloyl-glucose	2.486	C13 H16 O10		98.65	332.0748	-0.46	(M-H)-
	Gluco-syringic acid	2.486	C13 H16 O10		98.65	332.0748	-0.46	(M-H)-

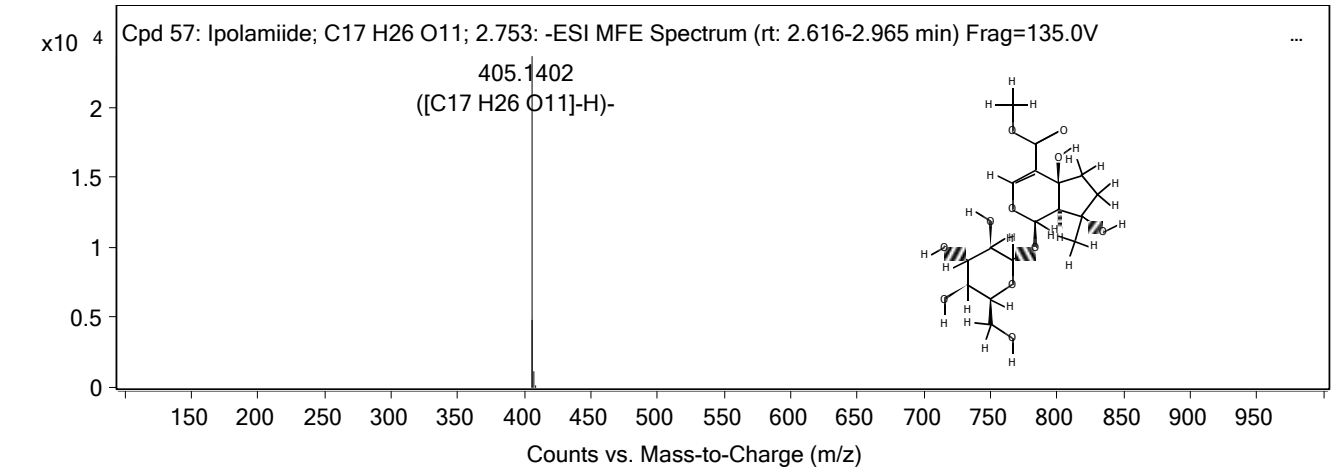
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 57: Ipolamiide; C17 H26 O11; 2.753	**Ipolamiide**	405.1402	2.753	Find by Molecular Feature	406.1476

Compound Chromatograms

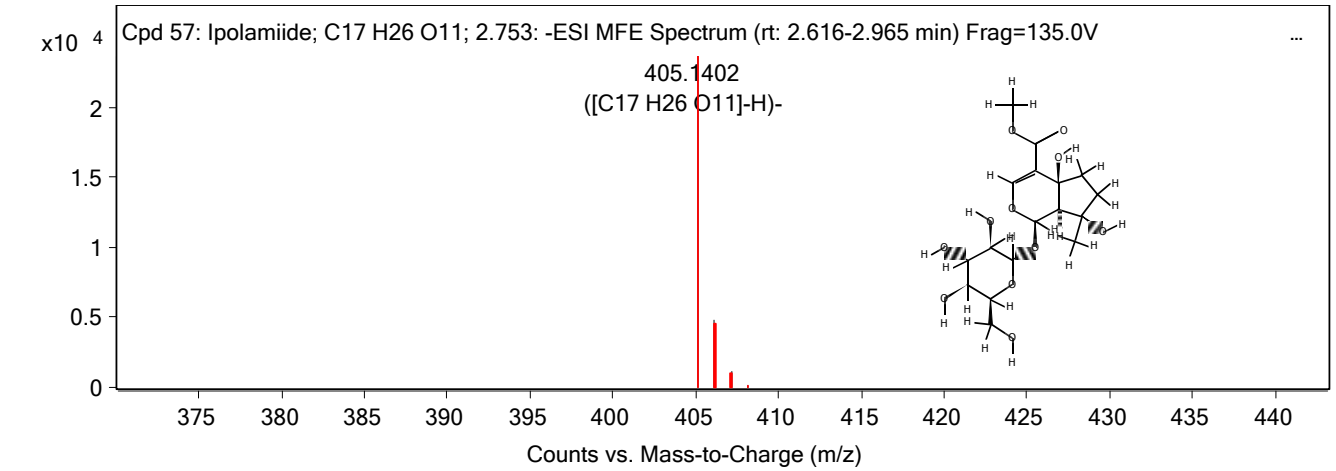




MFE MS Spectrum



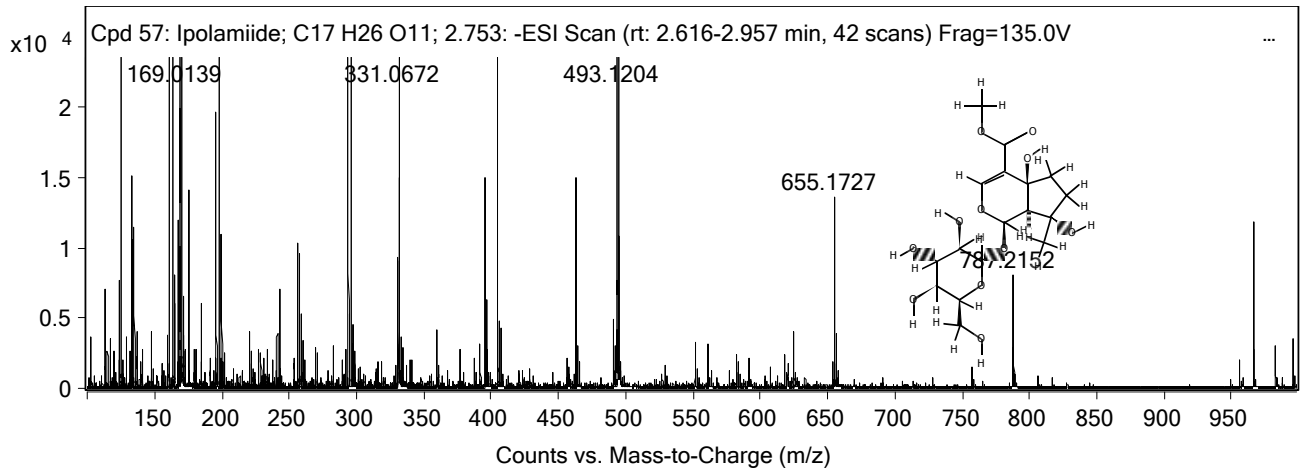
MFE MS Zoomed Spectrum



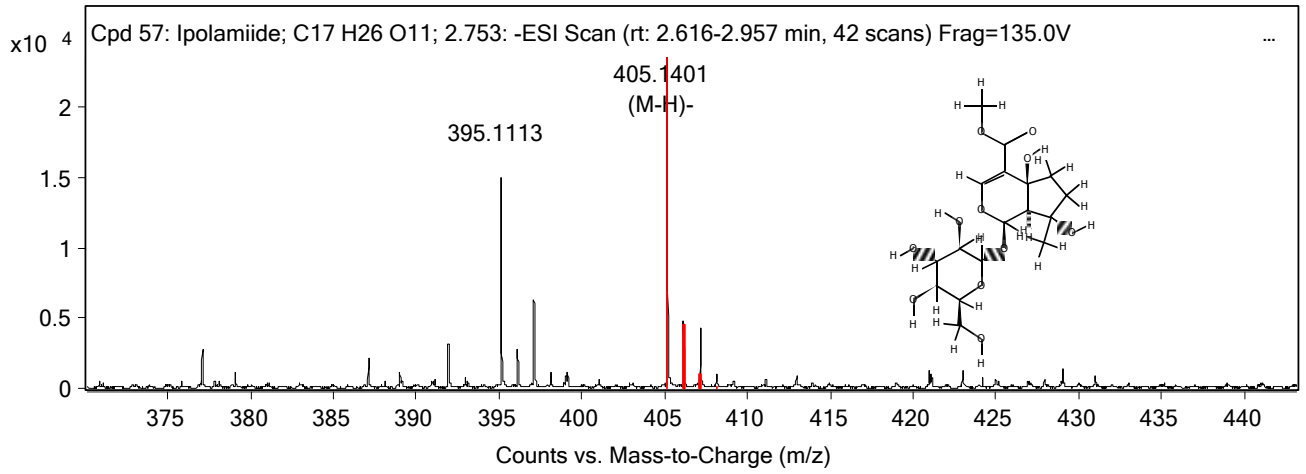
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
405.1402	-1	23663.09	C17 H26 O11	(M-H)-
406.1442	-1	4841.57	C17 H26 O11	(M-H)-
407.1462	-1	1163.43	C17 H26 O11	(M-H)-
408.1484	-1	87.61	C17 H26 O11	(M-H)-

MS Spectrum



MS Zoomed Spectrum

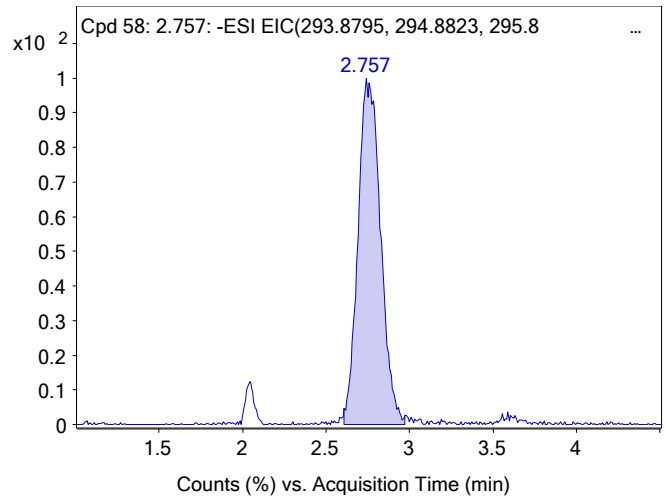


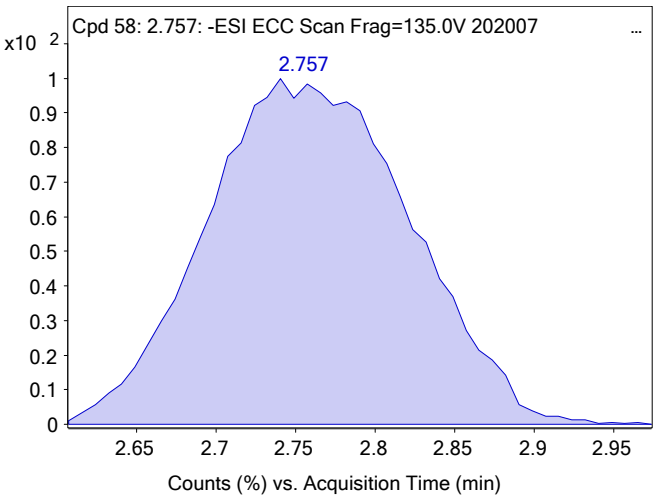
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Ipolamiide	2.753	C17 H26 O11		99.06	406.1476	-0.1	(M-H)-
	Caryoptoside	2.753	C17 H26 O11		99.06	406.1476	-0.1	(M-H)-
	Morroniside	2.753	C17 H26 O11		99.06	406.1476	-0.1	(M-H)-
	8-Acetylharpagide	2.753	C17 H26 O11		99.06	406.1476	-0.1	(M-H)-
	4,4'-Methylene bis[2,3,5,6-tetramethyl phenol]	2.753	C22 H30 O2		46.2	326.2217	2.83	(M+Br)-
	Bufadienolide	2.753	C22 H30 O2		46.2	326.2217	2.83	(M+Br)-

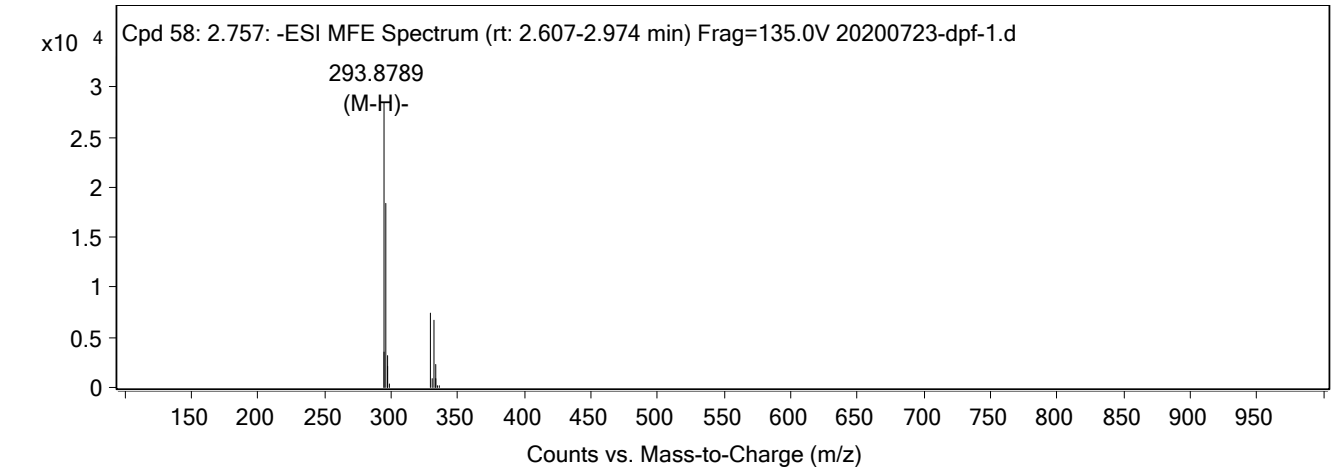
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 58: 2.757	293.8789	2.757	Find by Molecular Feature	294.8861

Compound Chromatograms

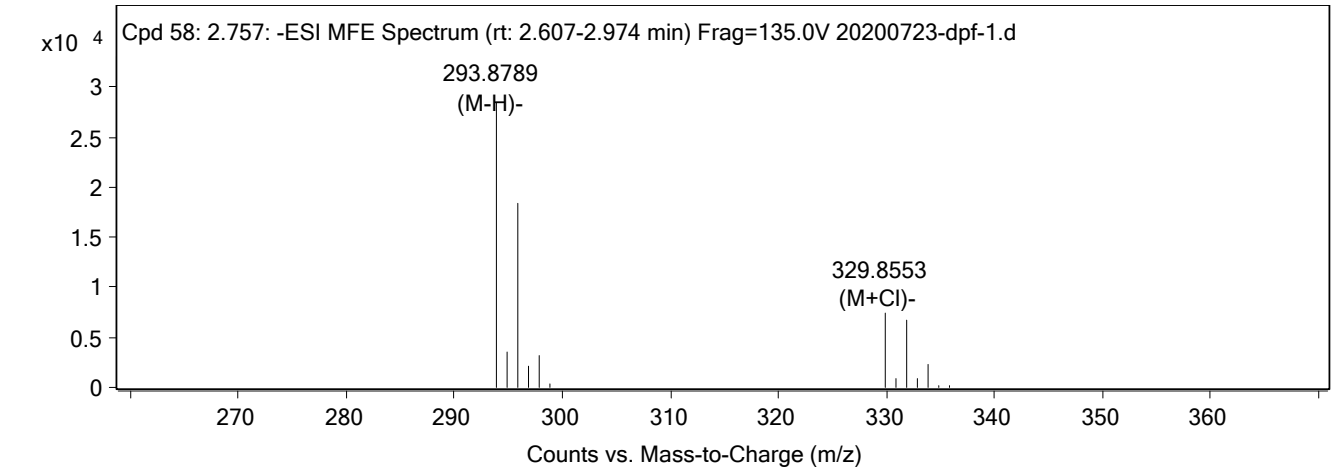




MFE MS Spectrum



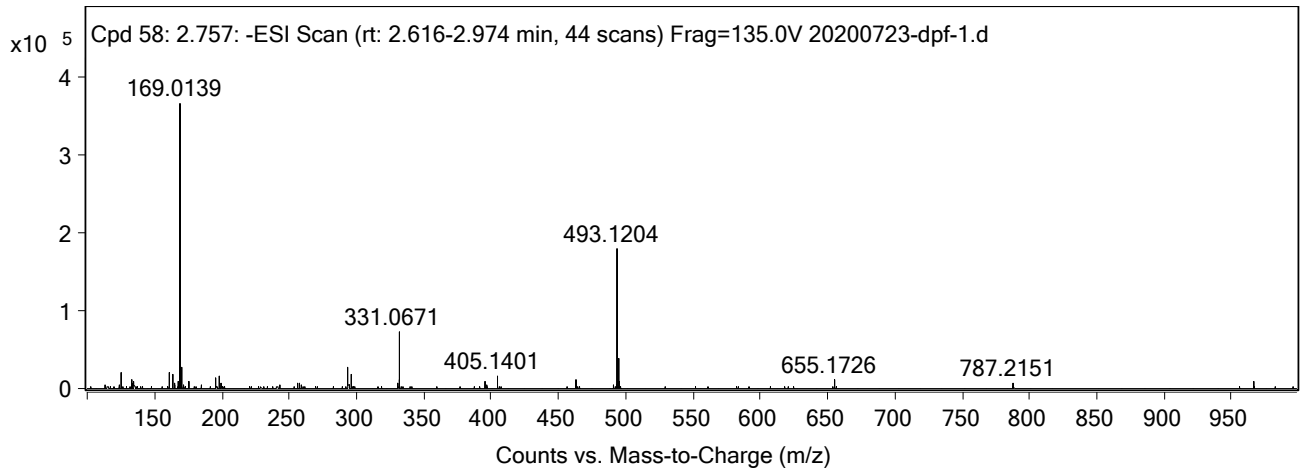
MFE MS Zoomed Spectrum



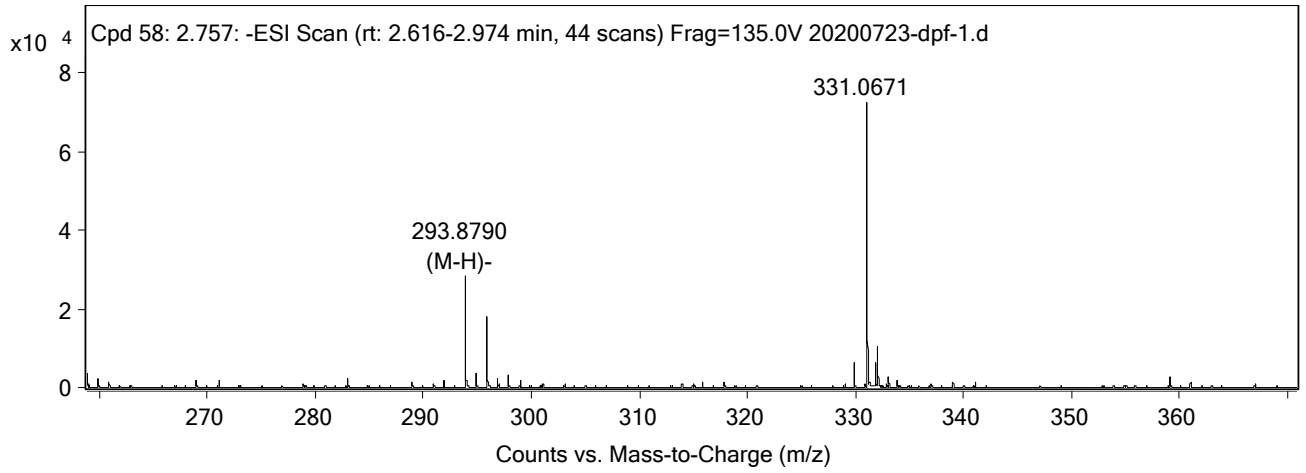
MS Spectrum Peak List

m/z	z	Abund	Ion
293.8789	-1	28522.72	(M-H)-
294.8823	-1	3472.48	(M-H)-
295.8759	-1	18430.4	(M-H)-
296.8793	-1	2143.71	(M-H)-
297.8737	-1	3224.42	(M-H)-
329.8553	-1	7360.7	(M+Cl)-
330.8606	-1	861.84	(M+Cl)-
331.8525	-1	6697.23	(M+Cl)-
332.8575	-1	827.3	(M+Cl)-
333.8499	-1	2270.73	(M+Cl)-

MS Spectrum

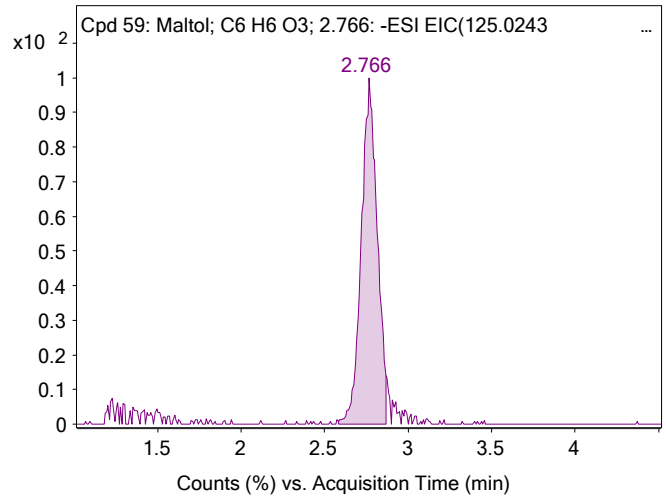


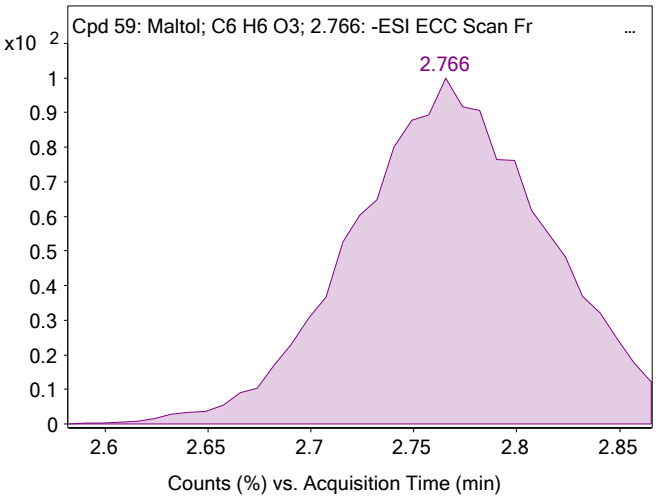
MS Zoomed Spectrum



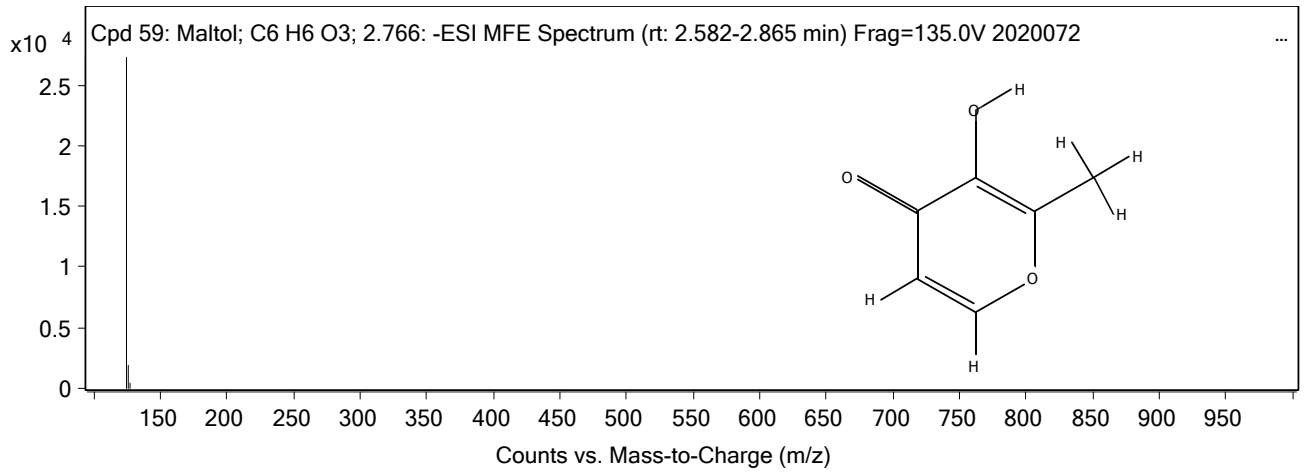
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 59: Maltol; C6 H6 O3; 2.766	**Maltol**	125.024	2.766	Find by Molecular Feature	126.0313

Compound Chromatograms

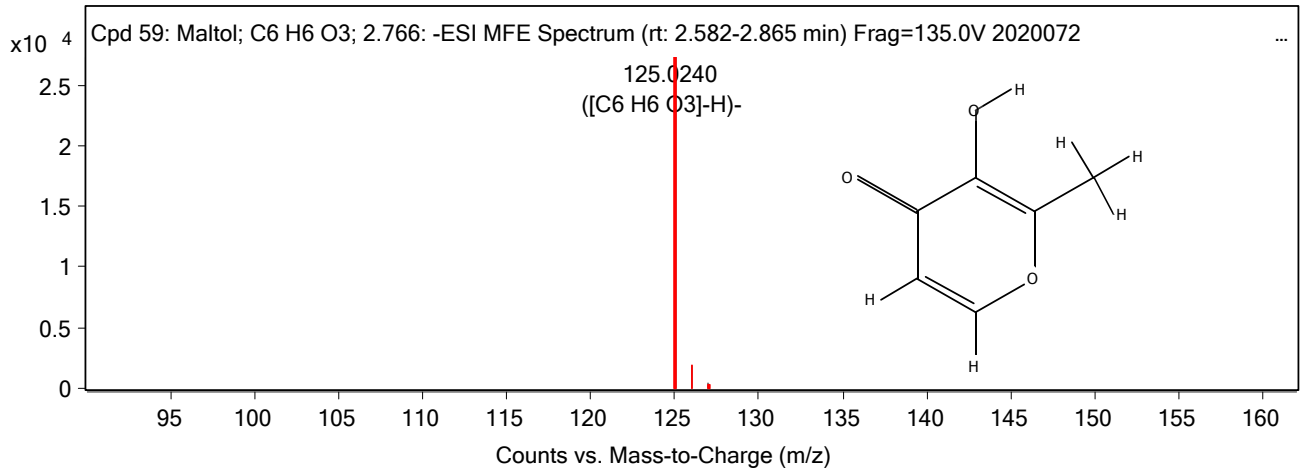




MFE MS Spectrum



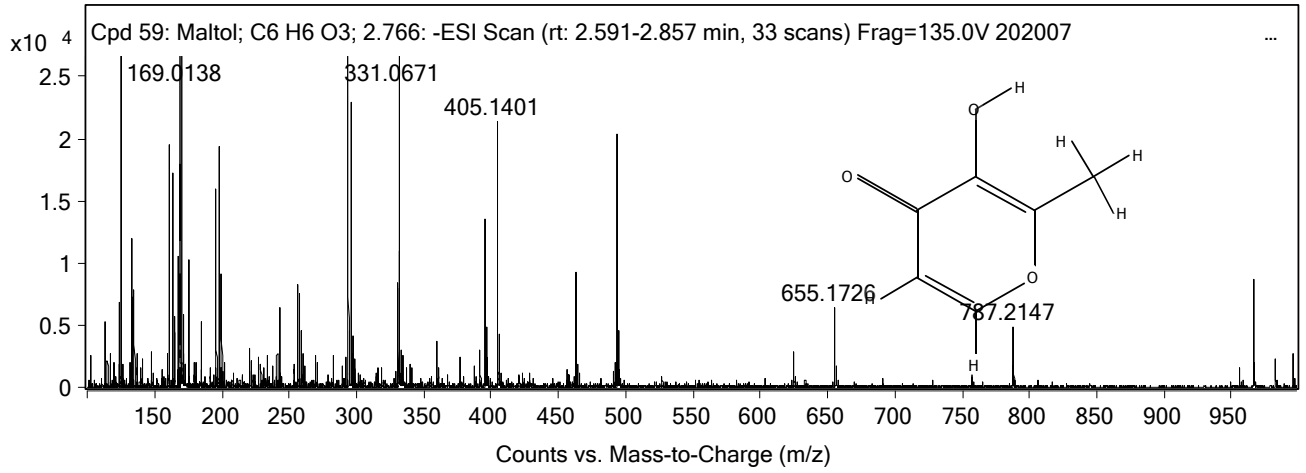
MFE MS Zoomed Spectrum



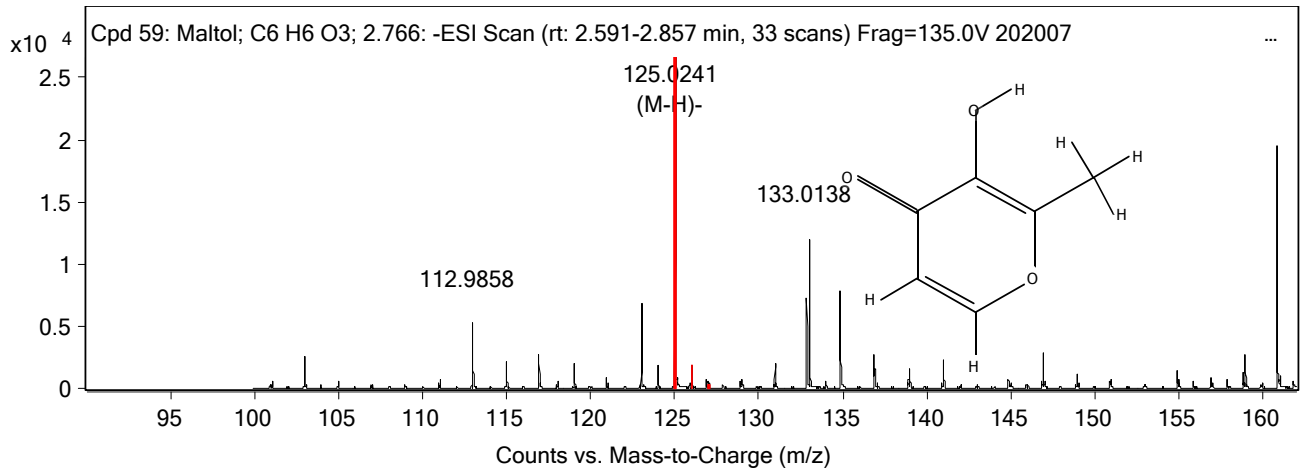
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
125.024	-1	27290.88	C6 H6 O3	(M-H)-
126.0281	-1	1918.51	C6 H6 O3	(M-H)-
127.0259	-1	382.08	C6 H6 O3	(M-H)-

MS Spectrum



MS Zoomed Spectrum

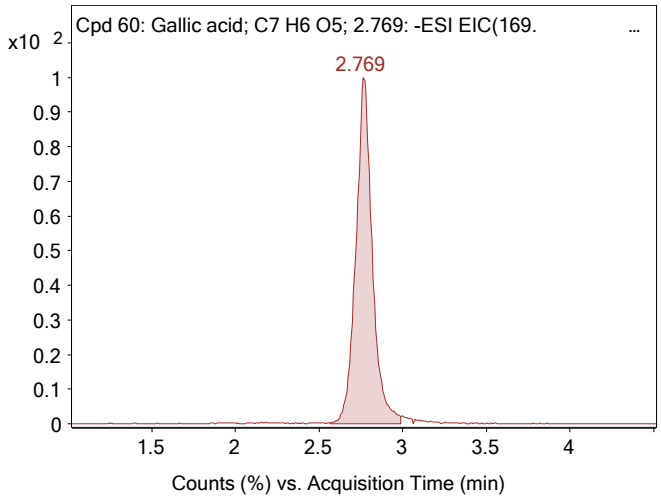


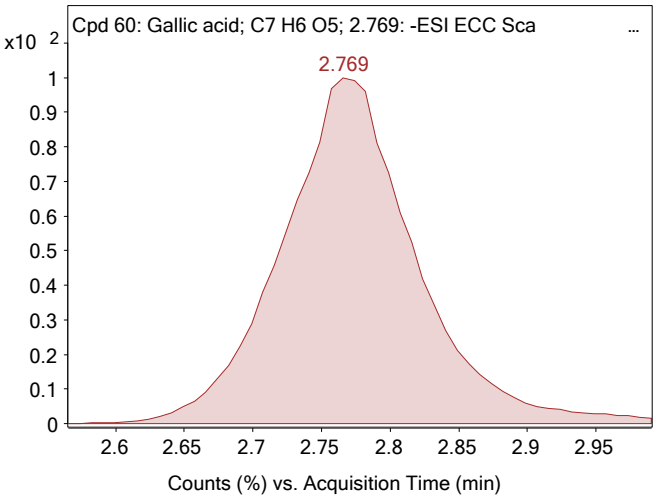
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Maltol	2.766	C6 H6 O3		97.82	126.0313	0.41	(M-H)-
	5-Hydroxymethyl furaldehyde	2.766	C6 H6 O3		97.82	126.0313	0.41	(M-H)-
	4-Hydroxymethyl-2-furaldehyde	2.766	C6 H6 O3		97.82	126.0313	0.41	(M-H)-
	Pyrogallol	2.766	C6 H6 O3		97.82	126.0313	0.41	(M-H)-
	Phloroglucinol	2.766	C6 H6 O3		97.82	126.0313	0.41	(M-H)-
	5-Methoxyfuraldehyde	2.766	C6 H6 O3		97.82	126.0313	0.41	(M-H)-

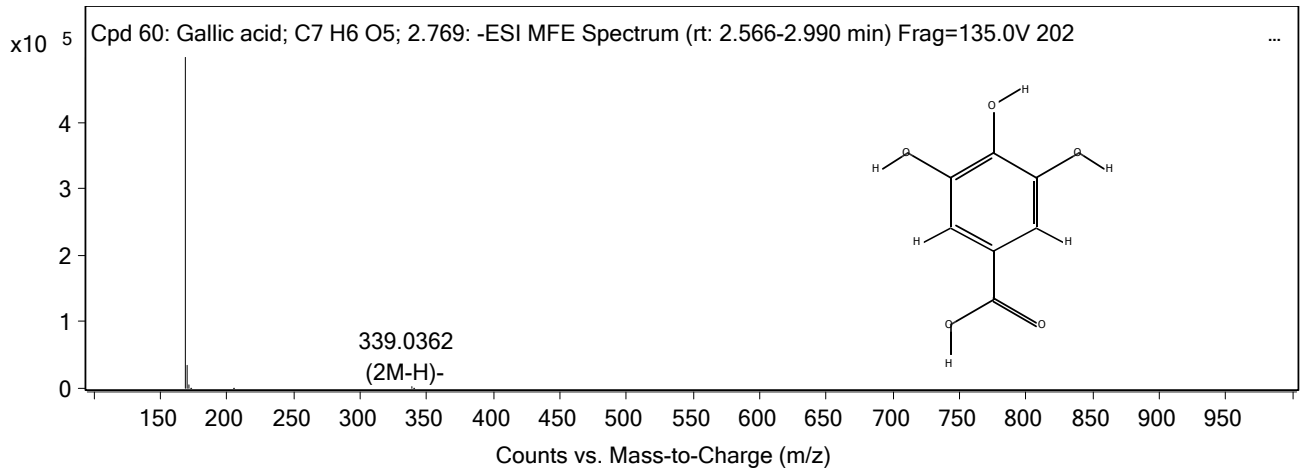
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 60: Gallic acid; C7 H6 O5; 2.769	**Gallic acid**	169.0135	2.769	Find by Molecular Feature	170.0208

Compound Chromatograms

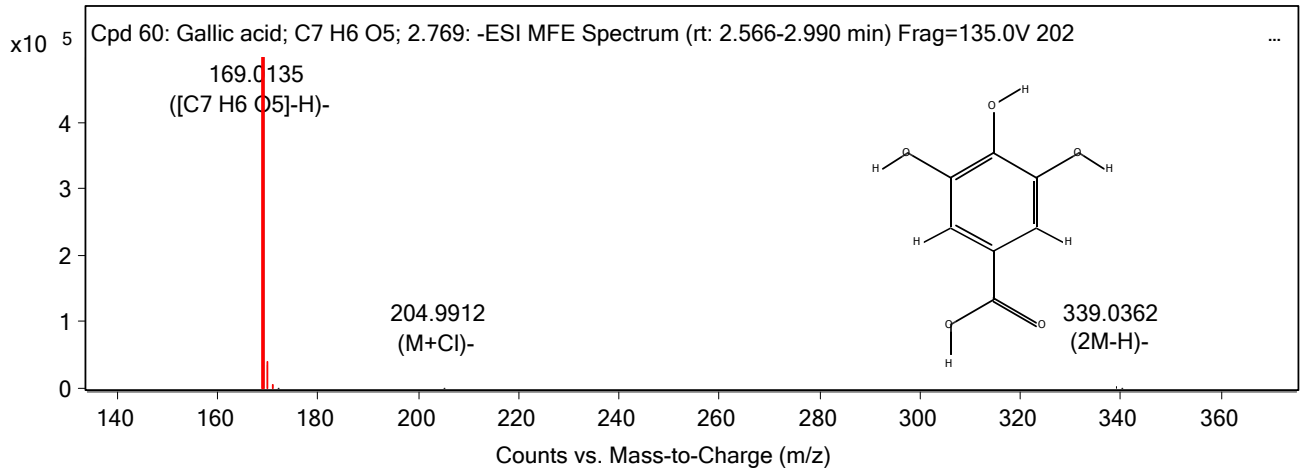




MFE MS Spectrum



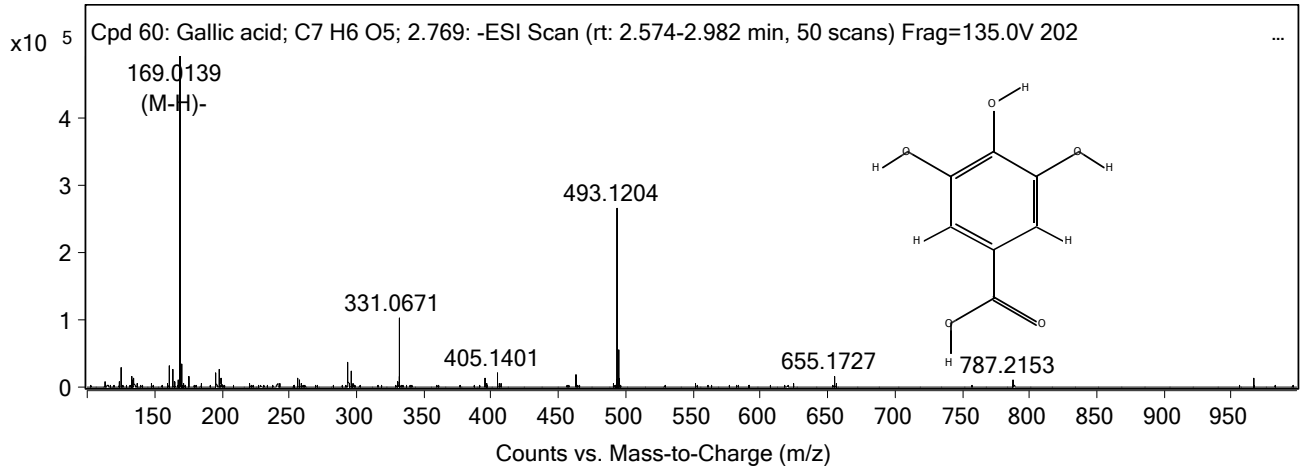
MFE MS Zoomed Spectrum



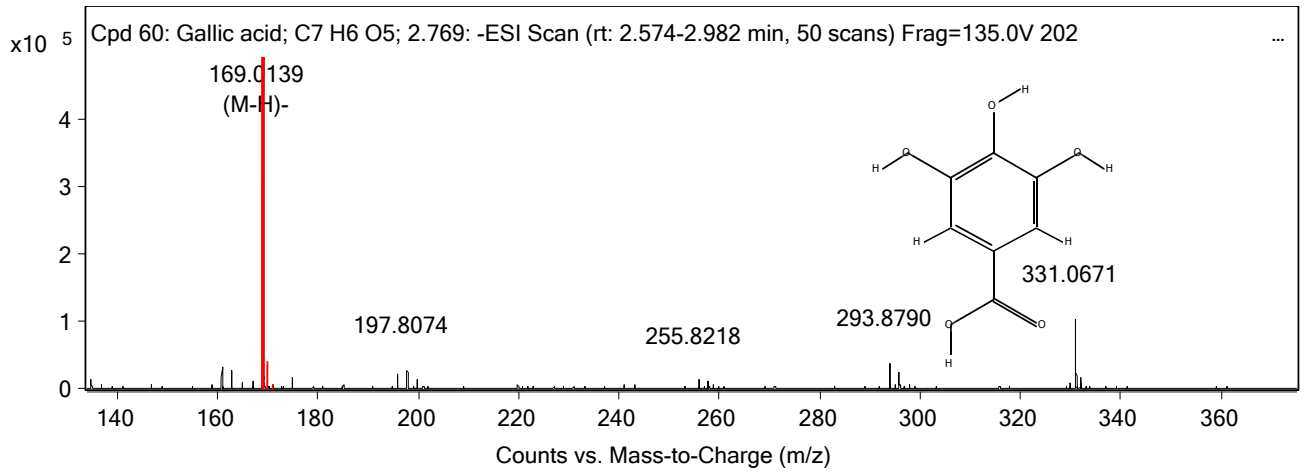
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
169.0135	-1	497807.94	C7 H6 O5	(M-H)-
170.0169	-1	35582.43	C7 H6 O5	(M-H)-
171.0182	-1	6079.76	C7 H6 O5	(M-H)-
172.0213	-1	429.89	C7 H6 O5	(M-H)-
204.9912	-1	512.38		(M+Cl)-
339.0362	-1	2180.25		(2M-H)-
340.0401	-1	383.46		(2M-H)-

MS Spectrum



MS Zoomed Spectrum

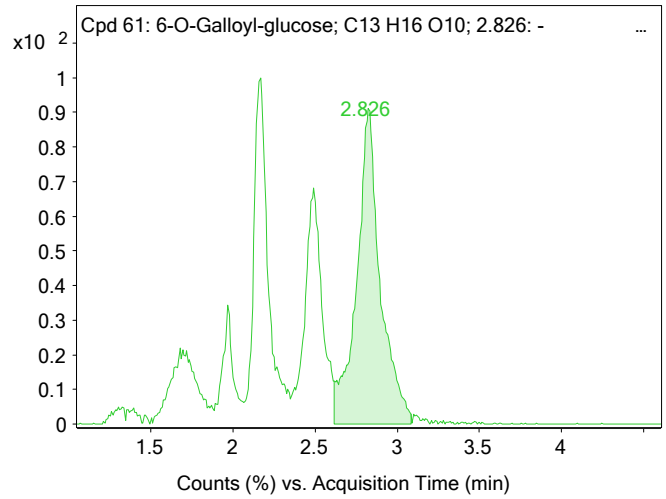


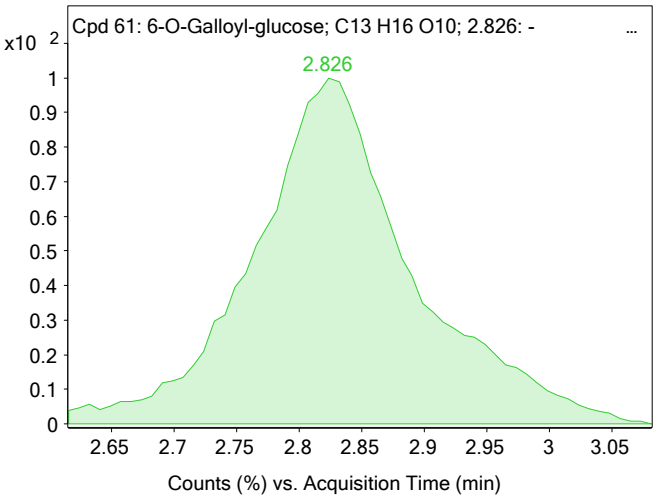
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Gallic acid	2.769	C7 H6 O5		97.02	170.0208	0.73	(M-H)-

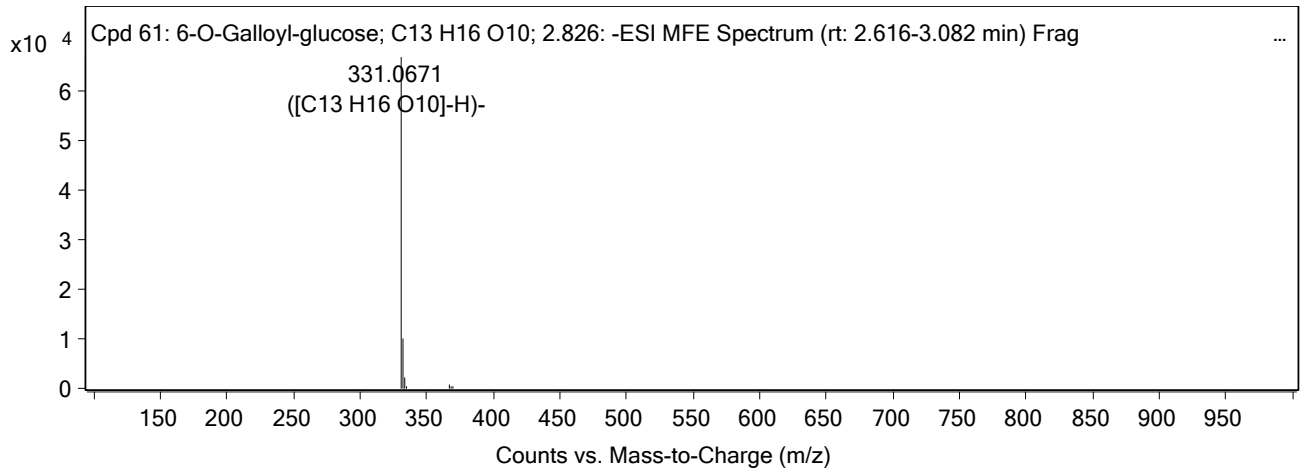
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 61: 6-O-Galloyl-glucose; C13 H16 O10; 2.826	**6-O-Galloyl-glucose**	331.0671	2.826	Find by Molecular Feature	332.0743

Compound Chromatograms

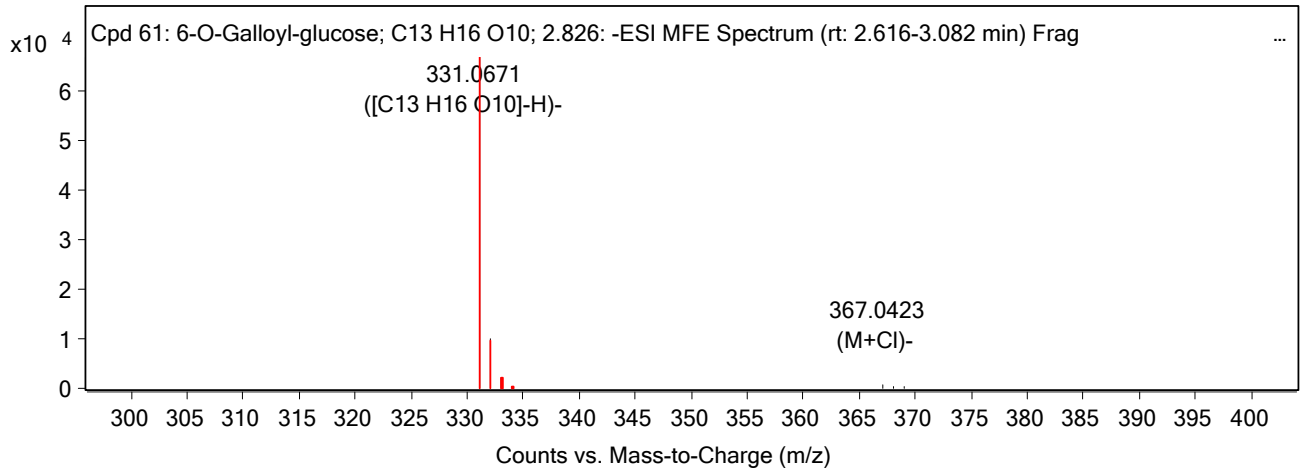




MFE MS Spectrum



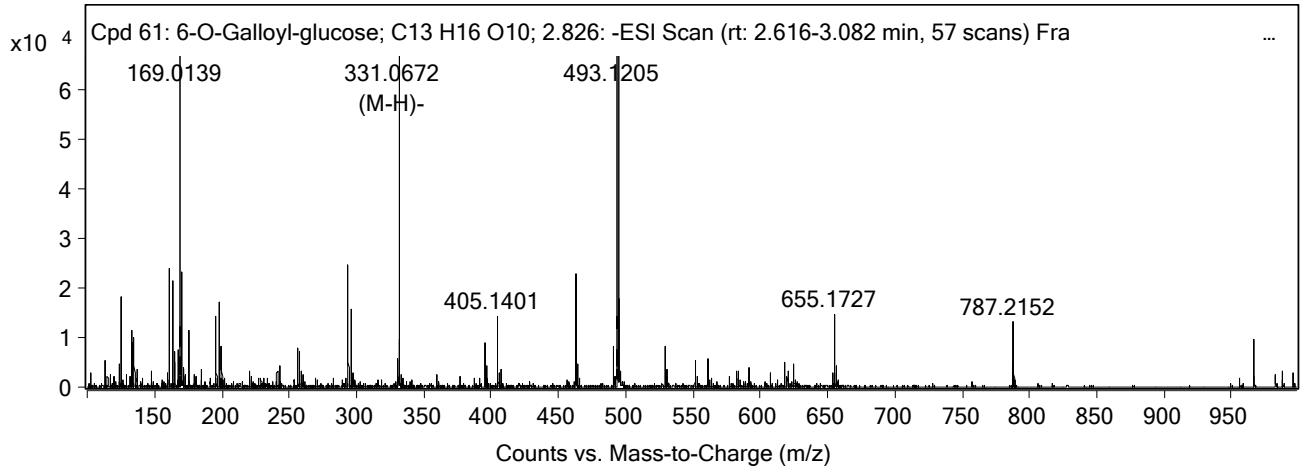
MFE MS Zoomed Spectrum



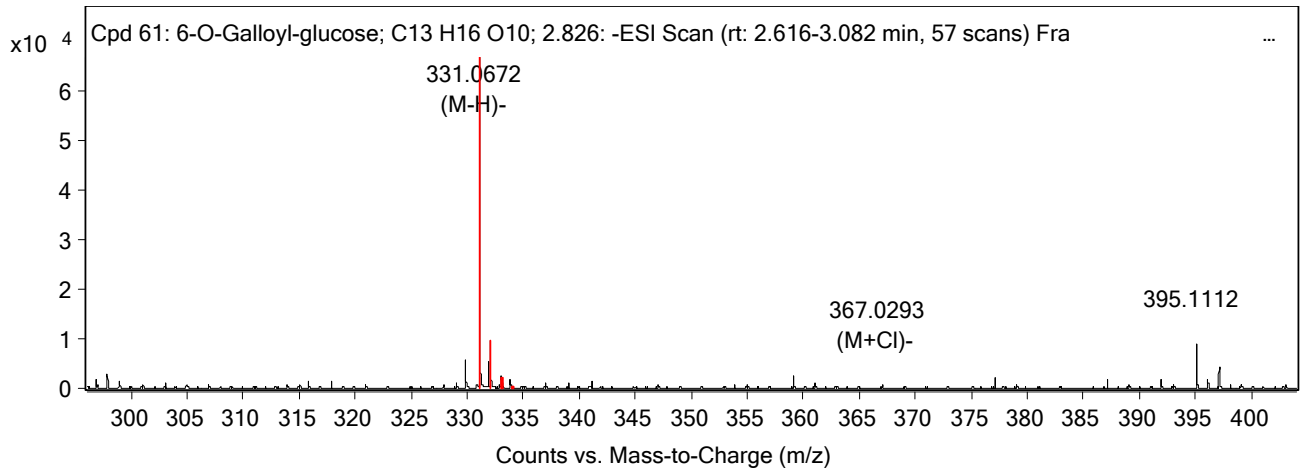
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
331.0671	-1	66916.05	C13 H16 O10	(M-H)-
332.0702	-1	9978.27	C13 H16 O10	(M-H)-
333.0725	-1	2073.69	C13 H16 O10	(M-H)-
334.0721	-1	303.36	C13 H16 O10	(M-H)-
367.0423	-1	900.15		(M+Cl)-
368.0478	-1	270.16		(M+Cl)-
369.0423	-1	443.22		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

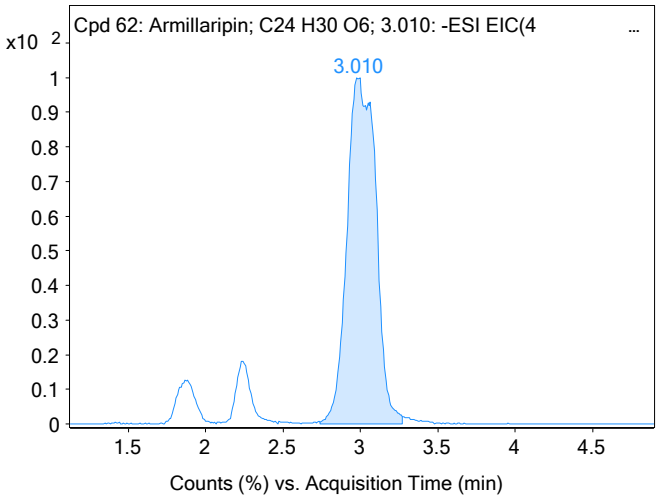


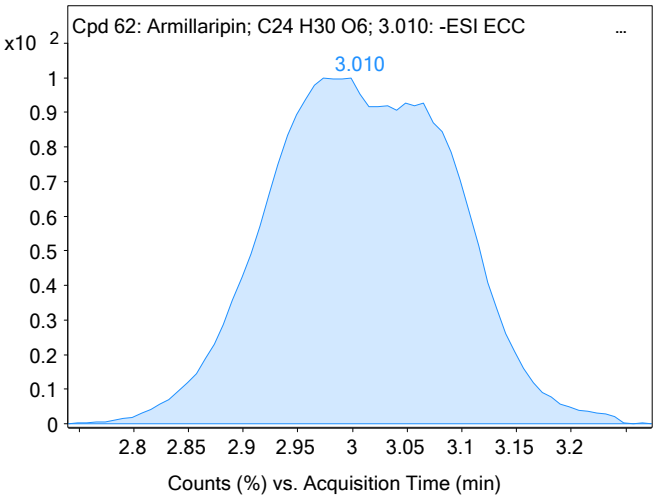
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	6-O-Galloyl-glucose	2.826	C13 H16 O10		99.85	332.0743	0.03	(M-H)-
	1-Galloyl-glucose	2.826	C13 H16 O10		99.85	332.0743	0.03	(M-H)-
	Gluco-syringic acid	2.826	C13 H16 O10		99.85	332.0743	0.03	(M-H)-

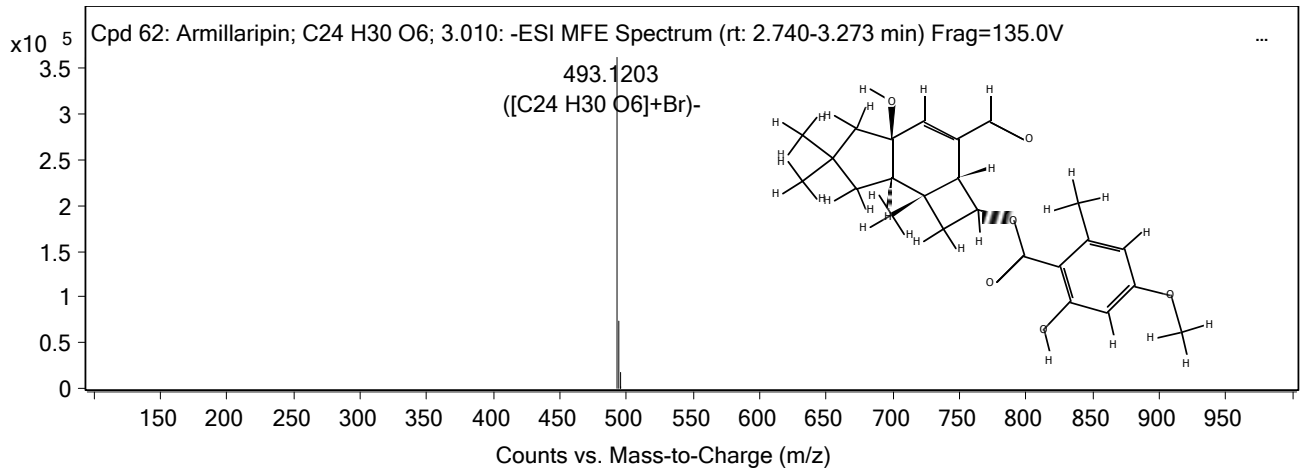
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 62: Armillaripin; C24 H30 O6; 3.010	**Armillaripin**	493.1203	3.01	Find by Molecular Feature	414.2017

Compound Chromatograms

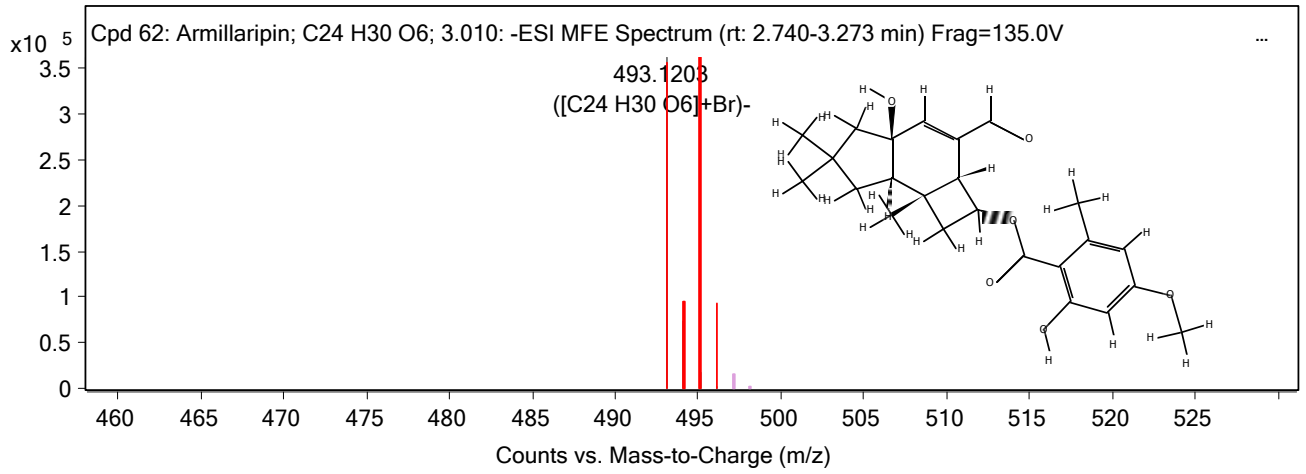




MFE MS Spectrum



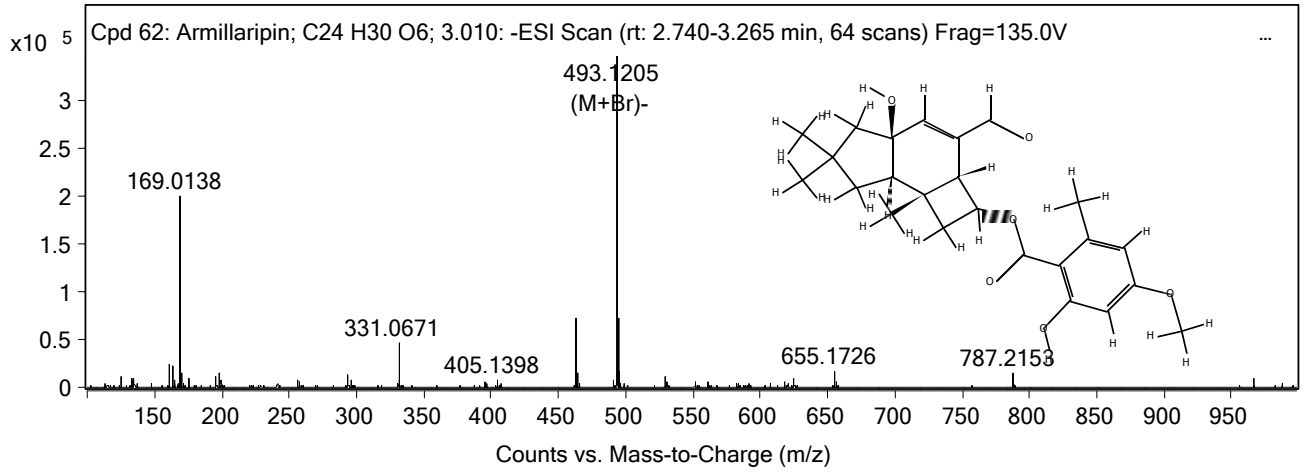
MFE MS Zoomed Spectrum



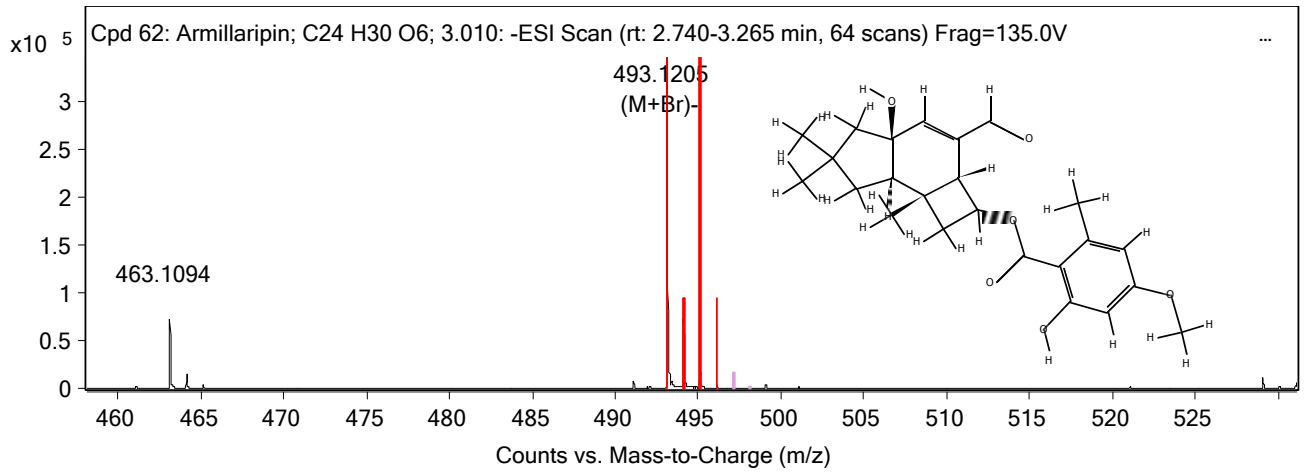
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
493.1203	-1	361972.56	C24 H30 O6	(M+Br)-
494.1233	-1	73106.52	C24 H30 O6	(M+Br)-
495.1251	-1	17291.67	C24 H30 O6	(M+Br)-
496.1281	-1	2697.42	C24 H30 O6	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

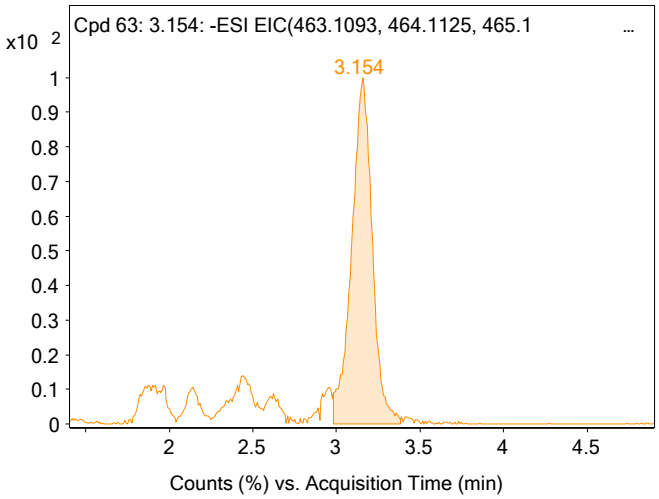


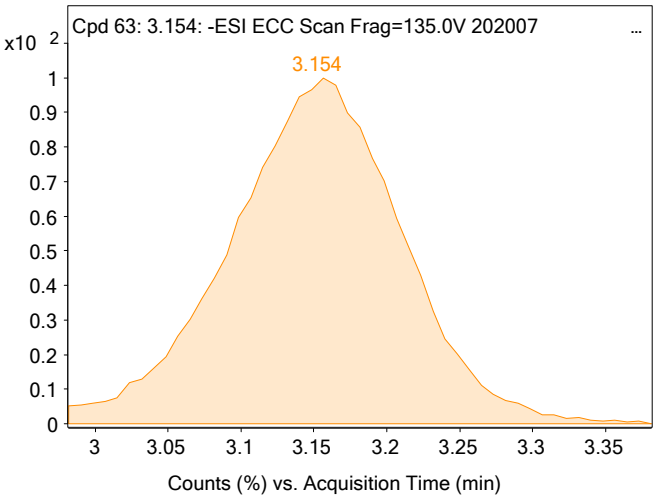
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Armillaripin	3.01	C24 H30 O6		54	414.2017	2.57	(M+Br)-
	Bufotalinin	3.01	C24 H30 O6		54	414.2017	2.57	(M+Br)-
	Magnoshinin	3.01	C24 H30 O6		54	414.2017	2.57	(M+Br)-

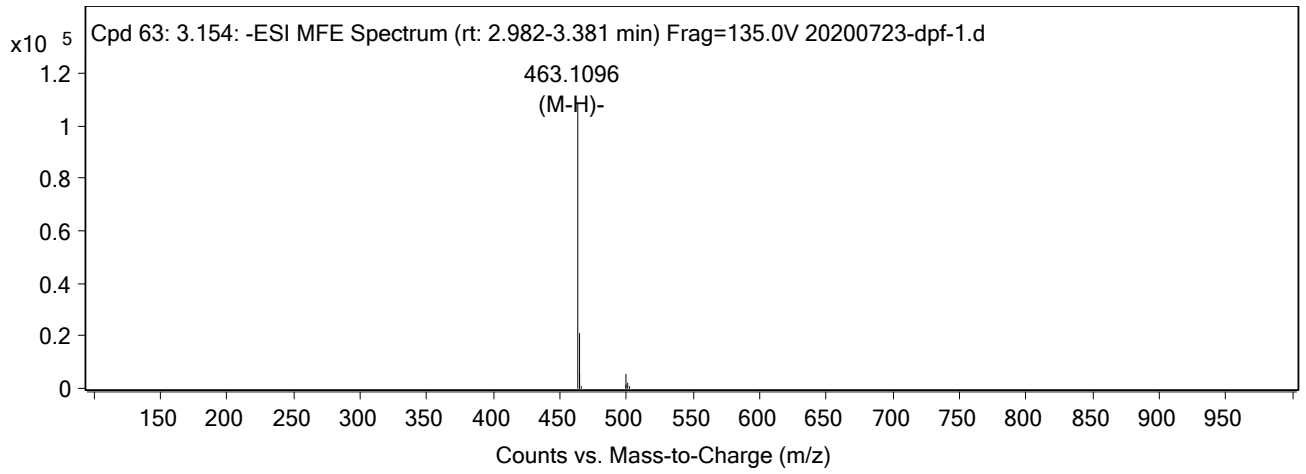
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 63: 3.154	463.1096	3.154	Find by Molecular Feature	464.1169

Compound Chromatograms

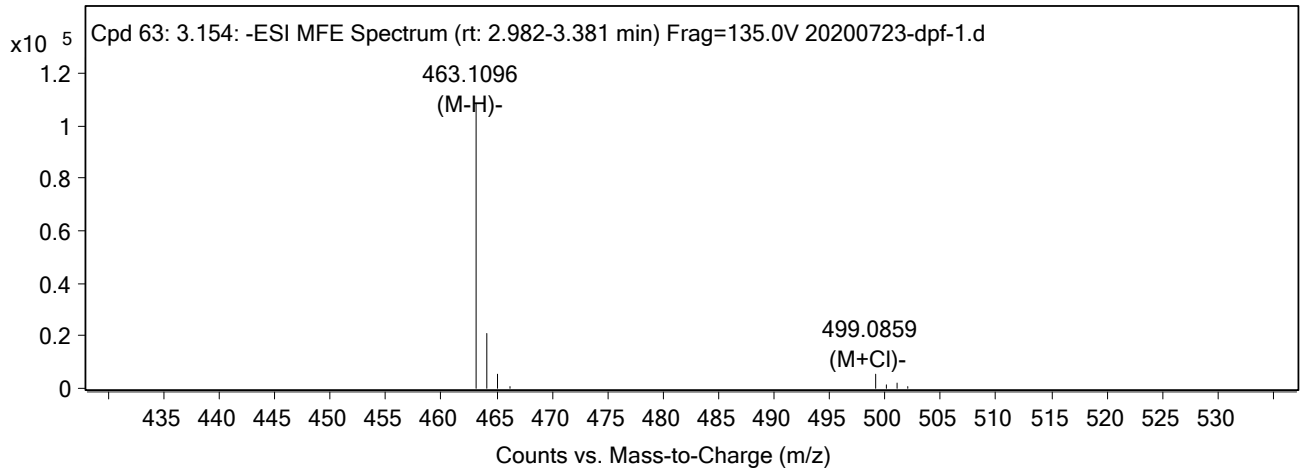




MFE MS Spectrum



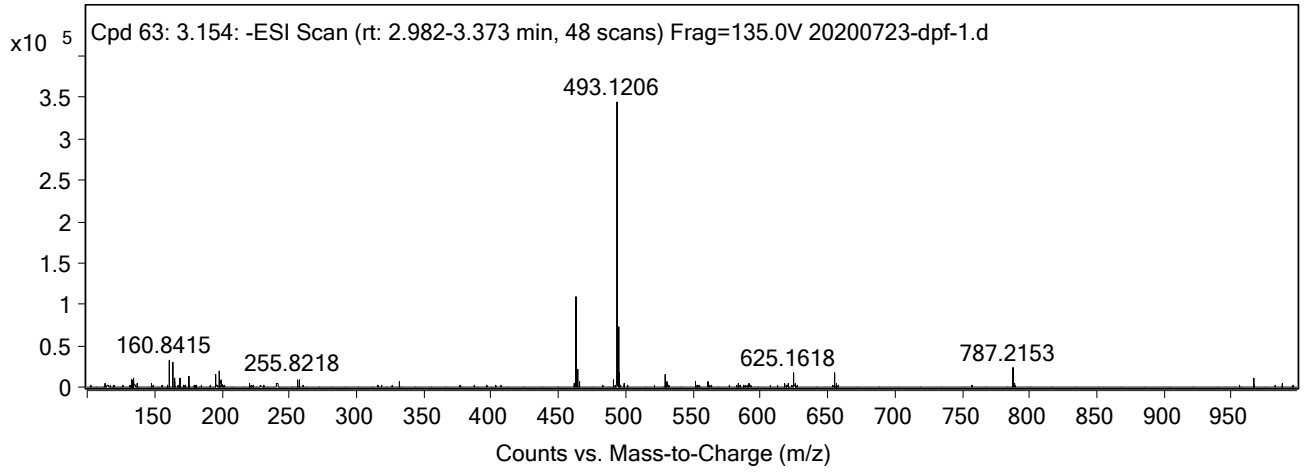
MFE MS Zoomed Spectrum



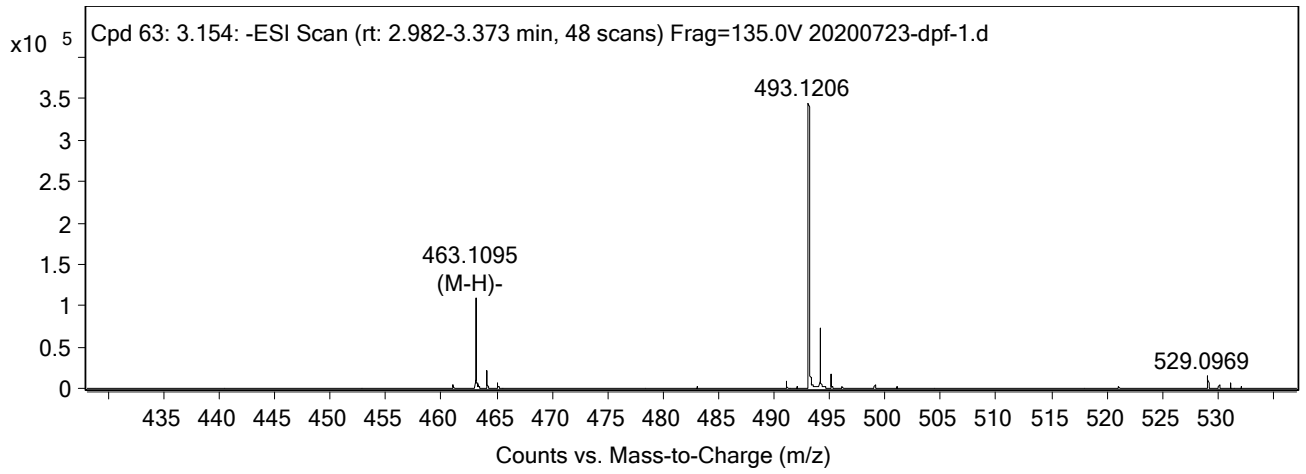
MS Spectrum Peak List

m/z	z	Abund	Ion
463.1096	-1	108739.02	(M-H)-
464.1129	-1	21160.06	(M-H)-
465.1155	-1	5540.88	(M-H)-
466.119	-1	919.82	(M-H)-
499.0859	-1	5248.09	(M+Cl)-
500.0892	-1	1256.98	(M+Cl)-
501.0842	-1	1981.09	(M+Cl)-
502.0899	-1	427.75	(M+Cl)-

MS Spectrum

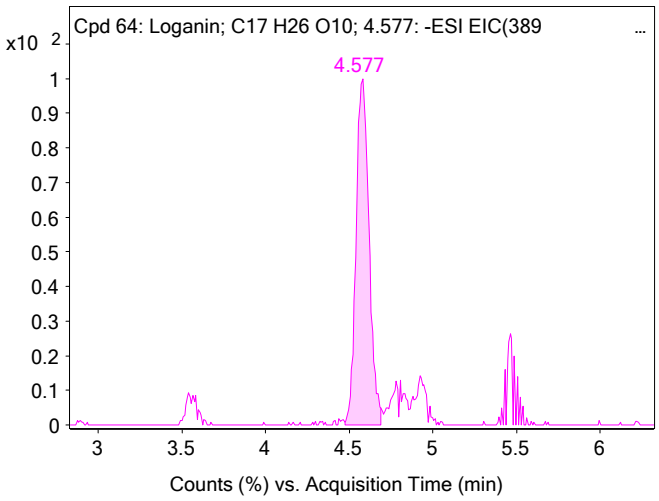


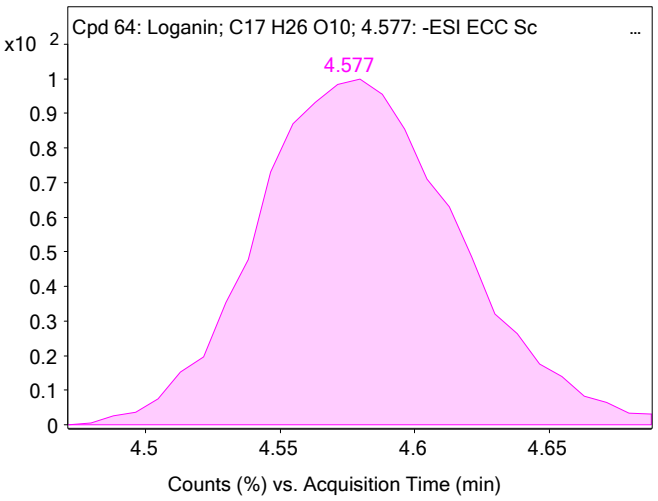
MS Zoomed Spectrum



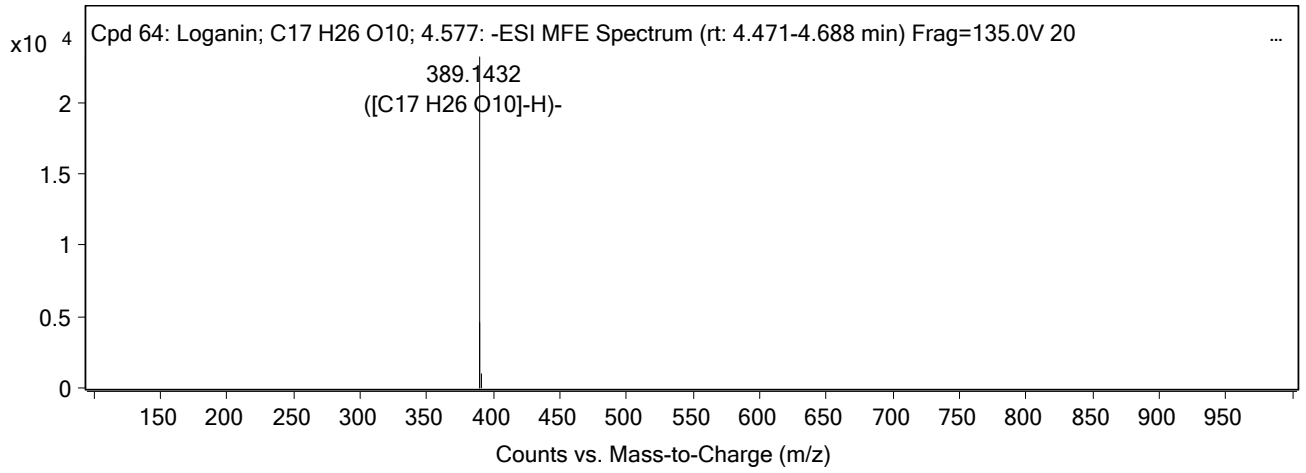
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 64: Loganin; C17 H26 O10; 4.577	**Loganin**	389.1432	4.577	Find by Molecular Feature	390.1505

Compound Chromatograms

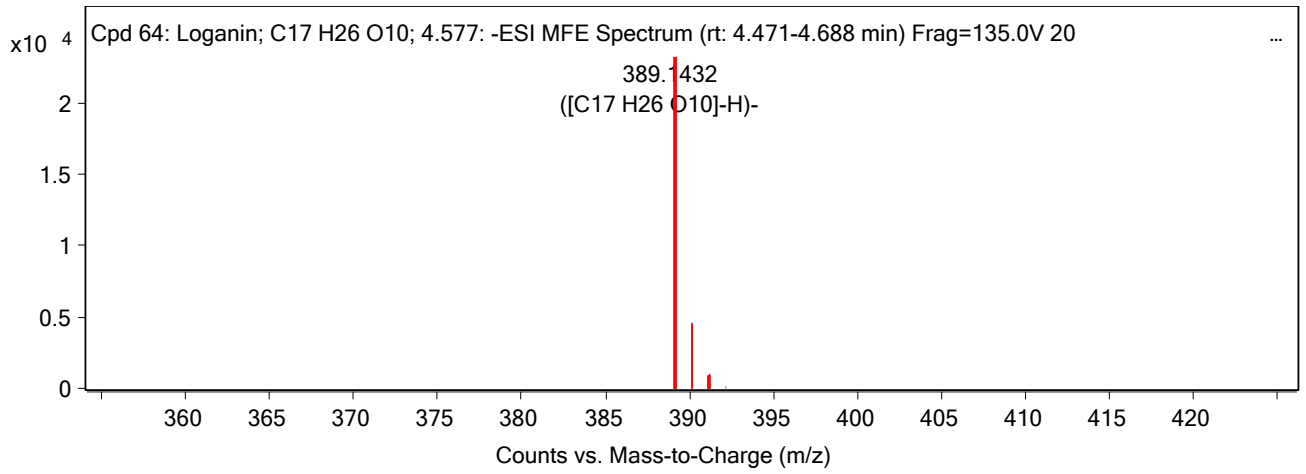




MFE MS Spectrum



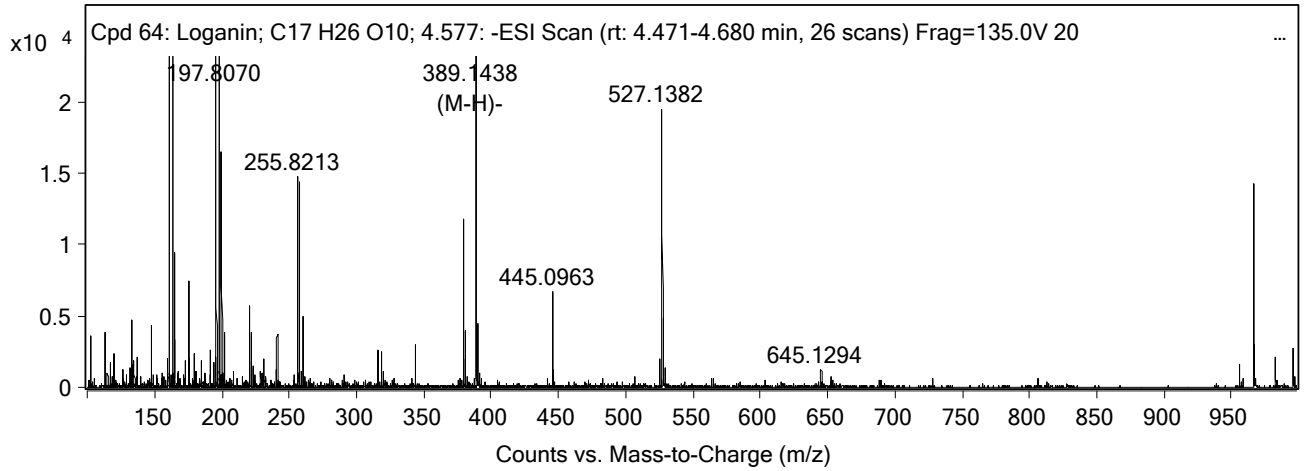
MFE MS Zoomed Spectrum



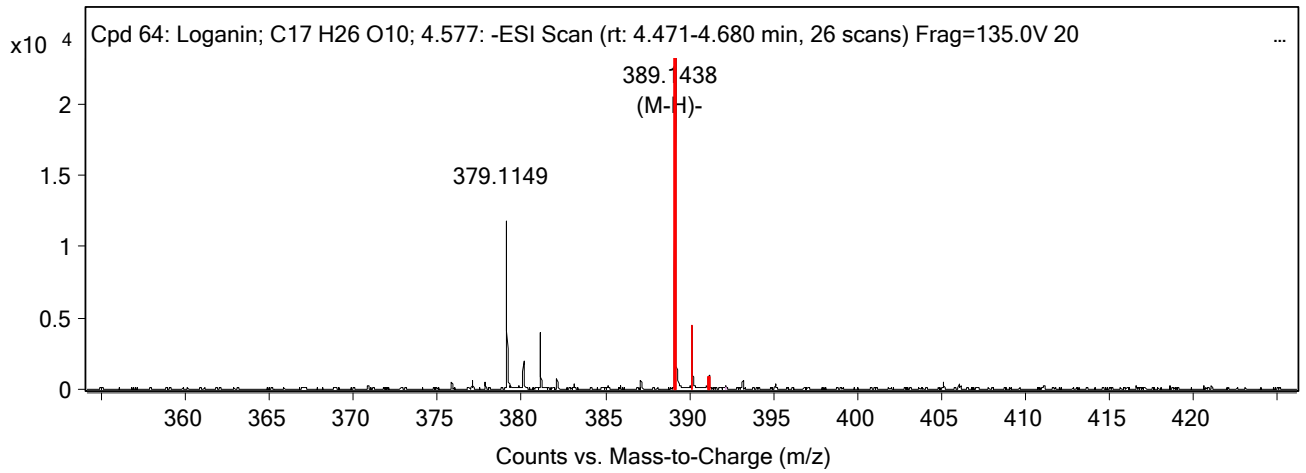
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
389.1432	-1	23205.21	C17 H26 O10	(M-H)-
390.1469	-1	4555.71	C17 H26 O10	(M-H)-
391.149	-1	949.42	C17 H26 O10	(M-H)-

MS Spectrum



MS Zoomed Spectrum



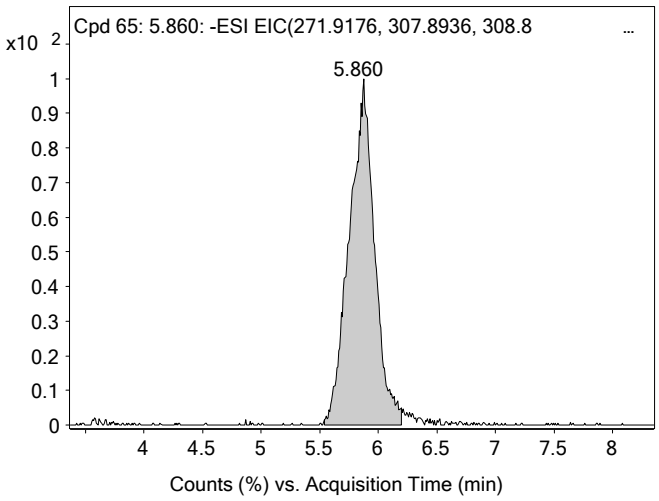
Identification Hit Table

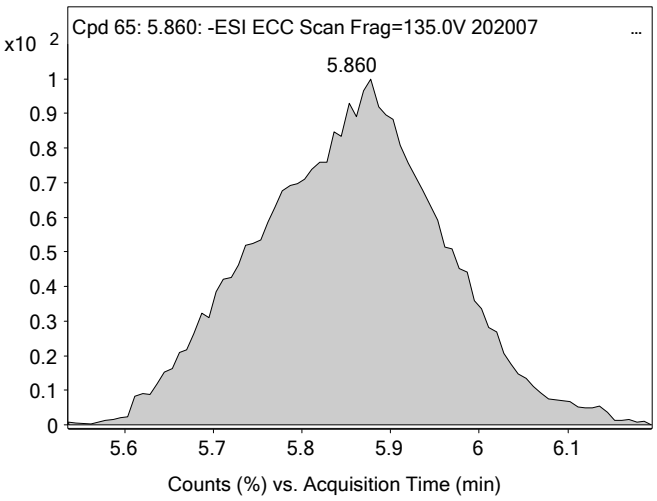
Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Loganin	4.577	C17 H26 O10		89.34	390.1505	2.07	(M-H)-
	3,4-Dihydroverbenalin	4.577	C17 H26 O10		89.34	390.1505	2.07	(M-H)-
	1-beta-Glucogeniposide	4.577	C17 H26 O10		89.34	390.1505	2.07	(M-H)-
	Harpagideacetate	4.577	C17 H26 O10		89.34	390.1505	2.07	(M-H)-
	Ajugoside	4.577	C17 H26 O10		89.34	390.1505	2.07	(M-H)-
	Loganoside	4.577	C17 H26 O10		89.34	390.1505	2.07	(M-H)-

	Mesuagin	4.577	C24 H22 O5		65.48	390.1505	-3.78	(M-H)-
	Takatonine	4.577	C21 H24 N O4		40.93	354.1741	-3.58	(M+Cl)-
	N-Methyl canadine	4.577	C21 H24 N O4		40.93	354.1741	-3.58	(M+Cl)-

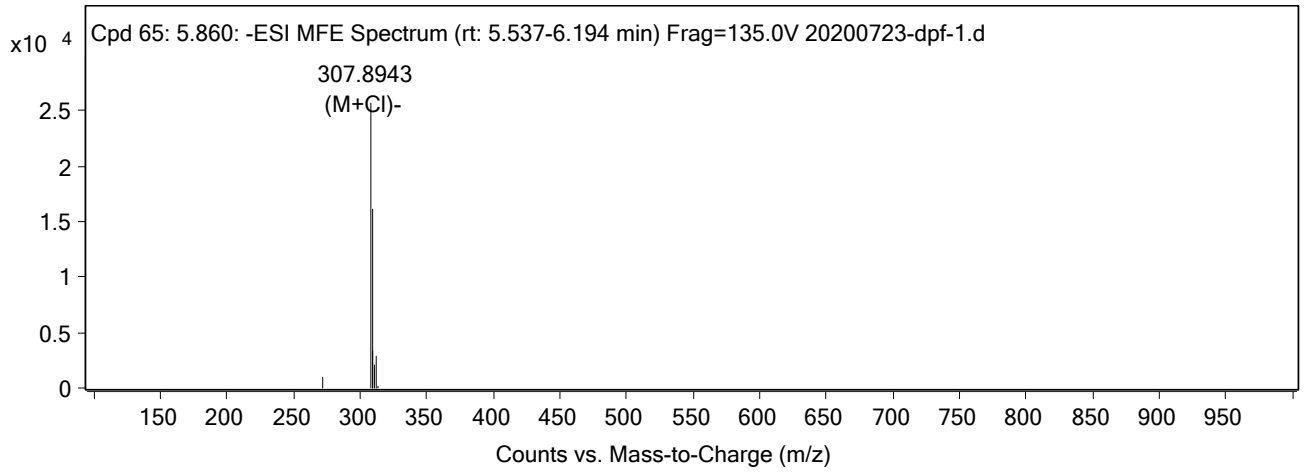
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 65: 5.860	307.8943	5.86	Find by Molecular Feature	272.9249

Compound Chromatograms

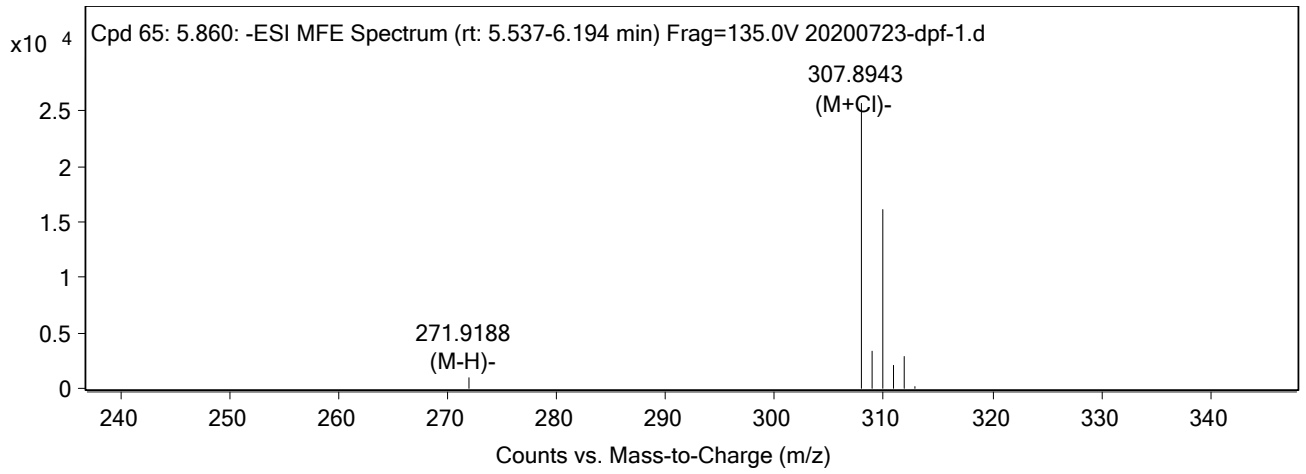




MFE MS Spectrum



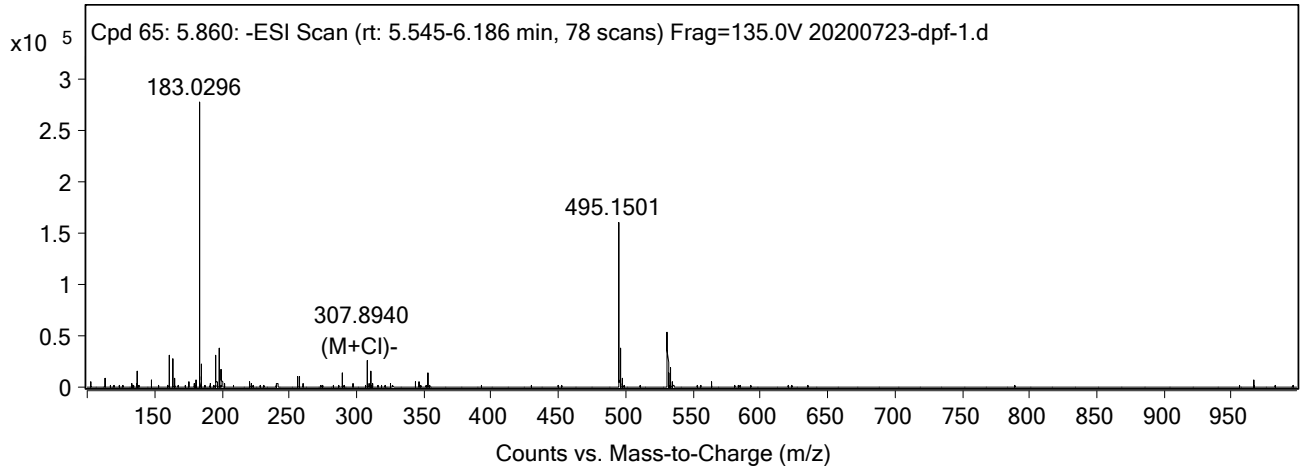
MFE MS Zoomed Spectrum



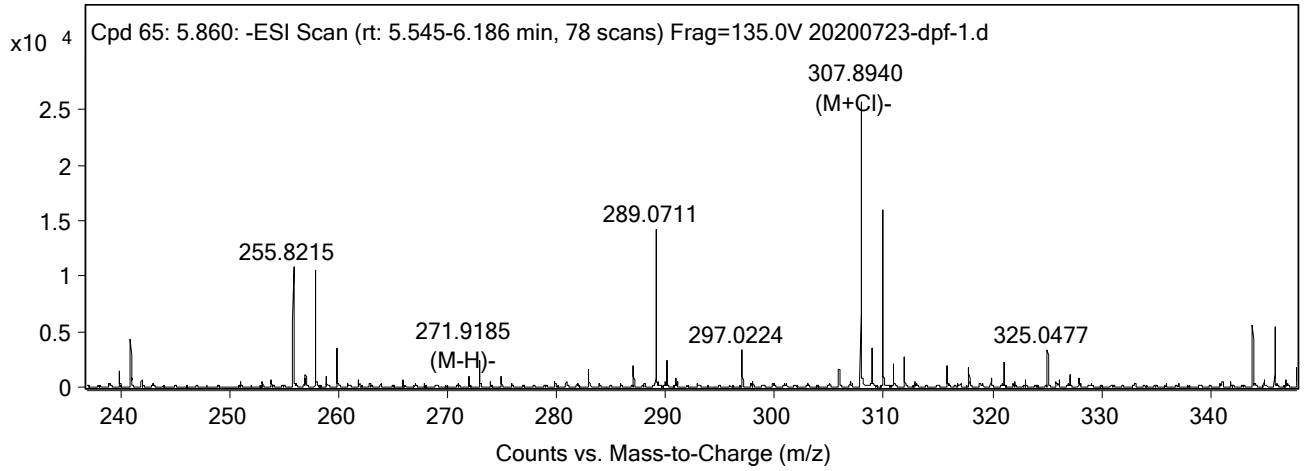
MS Spectrum Peak List

m/z	z	Abund	Ion
271.9188	-1	1043.47	(M-H)-
307.8943	-1	25729.72	(M+Cl)-
308.8969	-1	3285.39	(M+Cl)-
309.8913	-1	16193.08	(M+Cl)-
310.8938	-1	2103.89	(M+Cl)-
311.8887	-1	2821.72	(M+Cl)-
312.891	-1	238.35	(M+Cl)-

MS Spectrum



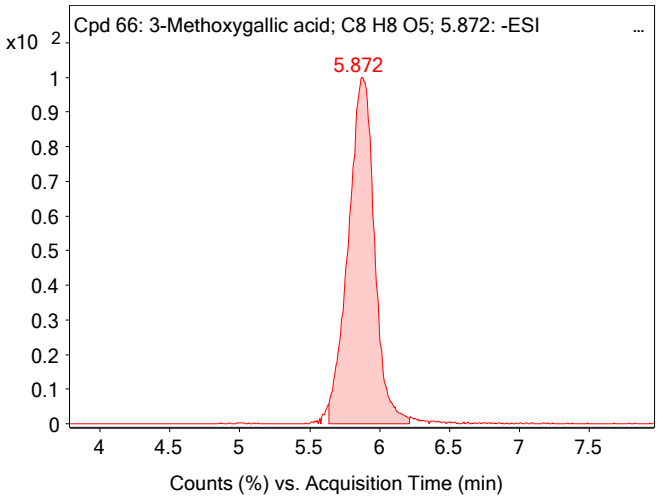
MS Zoomed Spectrum

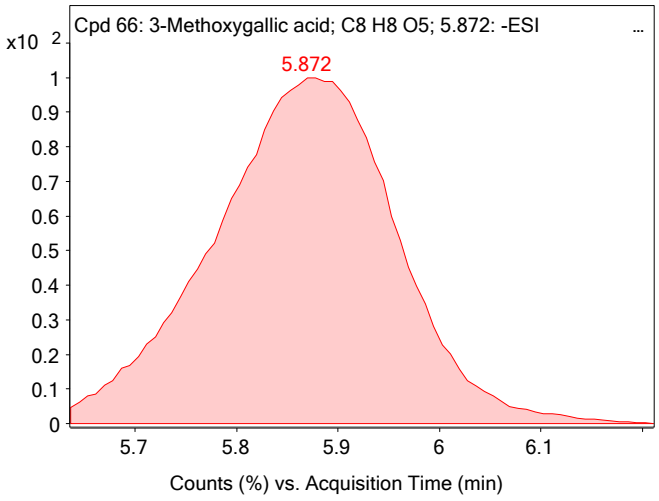


Qualitative Compound Identification Report

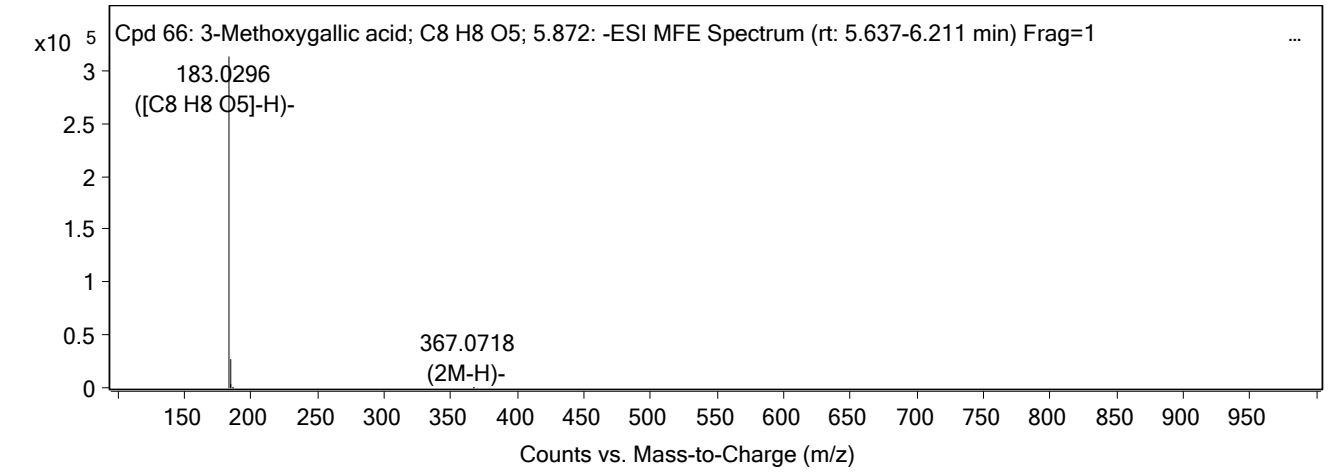
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 66: 3-Methoxygallic acid; C8 H8 O5; 5.872	**3-Methoxygallic acid**	183.0296	5.872	Find by Molecular Feature	184.0368

Compound Chromatograms

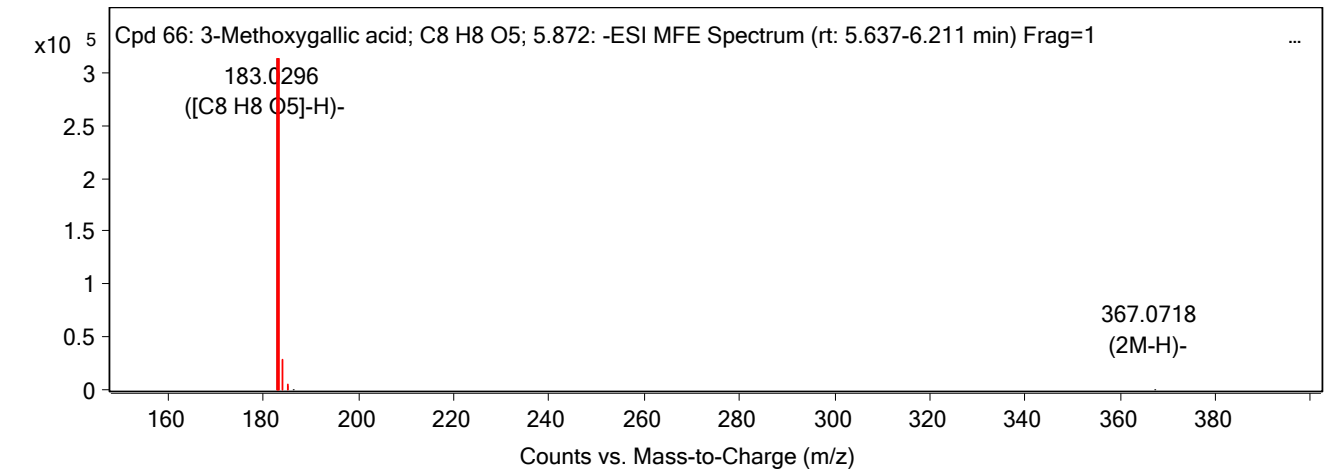




MFE MS Spectrum



MFE MS Zoomed Spectrum

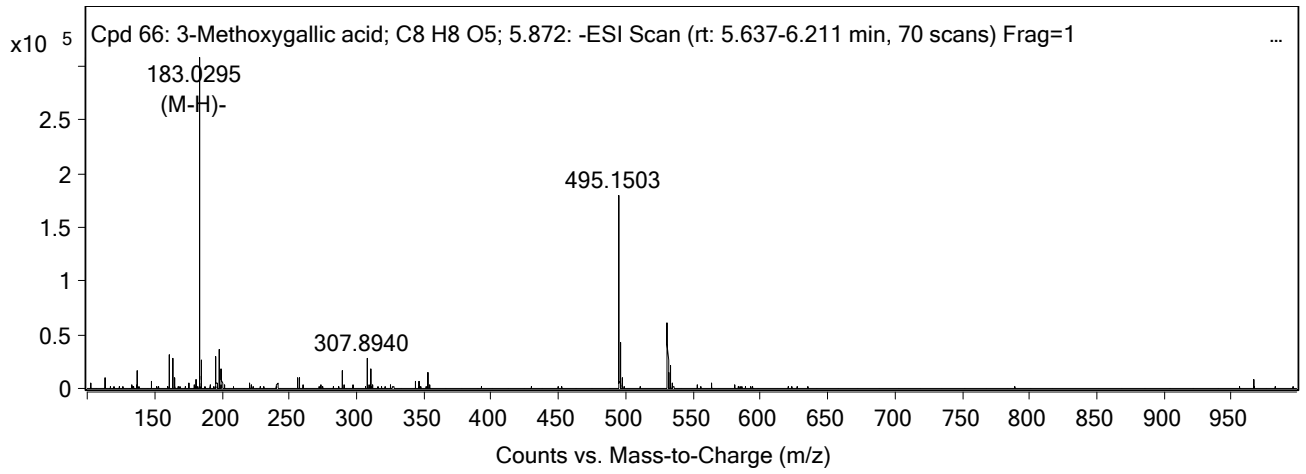


MS Spectrum Peak List

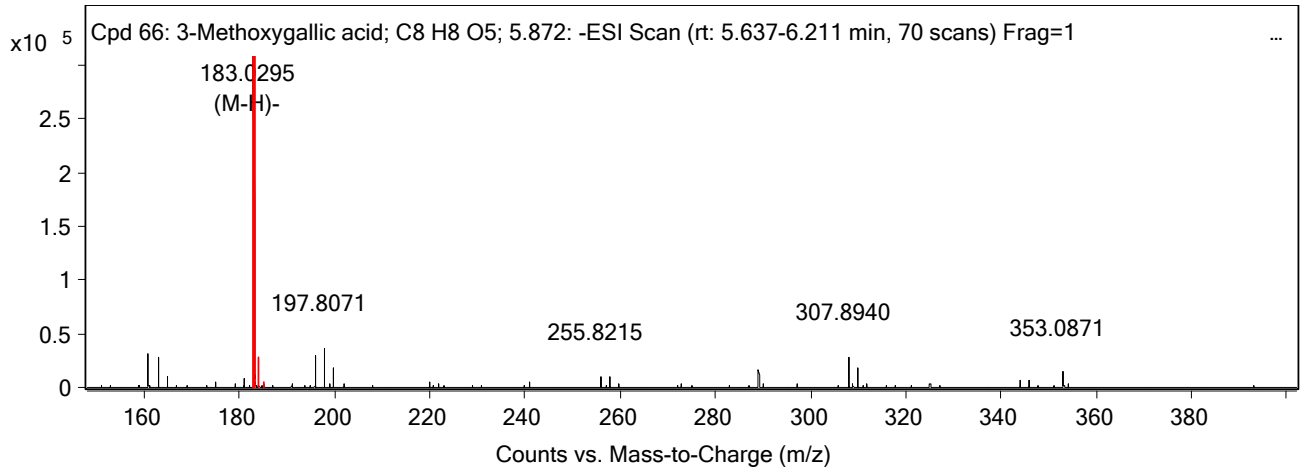
m/z	z	Abund	Formula	Ion
183.0296	-1	313345.38	C8 H8 O5	(M-H)-
184.0329	-1	26376.84	C8 H8 O5	(M-H)-
185.0344	-1	4220.81	C8 H8 O5	(M-H)-

186.0385	-1	232.49	C8 H8 O5	(M-H)-
367.0718	-1	874.86		(2M-H)-

MS Spectrum



MS Zoomed Spectrum

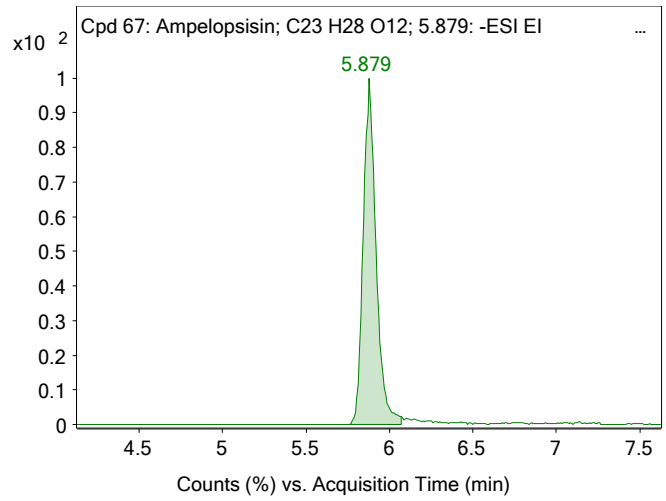


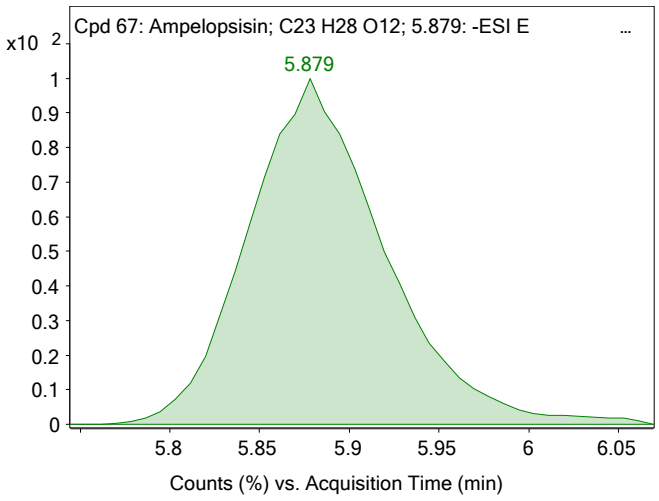
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	3-Methoxygallic acid	5.872	C8 H8 O5		99.31	184.0368	0.34	(M-H)-
	Methyl gallate	5.872	C8 H8 O5		99.31	184.0368	0.34	(M-H)-

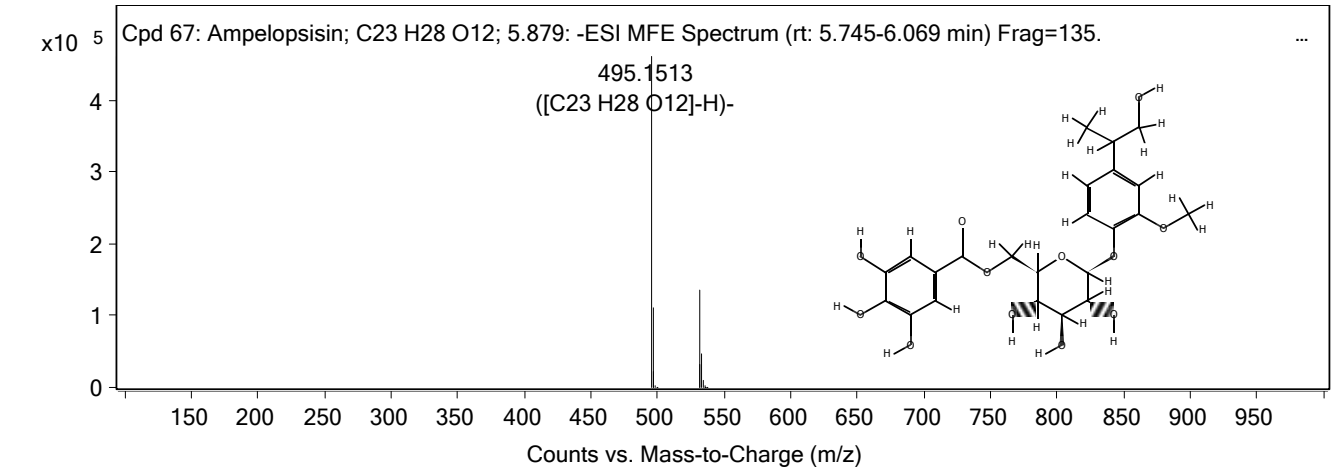
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 67: Ampelopsisin; C23 H28 O12; 5.879	**Ampelopsisin**	495.1513	5.879	Find by Molecular Feature	496.1584

Compound Chromatograms

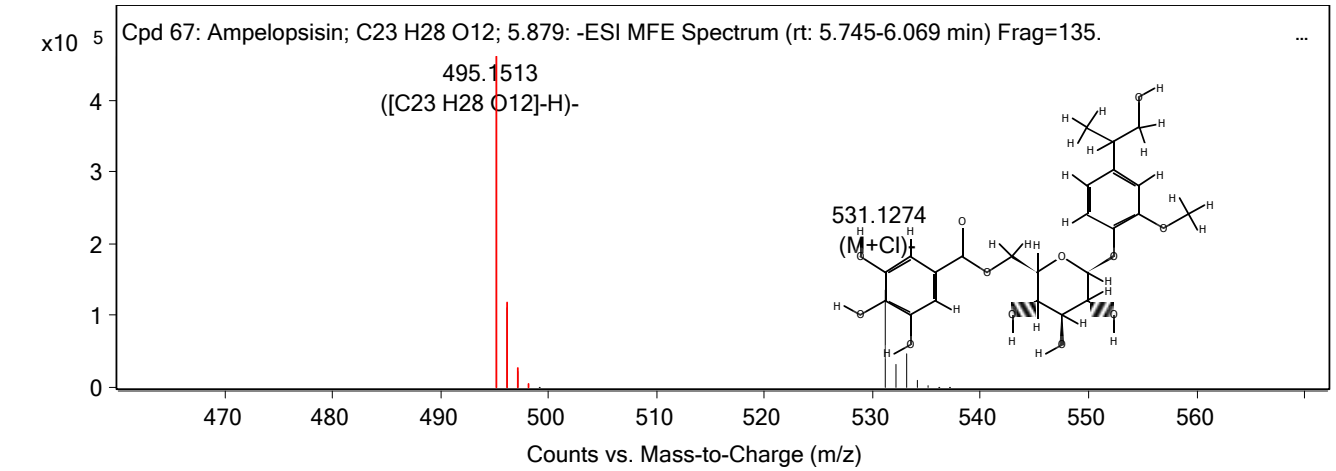




MFE MS Spectrum



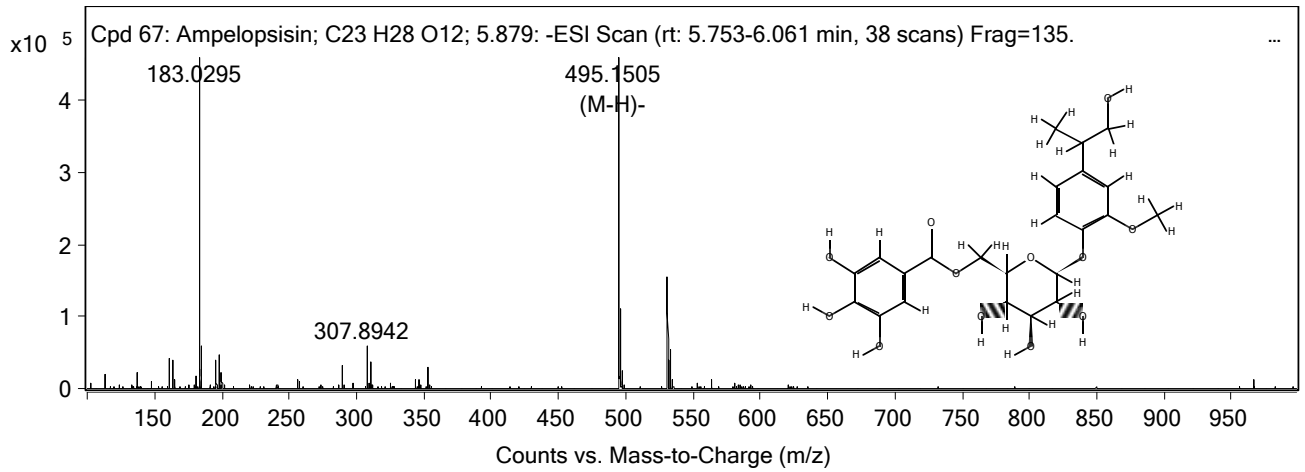
MFE MS Zoomed Spectrum



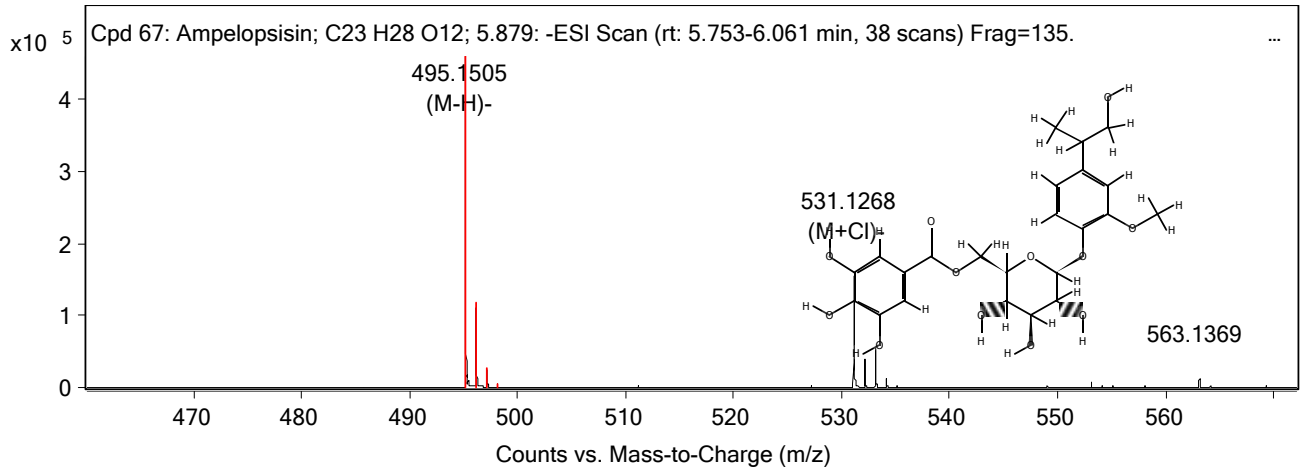
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
495.1513	-1	461211.22	C23 H28 O12	(M-H)-
496.1542	-1	110292.37	C23 H28 O12	(M-H)-
497.1562	-1	23535.29	C23 H28 O12	(M-H)-
498.1598	-1	3616.19	C23 H28 O12	(M-H)-
499.1622	-1	526.51	C23 H28 O12	(M-H)-
531.1274	-1	135819.83		(M+Cl)-
532.1305	-1	33206.85		(M+Cl)-
533.1256	-1	47038.75		(M+Cl)-
534.128	-1	11159.83		(M+Cl)-
535.1317	-1	2573.08		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

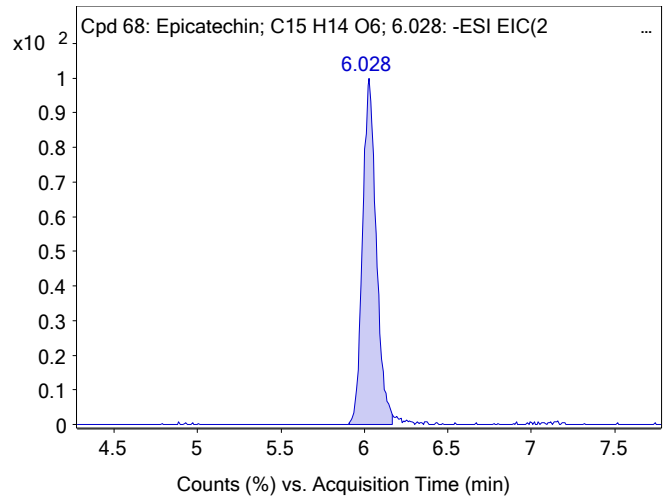


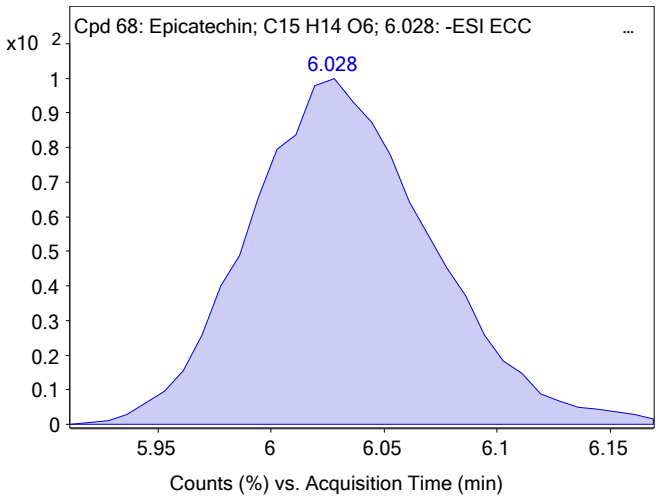
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Ampelopsisin	5.879	C23 H28 O12		98.93	496.1584	-0.36	(M-H)-
	Oxypaeoniflorin	5.879	C23 H28 O12		98.93	496.1584	-0.36	(M-H)-
	Tetracentronside A	5.879	C23 H28 O12		98.93	496.1584	-0.36	(M-H)-

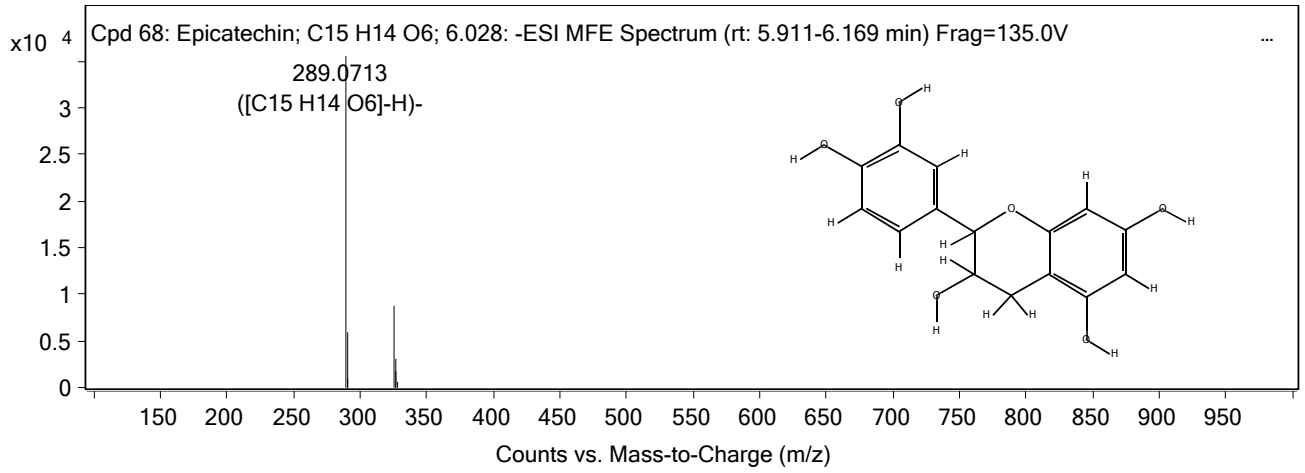
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 68: Epicatechin; C15 H14 O6; 6.028	**Epicatechin**	289.0713	6.028	Find by Molecular Feature	290.0786

Compound Chromatograms

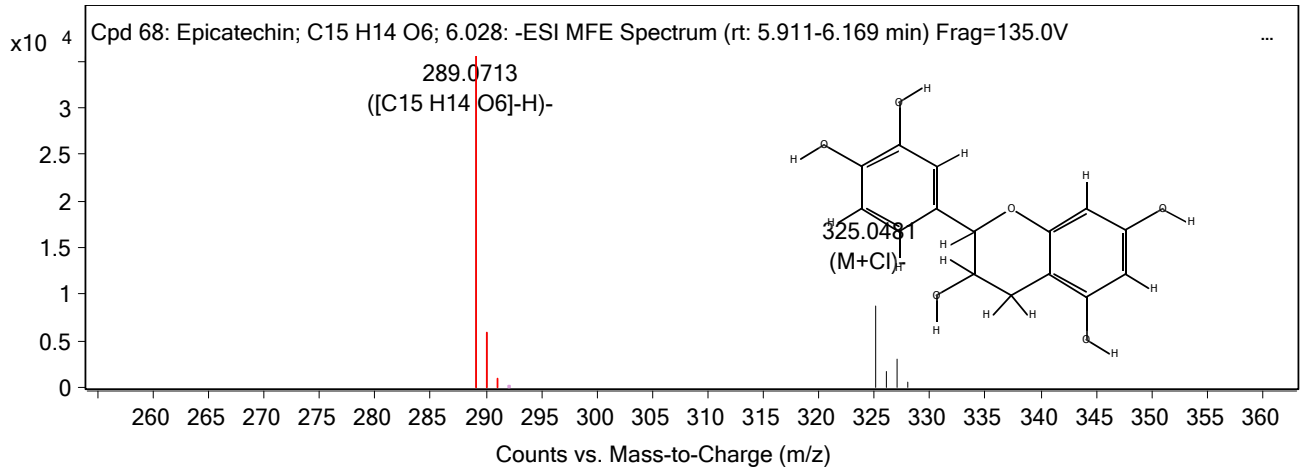




MFE MS Spectrum



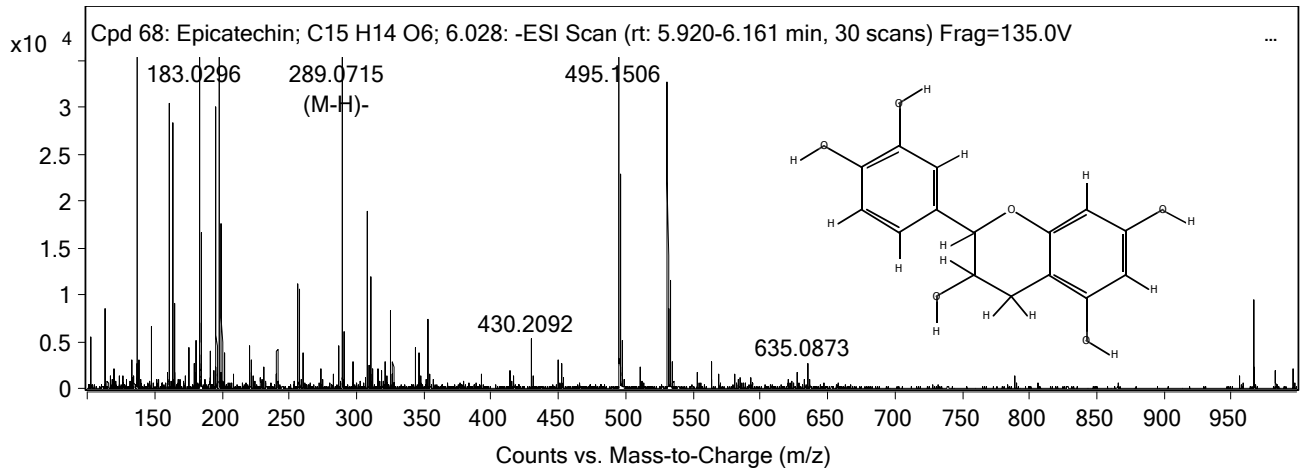
MFE MS Zoomed Spectrum



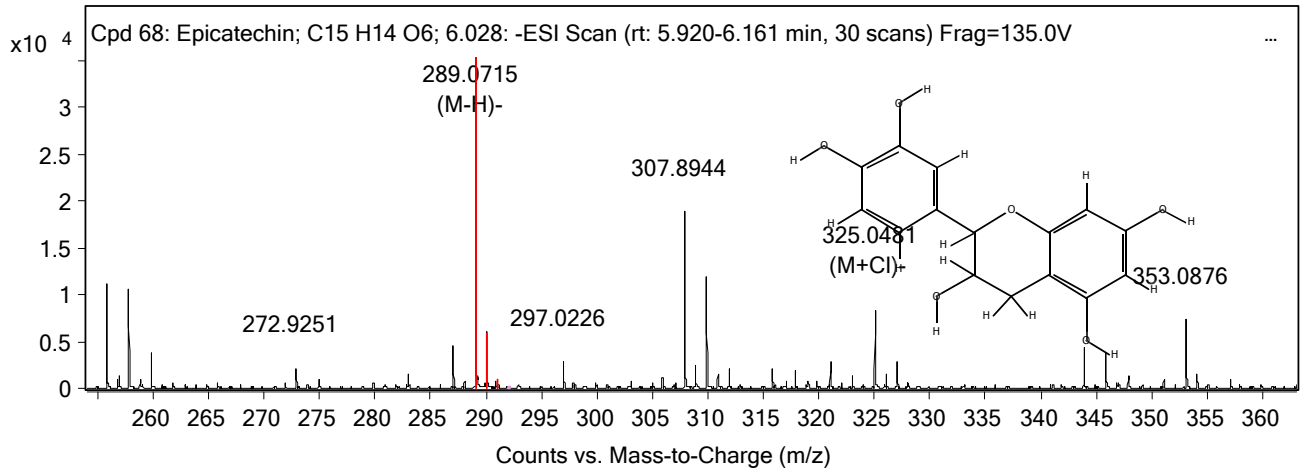
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
289.0713	-1	35526.19	C15 H14 O6	(M-H)-
290.075	-1	5993.75	C15 H14 O6	(M-H)-
291.0766	-1	988.84	C15 H14 O6	(M-H)-
325.0481	-1	8725.95		(M+Cl)-
326.0513	-1	1647.67		(M+Cl)-
327.046	-1	2965.43		(M+Cl)-
328.0478	-1	553.58		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

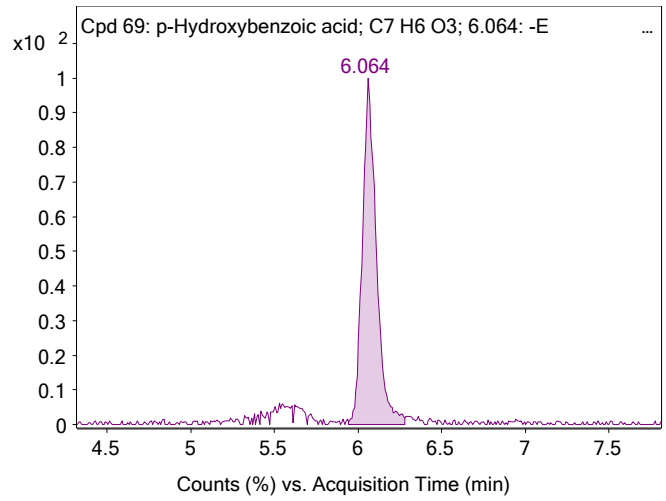


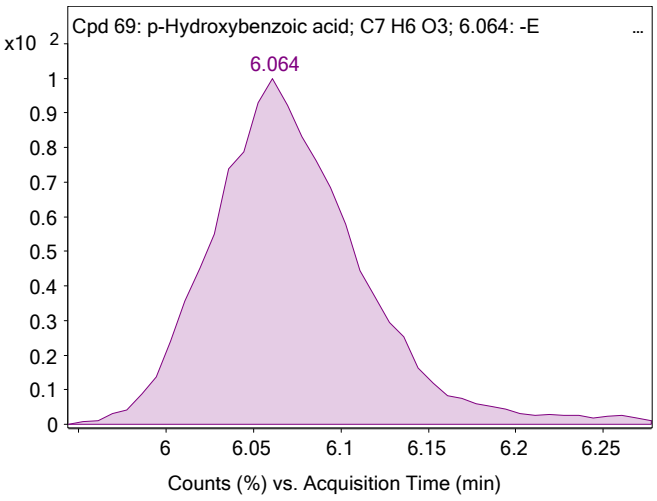
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Epicatechin	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-
	Fistucacidin	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-
	Catechin	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-
	(-)-Epicatechin	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-
	Isoplumericin	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-
	Plumericin	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-
	3',4',5,7-Tetrahydroxyflavanol	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-
	Leucopelargonidin	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-
	Mikanolide	6.028	C15 H14 O6		99.16	290.0786	0.41	(M-H)-

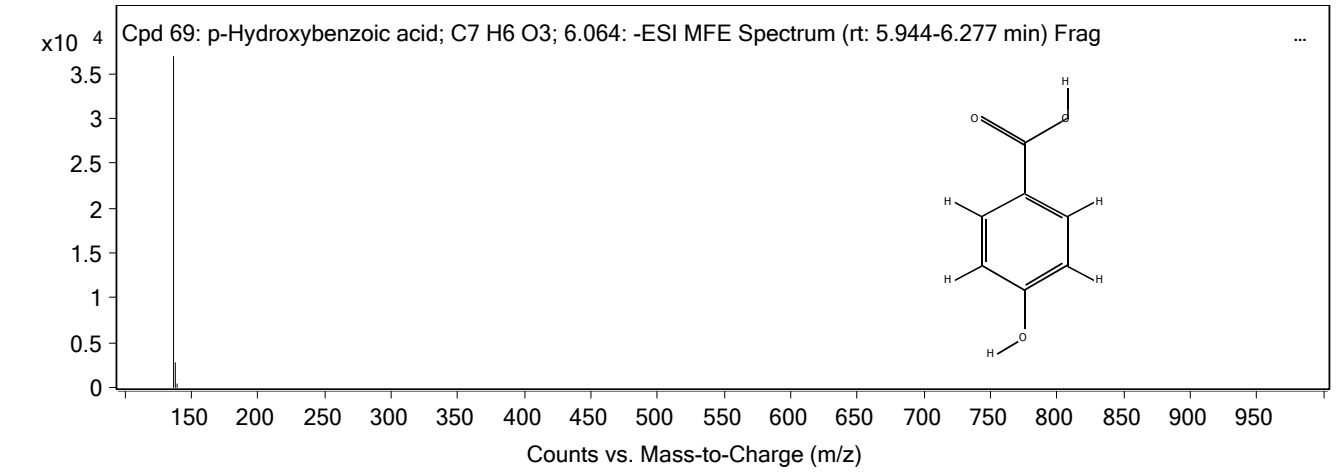
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 69: p-Hydroxybenzoic acid; C7 H6 O3; 6.064	**p-Hydroxybenzoic acid**	137.0244	6.064	Find by Molecular Feature	138.0317

Compound Chromatograms

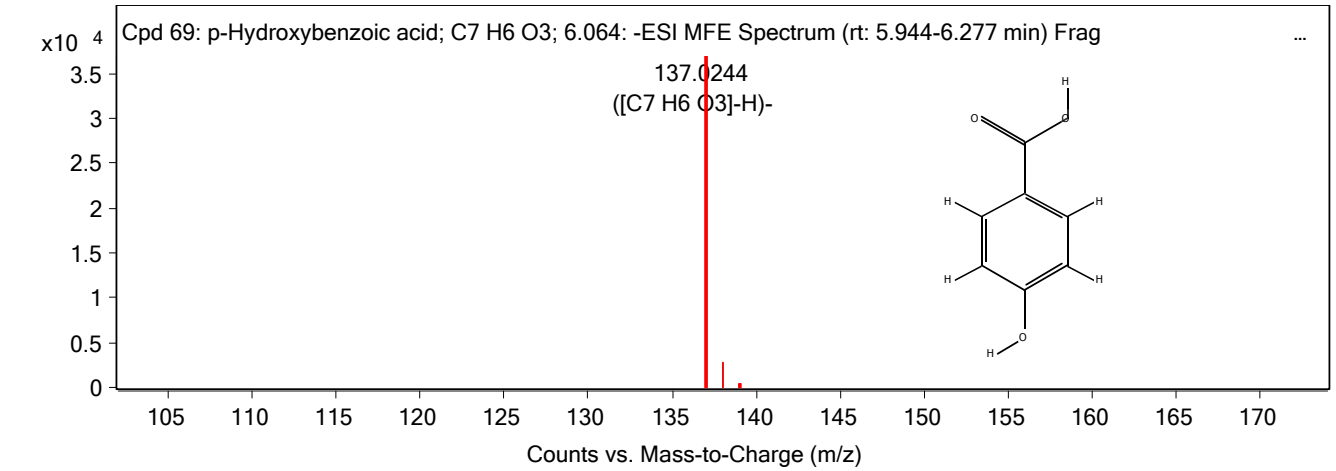




MFE MS Spectrum



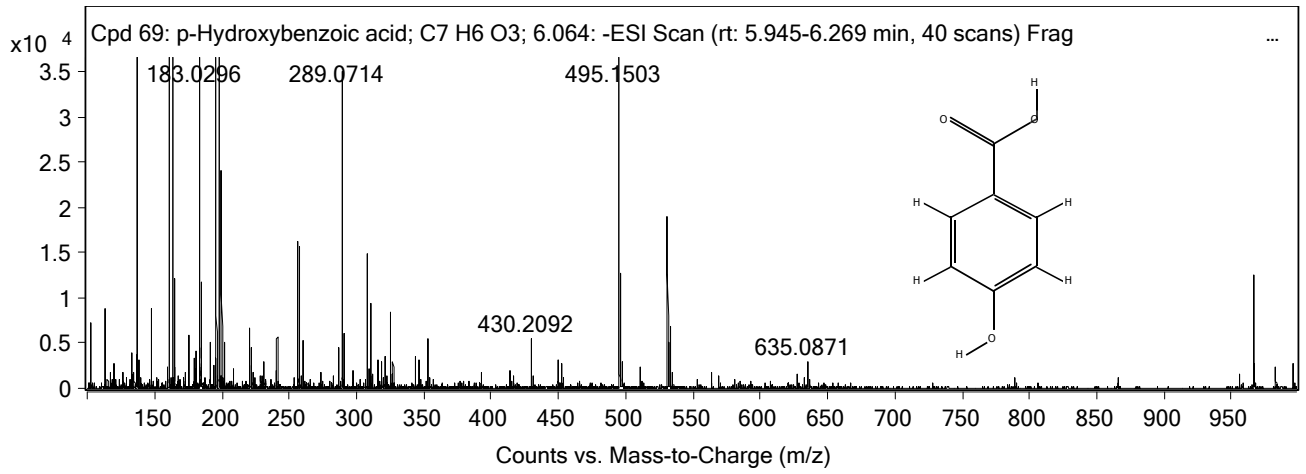
MFE MS Zoomed Spectrum



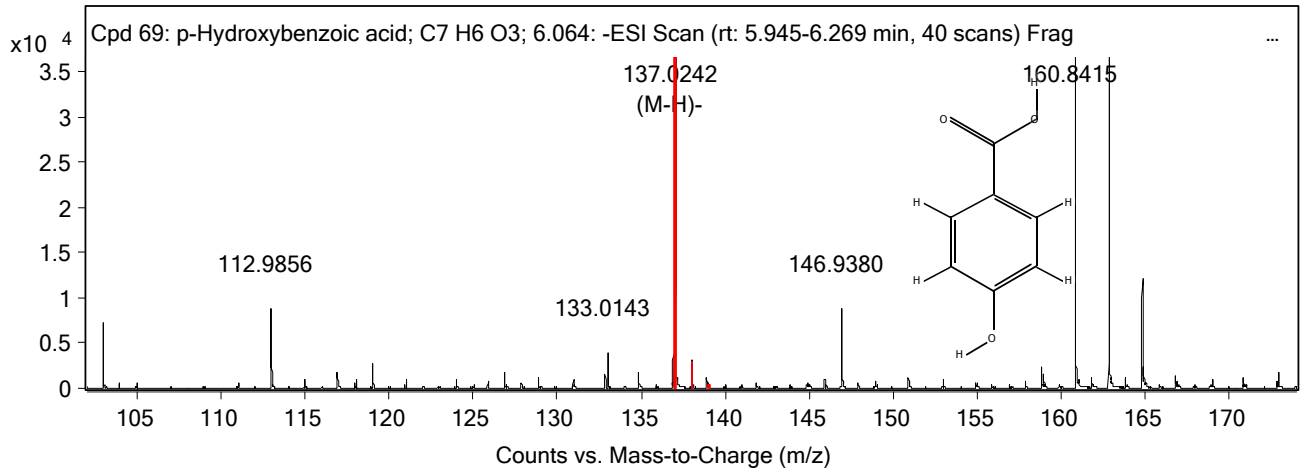
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
137.0244	-1	36918.55	C7 H6 O3	(M-H)-
138.0279	-1	2827.65	C7 H6 O3	(M-H)-
139.027	-1	392.1	C7 H6 O3	(M-H)-

MS Spectrum



MS Zoomed Spectrum

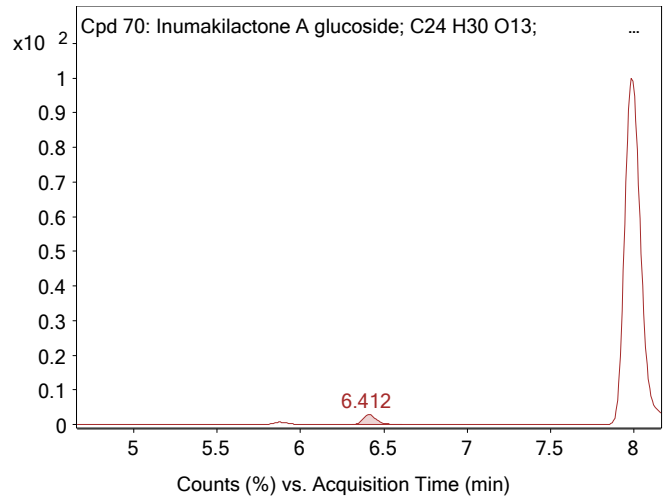


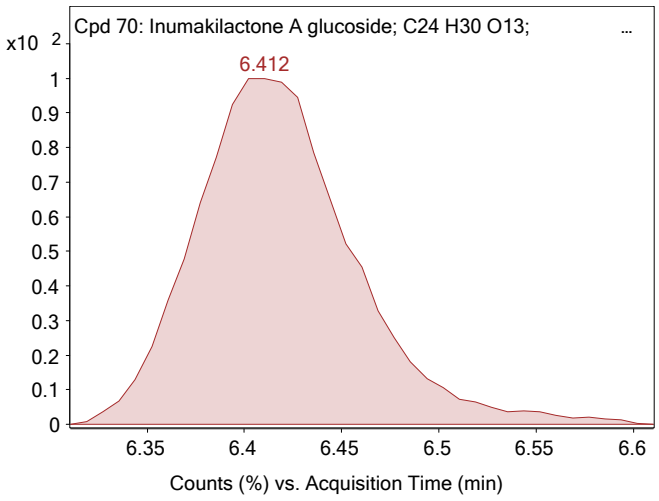
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	p-Hydroxybenzoic acid	6.064	C7 H6 O3		99.89	138.0317	0.02	(M-H)-
	m-Hydroxybenzoic acid	6.064	C7 H6 O3		99.89	138.0317	0.02	(M-H)-
	3,4-Dihydroxybenzyl aldehyde	6.064	C7 H6 O3		99.89	138.0317	0.02	(M-H)-
	Salicylic acid	6.064	C7 H6 O3		99.89	138.0317	0.02	(M-H)-
	Sesamol	6.064	C7 H6 O3		99.89	138.0317	0.02	(M-H)-
	Protocatechuic aldehyde	6.064	C7 H6 O3		99.89	138.0317	0.02	(M-H)-

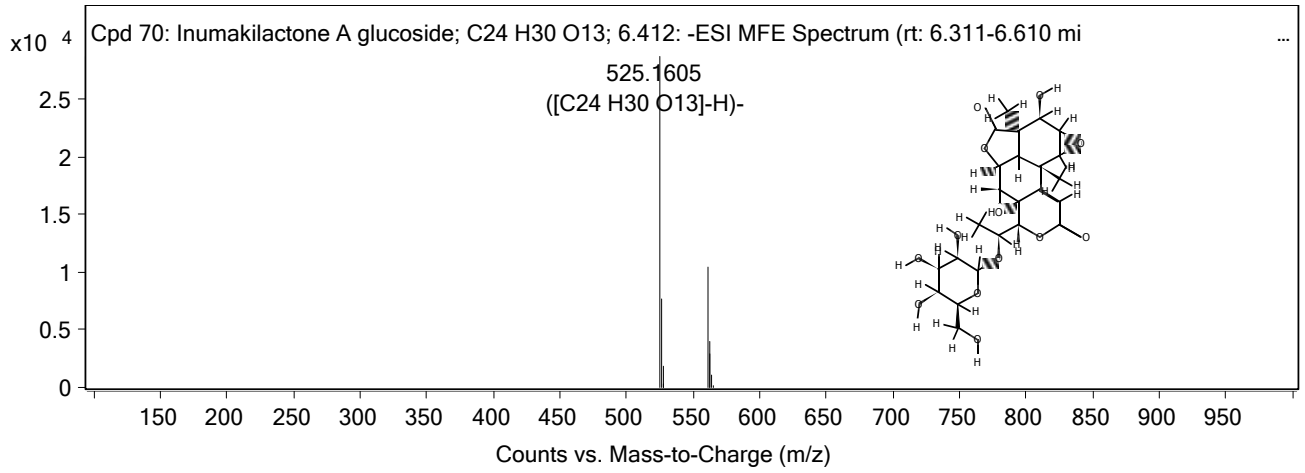
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 70: Inumakilactone A glucoside; C24 H30 O13; 6.412	**Inumakilactone A glucoside**	525.1605	6.412	Find by Molecular Feature	526.1679

Compound Chromatograms

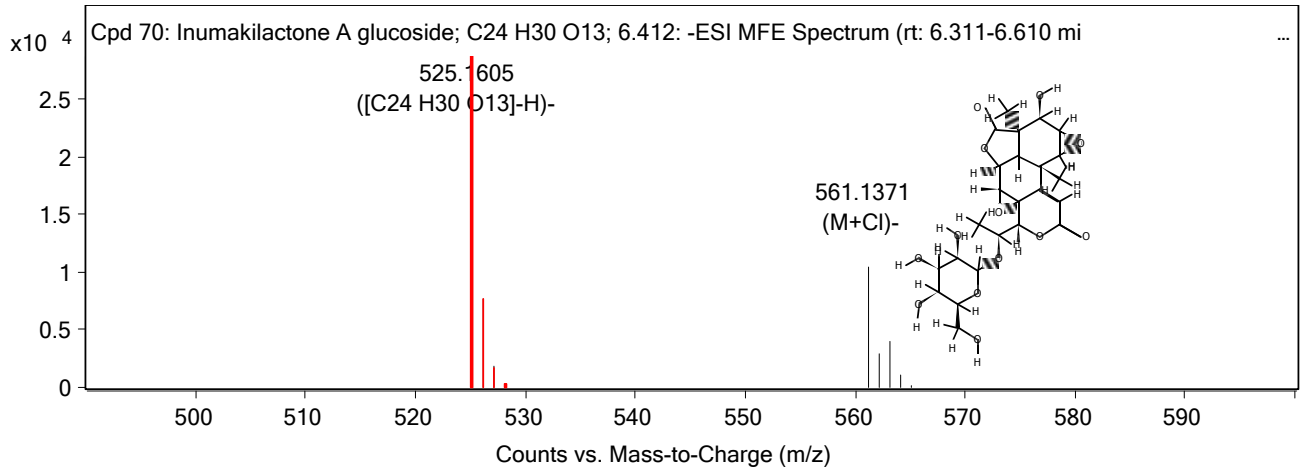




MFE MS Spectrum



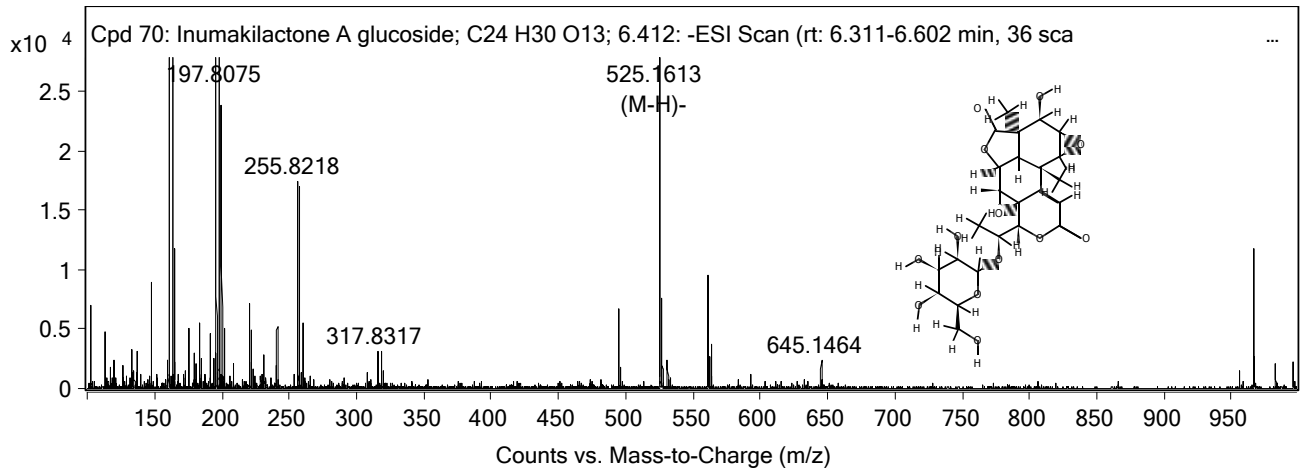
MFE MS Zoomed Spectrum



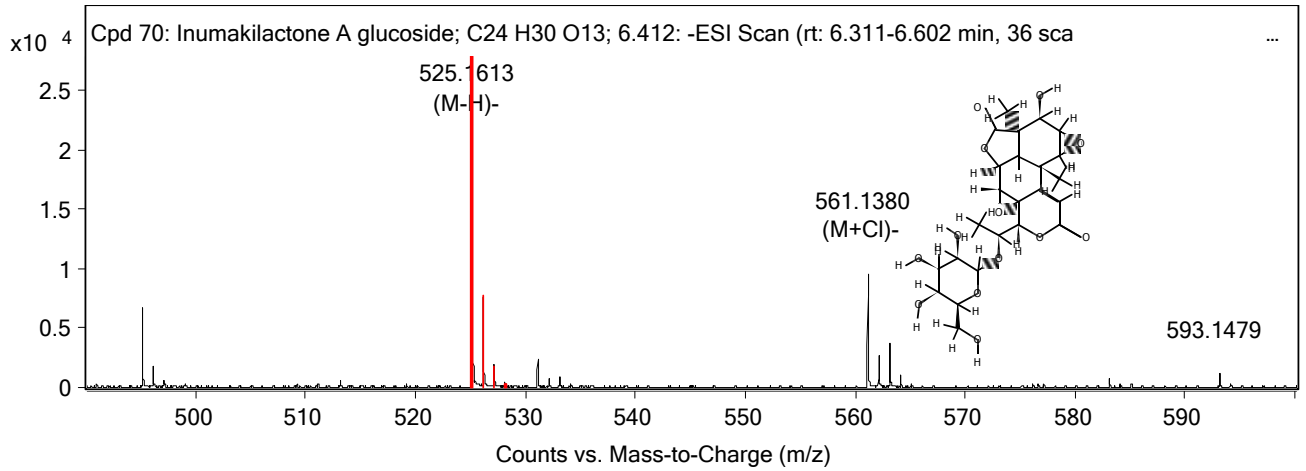
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
525.1605	-1	28765.23	C24 H30 O13	(M-H)-
526.1643	-1	7721.62	C24 H30 O13	(M-H)-
527.1663	-1	1878.23	C24 H30 O13	(M-H)-
528.173	-1	287.02	C24 H30 O13	(M-H)-
561.1371	-1	10484.68		(M+Cl)-
562.1404	-1	2926.68		(M+Cl)-
563.1348	-1	3978.38		(M+Cl)-
564.1383	-1	1078.36		(M+Cl)-
565.1441	-1	180.16		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

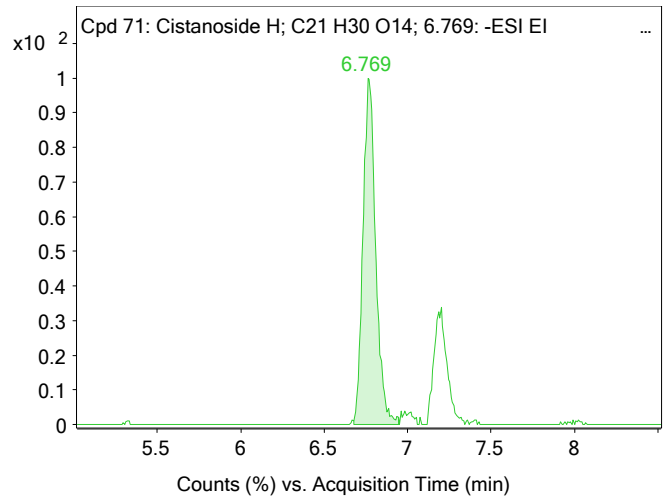


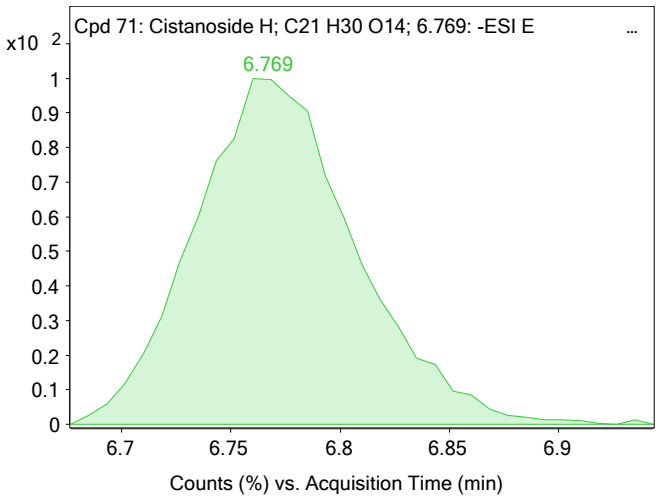
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Inumakilactone A glucoside	6.412	C24 H30 O13		98.87	526.1679	0.7	(M-H)-

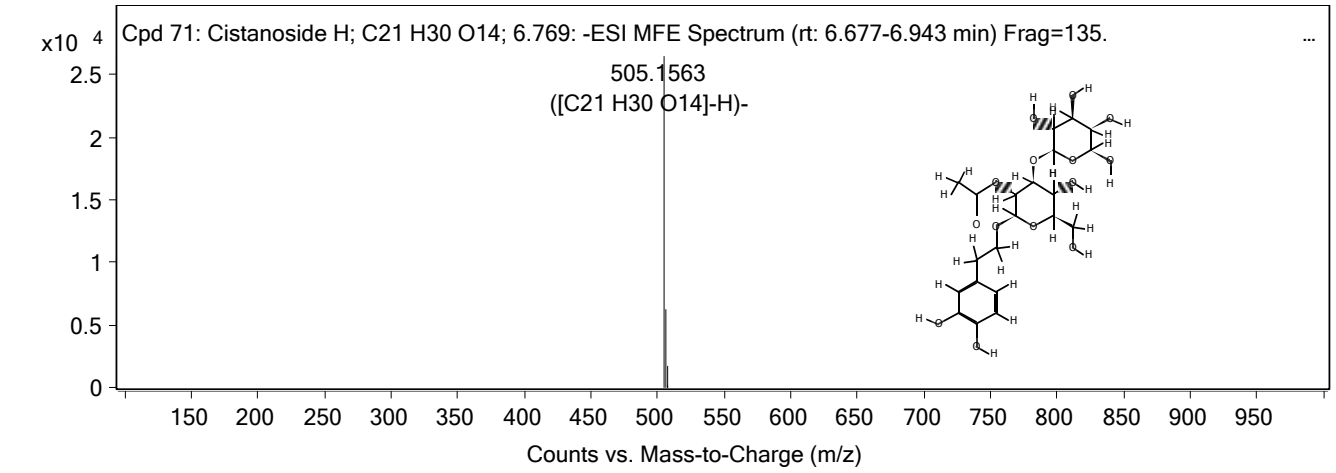
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 71: Cistanoside H; C21 H30 O14; 6.769	**Cistanoside H**	505.1563	6.769	Find by Molecular Feature	506.1636

Compound Chromatograms

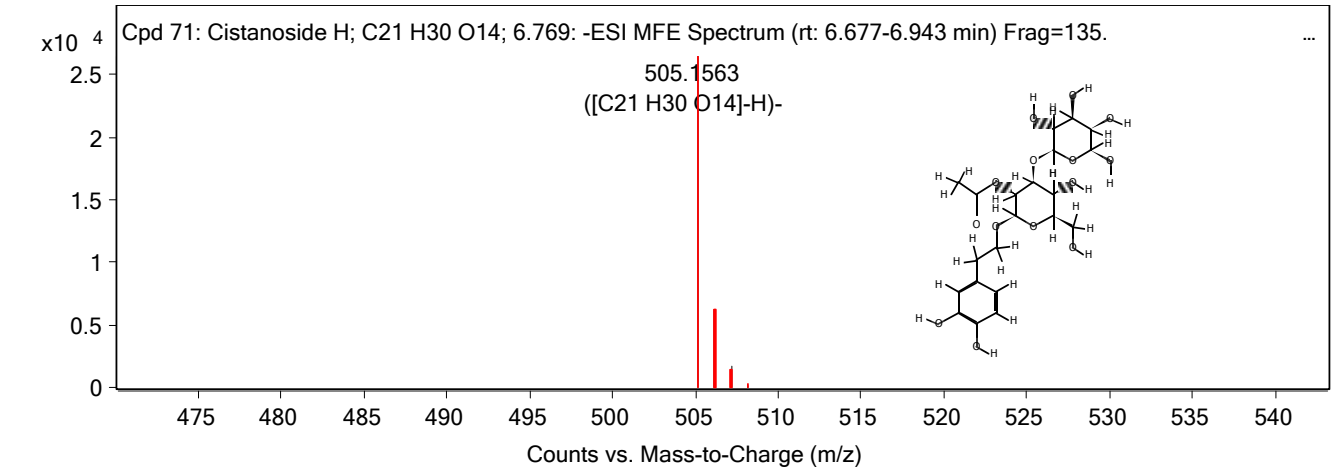




MFE MS Spectrum



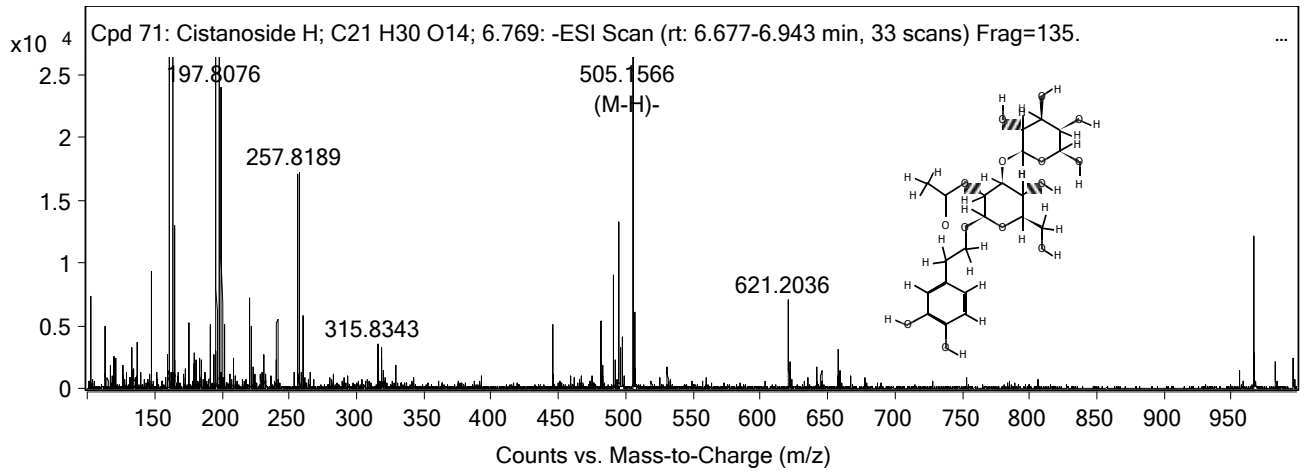
MFE MS Zoomed Spectrum



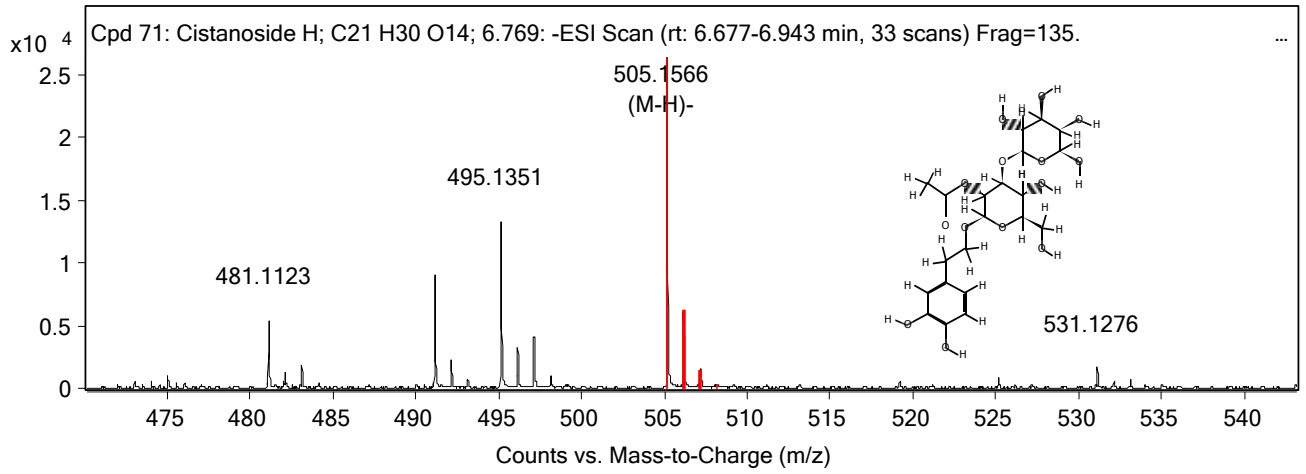
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
505.1563	-1	26453.78	C21 H30 O14	(M-H)-
506.1593	-1	6182.24	C21 H30 O14	(M-H)-
507.1651	-1	1646.77	C21 H30 O14	(M-H)-
508.1556	-1	88.15	C21 H30 O14	(M-H)-

MS Spectrum



MS Zoomed Spectrum

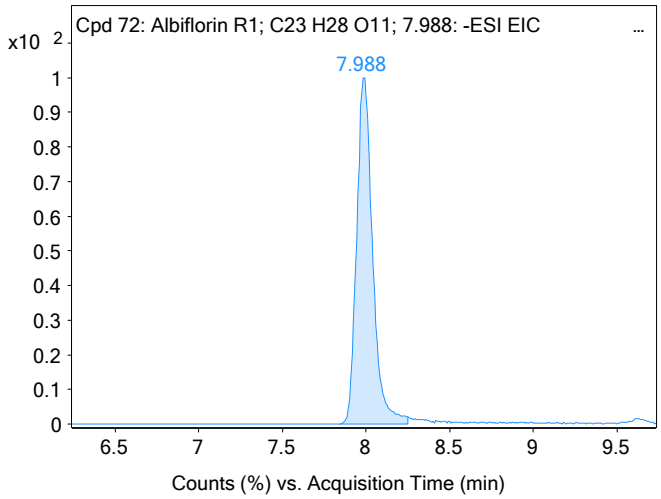


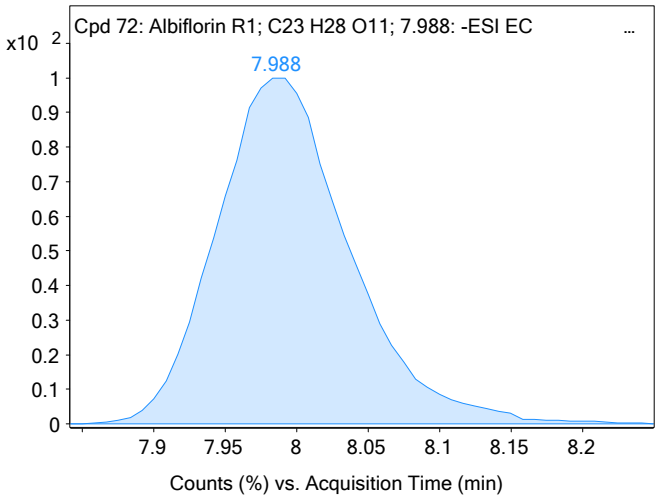
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Cistanoside H	6.769	C21 H30 O14		98.13	506.1636	-0.05	(M-H)-

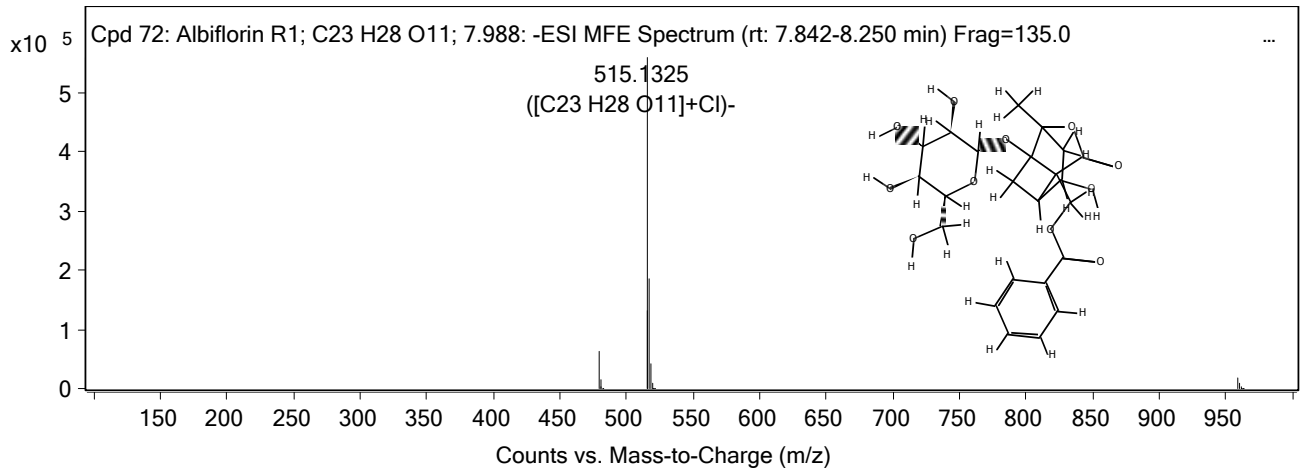
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 72: Albiflorin R1; C23 H28 O11; 7.988	**Albiflorin R1**	515.1325	7.988	Find by Molecular Feature	480.1633

Compound Chromatograms

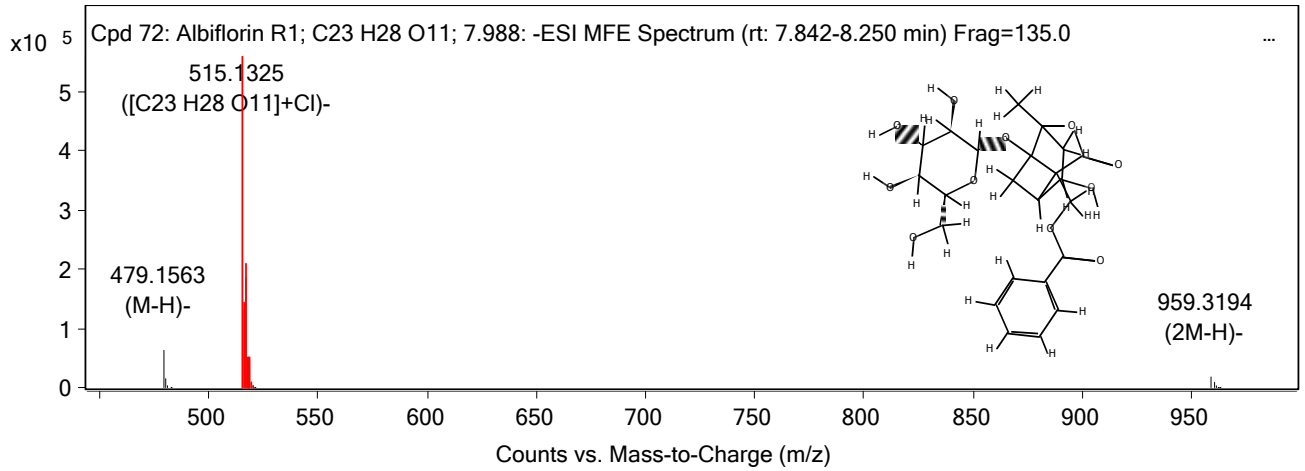




MFE MS Spectrum



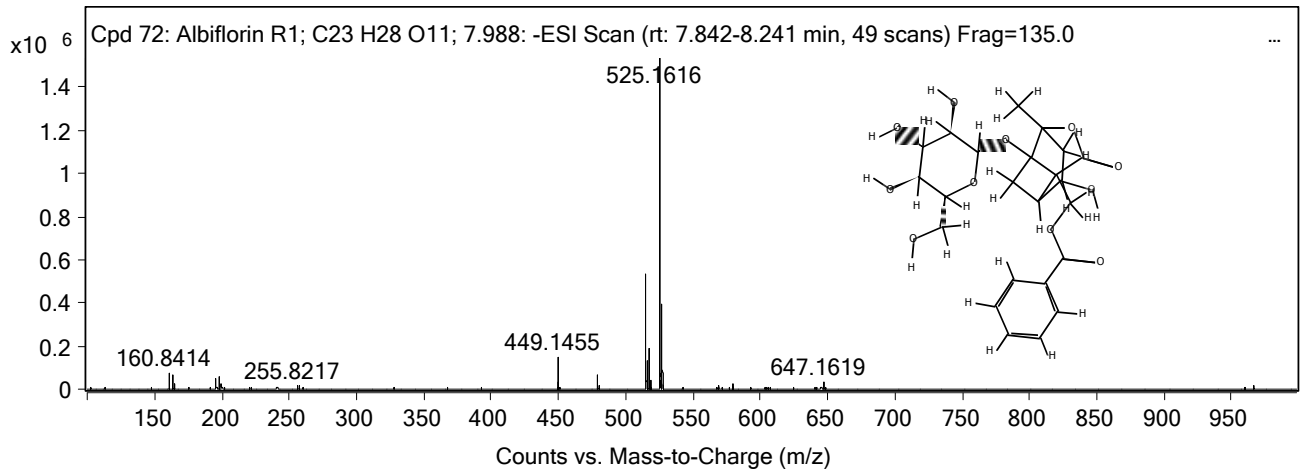
MFE MS Zoomed Spectrum



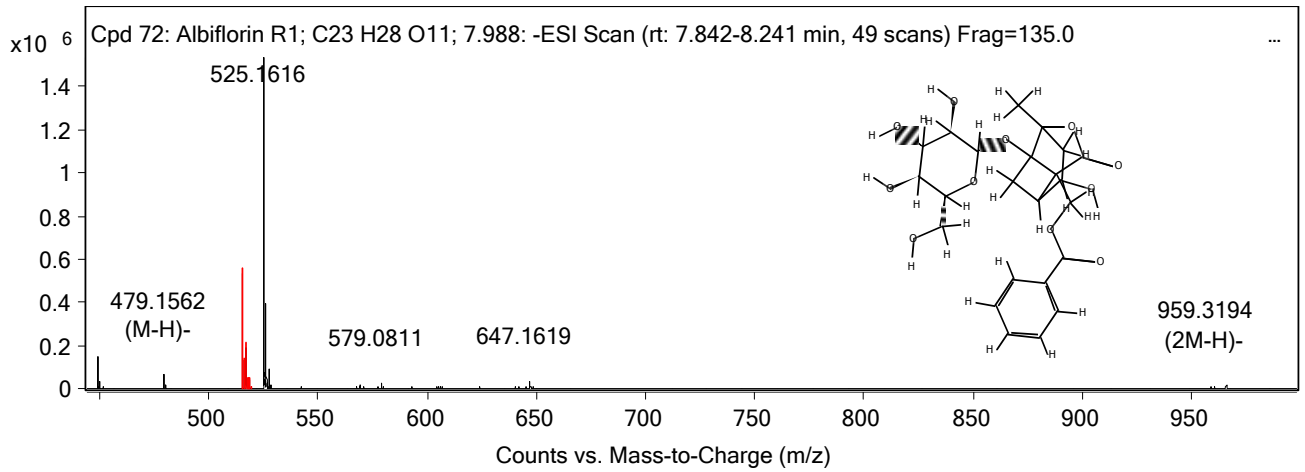
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
479.1563	-1	64139.05		(M-H)-
480.1594	-1	16290.84		(M-H)-
515.1325	-1	560282.56	C23 H28 O11	(M+Cl)-
516.1364	-1	130829.98	C23 H28 O11	(M+Cl)-
517.1313	-1	185433.43	C23 H28 O11	(M+Cl)-
518.1338	-1	43202.35	C23 H28 O11	(M+Cl)-
519.1358	-1	9363.12	C23 H28 O11	(M+Cl)-
959.3194	-1	18565.38		(2M-H)-
960.3229	-1	9692.59		(2M-H)-
961.3253	-1	3565.96		(2M-H)-

MS Spectrum



MS Zoomed Spectrum

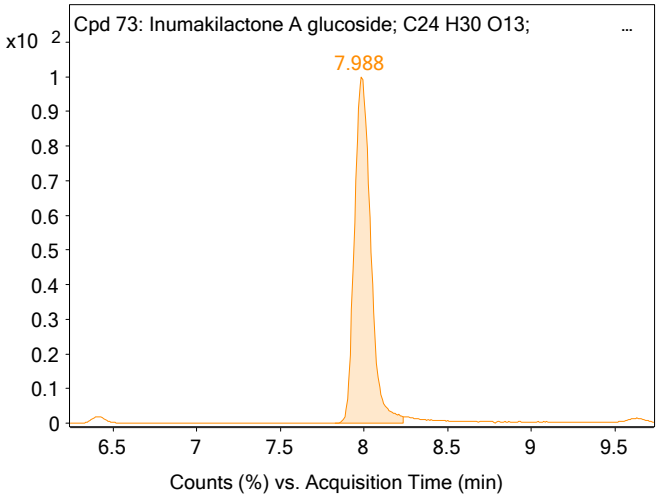


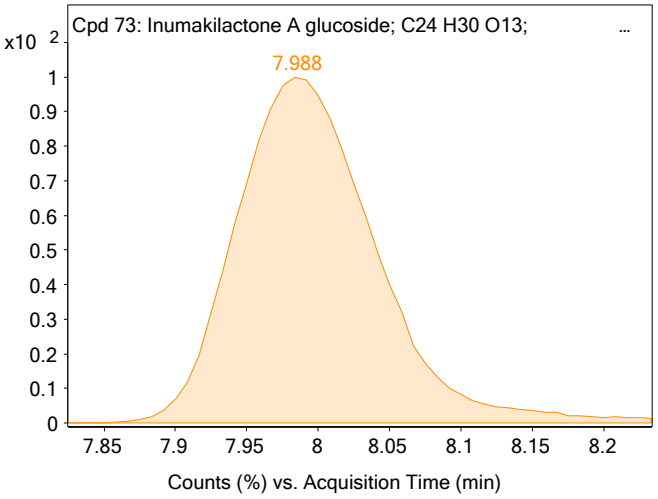
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Albiflorin R1	7.988	C23 H28 O11		98.2	480.1633	-0.13	(M+Cl)-
	Bruceine B	7.988	C23 H28 O11		98.2	480.1633	-0.13	(M+Cl)-
	Paeoniflorin	7.988	C23 H28 O11		98.2	480.1633	-0.13	(M+Cl)-

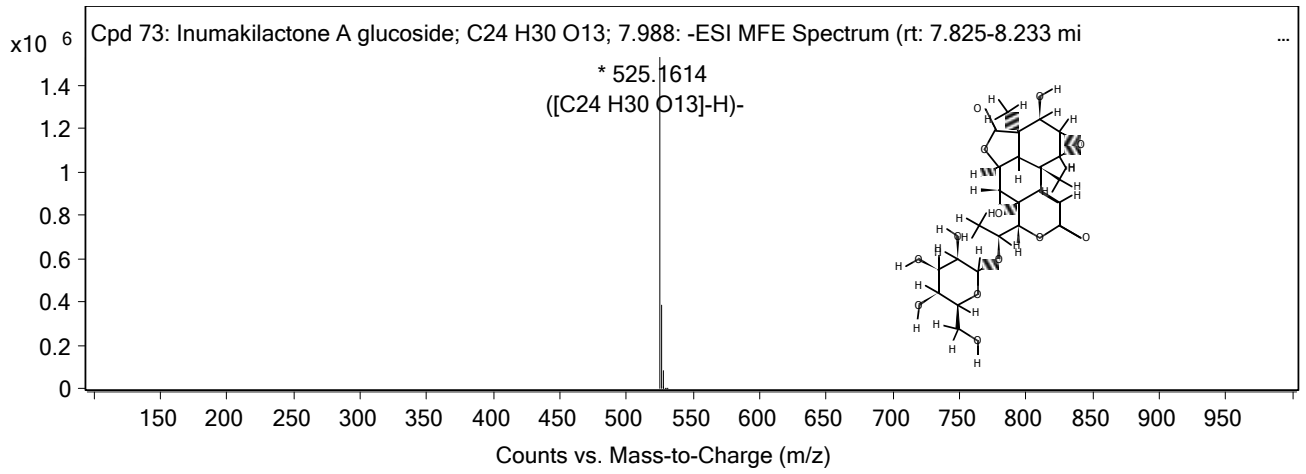
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 73: Inumakilactone A glucoside; C24 H30 O13; 7.988	**Inumakilactone A glucoside**	525.1614	7.988	Find by Molecular Feature	526.1688

Compound Chromatograms

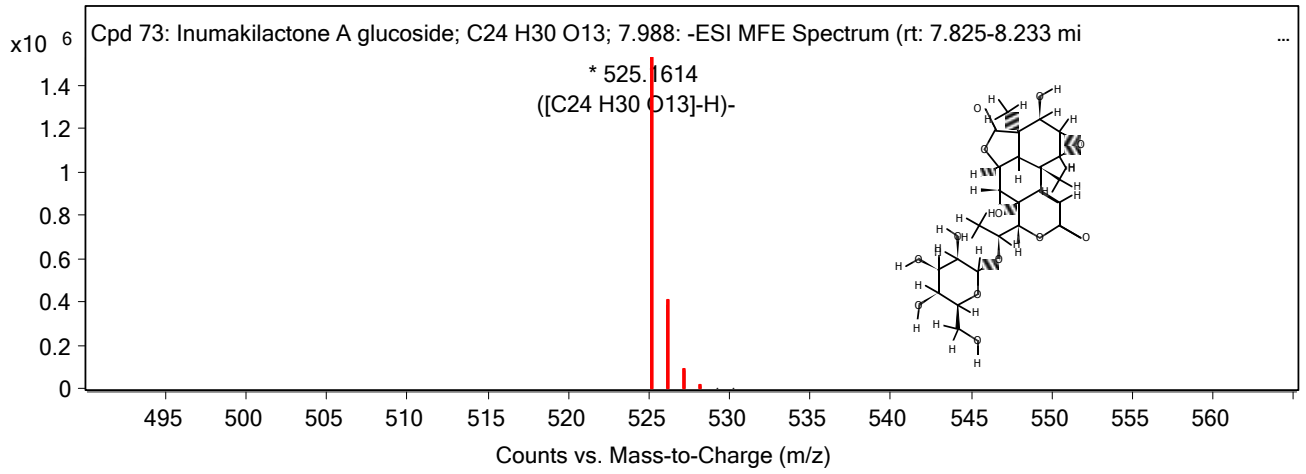




MFE MS Spectrum



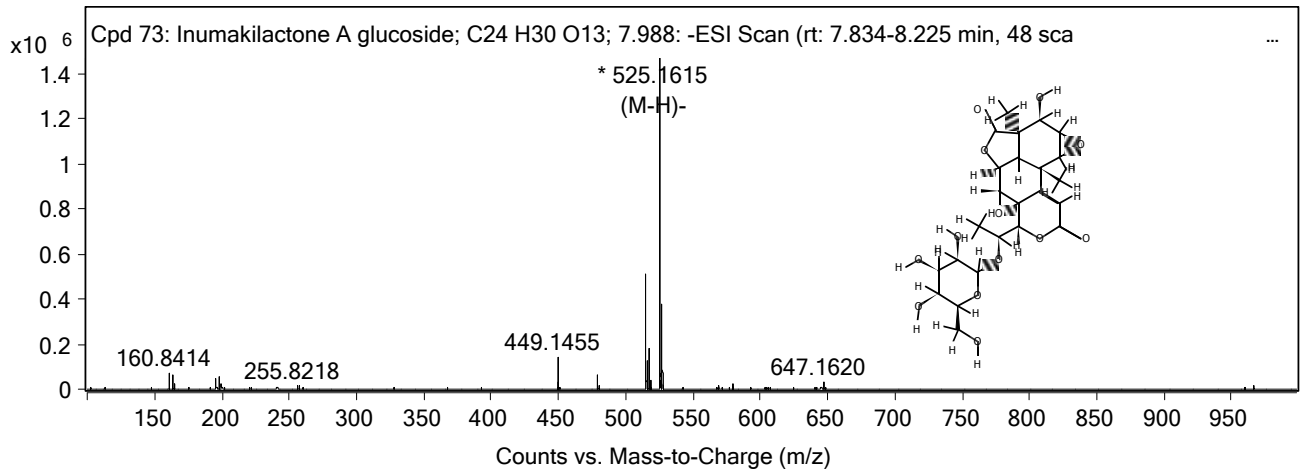
MFE MS Zoomed Spectrum



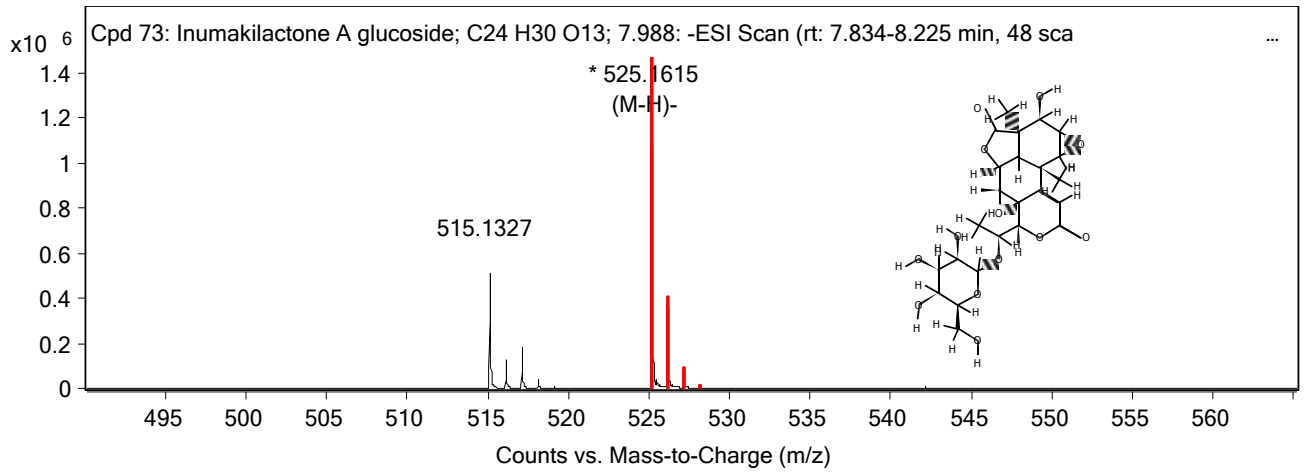
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
525.1614	-1	1527487.38	C24 H30 O13	(M-H)-
526.1655	-1	385331.59	C24 H30 O13	(M-H)-
527.1673	-1	84825.23	C24 H30 O13	(M-H)-
528.1695	-1	12675.97	C24 H30 O13	(M-H)-
529.1707	-1	2065.25	C24 H30 O13	(M-H)-
530.1733	-1	272.72	C24 H30 O13	(M-H)-

MS Spectrum



MS Zoomed Spectrum

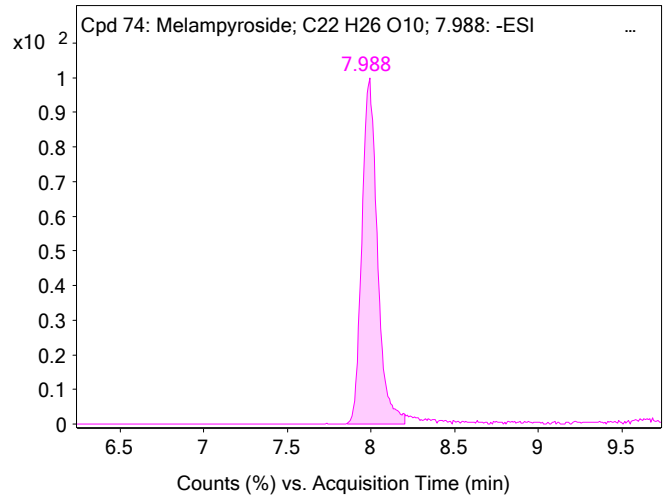


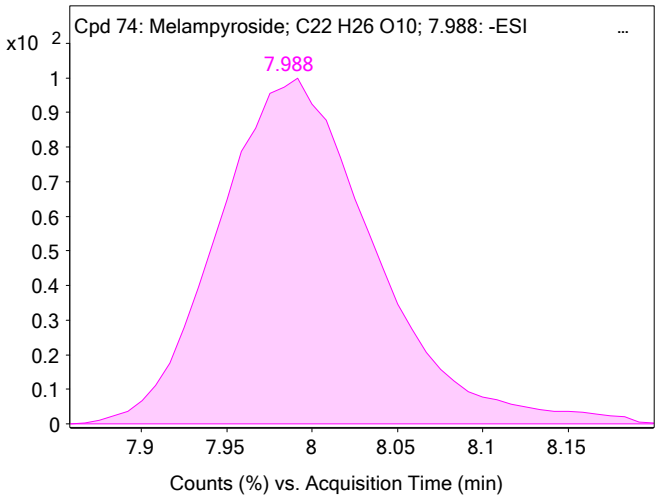
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Inumakilactone A glucoside	7.988	C24 H30 O13		99.17	526.1688	-0.19	(M-H)-

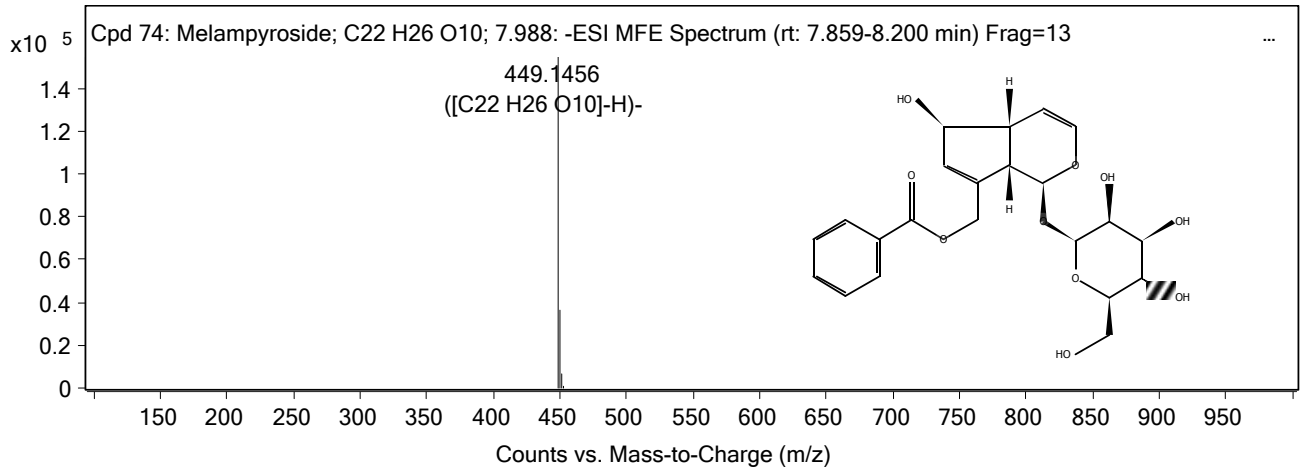
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 74: Melampyroside; C22 H26 O10; 7.988	**Melampyroside**	449.1456	7.988	Find by Molecular Feature	450.1528

Compound Chromatograms

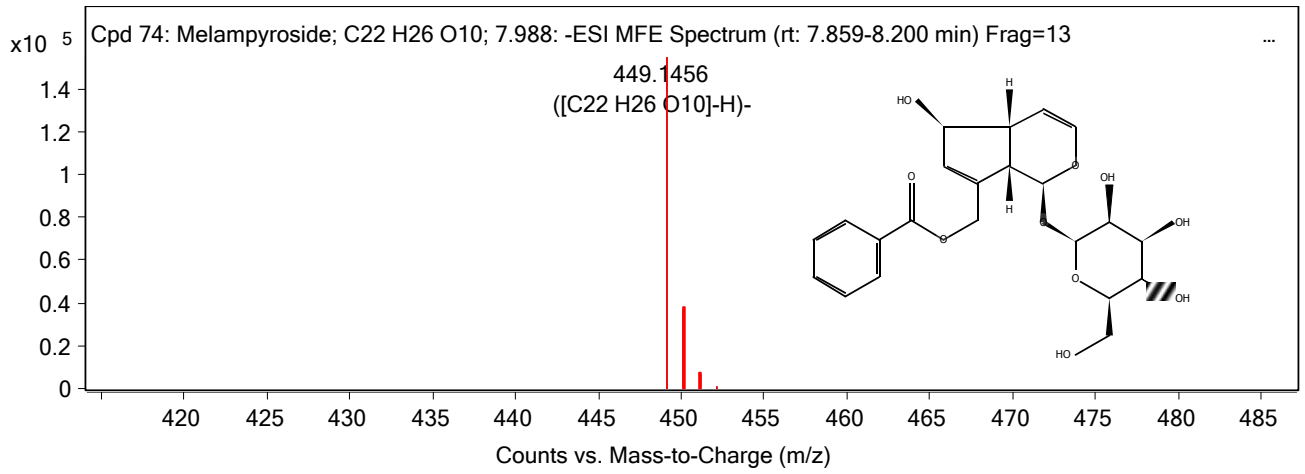




MFE MS Spectrum



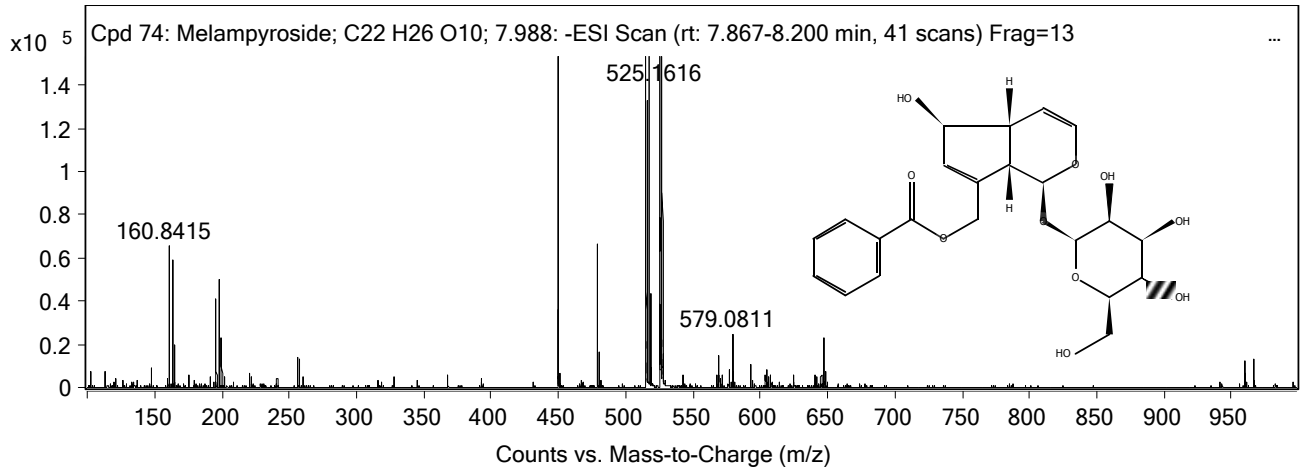
MFE MS Zoomed Spectrum



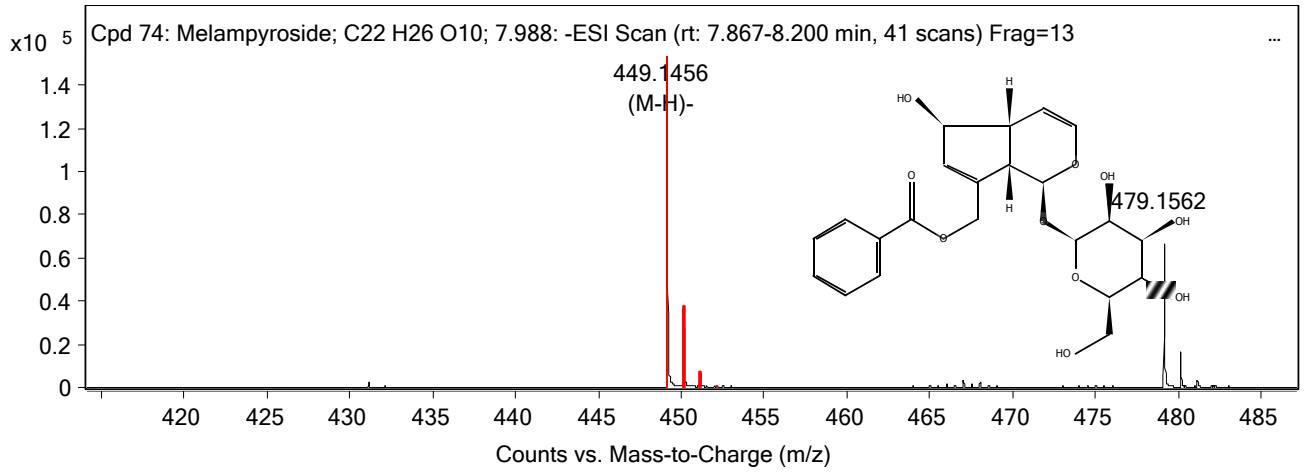
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
449.1456	-1	154550.22	C22 H26 O10	(M-H)-
450.1485	-1	36368.8	C22 H26 O10	(M-H)-
451.151	-1	7027.04	C22 H26 O10	(M-H)-
452.1554	-1	1039.8	C22 H26 O10	(M-H)-

MS Spectrum



MS Zoomed Spectrum



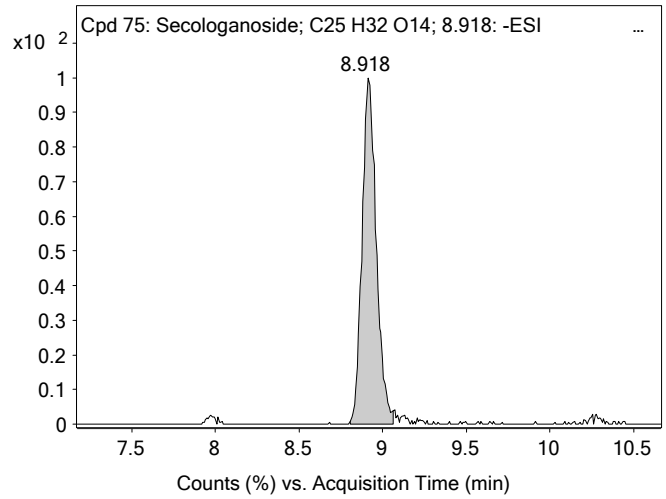
Identification Hit Table

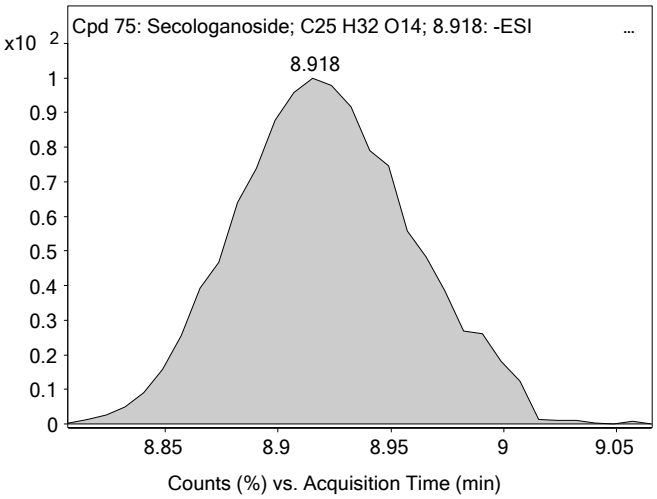
Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Melampyroside	7.988	C22 H26 O10		99.49	450.1528	-0.2	(M-H)-
	Auriculoside	7.988	C22 H26 O10		99.49	450.1528	-0.2	(M-H)-
	Aspidocarpine	7.988	C22 H30 N2 O3		62.95	370.227	-1.33	(M+Br)-

	11,12-Methylenedioxykopsinaline N(4)-oxide	7.988	C22 H26 N2 O6		53.02	414.1765	2.62	(M+Cl)-

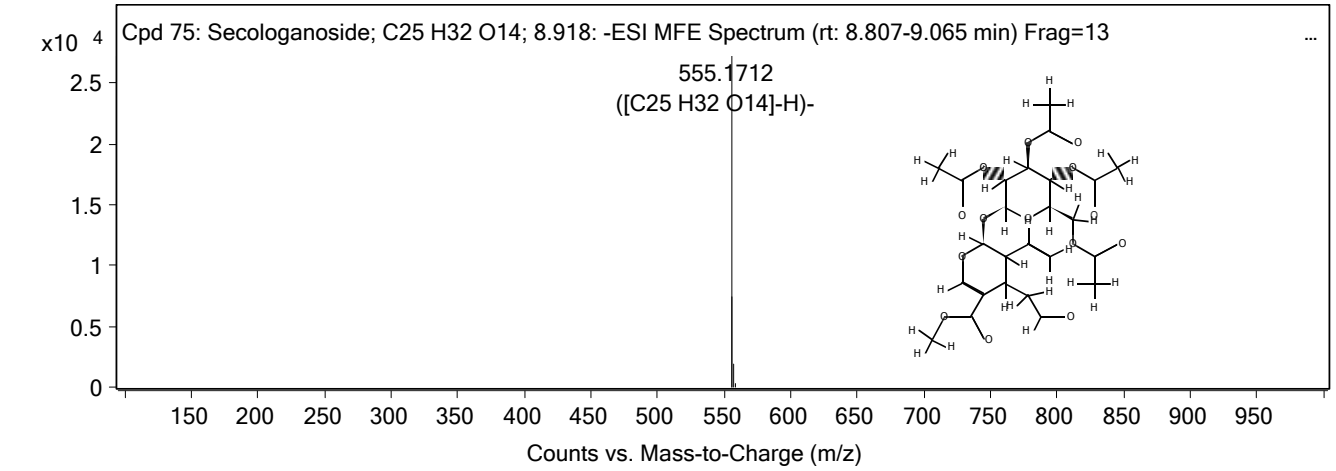
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 75: Secologanoside; C25 H32 O14; 8.918	**Secologanoside**	555.1712	8.918	Find by Molecular Feature	556.1783

Compound Chromatograms

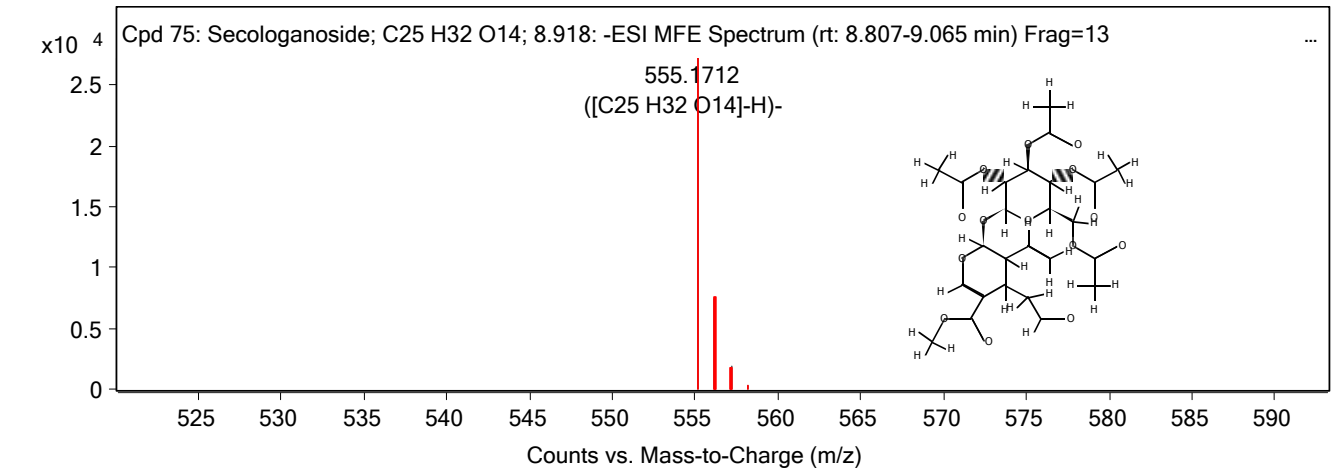




MFE MS Spectrum



MFE MS Zoomed Spectrum

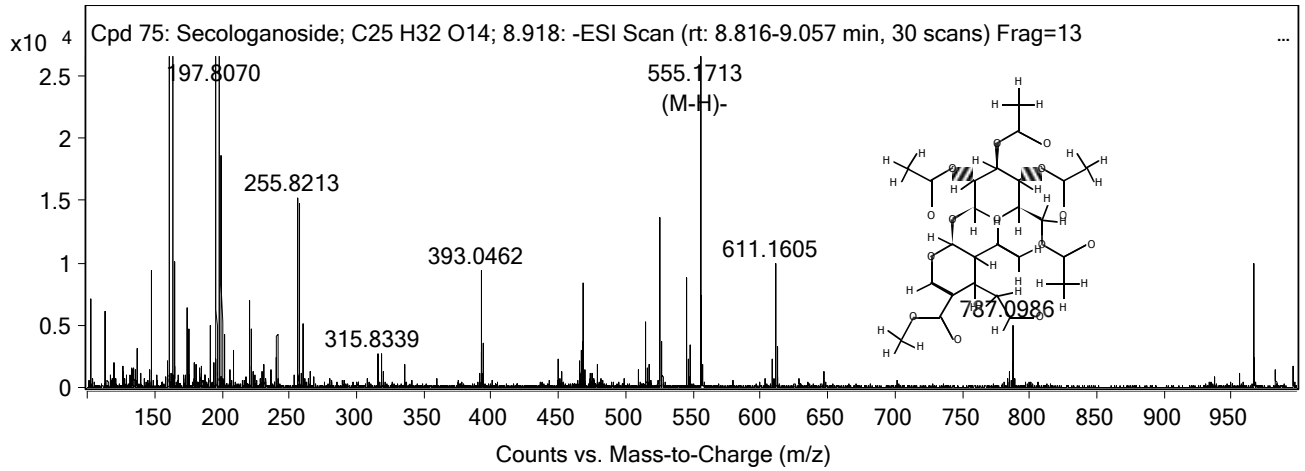


Qualitative Compound Identification Report

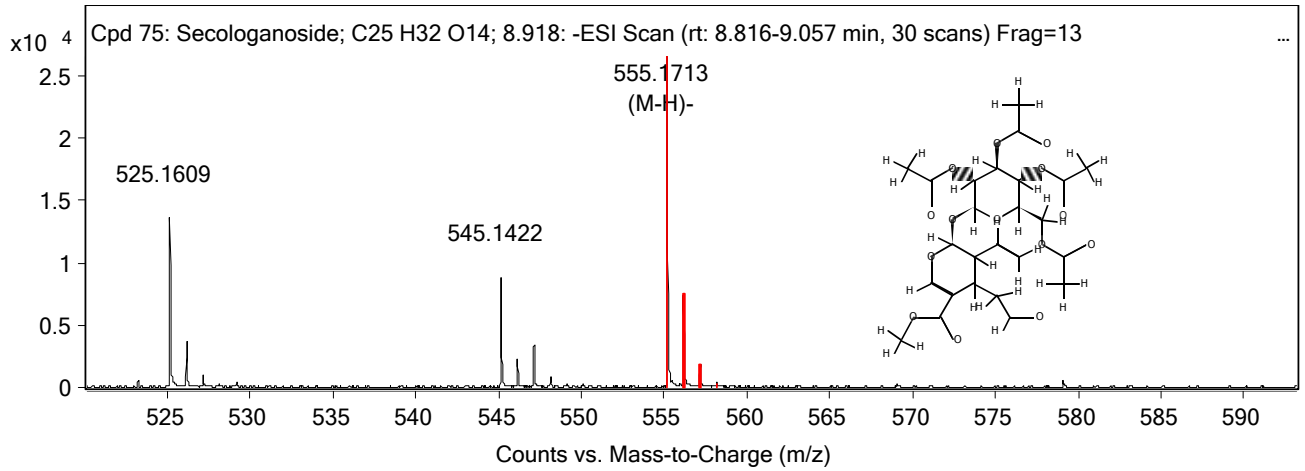
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
555.1712	-1	27227.23	C25 H32 O14	(M-H)-
556.1741	-1	7392.59	C25 H32 O14	(M-H)-
557.1753	-1	1932.21	C25 H32 O14	(M-H)-
558.1795	-1	323.33	C25 H32 O14	(M-H)-

MS Spectrum



MS Zoomed Spectrum

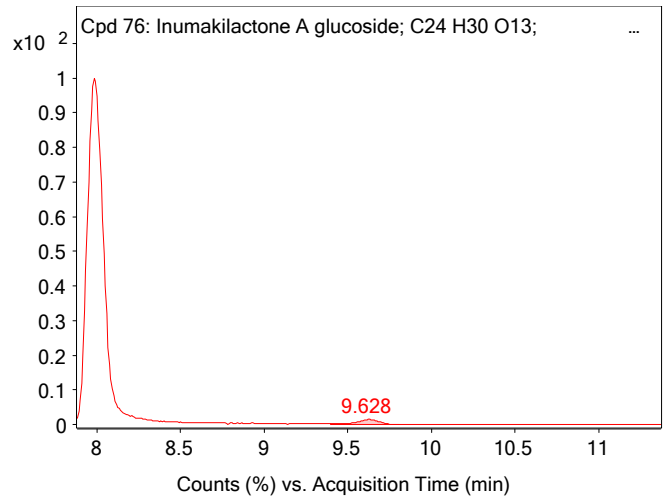


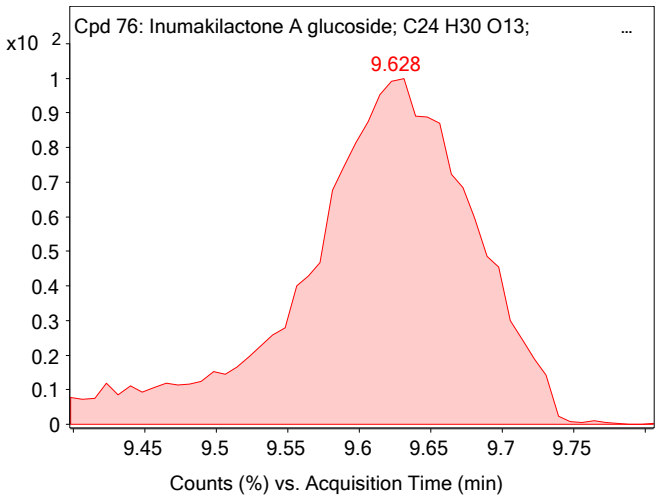
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Secologanoside	8.918	C25 H32 O14		97.64	556.1783	0.94	(M-H)-

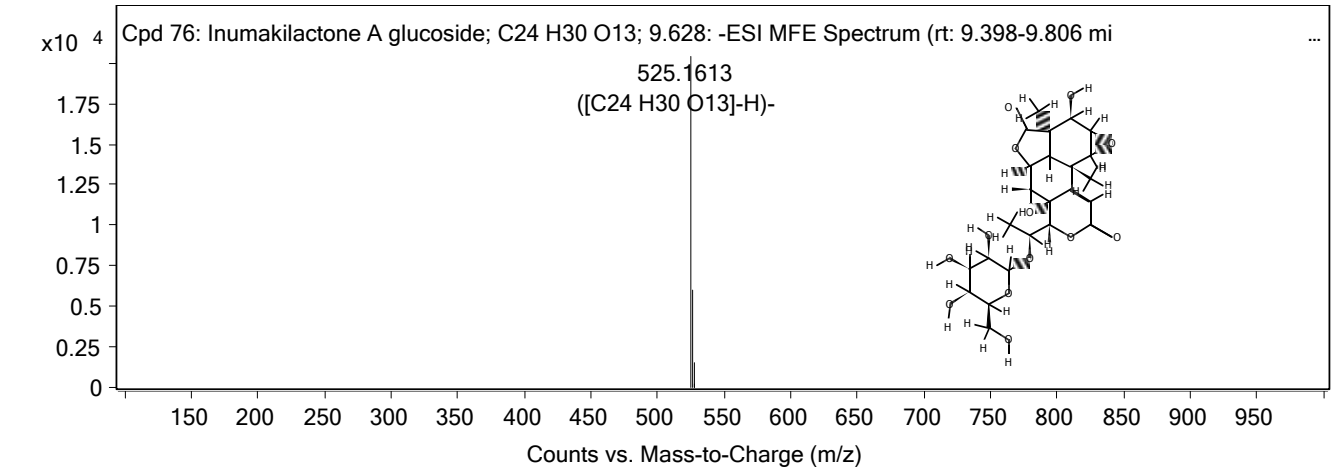
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 76: Inumakilactone A glucoside; C24 H30 O13; 9.628	**Inumakilactone A glucoside**	525.1613	9.628	Find by Molecular Feature	526.1684

Compound Chromatograms

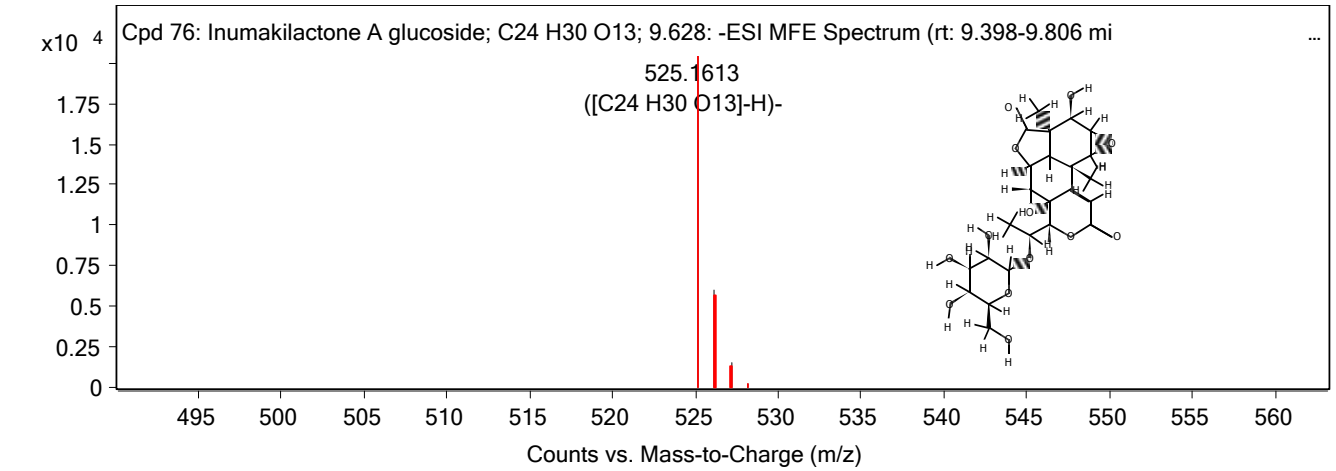




MFE MS Spectrum



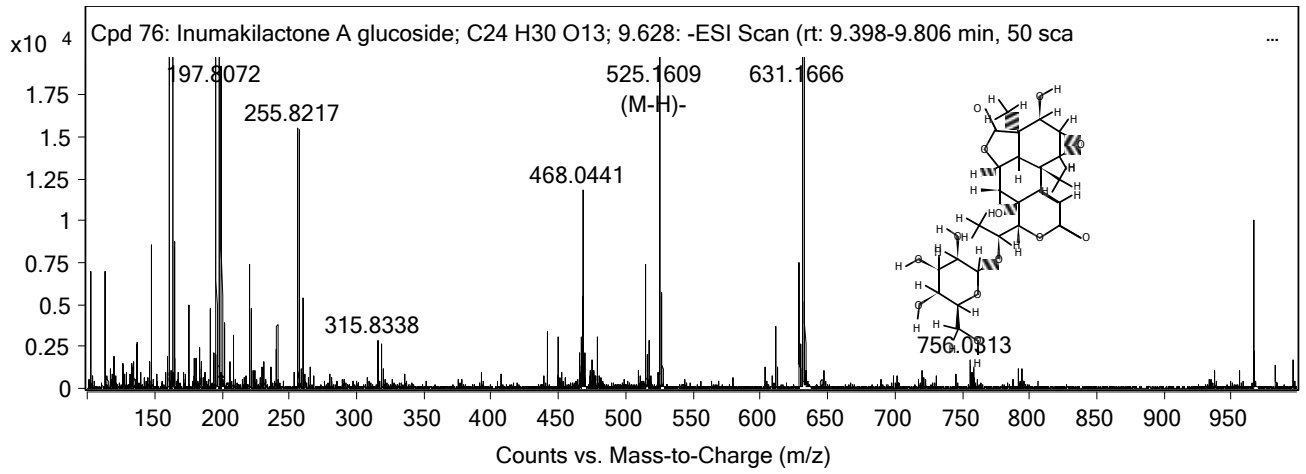
MFE MS Zoomed Spectrum



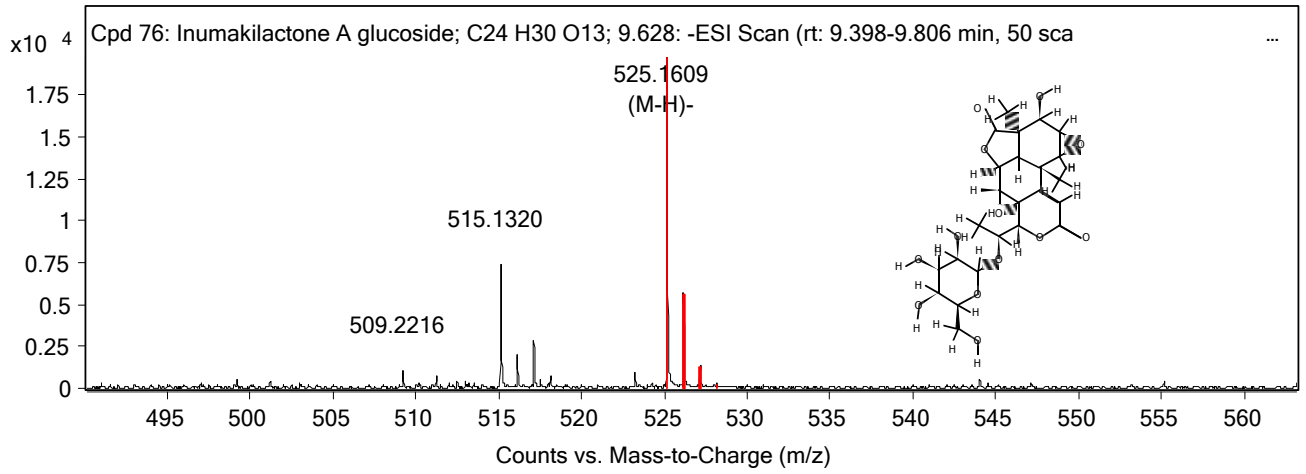
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
525.1613	-1	20402.04	C24 H30 O13	(M-H)-
526.1642	-1	5989.16	C24 H30 O13	(M-H)-
527.1661	-1	1524.41	C24 H30 O13	(M-H)-
528.1741	-1	189.64	C24 H30 O13	(M-H)-

MS Spectrum



MS Zoomed Spectrum

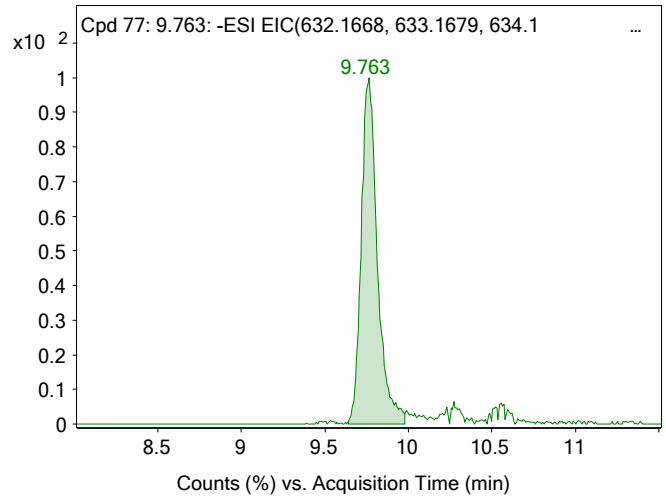


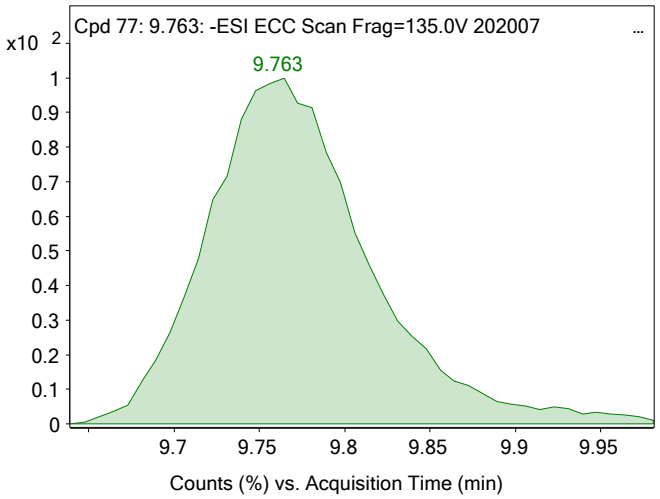
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Inumakilactone A glucoside	9.628	C24 H30 O13		98.3	526.1684	0.23	(M-H)-

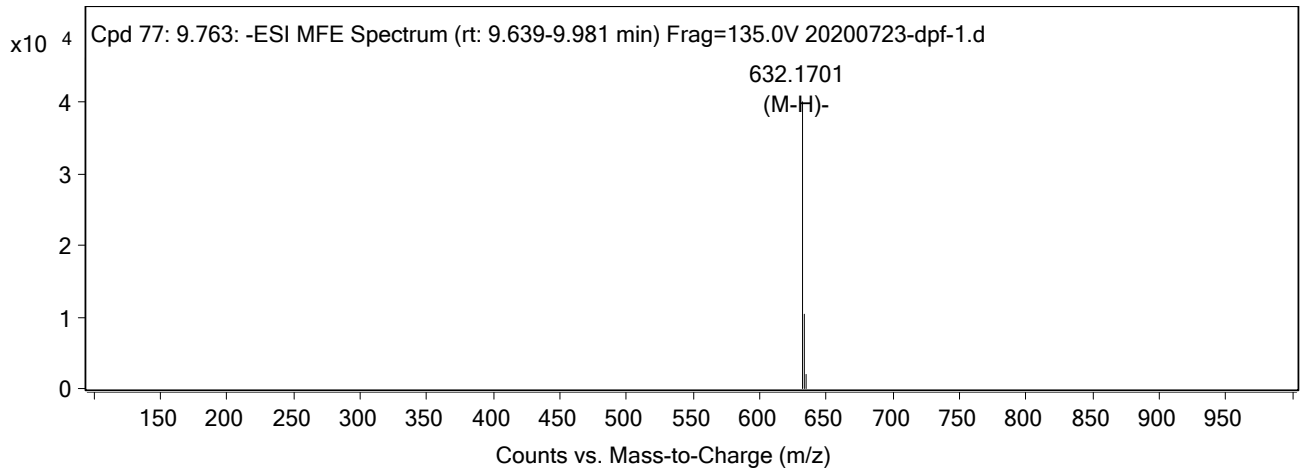
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 77: 9.763	632.1701	9.763	Find by Molecular Feature	633.1773

Compound Chromatograms

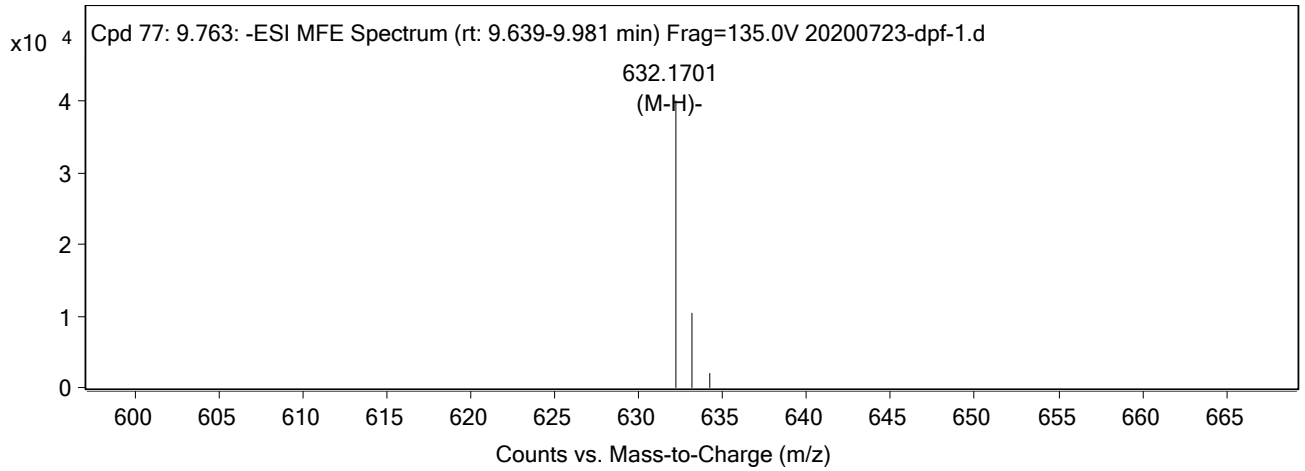




MFE MS Spectrum



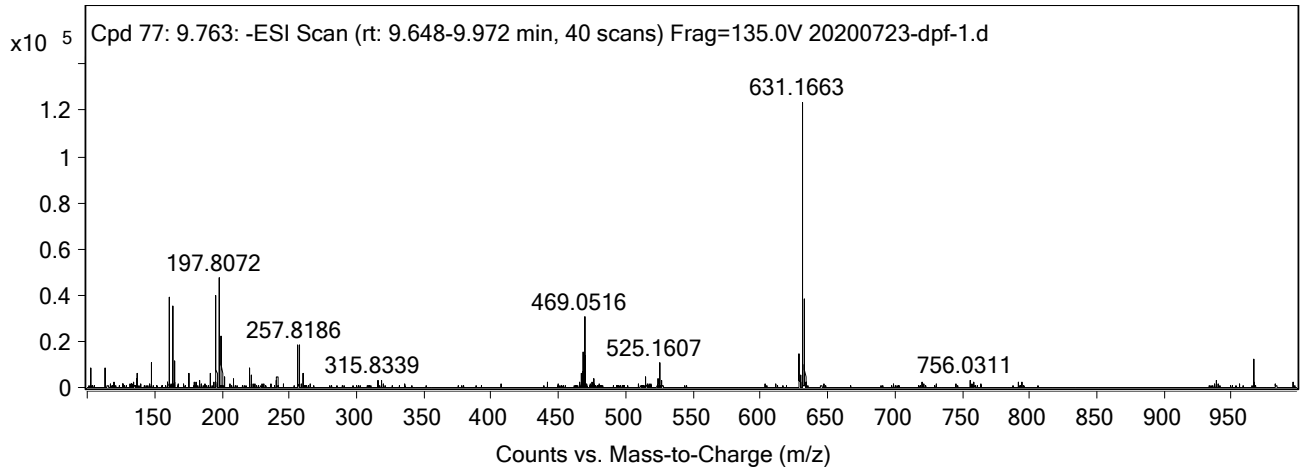
MFE MS Zoomed Spectrum



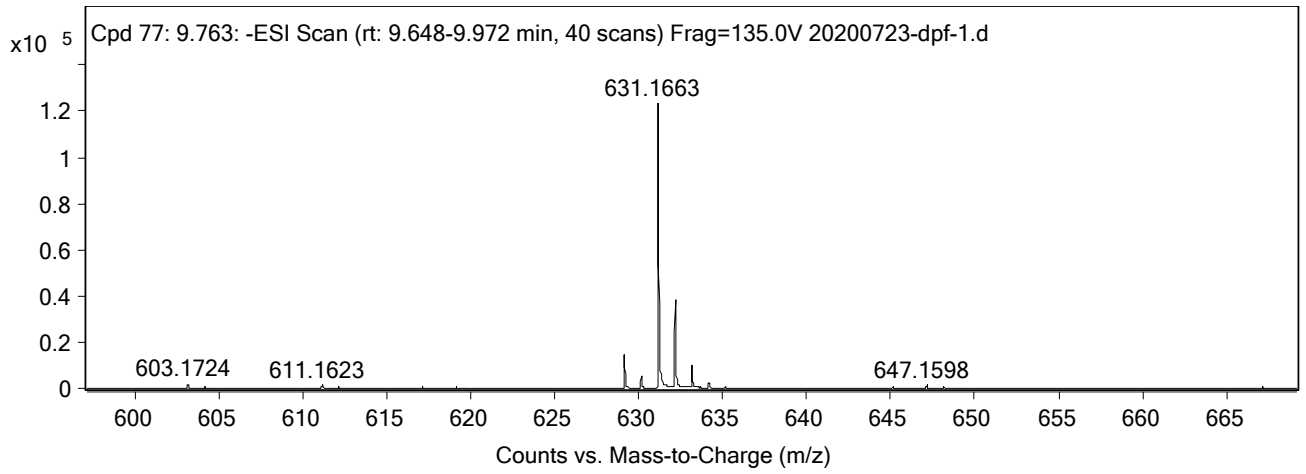
MS Spectrum Peak List

m/z	z	Abund	Ion
632.1701	-1	40143.98	(M-H)-
633.1723	-1	10315.24	(M-H)-
634.1756	-1	2030.72	(M-H)-

MS Spectrum

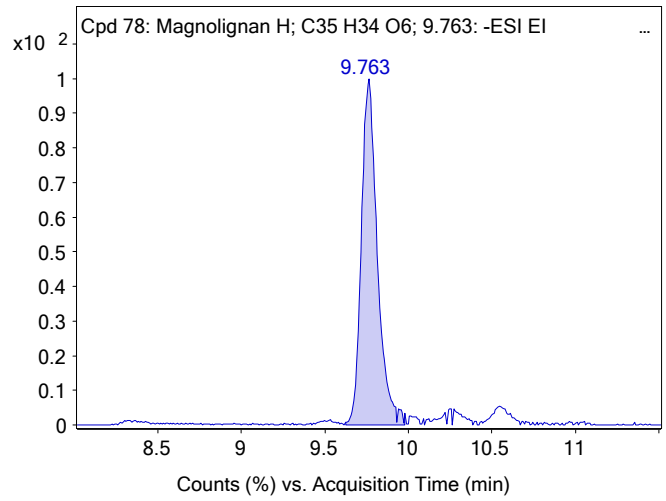


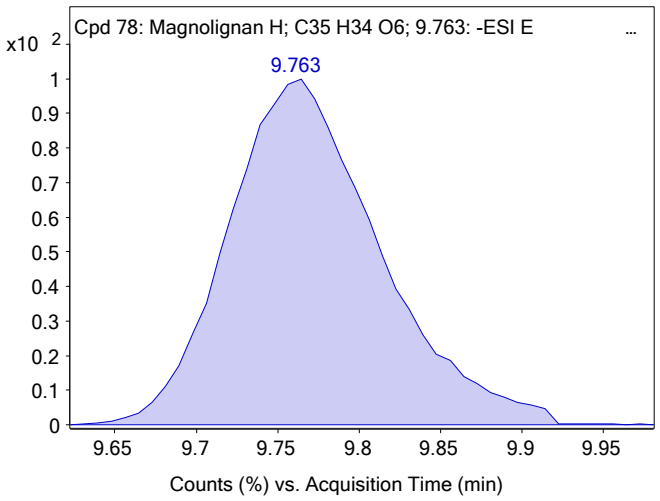
MS Zoomed Spectrum



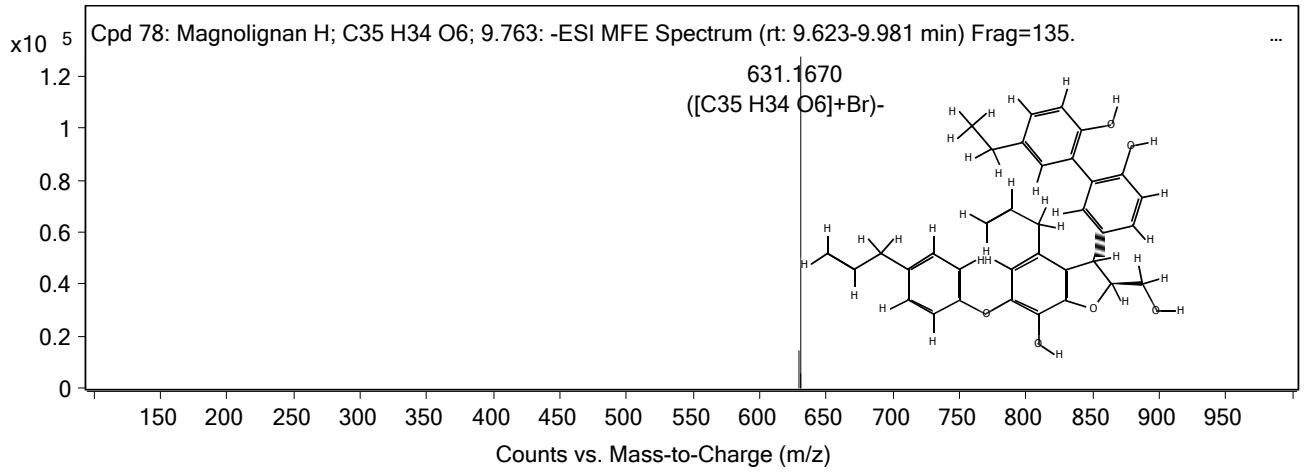
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 78: Magnolignan H; C35 H34 O6; 9.763	**Magnolignan H**	629.1513	9.763	Find by Molecular Feature	550.2471

Compound Chromatograms

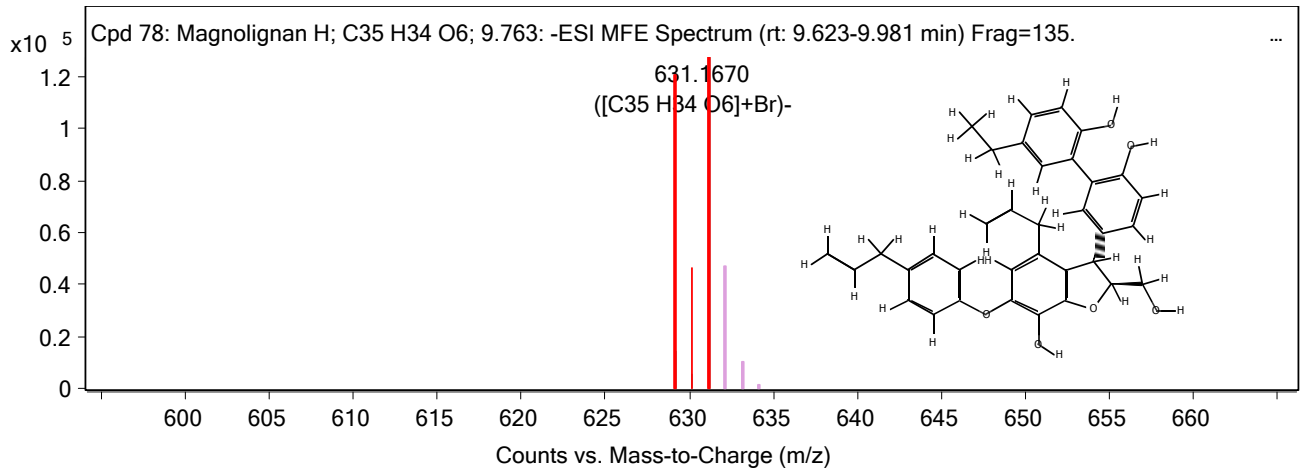




MFE MS Spectrum



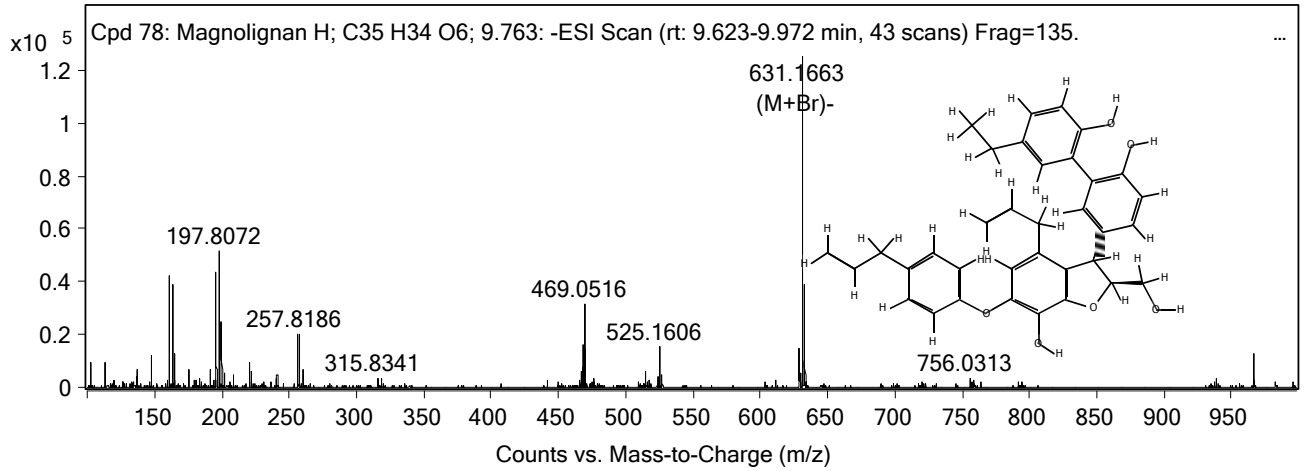
MFE MS Zoomed Spectrum



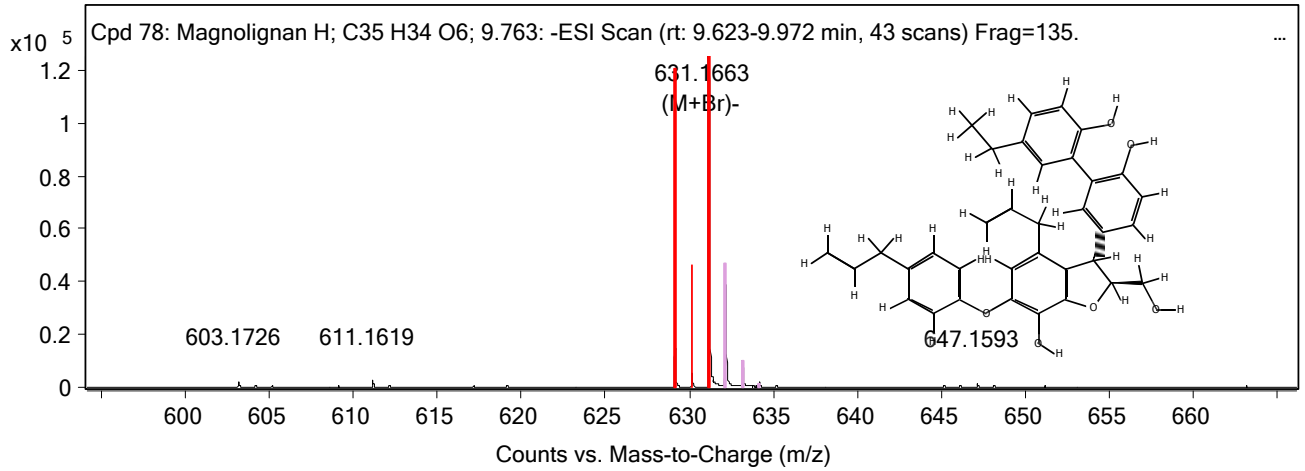
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
629.1513	-1	14543.19	C35 H34 O6	(M+Br)-
630.1547	-1	5423.77	C35 H34 O6	(M+Br)-
631.167	-1	127521.63	C35 H34 O6	(M+Br)-

MS Spectrum



MS Zoomed Spectrum



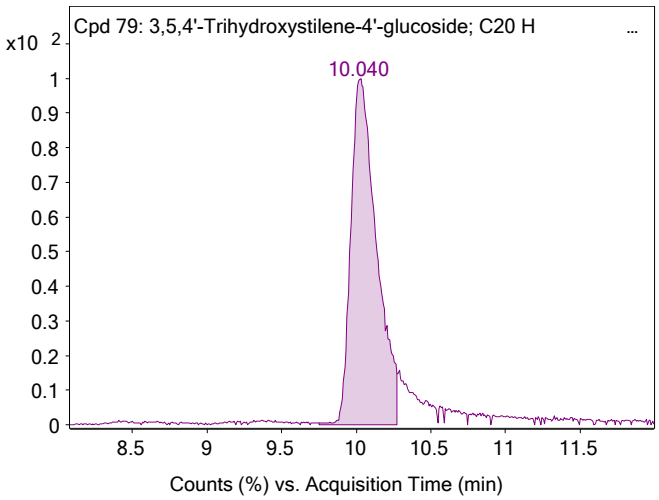
Identification Hit Table

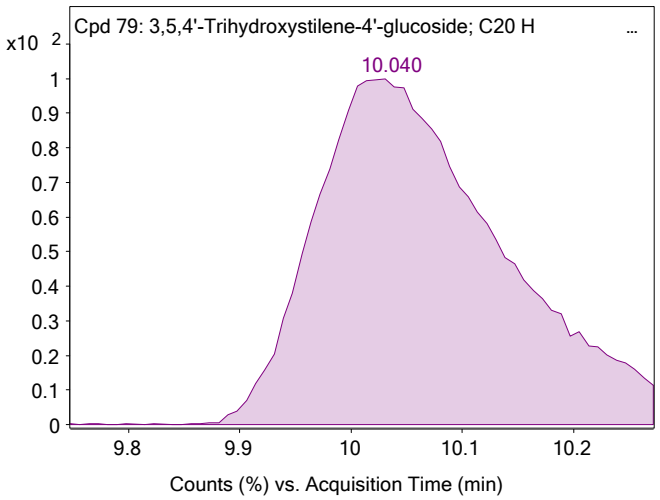
Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Magnolignan H	9.763	C35 H34 O6		14.55	550.2471	-11.6	(M+Br)-

Qualitative Compound Identification Report

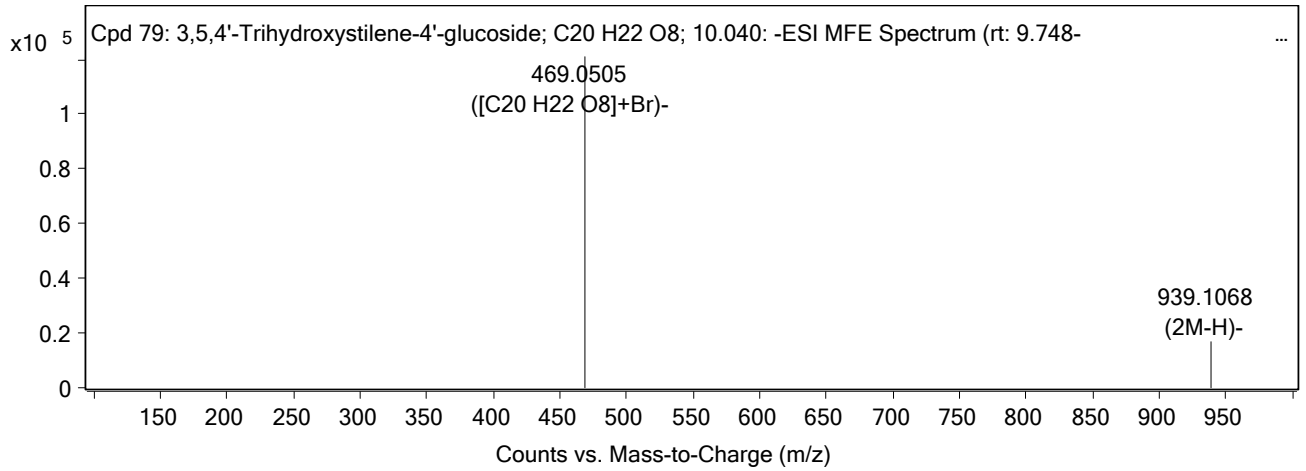
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 79: 3,5,4'-Trihydroxystilene-4'-glucoside; C20 H22 O8; 10.040	**3,5,4'-Trihydroxystilene-4'-glucoside**	469.0505	10.04	Find by Molecular Feature	390.1317

Compound Chromatograms

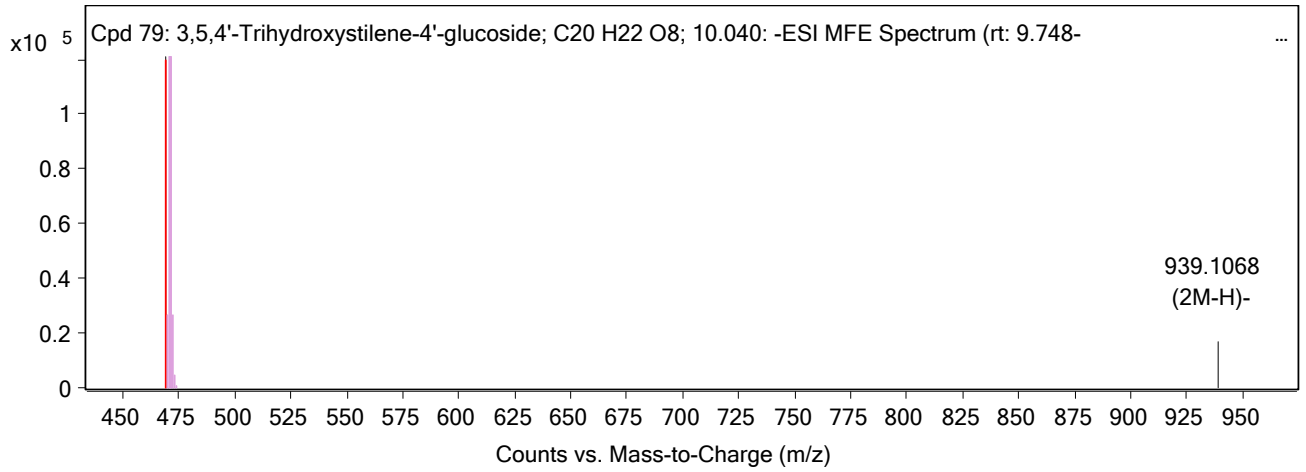




MFE MS Spectrum



MFE MS Zoomed Spectrum

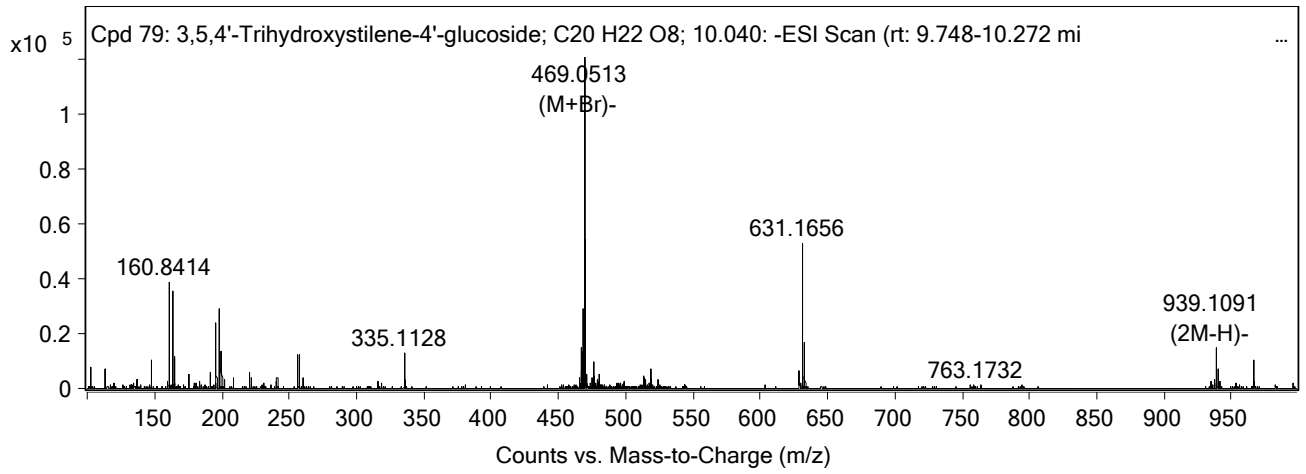


MS Spectrum Peak List

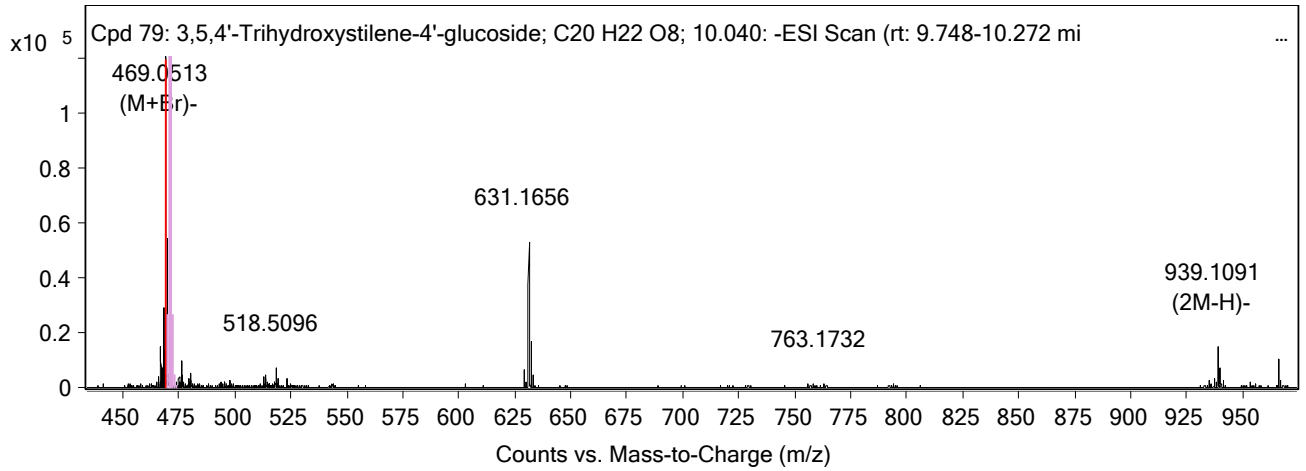
m/z	z	Abund	Formula	Ion
469.0505	-1	121025.33	C20 H22 O8	(M+Br)-

939.1068	-1	16792.98		(2M-H)-

MS Spectrum



MS Zoomed Spectrum

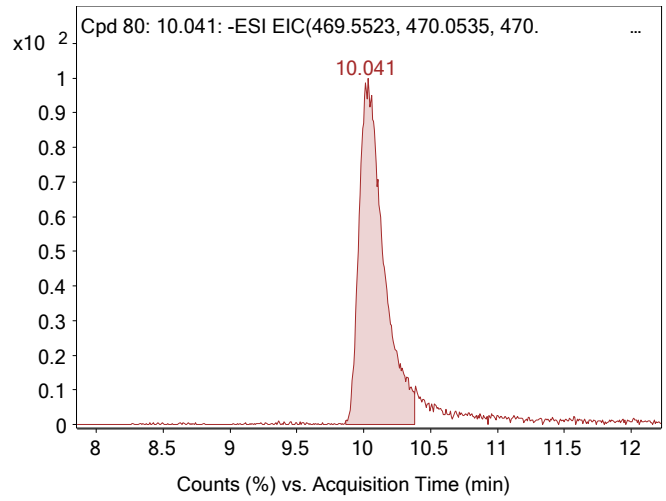


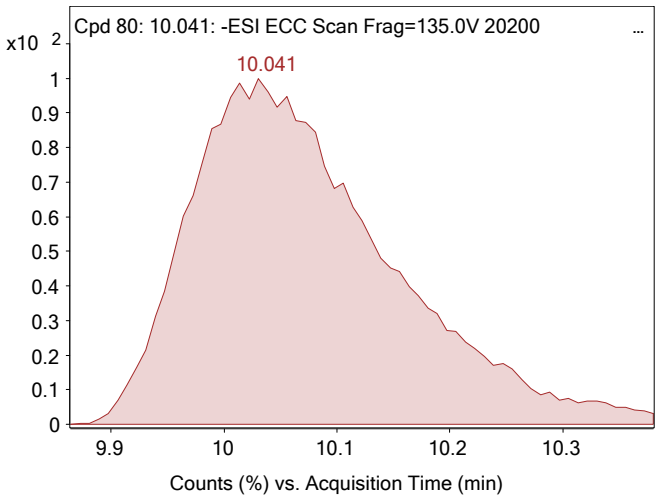
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	3,5,4'-Trihydroxystilene-4'-glucoside	10.04	C20 H22 O8		47.53	390.1317	-0.18	(M+Br)-
	Spiramongolin	10.04	C20 H22 O8		47.53	390.1317	-0.18	(M+Br)-
	Piceid	10.04	C20 H22 O8		47.53	390.1317	-0.18	(M+Br)-
	Abruquinone B	10.04	C20 H22 O8		47.53	390.1317	-0.18	(M+Br)-
	Polydatin	10.04	C20 H22 O8		47.53	390.1317	-0.18	(M+Br)-
	Polydatin	10.04	C20 H22 O8		47.53	390.1317	-0.18	(M+Br)-
	Quercetin-3-xyloside	10.04	C20 H18 O11		23.05	434.0811	3.77	(M+Cl)-
	Avicularin	10.04	C20 H18 O11		23.05	434.0811	3.77	(M+Cl)-
	Polystachoside	10.04	C20 H18 O11		23.05	434.0811	3.77	(M+Cl)-
	Guaijaverin	10.04	C20 H18 O11		23.05	434.0811	3.77	(M+Cl)-

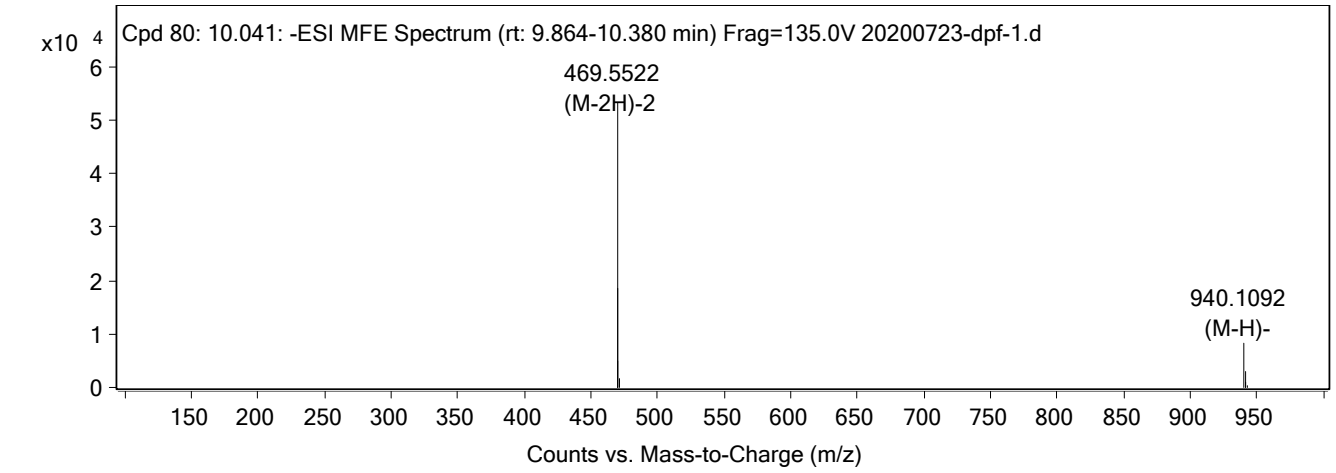
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 80: 10.041	469.5522	10.041	Find by Molecular Feature	941.1187

Compound Chromatograms

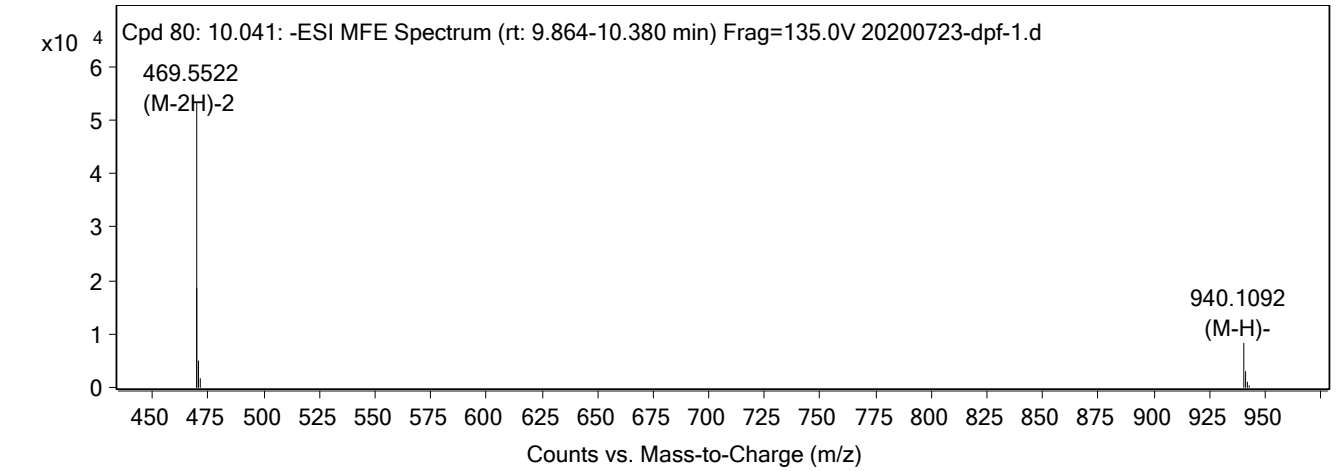




MFE MS Spectrum



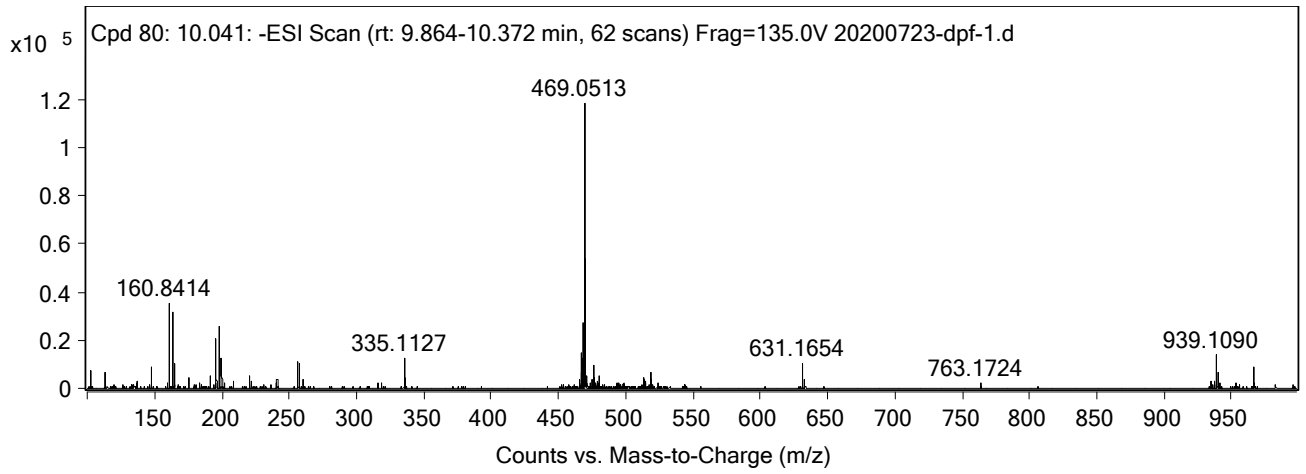
MFE MS Zoomed Spectrum



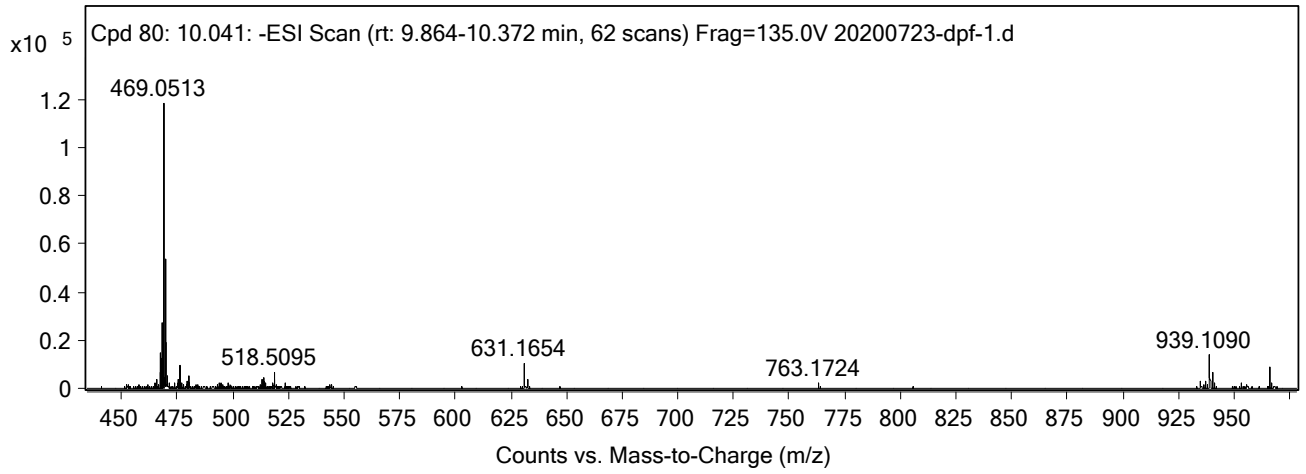
MS Spectrum Peak List

m/z	z	Abund	Ion
469.5522	-2	53439.6	(M-2H)-2
470.053	-2	18713.74	(M-2H)-2
470.5546	-2	4918.09	(M-2H)-2
471.0535	-2	1763.7	(M-2H)-2
940.1092	-1	8455.01	(M-H)-
941.1113	-1	2941.21	(M-H)-
942.1138	-1	913.6	(M-H)-
943.1118	-1	222.02	(M-H)-

MS Spectrum

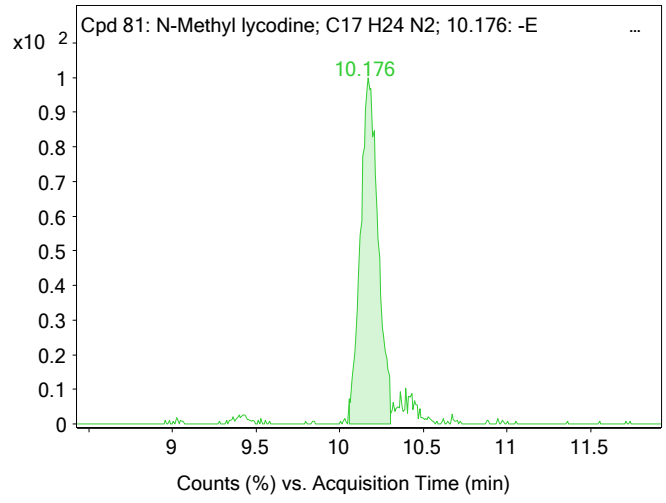


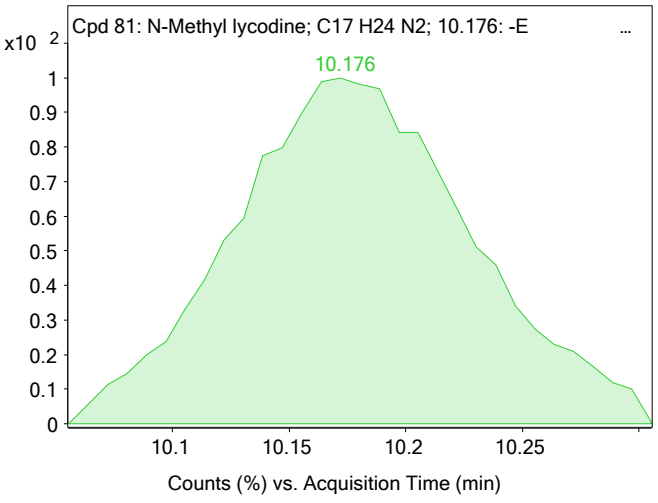
MS Zoomed Spectrum



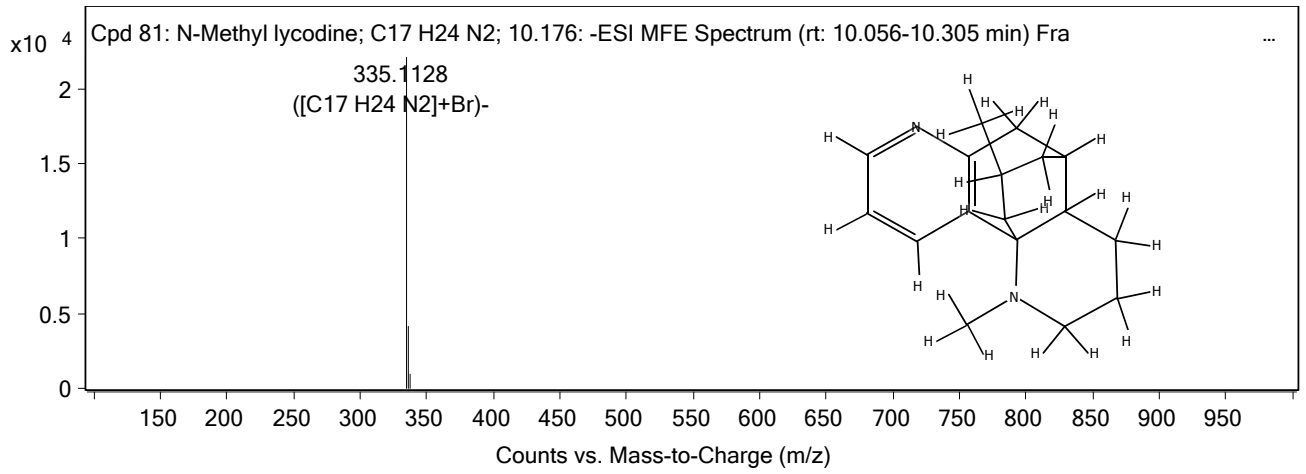
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 81: N-Methyl lycodine; C17 H24 N2; 10.176	**N-Methyl lycodine**	335.1128	10.176	Find by Molecular Feature	256.1942

Compound Chromatograms

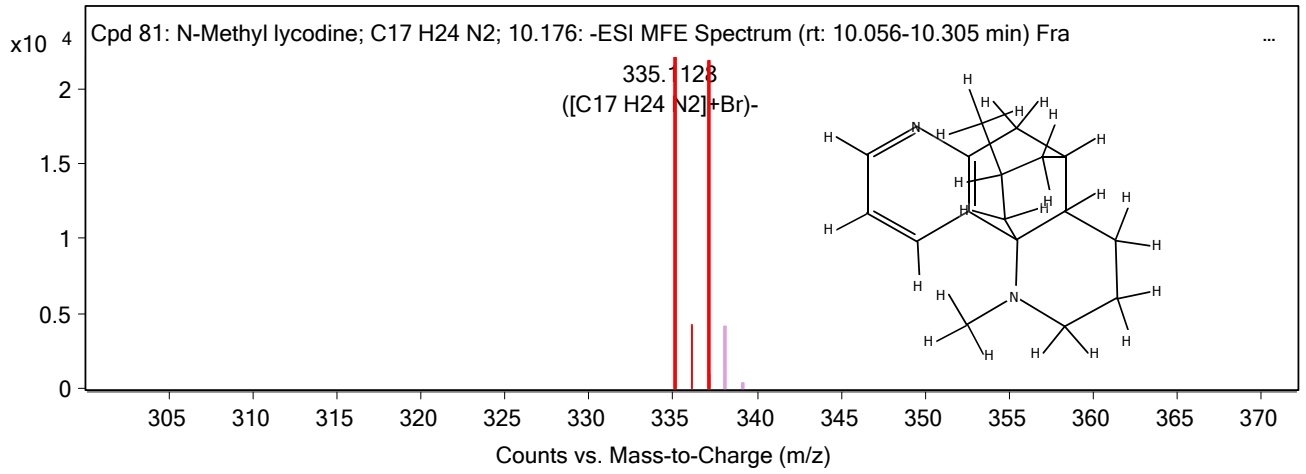




MFE MS Spectrum



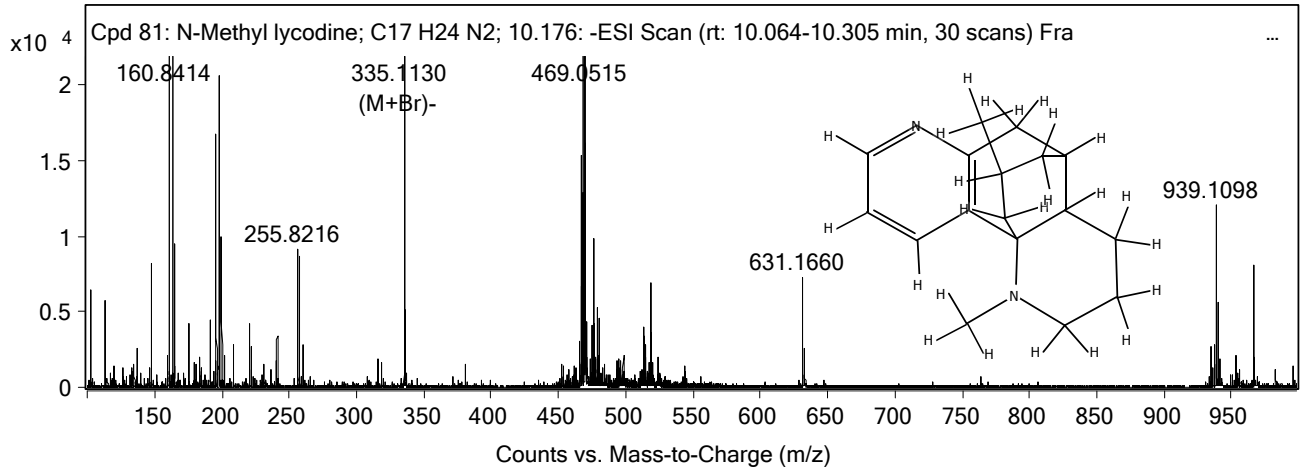
MFE MS Zoomed Spectrum



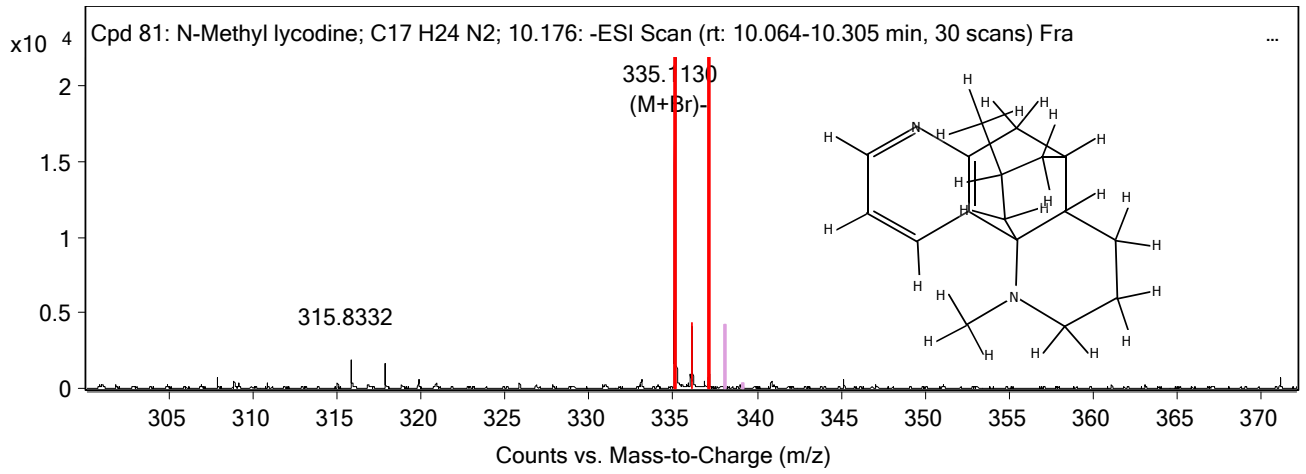
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
335.1128	-1	22124.33	C17 H24 N2	(M+Br)-
336.116	-1	4154.64	C17 H24 N2	(M+Br)-
337.1194	-1	897.66	C17 H24 N2	(M+Br)-

MS Spectrum



MS Zoomed Spectrum

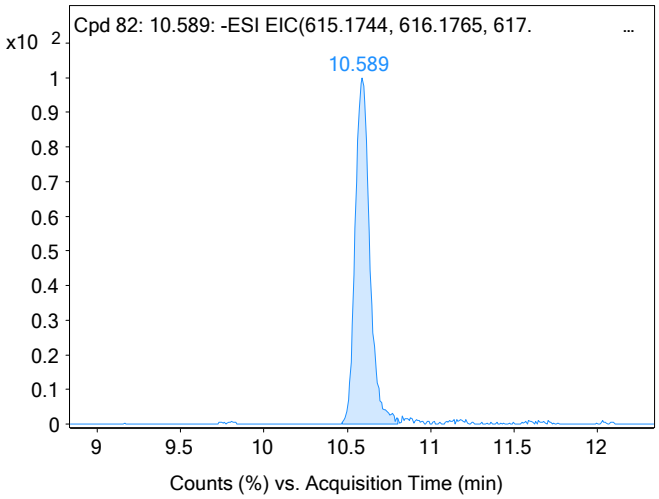


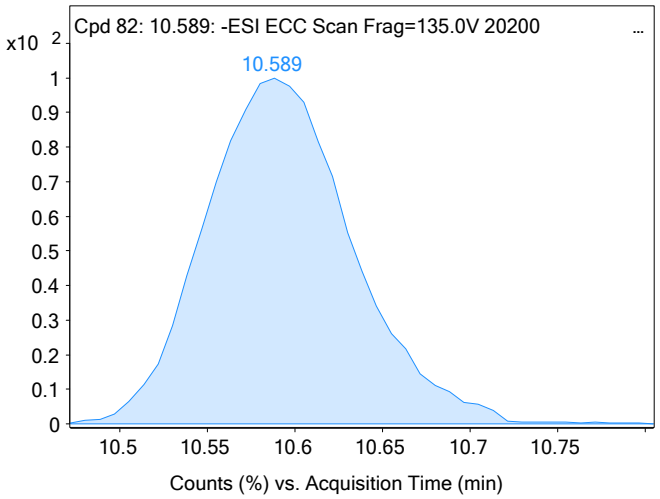
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	N-Methyl lycodine	10.176	C17 H24 N2		66.27	256.1942	-0.26	(M+Br)-

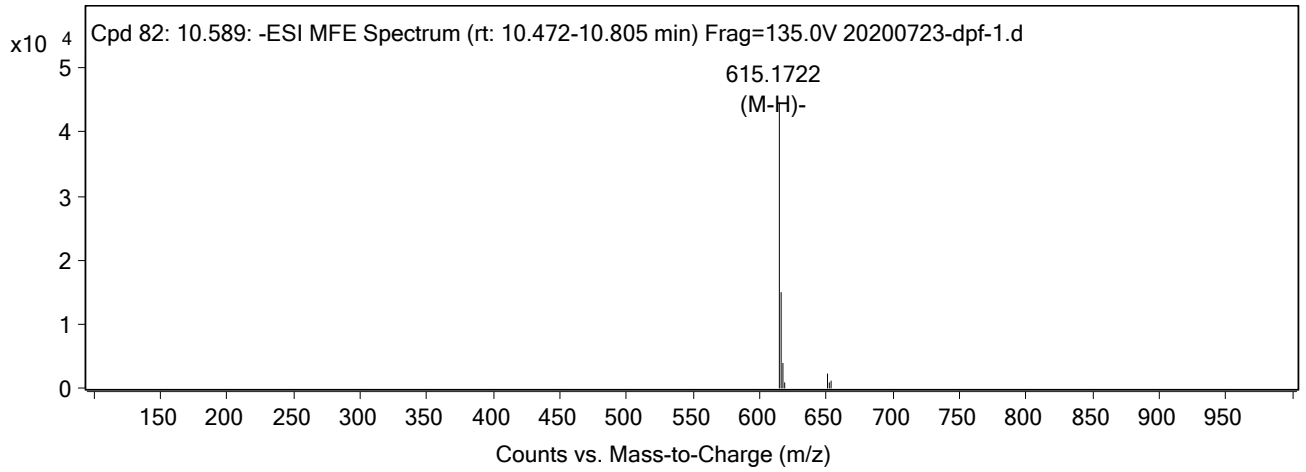
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 82: 10.589	615.1722	10.589	Find by Molecular Feature	616.1795

Compound Chromatograms

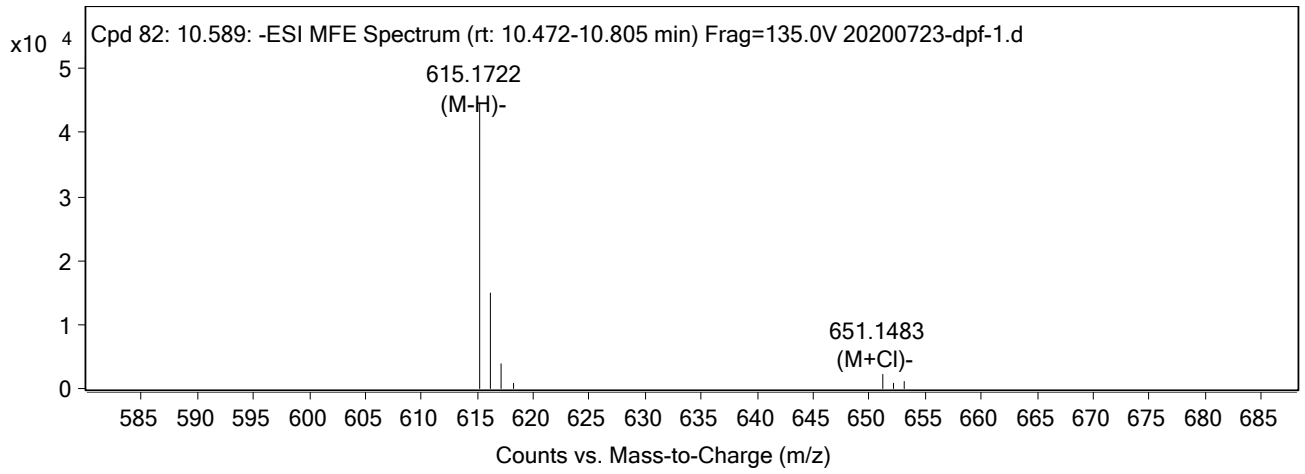




MFE MS Spectrum



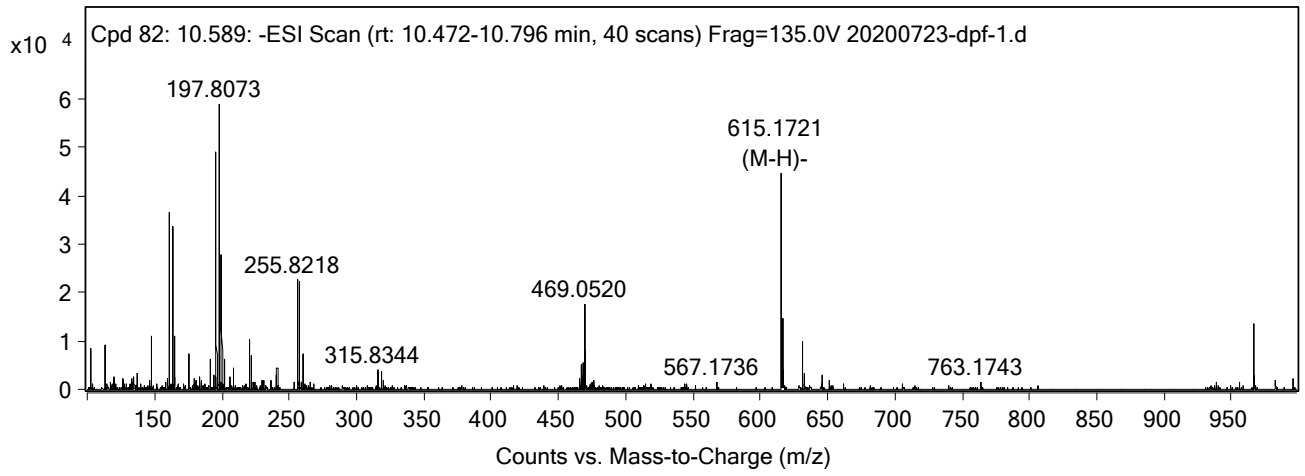
MFE MS Zoomed Spectrum



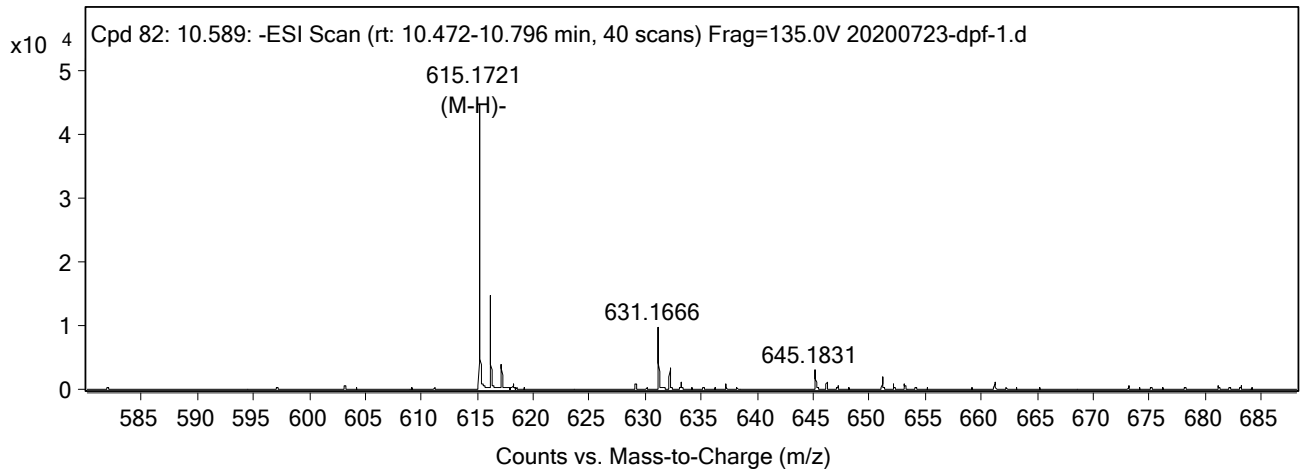
MS Spectrum Peak List

m/z	z	Abund	Ion
615.1722	-1	44691.88	(M-H)-
616.1752	-1	14856.9	(M-H)-
617.1775	-1	3858.13	(M-H)-
618.1788	-1	811.07	(M-H)-
651.1483	-1	2100.68	(M+Cl)-
652.1487	-1	741.22	(M+Cl)-
653.1466	-1	1017.32	(M+Cl)-

MS Spectrum



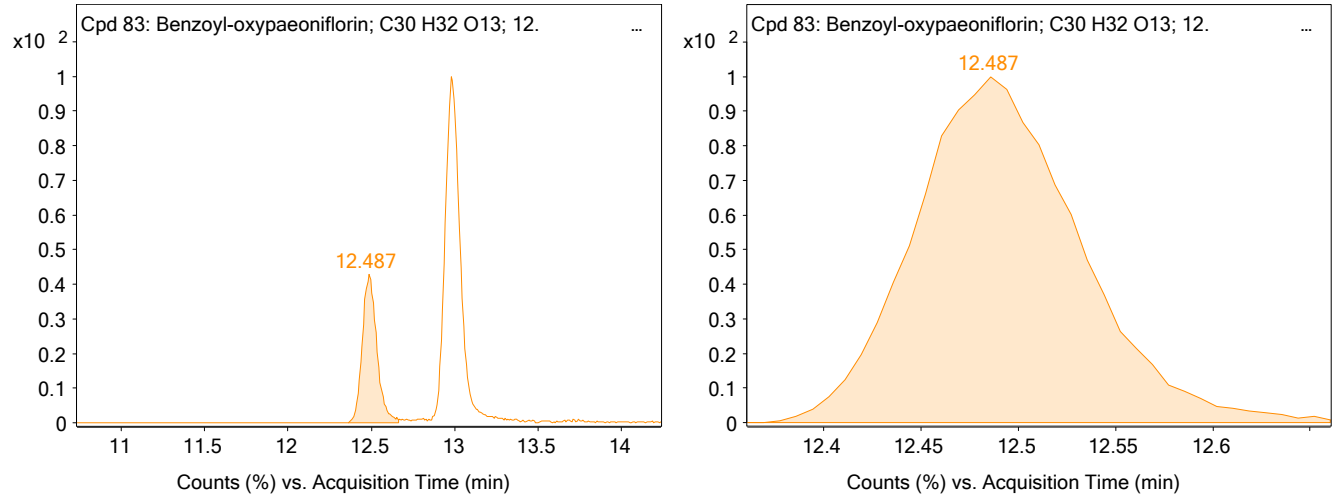
MS Zoomed Spectrum



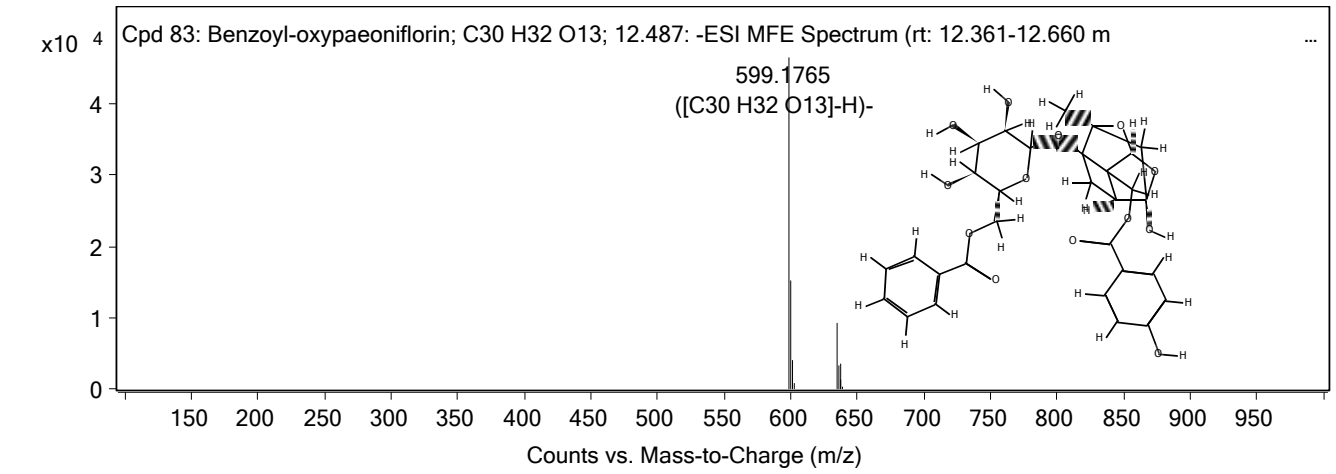
Qualitative Compound Identification Report

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 83: Benzoyl-oxypaeoniflorin; C30 H32 O13; 12.487	**Benzoyl-oxypaeoniflorin**	599.1765	12.487	Find by Molecular Feature	600.1838

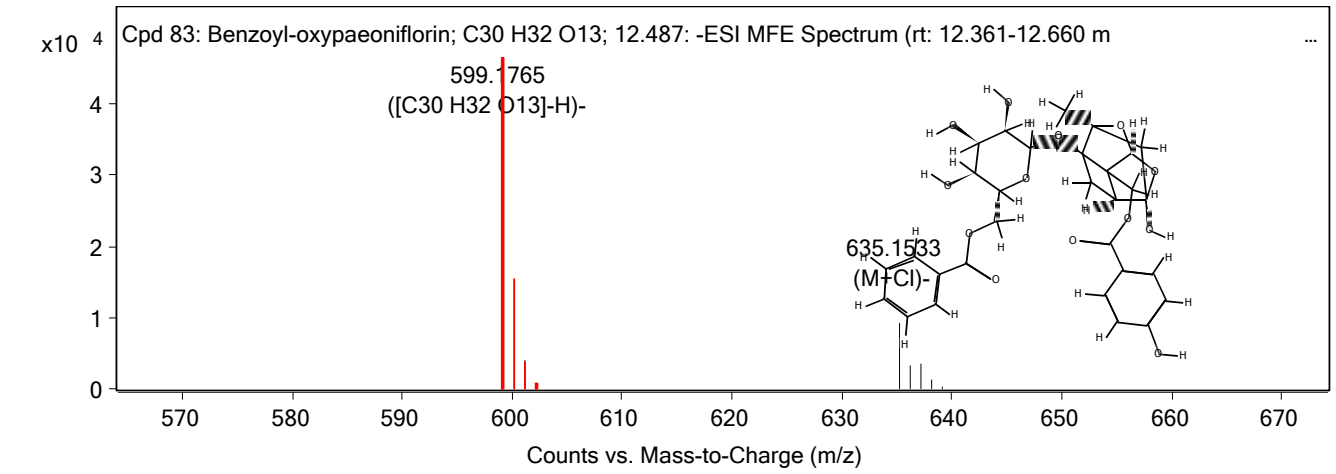
Compound Chromatograms



MFE MS Spectrum



MFE MS Zoomed Spectrum

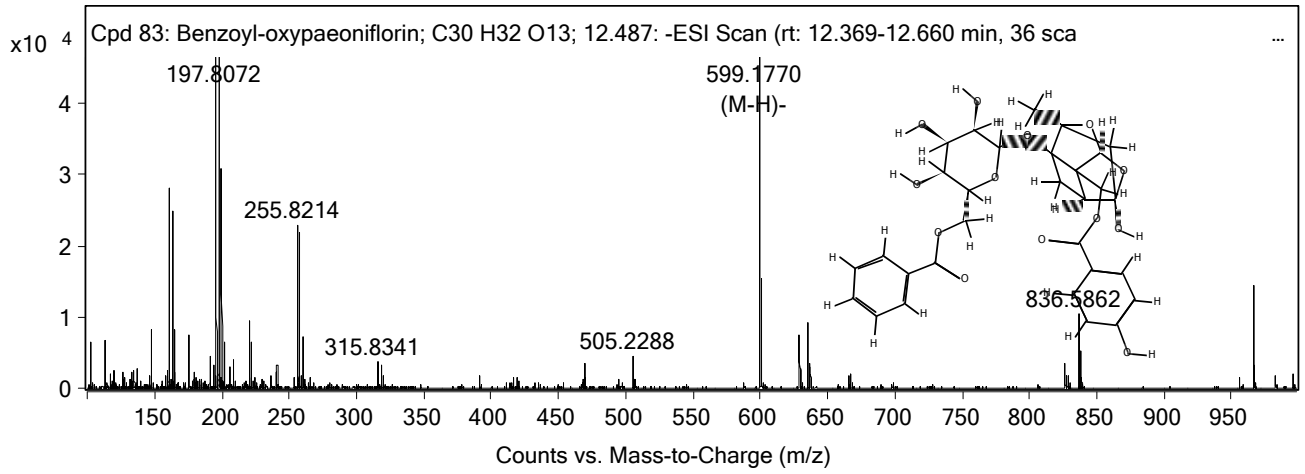


MS Spectrum Peak List

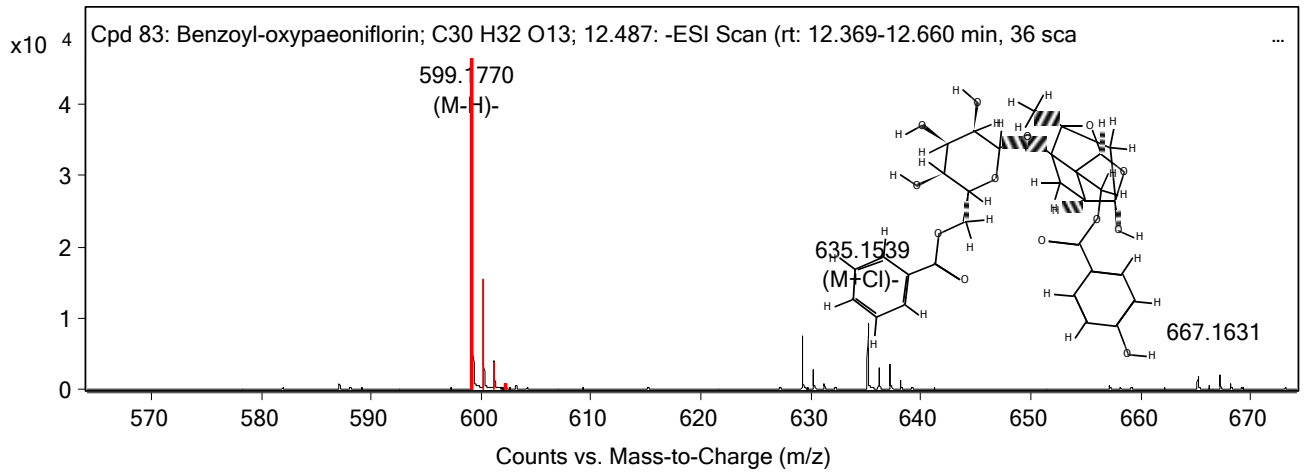
m/z	z	Abund	Formula	Ion
599.1765	-1	46553.53	C30 H32 O13	(M-H)-
600.1799	-1	15318.15	C30 H32 O13	(M-H)-

601.1825	-1	4013.47	C30 H32 O13	(M-H)-
602.1823	-1	746.24	C30 H32 O13	(M-H)-
635.1533	-1	9291.01		(M+Cl)-
636.1559	-1	3218.26		(M+Cl)-
637.151	-1	3531.63		(M+Cl)-
638.1545	-1	1149.75		(M+Cl)-
639.1536	-1	265.51		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

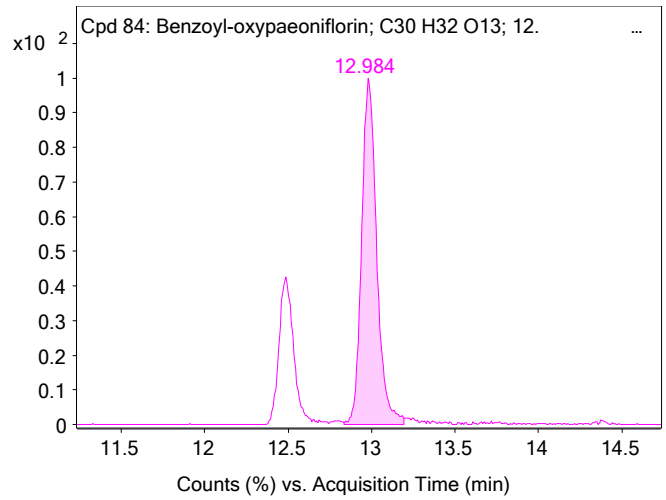


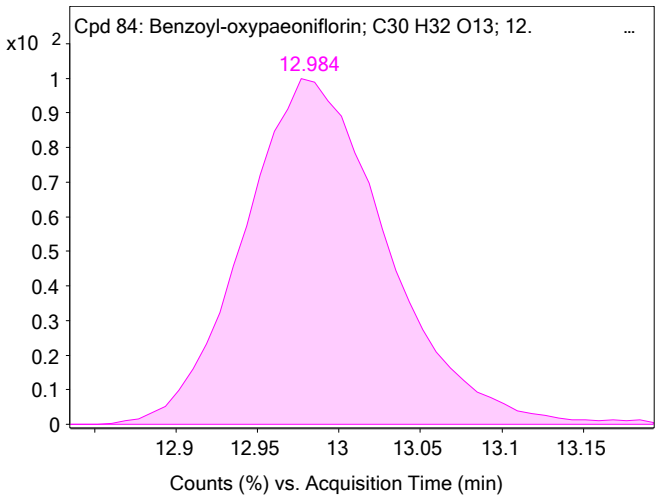
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Benzoyl-oxypaeoniflorin	12.487	C30 H32 O13		99.43	600.1838	0.51	(M-H)-

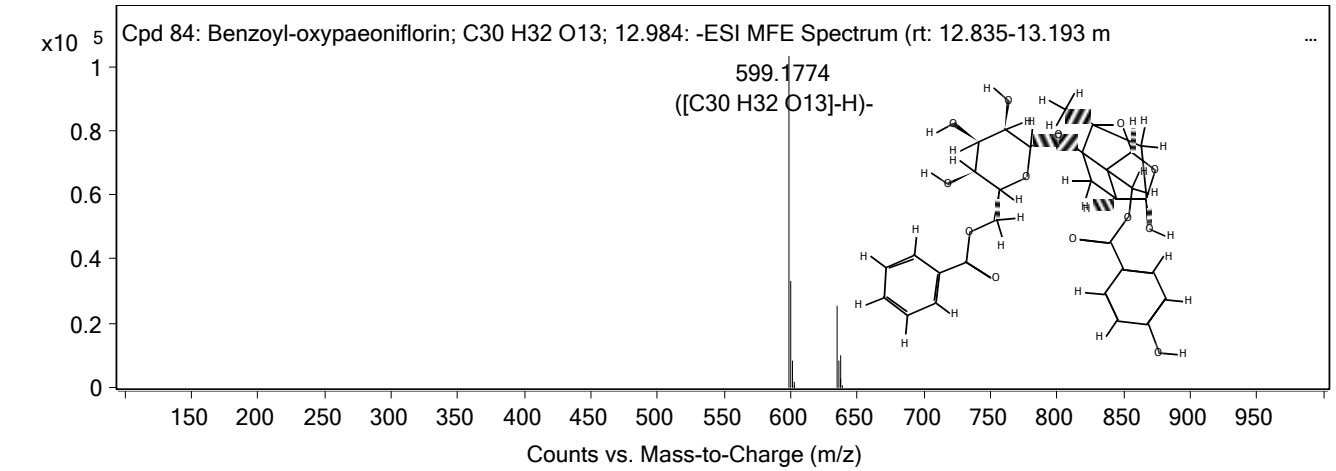
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 84: Benzoyl-oxypaeoniflorin; C30 H32 O13; 12.984	**Benzoyl-oxypaeoniflorin**	599.1774	12.984	Find by Molecular Feature	600.1845

Compound Chromatograms

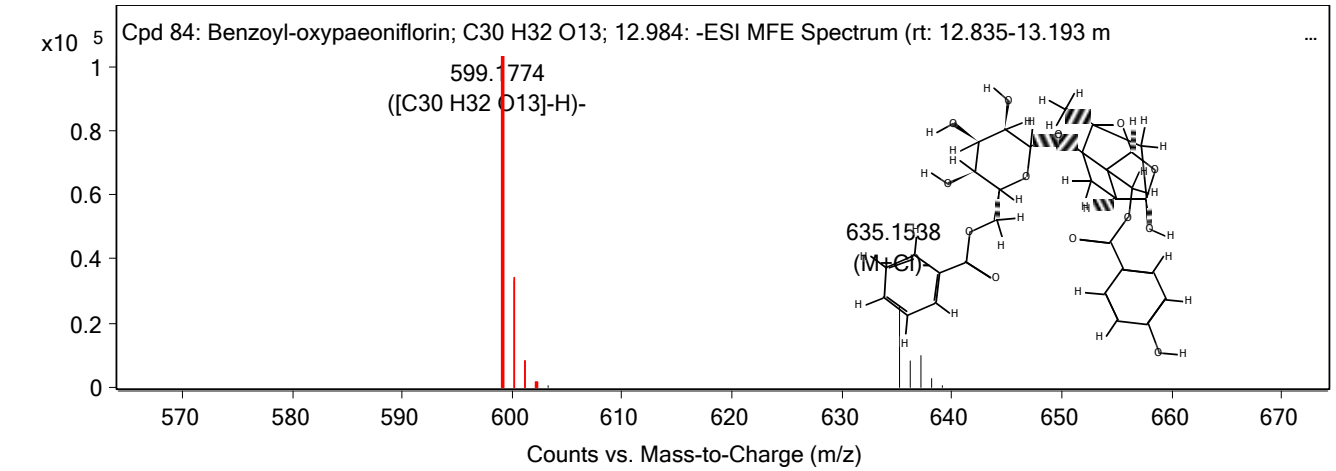




MFE MS Spectrum



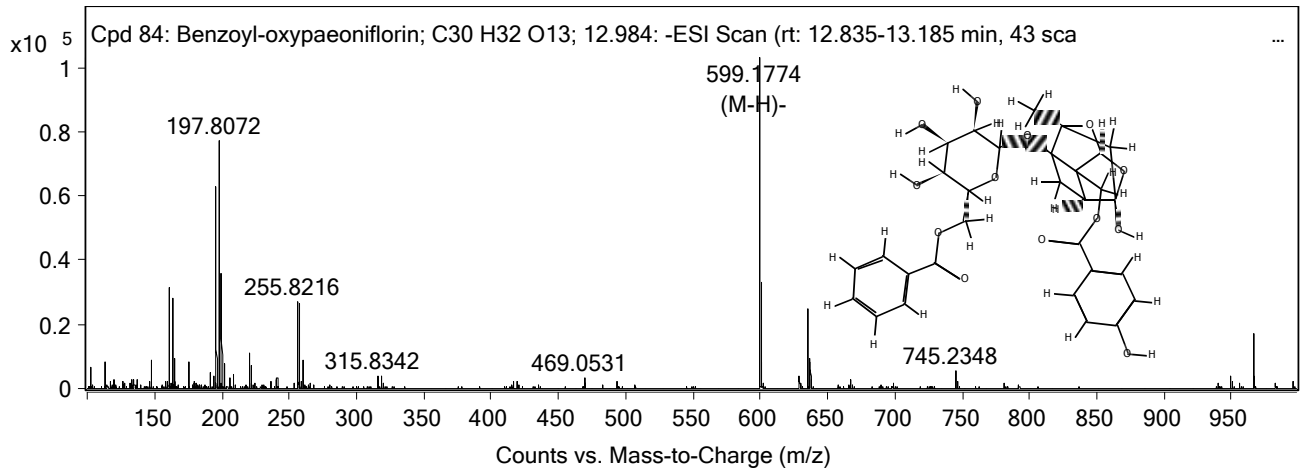
MFE MS Zoomed Spectrum



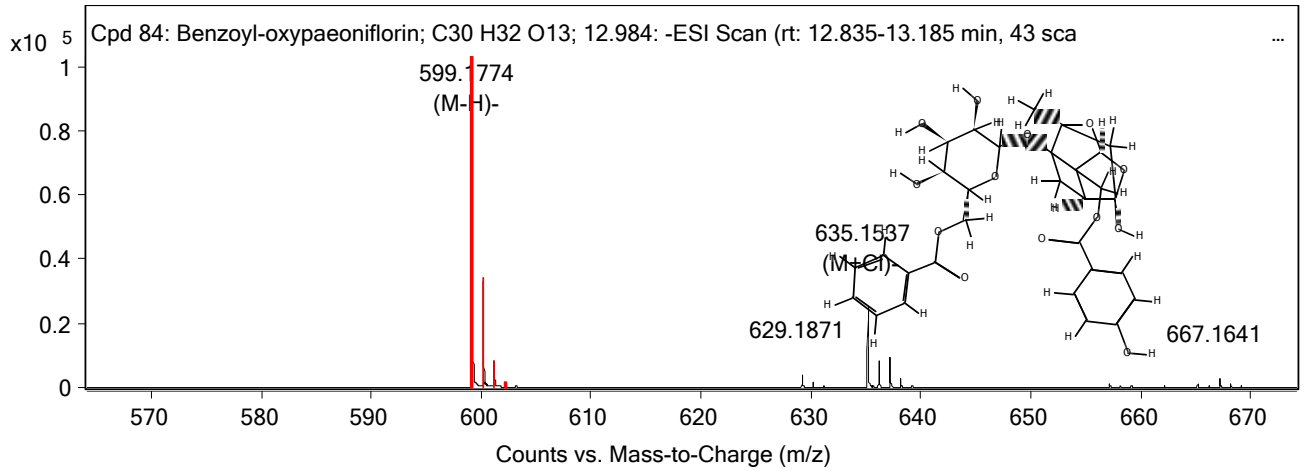
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
599.1774	-1	103152.35	C30 H32 O13	(M-H)-
600.1802	-1	32948.08	C30 H32 O13	(M-H)-
601.183	-1	8163.38	C30 H32 O13	(M-H)-
602.185	-1	1506.09	C30 H32 O13	(M-H)-
603.1832	-1	345.82	C30 H32 O13	(M-H)-
635.1538	-1	25201.38		(M+Cl)-
636.1574	-1	8386.55		(M+Cl)-
637.1522	-1	9907.53		(M+Cl)-
638.1544	-1	2919.92		(M+Cl)-
639.1568	-1	671.33		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

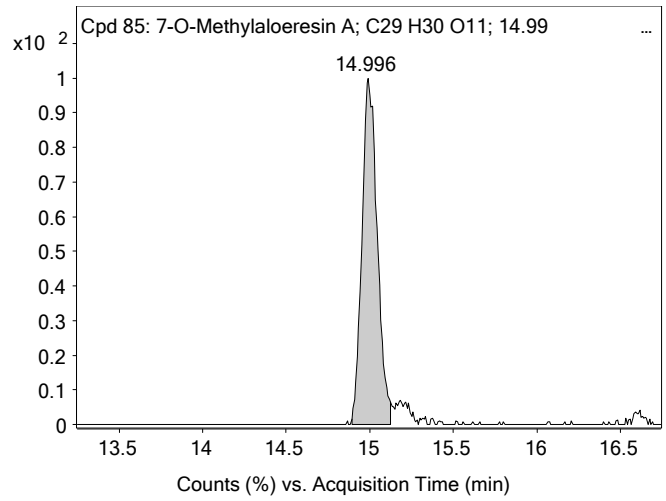


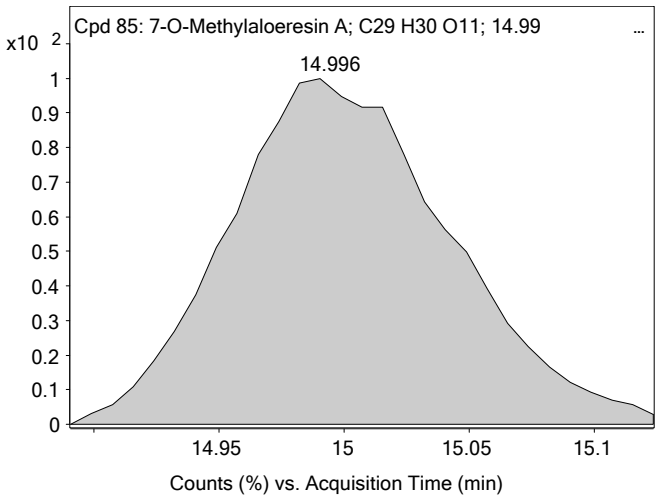
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Benzoyl-oxypaeoniflorin	12.984	C30 H32 O13		99.3	600.1845	-0.23	(M-H)-

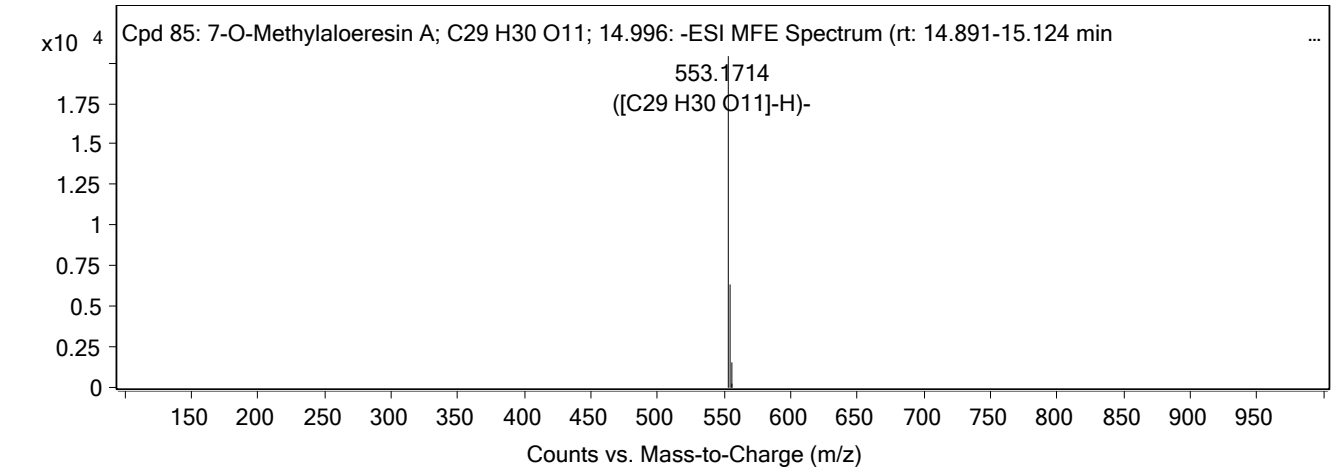
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 85: 7-O-Methylaloeresin A; C29 H30 O11; 14.996	**7-O-Methylaloeresin A**	553.1714	14.996	Find by Molecular Feature	554.1786

Compound Chromatograms

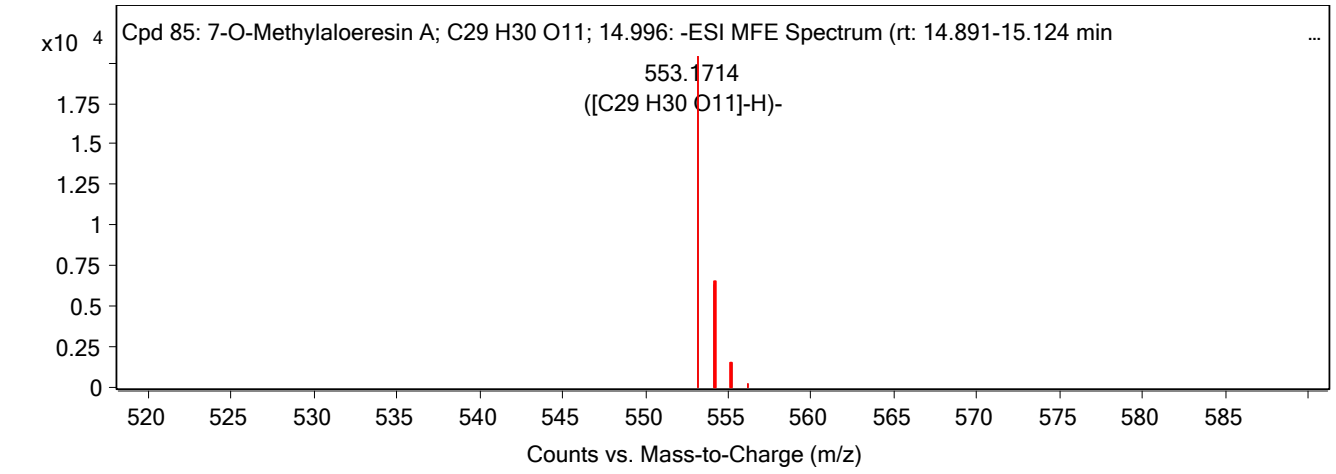




MFE MS Spectrum



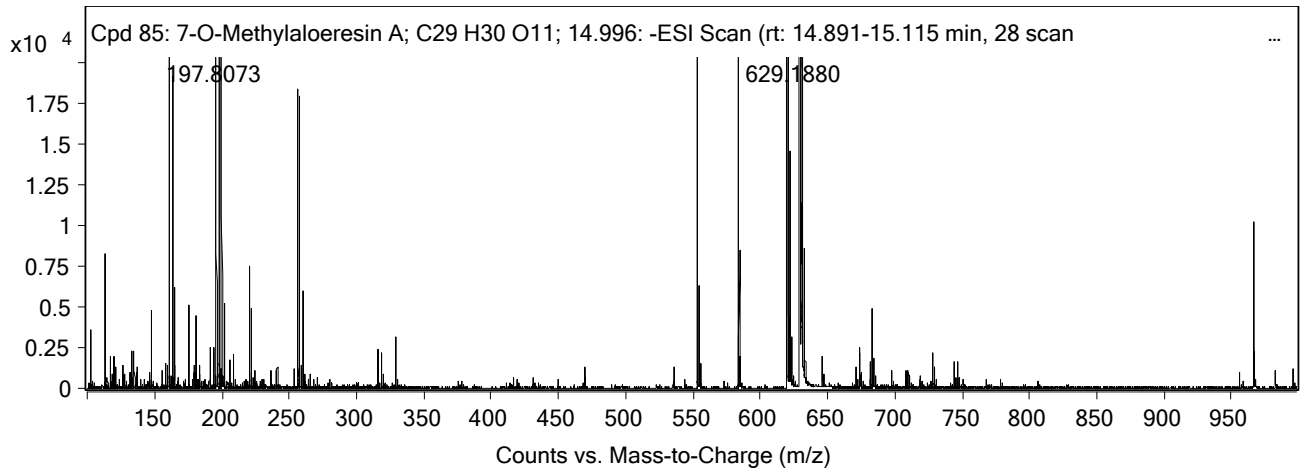
MFE MS Zoomed Spectrum



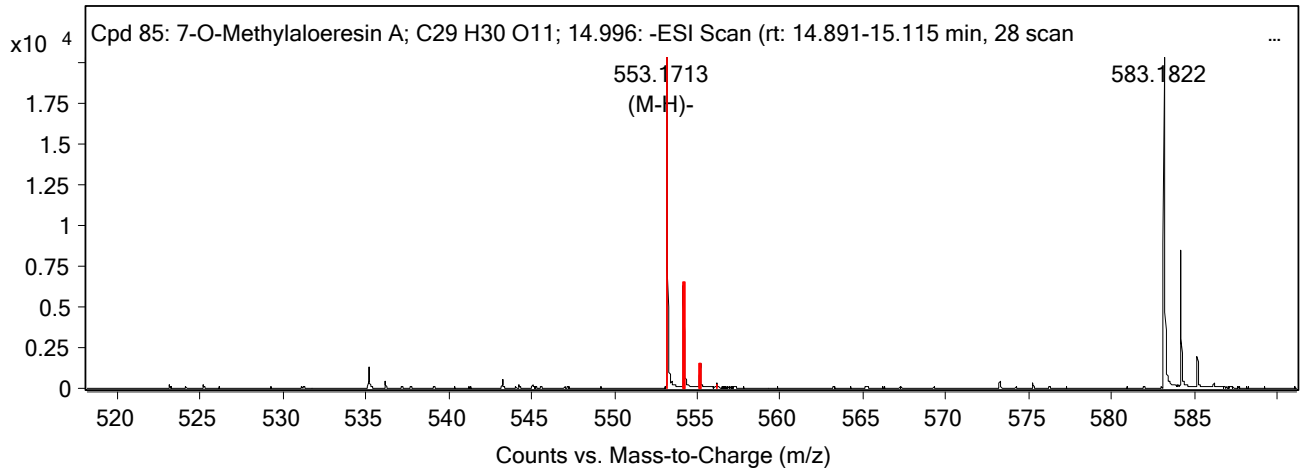
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
553.1714	-1	20394.02	C29 H30 O11	(M-H)-
554.1744	-1	6356.55	C29 H30 O11	(M-H)-
555.1774	-1	1501.69	C29 H30 O11	(M-H)-
556.1825	-1	191.15	C29 H30 O11	(M-H)-

MS Spectrum



MS Zoomed Spectrum

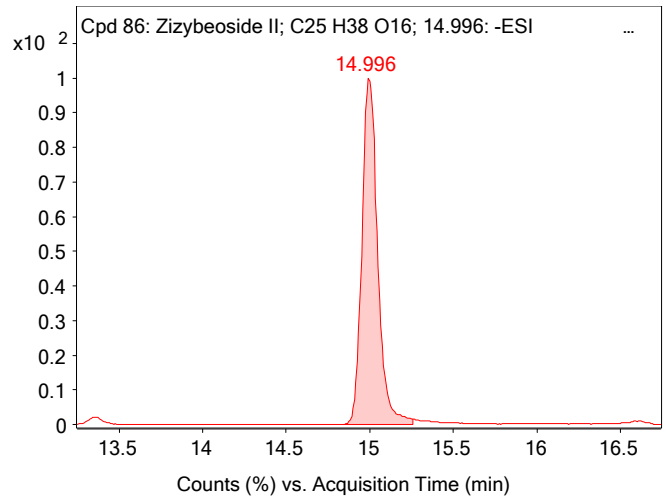


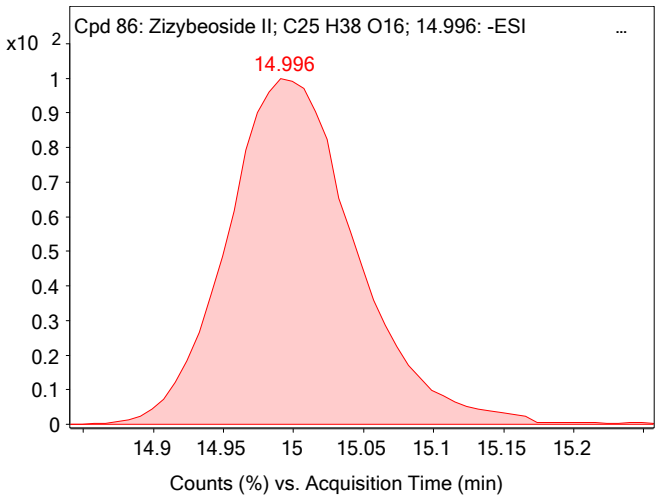
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	7-O-Methylaloeresin A	14.996	C29 H30 O11		99.65	554.1786	0.24	(M-H)-
	Jioglutoside B	14.996	C23 H34 O13		54.85	518.2023	-2.4	(M+Cl)-
	Ipobscurine B	14.996	C29 H30 N2 O7		51.03	518.2024	2.93	(M+Cl)-

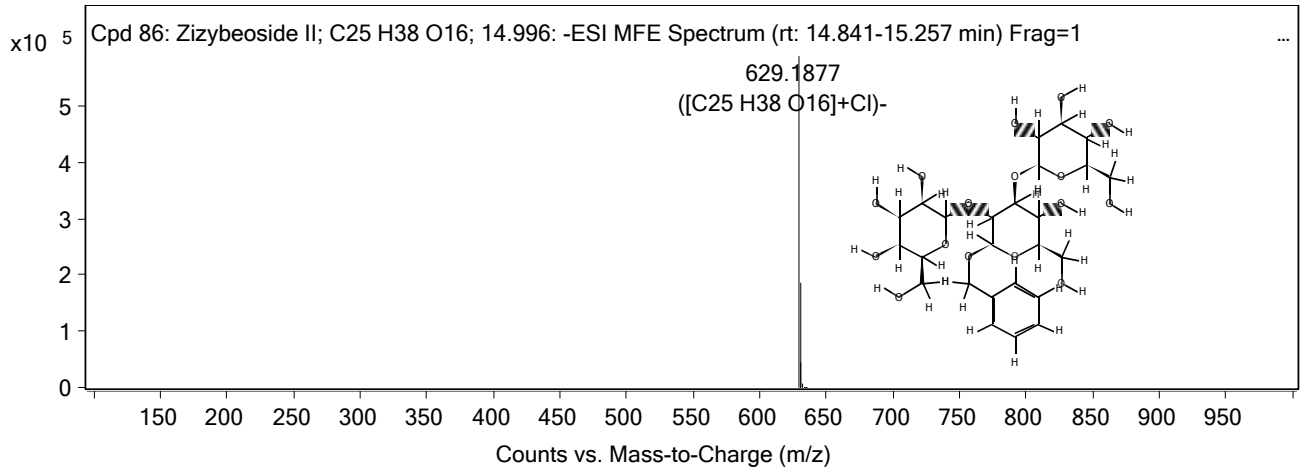
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 86: Zizybeoside II; C25 H38 O16; 14.996	**Zizybeoside II**	629.1877	14.996	Find by Molecular Feature	594.2189

Compound Chromatograms

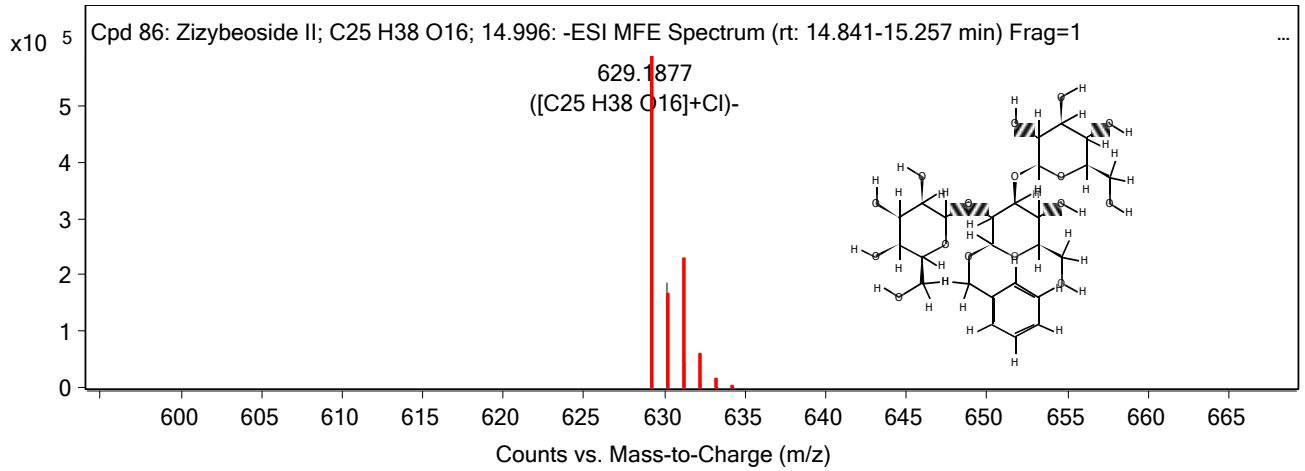




MFE MS Spectrum



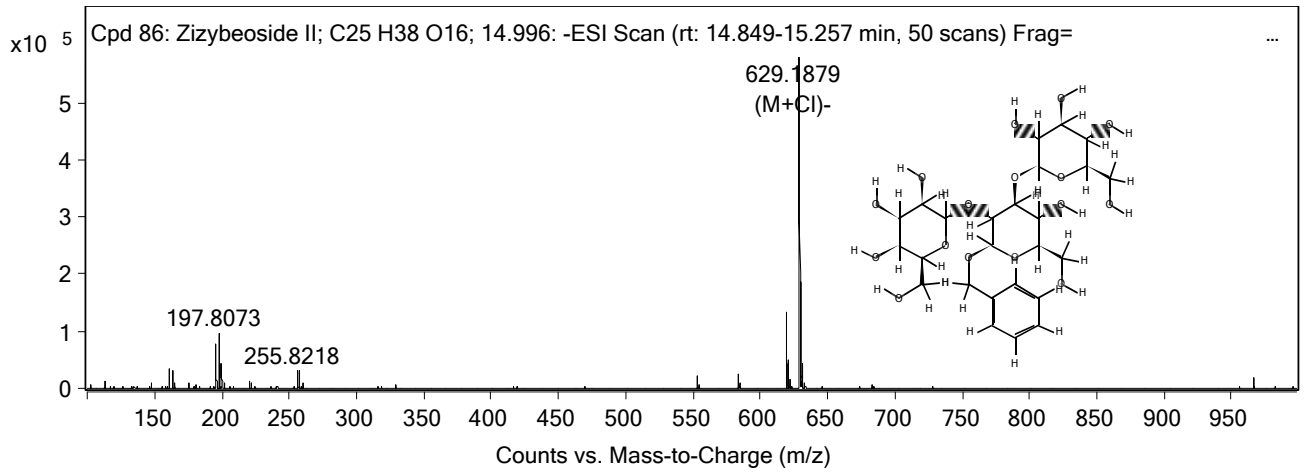
MFE MS Zoomed Spectrum



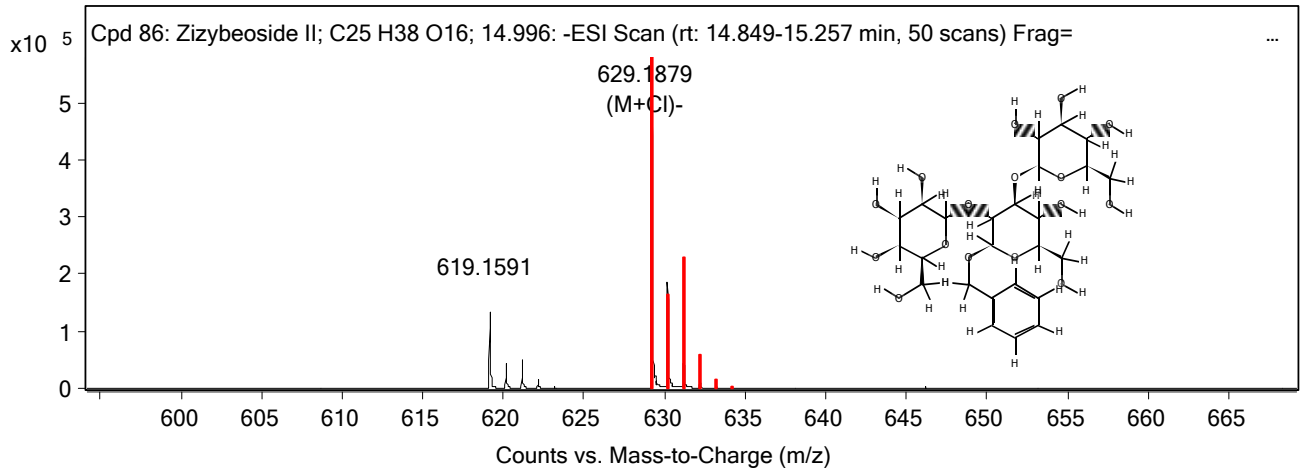
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
629.1877	-1	587841.25	C25 H38 O16	(M+Cl)-
630.1914	-1	185312.05	C25 H38 O16	(M+Cl)-
631.1936	-1	44287.34	C25 H38 O16	(M+Cl)-
632.1966	-1	7960.83	C25 H38 O16	(M+Cl)-
633.1992	-1	1337.52	C25 H38 O16	(M+Cl)-
634.2005	-1	274.92	C25 H38 O16	(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

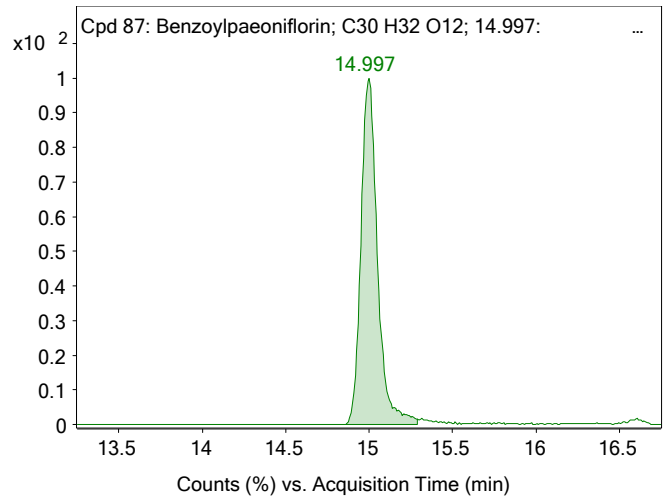


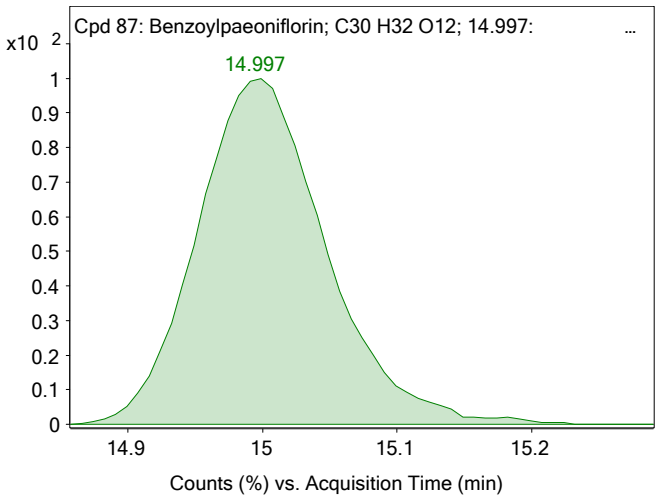
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Zizybeoside II	14.996	C25 H38 O16		53.85	594.2189	-2.88	(M+Cl)-

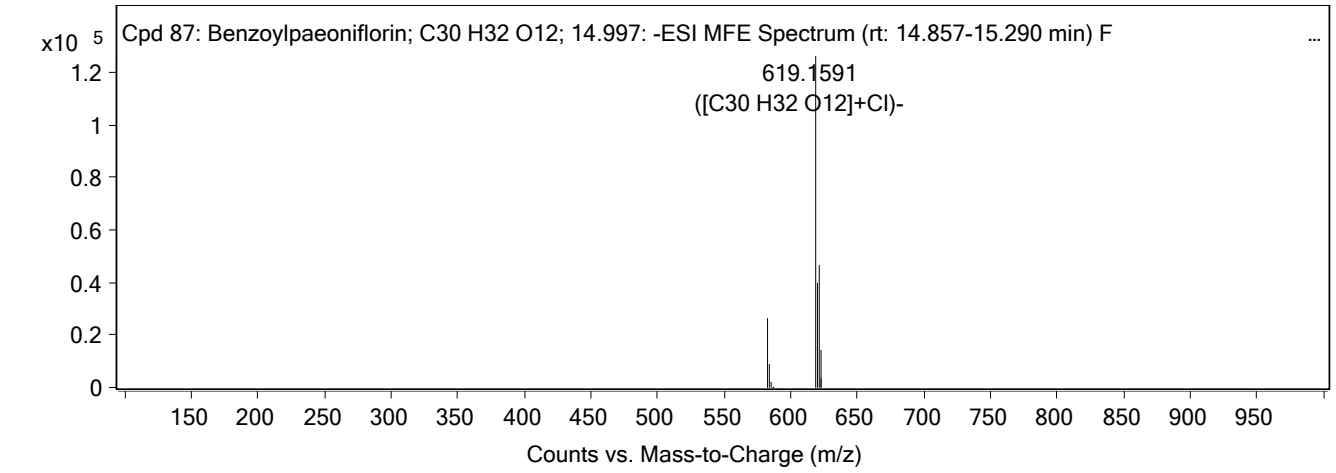
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 87: Benzoylpaeoniflorin; C30 H32 O12; 14.997	**Benzoylpaeoniflorin**	619.1591	14.997	Find by Molecular Feature	584.1896

Compound Chromatograms

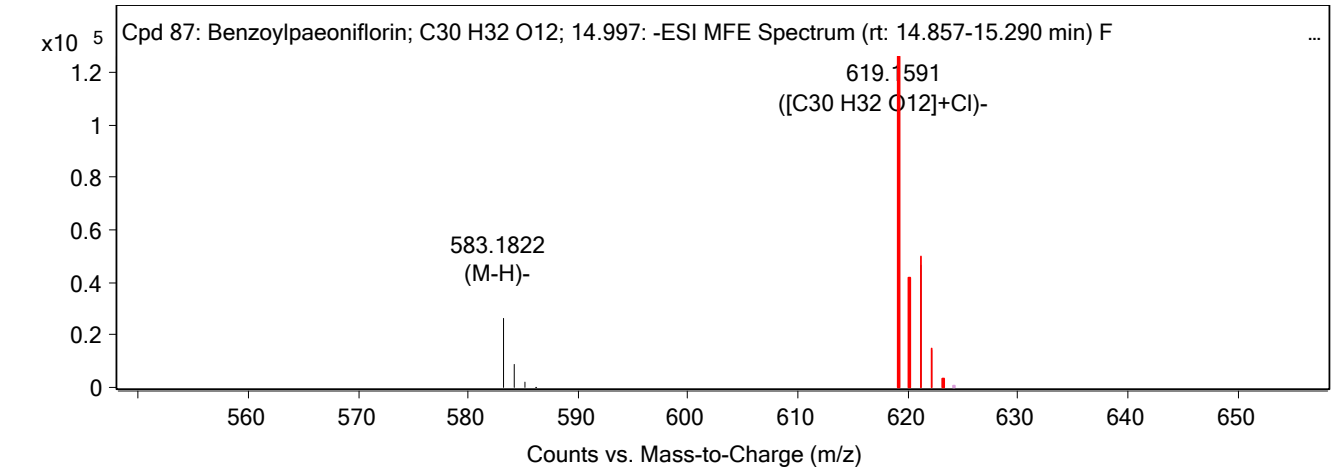




MFE MS Spectrum



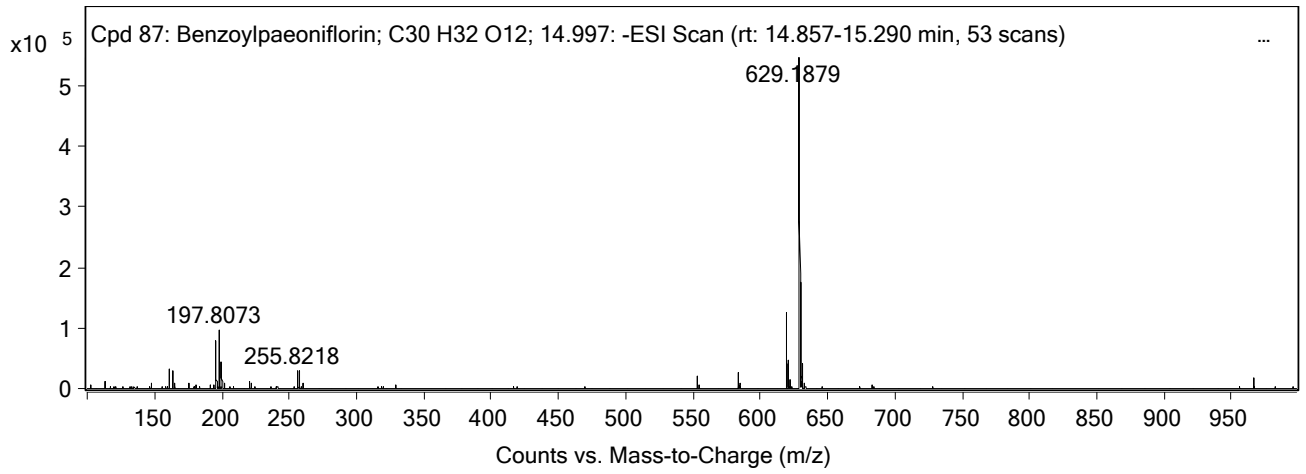
MFE MS Zoomed Spectrum



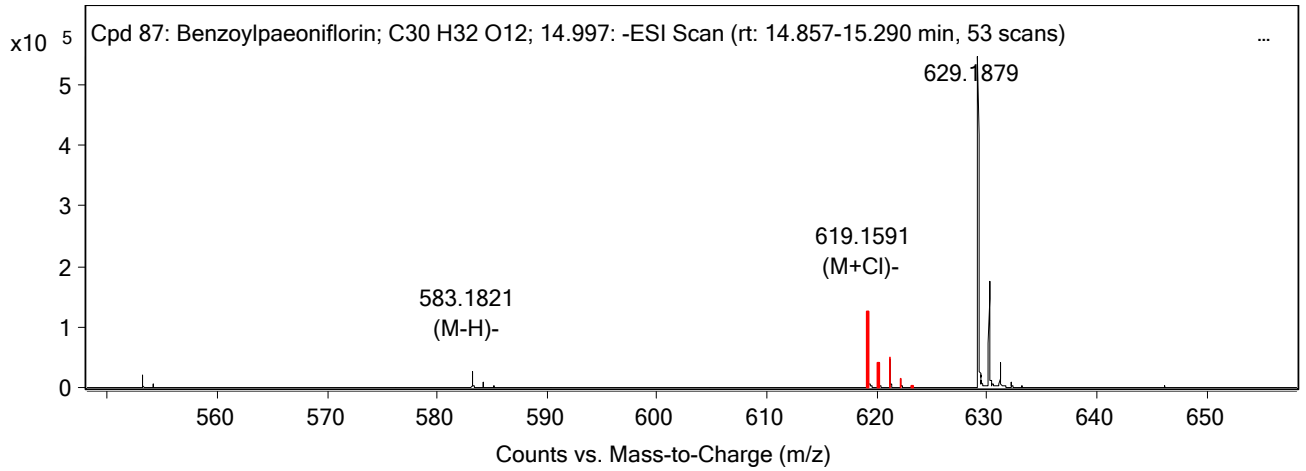
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
583.1822	-1	26179.15		(M-H)-
584.1853	-1	8768.7		(M-H)-
585.1874	-1	2069.24		(M-H)-
586.1896	-1	307.87		(M-H)-
619.1591	-1	126040.72	C30 H32 O12	(M+Cl)-
620.1621	-1	39962.82	C30 H32 O12	(M+Cl)-
621.1578	-1	46878.62	C30 H32 O12	(M+Cl)-
622.1601	-1	14172.72	C30 H32 O12	(M+Cl)-
623.1633	-1	3154.11	C30 H32 O12	(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

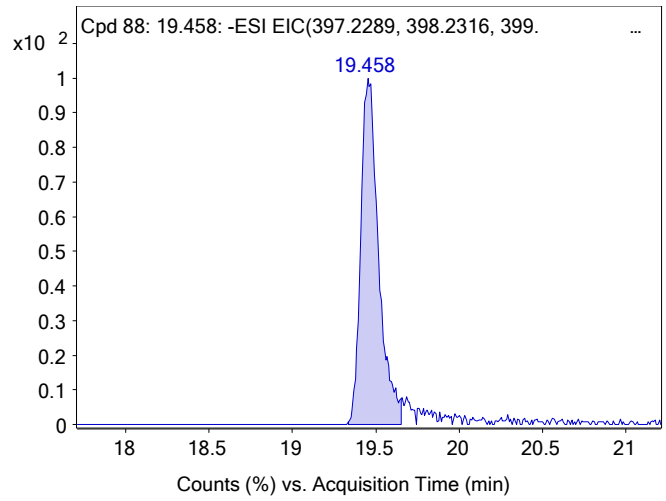


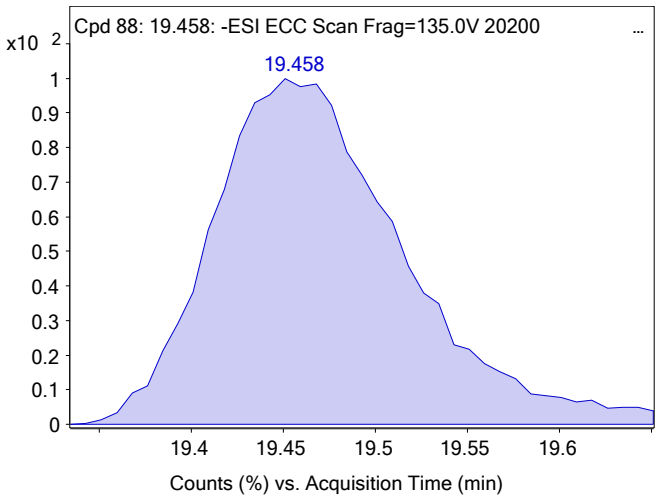
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Benzoylpaeoniflorin	14.997	C30 H32 O12		99.39	584.1896	-0.22	(M+Cl)-

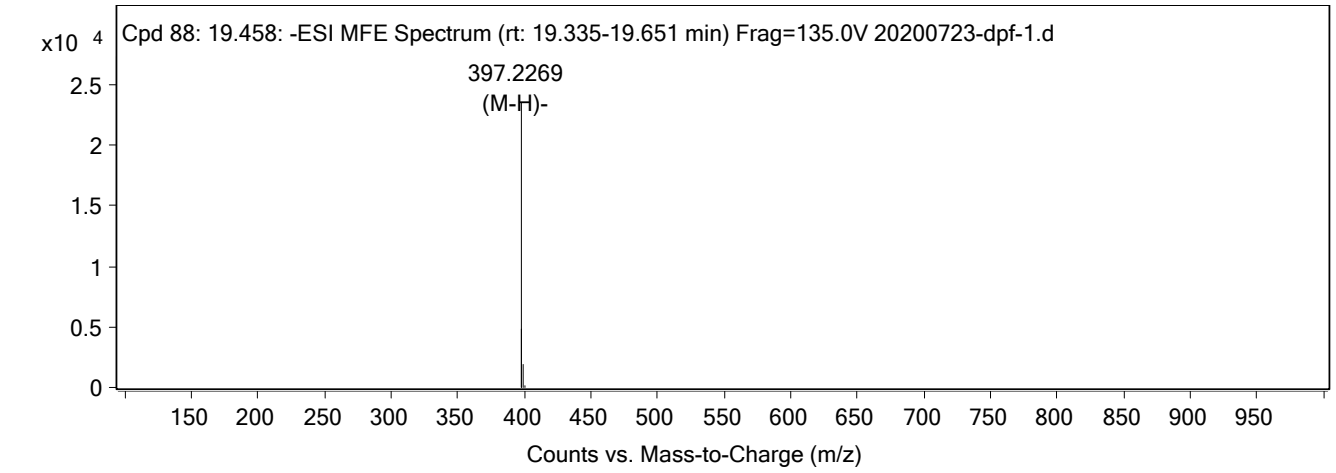
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 88: 19.458	397.2269	19.458	Find by Molecular Feature	398.2342

Compound Chromatograms

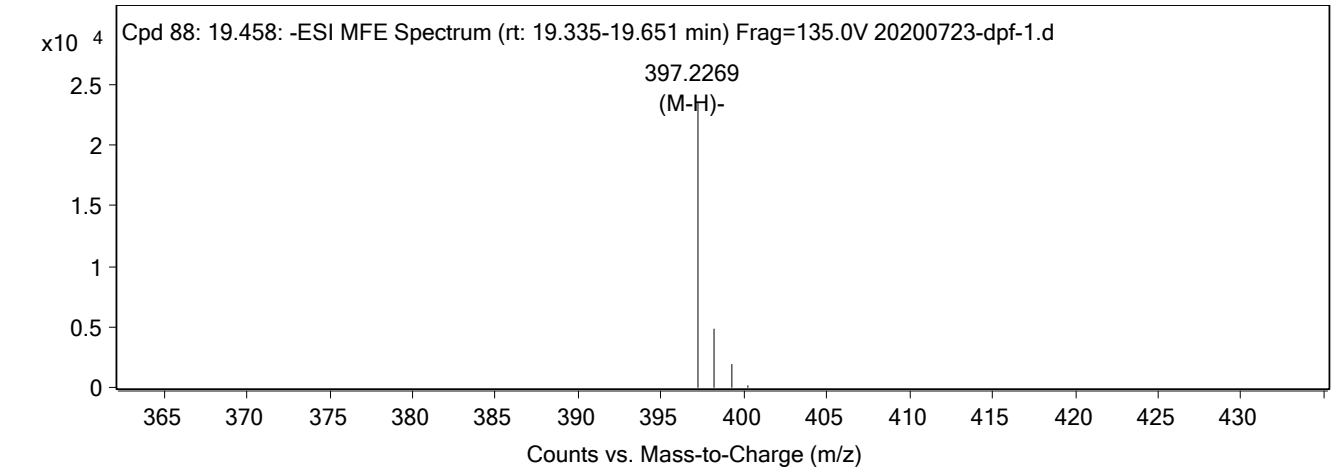




MFE MS Spectrum



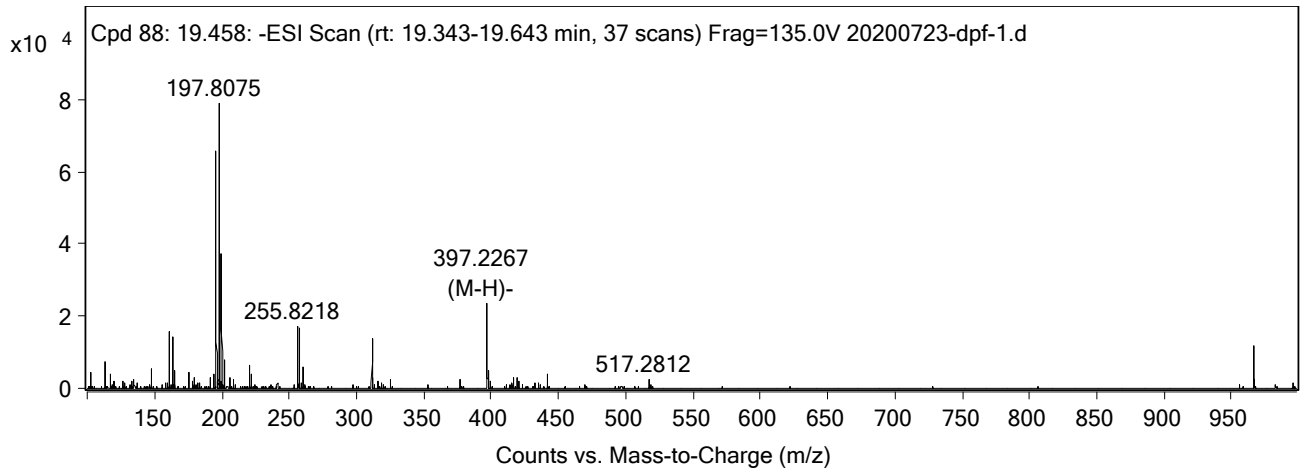
MFE MS Zoomed Spectrum



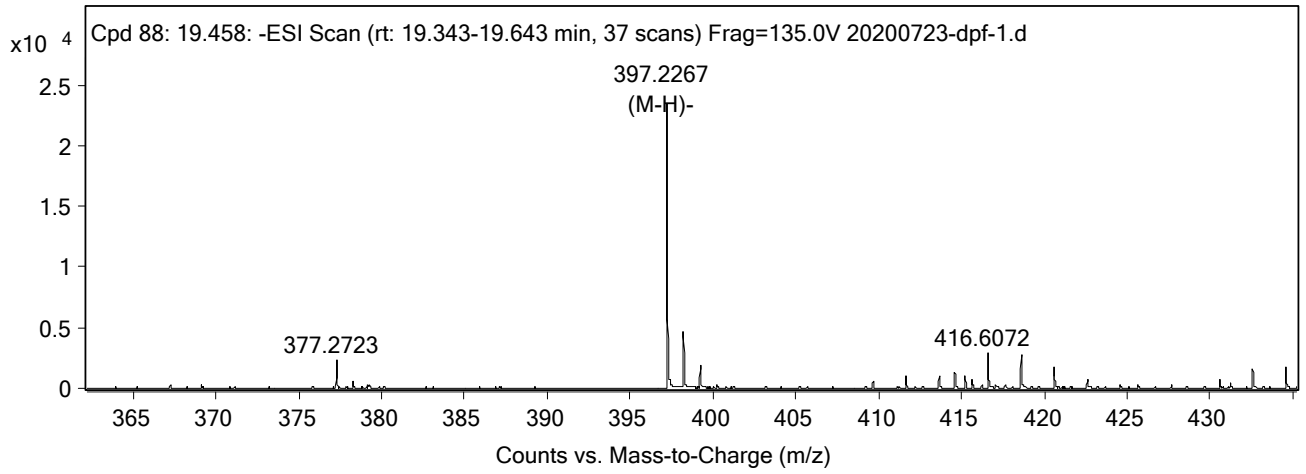
MS Spectrum Peak List

m/z	z	Abund	Ion
397.2269	-1	23601.84	(M-H)-
398.2299	-1	4813.96	(M-H)-
399.2281	-1	1877.52	(M-H)-
400.2309	-1	199.7	(M-H)-

MS Spectrum

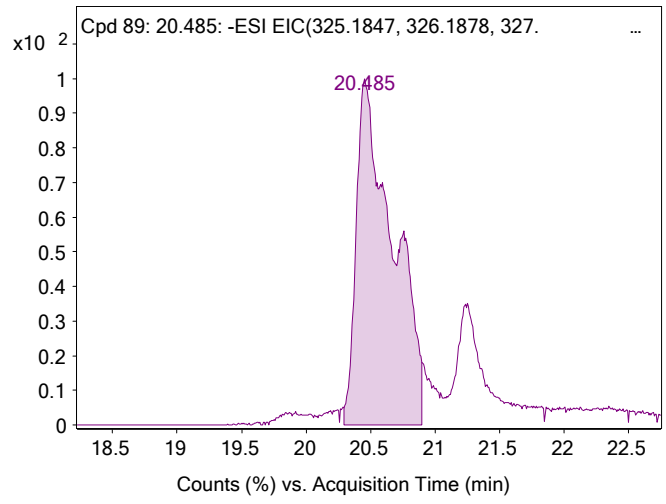


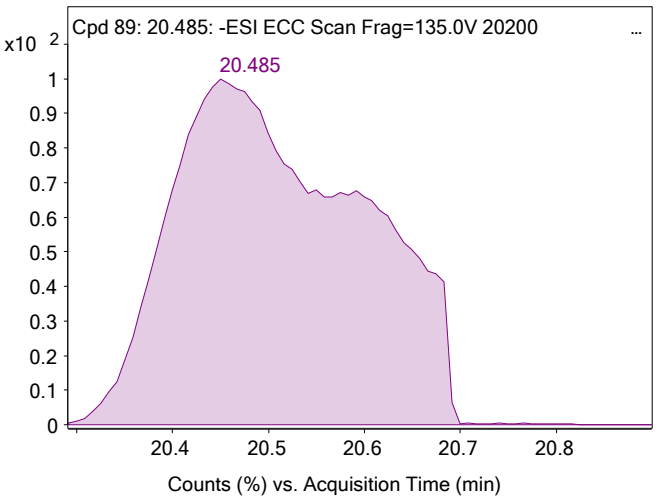
MS Zoomed Spectrum



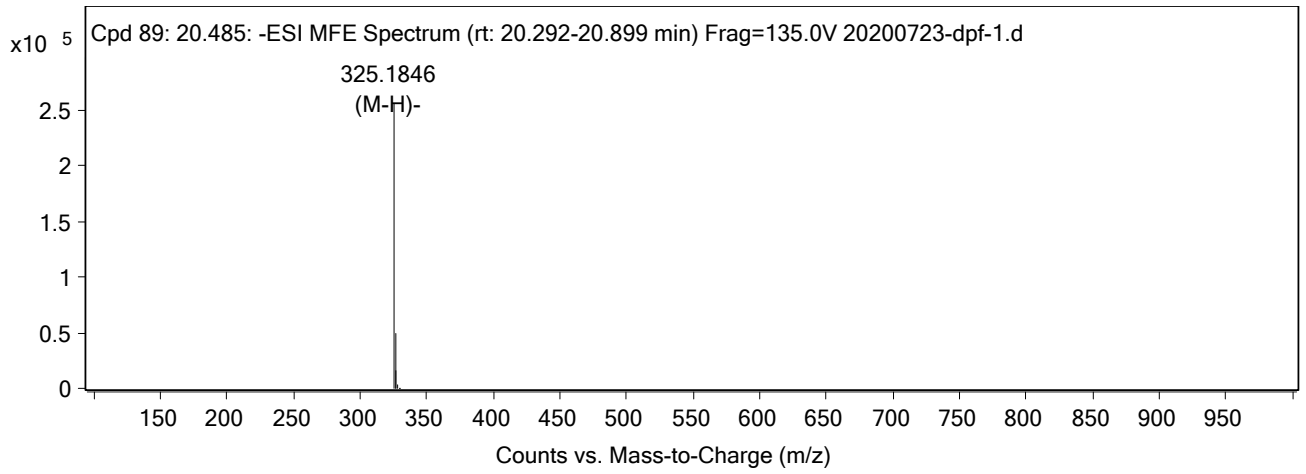
Compound Label	m/z	RT	Algorithm	Mass
Cpd 89: 20.485	325.1846	20.485	Find by Molecular Feature	326.1919

Compound Chromatograms

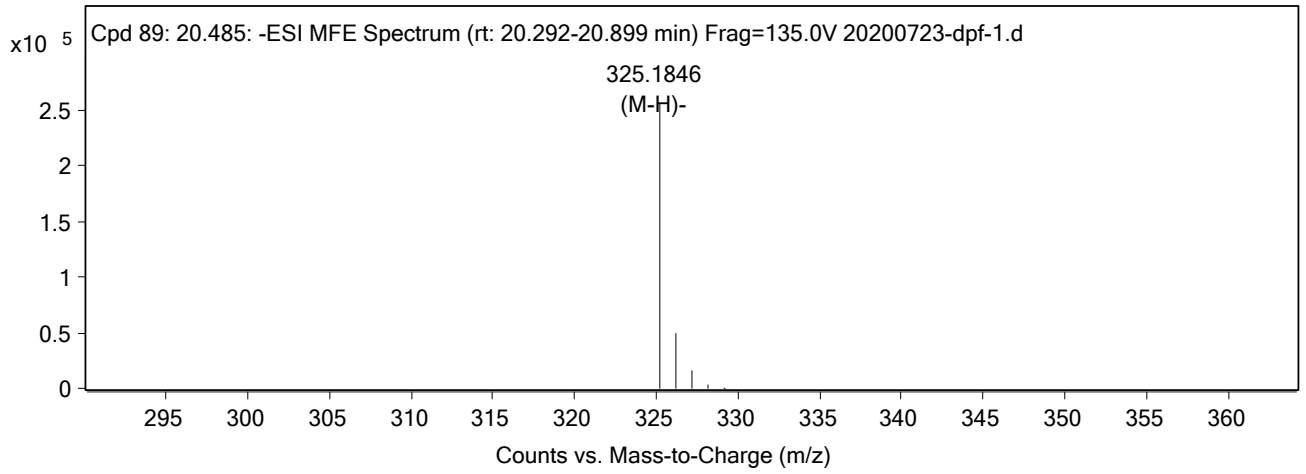




MFE MS Spectrum



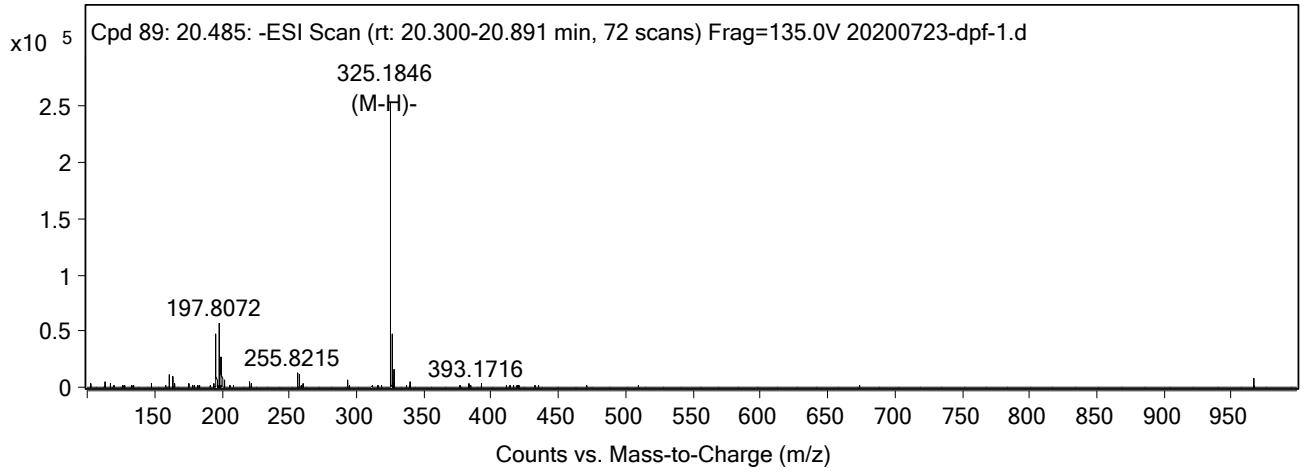
MFE MS Zoomed Spectrum



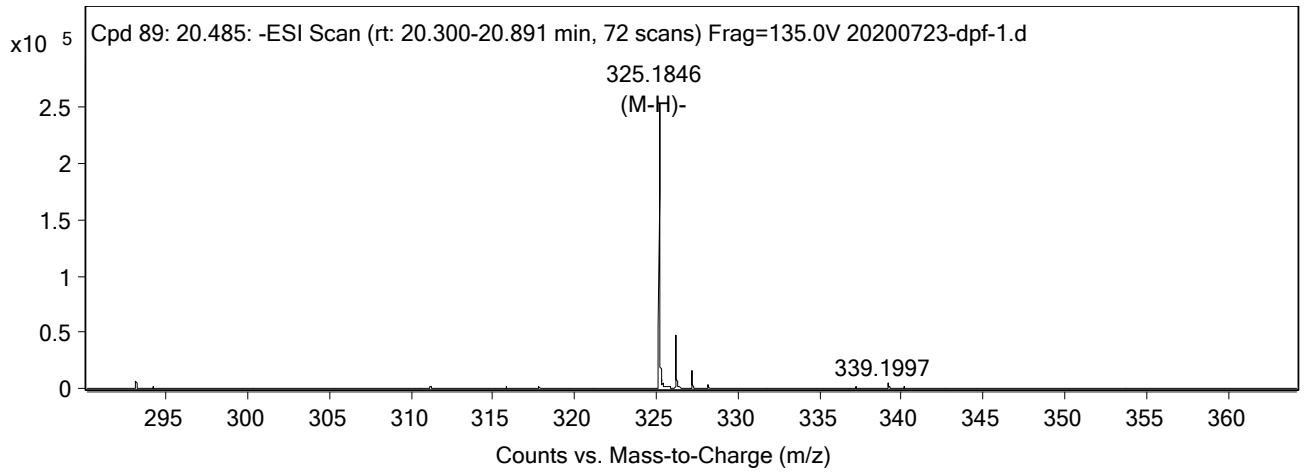
MS Spectrum Peak List

m/z	z	Abund	Ion
325.1846	-1	256236.23	(M-H)-
326.1876	-1	49413.48	(M-H)-
327.1842	-1	15769.63	(M-H)-
328.1864	-1	2926.77	(M-H)-
329.1887	-1	196.02	(M-H)-

MS Spectrum

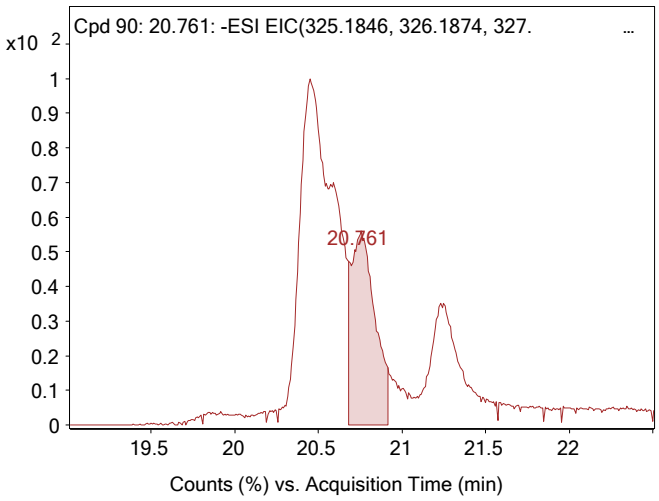


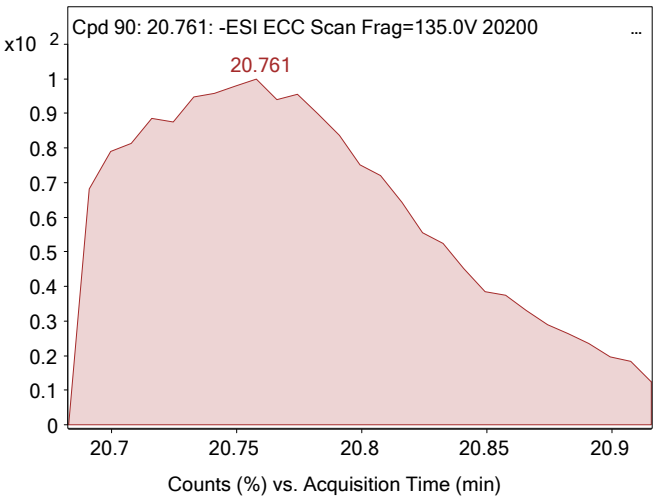
MS Zoomed Spectrum



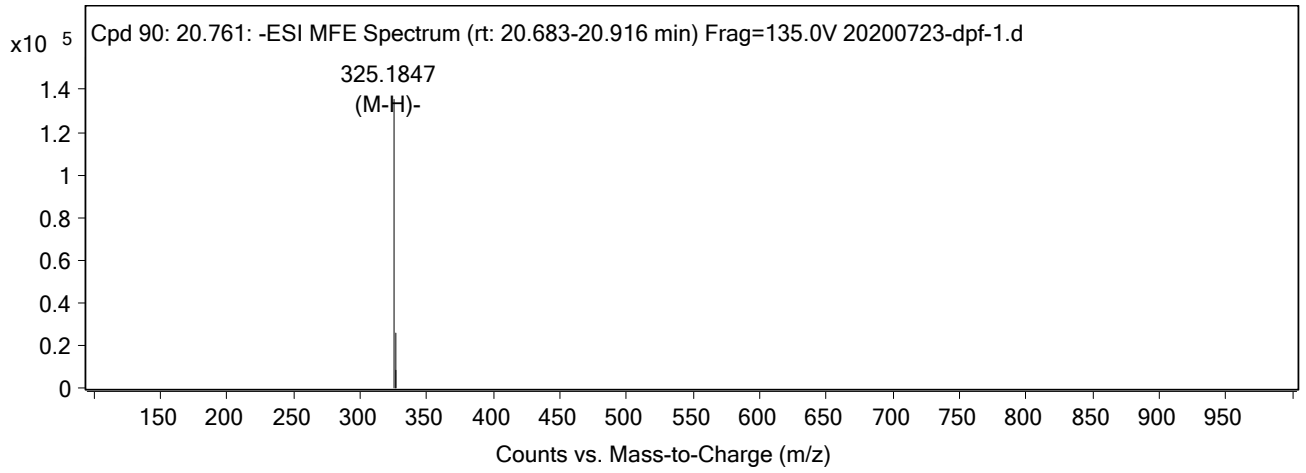
Compound Label	m/z	RT	Algorithm	Mass
Cpd 90: 20.761	325.1847	20.761	Find by Molecular Feature	326.192

Compound Chromatograms

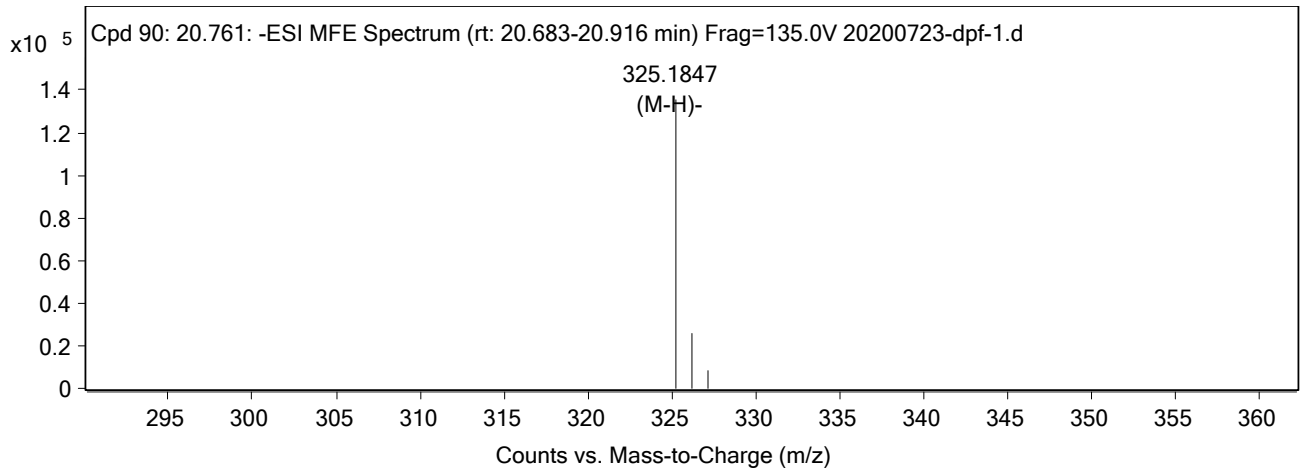




MFE MS Spectrum



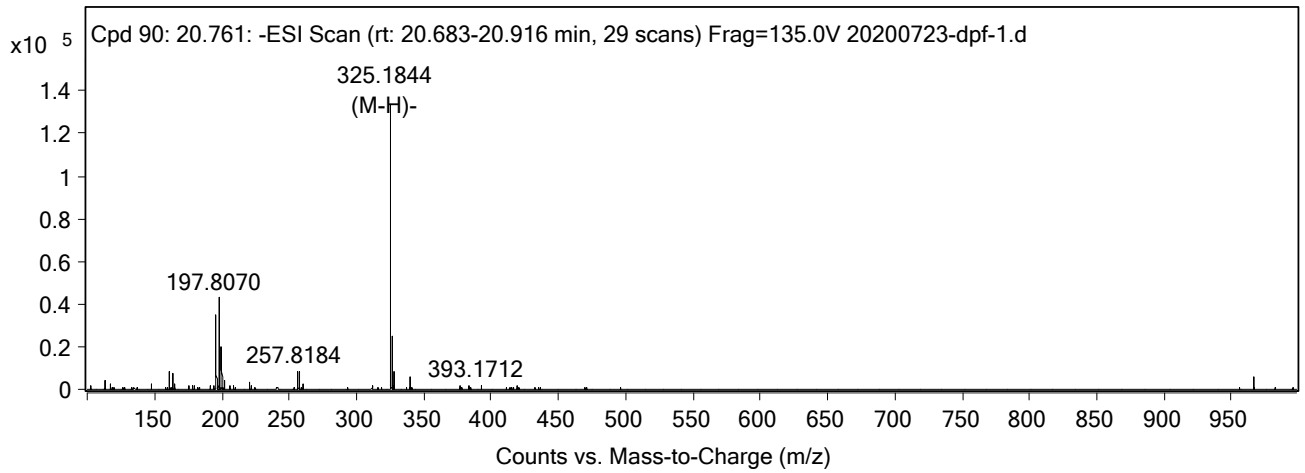
MFE MS Zoomed Spectrum



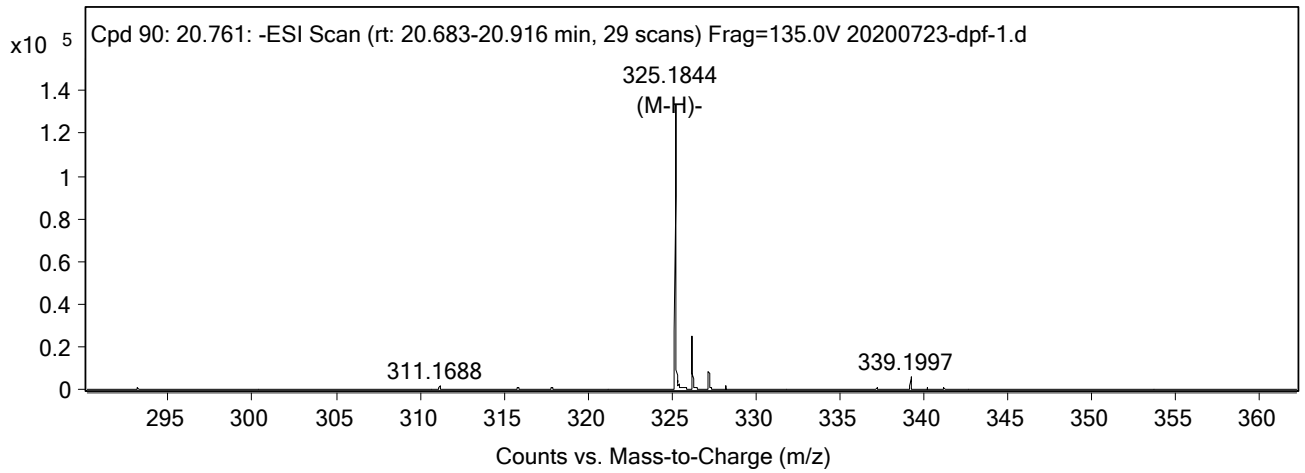
MS Spectrum Peak List

m/z	z	Abund	Ion
325.1847	-1	135031	(M-H)-
326.1876	-1	26112.17	(M-H)-
327.1844	-1	8575.39	(M-H)-

MS Spectrum

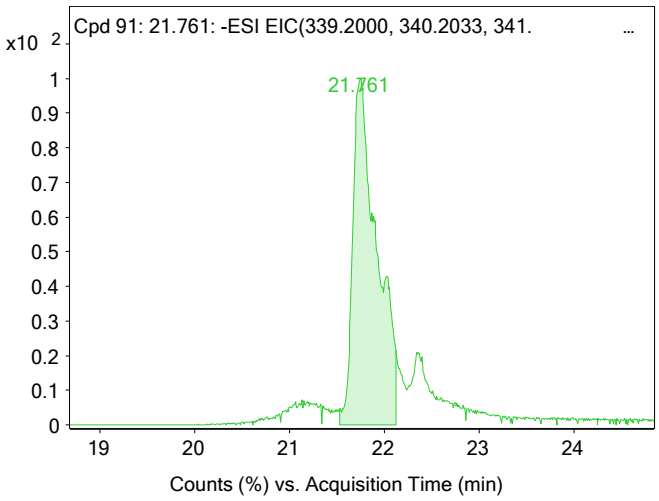


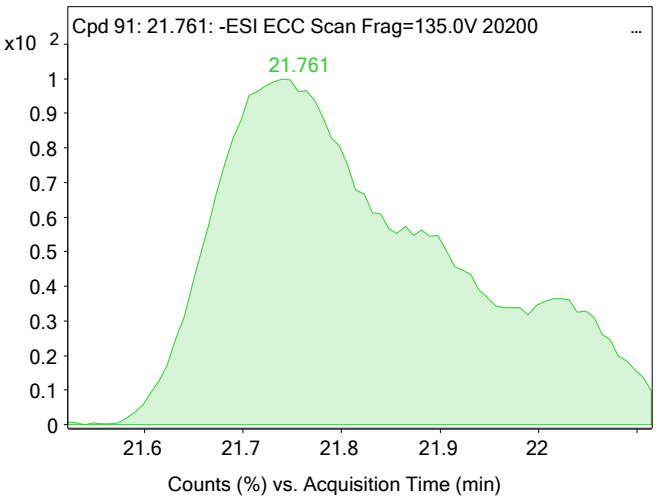
MS Zoomed Spectrum



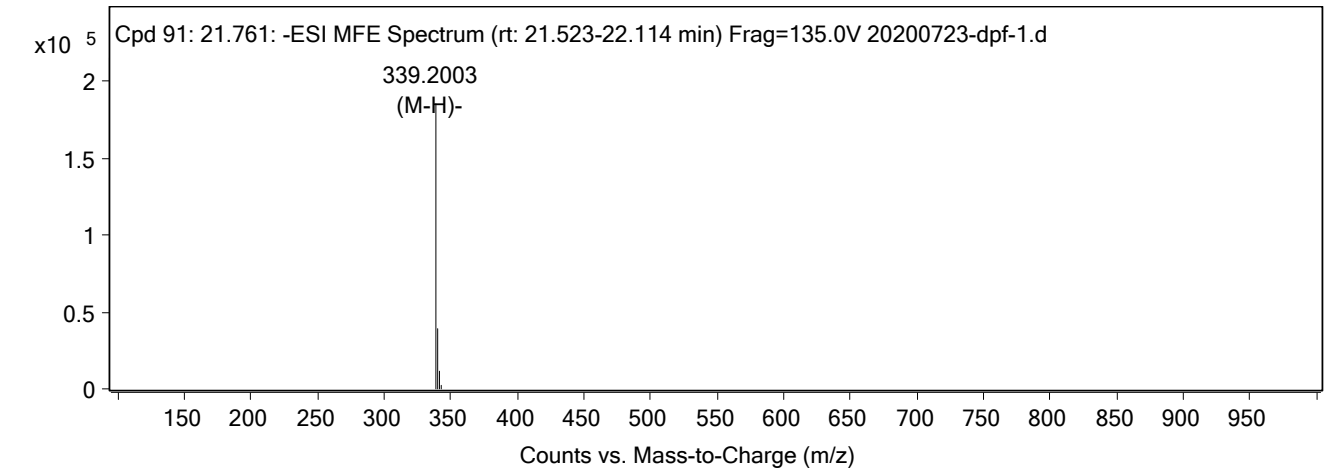
Compound Label	m/z	RT	Algorithm	Mass
Cpd 91: 21.761	339.2003	21.761	Find by Molecular Feature	340.2076

Compound Chromatograms

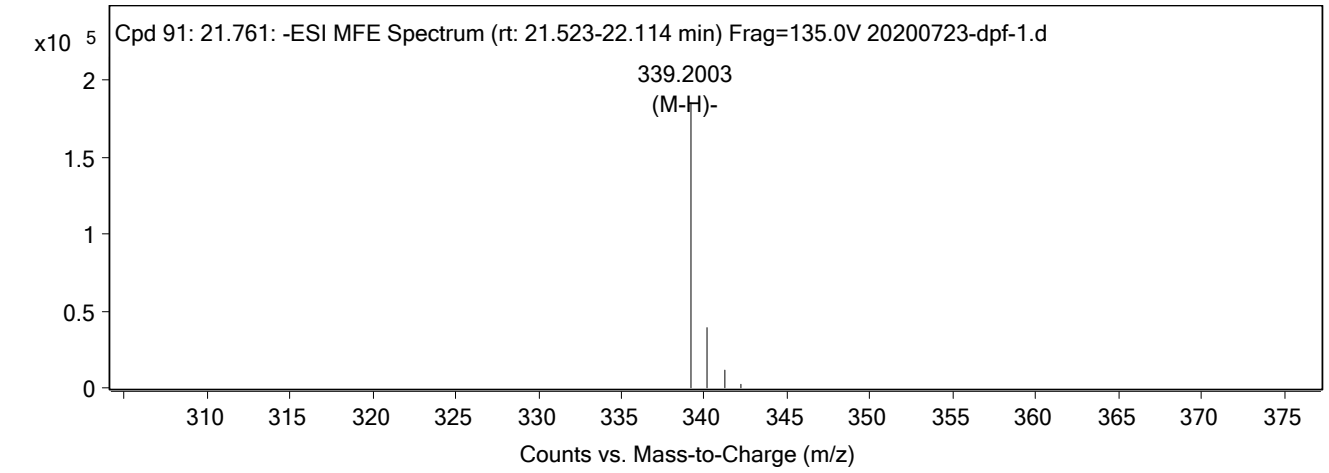




MFE MS Spectrum



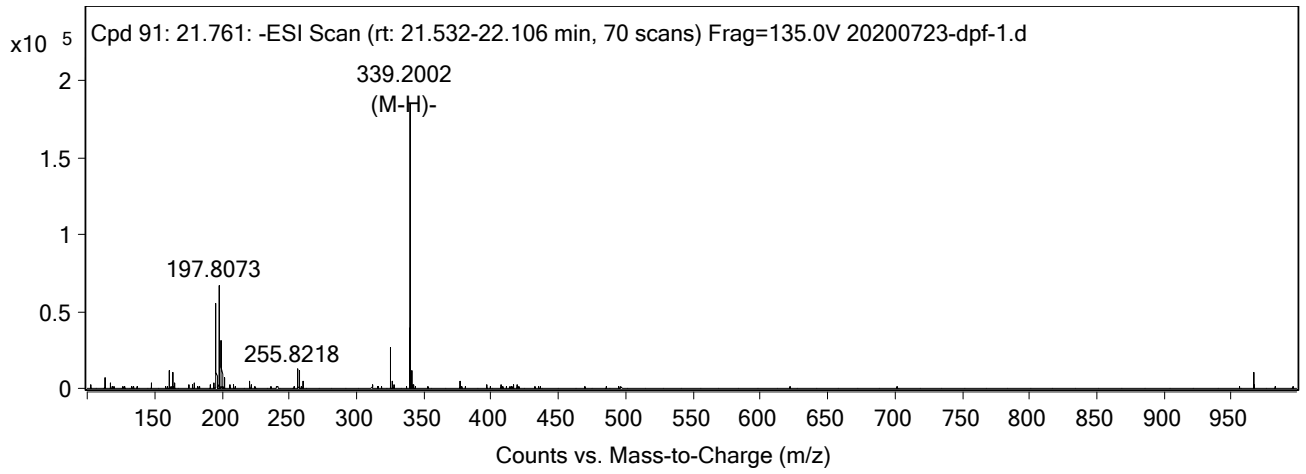
MFE MS Zoomed Spectrum



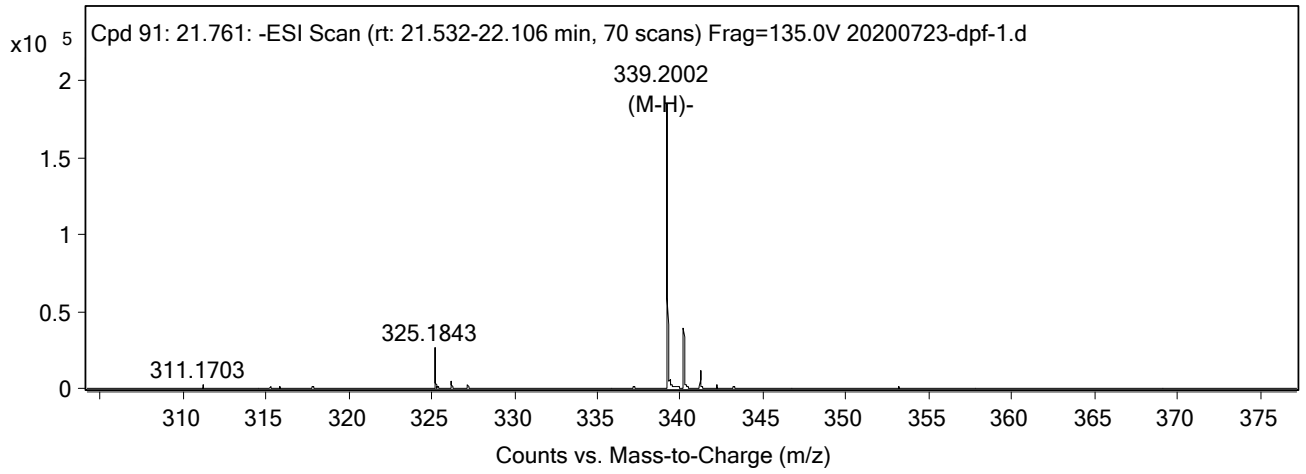
MS Spectrum Peak List

m/z	z	Abund	Ion
339.2003	-1	185840.8	(M-H)-
340.2034	-1	39558.89	(M-H)-
341.2002	-1	11857.62	(M-H)-
342.2013	-1	2213.63	(M-H)-

MS Spectrum

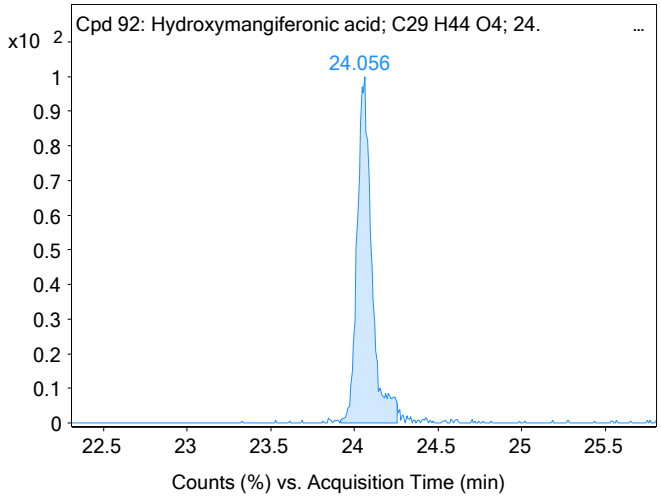


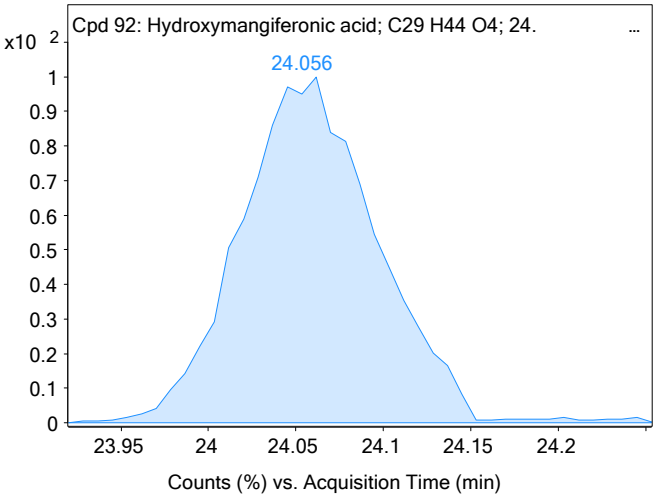
MS Zoomed Spectrum



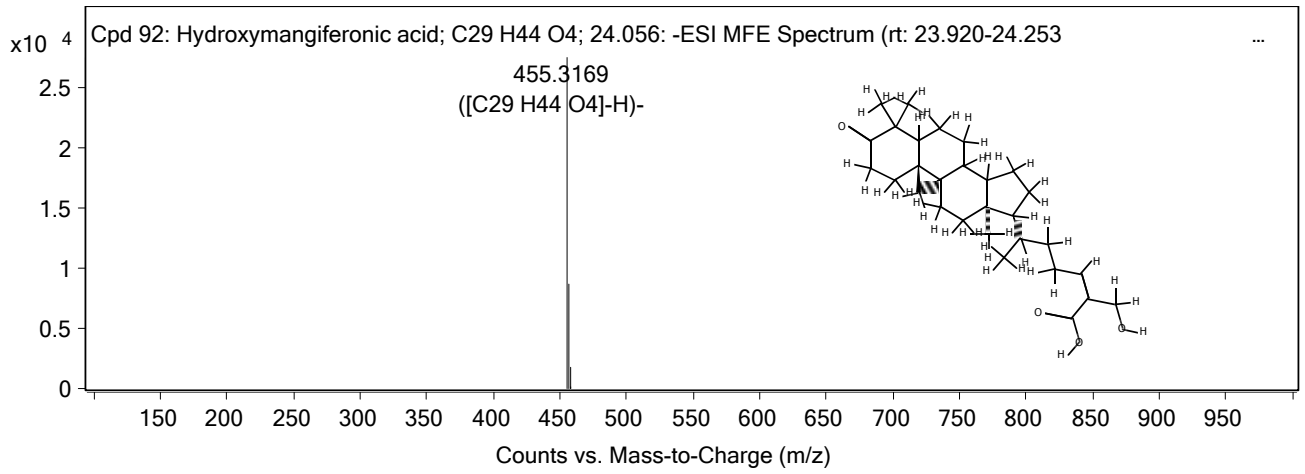
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 92: Hydroxymangiferonic acid; C29 H44 O4; 24.056	**Hydroxymangiferonic acid**	455.3169	24.056	Find by Molecular Feature	456.324

Compound Chromatograms

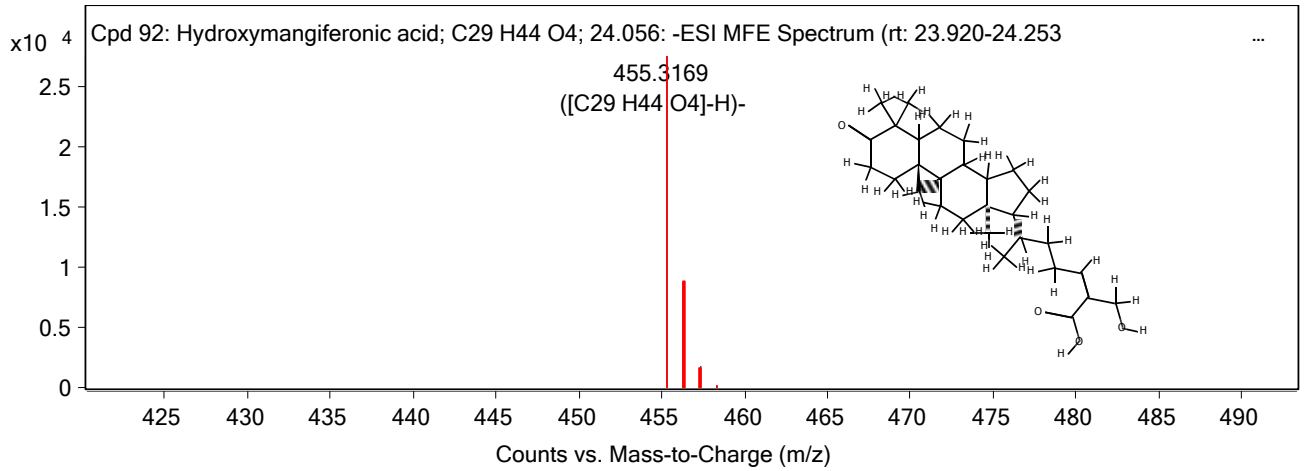




MFE MS Spectrum



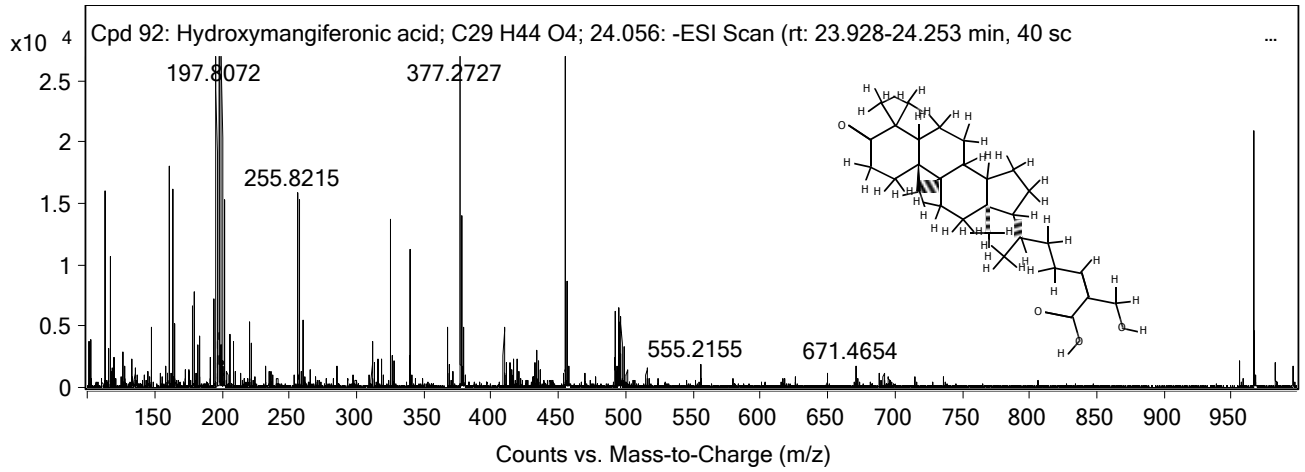
MFE MS Zoomed Spectrum



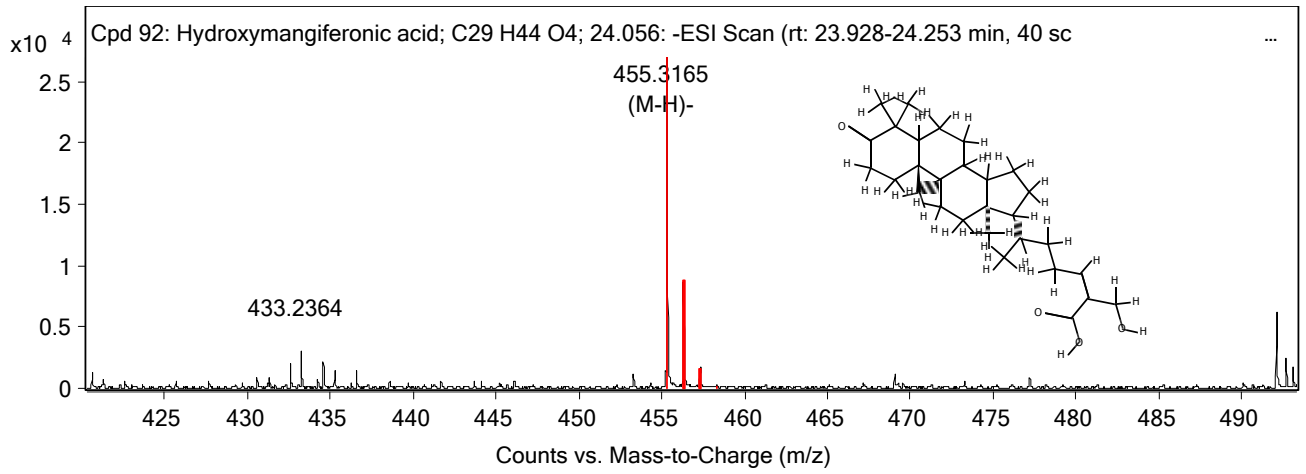
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
455.3169	-1	27504.92	C29 H44 O4	(M-H)-
456.32	-1	8710.52	C29 H44 O4	(M-H)-
457.3218	-1	1712.52	C29 H44 O4	(M-H)-
458.3249	-1	212.56	C29 H44 O4	(M-H)-

MS Spectrum



MS Zoomed Spectrum

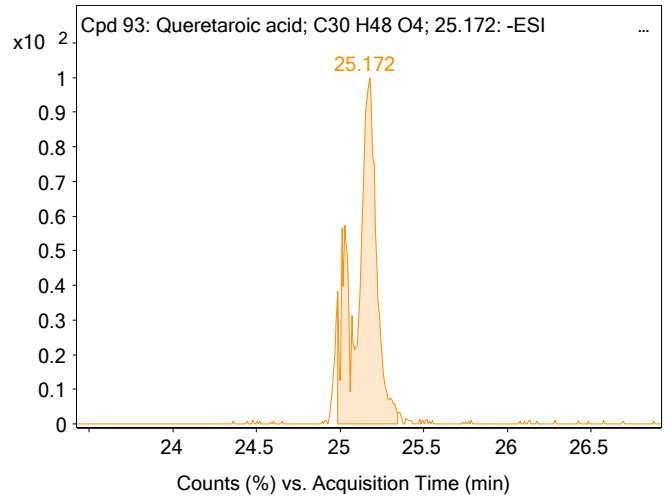


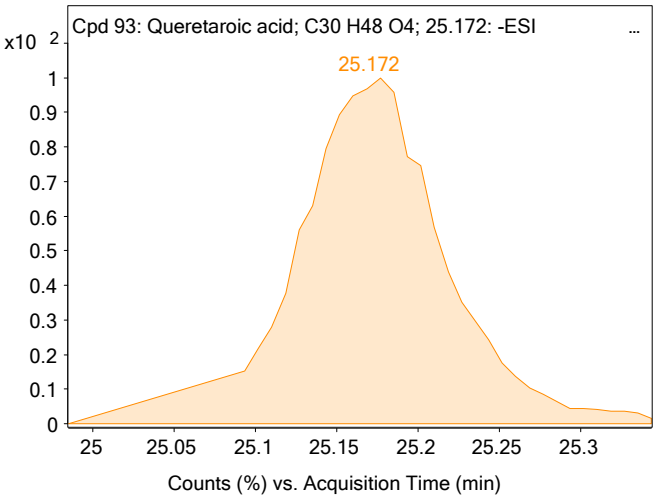
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Hydroxymangiferonic acid	24.056	C29 H44 O4		99.49	456.324	-0.04	(M-H)-
	Diosgenin acetate	24.056	C29 H44 O4		99.49	456.324	-0.04	(M-H)-
	Yamogenin acetate	24.056	C29 H44 O4		99.49	456.324	-0.04	(M-H)-
	Rutundanonic acid	24.056	C29 H44 O4		99.49	456.324	-0.04	(M-H)-

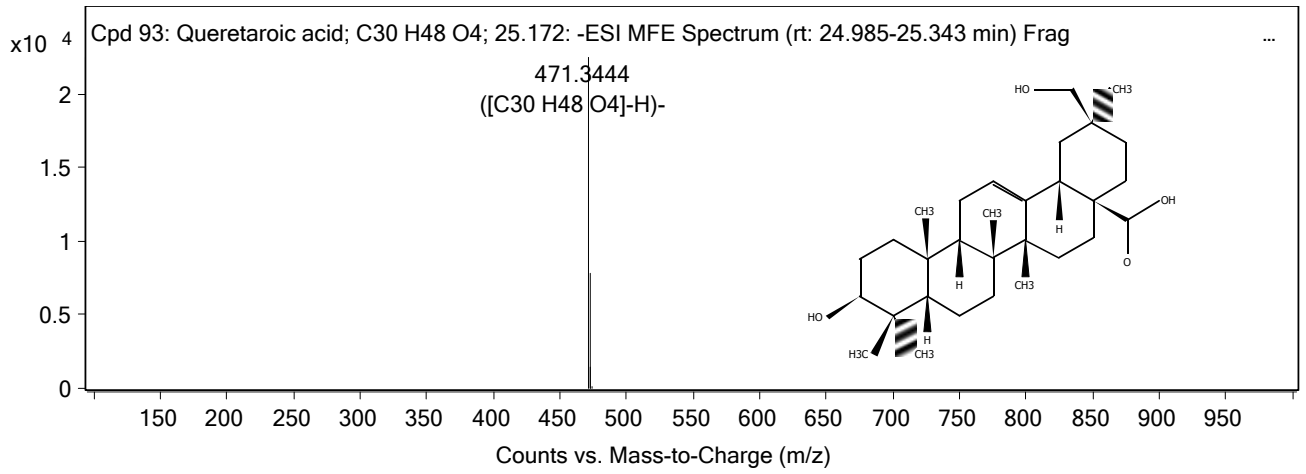
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 93: Queretaroic acid; C30 H48 O4; 25.172	**Queretaroic acid**	471.3444	25.172	Find by Molecular Feature	472.3515

Compound Chromatograms

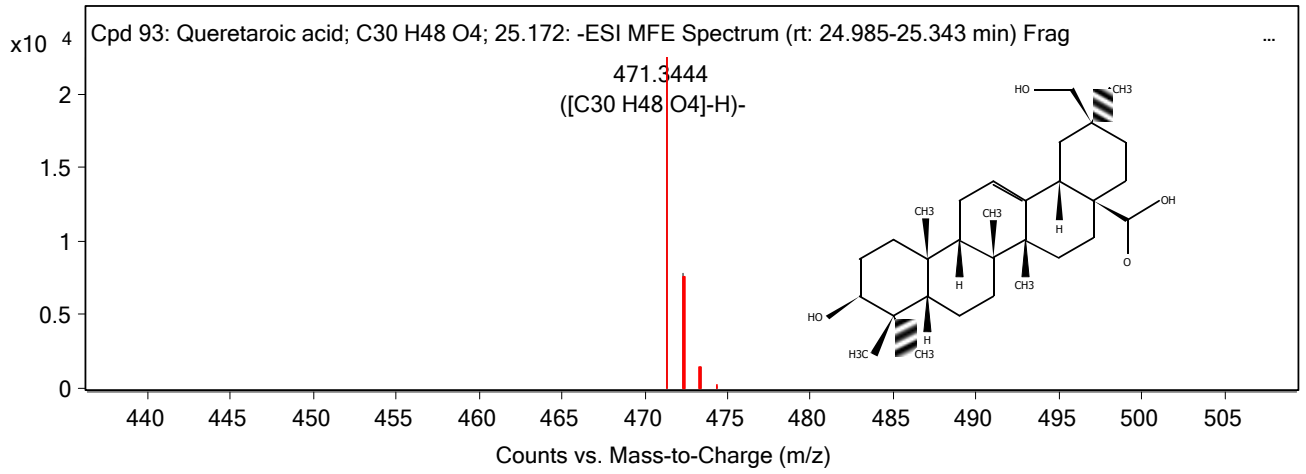




MFE MS Spectrum



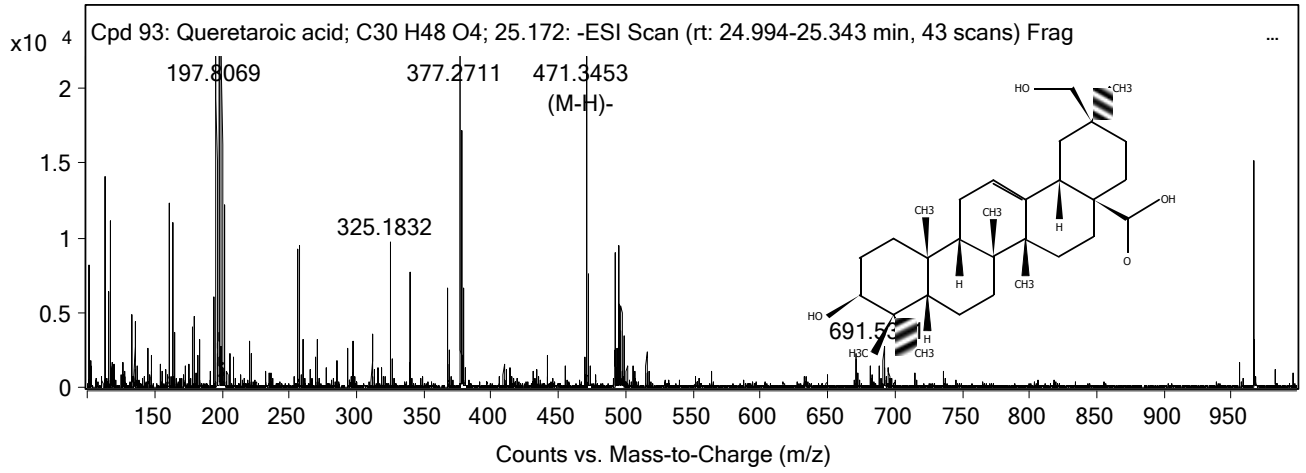
MFE MS Zoomed Spectrum



MS Spectrum Peak List

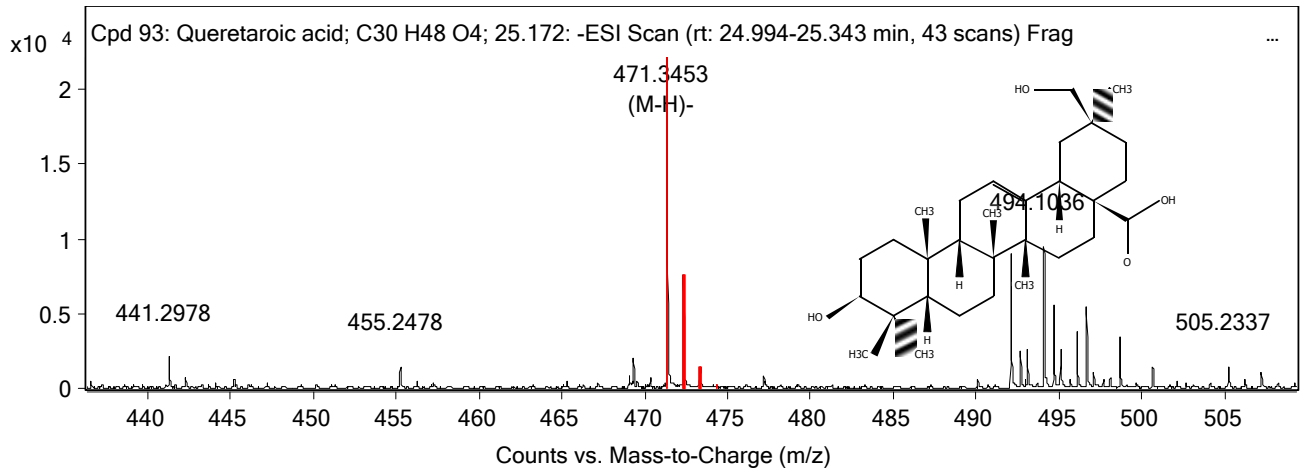
m/z	z	Abund	Formula	Ion
471.3444	-1	22516.91	C30 H48 O4	(M-H)-
472.3474	-1	7835.27	C30 H48 O4	(M-H)-
473.35	-1	1428.31	C30 H48 O4	(M-H)-
474.3512	-1	100	C30 H48 O4	(M-H)-

MS Spectrum



MS Zoomed Spectrum

Qualitative Compound Identification Report

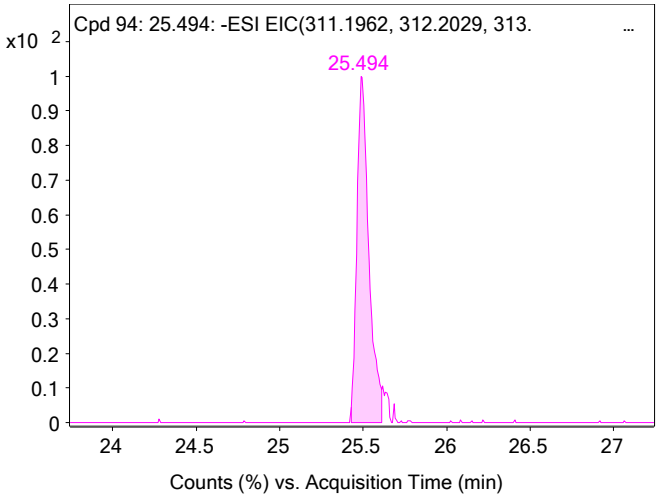


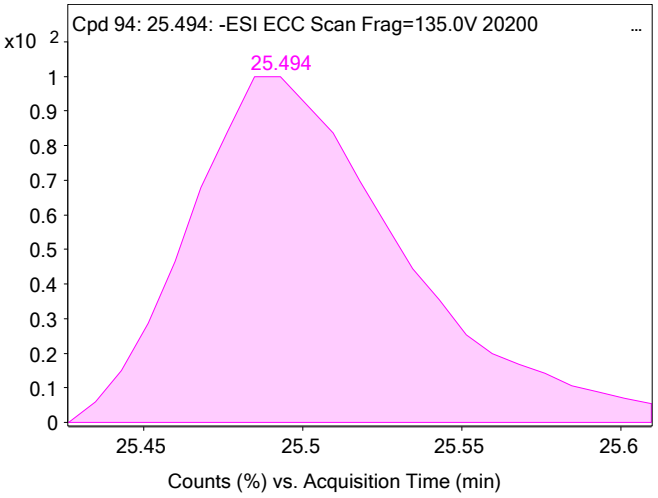
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Queretaroic acid	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	Rosacea acid A	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	Saikogenin D	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	Saikogenin F	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	Saikogenin G	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	Salaspermic acid	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	Siaresinolic acid	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	Sumaresinolic acid	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	3beta,15alpha,23-Trihydroxy-olean-12-en-16-one	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-
	Triptotin C	25.172	C30 H48 O4		76.76	472.3515	3.71	(M-H)-

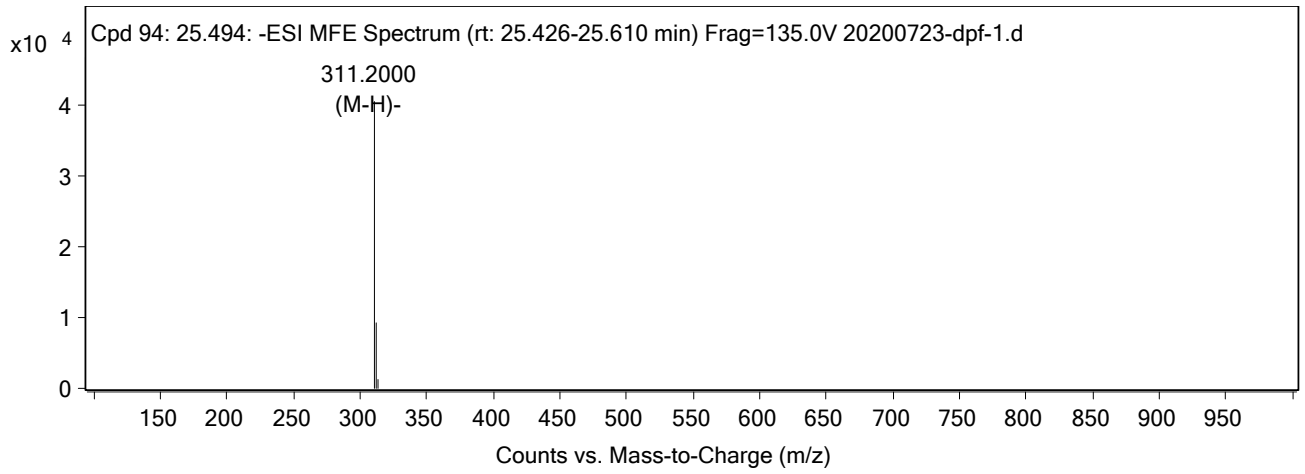
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 94: 25.494	311.2	25.494	Find by Molecular Feature	312.2073

Compound Chromatograms

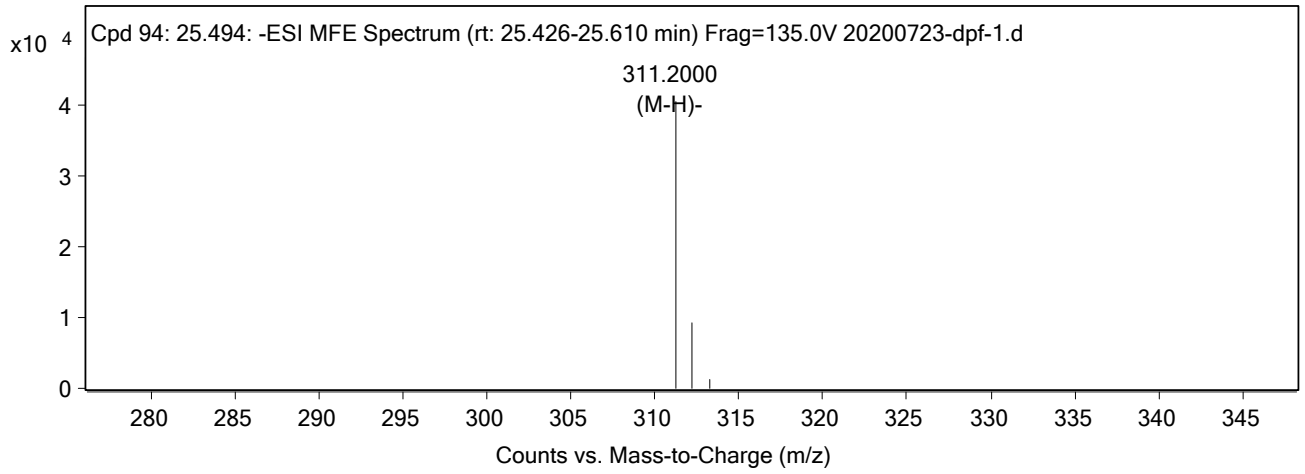




MFE MS Spectrum



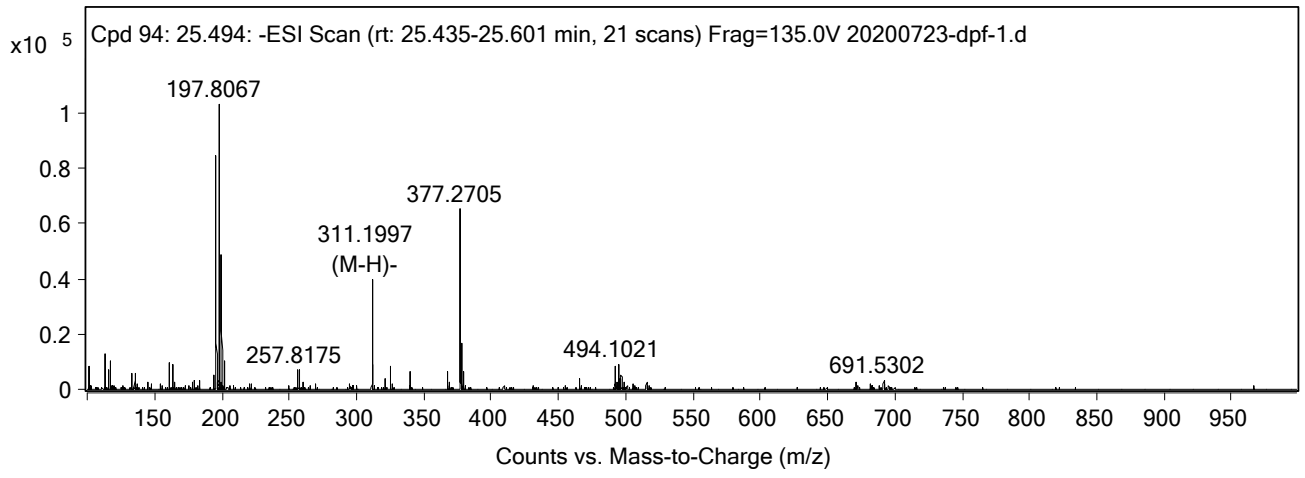
MFE MS Zoomed Spectrum



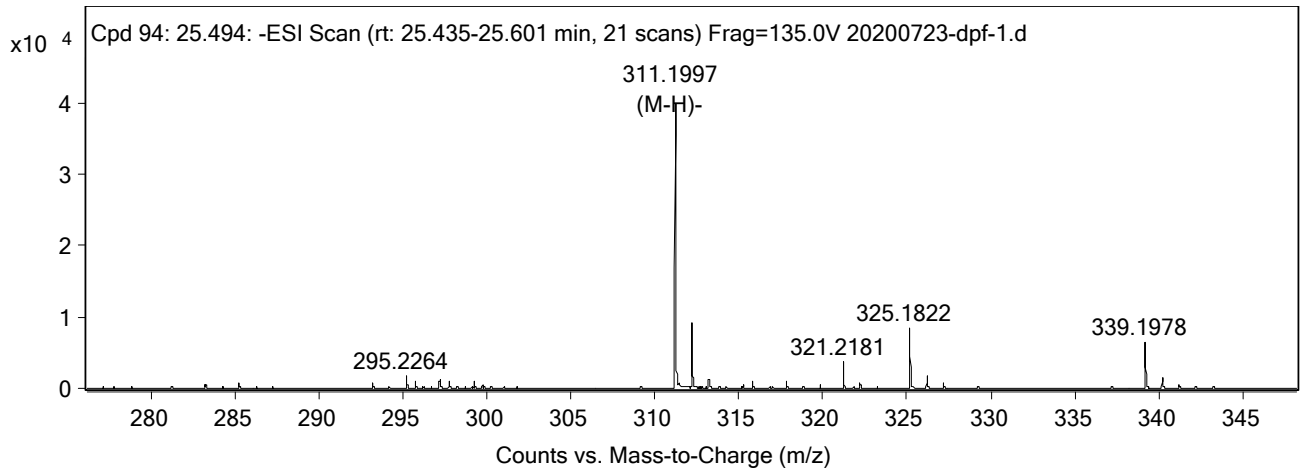
MS Spectrum Peak List

m/z	z	Abund	Ion
311.2	-1	40320.86	(M-H)-
312.2037	-1	9253.72	(M-H)-
313.2097	-1	1140.6	(M-H)-

MS Spectrum

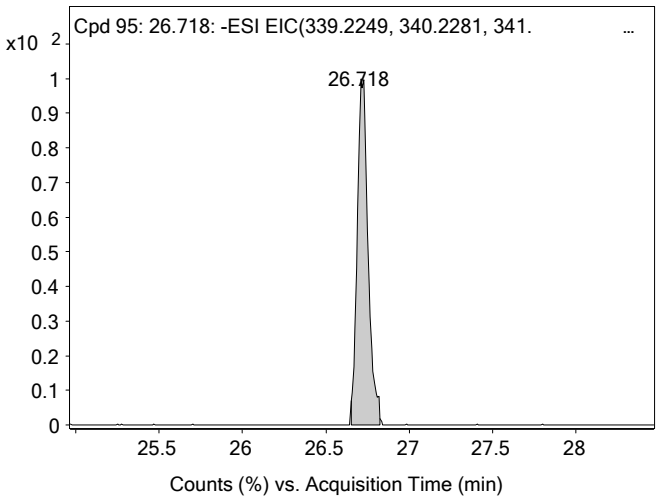


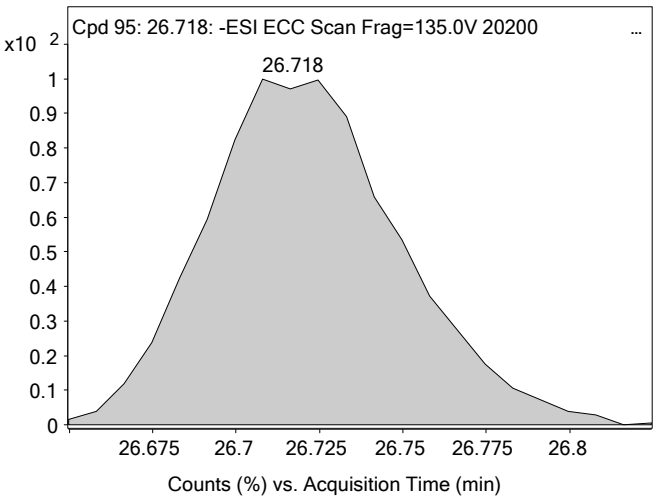
MS Zoomed Spectrum



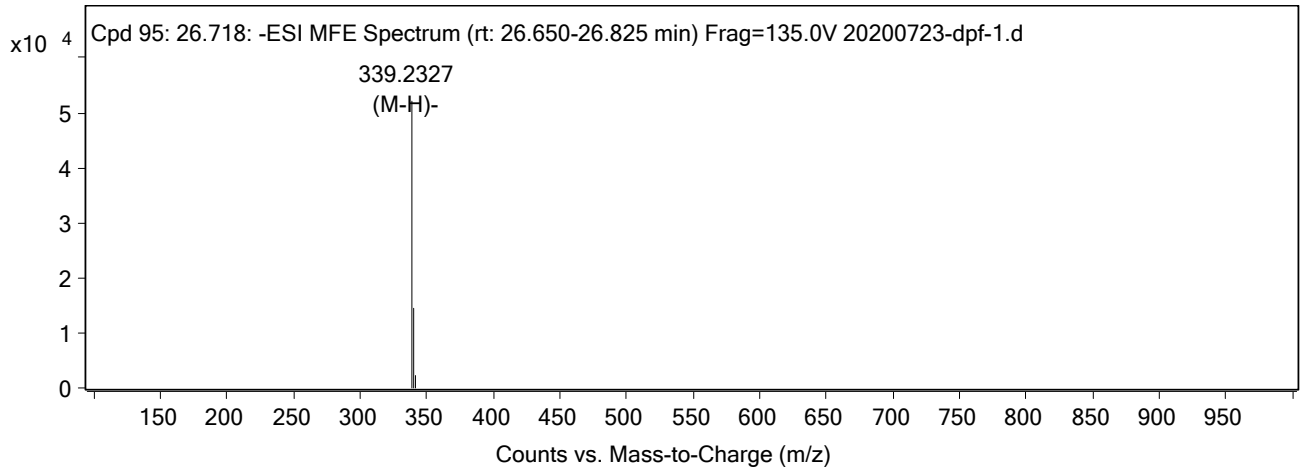
Compound Label	m/z	RT	Algorithm	Mass
Cpd 95: 26.718	339.2327	26.718	Find by Molecular Feature	340.2399

Compound Chromatograms

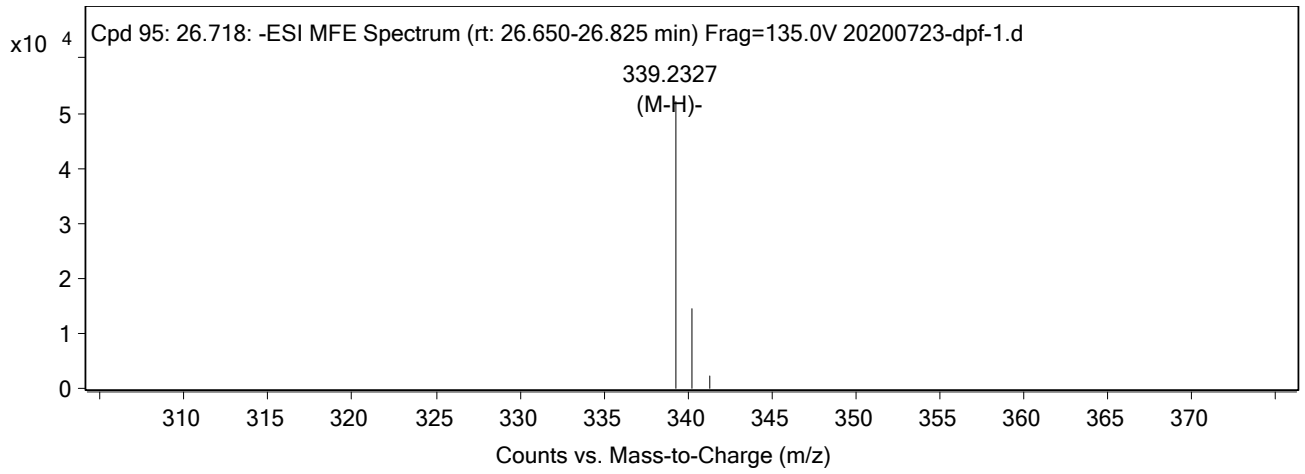




MFE MS Spectrum



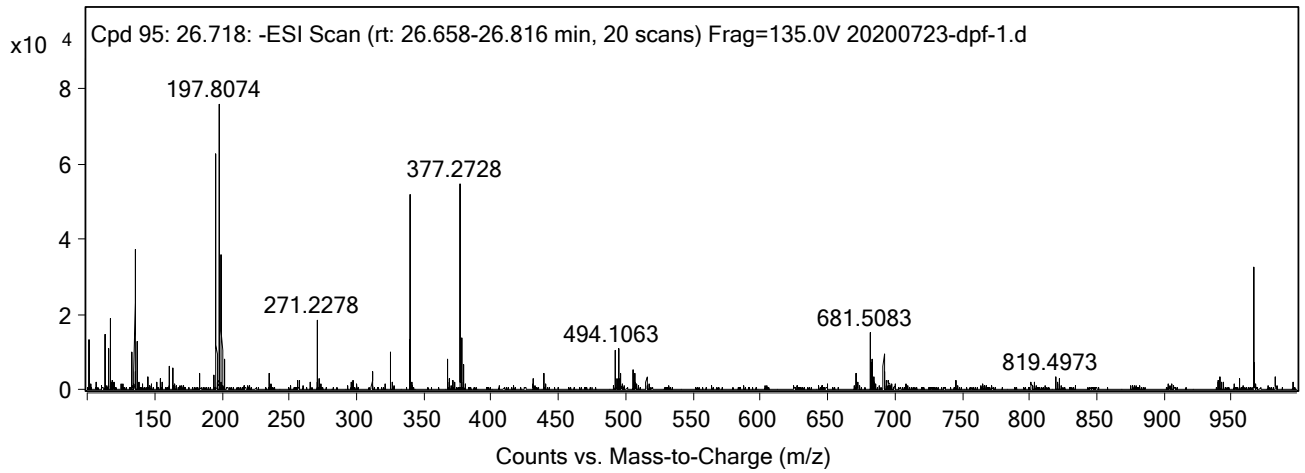
MFE MS Zoomed Spectrum



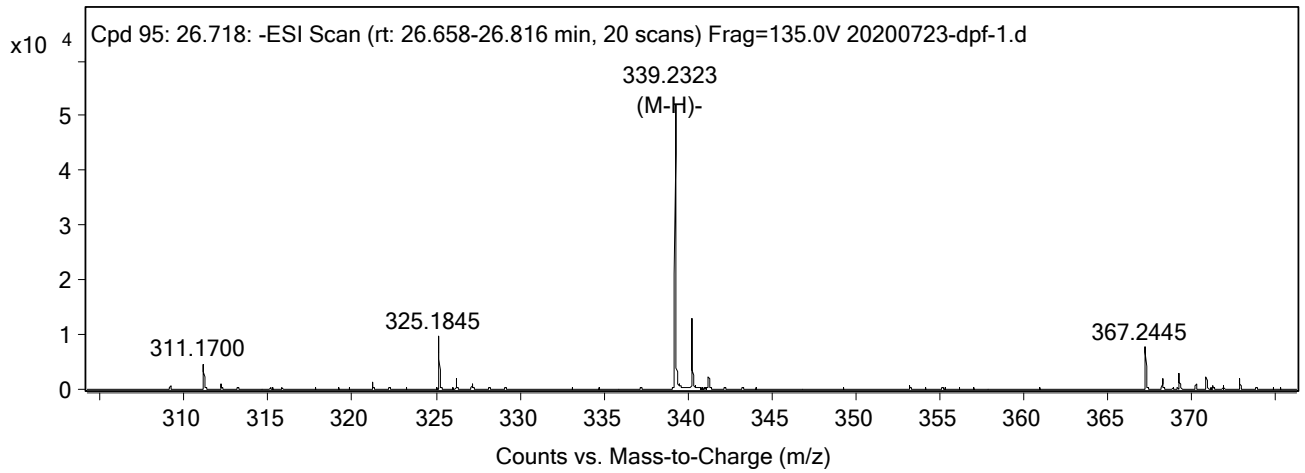
MS Spectrum Peak List

m/z	z	Abund	Ion
339.2327	-1	52162.85	(M-H)-
340.2359	-1	14584.36	(M-H)-
341.2397	-1	2386.8	(M-H)-

MS Spectrum

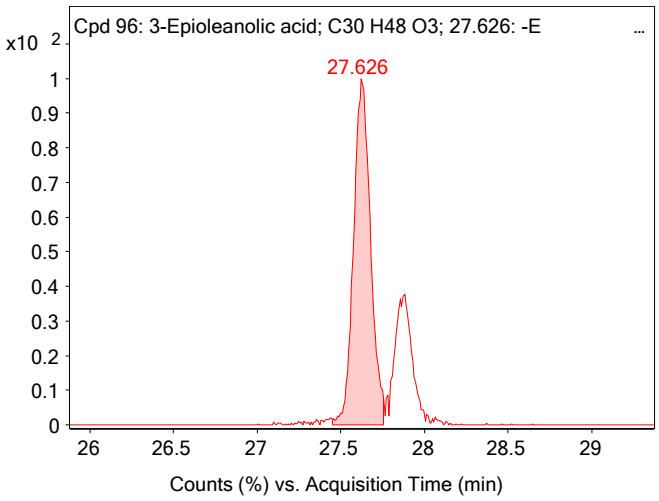


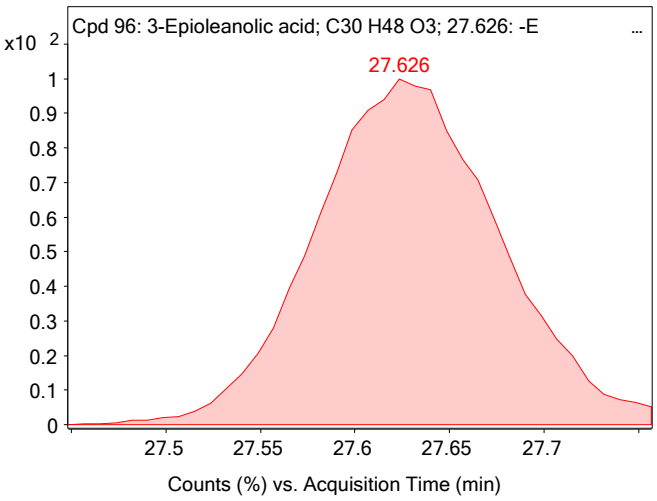
MS Zoomed Spectrum



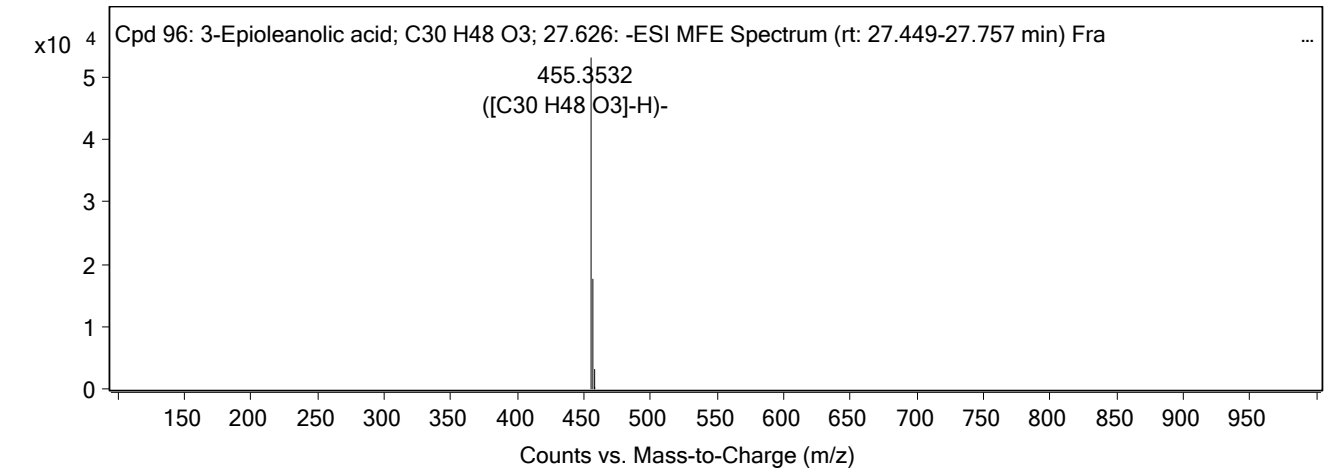
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 96: 3-Epioleanolic acid; C30 H48 O3; 27.626	**3-Epioleanolic acid**	455.3532	27.626	Find by Molecular Feature	456.3604

Compound Chromatograms

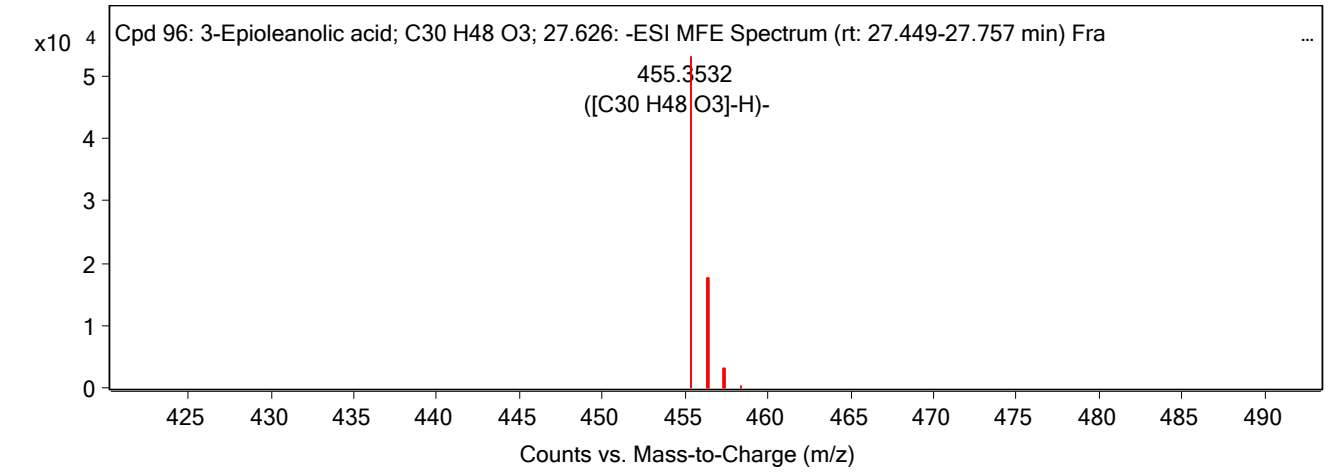




MFE MS Spectrum



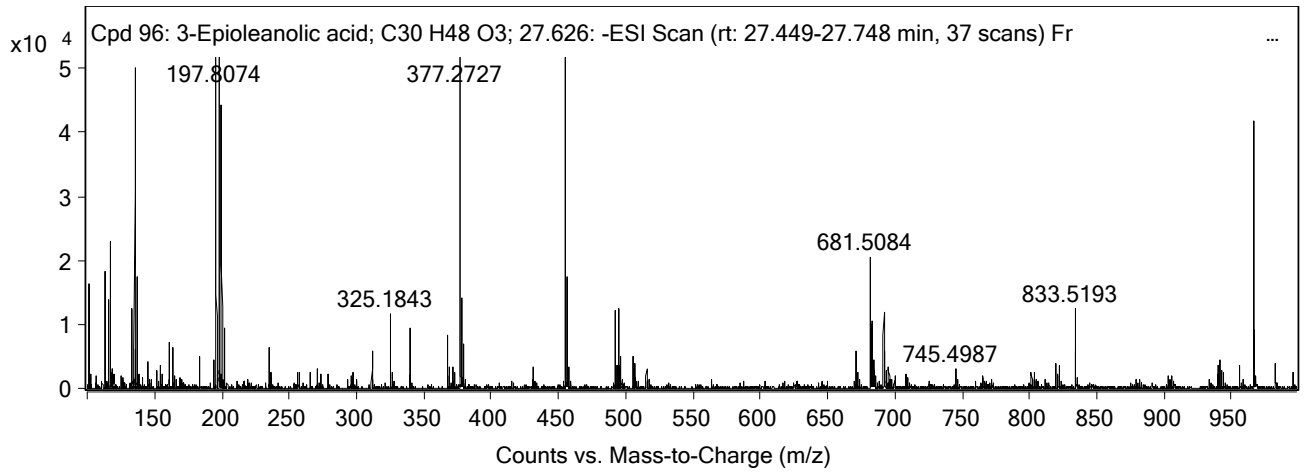
MFE MS Zoomed Spectrum



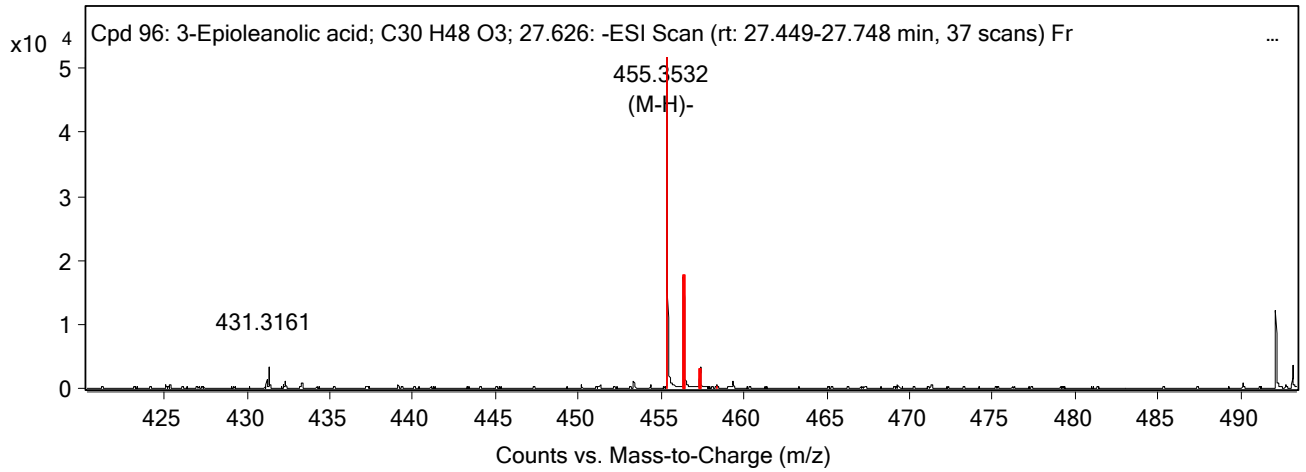
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
455.3532	-1	53175.3	C30 H48 O3	(M-H)-
456.3563	-1	17610.06	C30 H48 O3	(M-H)-
457.359	-1	3281.61	C30 H48 O3	(M-H)-
458.3603	-1	443.72	C30 H48 O3	(M-H)-

MS Spectrum



MS Zoomed Spectrum

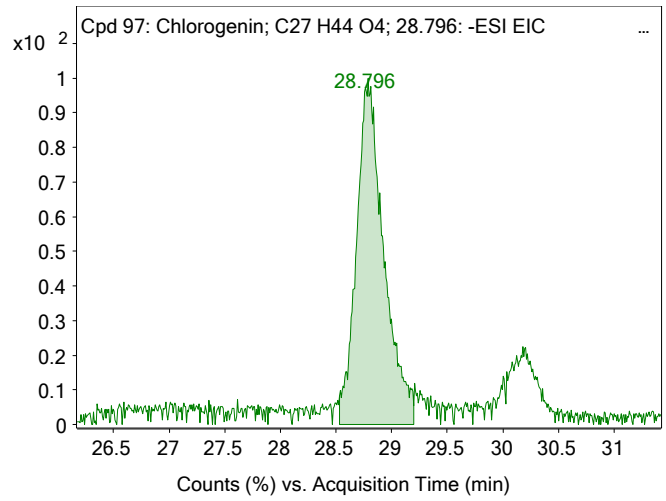


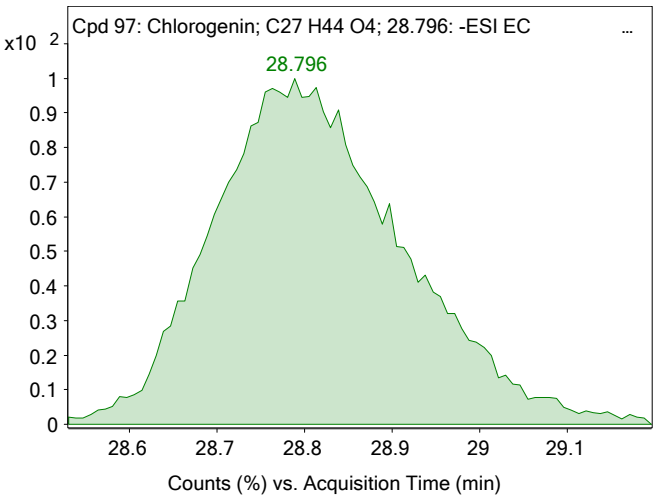
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	3-Epioleanolic acid	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	Ganoderic acid Z	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	3beta,16beta-Dihydroxy-olean-12-en-15-one	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	3-Epikatonic acid	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	(24Z)-3beta,27-Dihydroxy-7,24-titucalladien-21-al	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	Bryonolic acid	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	Betulinic acid	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	3beta,15alpha-Dihydroxy-olean-12-en-16-one	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	Friedelan-1,3-dion-7alpha-ol	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-
	Eriocarpin A	27.626	C30 H48 O3		99.82	456.3604	-0.01	(M-H)-

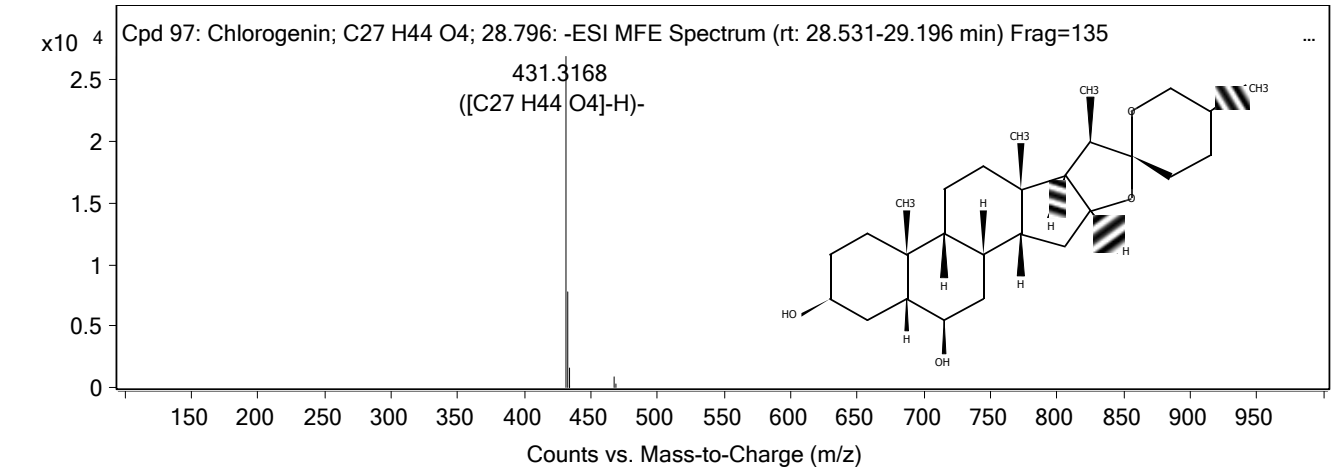
Compound Label	Name	*m/z*	RT	Algorithm	Mass
Cpd 97: Chlorogenin; C27 H44 O4; 28.796	**Chlorogenin**	431.3168	28.796	Find by Molecular Feature	432.324

Compound Chromatograms

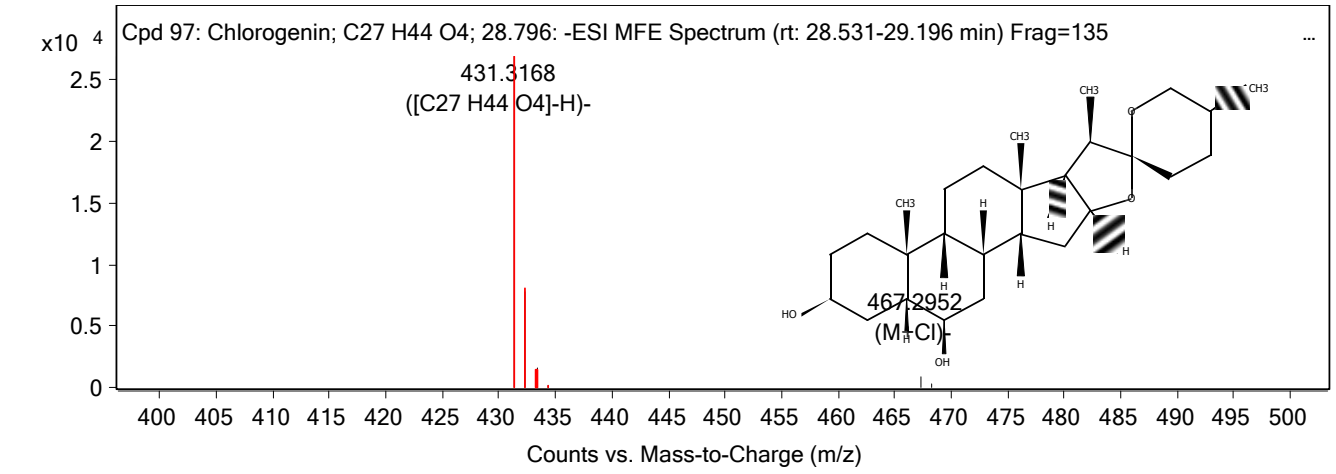




MFE MS Spectrum



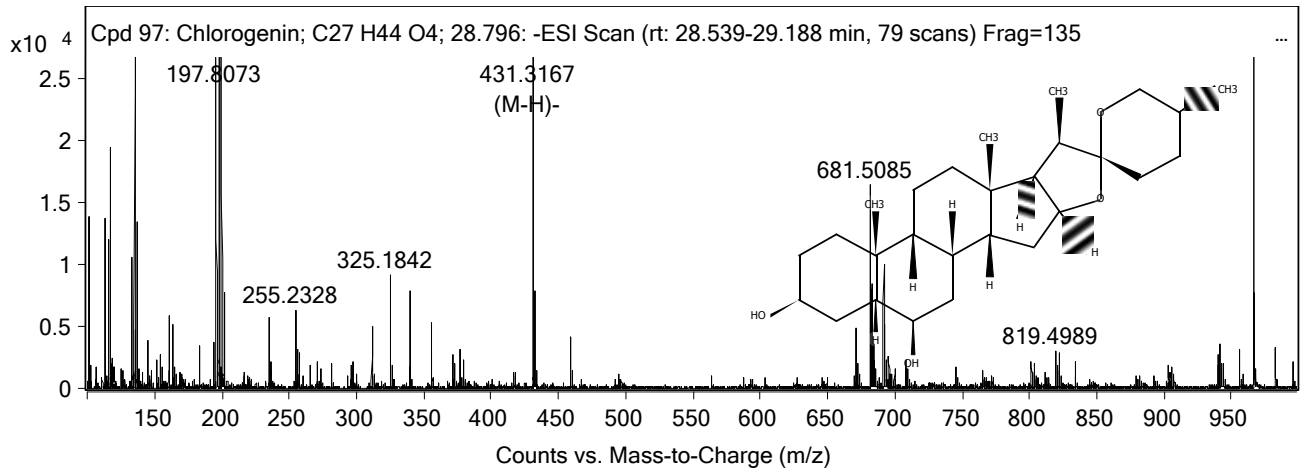
MFE MS Zoomed Spectrum



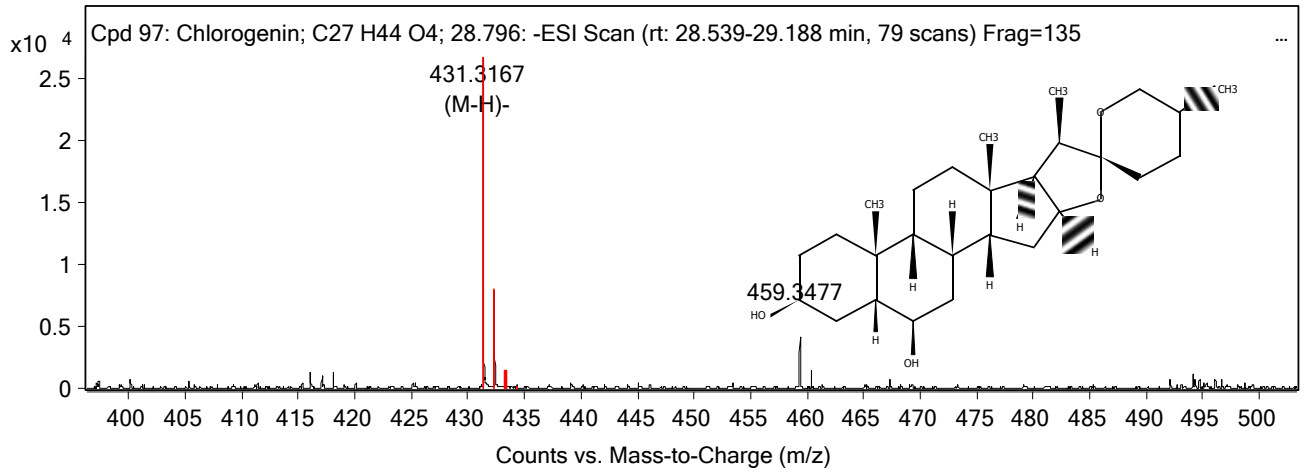
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
431.3168	-1	26923.06	C27 H44 O4	(M-H)-
432.3202	-1	7754.14	C27 H44 O4	(M-H)-
433.3232	-1	1543.56	C27 H44 O4	(M-H)-
434.3242	-1	113.71	C27 H44 O4	(M-H)-
467.2952	-1	858.44		(M+Cl)-
468.2903	-1	275.4		(M+Cl)-

MS Spectrum



MS Zoomed Spectrum

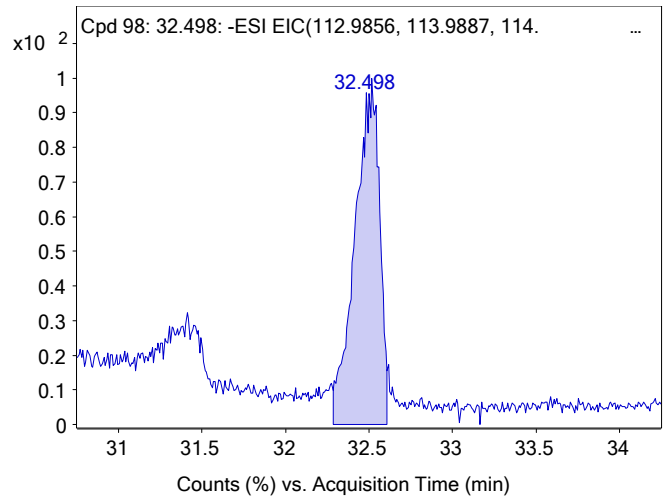


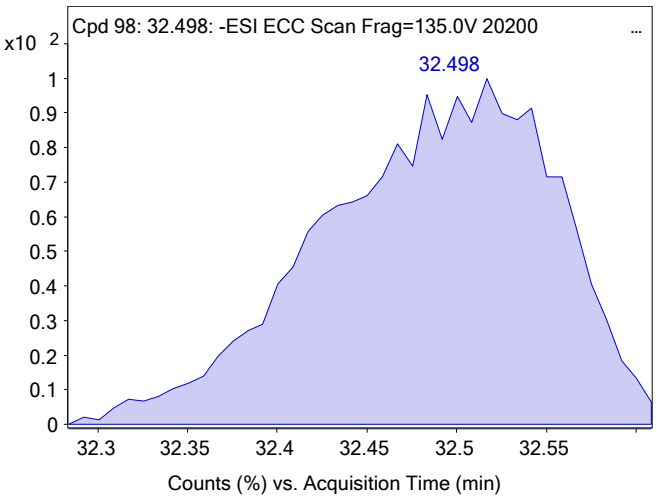
Identification Hit Table

Best Hit	Compound Name	RT	Formula	Notes	Match Score	Mass	Difference	Ion Species
✓	Chlorogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	Cordylagenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	Isorhodeasapogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	12-Epirockogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	Gitogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	Rockogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	Yonogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	Rhodeasapogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	Epirockogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-
	Markogenin	28.796	C27 H44 O4		99.64	432.324	-0.08	(M-H)-

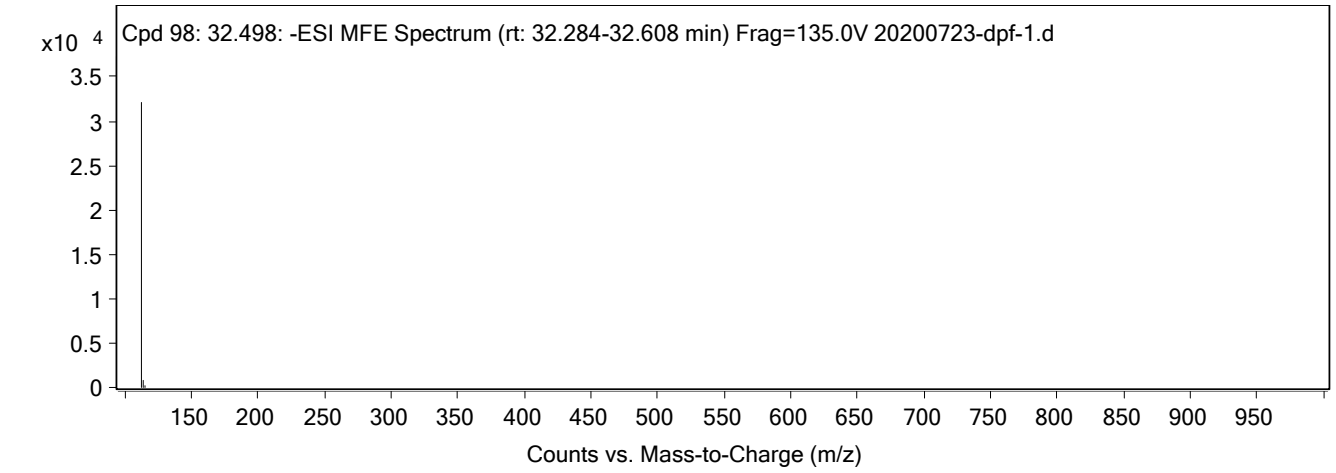
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 98: 32.498	112.9856	32.498	Find by Molecular Feature	113.9929

Compound Chromatograms

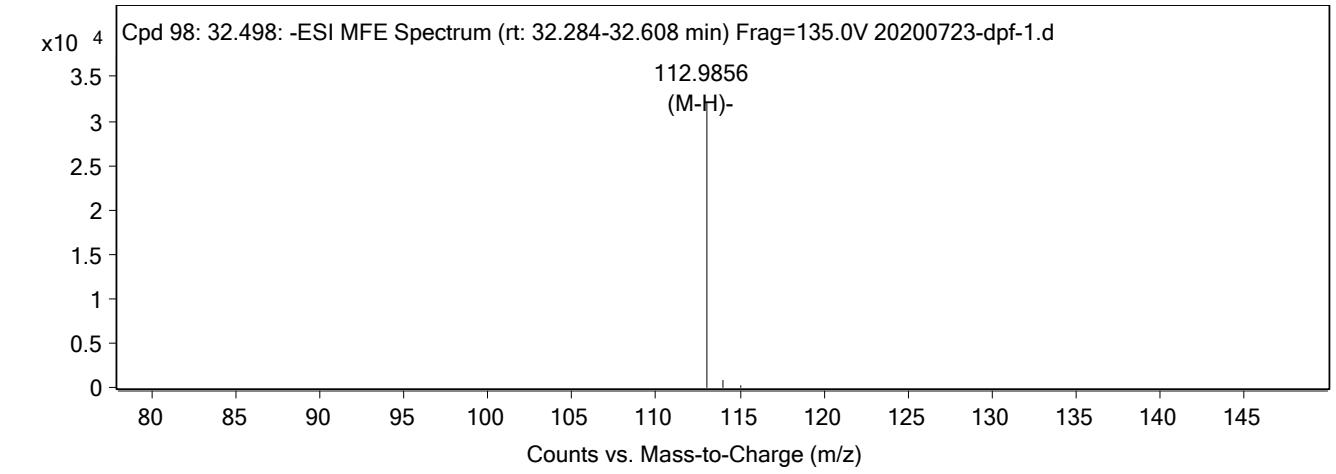




MFE MS Spectrum



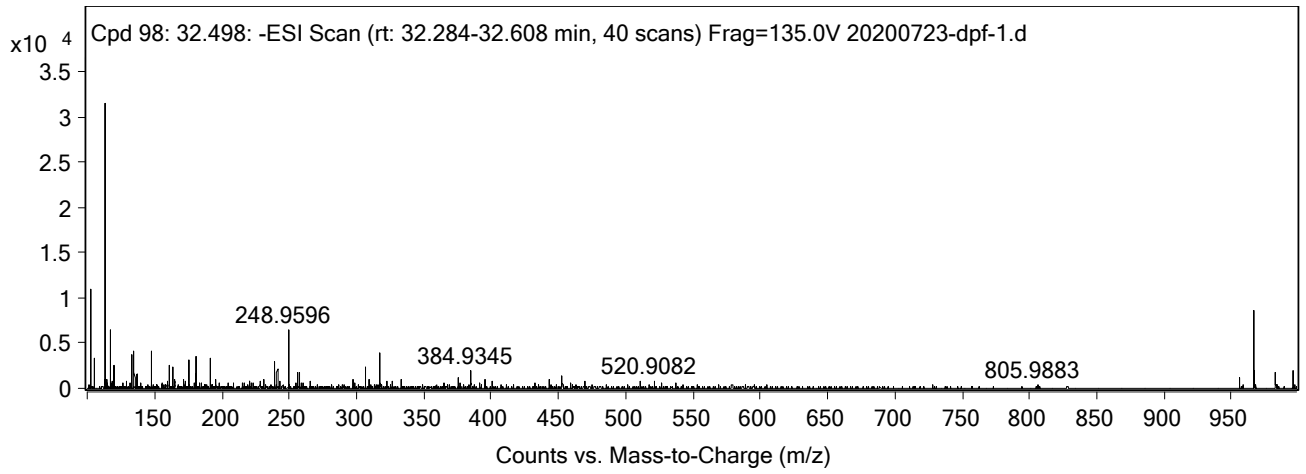
MFE MS Zoomed Spectrum



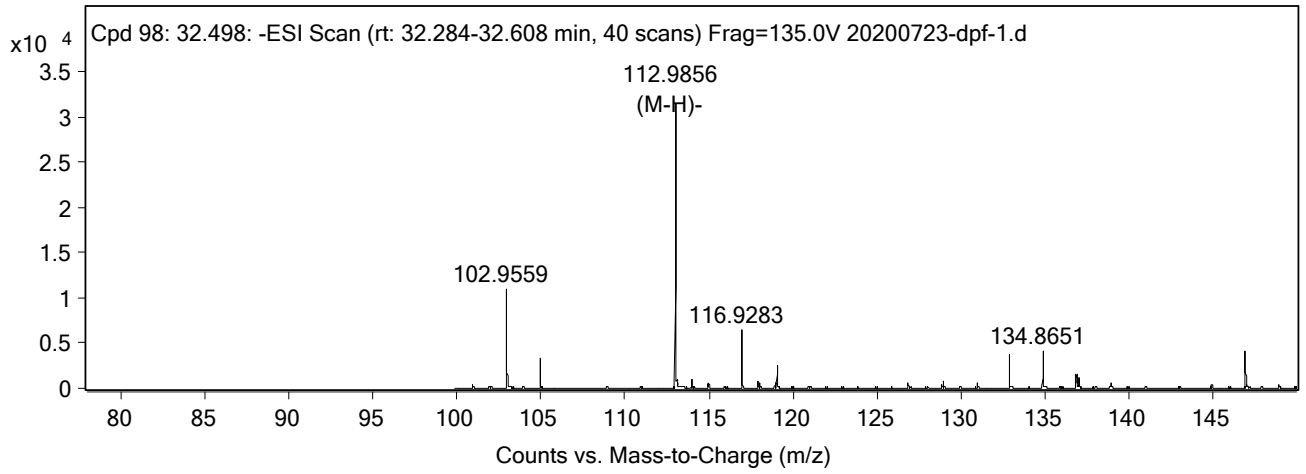
MS Spectrum Peak List

m/z	z	Abund	Ion
112.9856	-1	32161.03	(M-H)-
113.9893	-1	889.21	(M-H)-
114.9909	-1	265.34	(M-H)-

MS Spectrum



MS Zoomed Spectrum



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