

Qualitative Compound Report

Data File	SNP1.d	Sample Name	SNP1
Sample Type	Sample	Position	P1-B8
Instrument Name	QTOF	User Name	
Acq Method	metabolite_ESI_+VE_MSMS.m	Acquired Time	7/4/2025 6:36:30 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

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

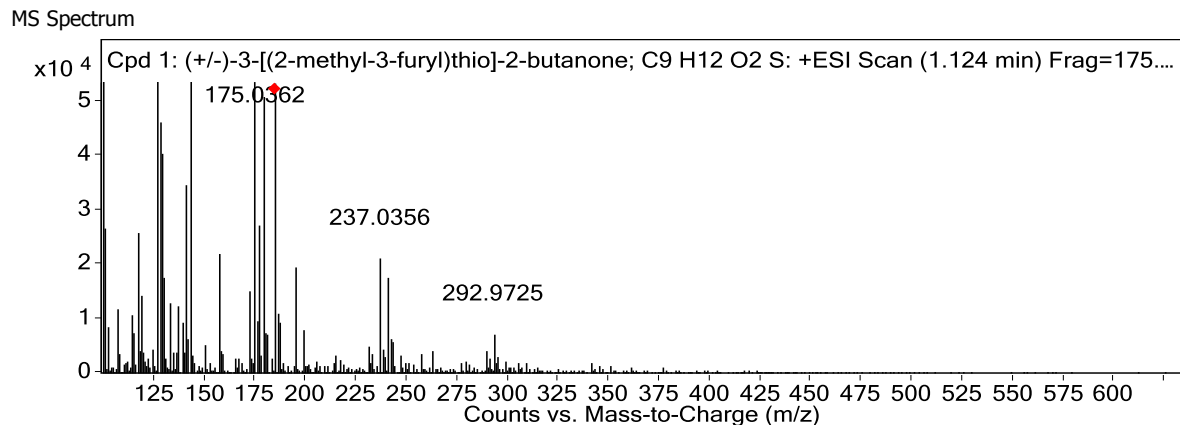
Compound Table

Compound Label	RT	Mass	Abund	Name	Formula	MFG Formula	DB Formula	DB Diff (ppm)	Hits (DB)
Cpd 1: (+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone; C9 H12 O2 S	1.138	184.0575		(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	C9 H12 O2 S	C9 H12 O2 S	C9 H12 O2 S	-8.99	1
Compound 2	1.212								
Cpd 3: 4-Amino-2,6-dinitrotoluene; C7 H7 N3 O4	1.299	197.0436		4-Amino-2,6-dinitrotoluene	C7 H7 N3 O4	C7 H7 N3 O4	C7 H7 N3 O4	0.27	10
Cpd 4: 3beta,6beta-Dihydroxynortropane; C7 H13 N O2	1.44	143.0944		3beta,6beta-Dihydroxynortropane	C7 H13 N O2	C7 H13 N O2	C7 H13 N O2	1.68	3
Compound 5	1.444								
Cpd 6: 3beta,6beta-Dihydroxynortropane; C7 H13 N O2	1.741	143.0944	473597	3beta,6beta-Dihydroxynortropane	C7 H13 N O2	C7 H13 N O2	C7 H13 N O2	1.72	3
Compound 7	1.886								
Cpd 8: 3beta,6beta-Dihydroxynortropane; C7 H13 N O2	2.052	143.0941	91187	3beta,6beta-Dihydroxynortropane	C7 H13 N O2	C7 H13 N O2	C7 H13 N O2	3.67	3
Cpd 9: Benzo[a]fluorene; C17 H12	2.371	216.0964	198698	Benzo[a]fluorene	C17 H12	C17 H12	C17 H12	-11.63	5
Cpd 10: Pirimicarb; C11 H18 N4 O2	2.863	238.1402		Pirimicarb	C11 H18 N4 O2	C11 H18 N4 O2	C11 H18 N4 O2	11.86	1
Compound 11	3.52								
Cpd 12: 4-Prenyldihydropinosylvin; C19 H22 O2	3.865	282.1655	60849	4-Prenyldihydropinosylvin	C19 H22 O2	C19 H22 O2	C19 H22 O2	-12.39	5
Cpd 13: 2-Dodecylbenzenesulfonic acid; C18 H30 O3 S	4.046	326.1919	795122	2-Dodecylbenzenesulfonic acid	C18 H30 O3 S	C18 H30 O3 S	C18 H30 O3 S	-0.97	10
Cpd 14: 2-Dodecylbenzenesulfonic acid; C18 H30 O3 S	4.434	326.1914		2-Dodecylbenzenesulfonic acid	C18 H30 O3 S	C18 H30 O3 S	C18 H30 O3 S	0.56	10
Cpd 15: Paramethasone; C22 H29 F O5	4.493	392.1998		Paramethasone	C22 H29 F O5	C22 H29 F O5	C22 H29 F O5	0.29	10
Cpd 16: Paramethasone; C22 H29 F O5	4.85	392.1993		Paramethasone	C22 H29 F O5	C22 H29 F O5	C22 H29 F O5	1.57	10
Cpd 17: Flurandrenolide; C24 H33 F O6	4.889	436.2257		Flurandrenolide	C24 H33 F O6	C24 H33 F O6	C24 H33 F O6	0.92	5
Cpd 18: Lucidenic acid A; C27 H38 O6	5.198	458.2701		Lucidenic acid A	C27 H38 O6	C27 H38 O6	C27 H38 O6	-7.03	3
Cpd 19: Progeldanamycin; C27 H41 N O6	5.239	475.2958		Progeldanamycin	C27 H41 N O6	C27 H41 N O6	C27 H41 N O6	-5.15	4
Cpd 20: Flurandrenolide; C24 H33 F O6	5.243	436.225		Flurandrenolide	C24 H33 F O6	C24 H33 F O6	C24 H33 F O6	2.58	4
Compound 21	5.53								
Cpd 22: Lucidenic acid A; C27 H38 O6	5.582	458.2689		Lucidenic acid A	C27 H38 O6	C27 H38 O6	C27 H38 O6	-4.58	3
Cpd 23: 5-Oxoavermectin "1b" aglycone; C33 H44 O8	5.798	568.3041		5-Oxoavermectin "1b" aglycone	C33 H44 O8	C33 H44 O8	C33 H44 O8	-0.86	6
Cpd 24: 5-Oxoavermectin "1b" aglycone; C33 H44 O8	6.052	568.3027		5-Oxoavermectin "1b" aglycone	C33 H44 O8	C33 H44 O8	C33 H44 O8	1.64	6
Compound 25	6.056								
Cpd 26: (+)-Prosopinine; C18 H35 N O3	7.671	313.2599		(+)-Prosopinine	C18 H35 N O3	C18 H35 N O3	C18 H35 N O3	5.8	1
Cpd 27: Apimaysin; C27 H28 O13	7.791	560.1485		Apimaysin	C27 H28 O13	C27 H28 O13	C27 H28 O13	8.08	1
Compound 28	7.932								
Cpd 29: Picrotoxinin; C15 H16 O6	8.049	292.0947	94473	Picrotoxinin	C15 H16 O6	C15 H16 O6	C15 H16 O6	-0.18	10
Cpd 30: (+)-Prosopinine; C18 H35 N O3	8.051	313.2595	147256	(+)-Prosopinine	C18 H35 N O3	C18 H35 N O3	C18 H35 N O3	6.85	1
Cpd 31: Cassine; C18 H35 N O2	8.054	297.2648		Cassine	C18 H35 N O2	C18 H35 N O2	C18 H35 N O2	6.68	2
Cpd 32: Apimaysin; C27 H28 O13	8.151	560.1485		Apimaysin	C27 H28 O13	C27 H28 O13	C27 H28 O13	7.98	1
Cpd 33: (2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol; C13 H12 O4	8.155	232.074		(2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol	C13 H12 O4	C13 H12 O4	C13 H12 O4	-1.97	10
Cpd 34: C16 Sphinganine; C16 H35 N O2	8.386	273.2667		C16 Sphinganine	C16 H35 N O2	C16 H35 N O2	C16 H35 N O2	0.36	1
Cpd 35: Cassine; C18 H35 N O2	8.424	297.265		Cassine	C18 H35 N O2	C18 H35 N O2	C18 H35 N O2	5.88	2
Cpd 36: (2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol; C13 H12 O4	8.487	232.0737		(2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol	C13 H12 O4	C13 H12 O4	C13 H12 O4	-0.7	10
Cpd 37: Cassine; C18 H35 N O2	8.781	297.2643	61294	Cassine	C18 H35 N O2	C18 H35 N O2	C18 H35 N O2	8.48	2
Compound 38	9.163								
Compound 39	9.506								
Compound 40	10.631								
Compound 41	10.81								

Qualitative Compound Report

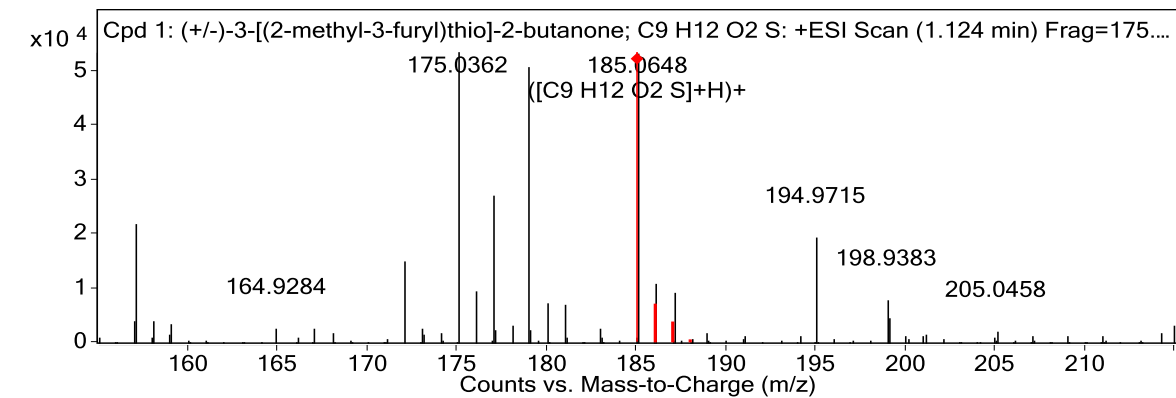
Cpd 42: Terbinafine; C21 H25 N	11.122	291.1959		Terbinafine	C21 H25 N	C21 H25 N	C21 H25 N	9.72	1
Cpd 43: Pseudouridine; C9 H12 N2 O6	12.99	244.0693	41716	Pseudouridine	C9 H12 N2 O6	C9 H12 N2 O6	C9 H12 N2 O6	0.86	10
Compound 44	14.216		45881						
Cpd 45: Alloimperatorin; C16 H14 O4	15.317	270.0893		Alloimperatorin	C16 H14 O4	C16 H14 O4	C16 H14 O4	-0.5	10
Cpd 46: Phthalic acid Mono-2-ethylhexyl Ester; C16 H22 O4	18.389	278.1499		Phthalic acid Mono-2-ethylhexyl Ester	C16 H22 O4	C16 H22 O4	C16 H22 O4	6.92	9
Compound 47	18.61								
Compound 48	18.708		35464						
Cpd 49: Phthalic acid Mono-2-ethylhexyl Ester; C16 H22 O4	18.767	278.1497		Phthalic acid Mono-2-ethylhexyl Ester	C16 H22 O4	C16 H22 O4	C16 H22 O4	7.75	9
Cpd 50: PI(16:0/18:1(11Z)); C43 H81 O13 P	18.857	836.5428		PI(16:0/18:1(11Z))	C43 H81 O13 P	C43 H81 O13 P	C43 H81 O13 P	-1.59	10
Compound 51	18.998								
Cpd 52: 7,8-Dehydroastaxanthianthin; C40 H50 O4	19.156	594.3692		7,8-Dehydroastaxanthianthin	C40 H50 O4	C40 H50 O4	C40 H50 O4	2.85	2
Cpd 53: Acetylvalerenolic acid; C17 H24 O4	19.535	292.1645		Acetylvalerenolic acid	C17 H24 O4	C17 H24 O4	C17 H24 O4	10.27	8
Compound 54	21.524								
Compound 55	21.865								
Cpd 56: Irinotecan; C33 H38 N4 O6	21.912	586.2774	160923	Irinotecan	C33 H38 N4 O6	C33 H38 N4 O6	C33 H38 N4 O6	2.99	5
Compound 57	22.269								
Cpd 58: Irinotecan; C33 H38 N4 O6	22.436	586.2779	176159	Irinotecan	C33 H38 N4 O6	C33 H38 N4 O6	C33 H38 N4 O6	2.12	5
Cpd 59: Irinotecan; C33 H38 N4 O6	22.805	586.2782	242408	Irinotecan	C33 H38 N4 O6	C33 H38 N4 O6	C33 H38 N4 O6	1.6	5
Cpd 60: Capsicum annuum Fluorescent chlorophyll catabolite; C35 H40 N4 O7	23.133	628.2873		Capsicum annuum Fluorescent chlorophyll catabolite	C35 H40 N4 O7	C35 H40 N4 O7	C35 H40 N4 O7	3.74	2
Cpd 61: Ganoderic acid F; C32 H42 O9	23.174	570.2828	1072922	Ganoderic acid F	C32 H42 O9	C32 H42 O9	C32 H42 O9	0.09	2
Cpd 62: Capsicum annuum Fluorescent chlorophyll catabolite; C35 H40 N4 O7	23.5	628.286		Capsicum annuum Fluorescent chlorophyll catabolite	C35 H40 N4 O7	C35 H40 N4 O7	C35 H40 N4 O7	5.95	2
Cpd 63: Ganoderic acid F; C32 H42 O9	23.562	570.2831	836745	Ganoderic acid F	C32 H42 O9	C32 H42 O9	C32 H42 O9	-0.33	2
Cpd 64: gamma-L-Glutamyl-butyrosin B; C26 H48 N6 O15	23.691	684.3103		gamma-L-Glutamyl-butyrosin B	C26 H48 N6 O15	C26 H48 N6 O15	C26 H48 N6 O15	10.95	1
Cpd 65: Ganoderic acid F; C32 H42 O9	23.917	570.2821	136758	Ganoderic acid F	C32 H42 O9	C32 H42 O9	C32 H42 O9	1.46	2
Cpd 66: Ganoderic acid F; C32 H42 O9	24.245	570.283		Ganoderic acid F	C32 H42 O9	C32 H42 O9	C32 H42 O9	-0.26	2
Compound 67	24.575		319436						
Cpd 68: Ganoderic acid F; C32 H42 O9	24.577	570.2817		Ganoderic acid F	C32 H42 O9	C32 H42 O9	C32 H42 O9	2.13	2
Compound 69	24.923		293875						
Cpd 70: 3-Hydroxyethylbacteriochlorophyllide a; C35 H38 Mg N4 O6	25.306	634.2738		3-Hydroxyethylbacteriochlorophyllide a	C35 H38 Mg N4 O6	C35 H38 Mg N4 O6	C35 H38 Mg N4 O6	-15.22	2
Compound 71	25.359								
Cpd 72: Ansamitocin P3; C32 H43 Cl N2 O9	25.687	634.2745	71116	Ansamitocin P3	C32 H43 Cl N2 O9	C32 H43 Cl N2 O9	C32 H43 Cl N2 O9	-13.89	1
Cpd 73: Harderoporphyrinogen; C35 H42 N4 O6	27.443	614.309	1213185	Harderoporphyrinogen	C35 H42 N4 O6	C35 H42 N4 O6	C35 H42 N4 O6	2.32	4
Cpd 74: Harderoporphyrinogen; C35 H42 N4 O6	27.831	614.3087	665532	Harderoporphyrinogen	C35 H42 N4 O6	C35 H42 N4 O6	C35 H42 N4 O6	2.86	4
Cpd 75: Harderoporphyrinogen; C35 H42 N4 O6	28.207	614.3077	110924	Harderoporphyrinogen	C35 H42 N4 O6	C35 H42 N4 O6	C35 H42 N4 O6	4.49	4
Cpd 76: Harderoporphyrinogen; C35 H42 N4 O6	28.6	614.3065	20594	Harderoporphyrinogen	C35 H42 N4 O6	C35 H42 N4 O6	C35 H42 N4 O6	6.41	4
Compound 77	28.693		51638						
Compound 78	29.04		114488						
Compound 79	29.301		22547						
Compound 80	29.478								

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 1: (+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone; C9 H12 O2 S	(+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone	185.0648	1.138	Auto MS/MS	184.0575



MS Zoomed Spectrum

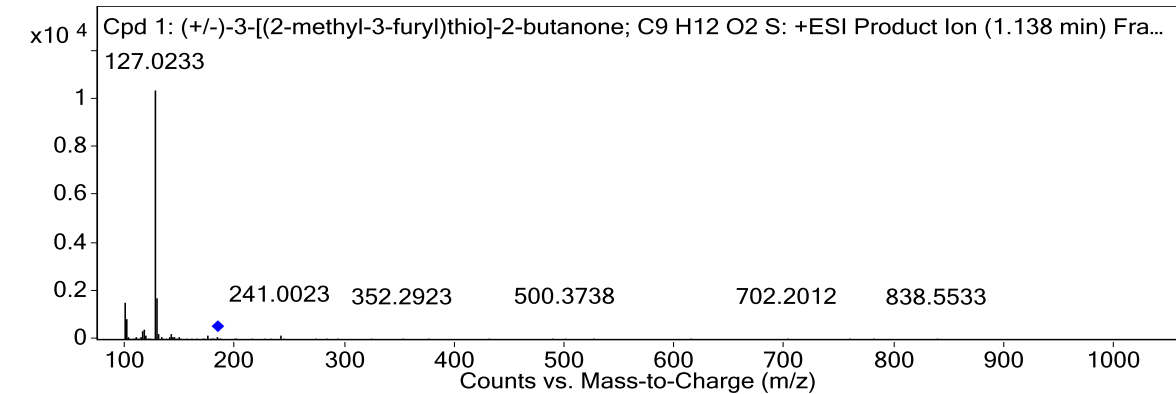
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
100.0536			2	64578.23		
127.0236			1	312246.56		
128.0246			1	46025.23		
143.0008			1	59593.51		
175.0362			1	53473.07		
178.9944			1	50785.68		
185.0648	185.0631	-9.47	1	53204.72	C9 H12 O2 S	(M+H)+
186.0663	186.0662	-0.41	1	10836.87	C9 H12 O2 S	(M+H)+
187.0633	187.0605	-15.04	1	9250.33	C9 H12 O2 S	(M+H)+
188.066	188.0633	-14.34	1	723.81	C9 H12 O2 S	(M+H)+

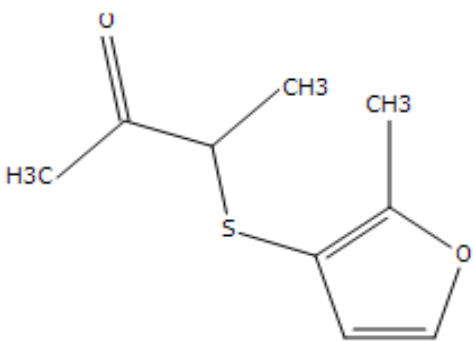
MS/MS Spectrum



MS/MS Spectrum Peak List

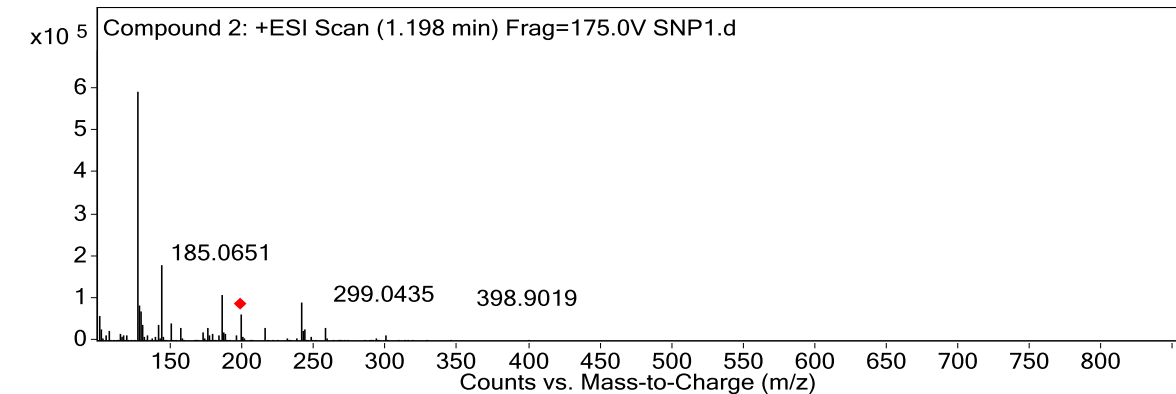
m/z	z	Abund
100.0287		1574.2
100.0522	2	579.21
101.026		842.15
115.0038		384.49
116.9936		437.68
127.0233	1	10371.4
128.0242	1	1764.09
129.0211	1	518.64
129.992		255.39
141.0382		239.27

Compound Structure

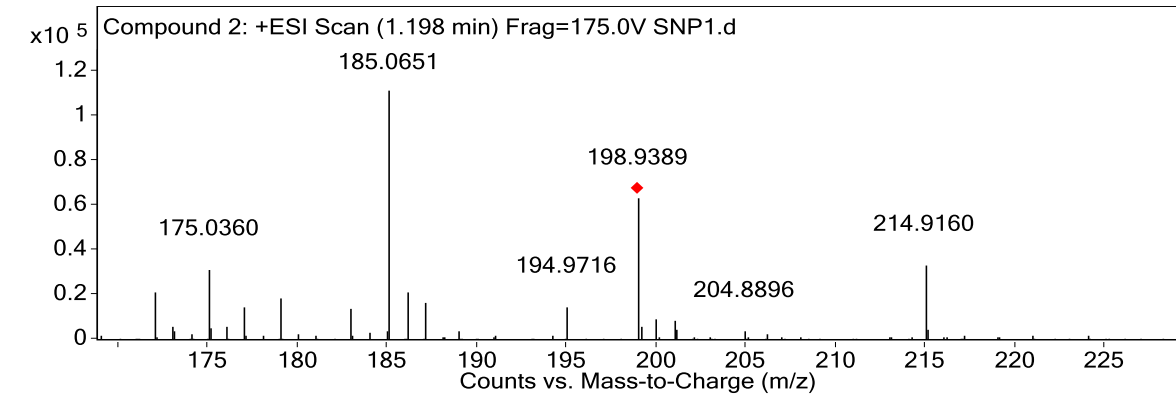


Compound Label	m/z	RT	Algorithm
Compound 2	198.9389	1.212	Auto MS/MS

MS Spectrum



MS Zoomed Spectrum



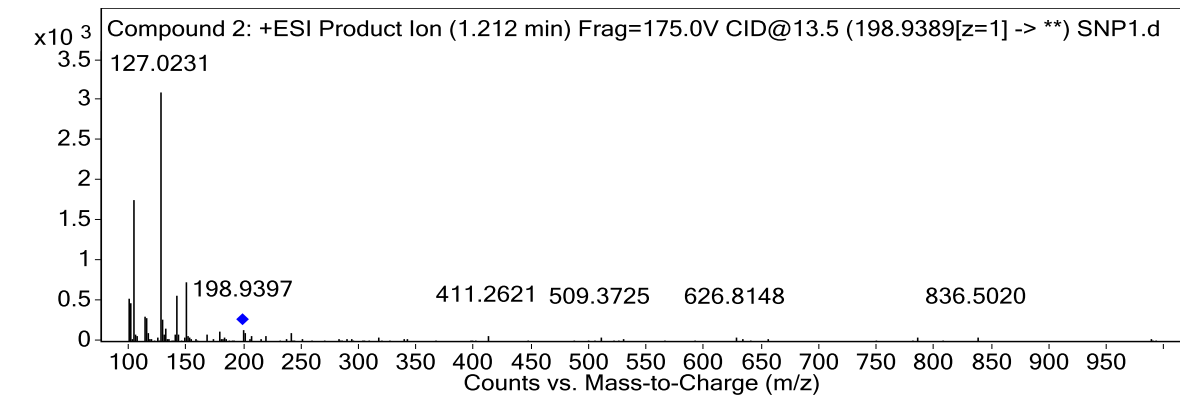
MS Spectrum Peak List

m/z	z	Abund
100.0537	2	60129.35
127.0236	1	594009.81

Qualitative Compound Report

128.025	1	86871.55
129.0213	1	72322.8
143.001	1	181065.31
185.0651	1	111229.05
198.9389	1	63156.89
199.94	1	9325.72
200.9371	1	8448.8
241.003	1	93081.44

MSMS Spectrum

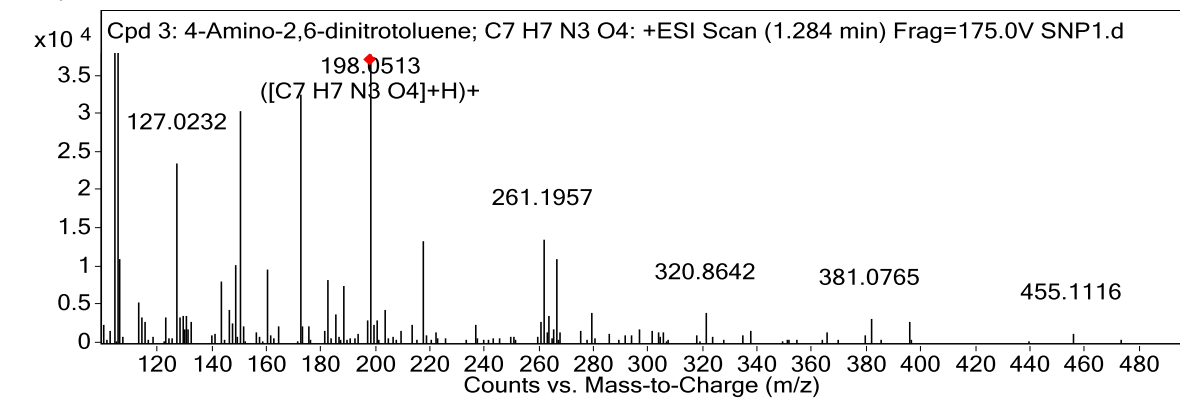


MS/MS Spectrum Peak List

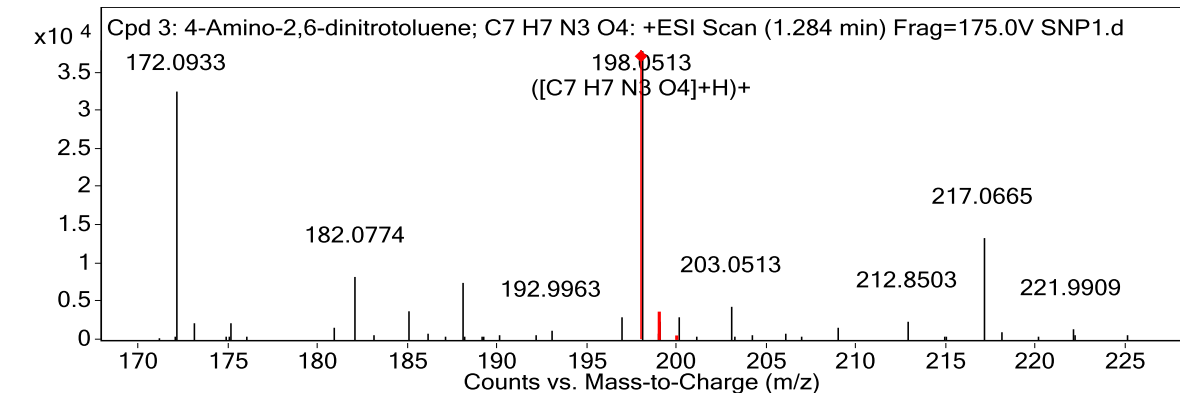
m/z	z	Abund
100.0294		535.09
101.0256		476.78
104.1067	1	1761.9
114.1025	1	324.39
115.0042		292.46
127.0231	1	3104.8
128.0237	1	455.77
129.0202	1	276.52
141.0388	1	584.35
150.1103	1	739.71

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 3: 4-Amino-2,6-dinitrotoluene; C7 H7 N3 O4	4-Amino-2,6-dinitrotoluene	198.0513	1.299	Auto MS/MS	197.0436

MS Spectrum



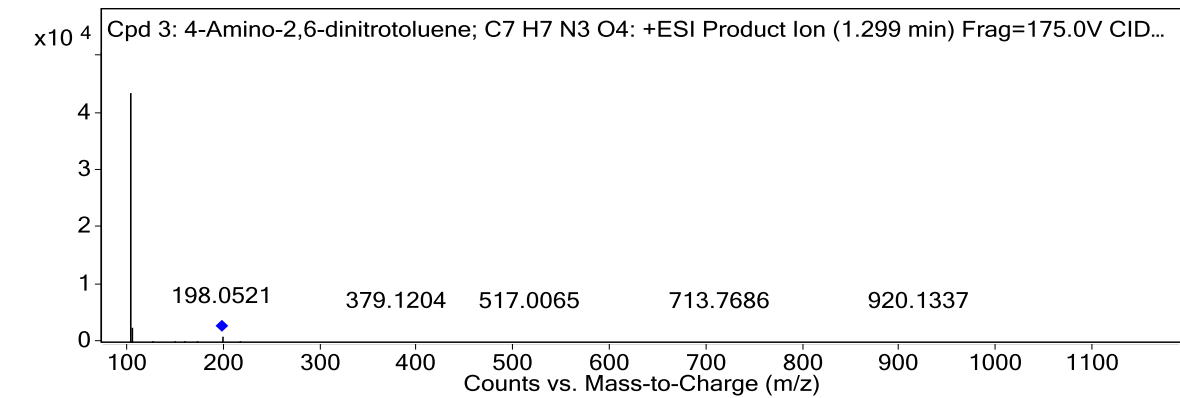
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
104.1068			1	4800697		
105.1101			1	236777.81		
127.0232			1	23652.93		
150.1116			1	30372.21		
172.0933			1	32483.1		
198.0513	198.0509	-2	1	37846.93	C7 H7 N3 O4	(M+H)+
199.0546	199.0536	-5.33	1	2506.04	C7 H7 N3 O4	(M+H)+
200.0503	200.0554	25.86	1	3063.31	C7 H7 N3 O4	(M+H)+
201.0494	201.0579	42.01	1	499.01	C7 H7 N3 O4	(M+H)+
261.1957			1	13743.34		

MSMS Spectrum



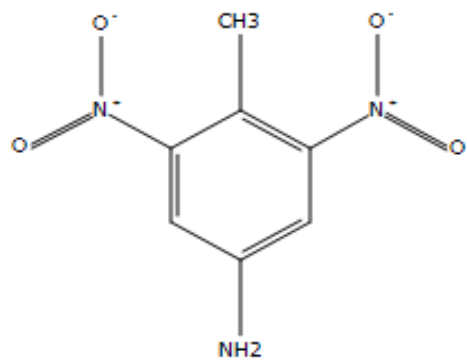
MS/MS Spectrum Peak List

m/z	z	Abund
104.1067	1	43642.1
105.1093	1	2492.41
127.0228		180.06
150.1122		179.31

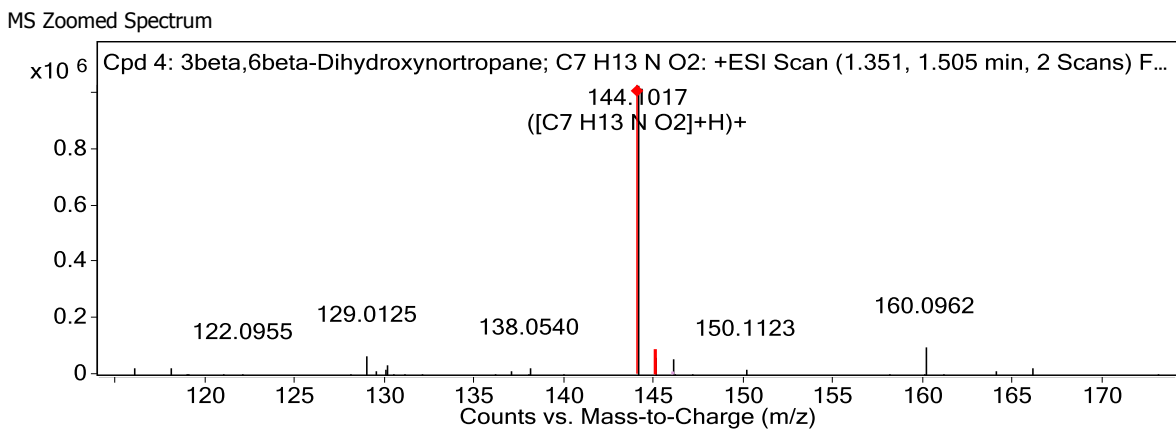
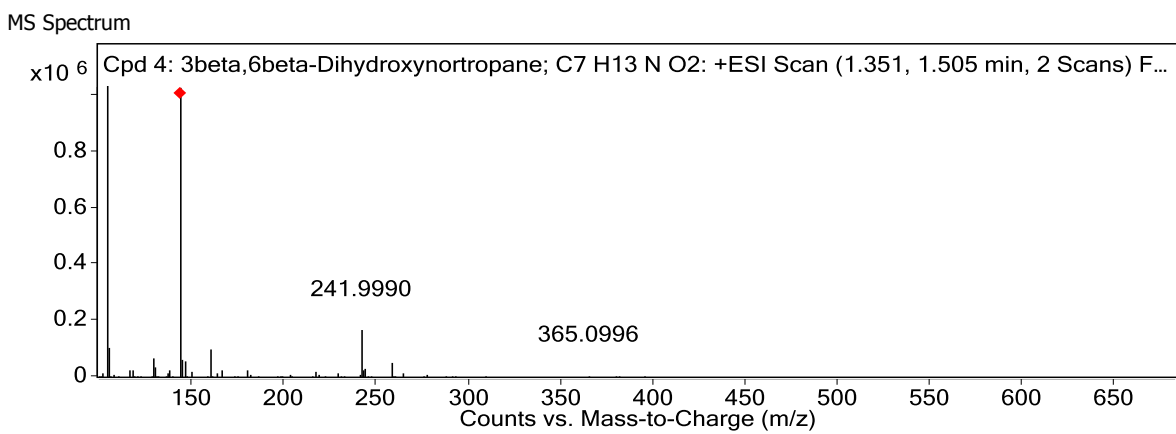
Qualitative Compound Report

160.0945	1	201.08
172.0945		144.64
198.0521	1	921.44
199.0583	1	140.22
203.0523	1	119.82
217.066		188.28

Compound Structure

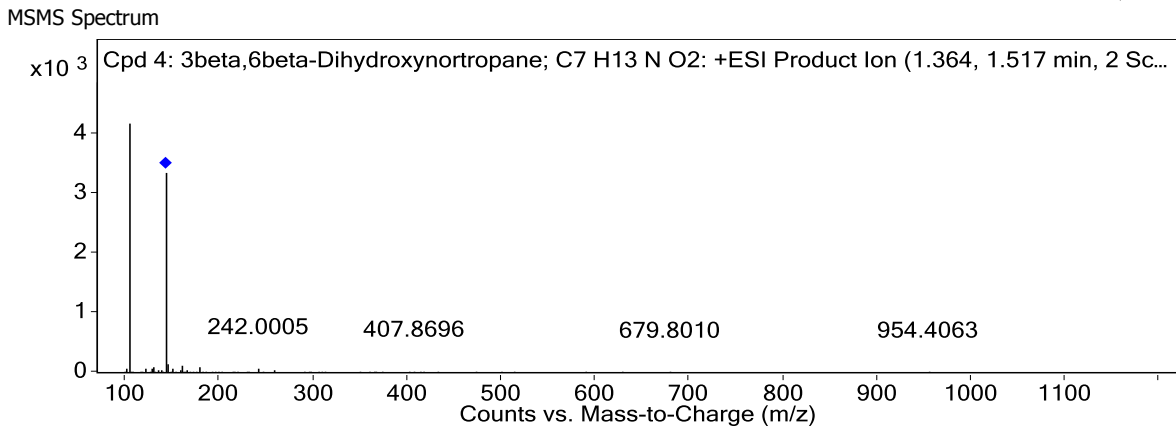


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 4: 3beta,6beta-Dihydroxynortropane; C7 H13 N O2	3beta,6beta-Dihydroxynortropane	144.1017	1.44	Auto MS/MS	143.0944



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
104.1067			1	2159616.5		
105.11			1	104024.83		
129.0125			2	69385.72		
130.0857			1	38520.84		
144.1017	144.1019	1.49	1	1026981.13	C7 H13 N O2	(M+H)+
145.1045	145.105	3.86	1	63009.96	C7 H13 N O2	(M+H)+
146.0805			1	60847.77		
160.0962			1	99768.11		
241.999			1	167962.73		
257.976			1	54213.1		

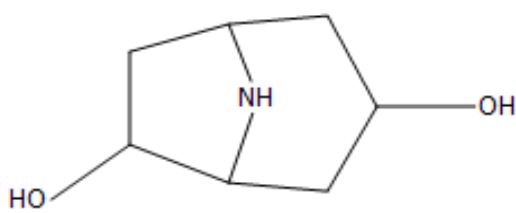


MS/MS Spectrum Peak List

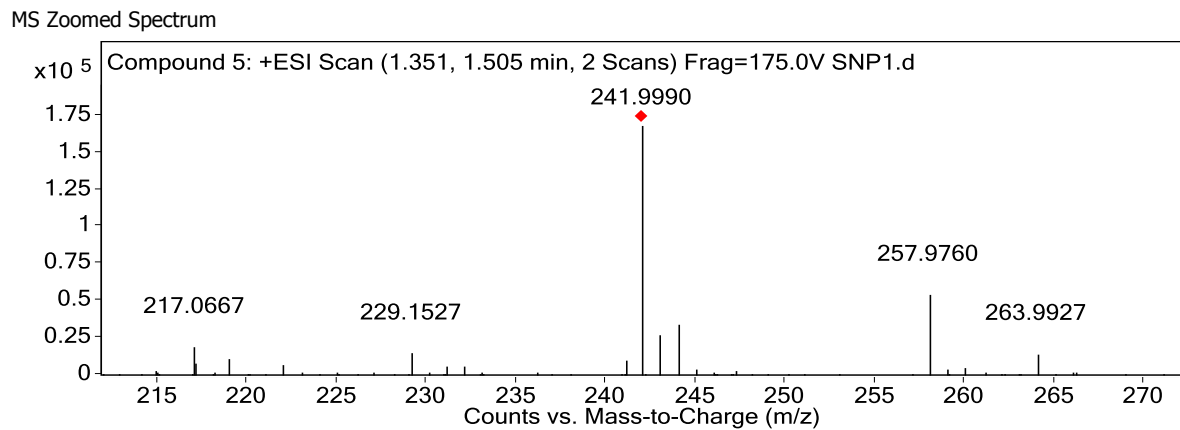
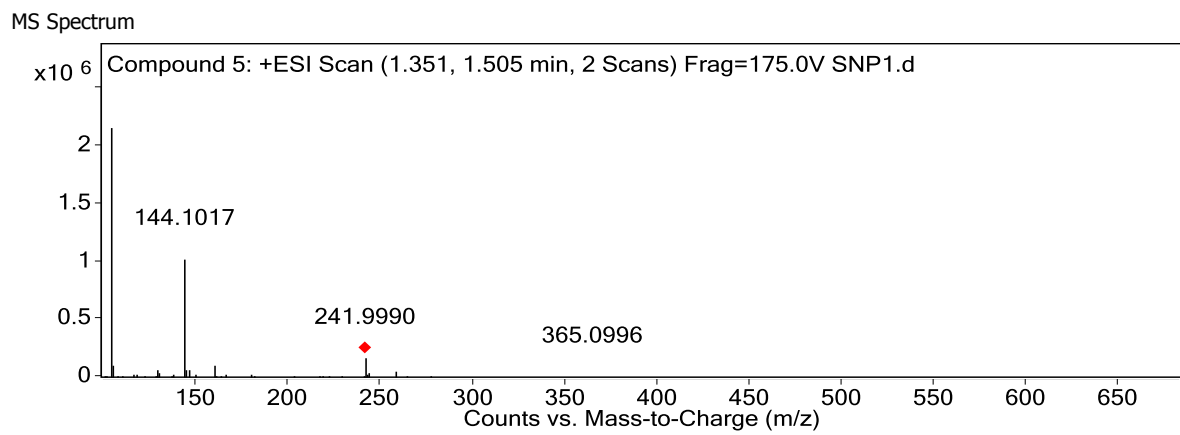
m/z	z	Abund
104.1063	1	4178.19
105.1085	1	358.76
130.0869		97.36
144.0775		85.03
144.1011	1	3345.34
145.1048	1	152.04
146.0787		86.05
160.097	1	116.03
179.9623		105.49
242.0005		78.61

Compound Structure

Qualitative Compound Report



Compound Label	m/z	RT	Algorithm
Compound 5	241.999	1.444	Auto MS/MS

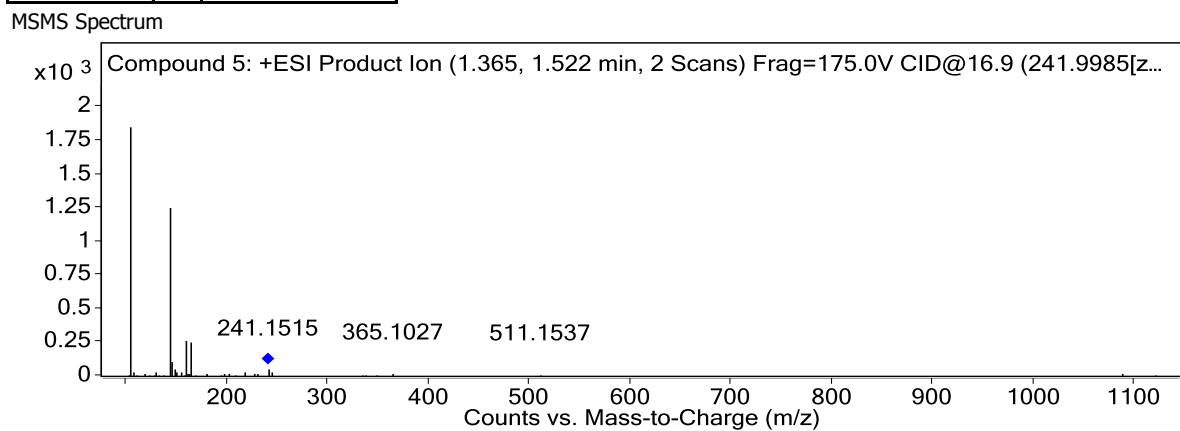


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m/z	z	Abund
104.1067	1	2159616.5
105.11	1	104024.83
129.0125	2	69385.72
144.1017	1	1026981.13
160.0962	1	99768.11
241.999	1	167962.73

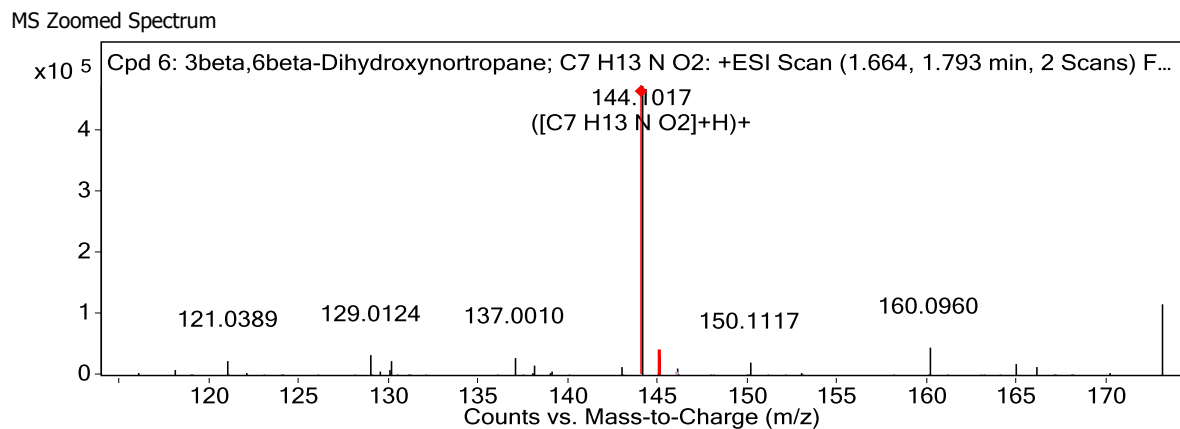
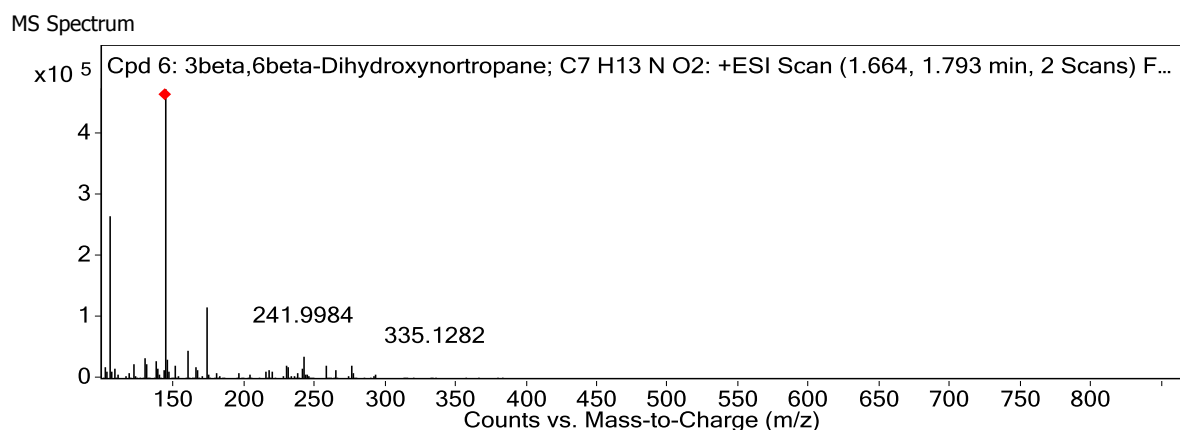
Qualitative Compound Report

m/z	z	Abund
242.9996	1	27568.76
243.9957	1	34139.23
244.9979	1	3971.76
245.9928	1	2478.02

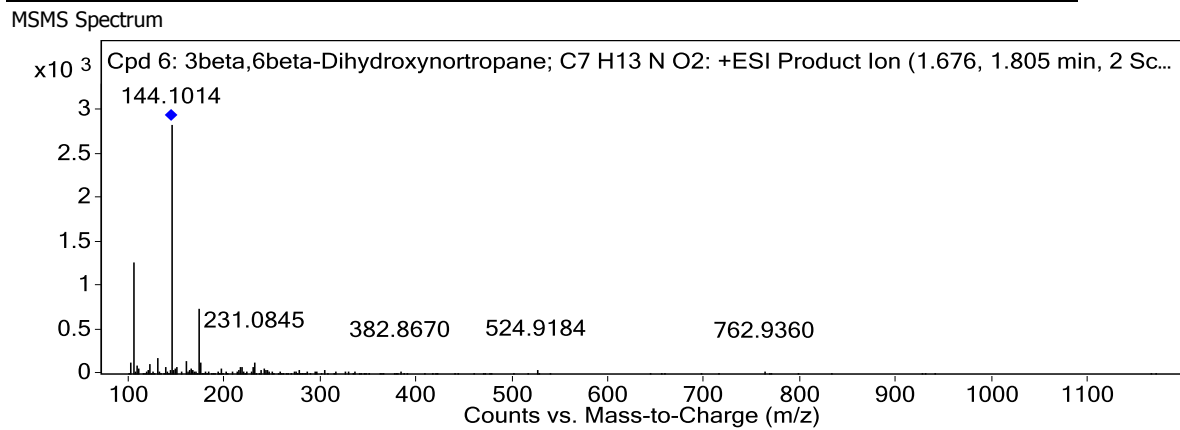


MS/MS Spectrum Peak List		
m/z	z	Abund
104.1063	1	1852.37
105.109	1	96.94
144.1012	1	1256.46
145.1022	1	111.11
146.0777		49.7
148.9585	1	56.13
160.0958	1	261.18
163.9855	1	255.55
164.9863	1	39.88
241.1515	1	52

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 6: 3beta,6beta-Dihydroxynortropane; C7 H13 N O2	3beta,6beta-Dihydroxynortropane	144.1017	1.741	Auto MS/MS	143.0944



m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
104.1066			1	266005.16		
121.0389				24380.23		
129.0124			2	33359.88		
130.1583				24590.8		
137.001			2	29939.02		
144.1017	144.1019	1.55	1	473596.69	C7 H13 N O2	(M+H)+
145.1044	145.105	4.3	1	31019.68	C7 H13 N O2	(M+H)+
160.096			1	45938.87		
173.078			1	118393.8		
241.9984			1	36305.45		

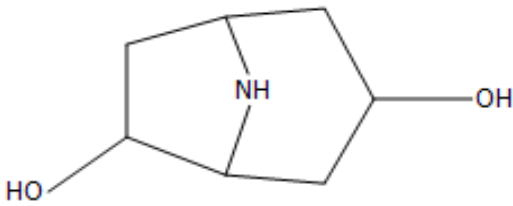


MS/MS Spectrum Peak List		
m/z	z	Abund
102.1267		129.94
104.1066	1	1275.7
121.0381		111.98
130.1582		192.2
144.1014	1	2835.46
145.1042	1	321.9
160.0964		146.89

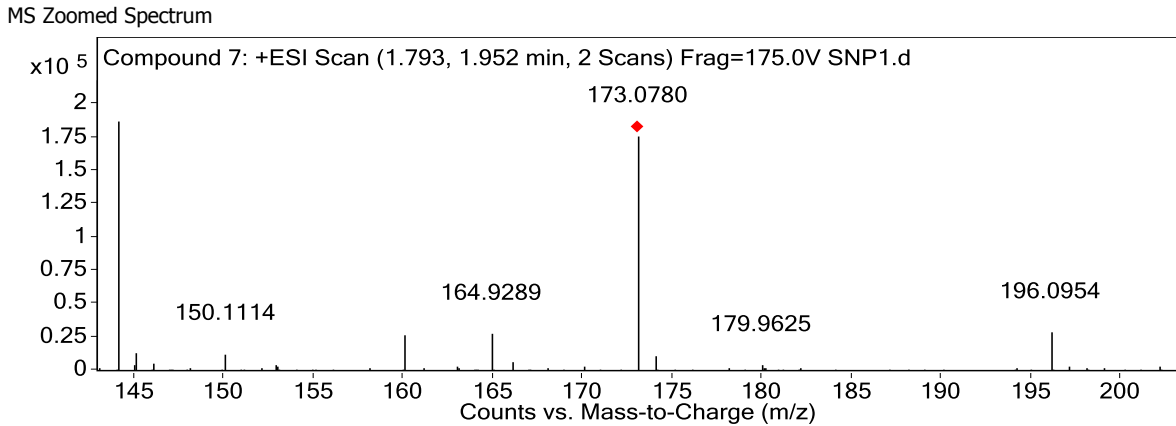
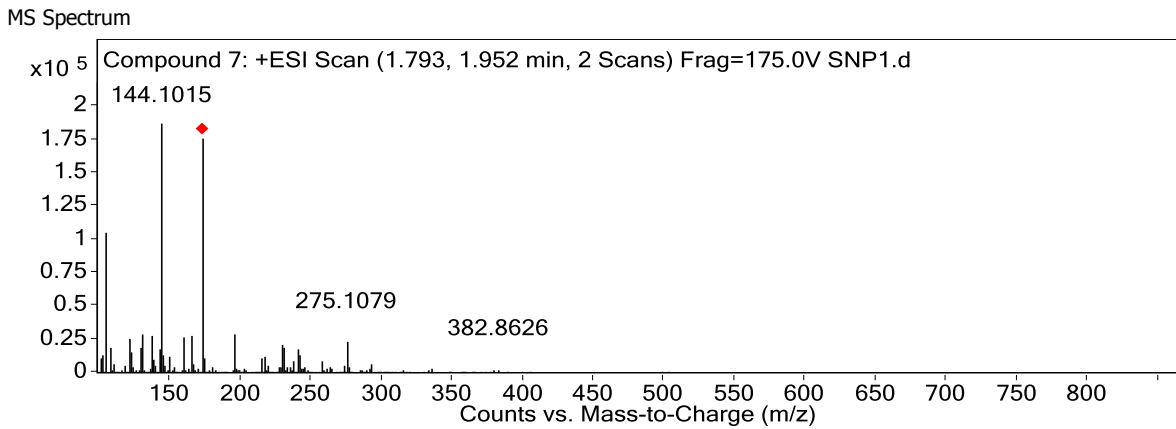
Qualitative Compound Report

173.0782	1	753.79
174.0804	1	139.83
231.0845		143.21

Compound Structure

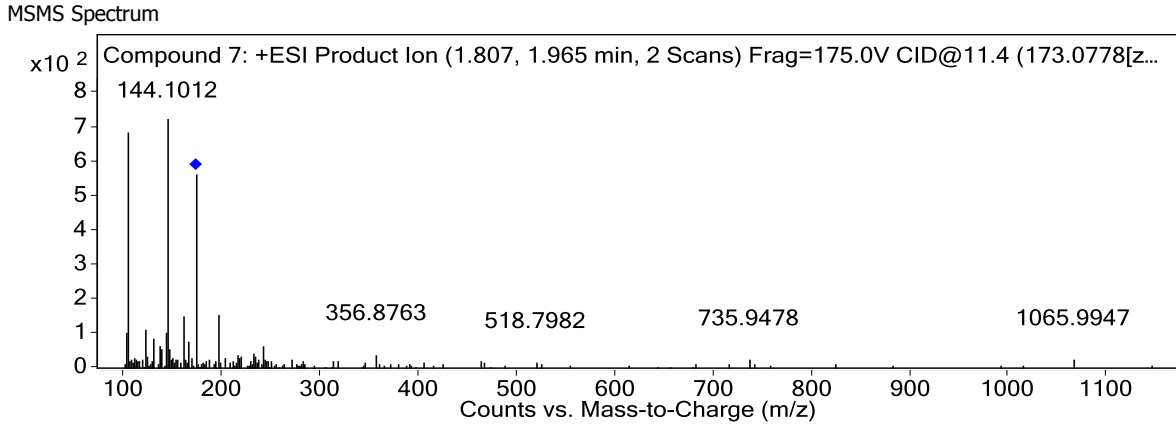


Compound Label	m/z	RT	Algorithm
Compound 7	173.078	1.886	Auto MS/MS



MS Spectrum Peak List

m/z	z	Abund
104.1064	1	105086.96
121.0389		25210.85
130.1583	1	28844.61
137.001	2	28112.53
144.1015	1	187121.94
160.096		26930.23
164.9289		27782.74
173.078	1	176276.69
174.0806	1	11325.69
196.0954	1	28926.47



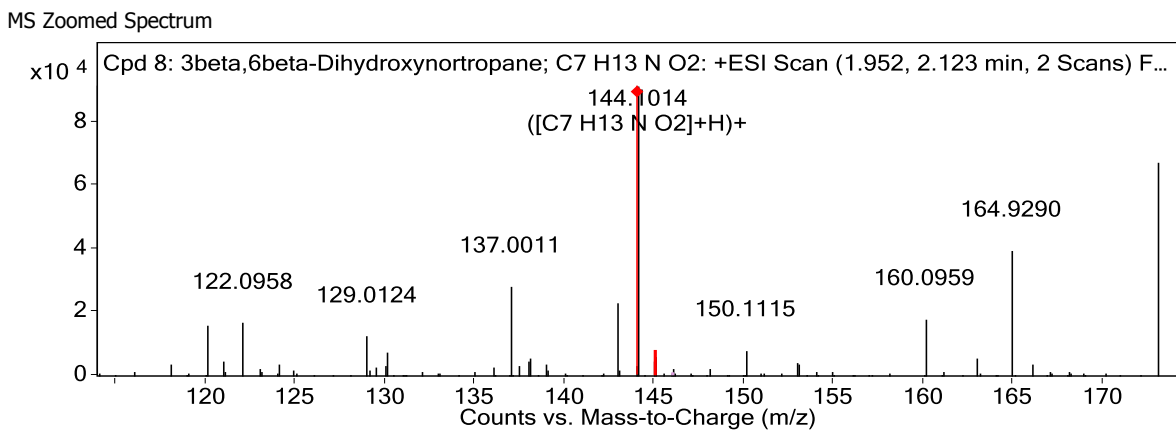
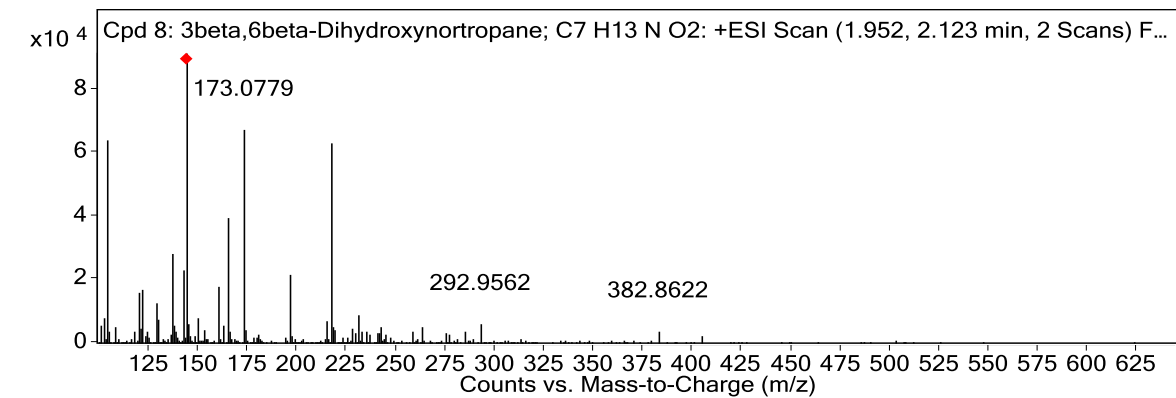
MS/MS Spectrum Peak List

m/z	z	Abund
102.1254	1	104.14
104.1053		683.3
122.0934		114.54
130.1575		86.83
142.9467		104.52
144.1012	1	725.07
145.1072	1	84.51
160.0953	1	152.63
173.0765	1	565.59
196.0946		154.07

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 8: 3beta,6beta-Dihydroxynortropane; C7 H13 N O2	3beta,6beta-Dihydroxynortropane	144.1014	2.052	Auto MS/MS	143.0941

MS Spectrum

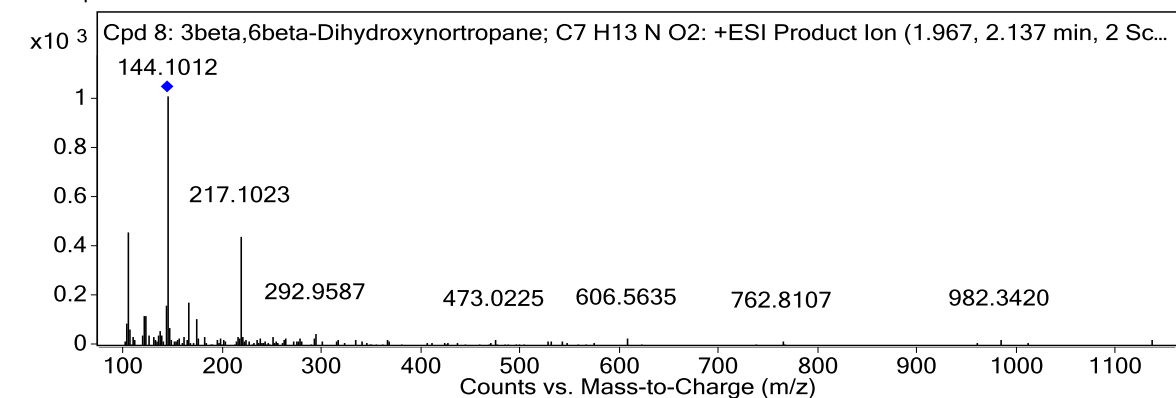
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
104.1064			1	64126.66		
137.0011			2	28285.26		
142.9472				23071.5		
144.1014	144.1019	3.57	1	91186.84	C7 H13 N O2	(M+H)+
145.1043	145.105	5.12	1	5907.04	C7 H13 N O2	(M+H)+
160.0959				17992.78		
164.929				39628.74		
173.0779			1	67386.73		
196.0955			1	21810.85		
217.1033			1	63182.15		

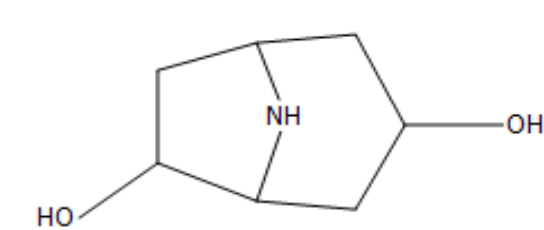
MSMS Spectrum



MS/MS Spectrum Peak List

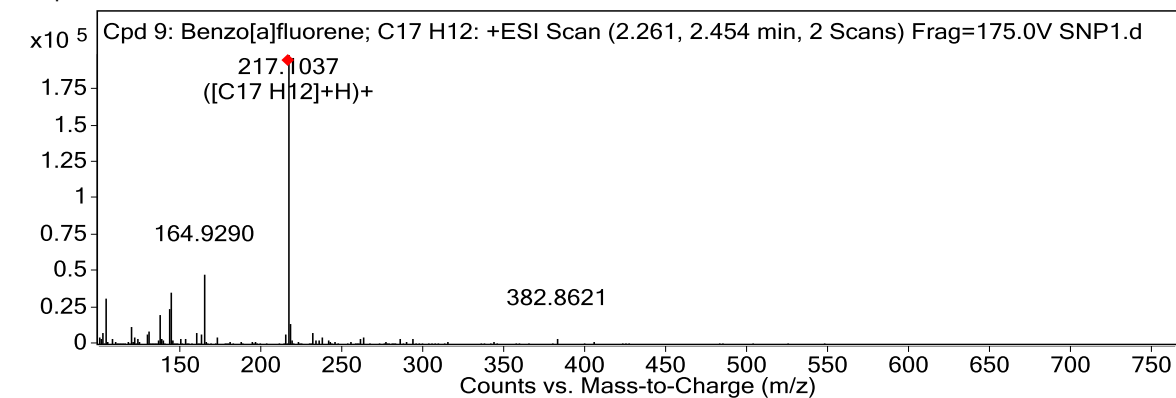
m/z	z	Abund
102.1269		91.08
104.1057	1	459.67
120.0802		121.03
122.0937		119.48
142.9467		166.67
144.047	1	87
144.1012	1	1014.57
164.927		176.16
173.0766	1	111.76
217.1023	1	445.62

Compound Structure



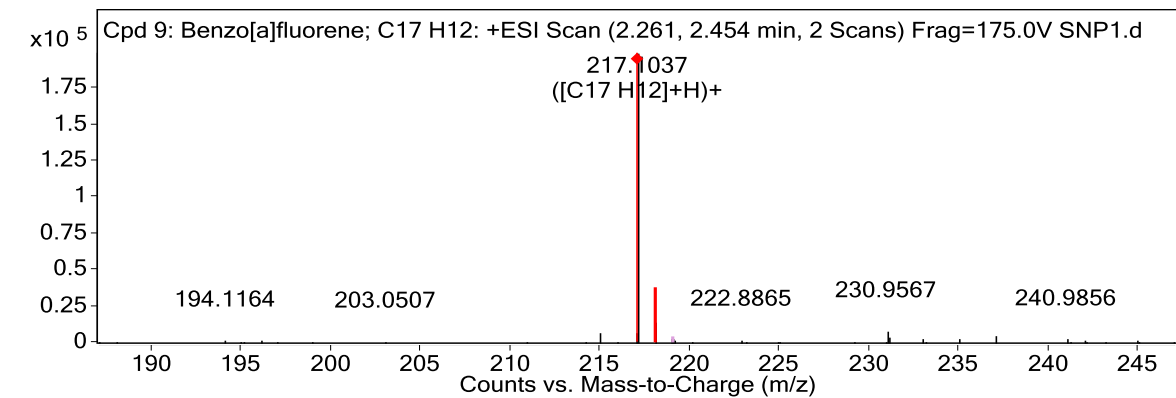
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 9: Benzo[a]fluorene; C17 H12	Benzo[a]fluorene	217.1037	2.371	Auto MS/MS	216.0964

MS Spectrum



MS Zoomed Spectrum

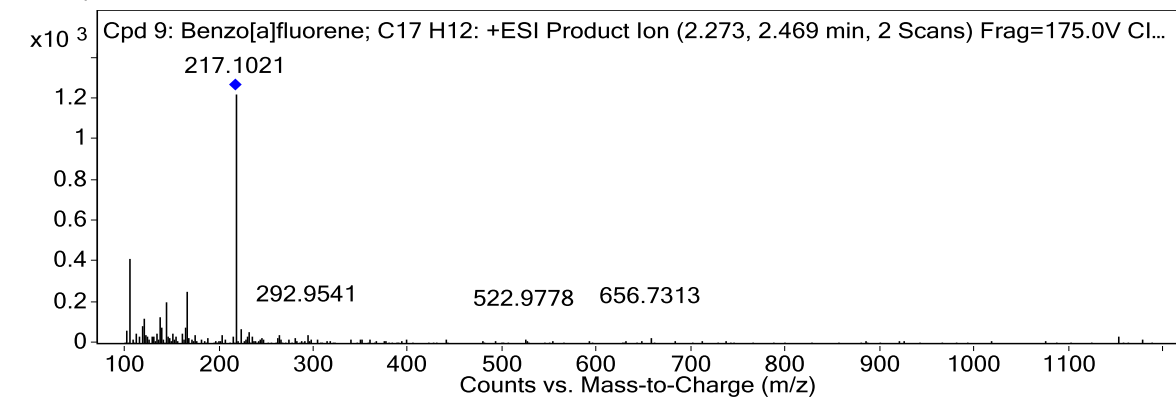
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
102.1271				8392.54		
104.1062			1	32237.74		
120.08				12719.21		
130.064				8966.16		
137.0011			2	20822.43		
142.947				24879.42		
144.1011			1	36181.73		
164.929				47719.03		
217.1037	217.1012	-11.74	1	198698.02	C17 H12	(M+H)+
218.1065	218.1046	-8.97	1	13865.13	C17 H12	(M+H)+

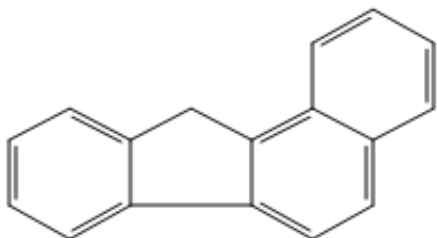
MSMS Spectrum



MS/MS Spectrum Peak List

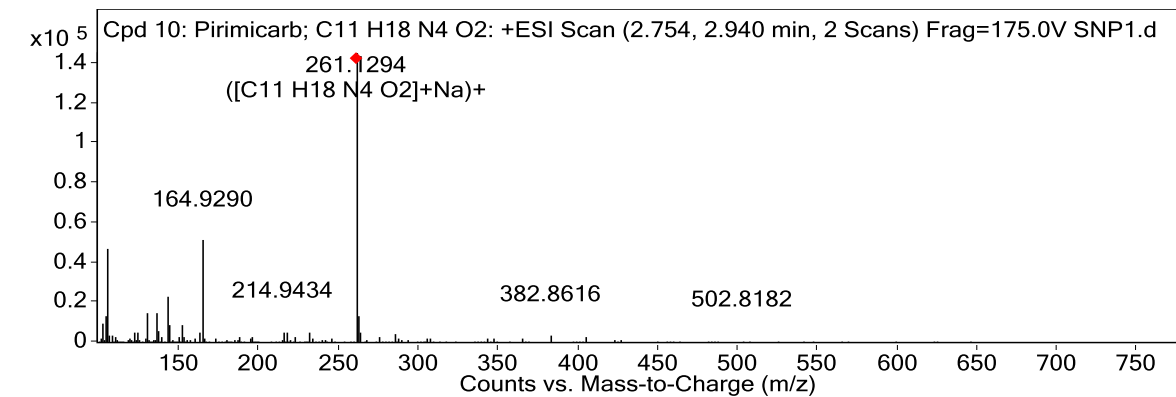
m/z	z	Abund
104.1057		420.35
118.0885		84.41
120.0808		123.05
137.0001		130.32
138.9988		82.53
142.9467		126.19
144.1006	1	207.18
164.9271		259.33
217.1021	1	1223.62
218.1082	1	124.92

Compound Structure

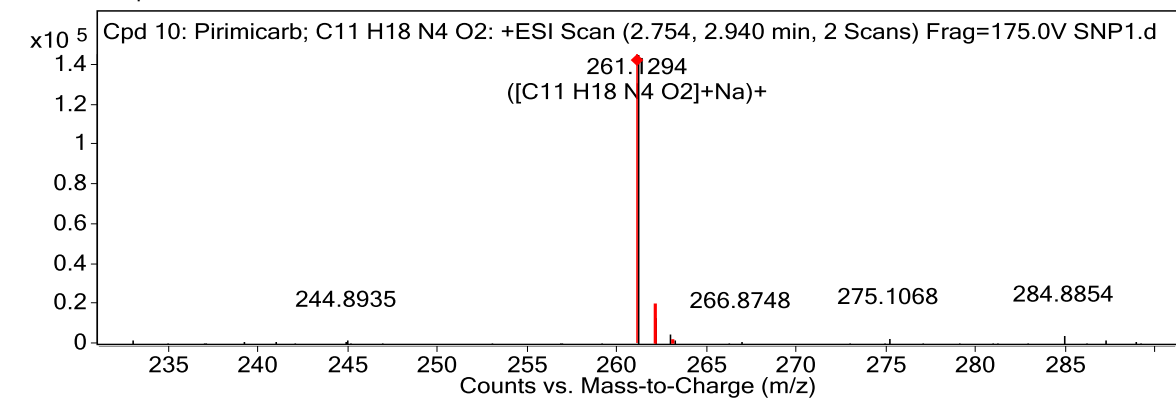


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 10: Pirimicarb; C11 H18 N4 O2	Pirimicarb	261.1294	2.863	Auto MS/MS	238.1402

MS Spectrum



MS Zoomed Spectrum

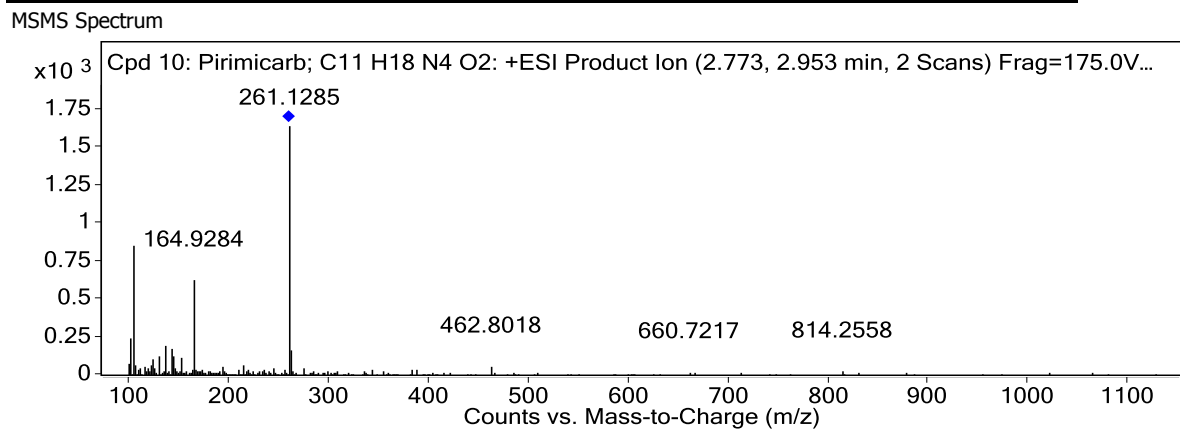


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
102.127				10001.97		

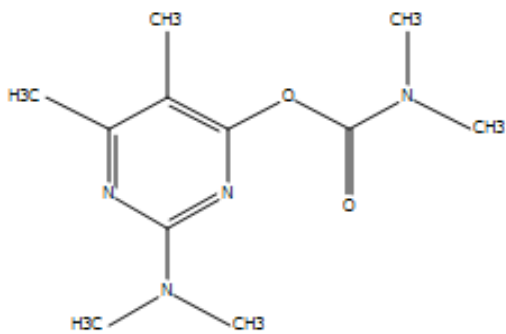
Qualitative Compound Report

104.106				13781.03		
105.0692			1	47148.38		
130.0642			1	14687.67		
136.1113			1	14951.92		
142.947				23423.37		
164.929				51376.29		
261.1294	261.1322	10.88	1	145263.23	C11 H18 N4 O2	(M+Na)+
262.1323	262.1349	9.99	1	13247.49	C11 H18 N4 O2	(M+Na)+
263.1338	263.1372	12.89	1	2001.24	C11 H18 N4 O2	(M+Na)+

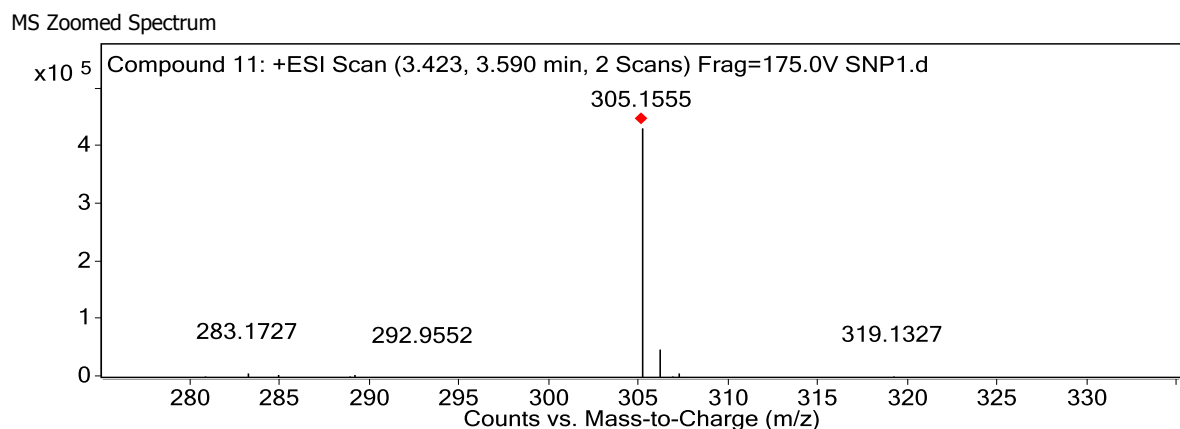
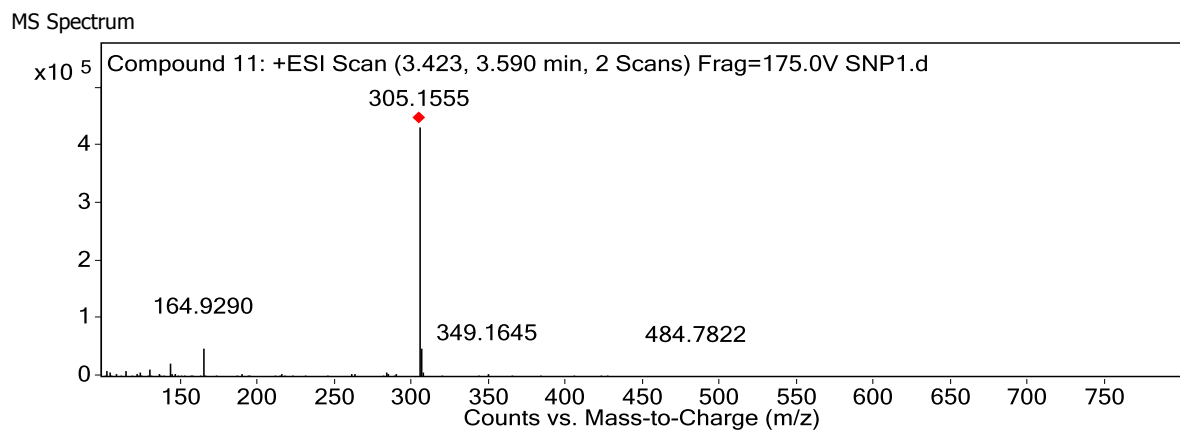


MS/MS Spectrum Peak List		
m/z	z	Abund
102.1264		245.04
104.1078		143.83
105.0687	1	856.43
130.0647		128.92
136.1112		194.84
142.948		180.79
144.1002		125.85
164.9284		625.96
261.1285	1	1642.77
262.1338	1	171.62

Compound Structure



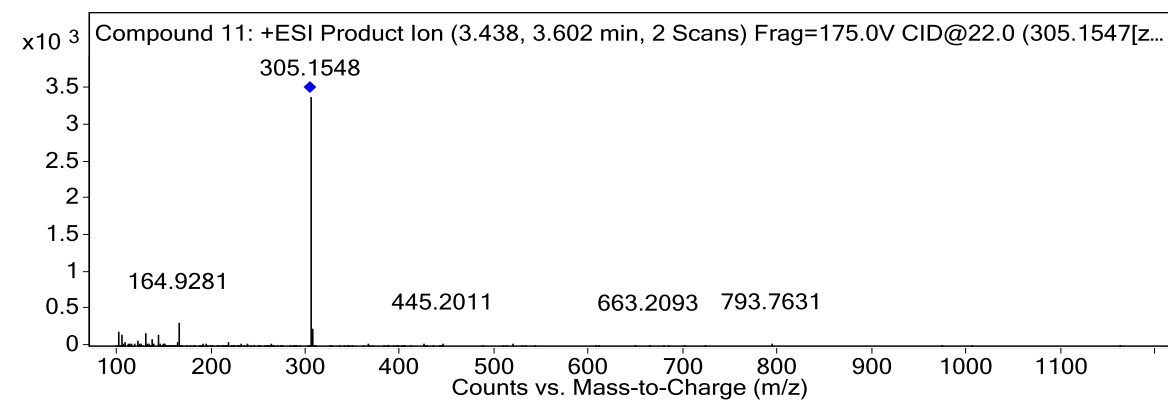
Compound Label	m/z	RT	Algorithm
Compound 11	305.1555	3.52	Auto MS/MS



MS Spectrum Peak List		
m/z	z	Abund
102.1271		10198.63
104.106		8816.01
114.0908		9692.38
130.0642	1	13265.23
142.9471		23097.95
164.929		50363.13
283.1727	1	7921.69
305.1555	1	432161.19
306.1583	1	48209.39
307.1593	1	6529.01

MSMS Spectrum

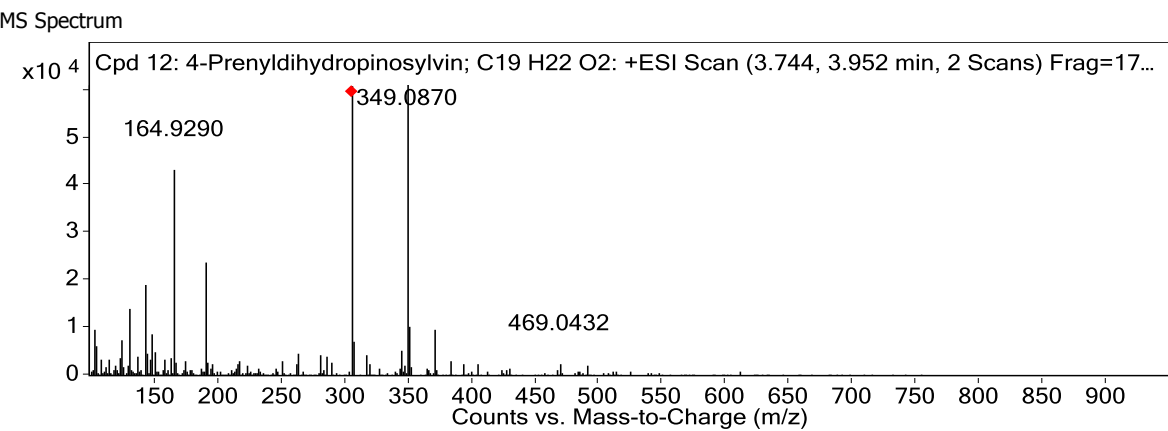
Qualitative Compound Report



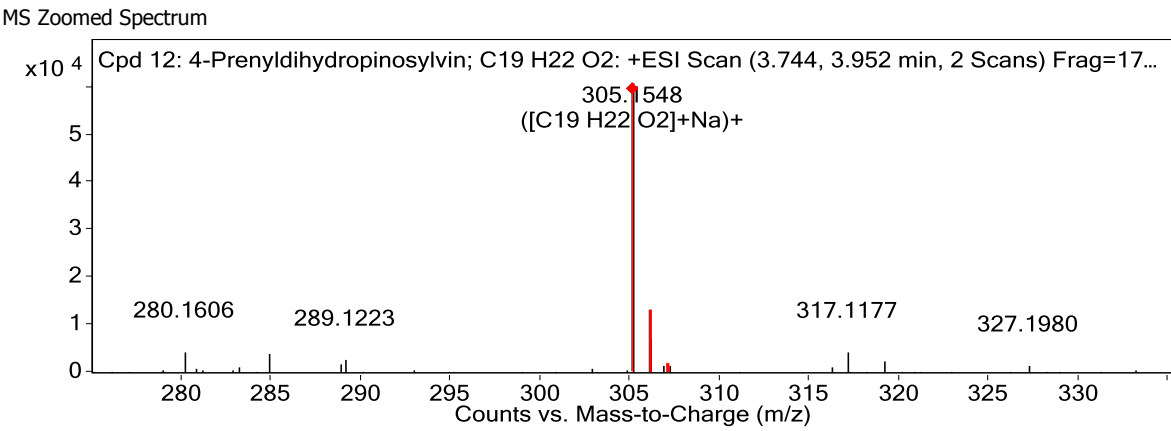
MS/MS Spectrum Peak List

m/z	z	Abund
102.1269		202.14
104.1057	1	161.27
122.0957		85.3
130.0642	1	173.3
136.0589		92.58
142.9466		155.7
144.0999		75.36
164.9281		317.19
305.1548	1	3391.4
306.1587	1	250.27

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 12: 4-Prenyldihydropinosylvin;	4-Prenyldihydropinosylvi	305.1548	3.865	Auto MS/MS	282.1655

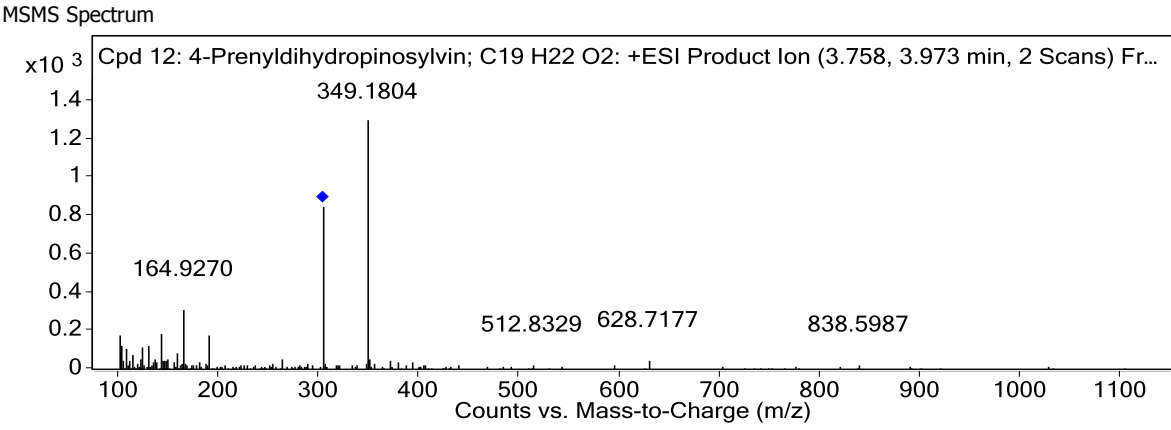


Qualitative Compound Report



MS Spectrum Peak List

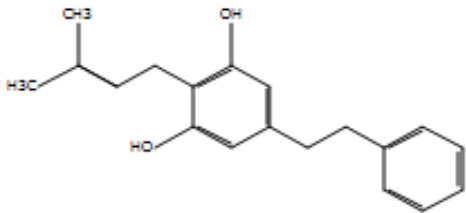
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
130.064			1	14072.67		
142.947				19257.91		
164.929				43302.91		
190.0488			1	23940.25		
305.1548	305.1512	-11.78	1	60849.07	C19 H22 O2	(M+Na)+
306.1576	306.1546	-9.86	1	7129.59	C19 H22 O2	(M+Na)+
307.1597	307.1576	-7.06	1	1569.79	C19 H22 O2	(M+Na)+
349.087			1	73689.5		
349.1806			1	36566.97		
350.0896			1	10366.04		



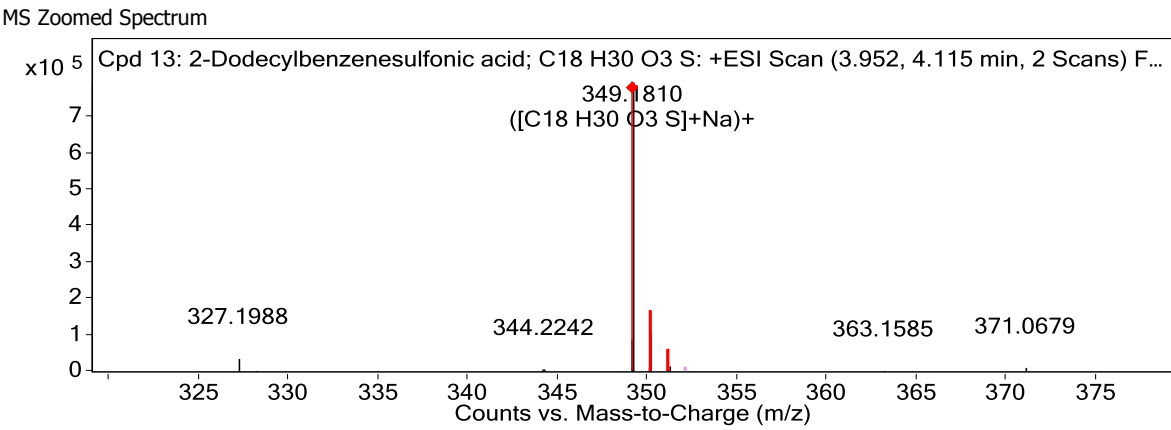
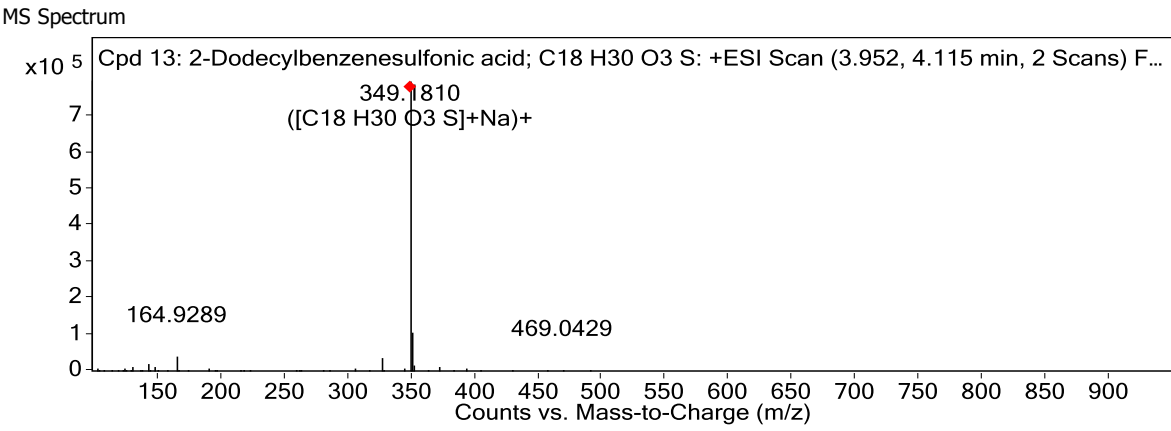
MS/MS Spectrum Peak List

m/z	z	Abund
102.1275		177.93
104.1056	1	122.67
124.0852		116.52
130.0653		126.45
142.9484		184.13
164.927		309.79
190.0487		176.86
305.1538	1	850.62
349.0875		114.73
349.1804	1	1299.15

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 13: 2-Dodecylbenzenesulfonic acid; C18 H30 O3 S	2-Dodecylbenzenesulfonic acid	349.181	4.046	Auto MS/MS	326.1919



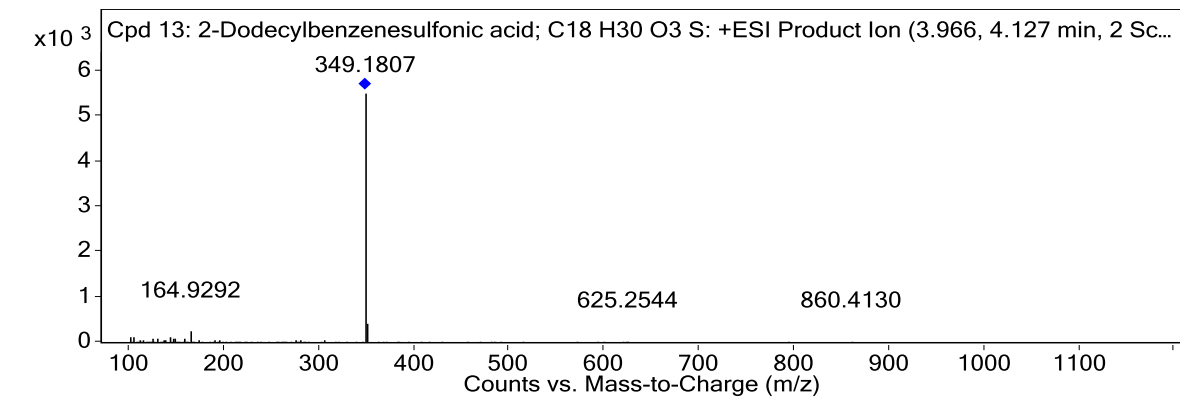
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
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Qualitative Compound Report

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
130.064			1	12207.18		
142.947				19011.26		
164.9289				41105.01		
327.1988			1	38755.22		
349.0868			1	91495.15		
349.181	349.1808	-0.74	1	795121.5	C18 H30 O3 S	(M+Na)+
350.0895			1	13171.76		
350.1843	350.184	-0.72	1	106446.11	C18 H30 O3 S	(M+Na)+
351.1849	351.1804	-12.91	1	15147.28	C18 H30 O3 S	(M+Na)+
371.0679			1	12301.16		

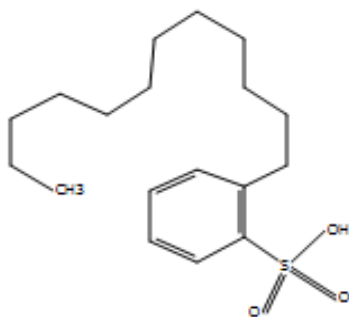
MSMS Spectrum



MS/MS Spectrum Peak List

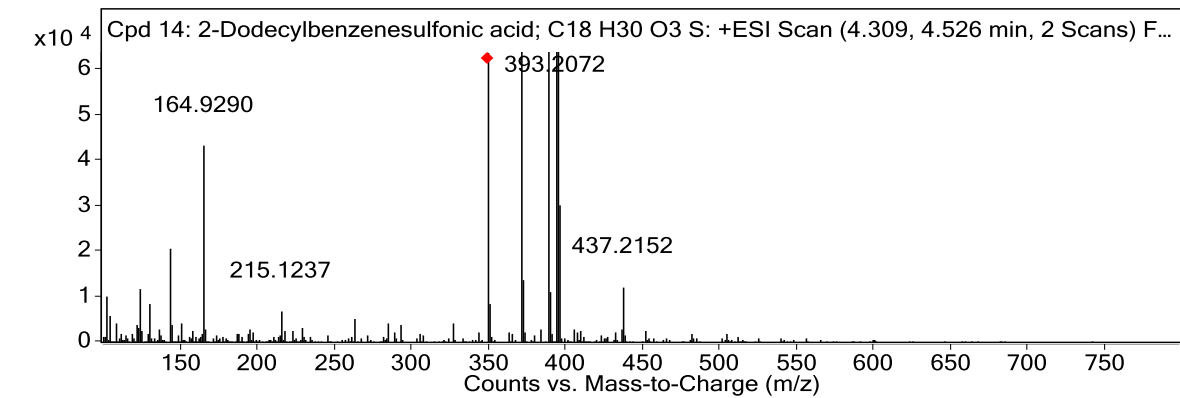
m/z	z	Abund
102.1277		117.94
104.1054		141.84
142.9458		124.4
147.0432		106.02
148.1093		102.43
164.9292		249.63
349.0871	1	564.15
349.1807	1	5504.21
350.0883	1	102.75
350.1842	1	426.65

Compound Structure

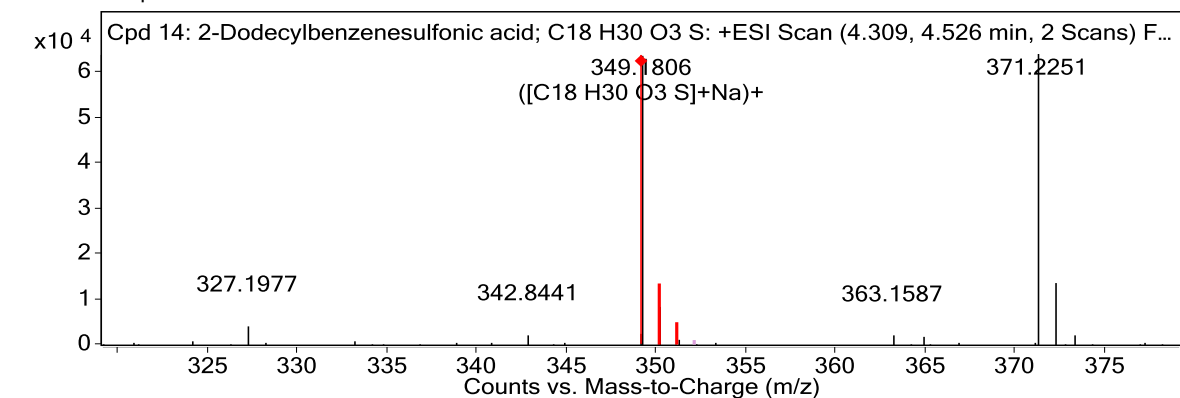


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 14: 2-Dodecylbenzenesulfonic acid; C18 H30 O3 S	2-Dodecylbenzenesulfonic acid	349.1806	4.434	Auto MS/MS	326.1914

MS Spectrum



MS Zoomed Spectrum

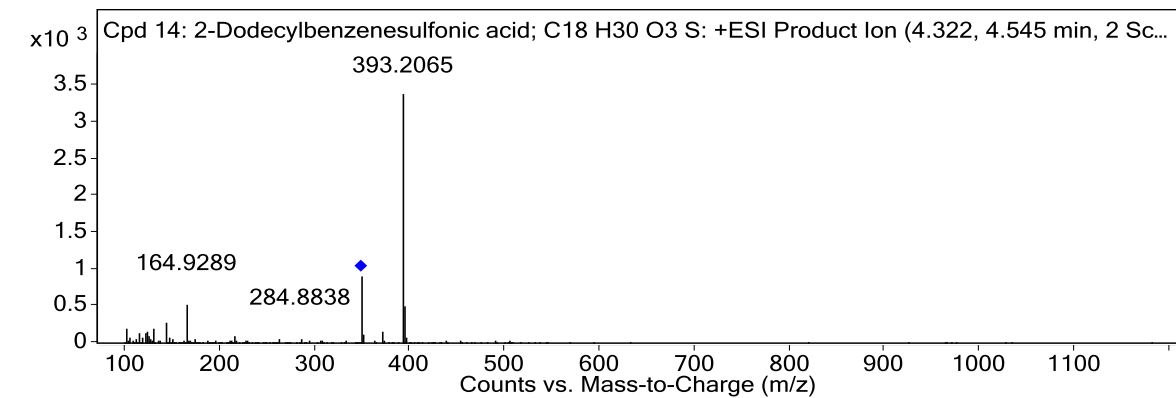


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
142.9471				20776.75		
164.929				43352		
349.1806	349.1808	0.62	1	63734.27	C18 H30 O3 S	(M+Na)+
350.1833	350.184	2.08	1	8415.26	C18 H30 O3 S	(M+Na)+
351.1849	351.1804	-12.96	1	1394.49	C18 H30 O3 S	(M+Na)+
371.2251			1	90250.01		
388.2514			1	74271.17		
393.2072			1	1330233		
394.2109			1	215508.77		
395.2121			1	30342.89		

MSMS Spectrum

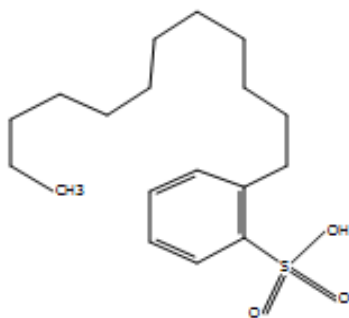
Qualitative Compound Report



MS/MS Spectrum Peak List

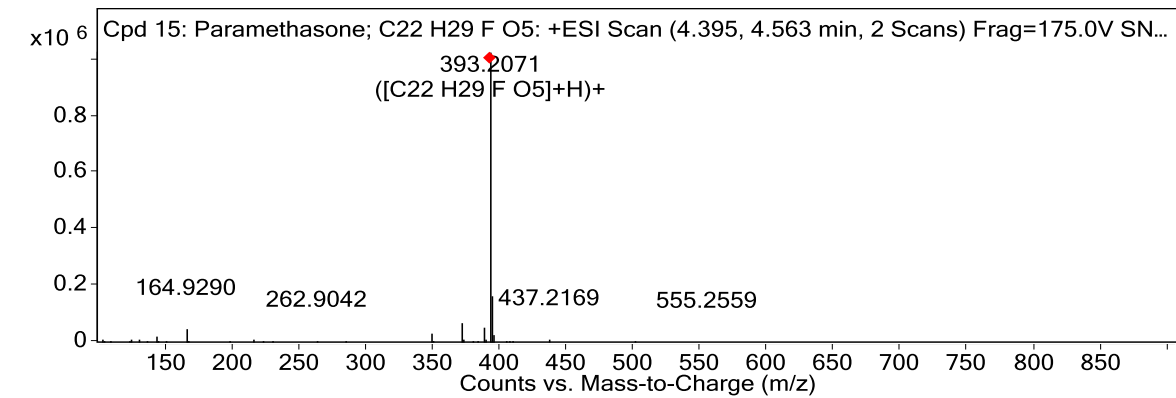
m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
102.1271			1	193.28		
122.0952				135.18		
124.0851			1	156.28		
130.0636				207.87		
142.9473				279.66		
164.9289				532.81		
349.1805	349.1808	0.71	1	913.33	C ₁₈ H ₃₀ O ₃ S	(M+Na) ⁺
371.2251			1	164.27		
393.2065			1	3390.51		
394.2095			1	508.73		

Compound Structure

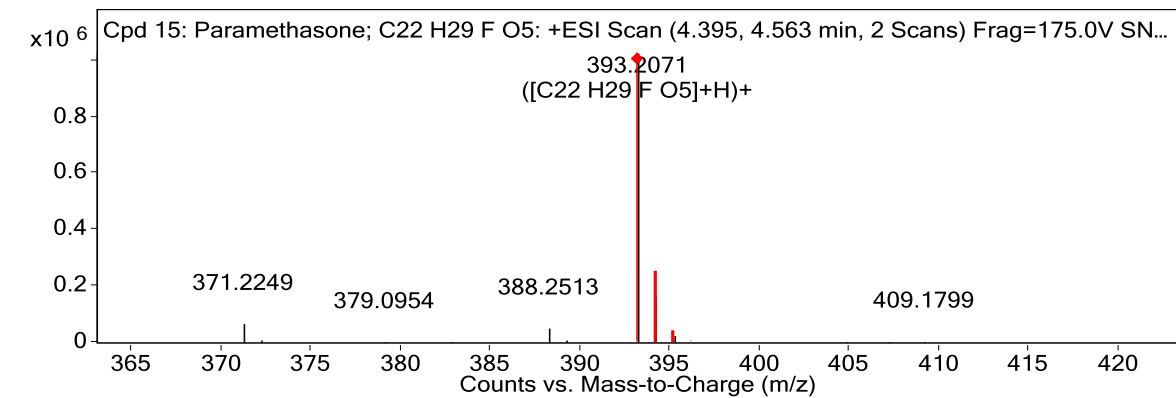


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 15: Paramethasone; C ₂₂ H ₂₉ F O ₅	Paramethasone	393.2071	4.493	Auto MS/MS	392.1998

MS Spectrum



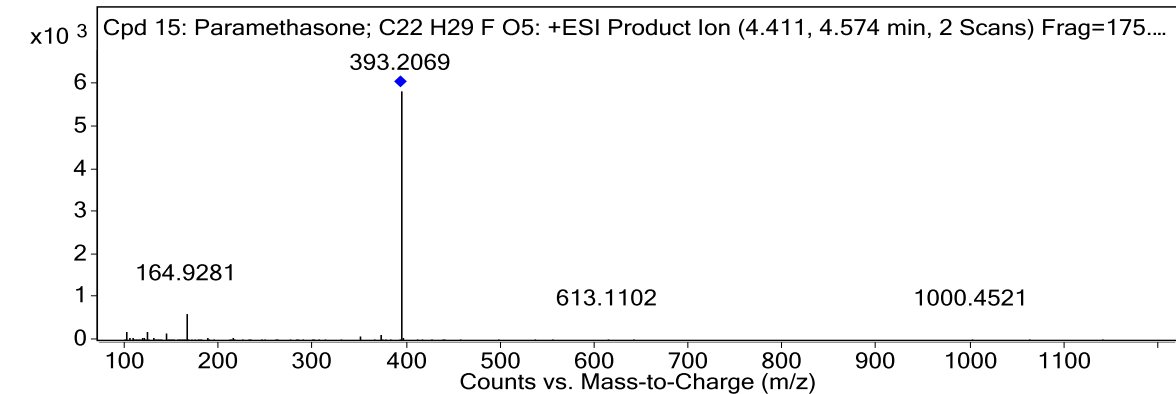
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
142.9469				19167.62		
164.929				47133.98		
349.18			1	29092.38		
371.2249			1	67889.23		
372.2276			1	10782.21		
388.2513			1	51846.6		
393.2071	393.2072	0.26	1	1024860.25	C ₂₂ H ₂₉ F O ₅	(M+H) ⁺
394.2107	394.2106	-0.31	1	162114.72	C ₂₂ H ₂₉ F O ₅	(M+H) ⁺
395.2119	395.2133	3.5	1	24488.8	C ₂₂ H ₂₉ F O ₅	(M+H) ⁺
437.2169			1	10443.2		

MSMS Spectrum



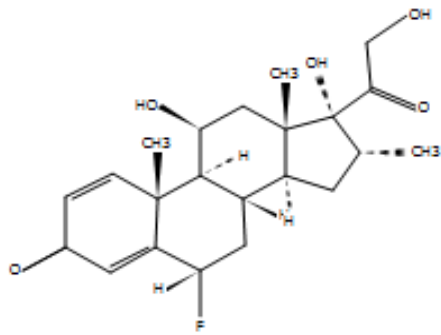
MS/MS Spectrum Peak List

m/z	z	Abund
102.127		208.38

Qualitative Compound Report

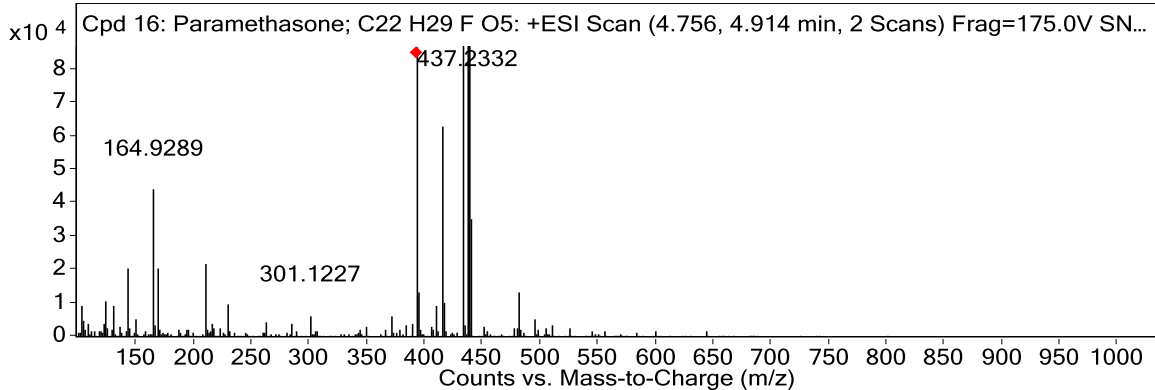
123.0895		105.91
124.0857		213.32
142.9473		182.37
144.0985		84.03
164.9281		616.79
349.1816	1	121.03
371.2249		122.67
393.2069	1	5846.93
394.2096	1	647.81

Compound Structure

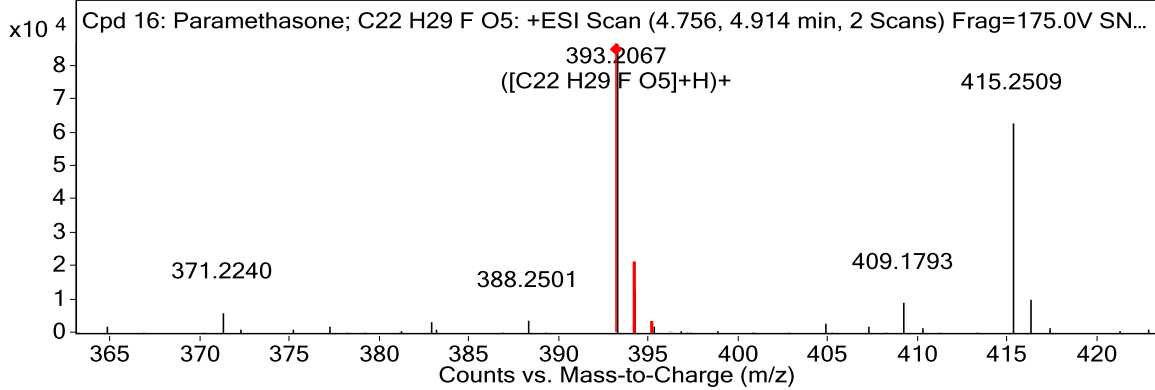


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 16: Paramethasone; C22 H29 F O5	Paramethasone	393.2067	4.85	Auto MS/MS	392.1993

MS Spectrum



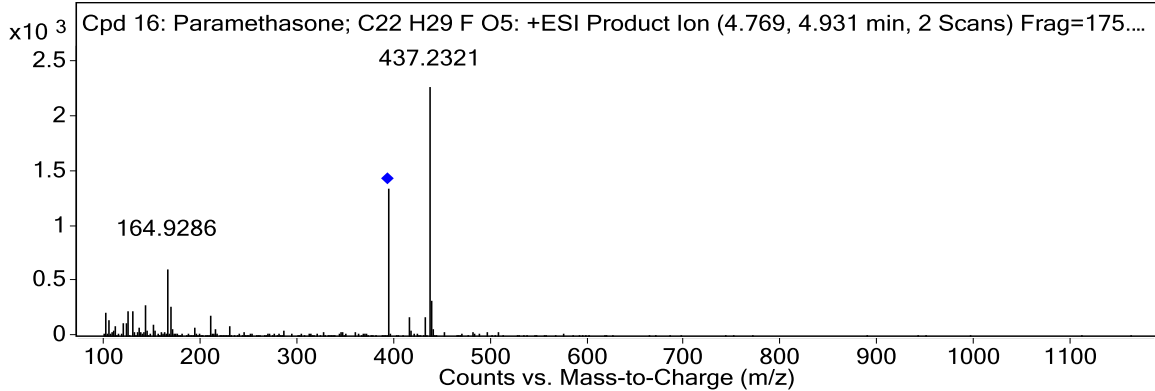
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
164.9289				44186.78		
393.2067	393.2072	1.27	1	86702.33	C22 H29 F O5	(M+H)+
394.2094	394.2106	2.87	1	13507.48	C22 H29 F O5	(M+H)+
395.2119	395.2133	3.54	1	2435.47	C22 H29 F O5	(M+H)+
415.2509			1	63154.39		
432.2778			1	132424.03		
433.2799			1	23618.03		
437.2332			1	1257102.13		
438.237			1	227733.39		
439.2377			1	35201.26		

MSMS Spectrum

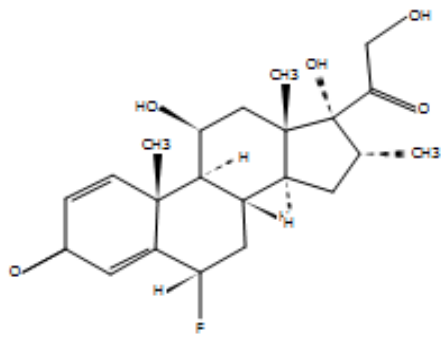


MS/MS Spectrum Peak List

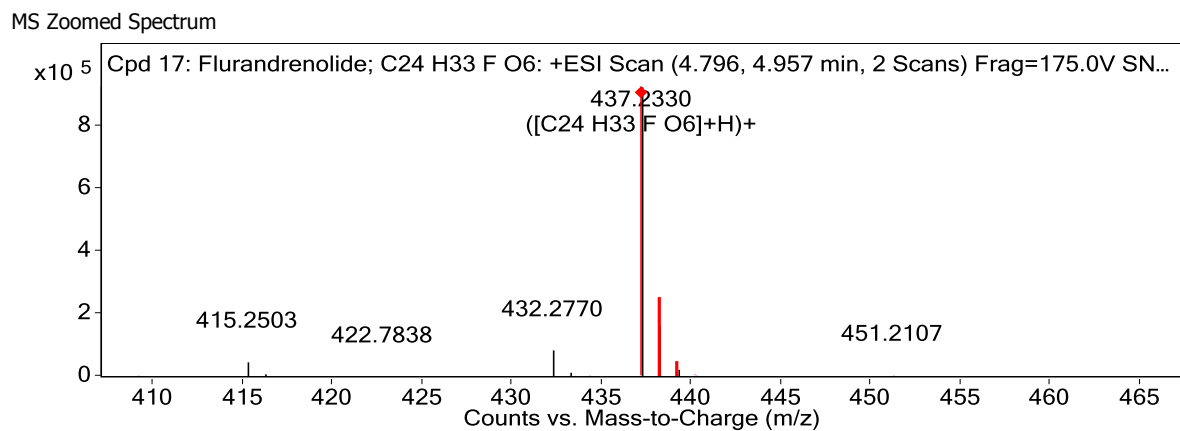
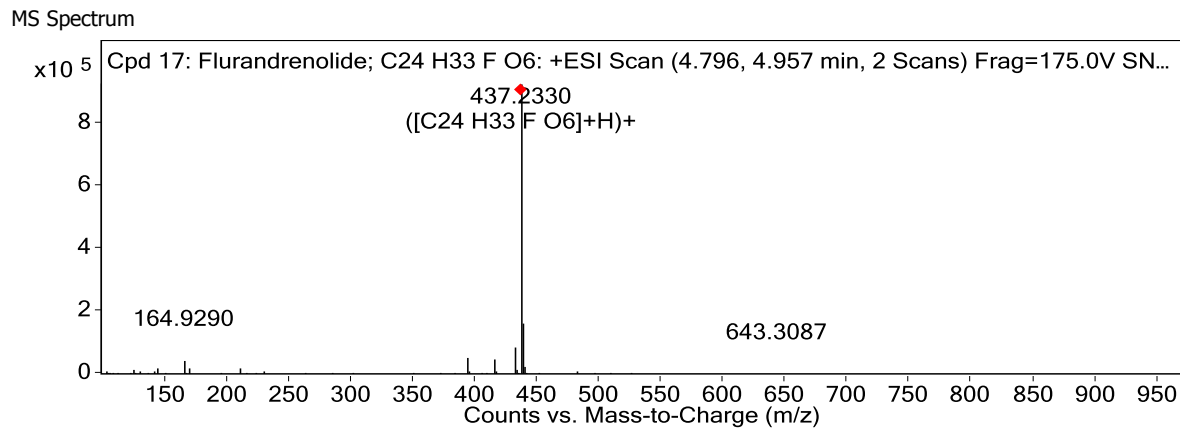
m/z	z	Abund
102.1275	1	217.97
124.0875		225.7
130.0627	1	228.23
142.946		285.38
164.9286		607.69
169.0741	1	265.58
210.134		185.29
393.2052	1	1347.87
437.2321	1	2275.52
438.2371	1	328.22

Compound Structure

Qualitative Compound Report

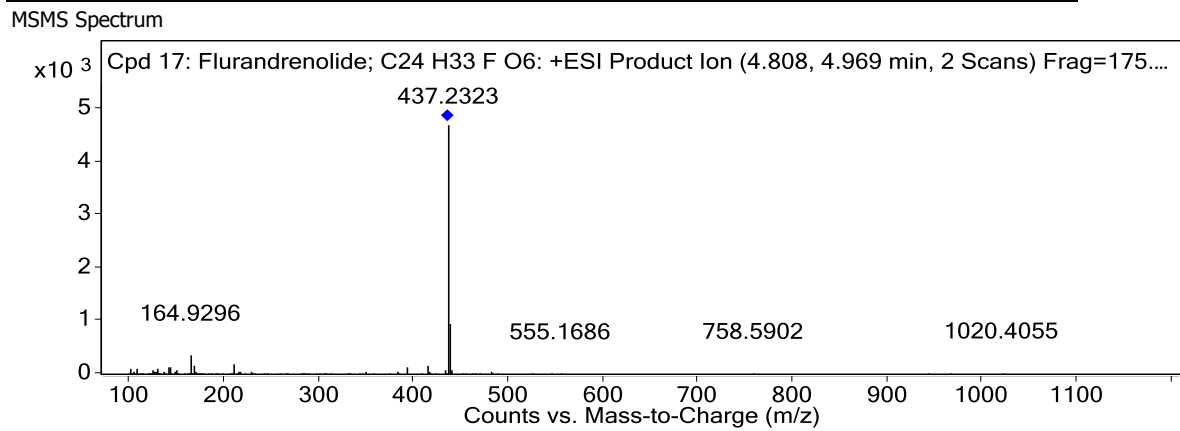


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 17: Flurandrenolide; C24 H33 F O6	Flurandrenolide	437.233	4.889	Auto MS/MS	436.2257



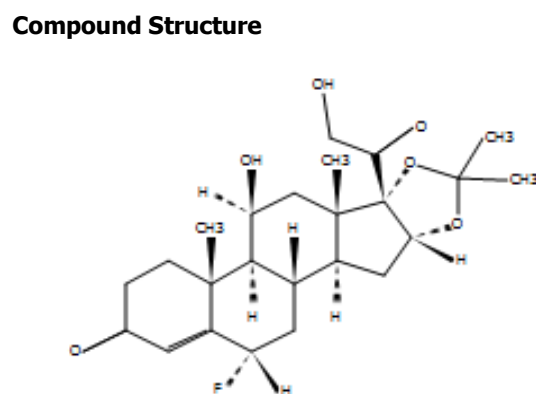
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
142.947				19980.25		
164.929				45068.98		
169.0749			1	17856.76		
210.1334			1	17818.95		
393.2064			1	54129.51		
415.2503			1	48569.85		
432.277			1	84782.7		
437.233	437.2334	0.86	1	922162.44	C24 H33 F O6	(M+H)+
438.2364	438.2368	0.85	1	163531.77	C24 H33 F O6	(M+H)+
439.2374	439.2395	4.88	1	24055.82	C24 H33 F O6	(M+H)+



MS/MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
102.1256				124.39		
141.0688				132.02		
142.9456				135.59		
164.9296				371.38		
169.0766			1	157.87		
210.1349				192.54		
393.2075				149.01		
415.246			1	159.36		
437.2323			1	4698.02		
438.2363	438.2368	1.06	1	958.93	C24 H33 F O6	(M+H)+

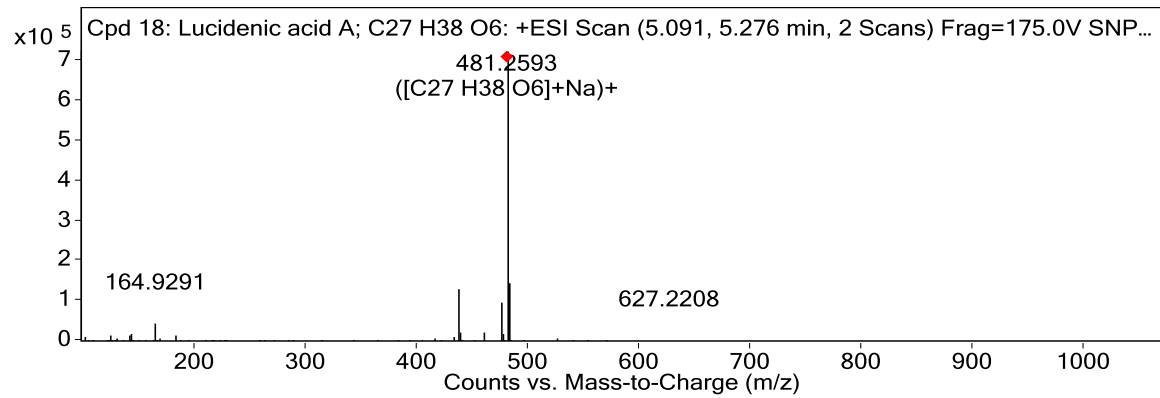


Compound Label	Name	m/z	RT	Algorithm	Mass
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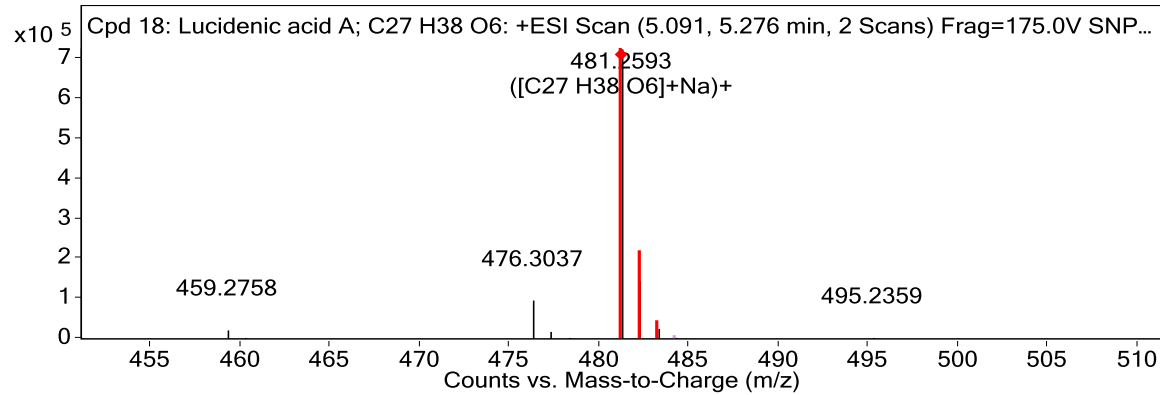
Qualitative Compound Report

Cpd 18: Lucidenic acid A; C27 H38 O6	Lucidenic acid A	481.2593	5.198	Auto MS/MS	458.2701
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MS Spectrum



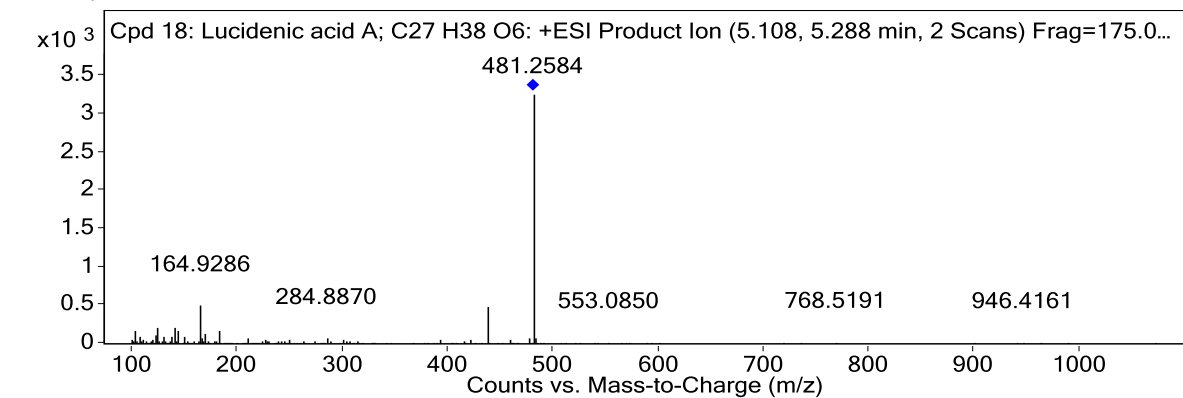
MS Zoomed Spectrum



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>z</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
142.9471				18971.8		
164.9291				44155.48		
437.2329			1	130725.66		
438.2355			1	22121.76		
459.2758			1	23871.38		
476.3037			1	97173.85		
477.3061			1	17756.7		
481.2593	481.2561	-6.74	1	724197.19	C27 H38 O6	(M+Na)+
482.2629	482.2595	-7.04	1	147317.58	C27 H38 O6	(M+Na)+
483.2638	483.2623	-3.12	1	24608.42	C27 H38 O6	(M+Na)+

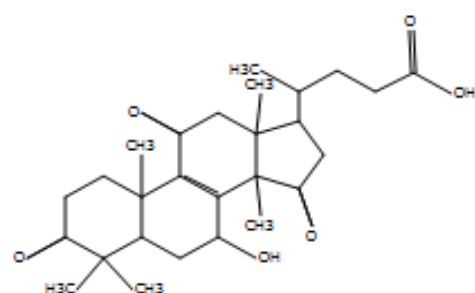
MSMS Spectrum



MS/MS Spectrum Peak List

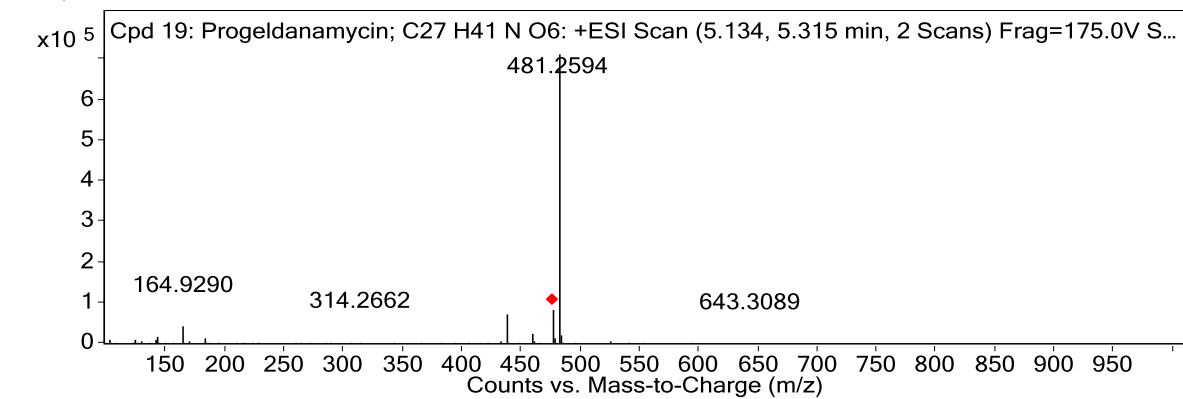
m/z	z	Abund
102.1265	1	166.36
124.0858		207.58
141.0697	1	216.45
142.9468		182.82
164.9286		505.04
183.0914		168.16
437.2306	1	478.48
438.2341	1	173.17
481.2584	1	3258.75
482.26	1	916.7

Compound Structure

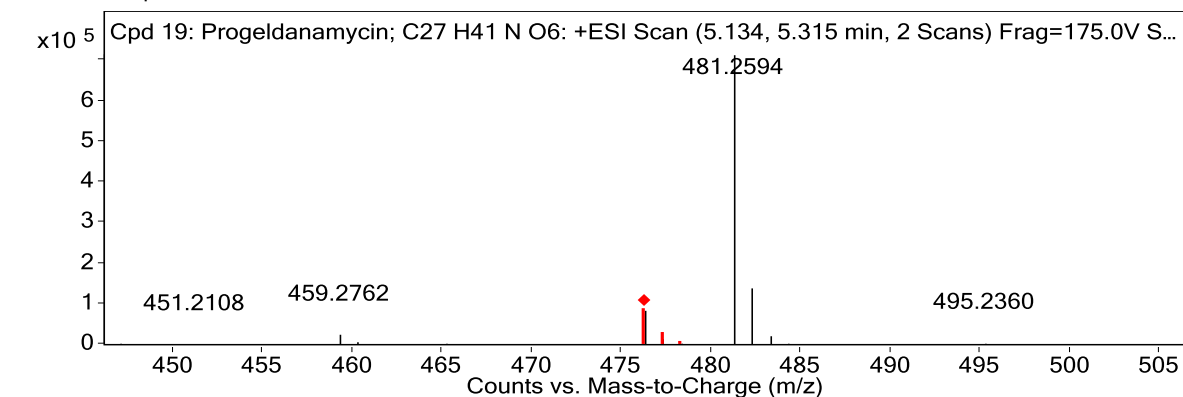


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 19: Progeldanamycin; C27 H41 N O6	Progeldanamycin	476.3033	5.239	Auto MS/MS	475.2958

MS Spectrum



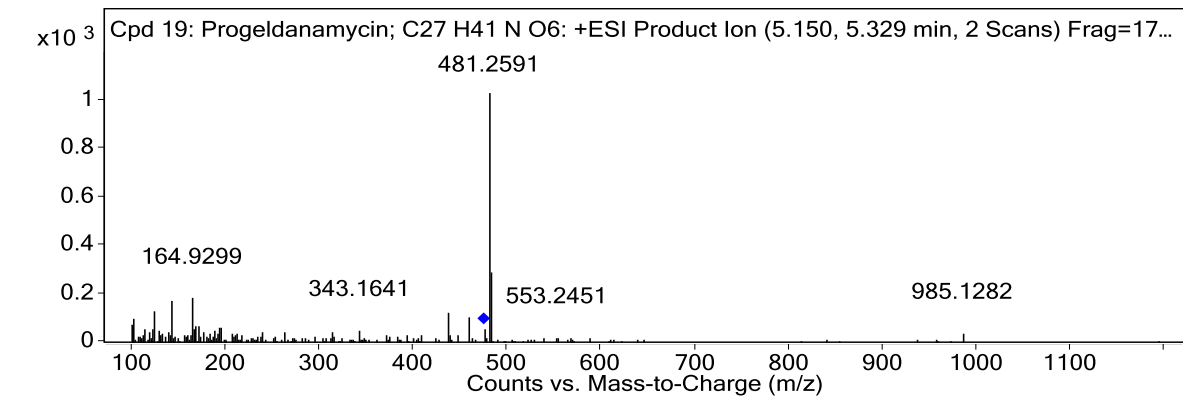
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
142.947				18130.63		
164.929				44073.57		
437.2324			1	73732.45		
459.2762			1	24991.09		
476.3033	476.3007	-5.6	1	85307.3	C27 H41 N O6	(M+H)+
477.3056	477.304	-3.43	1	16273.24	C27 H41 N O6	(M+H)+
478.3074	478.3068	-1.25	1	3498.22	C27 H41 N O6	(M+H)+
481.2594			1	712134.63		
482.2624			1	140228.58		
483.2633			1	23603.7		

MSMS Spectrum

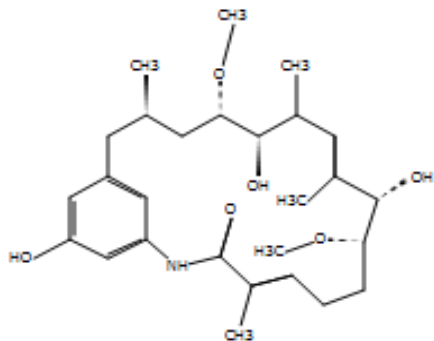


MS/MS Spectrum Peak List

<i>m/z</i>	<i>z</i>	Abund
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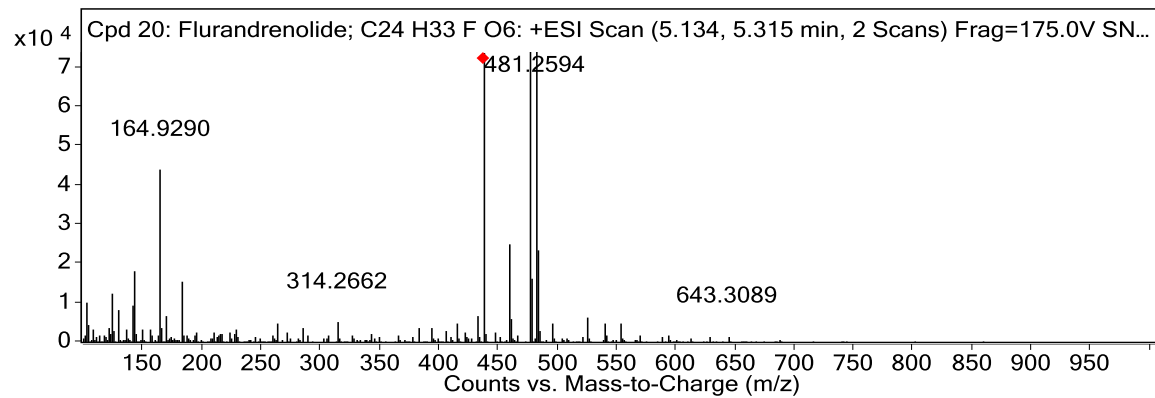
101.0693		74.25
102.1268		98.3
124.086	1	132.03
142.9476		174.4
164.9299		184.52
169.0762		67.33
437.233	1	121.11
459.2712		106.31
481.2591	1	1032.99
482.2623	1	291.53

Compound Structure

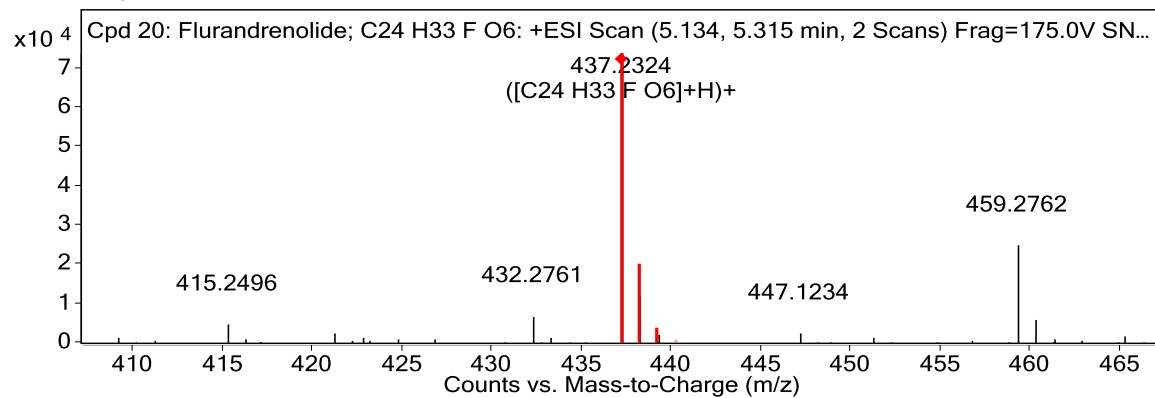


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 20: Flurandrenolide; C24 H33 F O6	Flurandrenolide	437.2324	5.243	Auto MS/MS	436.225

MS Spectrum



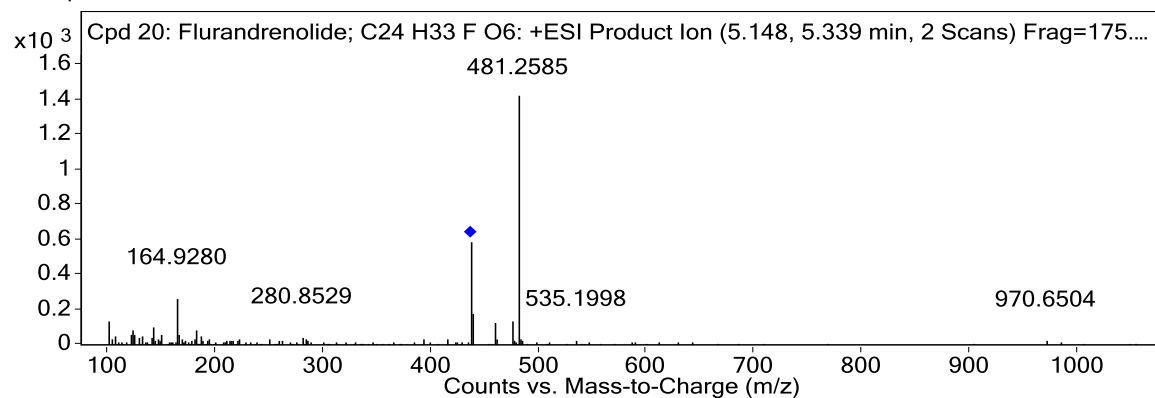
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
142.947				18130.63		
164.929				44073.57		
437.2324	437.2334	2.25	1	73732.45	C24 H33 F O6	(M+H)+
438.235	438.2368	4.11	1	12186.74	C24 H33 F O6	(M+H)+
439.237	439.2395	5.72	1	2169.04	C24 H33 F O6	(M+H)+
459.2762			1	24991.09		
476.3033			1	85307.3		
481.2594			1	712134.63		
482.2624			1	140228.58		
483.2633			1	23603.7		

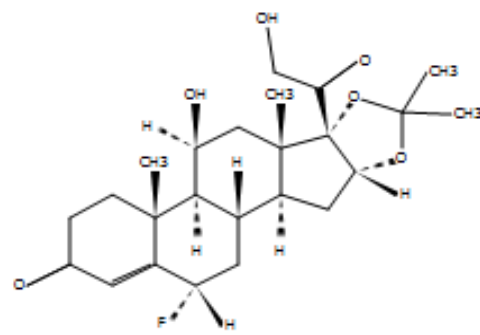
MSMS Spectrum



MS/MS Spectrum Peak List

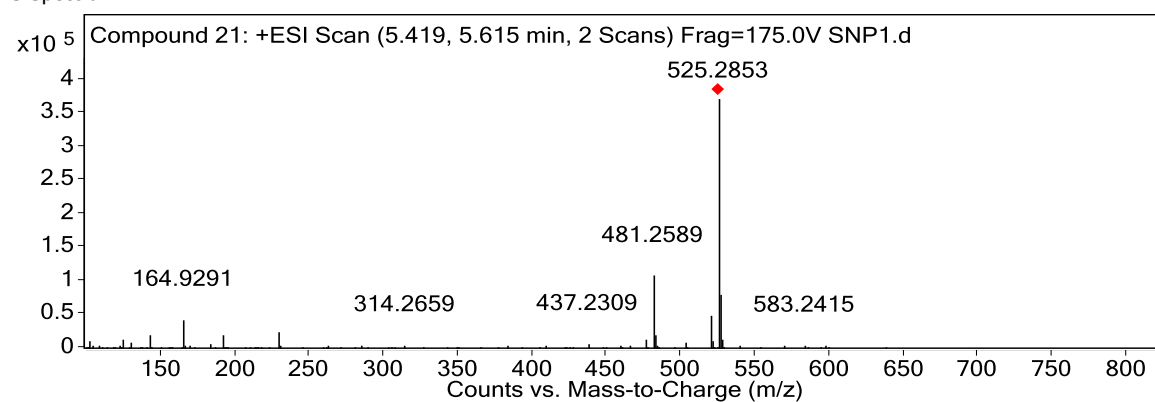
m/z	z	Abund
102.1257		140.41
124.0862		83.57
142.947		100.7
164.928		267.68
437.231	1	587.19
438.2328	1	182.1
459.275	1	125.55
476.301	1	138.13
481.2585	1	1425.41
482.2603	1	242.33

Compound Structure

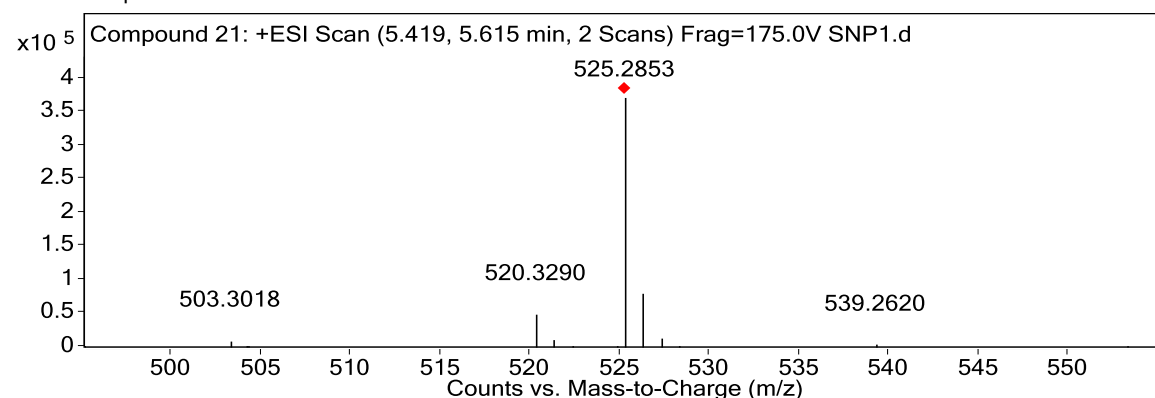


Compound Label	<i>m/z</i>	RT	Algorithm
Compound 21	525.2853	5.53	Auto MS/MS

MS Spectrum



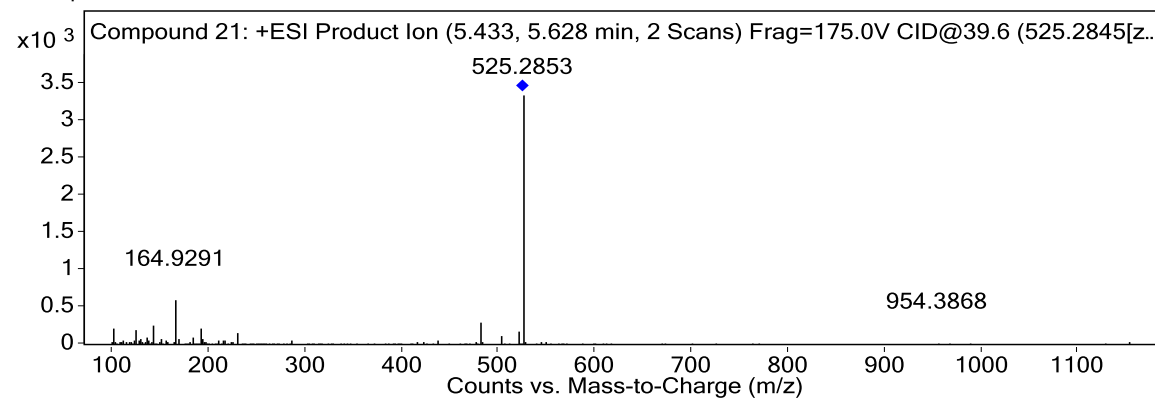
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
142.9469		19361.72
164.9291		42390.76
192.1005	1	19688.54
229.1392	1	23752.86
481.2589	1	107693.93
482.2612	1	20884.15
520.329	1	49225.63
525.2853	1	370936.75
526.2882	1	79921.53
527.2889	1	14196.97

MSMS Spectrum



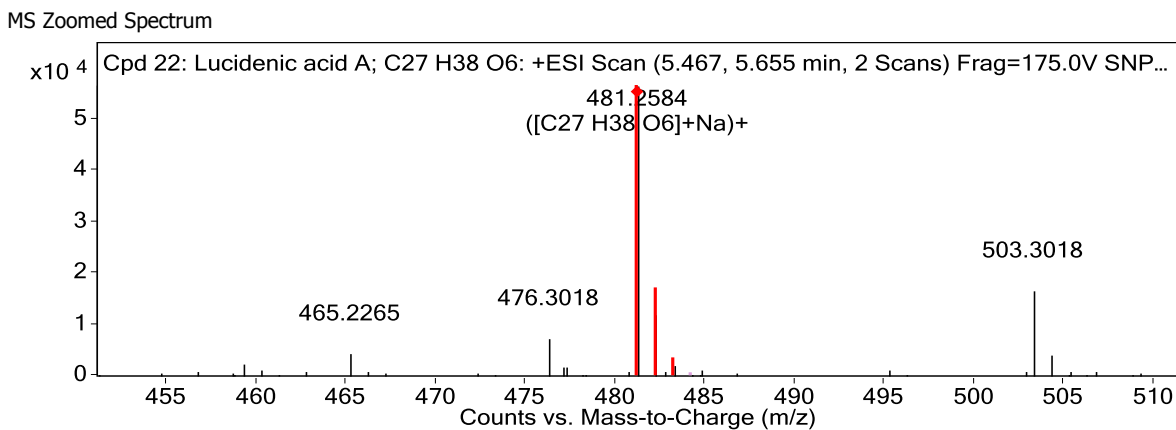
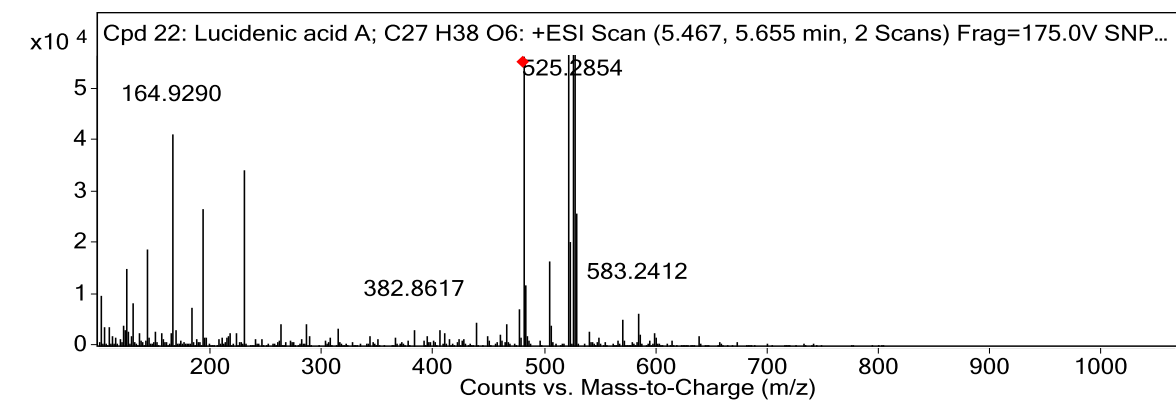
MS/MS Spectrum Peak List

m/z	z	Abund
102.1278	1	224.5
124.087		208.34
142.9463		262.8
164.9291		602.22
192.1002	1	229.41
229.1361	1	159.61
481.257	1	292.75
520.3249	1	170.76
525.2853	1	3344.06
526.2859	1	761.35

Compound Label	Name	<i>m/z</i>	RT	Algorithm	Mass
Cpd 22: Lucidenic acid A; C27 H38 O6	Lucidenic acid A	481.2584	5.582	Auto MS/MS	458.2689

MS Spectrum

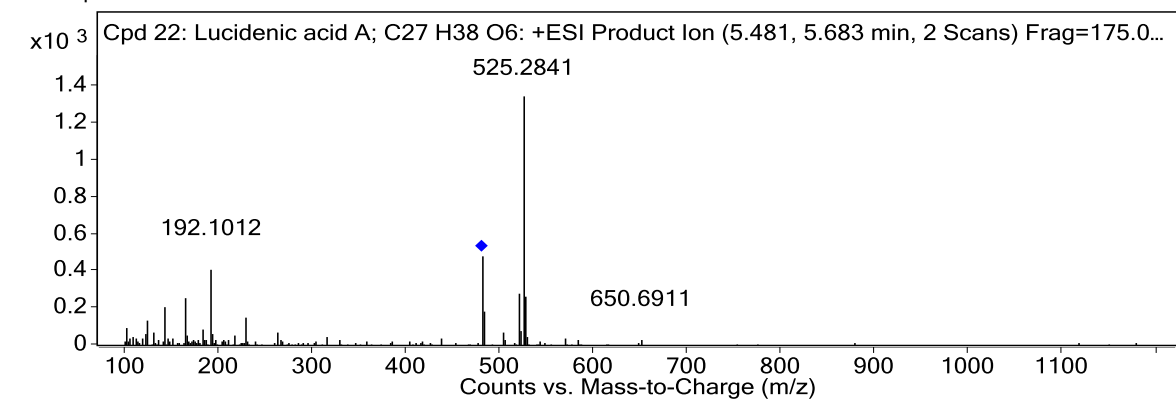
Qualitative Compound Report



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
164.929				41198.93		
192.1008			1	26629.88		
229.1393			1	34282.06		
481.2584	481.2561	-4.9	1	56340.16	C27 H38 O6	(M+Na)+
482.2607	482.2595	-2.66	1	11944.66	C27 H38 O6	(M+Na)+
483.262	483.2623	0.54	1	2166.38	C27 H38 O6	(M+Na)+
520.3294			1	97417.88		
525.2854			1	709510.63		
526.2886			1	157743.58		
527.2894			1	25891.41		

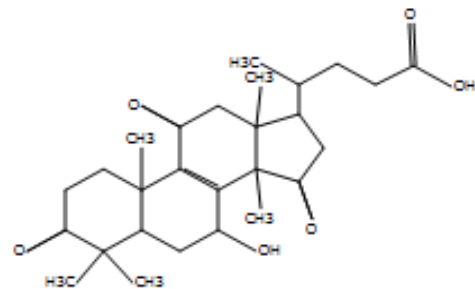
MSMS Spectrum



MS/MS Spectrum Peak List

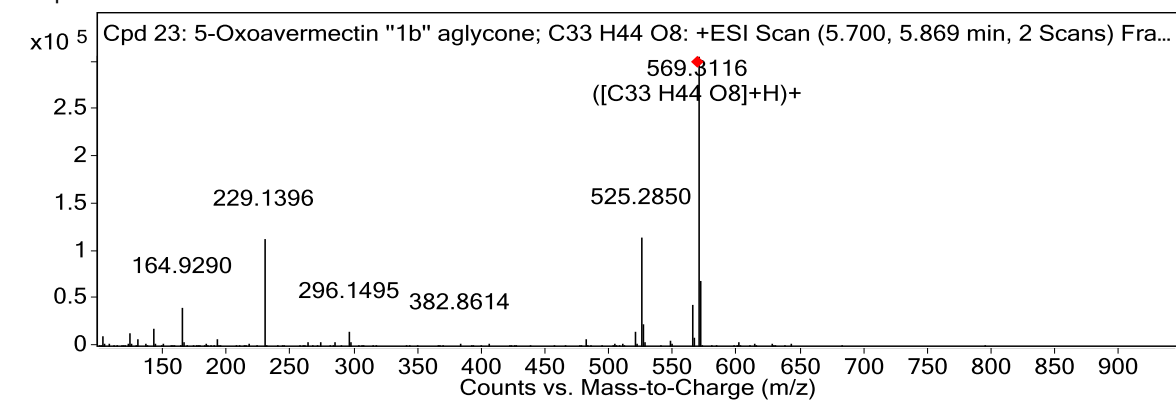
<i>m/z</i>	<i>z</i>	Abund
124.0874		137.57
142.9465		208.74
164.9282		257.31
192.1012	1	413.76
229.1377		150.85
481.2563	1	482.97
482.2556	1	182
520.3259	1	283.05
525.2841	1	1347.2
526.2881	1	263.12

Compound Structure

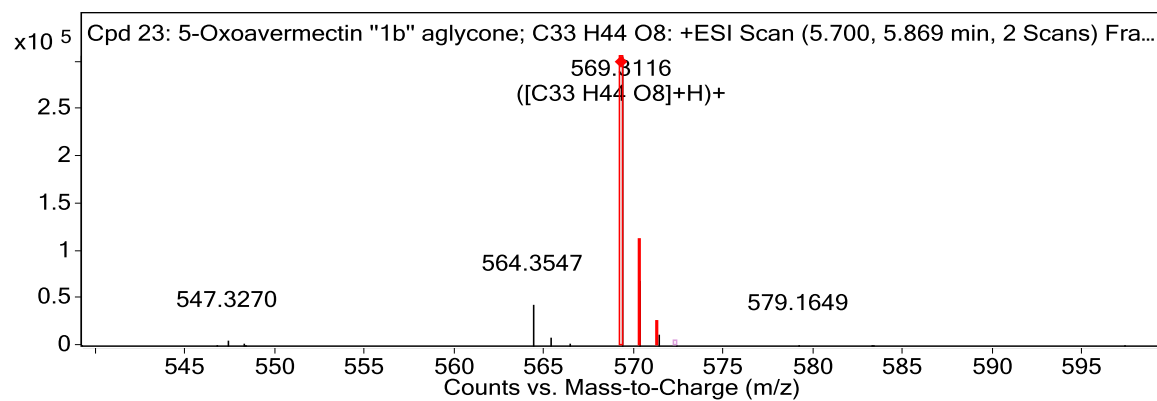


Compound Label	Name	<i>m/z</i>	RT	Algorithm	Mass
Cpd 23: 5-Oxoavermectin "1b" aglycone; C33 H44 O8	5-Oxoavermectin "1b" aglycone	569.3116	5.798	Auto MS/MS	568.3041

MS Spectrum



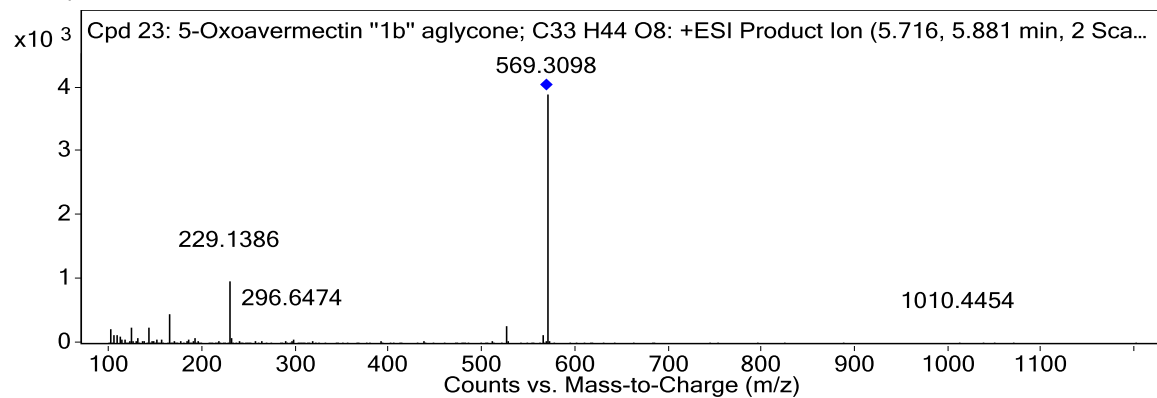
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
142.9469				18476.49		
164.929				41510.8		
229.1396			1	112823.39		
520.328			1	15528.78		
525.285			1	114492.27		
526.2869			1	24267.79		
564.3547			1	43980.86		
569.3116	569.3109	-1.16	1	305733.44	C33 H44 O8	(M+H)+
570.3142	570.3143	0.16	1	68764.44	C33 H44 O8	(M+H)+
571.3159	571.3172	2.27	1	13047.42	C33 H44 O8	(M+H)+

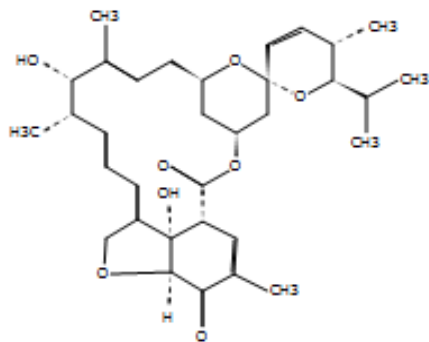
MSMS Spectrum



MS/MS Spectrum Peak List

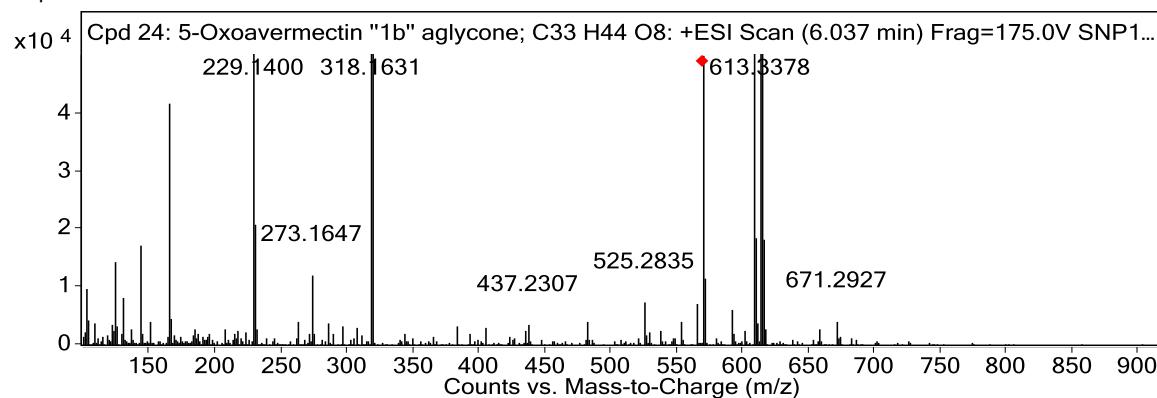
m/z	z	Abund
102.1271	1	241.12
104.1057		139.39
108.0805		151.17
124.086		266.61
142.9463		262.12
164.9288		467.02
229.1386	1	984.03
525.2866	1	290.52
569.3098	1	3900.45
570.3115	1	527.95

Compound Structure

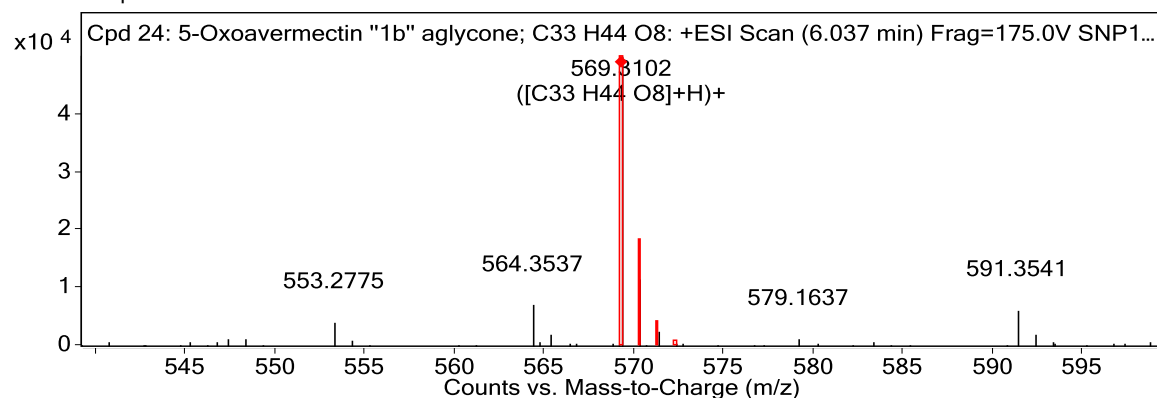


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 24: 5-Oxoavermectin "1b" aglycone; C33 H44 O8	5-Oxoavermectin "1b" aglycone	569.3102	6.052	Auto MS/MS	568.3027

MS Spectrum



MS Zoomed Spectrum



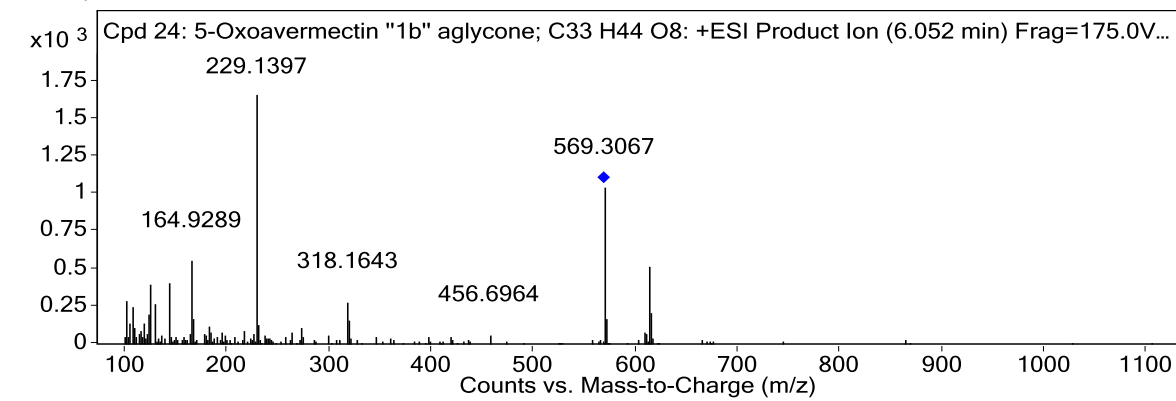
MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	z	Abund	Formula	Ion
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Qualitative Compound Report

229.14			1	211247.86		
318.1631			2	216950.27		
318.6643			2	60537.75		
569.3102	569.3109	1.18	1	49959.05	C33 H44 O8	(M+H)+
570.3127	570.3143	2.78	1	11595.58	C33 H44 O8	(M+H)+
571.3148	571.3172	4.16	1	2617.2	C33 H44 O8	(M+H)+
572.3151	572.32	8.53	1	584.26	C33 H44 O8	(M+H)+
608.3812			1	71482.13		
613.3378			1	412863.31		
614.3402			1	101598.99		

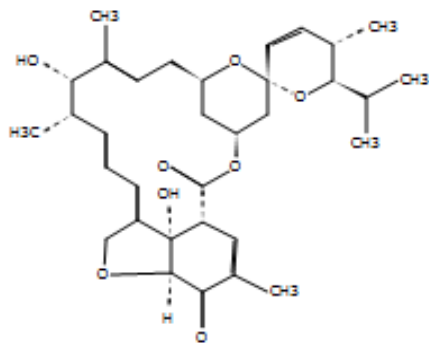
MSMS Spectrum



MS/MS Spectrum Peak List

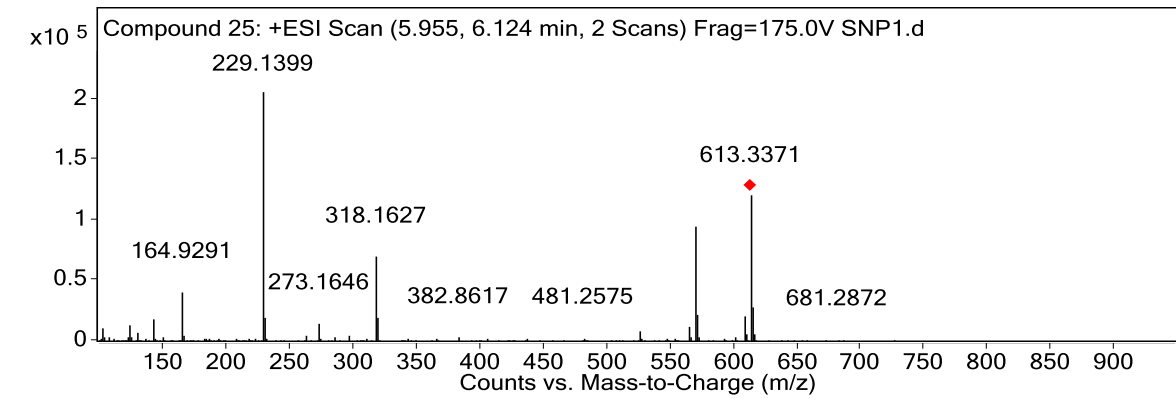
m/z	z	Abund
102.1262	1	285.97
108.0803		247
124.0866		396.4
130.0645		270.02
142.9471		405.39
164.9289		552.42
229.1397	1	1660.09
318.1643	2	280.77
569.3067	1	1041.44
613.3334	1	515.85

Compound Structure

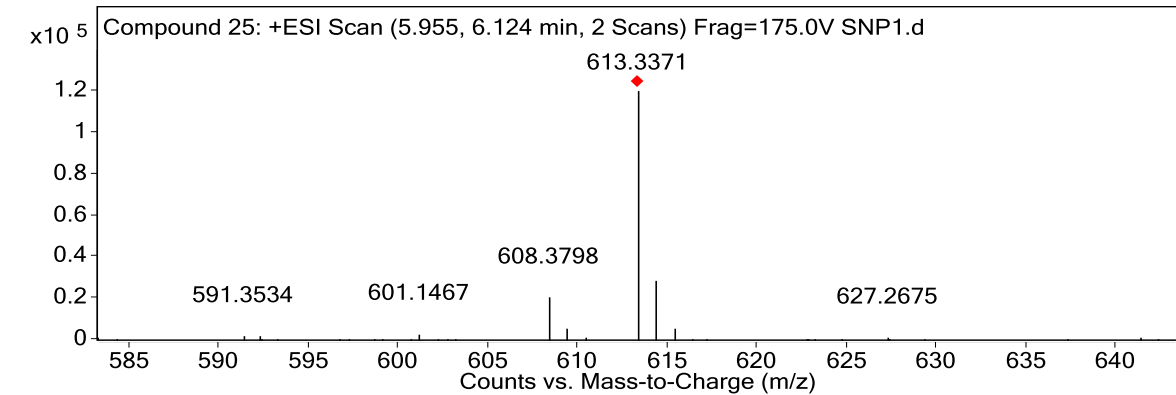


Compound Label	m/z	RT	Algorithm
Compound 25	613.3371	6.056	Auto MS/MS

MS Spectrum



MS Zoomed Spectrum

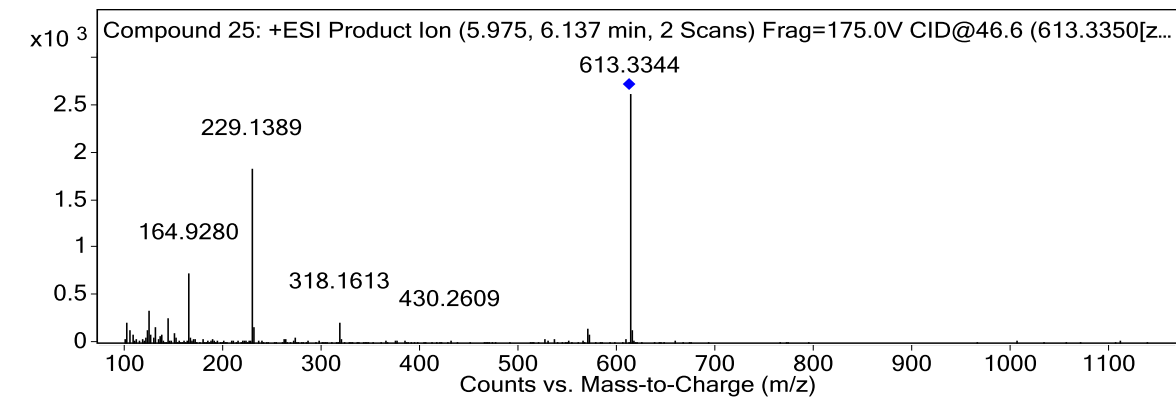


MS Spectrum Peak List

m/z	z	Abund
164.9291		40912.85
229.1399	1	206367.22
230.1426	1	20073.76
318.1627	2	70254.84
569.3109	1	95181.13
570.3126	1	21675.37
608.3798	1	20701.43
613.3371	1	120488.34
614.3396	1	28873.34
615.3406	1	5702.34

MSMS Spectrum

Qualitative Compound Report

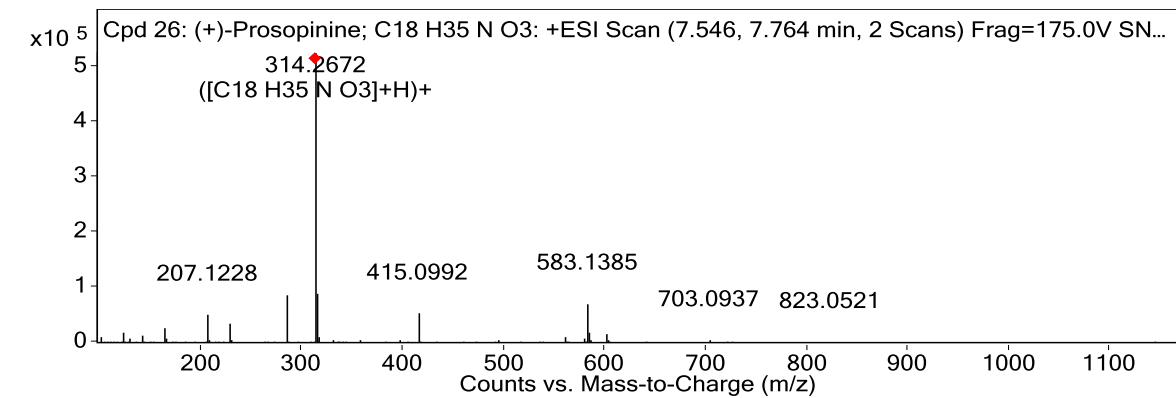


MS/MS Spectrum Peak List

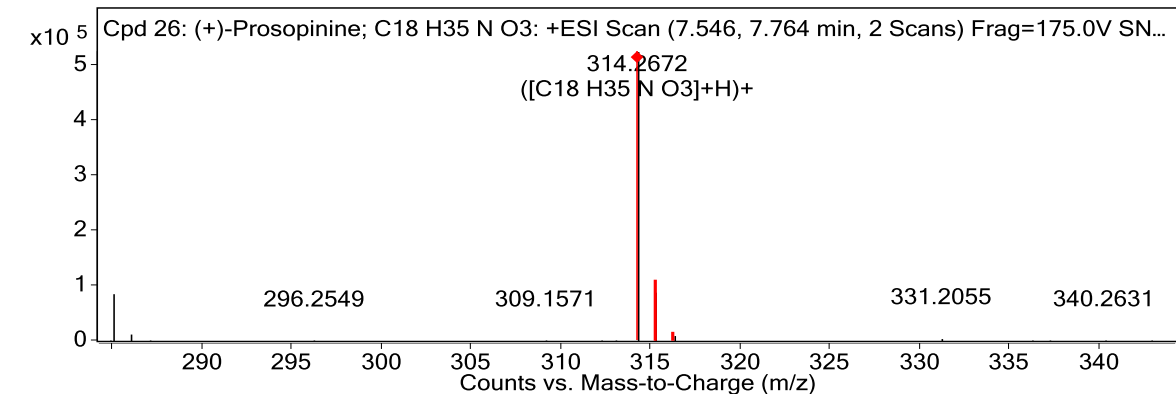
m/z	z	Abund
102.127		216.09
124.0866		344.36
130.0642		178.06
142.9471		266.62
164.928		737.93
229.1389	1	1837.76
230.1424	1	178.5
318.1613	2	219.21
569.3056	1	164.29
613.3344	1	2626.71

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 26: (+)-Prosopinine; C18 H35 N O3	(+)-Prosopinine	314.2672	7.671	Auto MS/MS	313.2599

MS Spectrum



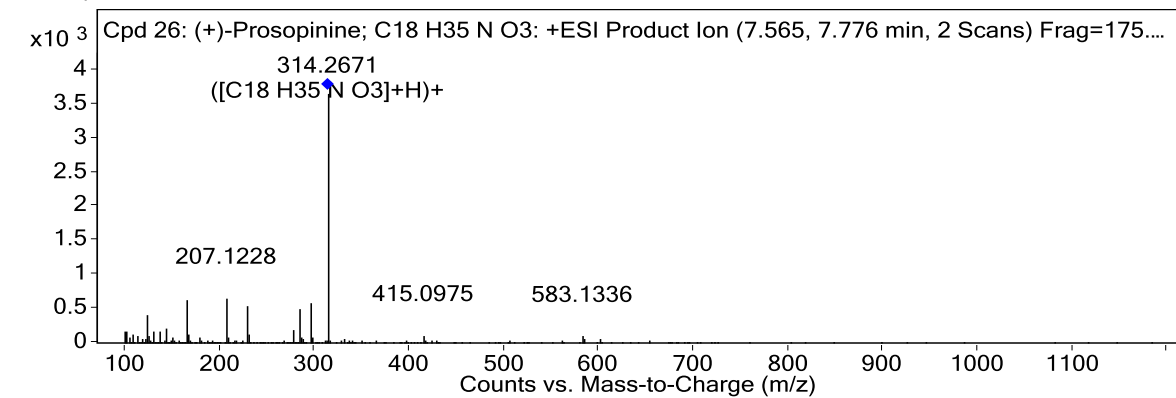
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0864			1	18357.38		
164.929				27463.03		
207.1228			1	50830.38		
229.139			1	34586.32		
285.0738			1	85614.3		
314.2672	314.269	5.57	1	523114.16	C18 H35 N O3	(M+H)+
315.2702	315.2723	6.47	1	89779.88	C18 H35 N O3	(M+H)+
316.2721	316.275	9.26	1	9642.31	C18 H35 N O3	(M+H)+
415.0992			1	52816.63		
583.1385			1	70852.07		

MSMS Spectrum

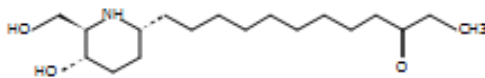


MS/MS Spectrum Peak List

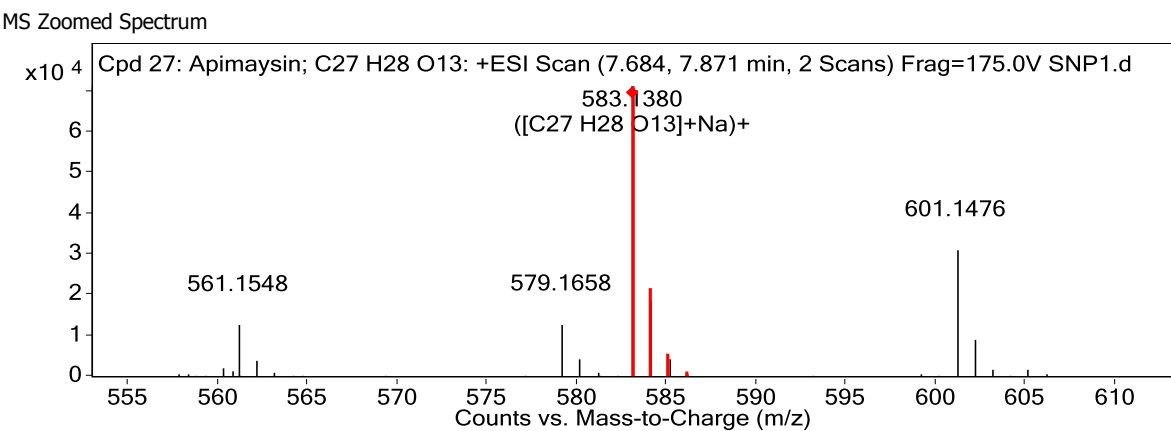
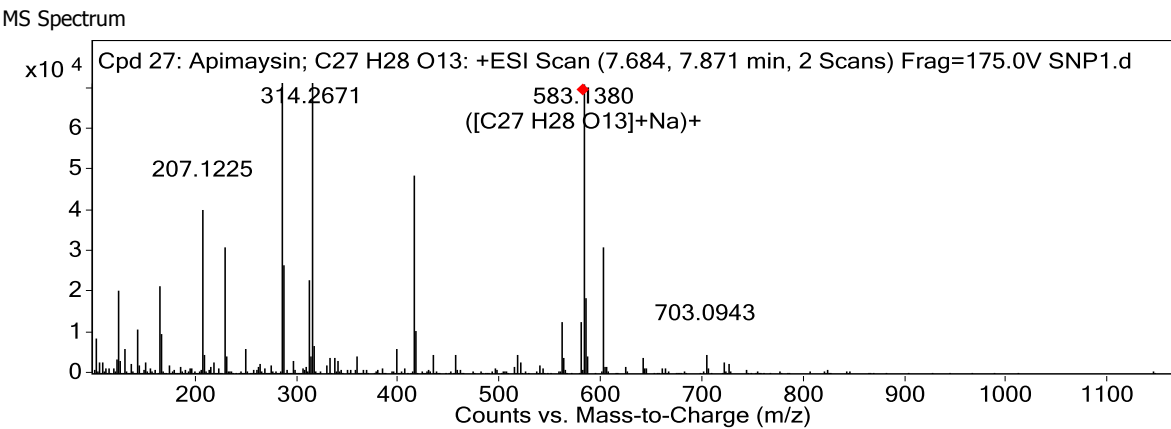
m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
124.0858			1	408.3		
142.9477				212.72		
164.9283				635.41		
165.1112				207.61		
207.1228			1	666.01		
229.1381			1	553.48		
285.0727			1	500.36		
296.2549			1	595.72		
314.2671	314.269	5.83	1	3653.74	C18 H35 N O3	(M+H)+
315.2701			1	433.8		

Compound Structure

Qualitative Compound Report

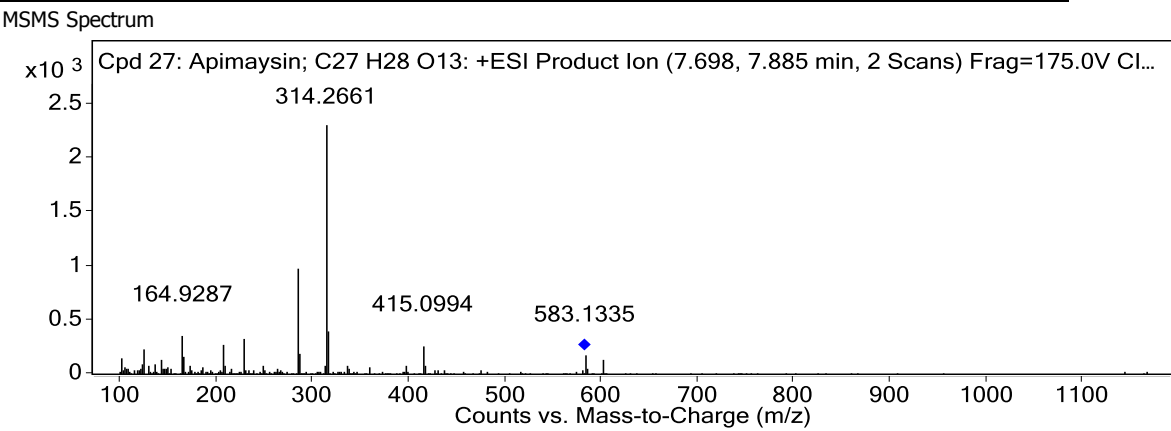


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 27: Apimaysin; C27 H28 O13	Apimaysin	583.138	7.791	Auto MS/MS	560.1485



MS Spectrum Peak List

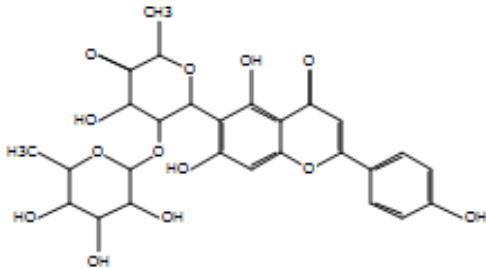
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
207.1225			1	40120.2		
285.074			1	183492.55		
314.2671			1	383224.72		
315.0836			1	36309.54		
315.2696			1	61946.42		
415.0987			1	48536.59		
583.138	583.1422	7.27	1	70921.27	C27 H28 O13	(M+Na)+
584.14	584.1456	9.57	1	18463.4	C27 H28 O13	(M+Na)+
585.1432	585.148	8.28	1	4430.93	C27 H28 O13	(M+Na)+
586.1452	586.1507	9.41	1	837.42	C27 H28 O13	(M+Na)+



MS/MS Spectrum Peak List

m/z	z	Abund
124.0863		235.43
164.9287		361.18
207.1222	1	274.77
229.1384	1	337.94
285.073	1	980.95
286.076	1	187.16
314.2661	1	2309.47
315.0814	1	324.63
315.2696	1	403.75
415.0994	1	269.16

Compound Structure

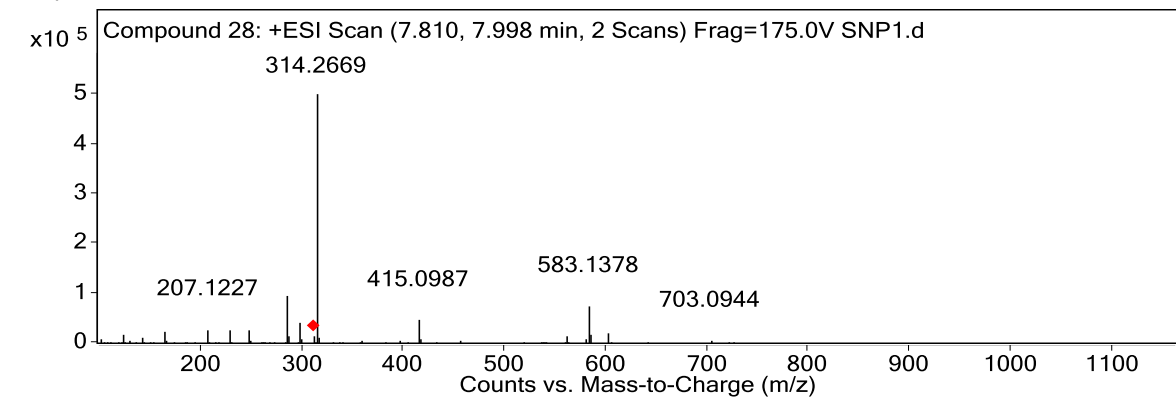


Compound Label	m/z	RT	Algorithm
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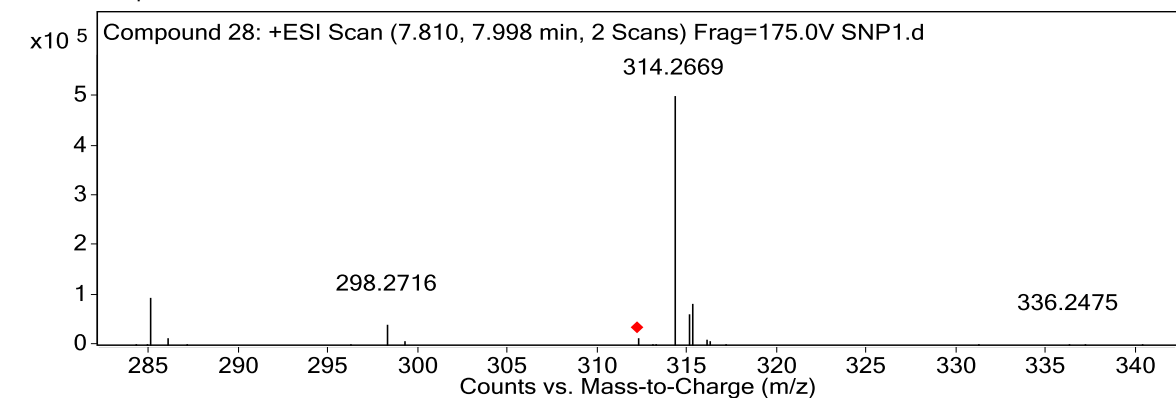
Qualitative Compound Report

Compound 28	312.2503	7.932	Auto MS/MS
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MS Spectrum



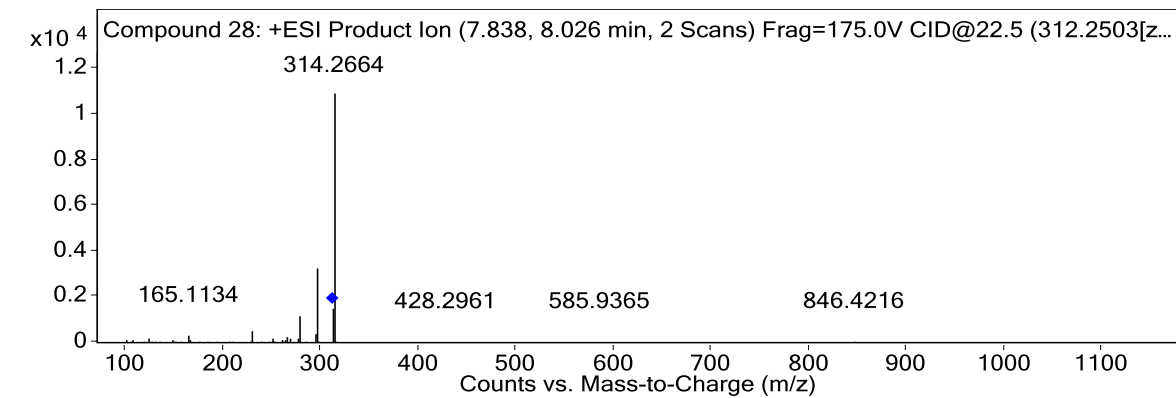
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
207.1227	1	28369.16
285.0736	1	96515.73
298.2716	1	41631.5
312.2503	1	16098.47
313.2535	1	3179.03
314.2669	1	501216.5
315.084	1	62616.34
315.27	1	84286.27
415.0987	1	46561.72
583.1378	1	75040.25

MSMS Spectrum

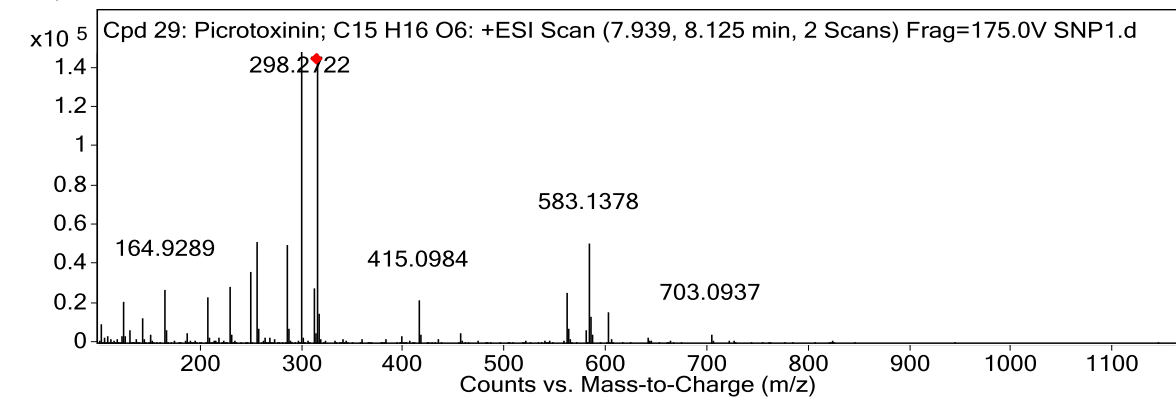


MS/MS Spectrum Peak List

m/z	z	Abund
165.1134		298.53
229.1386	1	508.52
266.2452		235.97
268.2627		217.61
276.228		211.01
278.245	1	1194.87
294.2396	1	361
296.2563	1	3269.16
312.2503	1	1488.62
314.2664		10918.82

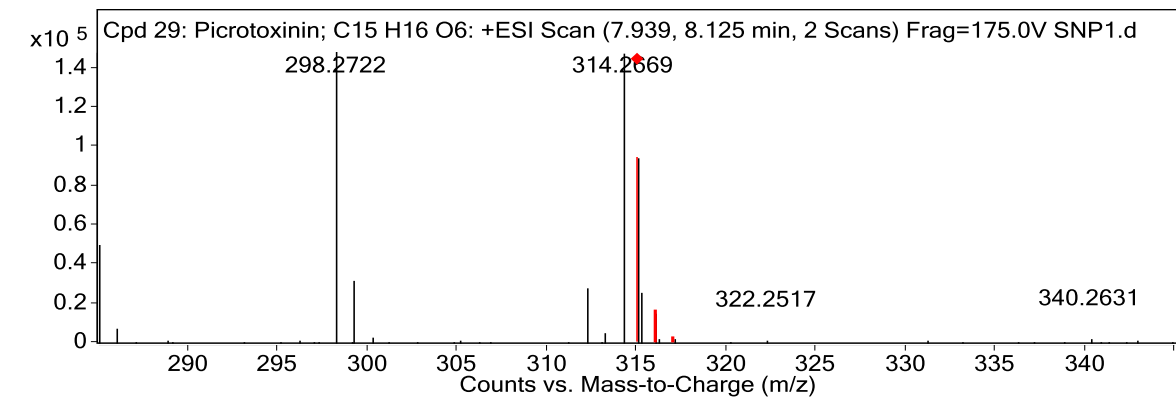
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 29: Picrotoxinin; C15 H16 O6	Picrotoxinin	315.084	8.049	Auto MS/MS	292.0947

MS Spectrum



MS Zoomed Spectrum

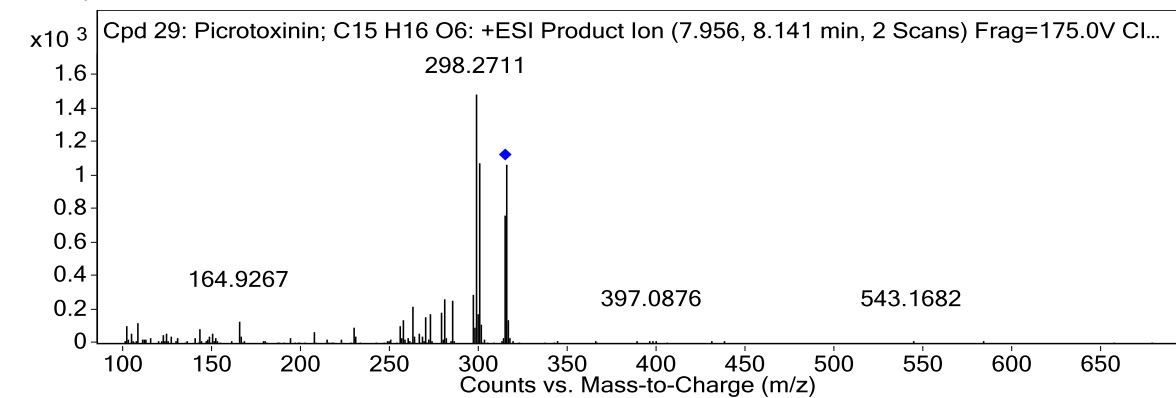
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
248.1988			1	36177.88		
255.0632			1	51454.19		
285.0733			1	49780.95		
298.2722			1	182862.84		
299.2748			1	32256.11		
314.2669			1	147256.16		
315.084	315.0839	-0.43	1	94472.83	C15 H16 O6	(M+Na)+
316.087	316.0873	0.98	1	15009.68	C15 H16 O6	(M+Na)+
317.0884	317.0895	3.32	1	2415.83	C15 H16 O6	(M+Na)+
583.1378			1	51107.16		

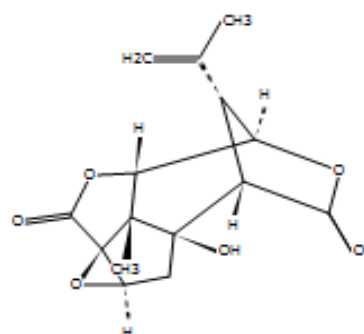
MSMS Spectrum



MS/MS Spectrum Peak List

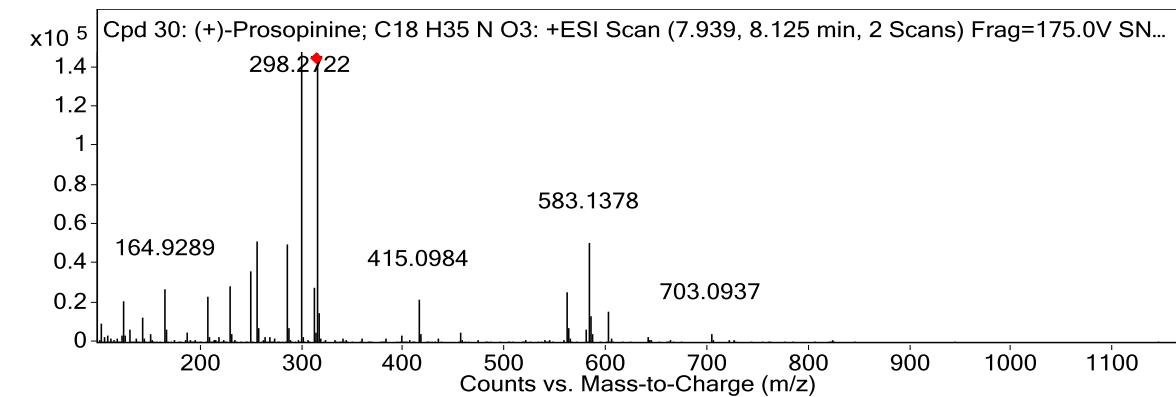
m/z	z	Abund
262.2506	1	220.63
278.2442	1	187.62
280.2609	1	267.38
285.0723	1	259.5
296.256	1	290.73
298.2711	1	1488.97
299.2743	1	179.75
300.0585	1	1076.79
314.2662	1	764.66
315.0822	1	1069.53

Compound Structure

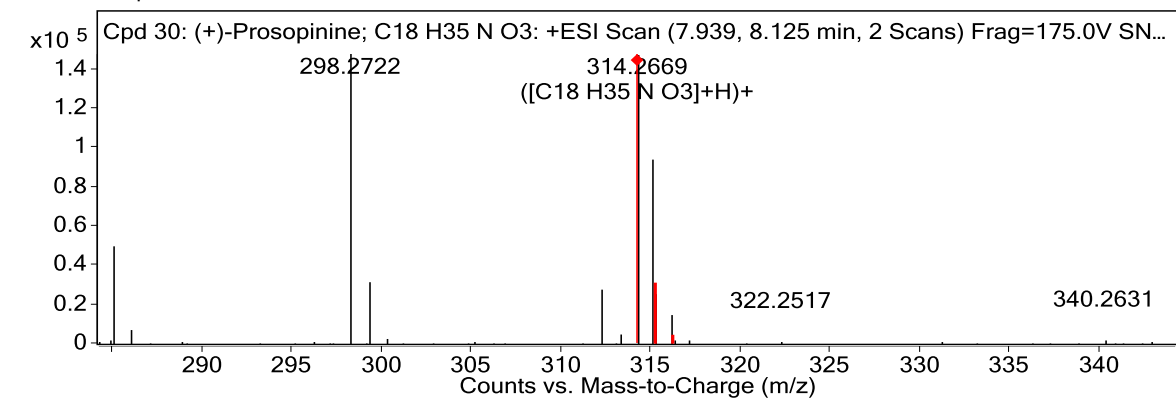


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 30: (+)-Prosopinine; C18 H35 N O3	(+)-Prosopinine	314.2669	8.051	Auto MS/MS	313.2595

MS Spectrum



MS Zoomed Spectrum

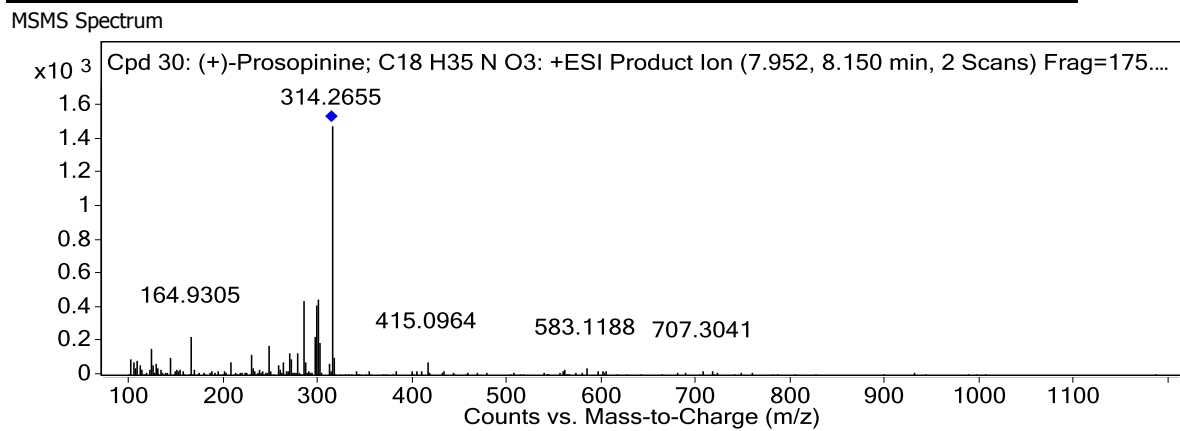


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
248.1988			1	36177.88		

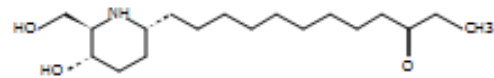
Qualitative Compound Report

255.0632			1	51454.19		
285.0733			1	49780.95		
298.2722			1	182862.84		
299.2748			1	32256.11		
314.2669	314.269	6.52	1	147256.16	C18 H35 N O3	(M+H)+
315.084			1	94472.83		
315.2697	315.2723	8.1	1	25655.72	C18 H35 N O3	(M+H)+
316.2724	316.275	8.31	1	2498.22	C18 H35 N O3	(M+H)+
583.1378			1	51107.16		

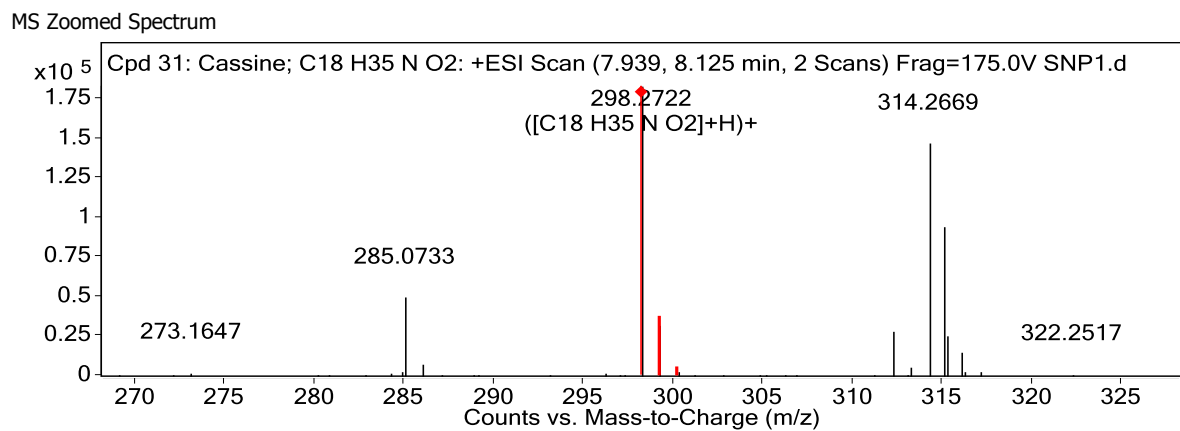
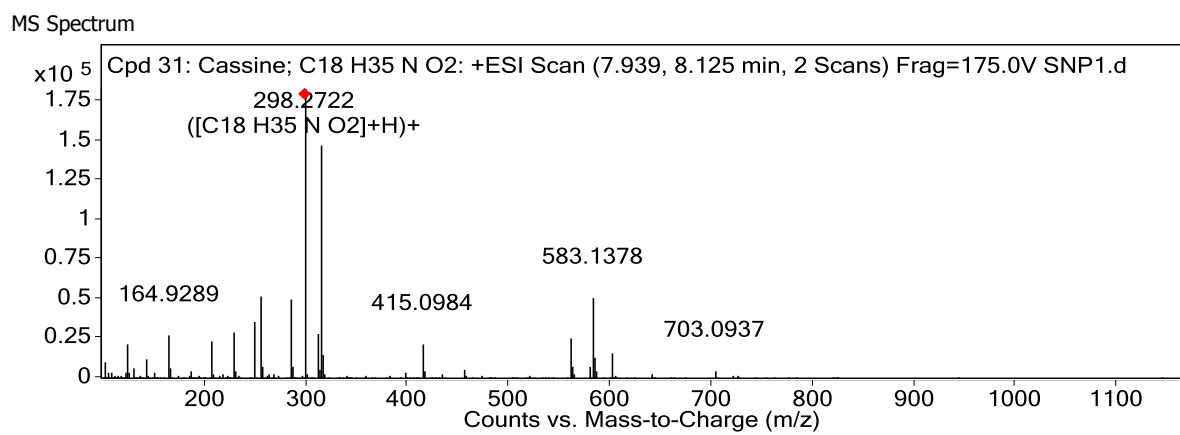


MS/MS Spectrum Peak List		
m/z	z	Abund
124.0855	1	161.58
164.9305		230.21
248.1996	1	175.86
285.0731	1	438.49
296.2554	1	226.65
298.2697	1	417.94
300.0599	1	448.8
301.0623	1	191.41
314.2655	1	1480.13
315.0823	1	837.39

Compound Structure



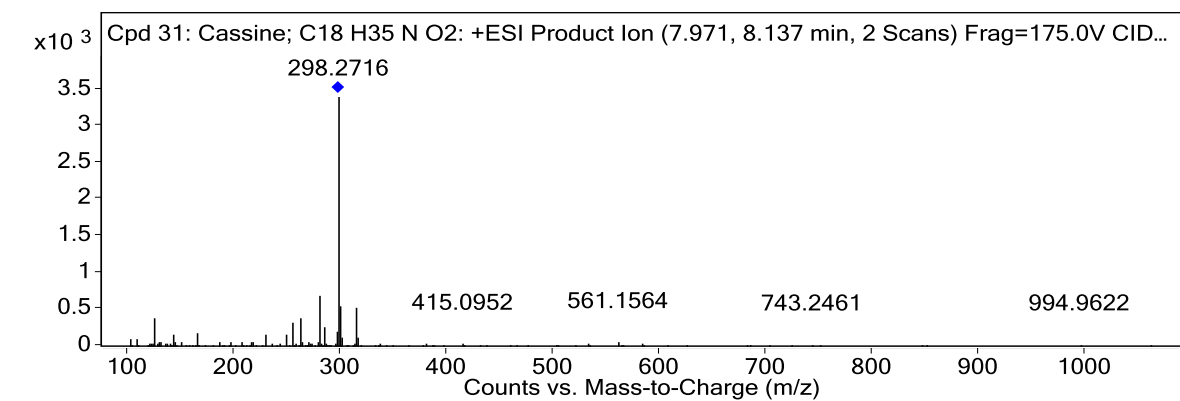
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 31: Cassine; C18 H35 N O2 N O2	Cassine	298.2722	8.054	Auto MS/MS	297.2648



MS Spectrum Peak List						
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
229.1392			1	29078.47		
248.1988			1	36177.88		
255.0632			1	51454.19		
285.0733			1	49780.95		
298.2722	298.2741	6.31	1	182862.84	C18 H35 N O2	(M+H)+
299.2748	299.2774	8.5	1	32256.11	C18 H35 N O2	(M+H)+
300.2774	300.2803	9.64	1	3290.76	C18 H35 N O2	(M+H)+
314.2669			1	147256.16		
315.084			1	94472.83		
583.1378			1	51107.16		

MSMS Spectrum

Qualitative Compound Report



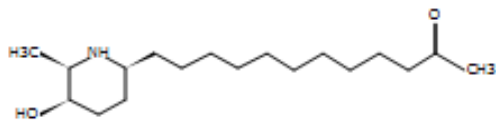
MS/MS Spectrum Peak List

m/z	z	Abund
124.0858	1	384
255.061		325.79
262.2503		392.27
280.2612	1	681.75
285.0729	1	254.64

Qualitative Compound Report

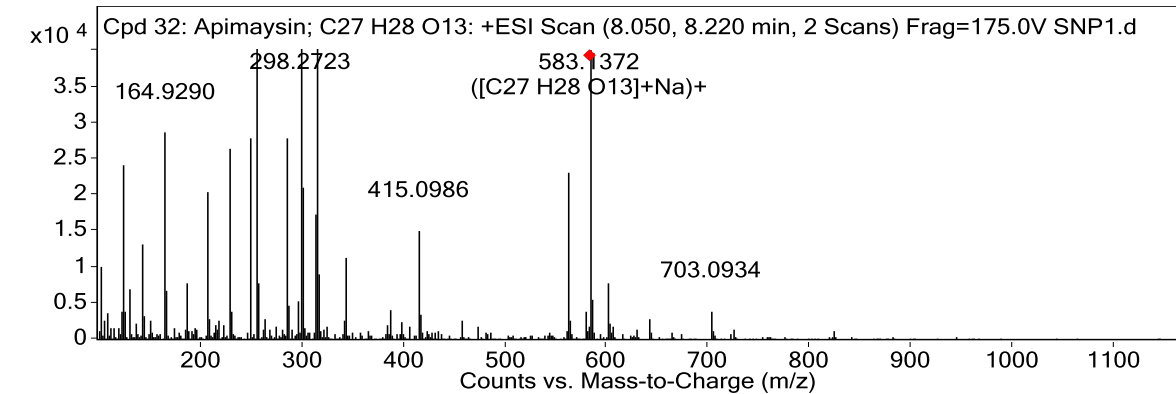
<i>m/z</i>	<i>z</i>	Abund
298.2716	1	3394.64
299.2742	1	539.33
300.0601	1	295.89
314.2667	1	523.54
315.0845	1	526.88

Compound Structure

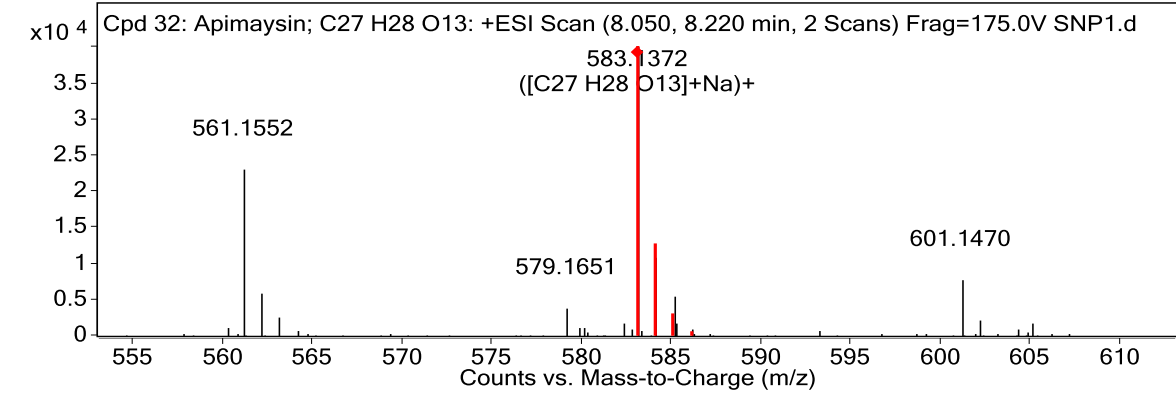


Compound Label	Name	<i>m/z</i>	RT	Algorithm	Mass
Cpd 32: Apimaysin; C27 H28 O13	Apimaysin	583.1372	8.151	Auto MS/MS	560.1485

MS Spectrum



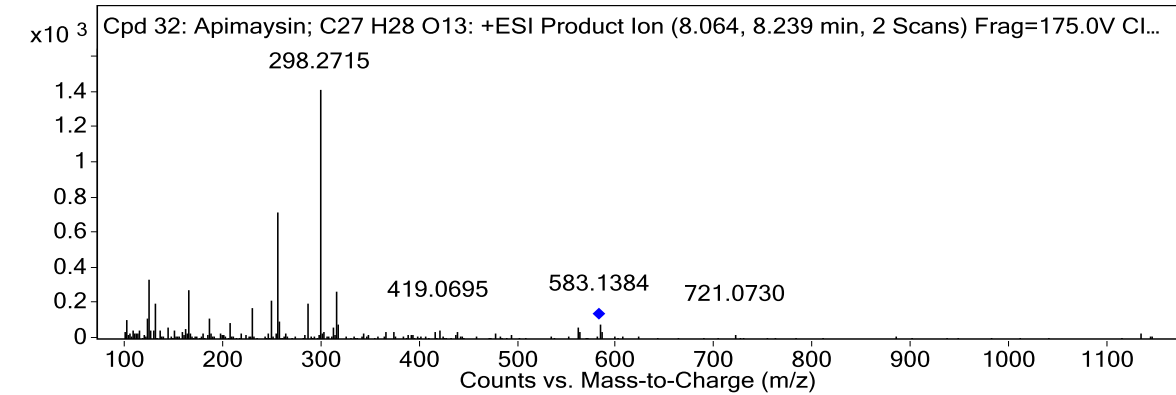
MS Zoomed Spectrum



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
164.929				28682.96		
255.0633			1	53993.47		
298.2723			1	1315179.13		
299.2759			1	245025.05		
314.2665			1	46605.38		
315.0838			1	53923.34		
583.1372	583.1422	8.55	1	40098.92	C27 H28 O13	(M+Na)+
584.1401	584.1456	9.37	1	10976.94	C27 H28 O13	(M+Na)+
585.148	585.148	0	1	5556.72	C27 H28 O13	(M+Na)+
586.153	586.1507	-3.95	1	1120.97	C27 H28 O13	(M+Na)+

MSMS Spectrum

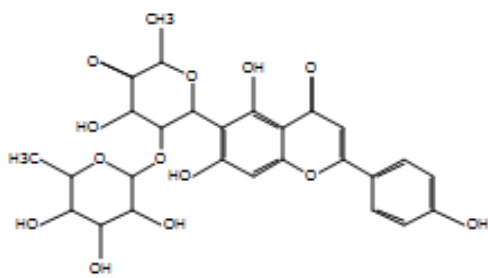


MS/MS Spectrum Peak List

<i>m/z</i>	<i>z</i>	Abund
124.0861		337.13
130.0639	1	207.06
164.928		281.55
248.1989		222.63
255.0632	1	717.47
285.0722		205.7
298.2715	1	1415.85
299.2728	1	211.87
314.264	1	271.09
315.0828	1	237.38

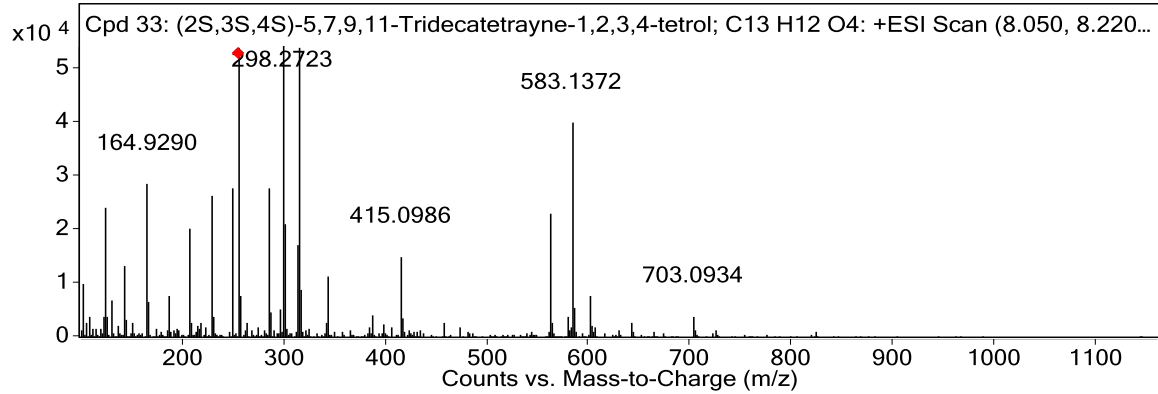
Compound Structure

Qualitative Compound Report

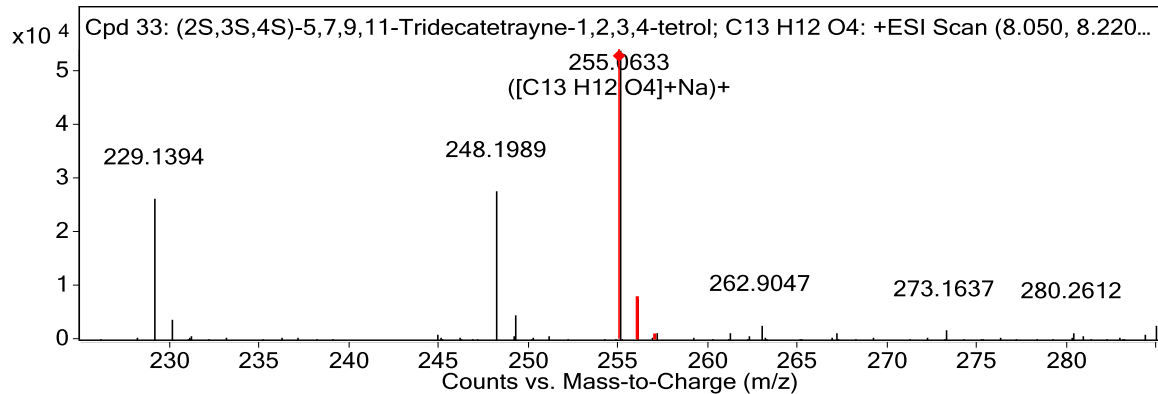


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 33: (2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol; C13 H12 O4	(2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol	255.0633	8.155	Auto MS/MS	232.074

MS Spectrum



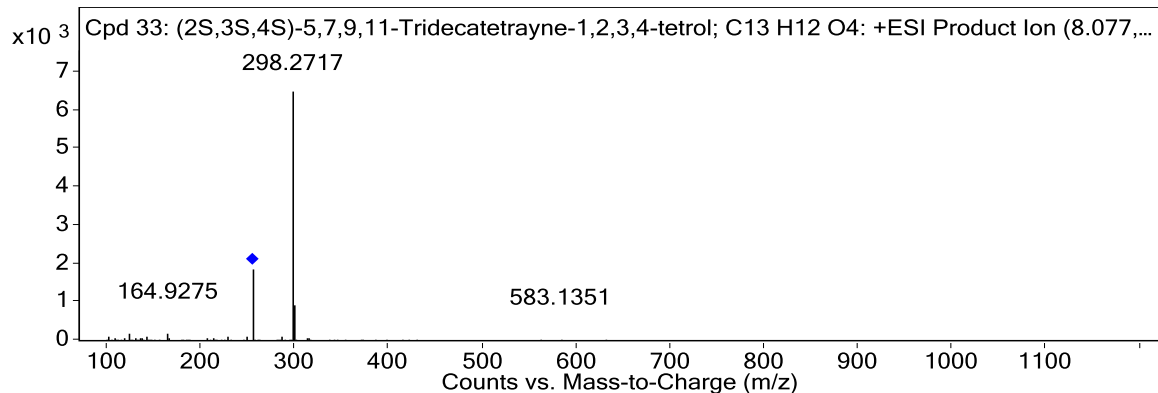
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
164.929				28682.96		
248.1989			1	27892.14		
255.0633	255.0628	-2.12	1	53993.47	C13 H12 O4	(M+Na)+
256.0662	256.0662	-0.14	1	7763.39	C13 H12 O4	(M+Na)+
257.0679	257.0684	1.75	1	1338.52	C13 H12 O4	(M+Na)+
298.2723			1	1315179.13		
299.2759			1	245025.05		
314.2665			1	46605.38		
315.0838			1	53923.34		
583.1372			1	40098.92		

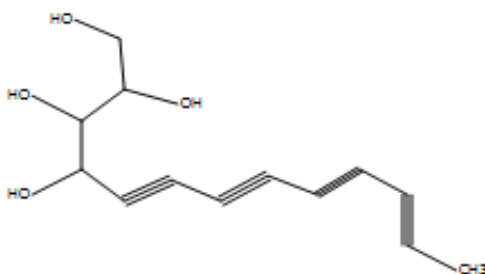
MSMS Spectrum



MS/MS Spectrum Peak List

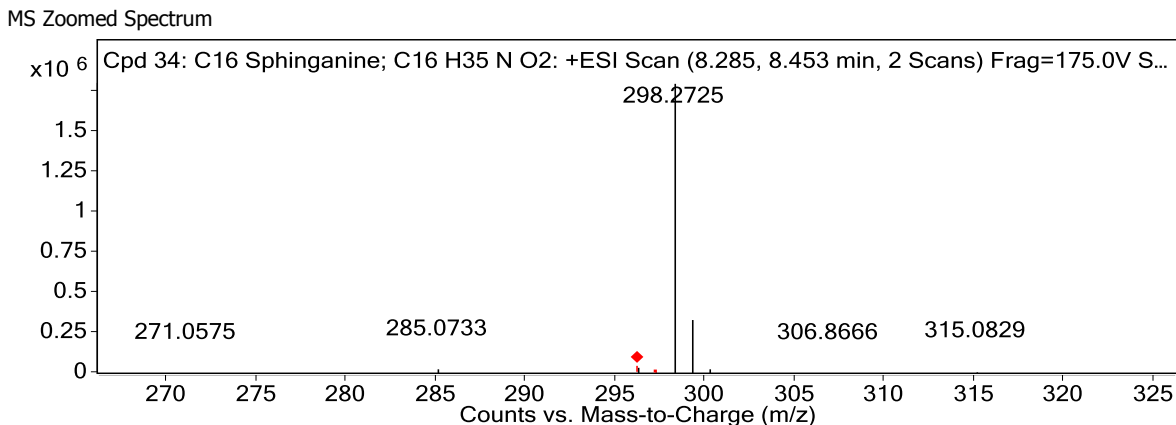
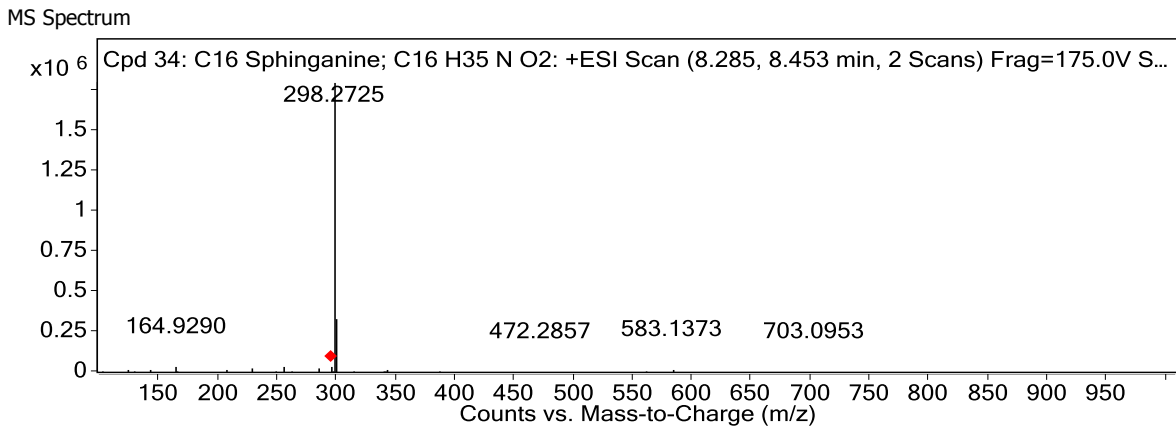
m/z	z	Abund
102.1274		102.31
124.0857	1	184.43
142.9484		103.91
164.9275		212.12
229.1391		109.29
248.1964	1	122.56
255.0632	1	1861.51
256.065	1	232.11
298.2717	1	6493.37
299.2758	1	932.65

Compound Structure



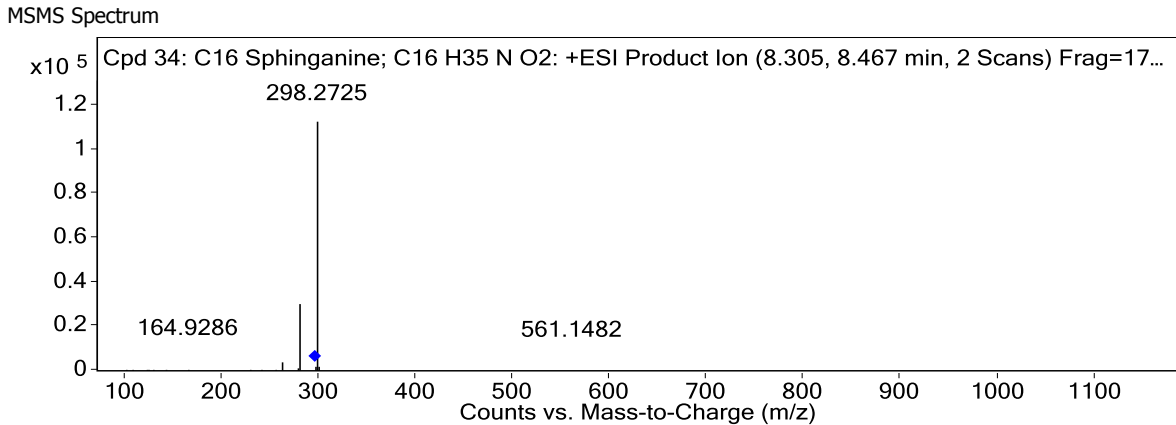
Qualitative Compound Report

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 34: C16 Sphinganine; C16 H35 N O2	C16 Sphinganine	296.2559	8.386	Auto MS/MS	273.2667



MS Spectrum Peak List

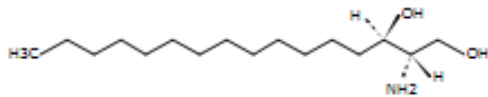
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0864			1	22327.19		
164.929				32451.92		
229.1394			1	25359.67		
255.0633			1	38150.43		
285.0733			1	25019.15		
296.2559	296.256	0.17	1	40062.66	C16 H35 N O2	(M+Na)+
297.2589	297.2593	1.21	1	7650.32	C16 H35 N O2	(M+Na)+
298.2725			1	1792343.38		
299.2759			1	331956.31		
300.2779			1	29792.43		



MS/MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
122.0955			1	522.13		
124.0867			1	707.94		
142.9467				498.8		
164.9286				848.43		
262.2509				3865.84		
278.2447			1	1416.86		
280.2613				30051.2		
296.2559	296.256	0.36	1	2352.58	C16 H35 N O2	(M+Na)+
298.2725			1	112804.59		
299.2745			1	2247.71		

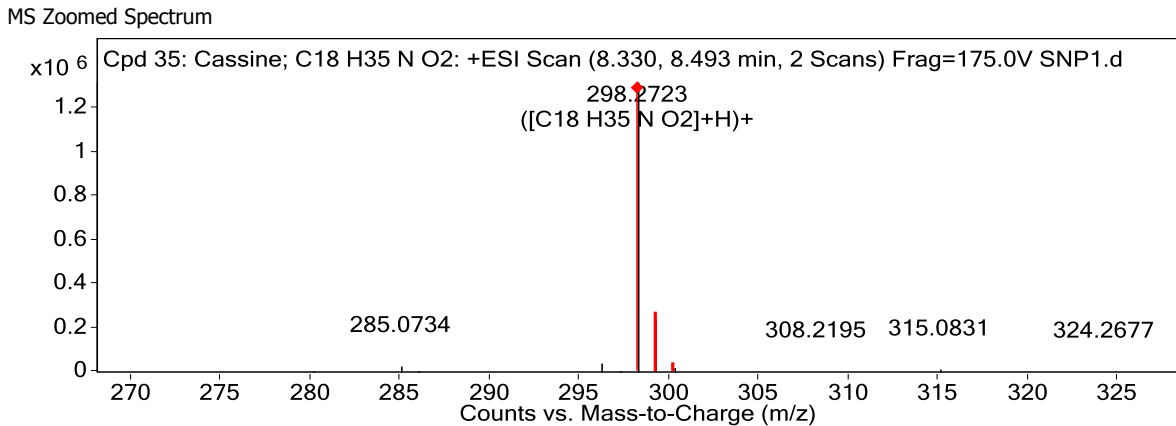
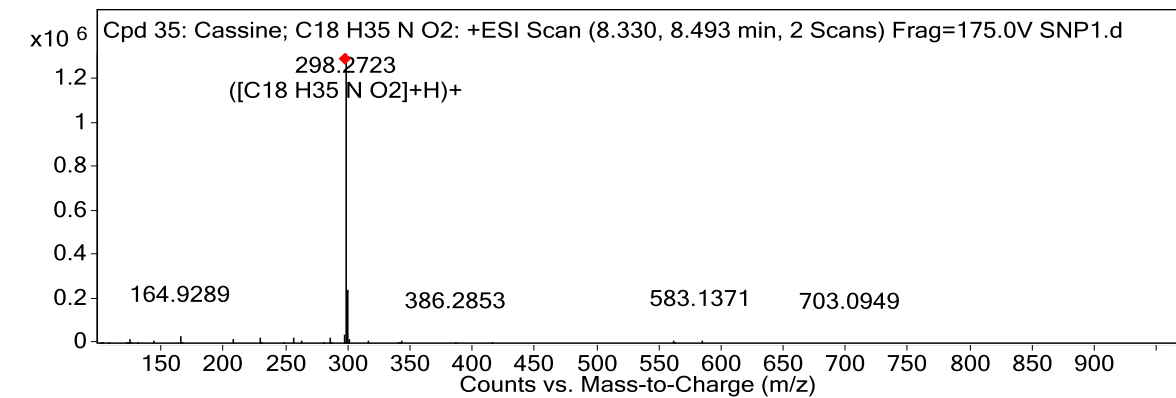
Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 35: Cassine; C18 H35 N O2	Cassine	298.2723	8.424	Auto MS/MS	297.265

MS Spectrum

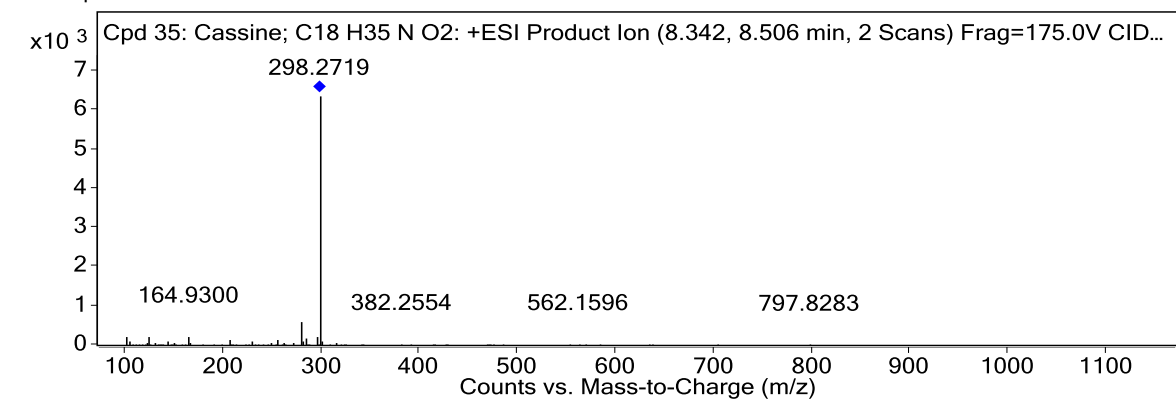
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0862			1	22348.13		
164.9289				33588.82		
207.1226			1	18942.63		
229.1393			1	25923.4		
255.0631			1	27443.32		
285.0734			1	27743.55		
296.2557			1	38043.04		
298.2723	298.2741	5.91	1	1316381.88	C18 H35 N O2	(M+H)+
299.2757	299.2774	5.52	1	242183.05	C18 H35 N O2	(M+H)+
300.2776	300.2803	8.91	1	22229.57	C18 H35 N O2	(M+H)+

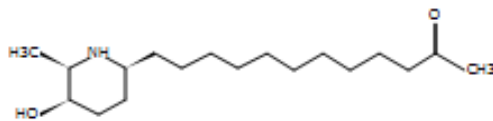
MSMS Spectrum



MS/MS Spectrum Peak List

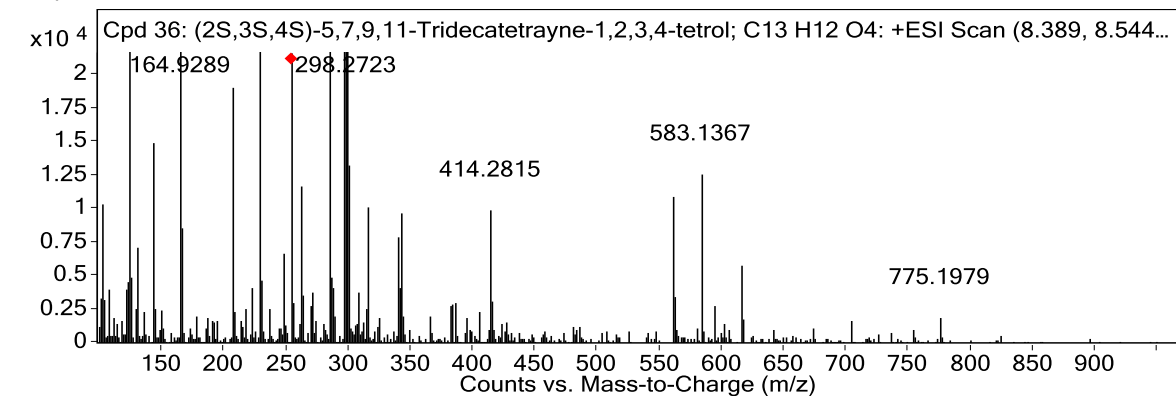
m/z	z	Abund
102.1266		215.84
124.086	1	227.59
164.93		231.33
207.1214		160.36
255.063		166.46
280.261	1	623.8
285.0732	1	199.9
296.2546	1	223.31
298.2719	1	6368.19
299.2752	1	858.58

Compound Structure



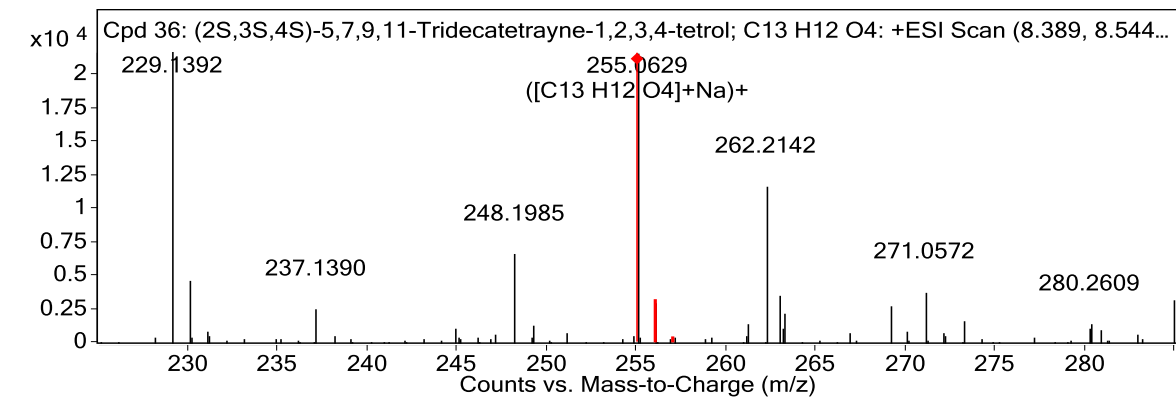
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 36: (2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol; C13 H12 O4	(2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol	255.0629	8.487	Auto MS/MS	232.0737

MS Spectrum



MS Zoomed Spectrum

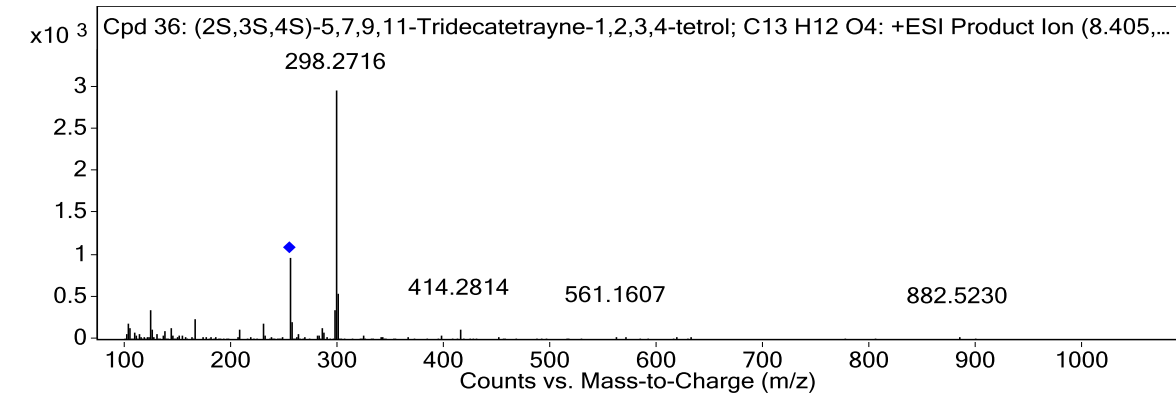
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0862			1	27686.91		
164.9289				33430.28		
229.1392			1	25561.93		
255.0629	255.0628	-0.62	1	21588.05	C13 H12 O4	(M+Na)+
256.0663	256.0662	-0.48	1	2968.59	C13 H12 O4	(M+Na)+
257.0689	257.0684	-1.97	1	399.21	C13 H12 O4	(M+Na)+
285.0733			1	31934.47		
296.2559			1	48772.21		
298.2723			1	794108.88		
299.2755			1	145397.66		

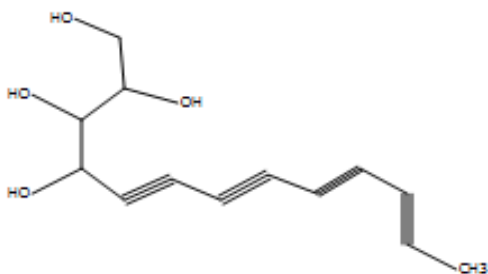
MS/MS Spectrum



MS/MS Spectrum Peak List

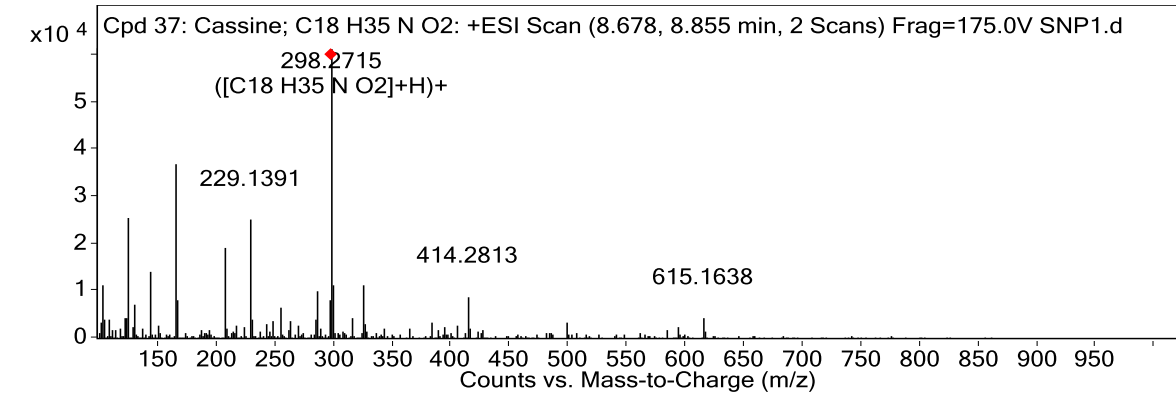
m/z	z	Abund
102.1263		195.46
104.1061	1	149.34
124.0864		347.46
164.9305		251.96
229.1398	1	189.92
255.0635	1	983.46
256.0683	1	205.81
296.256		346.49
298.2716	1	2962.77
299.2754	1	544.79

Compound Structure

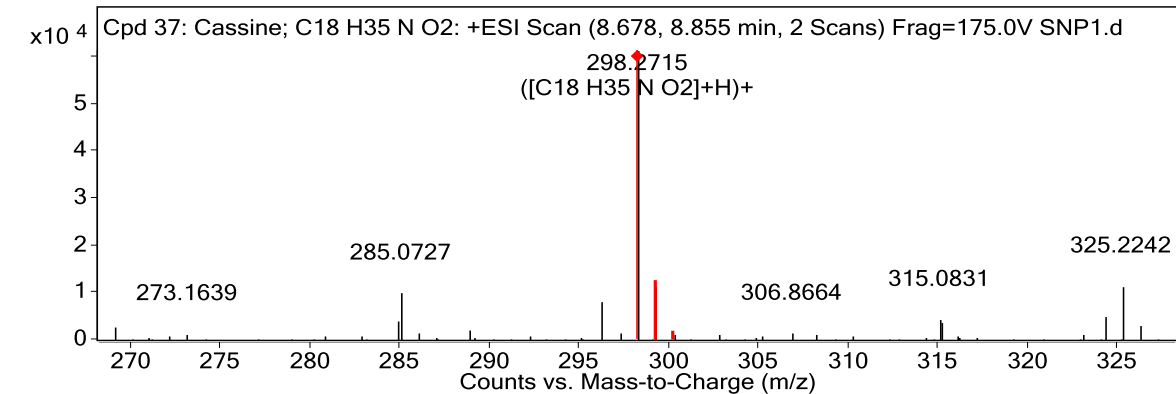


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 37: Cassine; C18 H35 N O2 N O2	Cassine	298.2715	8.781	Auto MS/MS	297.2643

MS Spectrum



MS Zoomed Spectrum



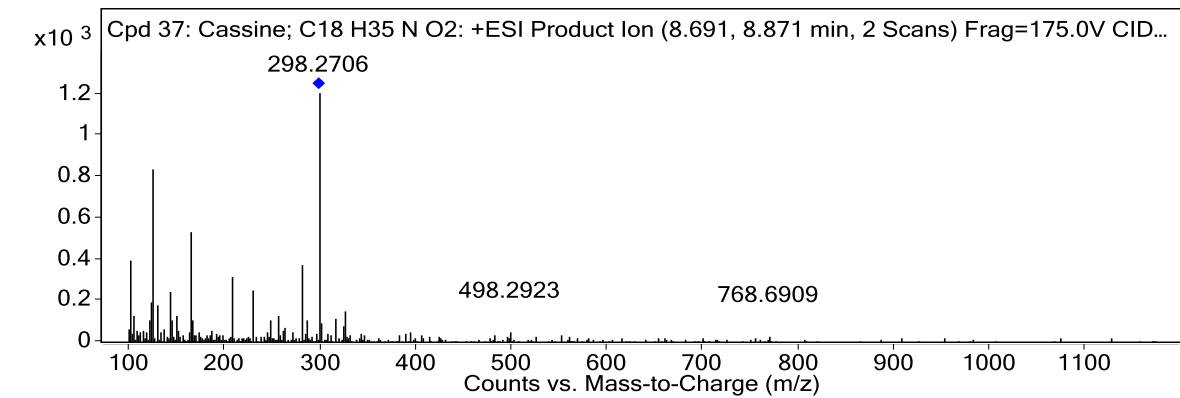
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
102.1271				11318.53		

Qualitative Compound Report

124.0862			1	25722.97		
142.9468				14228.95		
164.9289				36850.79		
207.1225			1	19223.5		
229.1391			1	25188.27		
298.2715	298.2741	8.43	1	61293.59	C18 H35 N O2	(M+H)+
299.2746	299.2774	9.24	1	11430.95	C18 H35 N O2	(M+H)+
300.2793	300.2803	3.18	1	1308.23	C18 H35 N O2	(M+H)+
325.2242			1	11470.97		

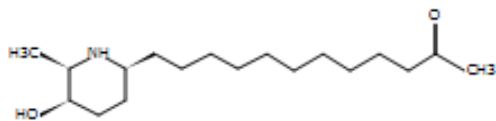
MSMS Spectrum



MS/MS Spectrum Peak List

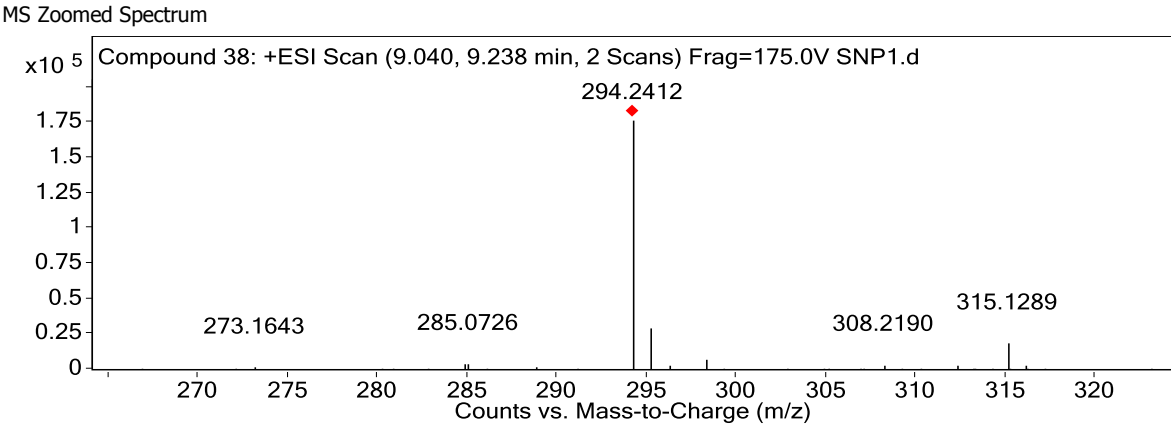
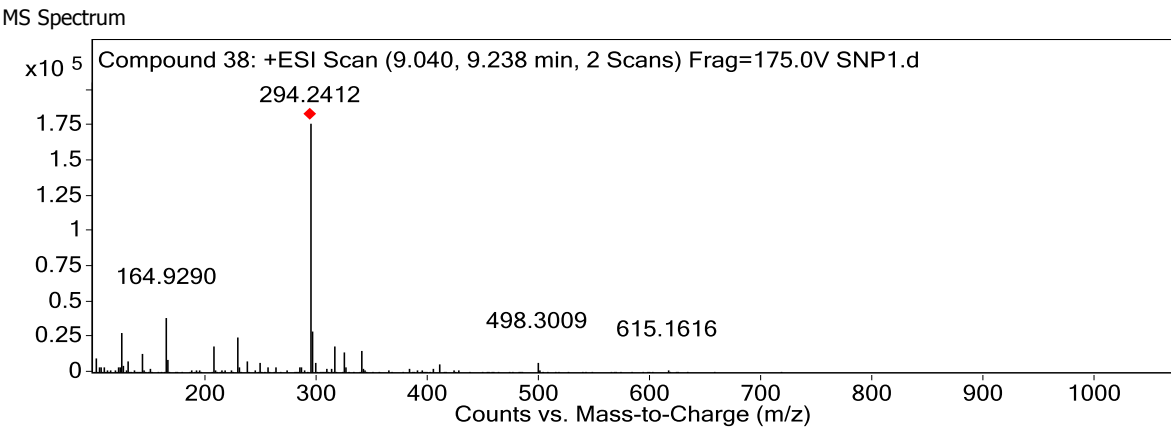
m/z	z	Abund
102.1272	1	393.89
123.0914		195.87
124.0862	1	836.67
142.9478		245.31
164.929		536.87
165.1138		225.52
207.1223	1	319.06
229.139	1	254.35
280.2589	1	373.14
298.2706	1	1206.34

Compound Structure



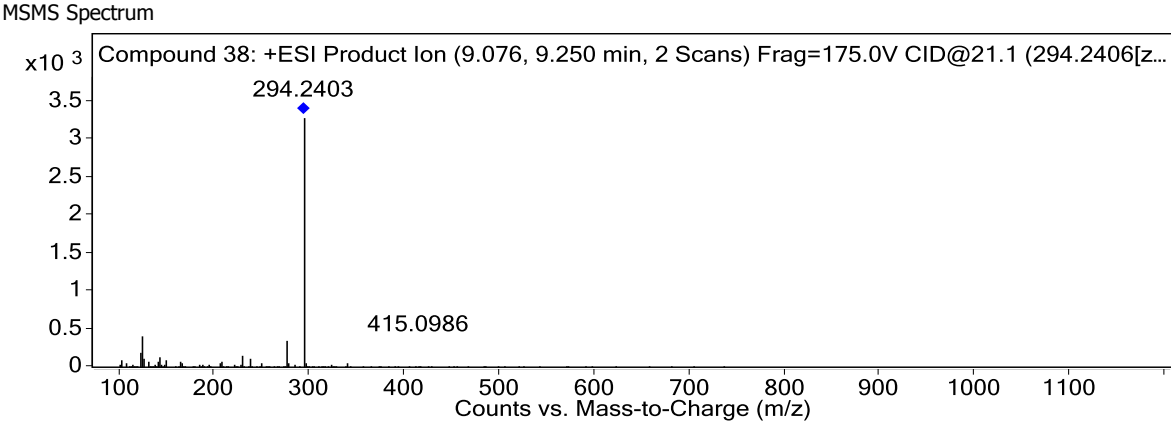
Compound Label	m/z	RT	Algorithm
Compound 38	294.2412	9.163	Auto MS/MS

Qualitative Compound Report



MS Spectrum Peak List

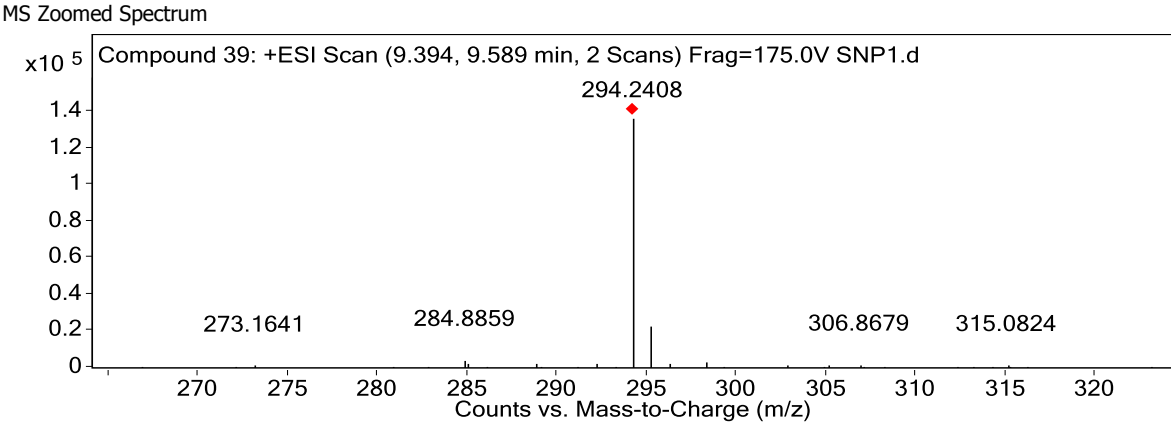
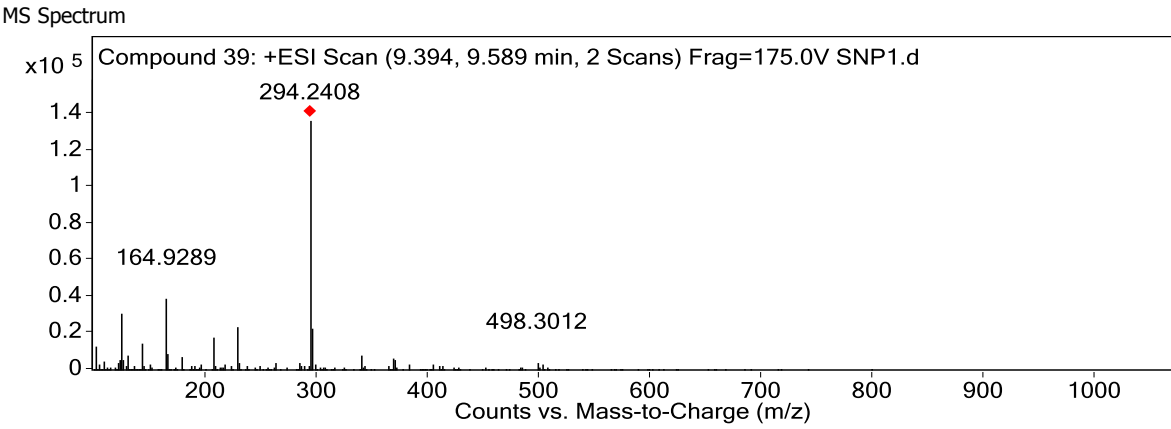
m/z	z	Abund
124.0864	1	28661.89
164.929		39011.25
207.1226	1	18582.73
229.1391	1	25062.63
294.2412	1	176632.22
295.2438	1	29505.28
296.2481	1	3427.07
315.1289	1	18733.06
324.2866	1	14707.64
340.2817	1	15969.22



MS/MS Spectrum Peak List

m/z	z	Abund
122.0591		201.25
123.0657		110.74
124.0863		414.26
125.0701	1	113.33
142.9468		135.92
229.1385	1	164.58
237.1481	1	113.64
276.2312	1	362.55
294.2403	1	3285.17
295.2433	1	343.6

Compound Label	m/z	RT	Algorithm
Compound 39	294.2408	9.506	Auto MS/MS

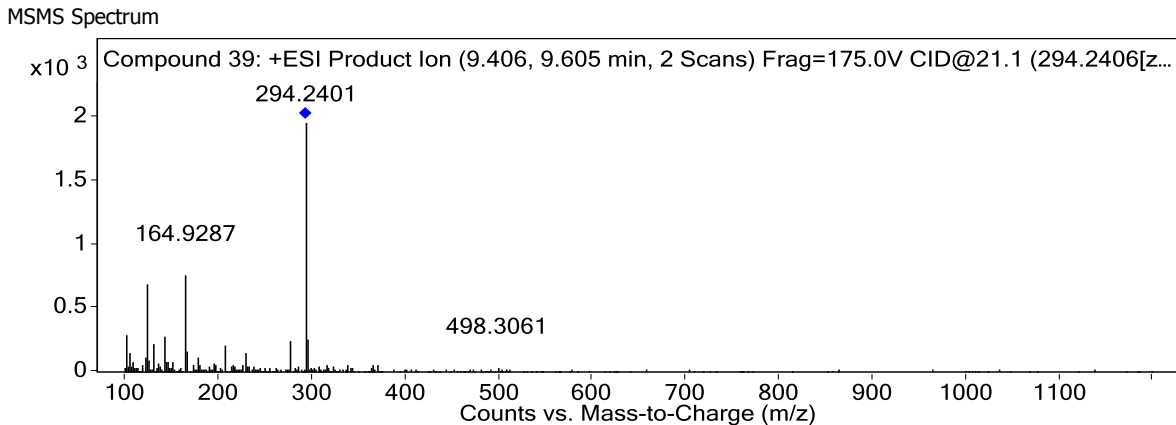


MS Spectrum Peak List

m/z	z	Abund
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Qualitative Compound Report

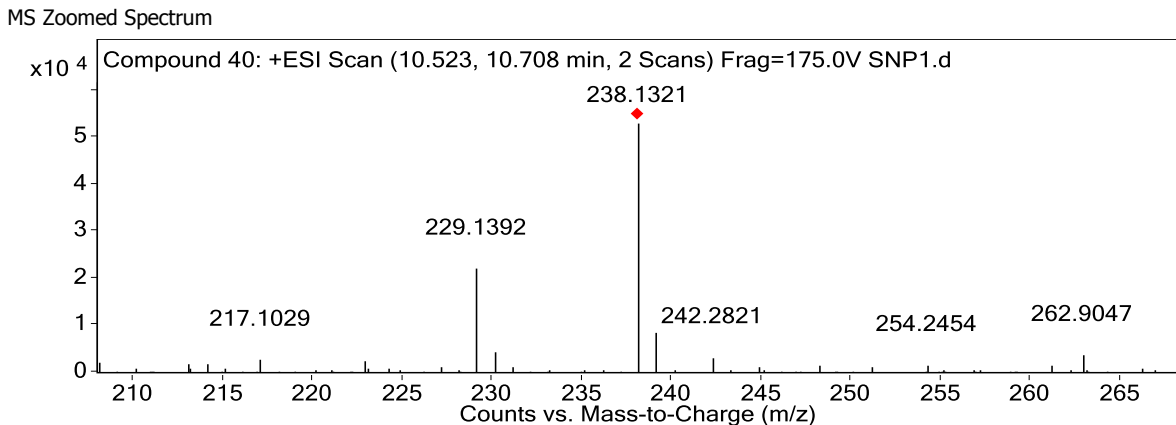
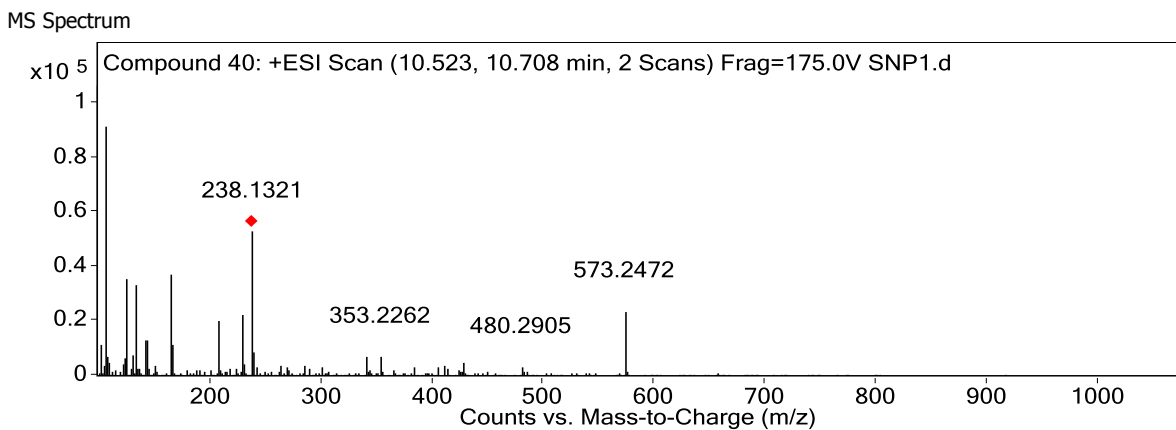
102.127		12892.05
124.0864	1	31132.27
142.9472		14690.99
164.9289		38994.1
166.0966		8802.28
207.1226	1	18259.66
229.1392	1	23658.09
294.2408	1	136206.7
295.2436	1	22476
296.2469	1	2233.36



MS/MS Spectrum Peak List

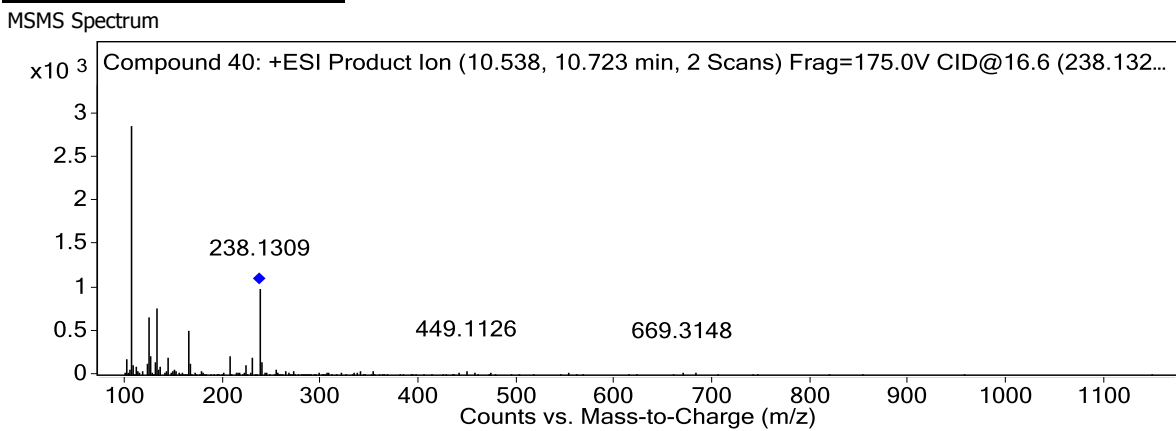
m/z	z	Abund
102.1273	1	293.58
124.0863		691.2
130.0643		228.02
142.9465		281.06
164.9287		764.55
166.0967		160.63
207.1222		213.26
276.229	1	248.8
294.2401	1	1959.39
295.2438	1	261.36

Compound Label	m/z	RT	Algorithm
Compound 40	238.1321	10.631	Auto MS/MS



MS Spectrum Peak List

m/z	z	Abund
106.0646	1	91340.03
124.0863	1	35311.08
133.0753	1	33200.25
164.9291		36961.68
207.1226	1	20178.99
229.1392	1	22154.93
238.1321	1	52957.44
239.1349	1	8509.25
240.1383	1	772.28
573.2472	1	23692.54



MS/MS Spectrum Peak List

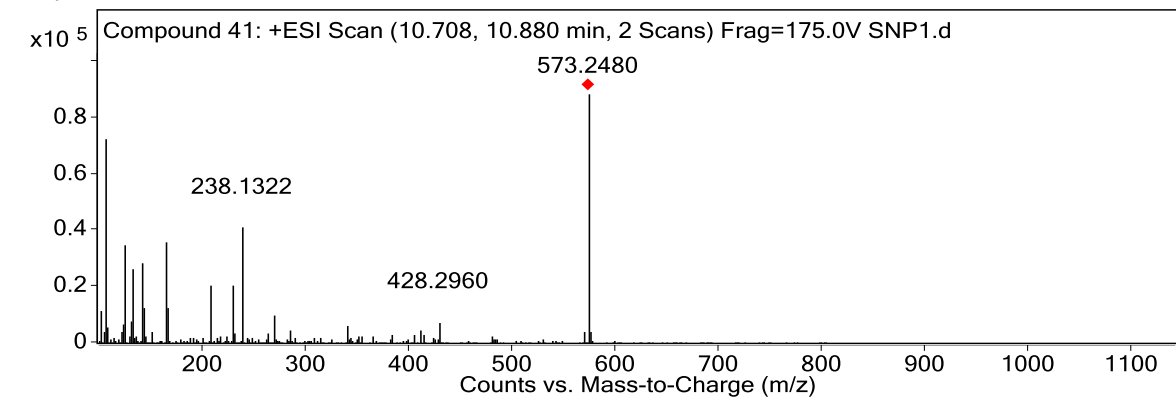
m/z	z	Abund
106.0642	1	2862.99
107.0667	1	263.57
124.0867	1	665.37
125.0684		223.5

Qualitative Compound Report

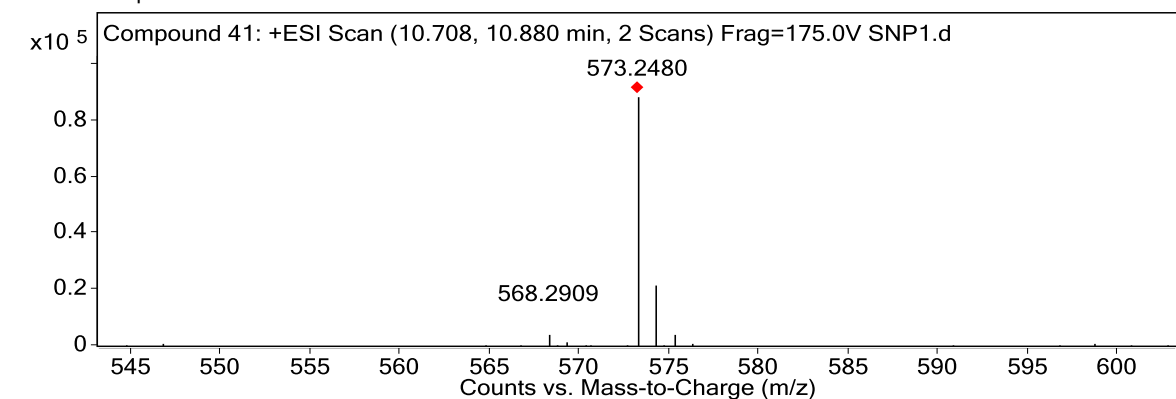
133.0759	1	778.06
142.9465		213.92
164.9278		512.19
207.1244		225.33
229.1399		212.84
238.1309	1	986.21

Compound Label	m/z	RT	Algorithm
Compound 41	573.248	10.81	Auto MS/MS

MS Spectrum



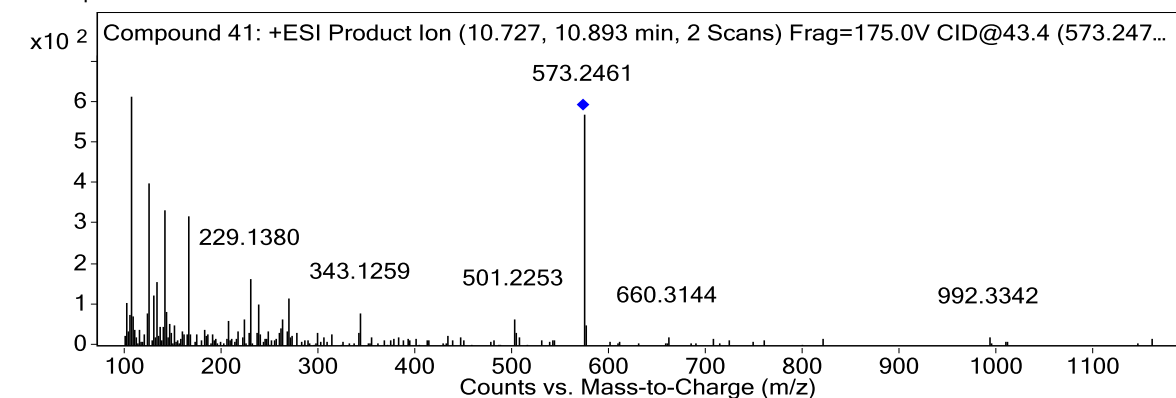
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
106.0646	1	72567.2
124.0863	1	35034.78
133.0752	1	26236.15
141.0691	1	28811.6
164.929		36206.19
207.1226	1	20526.07
238.1322	1	41134.3
573.248	1	88473.51
574.2502	1	21528.62
575.2521	1	4395.05

MSMS Spectrum

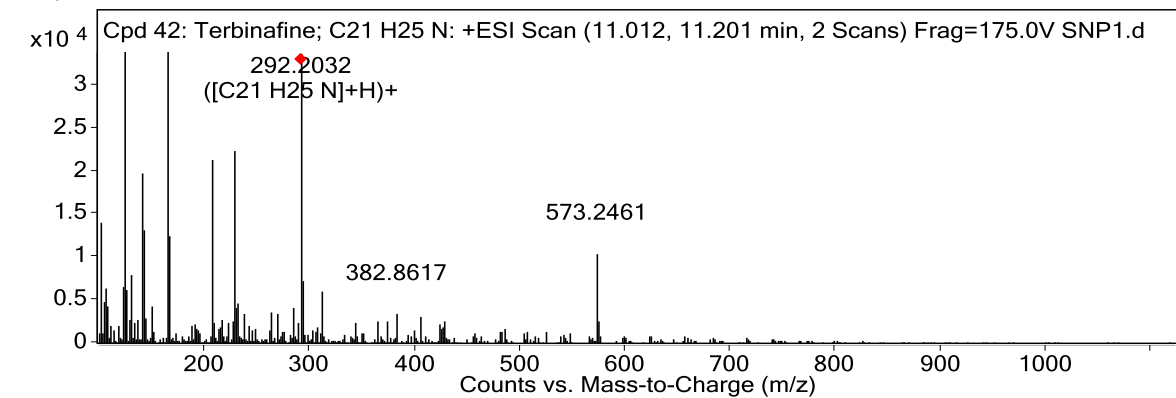


MS/MS Spectrum Peak List

m/z	z	Abund
106.0634	1	615.34
124.0863	1	399.82
130.0636	1	126.27
133.0757		158.38
141.0684	1	335.51
164.9293		321.13
166.0961	1	129.53
229.138	1	165.55
269.0803		119.29
573.2461	1	570.96

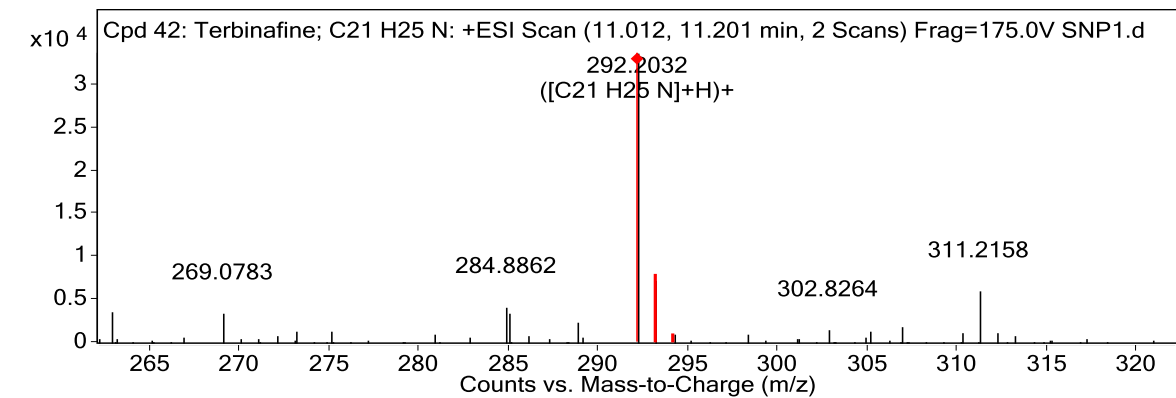
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 42: Terbinafine; C21 H25 N	Terbinafine	292.2032	11.122	Auto MS/MS	291.1959

MS Spectrum



MS Zoomed Spectrum

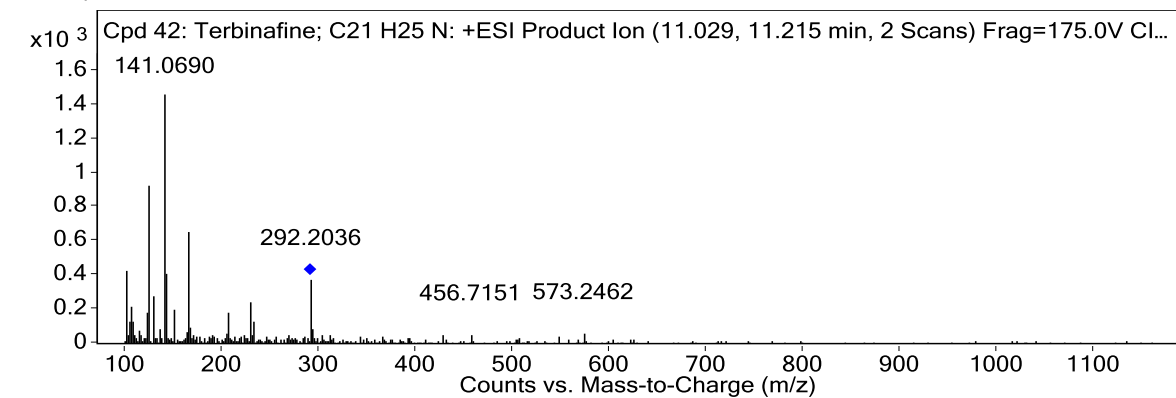
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
102.1271			1	13995.63		
124.0864			1	39558.41		
141.0689			1	19681.7		
142.947				13214.18		
164.9289				37478.7		
207.1225			1	21307.57		
229.1393			1	22342.48		
292.2032	292.206	9.59	1	33598.63	C21 H25 N	(M+H)+
293.2063	293.2093	10.22	1	7344.54	C21 H25 N	(M+H)+
294.2096	294.2126	10.12	1	959.62	C21 H25 N	(M+H)+

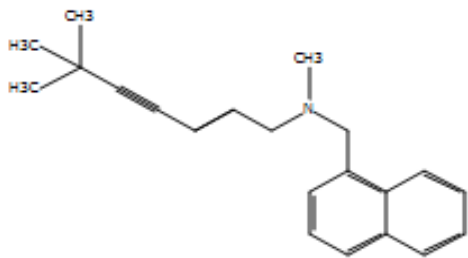
MSMS Spectrum



MS/MS Spectrum Peak List

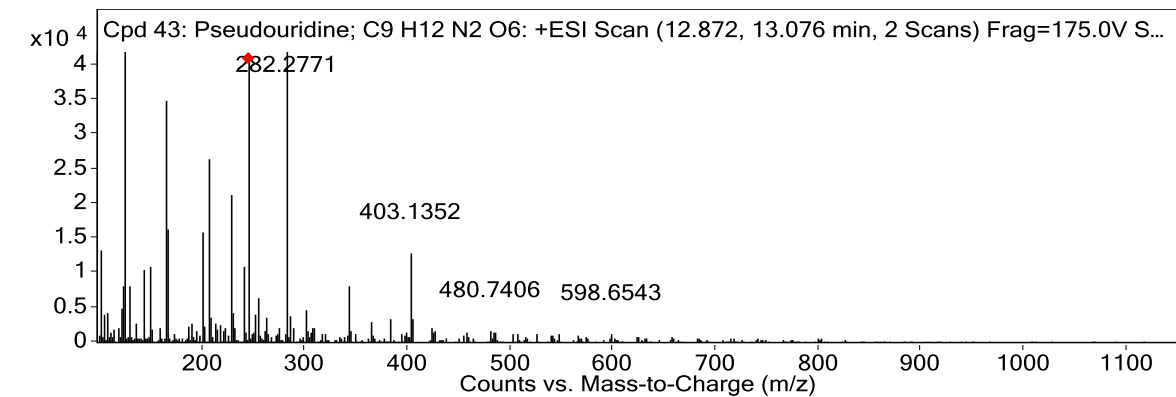
m/z	z	Abund
102.1272	1	424.79
106.0643		222.63
124.0859	1	925.48
130.0641	1	275.82
141.069	1	1461.28
142.9463		412.24
164.9292		652.1
166.0959	1	314.24
229.1399	1	241.43
292.2036	1	379.53

Compound Structure

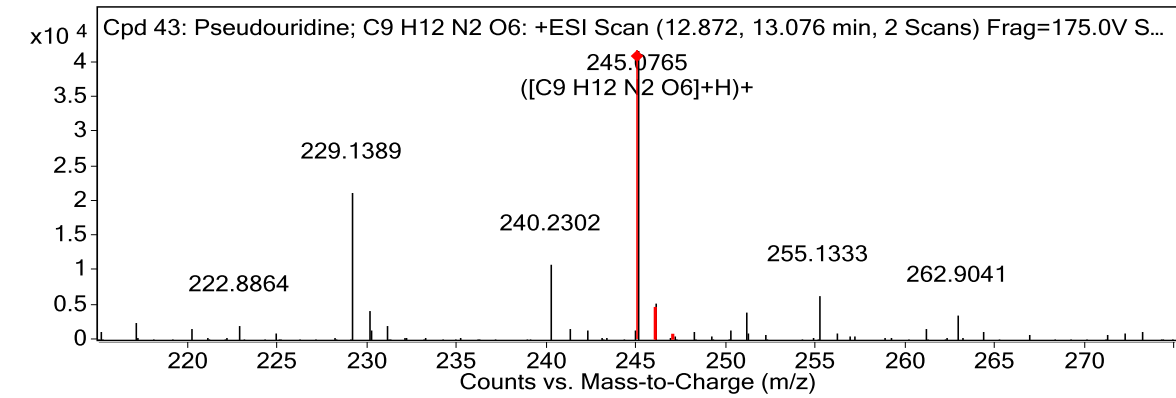


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 43: Pseudouridine; C9 H12 N2 O6	Pseudouridine	245.0765	12.99	Auto MS/MS	244.0693

MS Spectrum



MS Zoomed Spectrum



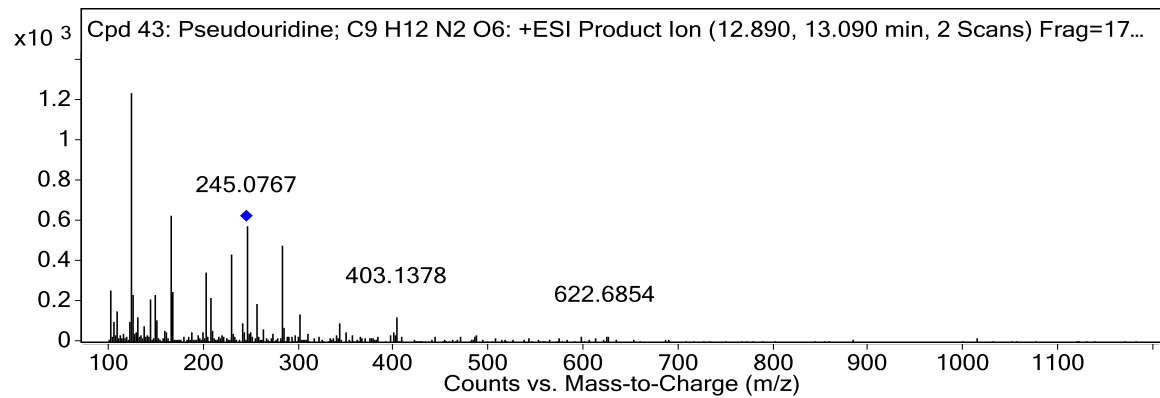
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0864			1	54306.49		

Qualitative Compound Report

164.929				34829.41		
166.0966			1	16365.19		
201.1262			1	15884.83		
207.1225			1	26455.17		
229.1389			1	21375.23		
245.0765	245.0768	1.07	1	41715.5	C9 H12 N2 O6	(M+H)+
246.0799	246.0798	-0.24	1	5451.9	C9 H12 N2 O6	(M+H)+
247.0822	247.0816	-2.38	1	639.48	C9 H12 N2 O6	(M+H)+
282.2771			1	55664.43		

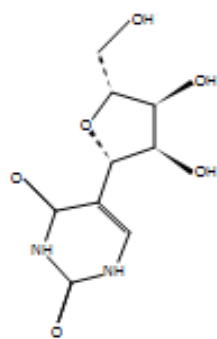
MSMS Spectrum



MS/MS Spectrum Peak List

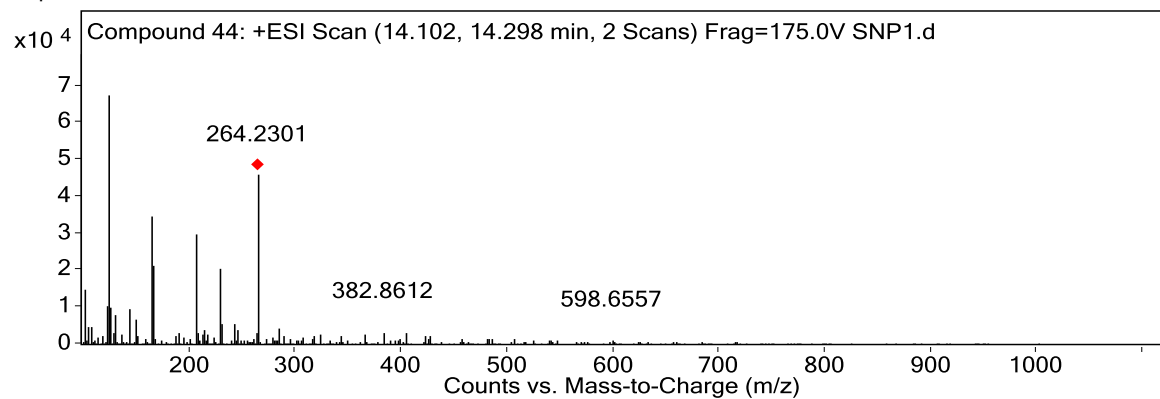
m/z	z	Abund
102.1262	1	263.34
124.0865	1	1241
125.0702	1	236.17
149.0221		238.24
164.9297		631.58
166.0968		254.61
201.1251	1	349.79
229.138	1	434.37
245.0767	1	579.35
282.2762	1	484.22

Compound Structure

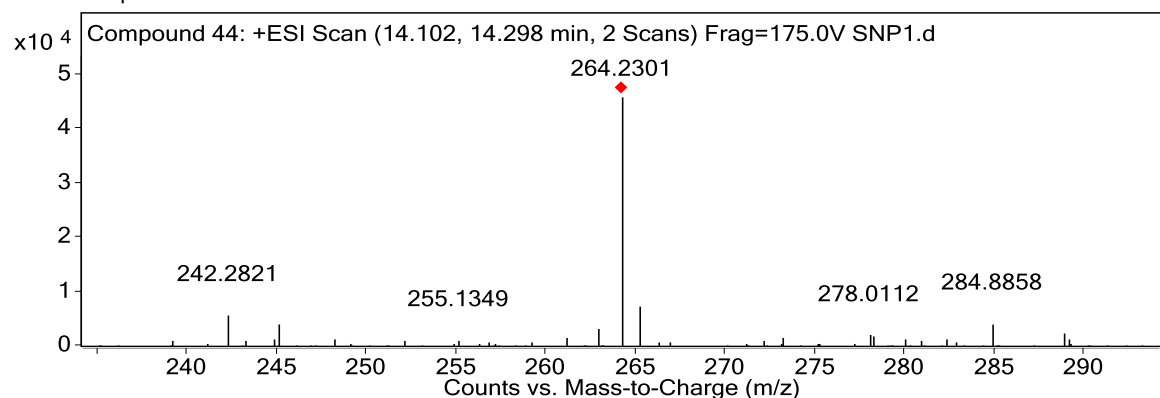


Compound Label	m/z	RT	Algorithm
Compound 44	264.2301	14.216	Auto MS/MS

MS Spectrum



MS Zoomed Spectrum

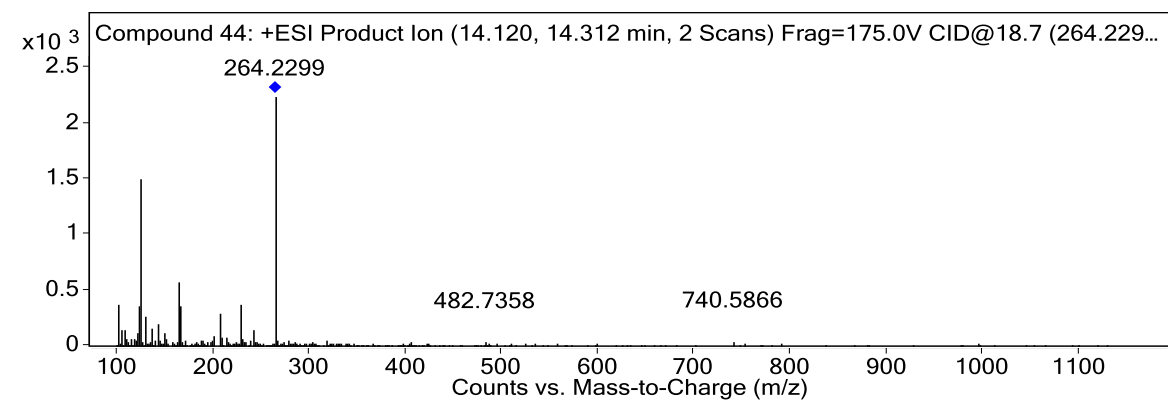


MS Spectrum Peak List

m/z	z	Abund
102.1271	1	14907.8
123.0911		10407.33
124.0863	1	67474.91
164.9286		34771.27
166.0966	1	21256.03
207.1226	1	30051.54
229.1392	1	20772.19
264.2301	1	45880.62
265.2329	1	7434.82
266.2359	1	736.43

MSMS Spectrum

Qualitative Compound Report

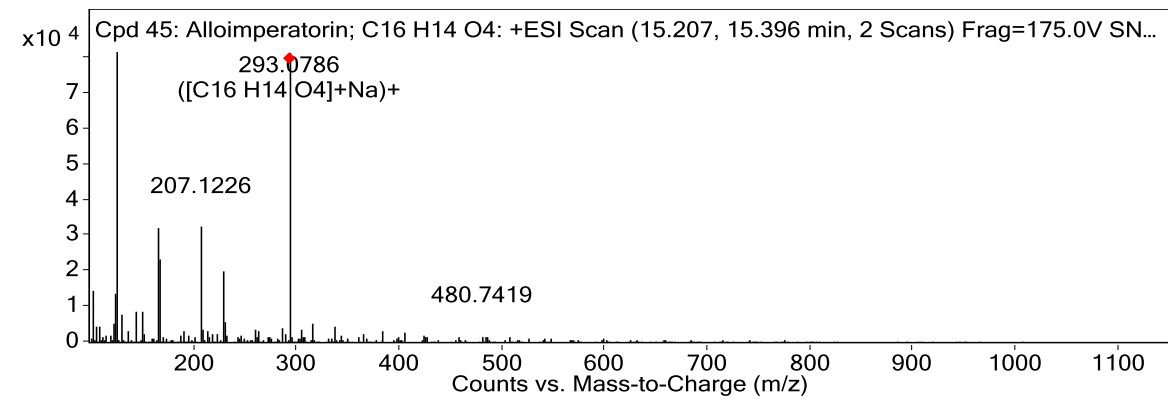


MS/MS Spectrum Peak List

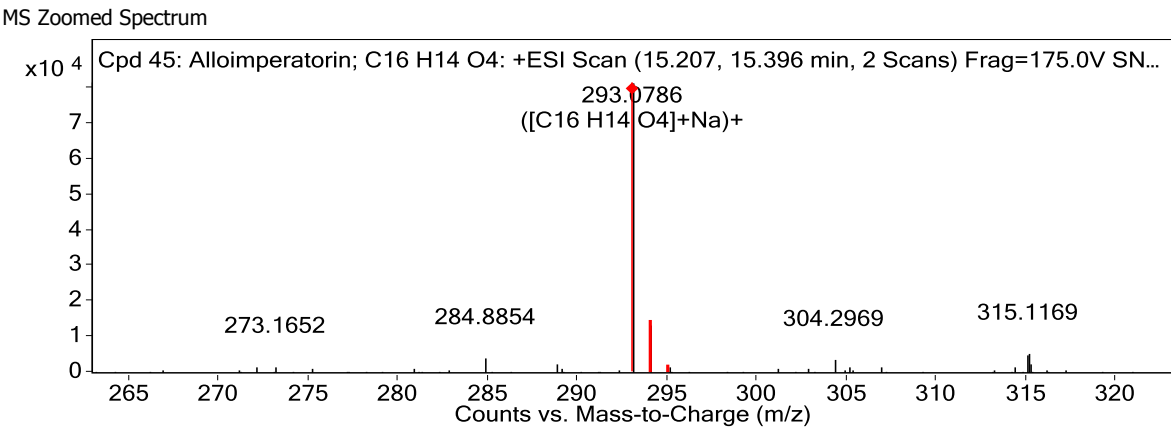
m/z	z	Abund
102.1265		379.47
123.0897		359.86
124.0864	1	1505.89
125.0718	1	383.84
130.063		273.02
164.9294		575.94
166.0958		364.75
207.1232	1	298.14
229.1396	1	378.27
264.2299	1	2240.32

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 45: Alloimperatorin; C16 H14 O4	Alloimperatorin	293.0786	15.317	Auto MS/MS	270.0893

MS Spectrum

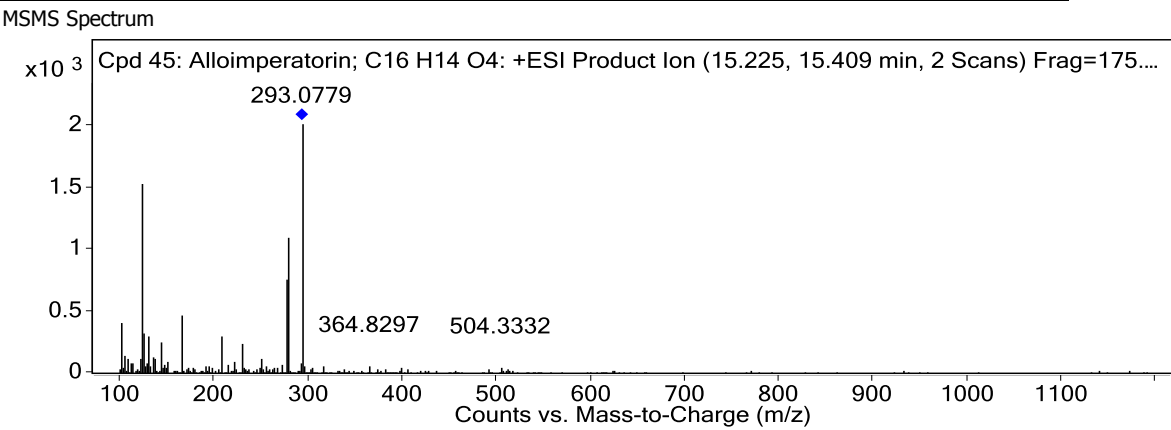


Qualitative Compound Report



MS Spectrum Peak List

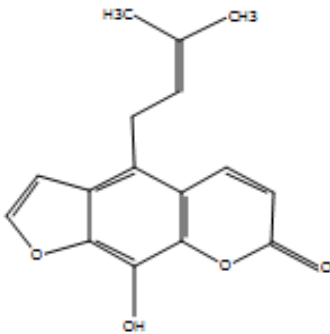
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
102.127				14683.71		
123.091				13726.64		
124.0864			1	81970.04		
164.9289				32222.94		
166.0966			1	23320.67		
207.1226			1	32534.79		
229.1393			1	20260.95		
293.0786	293.0784	-0.69	1	81286.45	C16 H14 O4	(M+Na)+
294.0814	294.0818	1.29	1	13432.08	C16 H14 O4	(M+Na)+
295.0847	295.0843	-1.22	1	1709.41	C16 H14 O4	(M+Na)+



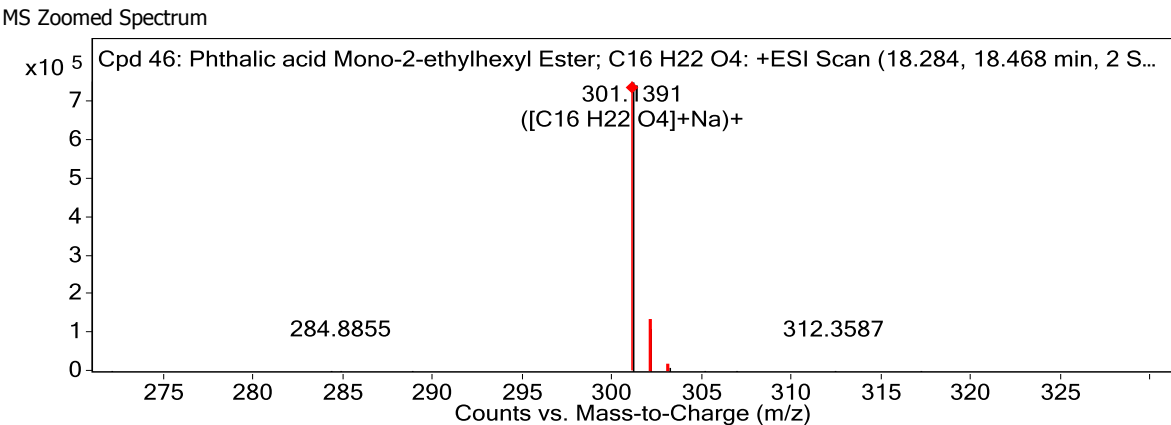
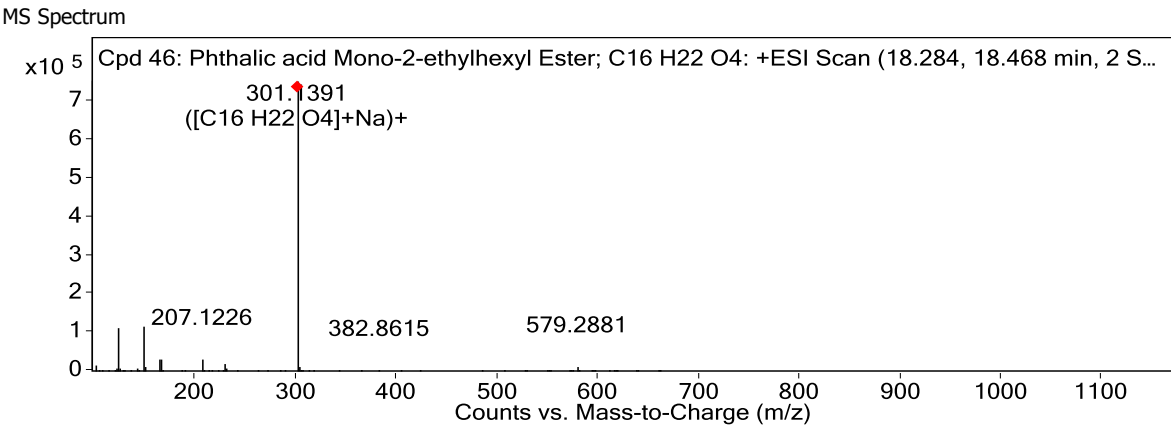
MS/MS Spectrum Peak List

m/z	z	Abund
102.127	1	403.76
123.091		353.78
124.0861	1	1528.55
125.0695	1	320.52
164.9283		466.67
166.0959		350.4
207.1228		304.81
277.0465		756.77
278.0543	1	1098.15
293.0779	1	2015.01

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 46: Phthalic acid Mono-2-ethylhexyl Ester; C16 H22 O4	Phthalic acid Mono-2-ethylhexyl Ester	301.1391	18.389	Auto MS/MS	278.1499

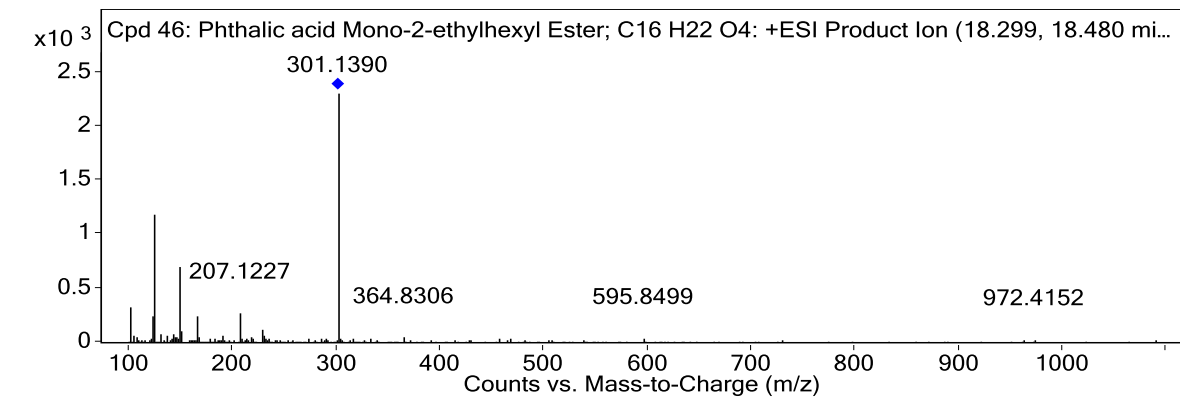


MS Spectrum Peak List

Qualitative Compound Report

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	z	Abund	Formula	Ion
123.0909				16487.39		
124.0864			1	112834.79		
149.023			1	117407.91		
164.9289				29874.71		
166.0966			1	30431.14		
207.1226			1	31810.81		
229.1391			1	18896.2		
301.1391	301.141	6.35	1	751681.56	C16 H22 O4	(M+Na)+
302.1425	302.1444	6.54	1	113921.02	C16 H22 O4	(M+Na)+
303.144	303.1469	9.65	1	12638.42	C16 H22 O4	(M+Na)+

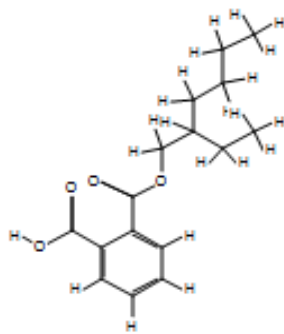
MSMS Spectrum



MS/MS Spectrum Peak List

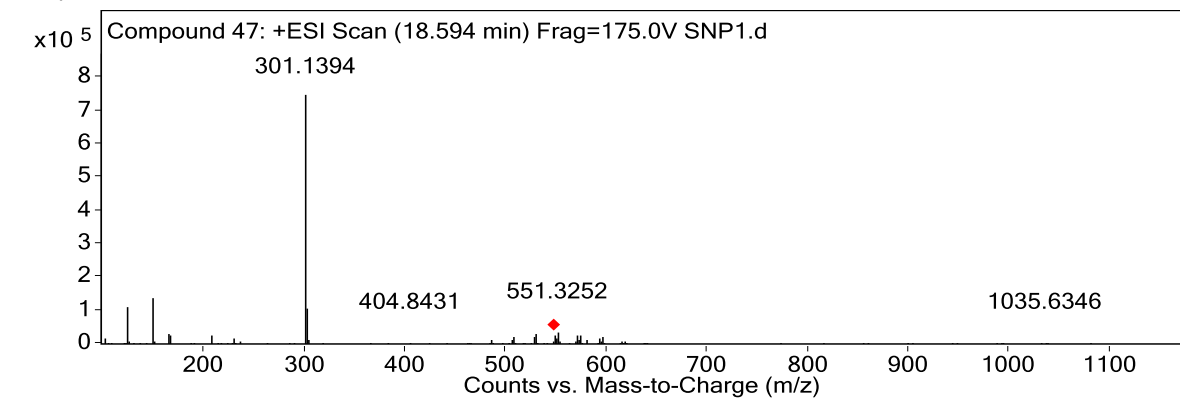
<i>m/z</i>	z	Abund
101.0706	1	326.96
102.127		283.34
123.0906		252.08
124.0862	1	1184.86
149.0214	1	701.69
164.9286		237.03
166.0971	1	250.81
207.1227	1	279.02
301.139	1	2303.13
302.1422	1	293.6

Compound Structure

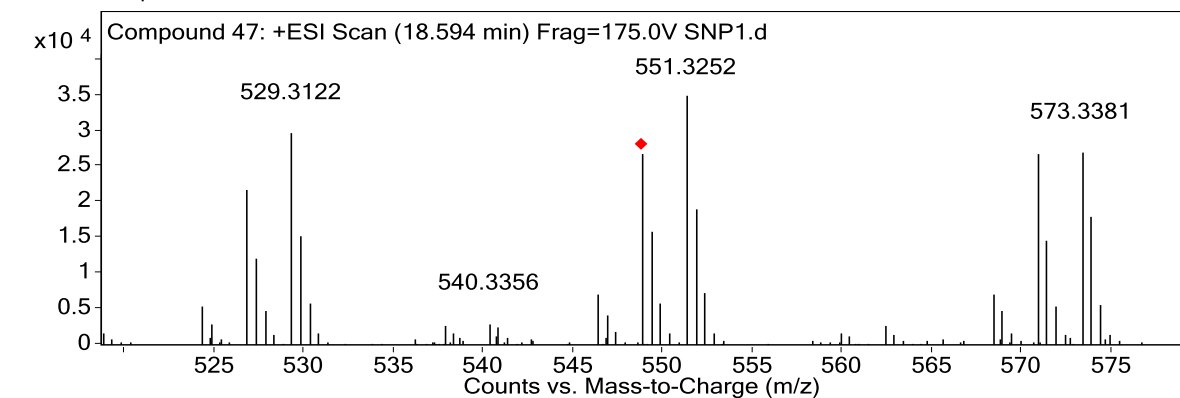


Compound Label	<i>m/z</i>	RT	Algorithm
Compound 47	548.8481	18.61	Auto MS/MS

MS Spectrum



MS Zoomed Spectrum

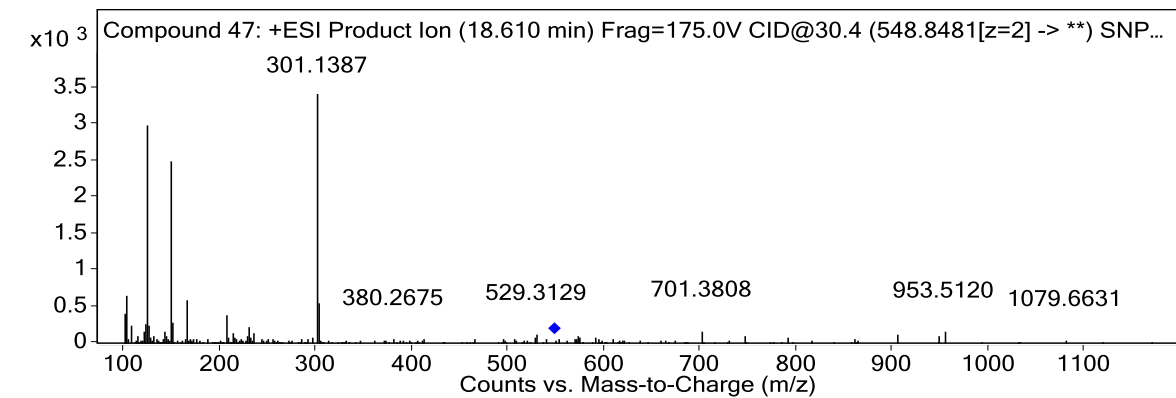


MS Spectrum Peak List

<i>m/z</i>	z	Abund
124.0865	1	113402.22
149.0229	1	140105.61
301.1394	1	748059.56
302.1422	1	106170.83
548.8481	2	26827.56
549.3493	2	15864.56
549.8509	2	5889.69
550.3495	2	1624.98
550.8567	2	339.75
551.3252	2	34983.19

MSMS Spectrum

Qualitative Compound Report

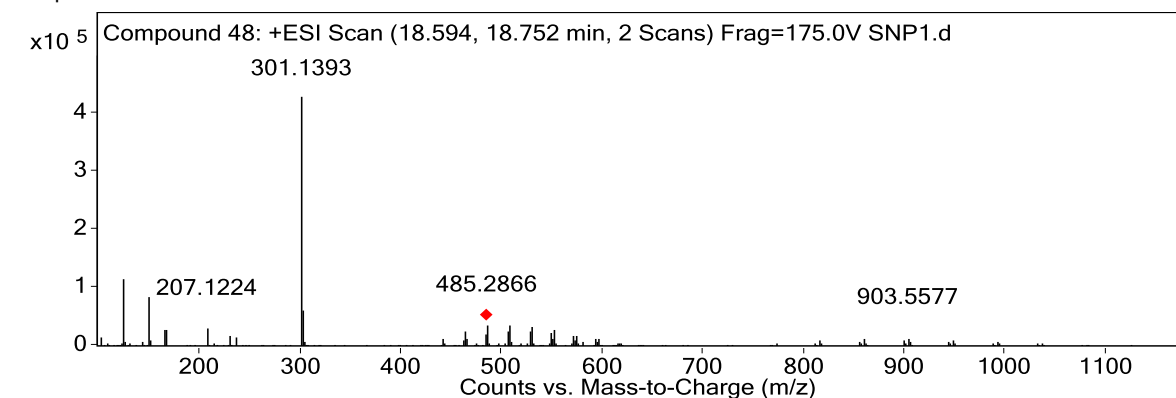


MS/MS Spectrum Peak List

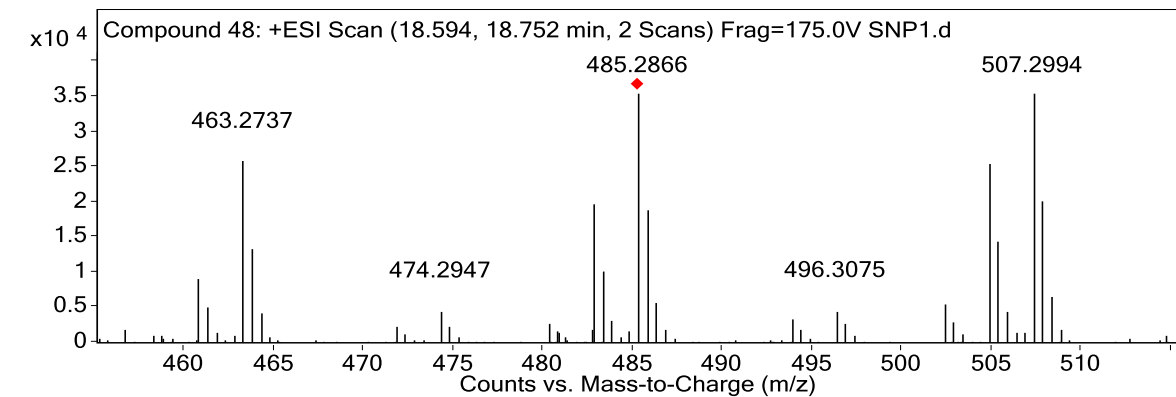
m/z	z	Abund
101.0703		398.24
102.1267		646.86
124.0863	1	2969.8
149.0223	1	2492.23
150.0253	1	288.09
164.9279		308.48
166.0962		586.86
207.1217	1	384.01
301.1387	1	3412.71
302.1396	1	552.08

Compound Label	m/z	RT	Algorithm
Compound 48	485.2866	18.708	Auto MS/MS

MS Spectrum



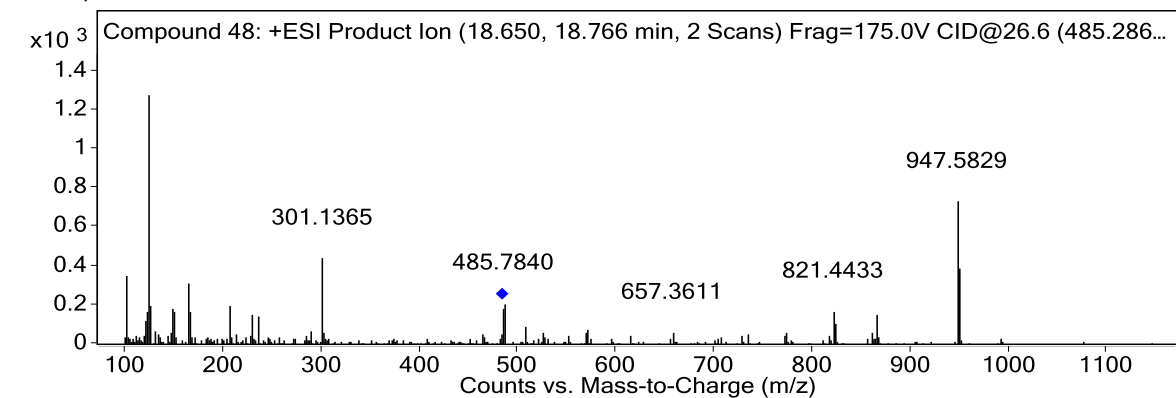
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
124.0865	1	115018.92
149.0228	1	84387.95
301.1393	1	429243.28
302.1421	1	61840.07
485.2866	2	35464.48
485.7881	2	18791.23
486.2883	2	5765.84
486.7874	2	1914.68
507.2994	2	35425.38
529.3125	2	33082.18

MSMS Spectrum



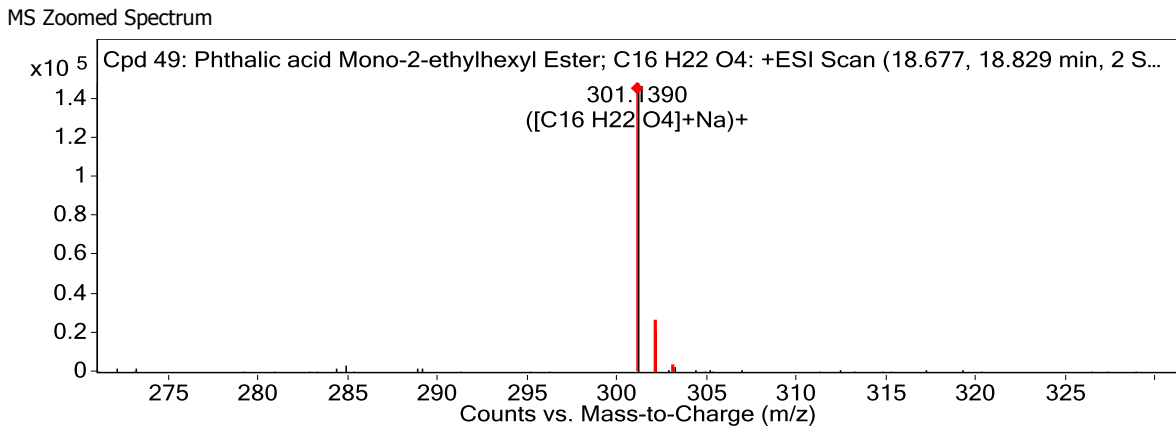
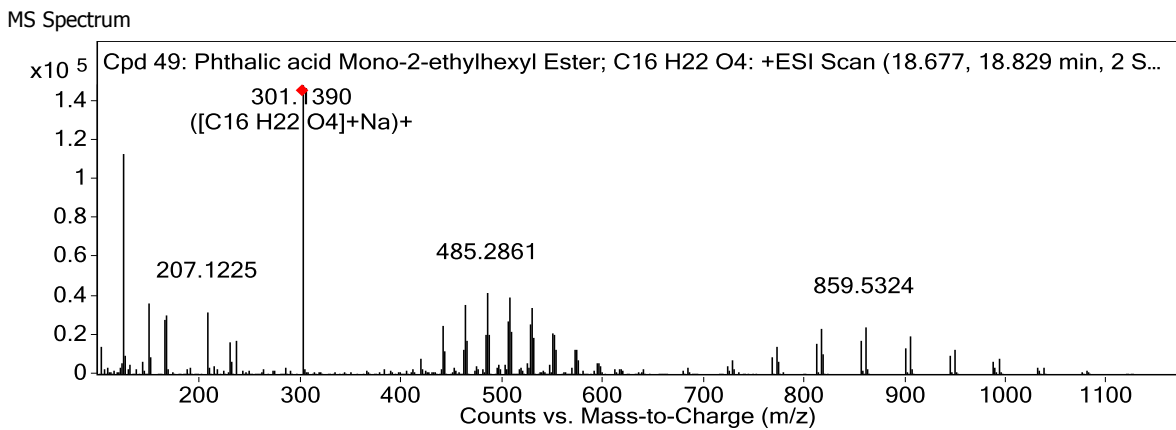
MS/MS Spectrum Peak List

m/z	z	Abund
101.0707	1	186.51
102.1275	1	354.11
124.0864	1	1275.95
125.0697		201.63
164.929		314.21
207.1229	1	199.54
301.1365	1	439.76
485.784	2	209.71
947.5829	1	730.33
948.5844	1	392.29

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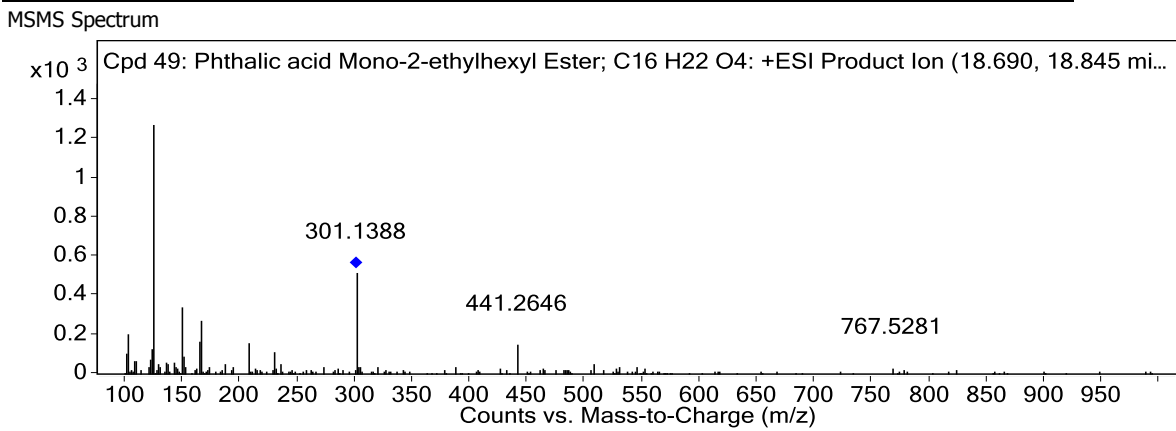
Qualitative Compound Report

Cpd 49: Phthalic acid Mono-2-ethylhexyl Ester; C16 H22 O4	Phthalic acid Mono-2-ethylhexyl Ester	301.139	18.767	Auto MS/MS	278.1497
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MS Spectrum Peak List

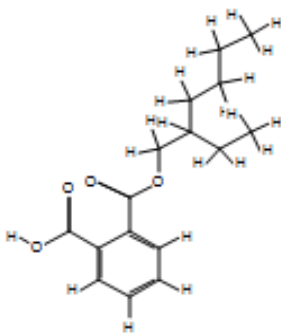
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0865			1	112702.12		
149.0226				36972.93		
207.1225			1	32426.76		
301.139	301.141	6.75	1	148206.75	C16 H22 O4	(M+Na)+
302.1416	302.1444	9.51	1	21609.45	C16 H22 O4	(M+Na)+
303.1433	303.1469	12.11	1	2940.39	C16 H22 O4	(M+Na)+
463.2731			2	35635.27		
485.2861			2	41892.16		
507.2995			2	39393.55		
529.3121			2	34280.44		



MS/MS Spectrum Peak List

m/z	z	Abund
102.1279		206.18
124.0866	1	1273.03
125.0691		156.88
125.088	1	165.62
149.0219	1	340.36
164.9285		169.71
166.0972		271.55
207.1229		163.47
301.1388	1	518.99
441.2646		150.84

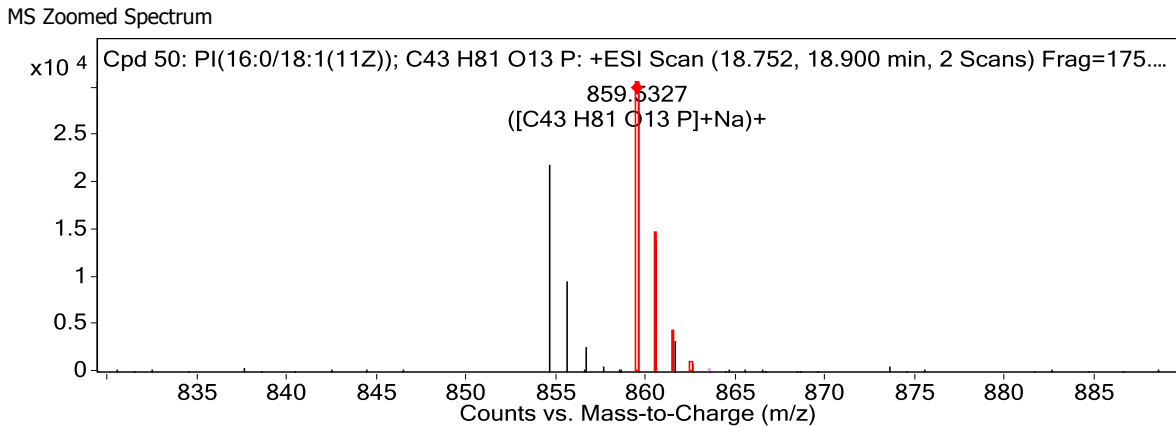
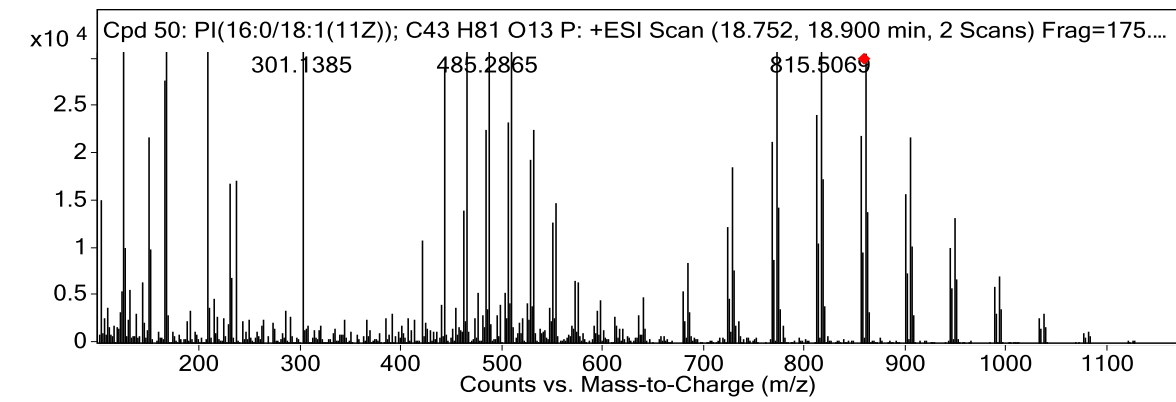
Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 50: PI(16:0/18:1(11Z)); C43	PI(16:0/18:1(11Z))	859.5327	18.857	Auto MS/MS	836.5428

MS Spectrum

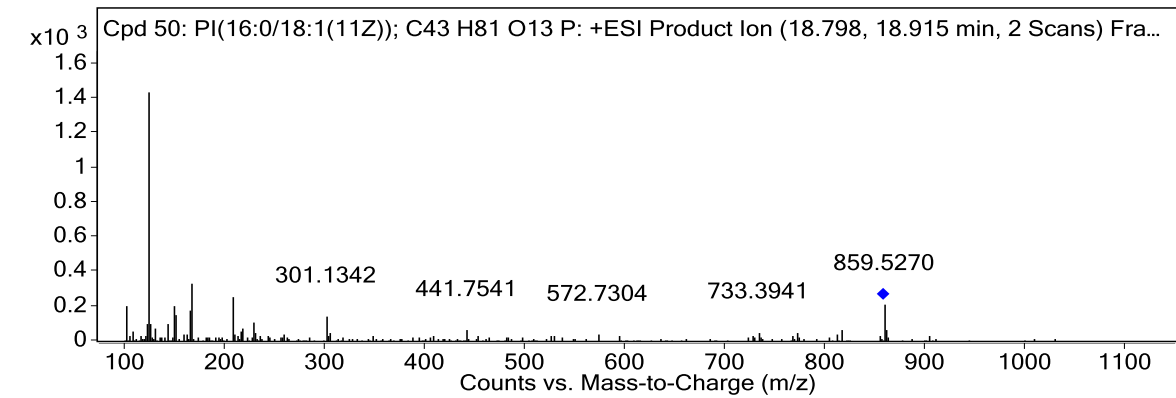
Qualitative Compound Report



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
124.0864			1	118459.53		
301.1385			1	81294.66		
463.2735			2	39761.22		
485.2865			2	41481.45		
771.4807			1	35654.38		
815.5069			1	40134.78		
859.5327	859.5307	-2.27	1	30572.08	C43 H81 O13 P	(M+Na)+
860.5348	860.5341	-0.74	1	13885.26	C43 H81 O13 P	(M+Na)+
861.5358	861.537	1.41	1	3308.78	C43 H81 O13 P	(M+Na)+
862.5407	862.5399	-0.99	1	951.7	C43 H81 O13 P	(M+Na)+

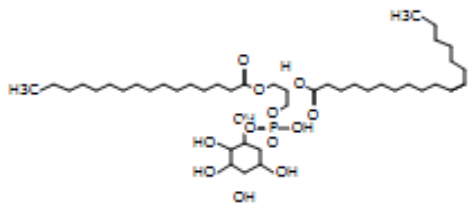
MSMS Spectrum



MS/MS Spectrum Peak List

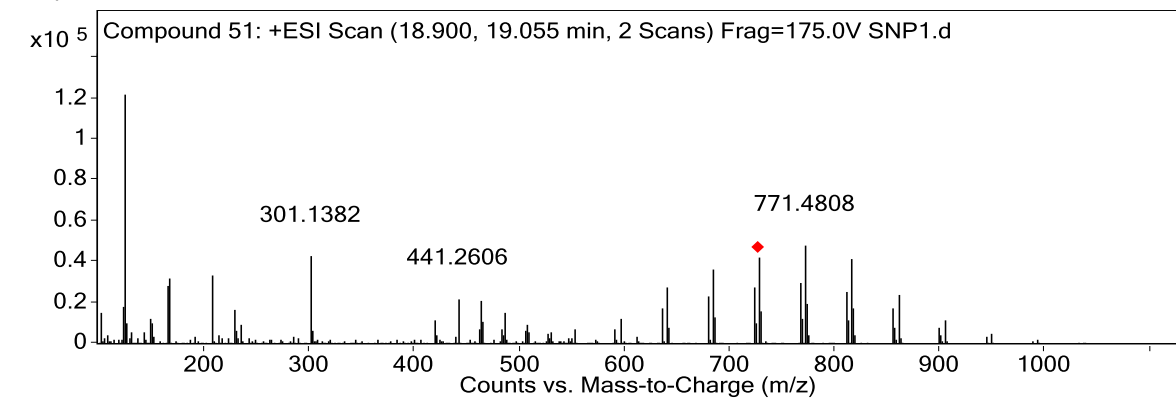
<i>m/z</i>	<i>z</i>	Abund
102.1267		207.44
123.0907		237.01
124.087	1	1435.88
149.0218		206.35
150.0654		158.67
164.9279		176.76
166.0951	1	331.94
207.1215	1	258.66
301.1342	1	144.47
859.527	1	216.29

Compound Structure



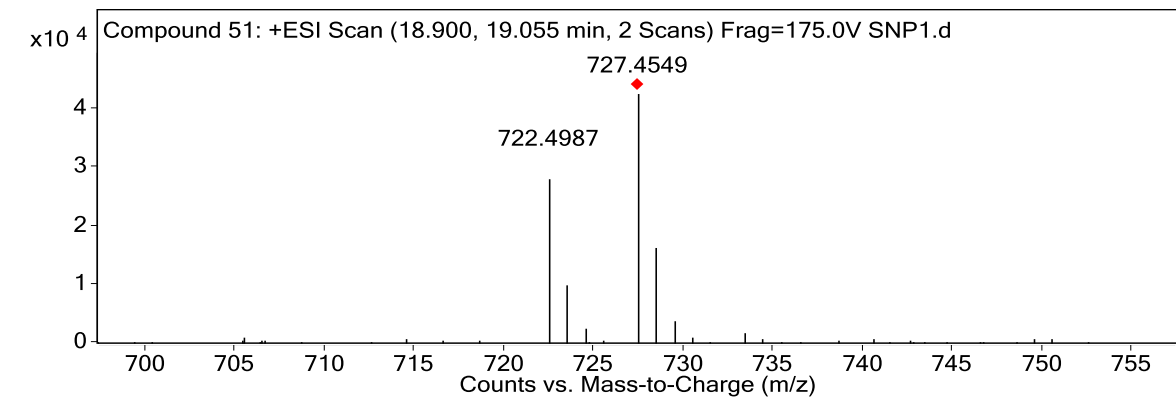
Compound Label	<i>m/z</i>	RT	Algorithm
Compound 51	727.4549	18.998	Auto MS/MS

MS Spectrum



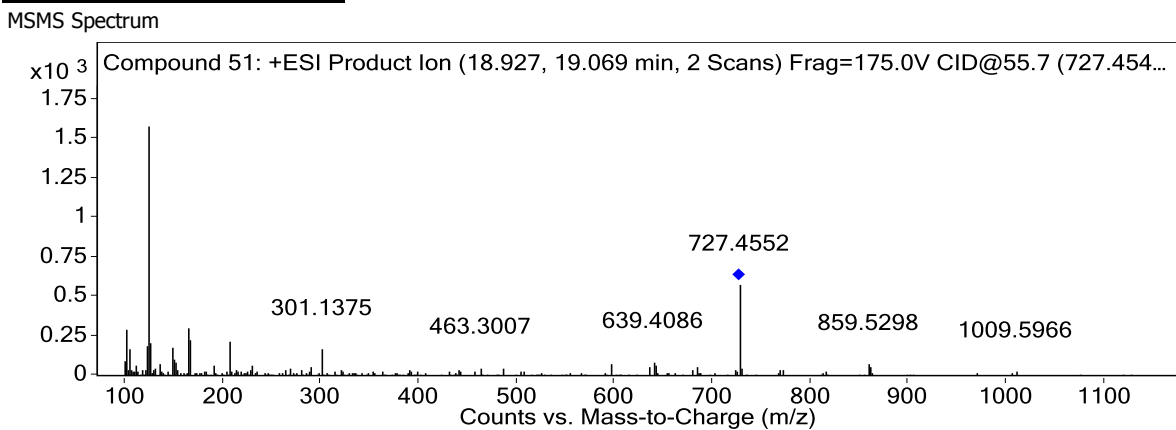
MS Zoomed Spectrum

Qualitative Compound Report



MS Spectrum Peak List

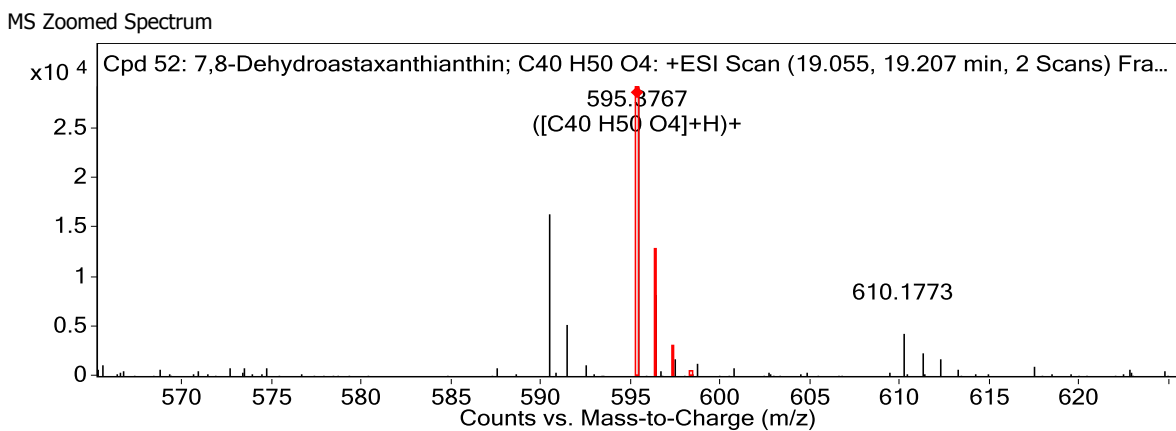
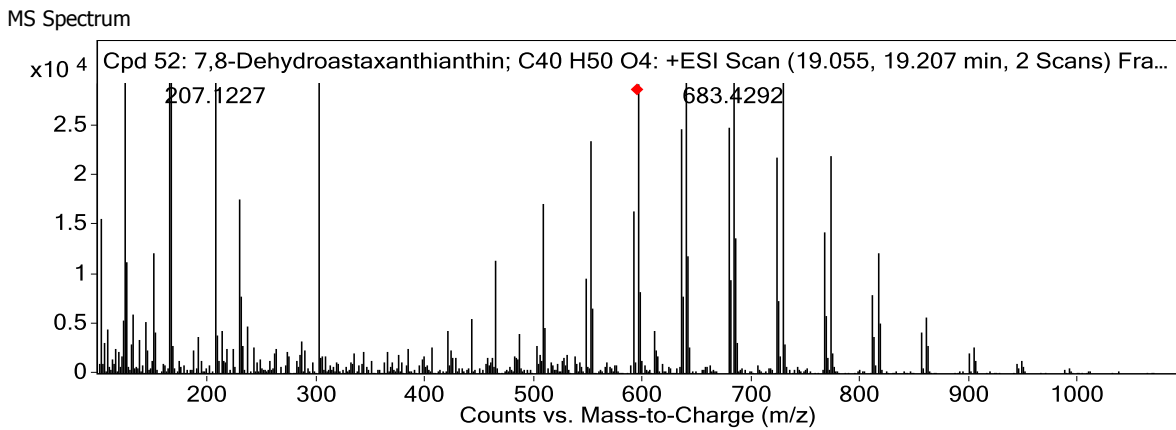
m/z	z	Abund
124.0865	1	122018.1
207.1227	1	33583.38
301.1382	1	43117.96
683.4289	1	36669.62
727.4549	1	42627.29
728.4569	1	16197.07
729.4592	1	3787.34
730.4652	1	957.14
771.4808	1	48520.23
815.5067	1	41951.34



MS/MS Spectrum Peak List

m/z	z	Abund
101.0707	1	288.75
102.1275	1	211.37
123.0906		186.51
124.0865	1	1577.44
125.0891	1	205.06
149.0235	1	182.53
164.9296		298.92
166.0975		228.83
207.1217	1	215.57
727.4552	1	577.11

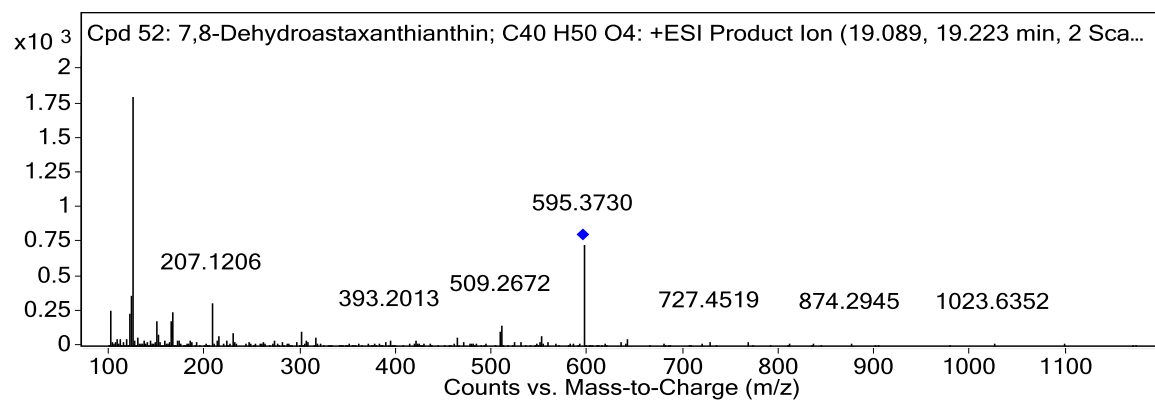
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 52: 7,8-Dehydroastaxanthianthin; C40 H50 O4	7,8-Dehydroastaxanthianthin	595.3767	19.156	Auto MS/MS	594.3692



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0865			1	127662.81		
166.0966			1	34539.58		
207.1227			1	34979.52		
595.3767	595.3782	2.53	1	29201.05	C40 H50 O4	(M+H)+
596.3794	596.3816	3.64	1	8242.76	C40 H50 O4	(M+H)+
597.3819	597.3848	4.76	1	1865.29	C40 H50 O4	(M+H)+
598.3859	598.3878	3.16	1	297.16	C40 H50 O4	(M+H)+
639.4028			1	37520.13		
683.4292			1	37956.55		
727.4548			1	32211.14		

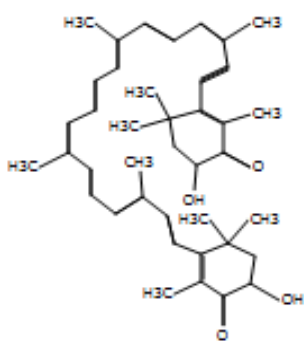
MSMS Spectrum



MS/MS Spectrum Peak List

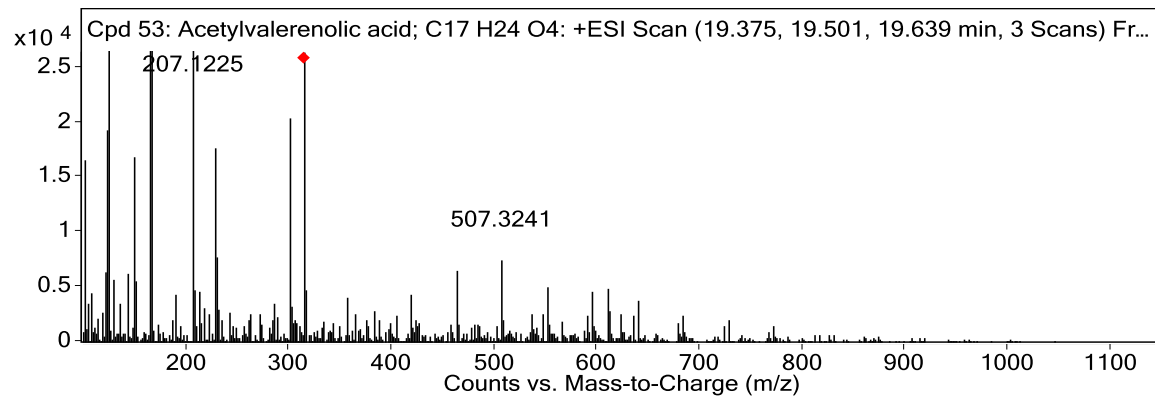
m/z	z	Abund
101.0705		196.7
102.1263	1	259.51
122.0936		235.73
123.0903		367.85
124.0864	1	1801.69
125.0697		293.77
164.9295		185.43
166.0961		243.02
207.1206	1	309.79
595.373	1	737.43

Compound Structure

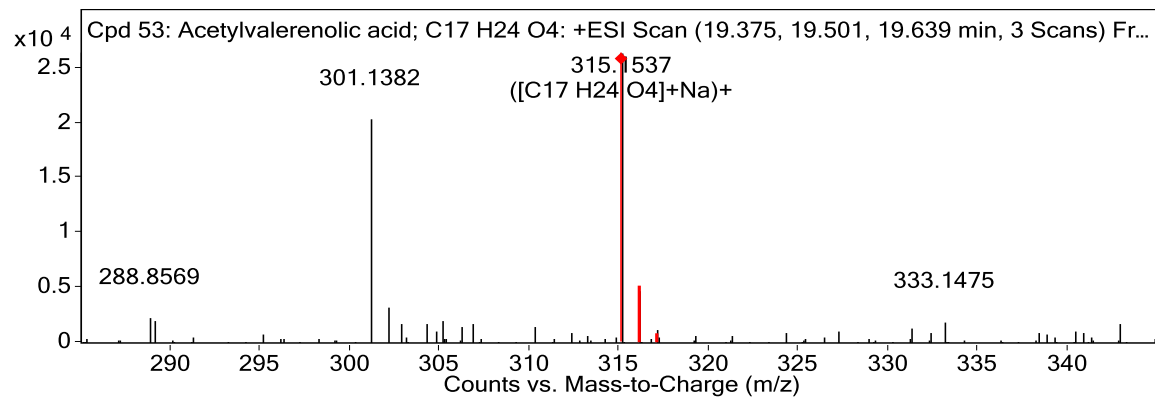


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 53: Acetylvalerenolic acid; C17 H24 O4	Acetylvalerenolic acid	315.1537	19.535	Auto MS/MS	292.1645

MS Spectrum



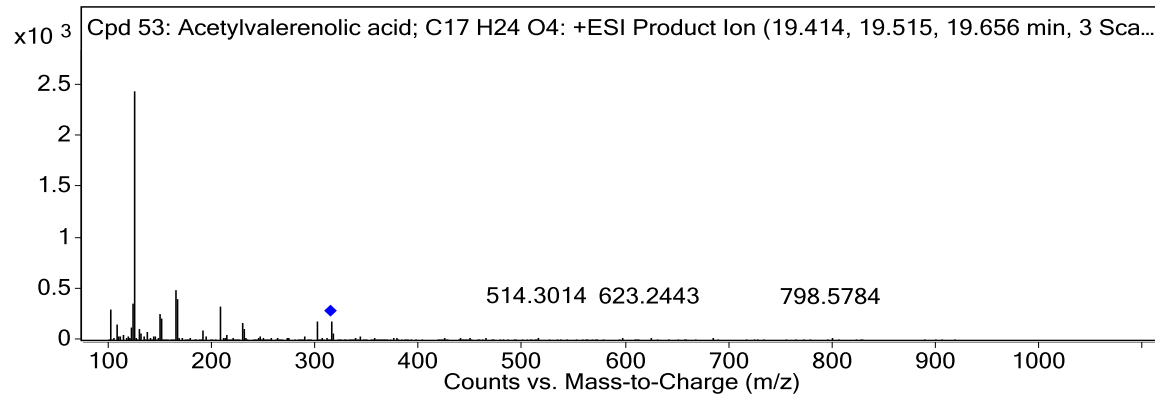
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
123.0911				19287.67		
124.0865			1	136960.08		
164.9289				27186.1		
166.0967			1	35128.92		
207.1225			1	37343.93		
229.1392				17582.08		
301.1382			1	20392.87		
315.1537	315.1567	9.43	1	26314.35	C17 H24 O4	(M+Na)+
316.1569	316.1601	10.07	1	4798.3	C17 H24 O4	(M+Na)+
317.1595	317.1626	9.89	1	532.58	C17 H24 O4	(M+Na)+

MSMS Spectrum

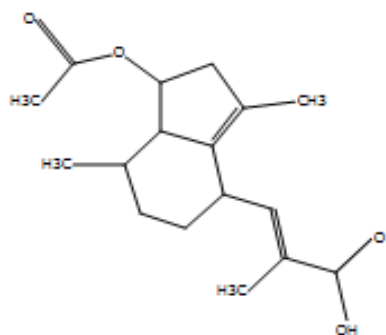


MS/MS Spectrum Peak List

<i>m/z</i>	<i>z</i>	Abund
101.0706		305.97

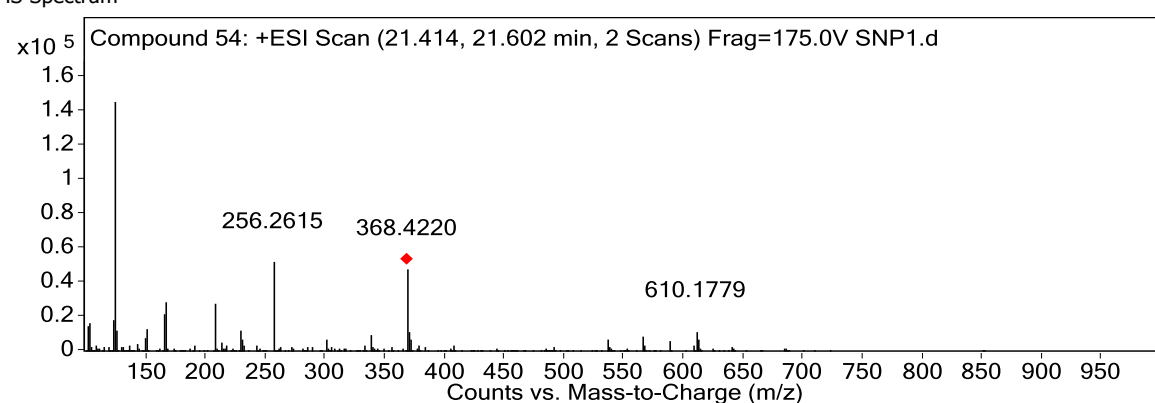
102.1273		266.74
123.0912		361.41
124.0864	1	2442.91
125.0702	1	360.75
125.0907	1	299.13
149.0218	1	259.69
164.9291		496.8
166.0967	1	409.67
207.1205	1	343.19

Compound Structure

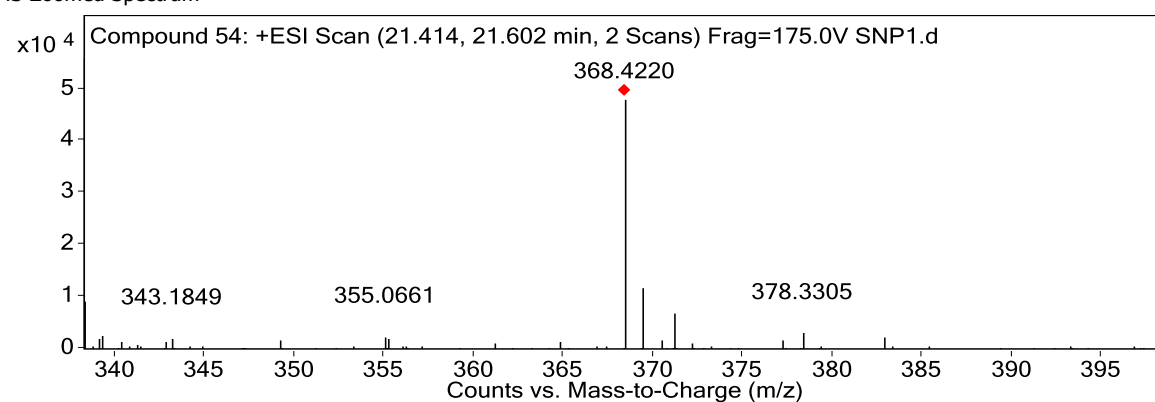


Compound Label	<i>m/z</i>	RT	Algorithm
Compound 54	368.422	21.524	Auto MS/MS

MS Spectrum



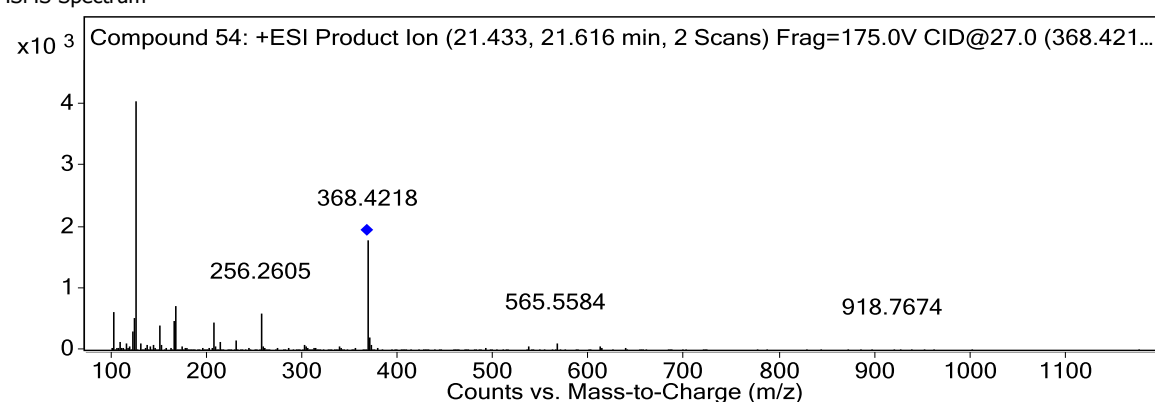
MS Zoomed Spectrum



MS Spectrum Peak List

<i>m/z</i>	<i>z</i>	Abund
102.1271		16589.45
123.0912		18691.96
124.0865	1	145553.72
164.9289		21854.4
166.0966	1	28920.21
207.1226	1	27610.59
256.2615	1	51991.69
368.422	1	47938.04
369.4249	1	11673.97
370.4281	1	1832.02

MSMS Spectrum



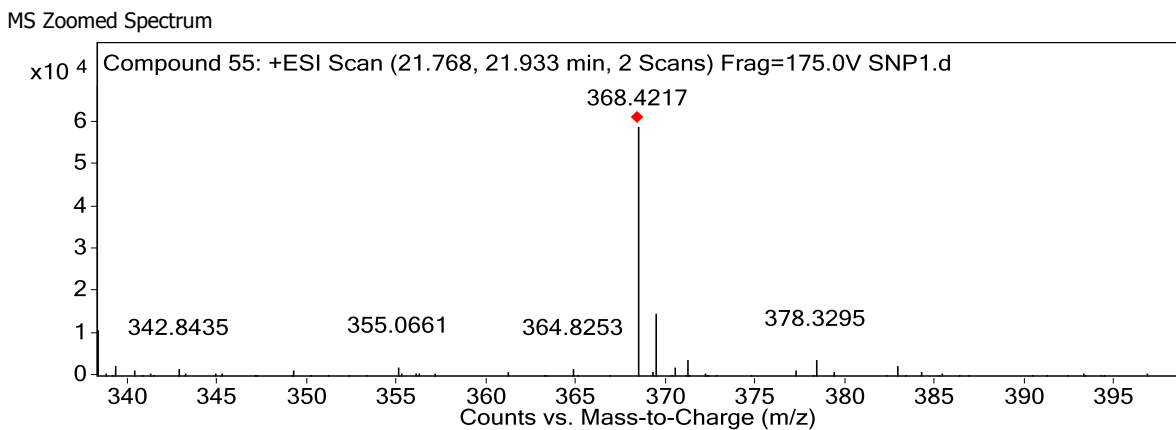
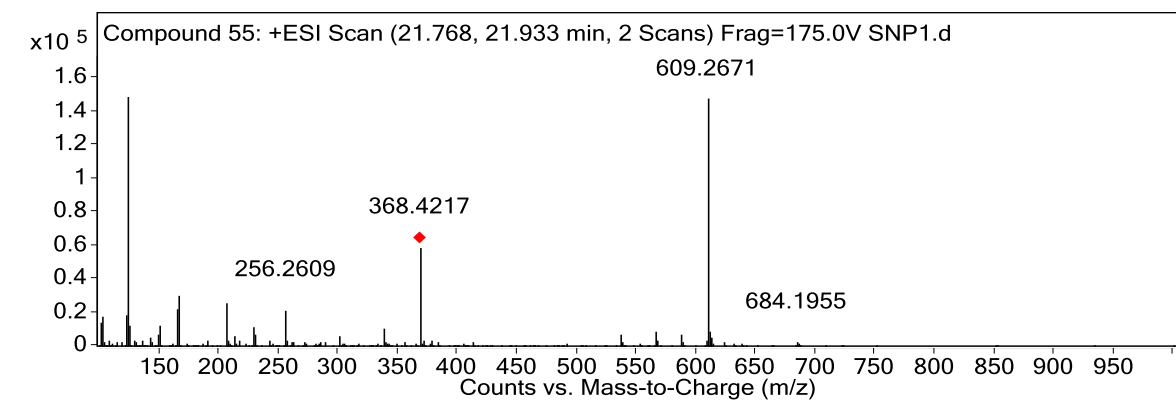
MS/MS Spectrum Peak List

<i>m/z</i>	<i>z</i>	Abund
101.07	1	406.02
102.1269		634.24
123.0914		534.54
124.0862	1	4053.02
150.0645		413.22
164.9281		475.8
166.0966	1	716.49
207.1235	1	455.92
256.2605	1	616.28
368.4218	1	1805.26

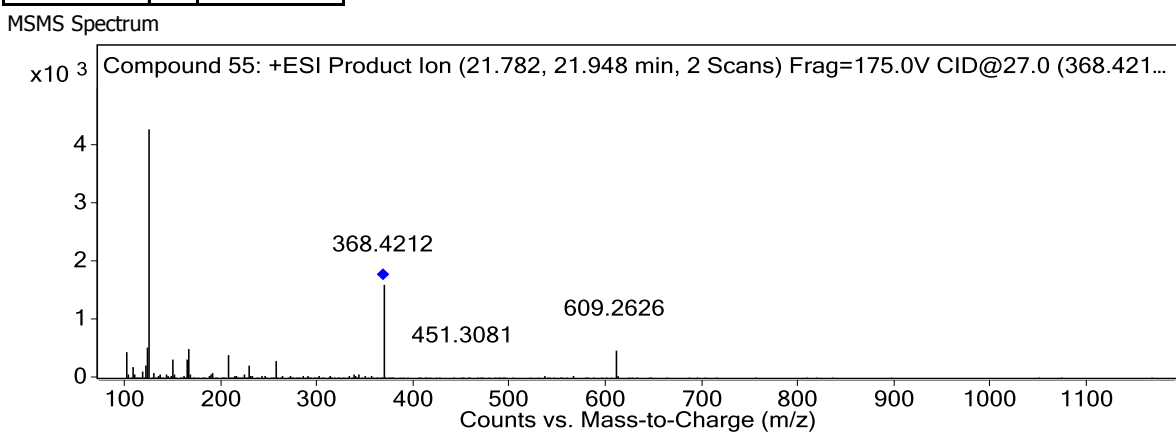
Compound Label	<i>m/z</i>	RT	Algorithm
Compound 55	368.4217	21.865	Auto MS/MS

MS Spectrum

Qualitative Compound Report

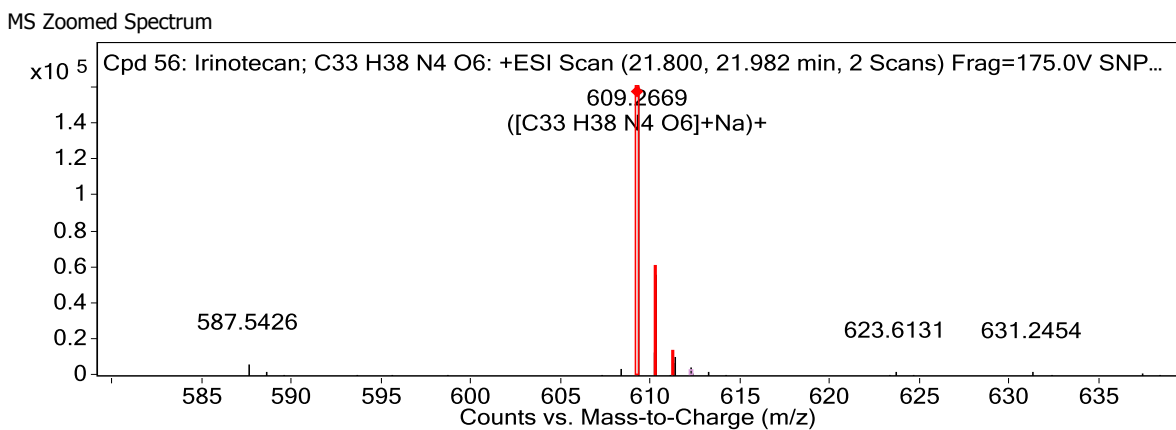
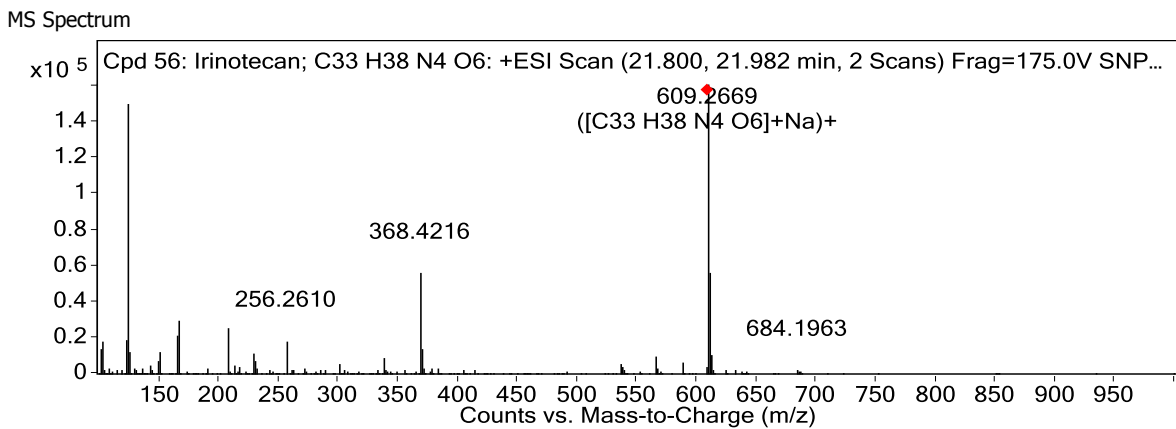


MS Spectrum Peak List		
m/z	z	Abund
124.0864	1	148735.47
164.9287		21943.53
166.0964	1	30508.1
207.1225	1	25771.44
256.2609	1	21522.91
368.4217	1	59033.88
369.4245	1	14749.85
370.4274	1	2136.43
609.2671	1	147280.75
610.2695	1	51591.8



MS/MS Spectrum Peak List		
m/z	z	Abund
101.0702		434.1
102.1264	1	462.27
123.0912		544.96
124.0865	1	4295.51
125.0692		400.29
164.9274		342.63
166.0968	1	514.68
207.1228	1	417.01
368.4212	1	1606.9
609.2626	1	499.49

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 56: Irinotecan; C33 H38 N4 O6	Irinotecan	609.2669	21.912	Auto MS/MS	586.2774

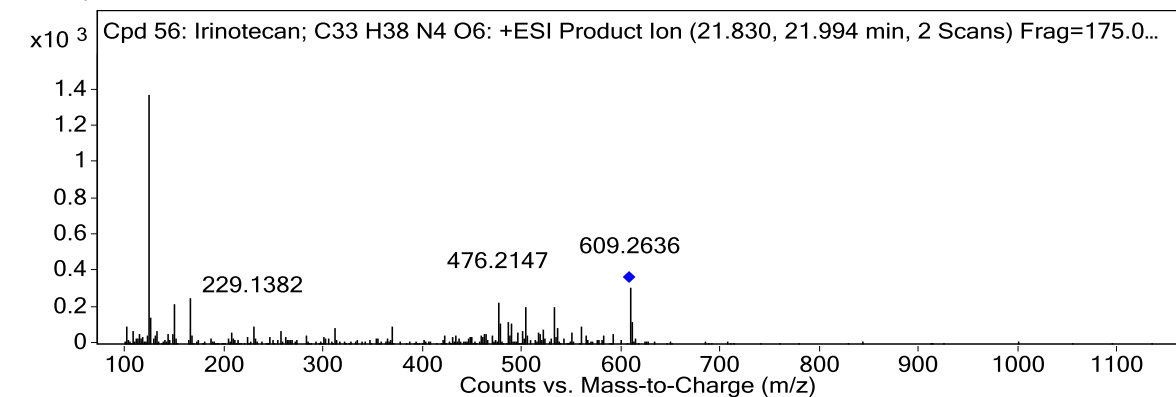


MS Spectrum Peak List						
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion

Qualitative Compound Report

123.091				19391.59		
124.0864			1	150167.06		
164.9286				21955.46		
166.0964			1	30121.55		
207.1226			1	25406.03		
256.261			1	18605.59		
368.4216			1	56467.06		
609.2669	609.2684	2.38	1	160923.03	C33 H38 N4 O6	(M+Na)+
610.2693	610.2715	3.59	1	56309.29	C33 H38 N4 O6	(M+Na)+
611.2704	611.2743	6.42	1	10554.95	C33 H38 N4 O6	(M+Na)+

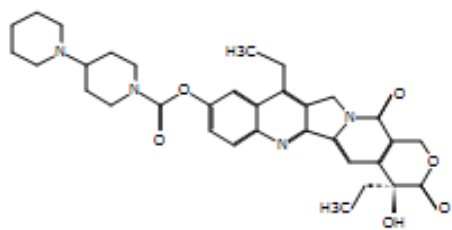
MSMS Spectrum



MS/MS Spectrum Peak List

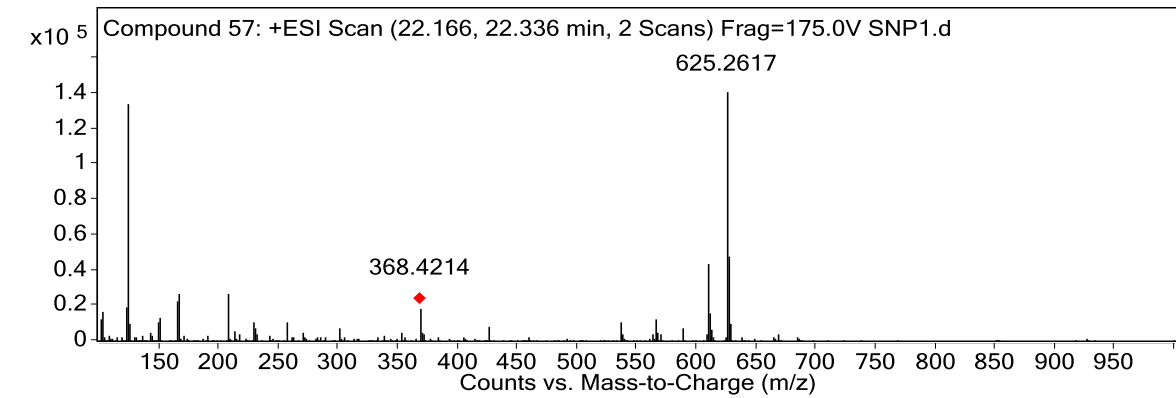
<i>m/z</i>	<i>z</i>	Abund
123.0897		186.03
124.0859	1	1374.84
125.0691		147.04
150.0648		219.1
166.0956	1	251.34
475.2089		143.95
476.2147		231.86
503.2338	1	206.4
531.2376		201.85
609.2636	1	314.09

Compound Structure

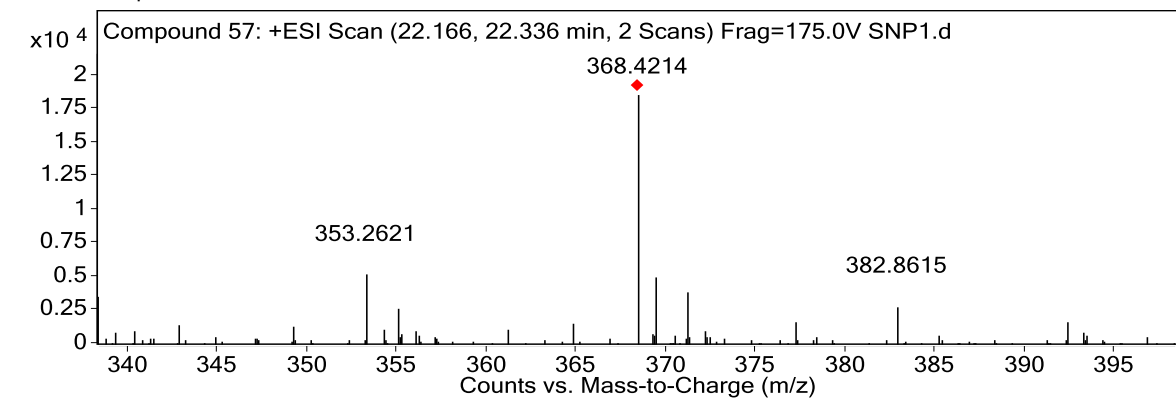


Compound Label	<i>m/z</i>	RT	Algorithm
Compound 57	368.4214	22.269	Auto MS/MS

MS Spectrum



MS Zoomed Spectrum

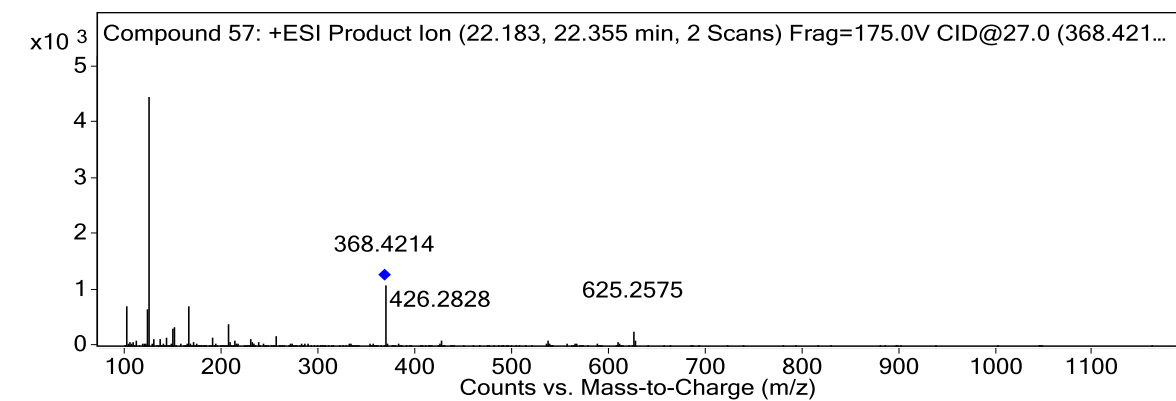


MS Spectrum Peak List

<i>m/z</i>	<i>z</i>	Abund
124.0864	1	134200.16
164.9287		22413.27
166.0965	1	27366.93
207.1226	1	27104.33
368.4214	1	18573.22
369.4239	1	4948.94
370.4284	1	630.54
609.2658	1	43560.84
625.2617	1	140981.31
626.2642	1	48420.9

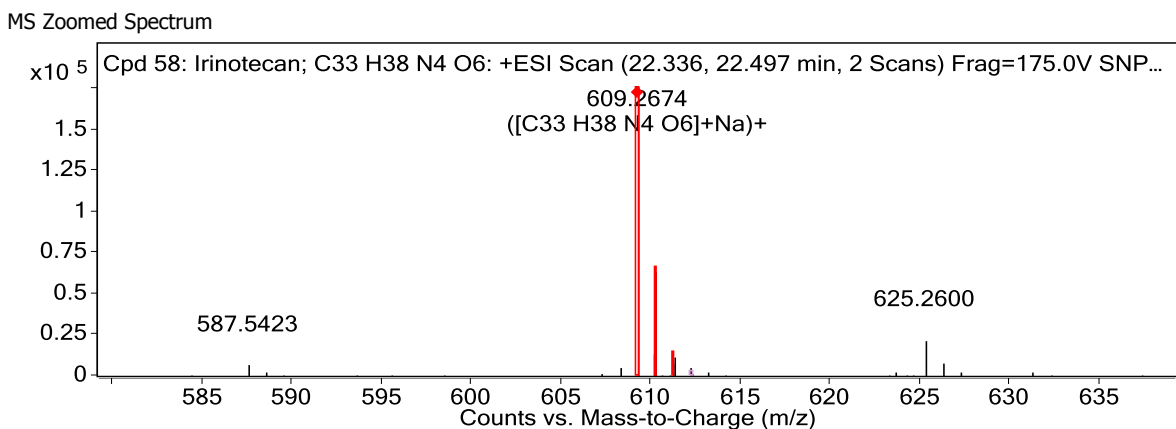
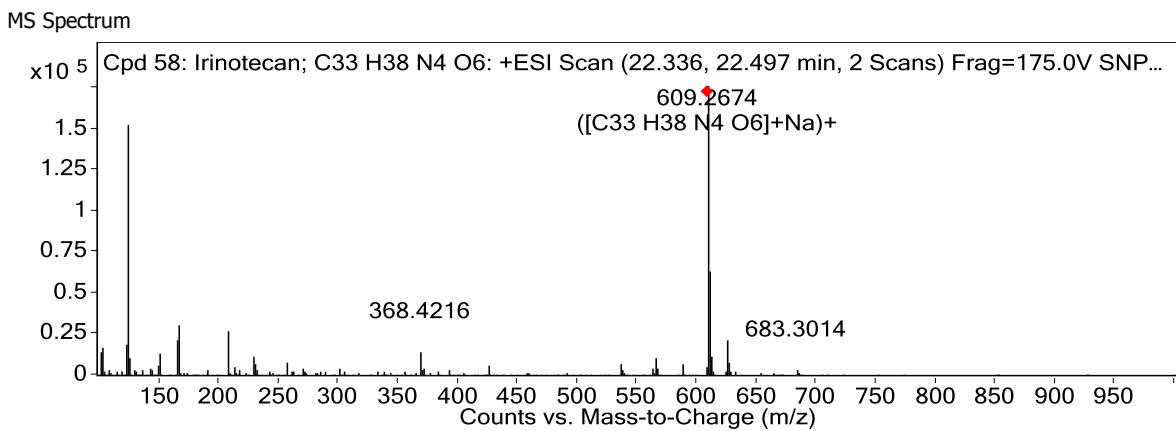
MSMS Spectrum

Qualitative Compound Report

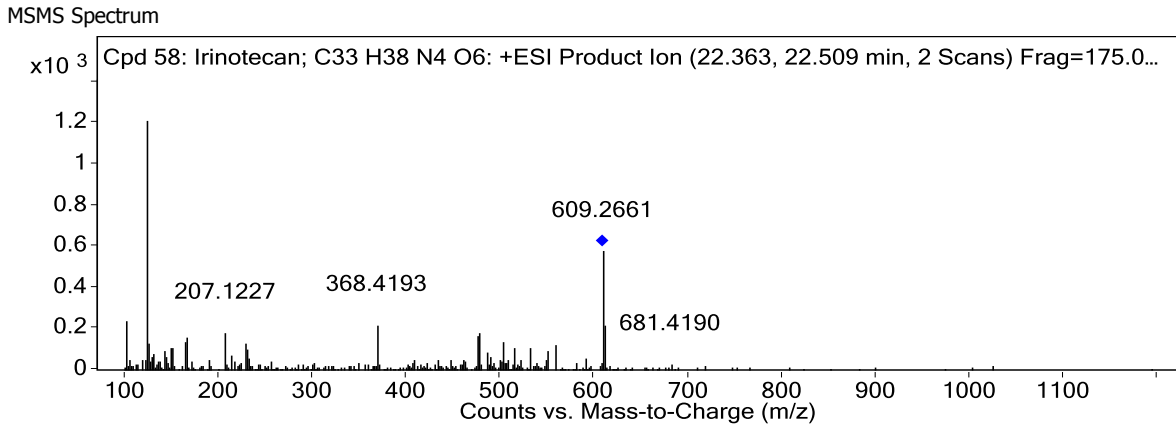


MS/MS Spectrum Peak List		
m/z	z	Abund
101.0702	1	425.7
102.1271	1	707.62
123.0909		680.41
124.0861	1	4462.73
125.0708		331.97
150.066		333.69
164.9298		432.44
166.0963	1	729.19
207.1225		407.9
368.4214	1	1087

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 58: Irinotecan; C33 H38 N4 O6	Irinotecan	609.2674	22.436	Auto MS/MS	586.2779



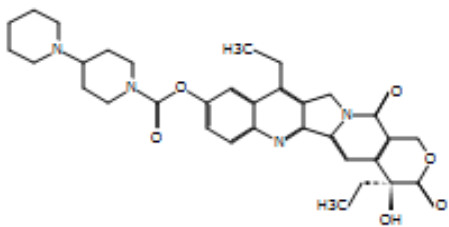
MS Spectrum Peak List						
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
102.127				16900.43		
123.0911				18944.98		
124.0864			1	152869.91		
164.9286				21388.68		
166.0965			1	30847.17		
207.1225			1	26921.88		
609.2674	609.2684	1.55	1	176159.14	C33 H38 N4 O6	(M+Na)+
610.2697	610.2715	2.88	1	63242.74	C33 H38 N4 O6	(M+Na)+
611.2715	611.2743	4.6	1	11677.92	C33 H38 N4 O6	(M+Na)+
625.26			1	22231.27		



MS/MS Spectrum Peak List		
m/z	z	Abund
101.0704		191.81
102.1271		236.43
123.0901		289.79
124.0859	1	1210.74
207.1227		181.88
368.4193	1	219.87
475.2079		168.16
477.2274	1	177.39
609.2661	1	578.83
610.2665	1	219.91

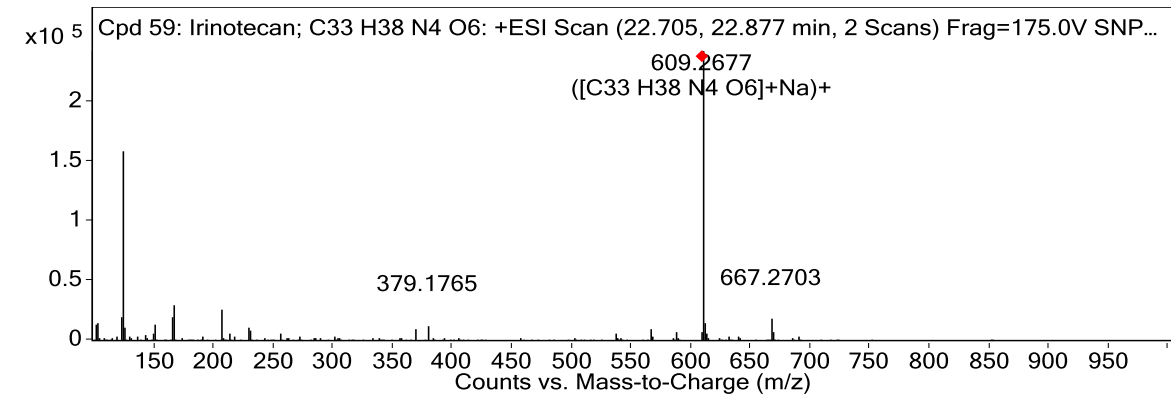
Qualitative Compound Report

Compound Structure

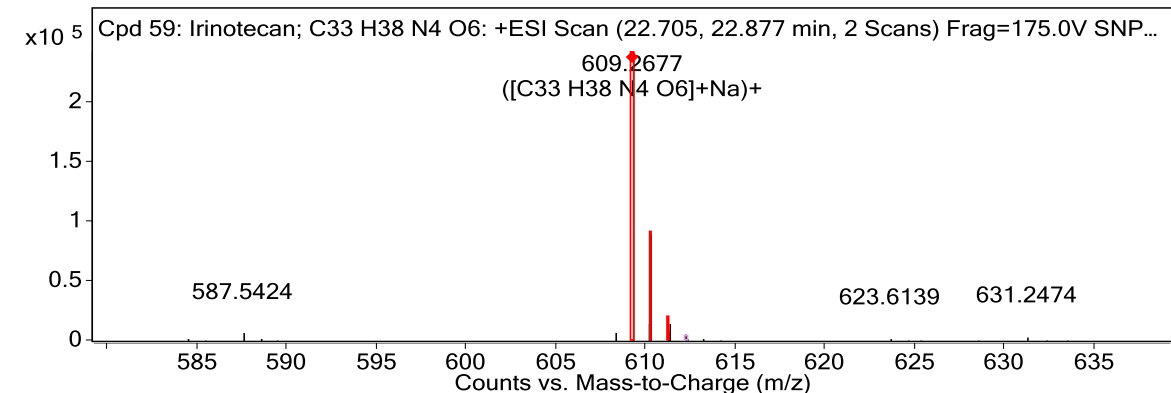


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 59: Irinotecan; C33 H38 N4 O6	Irinotecan	609.2677	22.805	Auto MS/MS	586.2782

MS Spectrum



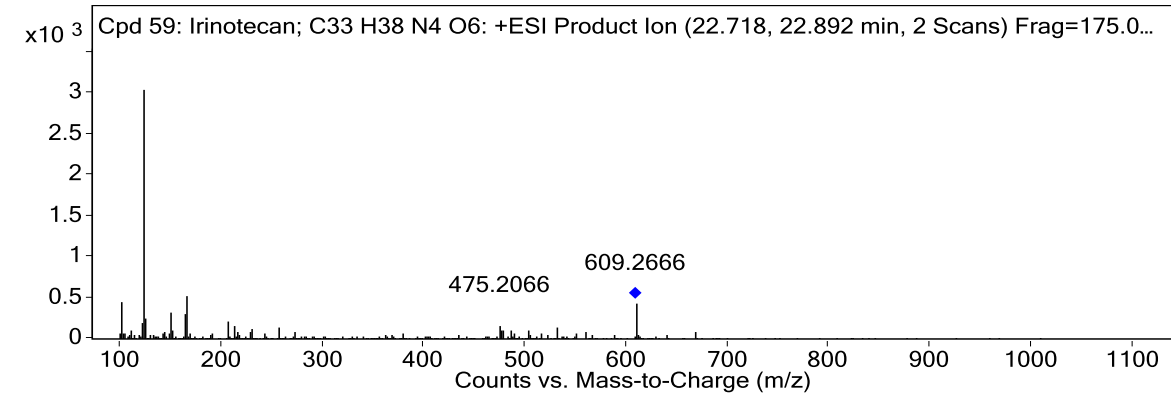
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
102.1271				15531.72		
123.0909				20426.82		
124.0864			1	159000.34		
164.9288				19987.75		
166.0965			1	29617.63		
207.1225			1	25882.16		
609.2677	609.2684	1.03	1	242408.27	C33 H38 N4 O6	(M+Na)+
610.2699	610.2715	2.61	1	89993.45	C33 H38 N4 O6	(M+Na)+
611.2719	611.2743	4.01	1	15564.16	C33 H38 N4 O6	(M+Na)+
667.2703			1	18146.31		

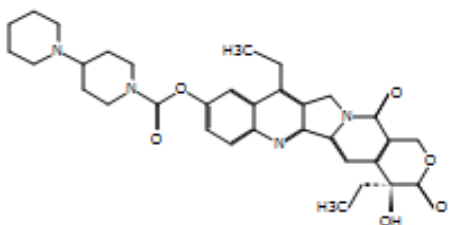
MSMS Spectrum



MS/MS Spectrum Peak List

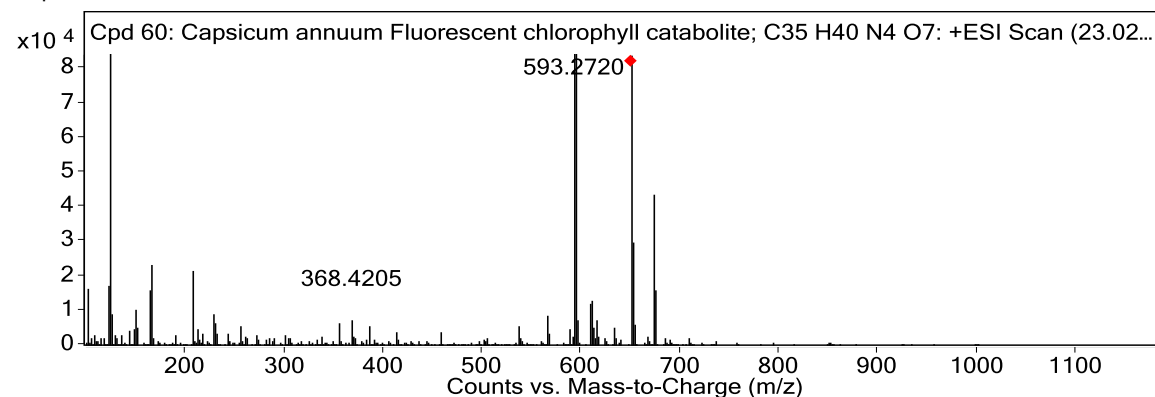
m/z	z	Abund
101.0698		430.33
102.1268	1	451.49
123.0913		404.3
124.0862	1	3041.45
125.0885	1	247.43
150.0664		334.75
164.9289		313.11
166.0963	1	529.69
207.1219		219.24
609.2666	1	429.38

Compound Structure

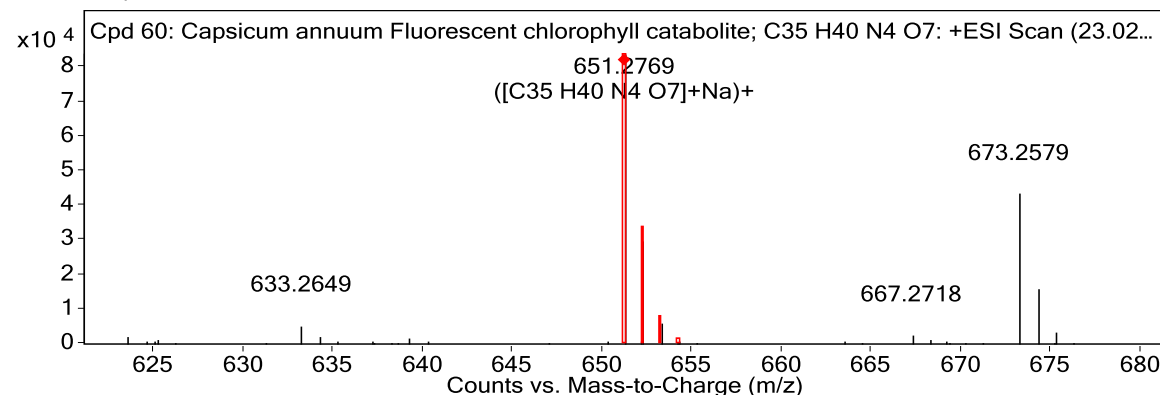


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 60: Capsicum annuum Fluorescent chlorophyll catabolite; C35 H40 N4 O7	Capsicum annuum Fluorescent chlorophyll catabolite	651.2769	23.133	Auto MS/MS	628.2873

MS Spectrum



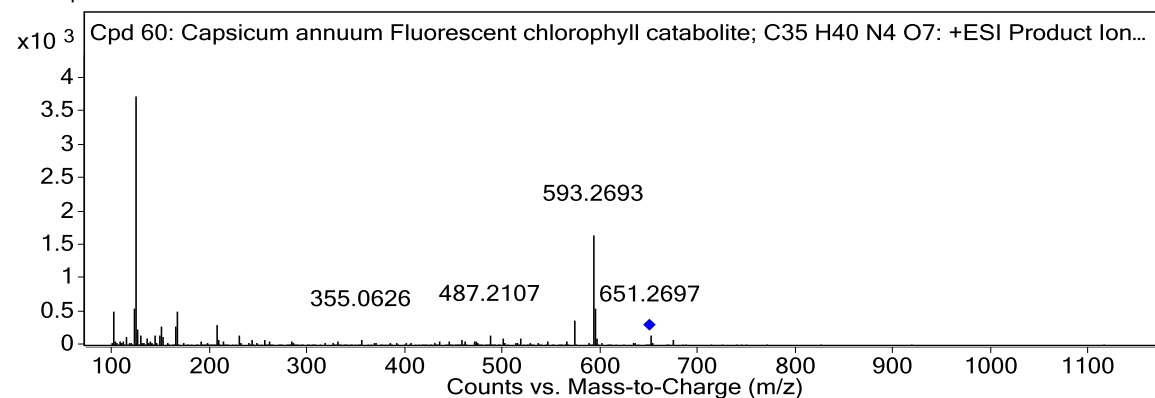
MS Zoomed Spectrum



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	z	Abund	Formula	Ion
124.0864			1	128578.53		
166.0963			1	23250.27		
593.272			1	823627.25		
594.2759			1	310668.16		
595.2777			1	57150.39		
651.2769	651.2789	3.14	1	83644.96	C35 H40 N4 O7	(M+Na)+
652.2792	652.2821	4.35	1	29728.55	C35 H40 N4 O7	(M+Na)+
653.2814	653.2849	5.46	1	6139.13	C35 H40 N4 O7	(M+Na)+
654.2835	654.2876	6.34	1	1034.27	C35 H40 N4 O7	(M+Na)+
673.2579			1	43456.39		

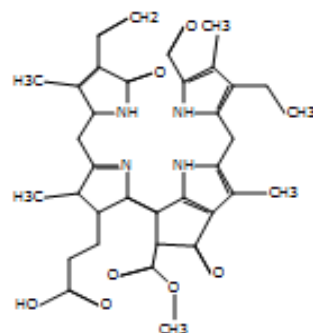
MSMS Spectrum



MS/MS Spectrum Peak List

m/z	z	Abund
101.0692		377.05
102.127	1	524.37
123.0909		553.63
124.0858	1	3738.49
164.9281		282.35
166.0969		522.49
207.1228	1	307.66
573.2454		390.88
593.2693	1	1664.87
594.2735	1	549.81

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 61: Ganoderic acid F; C32 H42 O9	Ganoderic acid F	593.2721	23.174	Auto MS/MS	570.2828

MS Spectrum

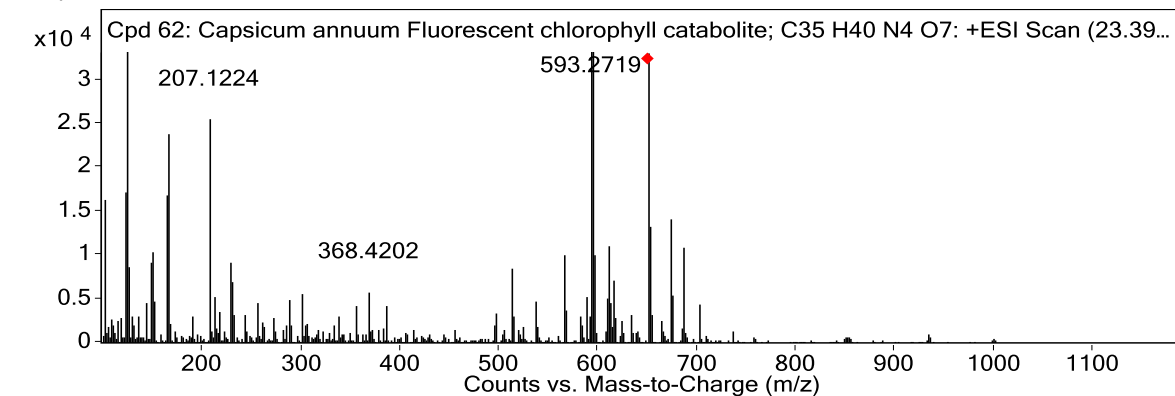


m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0864			1	123466.35		
166.0966			1	22631.5		
207.1224			1	21127.34		
593.2721	593.2721	-0.01	1	1072922.25	C32 H42 O9	(M+Na)+
594.2754	594.2755	0.17	1	406208.19	C32 H42 O9	(M+Na)+
595.278	595.2783	0.54	1	77177.59	C32 H42 O9	(M+Na)+
651.2767			1	90935.6		
652.2792			1	33867.04		
673.2576			1	46562.82		
674.2602			1	17716		

Cpd 61: Ganoderic acid F; C32 H42 O9: +ESI Product Ion (23.080, 23.268 min, 2 Scans) Frag=17...

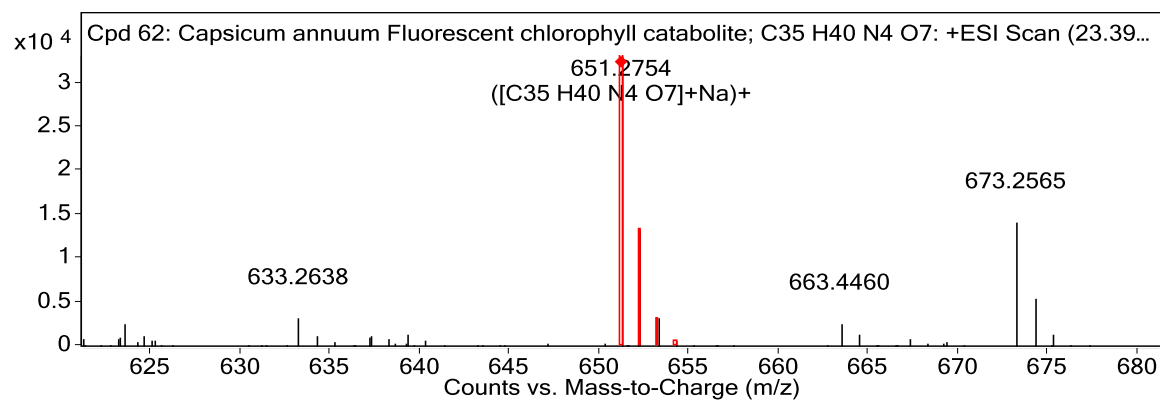
m/z	Relative Intensity (x10 ³)
289.1197	~0.4
460.2203	~0.8
533.2513	~1.4
593.2723	2.0

m/z	z	Abund
102.1276		430.2
123.0922		327.61
124.0863	1	2532.9
166.0963		573.12
207.1231	1	343.91
460.2203		433.8
461.2266	1	401.88
533.2513	1	1039.59
593.2723	1	1949.77
594.2738	1	525.77

CC(C)C(=O)CC(C)C1C(=O)C2C(C1)C(=O)C3C(C2)C(=O)C4C(C3)C(=O)C5C(C4)C(=O)C6C(C5)C(=O)C7C(C6)C(=O)C8C(C7)C(=O)C9C(C8)C(=O)C10C(C9)C(=O)C11C(C10)C(=O)C12C(C11)C(=O)C13C(C12)C(=O)C14C(C13)C(=O)C15C(C14)C(=O)C16C(C15)C(=O)C17C(C16)C(=O)C18C(C17)C(=O)C19C(C18)C(=O)C20C(C19)C(=O)C21C(C20)C(=O)C22C(C21)C(=O)C23C(C22)C(=O)C24C(C23)C(=O)C25C(C24)C(=O)C26C(C25)C(=O)C27C(C26)C(=O)C28C(C27)C(=O)C29C(C28)C(=O)C30C(C29)C(=O)C31C(C30)C(=O)C32C(C31)C(=O)C33C(C32)C(=O)C34C(C33)C(=O)C35C(C34)C(=O)C36C(C35)C(=O)C37C(C36)C(=O)C38C(C37)C(=O)C39C(C38)C(=O)C40C(C39)C(=O)C41C(C40)C(=O)C42C(C41)C(=O)C43C(C42)C(=O)C44C(C43)C(=O)C45C(C44)C(=O)C46C(C45)C(=O)C47C(C46)C(=O)C48C(C47)C(=O)C49C(C48)C(=O)C50C(C49)C(=O)C51C(C50)C(=O)C52C(C51)C(=O)C53C(C52)C(=O)C54C(C53)C(=O)C55C(C54)C(=O)C56C(C55)C(=O)C57C(C56)C(=O)C58C(C57)C(=O)C59C(C58)C(=O)C60C(C59)C(=O)C61C(C60)C(=O)C62C(C61)C(=O)C63C(C62)C(=O)C64C(C63)C(=O)C65C(C64)C(=O)C66C(C65)C(=O)C67C(C66)C(=O)C68C(C67)C(=O)C69C(C68)C(=O)C70C(C69)C(=O)C71C(C70)C(=O)C72C(C71)C(=O)C73C(C72)C(=O)C74C(C73)C(=O)C75C(C74)C(=O)C76C(C75)C(=O)C77C(C76)C(=O)C78C(C77)C(=O)C79C(C78)C(=O)C80C(C79)C(=O)C81C(C80)C(=O)C82C(C81)C(=O)C83C(C82)C(=O)C84C(C83)C(=O)C85C(C84)C(=O)C86C(C85)C(=O)C87C(C86)C(=O)C88C(C87)C(=O)C89C(C88)C(=O)C90C(C89)C(=O)C91C(C90)C(=O)C92C(C91)C(=O)C93C(C92)C(=O)C94C(C93)C(=O)C95C(C94)C(=O)C96C(C95)C(=O)C97C(C96)C(=O)C98C(C97)C(=O)C99C(C98)C(=O)C100C(C99)C(=O)C101C(C100)C(=O)C102C(C101)C(=O)C103C(C102)C(=O)C104C(C103)C(=O)C105C(C104)C(=O)C106C(C105)C(=O)C107C(C106)C(=O)C108C(C107)C(=O)C109C(C108)C(=O)C110C(C109)C(=O)C111C(C110)C(=O)C112C(C111)C(=O)C113C(C112)C(=O)C114C(C113)C(=O)C115C(C114)C(=O)C116C(C115)C(=O)C117C(C116)C(=O)C118C(C117)C(=O)C119C(C118)C(=O)C120C(C119)C(=O)C121C(C120)C(=O)C122C(C121)C(=O)C123C(C122)C(=O)C124C(C123)C(=O)C125C(C124)C(=O)C126C(C125)C(=O)C127C(C126)C(=O)C128C(C127)C(=O)C129C(C128)C(=O)C130C(C129)C(=O)C131C(C130)C(=O)C132C(C131)C(=O)C133C(C132)C(=O)C134C(C133)C(=O)C135C(C134)C(=O)C136C(C135)C(=O)C137C(C136)C(=O)C138C(C137)C(=O)C139C(C138)C(=O)C140C(C139)C(=O)C141C(C140)C(=O)C142C(C141)C(=O)C143C(C142)C(=O)C144C(C143)C(=O)C145C(C144)C(=O)C146C(C145)C(=O)C147C(C146)C(=O)C148C(C147)C(=O)C149C(C148)C(=O)C150C(C149)C(=O)C151C(C150)C(=O)C152C(C151)C(=O)C153C(C152)C(=O)C154C(C153)C(=O)C155C(C154)C(=O)C156C(C155)C(=O)C157C(C156)C(=O)C158C(C157)C(=O)C159C(C158)C(=O)C160C(C159)C(=O)C161C(C160)C(=O)C162C(C161)C(=O)C163C(C162)C(=O)C164C(C163)C(=O)C165C(C164)C(=O)C166C(C165)C(=O)C167C(C166)C(=O)C168C(C167)C(=O)C169C(C168)C(=O)C170C(C169)C(=O)C171C(C170)C(=O)C172C(C171)C(=O)C173C(C172)C(=O)C174C(C173)C(=O)C175C(C174)C(=O)C176C(C175)C(=O)C177C(C176)C(=O)C178C(C177)C(=O)C179C(C178)C(=O)C180C(C179)C(=O)C181C(C180)C(=O)C182C(C181)C(=O)C183C(C182)C(=O)C184C(C183)C(=O)C185C(C184)C(=O)C186C(C185)C(=O)C187C(C186)C(=O)C188C(C187)C(=O)C189C(C188)C(=O)C190C(C189)C(=O)C191C(C190)C(=O)C192C(C191)C(=O)C193C(C192)C(=O)C194C(C193)C(=O)C195C(C194)C(=O)C196C(C195)C(=O)C197C(C196)C(=O)C198C(C197)C(=O)C199C(C198)C(=O)C200C(C199)C(=O)C201C(C200)C(=O)C202C(C201)C(=O)C203C(C202)C(=O)C204C(C203)C(=O)C205C(C204)C(=O)C206C(C205)C(=O)C207C(C206)C(=O)C208C(C207)C(=O)C209C(C208)C(=O)C210C(C209)C(=O)C211C(C210)C(=O)C212C(C211)C(=O)C213C(C212)C(=O)C214C(C213)C(=O)C215C(C214)C(=O)C216C(C215)C(=O)C217C(C216)C(=O)C218C(C217)C(=O)C219C(C218)C(=O)C220C(C219)C(=O)C221C(C220)C(=O)C222C(C221)C(=O)C223C(C222)C(=O)C224C(C223)C(=O)C225C(C224)C(=O)C226C(C225)C(=O)C227C(C226)C(=O)C228C(C227)C(=O)C229C(C228)C(=O)C230C(C229)C(=O)C231C(C230)C(=O)C232C(C231)C(=O)C233C(C232)C(=O)C234C(C233)C(=O)C235C(C234)C(=O)C236C(C235)C(=O)C237C(C236)C(=O)C238C(C237)C(=O)C239C(C238)C(=O)C240C(C239)C(=O)C241C(C240)C(=O)C242C(C241)C(=O)C243C(C242)C(=O)C244C(C243)C(=O)C245C(C244)C(=O)C246C(C245)C(=O)C247C(C246)C(=O)C248C(C247)C(=O)C249C(C248)C(=O)C250C(C249)C(=O)C251C(C250)C(=O)C252C(C251)C(=O)C253C(C252)C(=O)C254C(C253)C(=O)C255C(C254)C(=O)C256C(C255)C(=O)C257C(C256)C(=O)C258C(C257)C(=O)C259C(C258)C(=O)C260C(C259)C(=O)C261C(C260)C(=O)C262C(C261)C(=O)C263C(C262)C(=O)C264C(C263)C(=O)C265C(C264)C(=O)C266C(C265)C(=O)C267C(C266)C(=O)C268C(C267)C(=O)C269C(C268)C(=O)C270C(C269)C(=O)C271C(C270)C(=O)C272C(C271)C(=O)C273C(C272)C(=O)C274C(C273)C(=O)C275C(C274)C(=O)C276C(C275)C(=O)C277C(C276)C(=O)C278C(C277)C(=O)C279C(C278)C(=O)C280C(C279)C(=O)C281C(C280)C(=O)C282C(C281)C(=O)C283C(C282)C(=O)C284C(C283)C(=O)C285C(C284)C(=O)C286C(C285)C(=O)C287C(C286)C(=O

Agilent Technologies

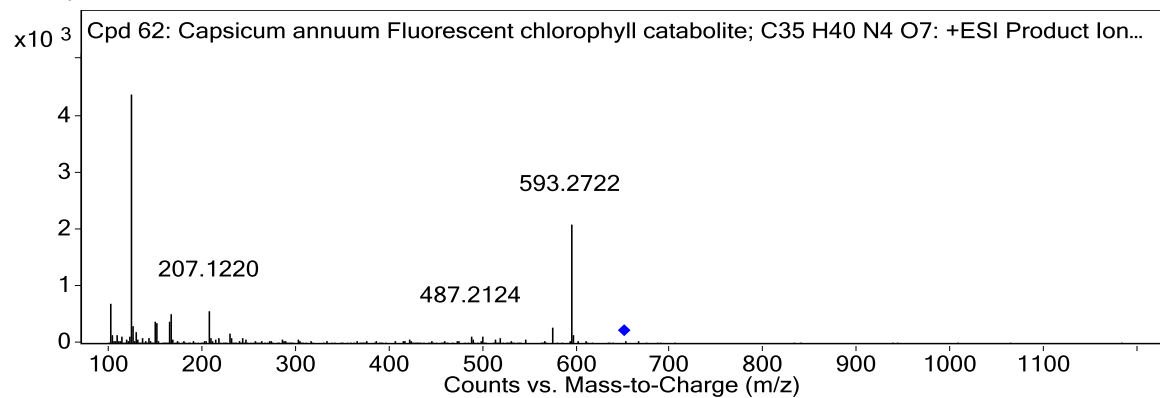
Page 56 of 73



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0863			1	124368.56		
166.0964			1	23838.29		
207.1224			1	25514.34		
593.2719			1	1161416.88		
594.2755			1	431890.25		
595.2772			1	78469.91		
651.2754	651.2789	5.44	1	33002.7	C35 H40 N4 O7	(M+Na)+
652.2776	652.2821	6.85	1	13221.99	C35 H40 N4 O7	(M+Na)+
653.2816	653.2849	5.15	1	3267.96	C35 H40 N4 O7	(M+Na)+
654.2874	654.2876	0.42	1	597.65	C35 H40 N4 O7	(M+Na)+

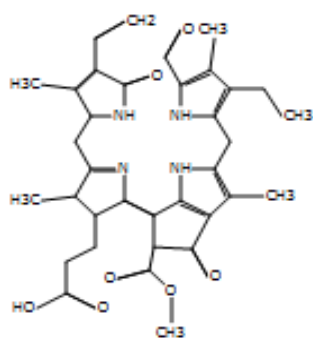
MSMS Spectrum



MS/MS Spectrum Peak List

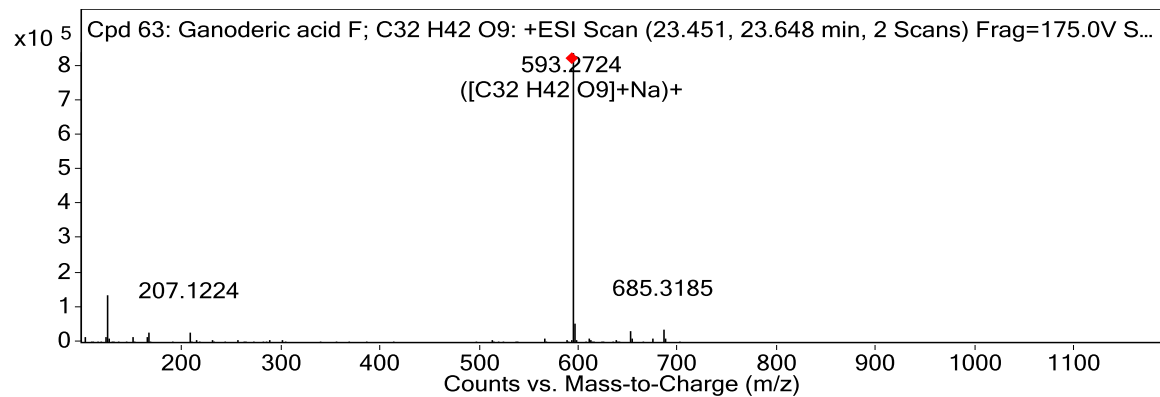
m/z	z	Abund
101.0707		464.91
102.1264	1	698.29
123.0909		524.02
124.0861	1	4386.79
149.0217	1	400.39
164.9301		381.03
166.0952	1	528.44
207.122	1	585.09
593.2722	1	2093
594.2733	1	742.56

Compound Structure

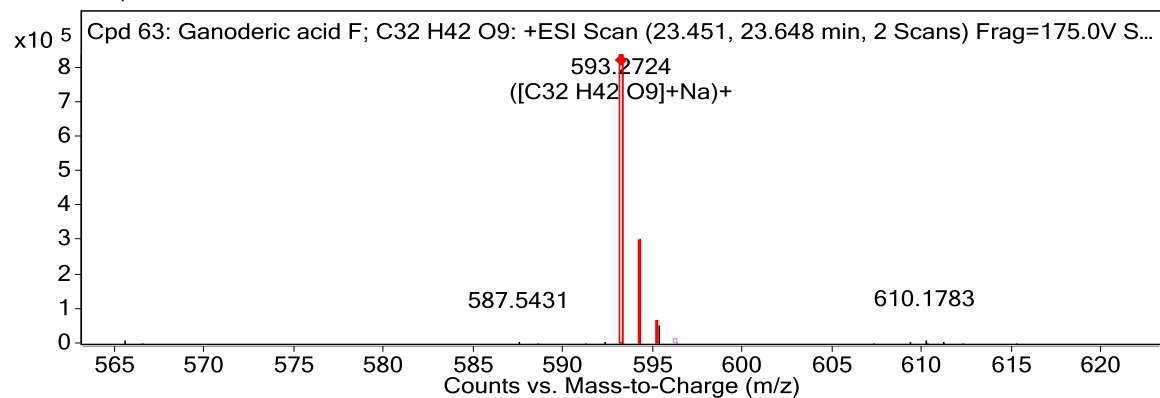


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 63: Ganoderic acid F; C32 H42 O9	Ganoderic acid F	593.2724	23.562	Auto MS/MS	570.2831

MS Spectrum



MS Zoomed Spectrum



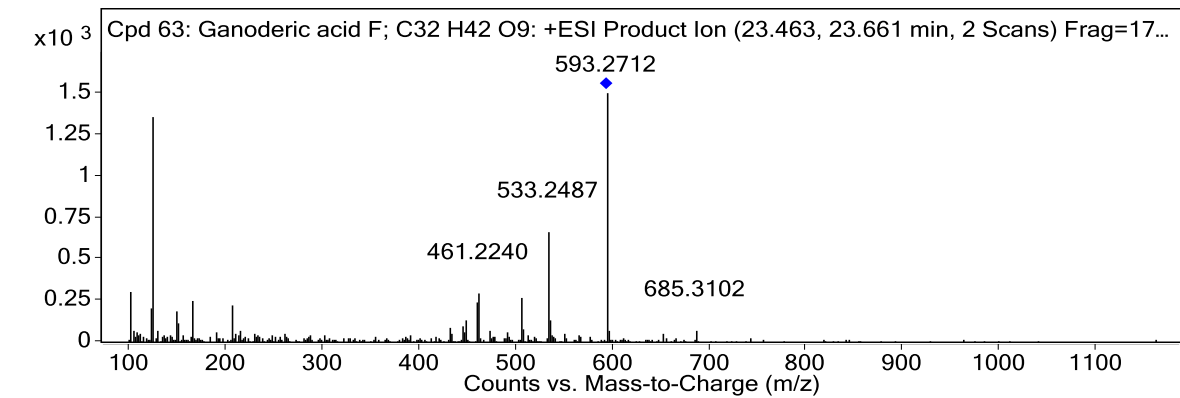
MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	z	Abund	Formula	Ion
124.0864			1	138990.16		

Qualitative Compound Report

149.0224				17230.75		
164.9287				18041.18		
166.0966			1	29346.79		
207.1224			1	30107.19		
593.2724	593.2721	-0.5	1	836745.25	C32 H42 O9	(M+Na)+
594.2756	594.2755	-0.22	1	306393.25	C32 H42 O9	(M+Na)+
595.2772	595.2783	1.86	1	55271.81	C32 H42 O9	(M+Na)+
651.2759			1	33024.04		
685.3185			1	37239.72		

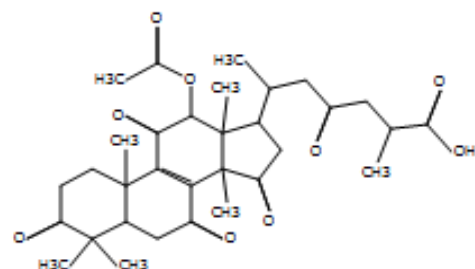
MSMS Spectrum



MS/MS Spectrum Peak List

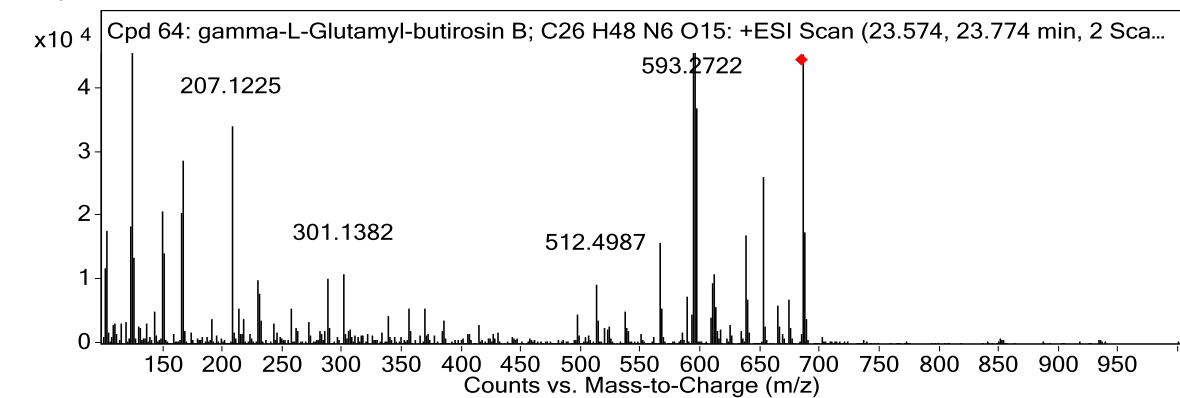
m/z	z	Abund
102.1273		302.84
124.0862	1	1359.19
164.9277		226
166.0983		250.36
460.2194		244.98
461.224	1	297.03
505.2152	1	266.32
533.2487	1	669.01
593.2712	1	1503.1
594.2749	1	427.25

Compound Structure

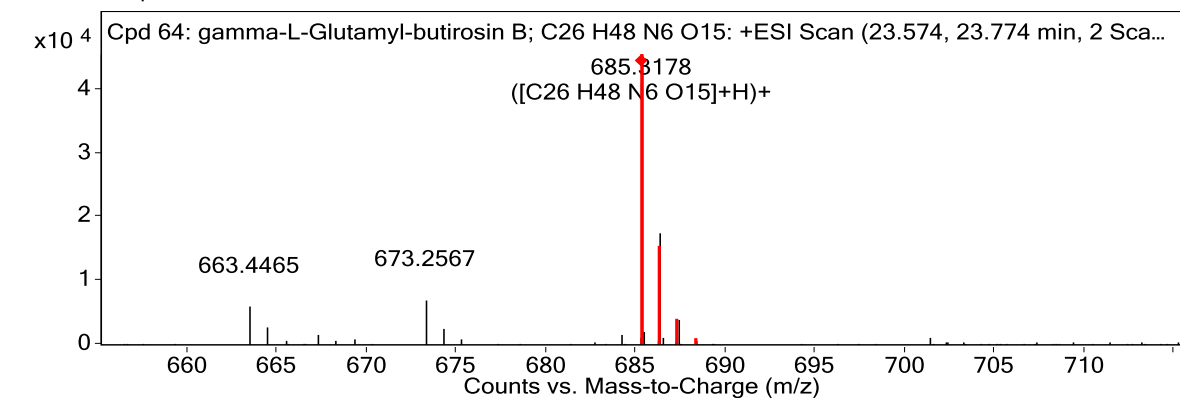


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 64: gamma-L-Glutamyl-butirosin B; C26 H48 N6 O15	gamma-L-Glutamyl-butirosin B	685.3178	23.691	Auto MS/MS	684.3103

MS Spectrum



MS Zoomed Spectrum

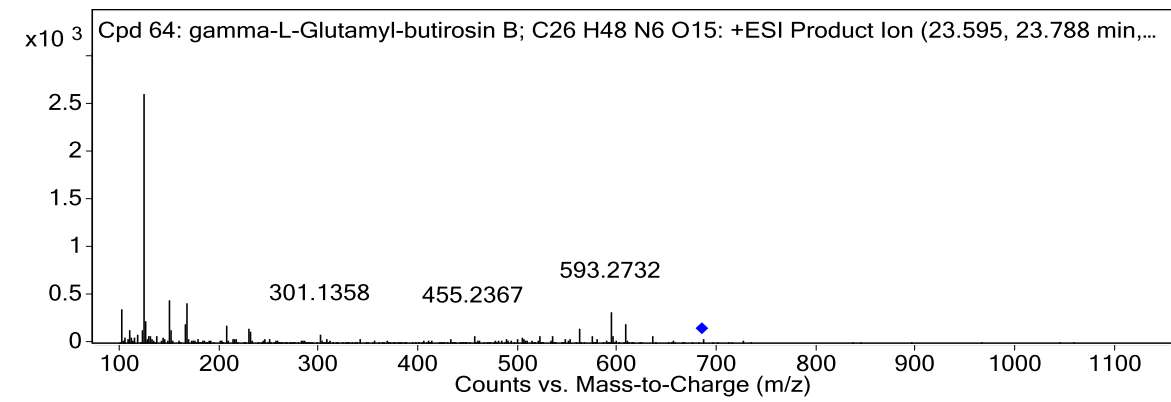


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0864			1	138542.53		
166.0965			1	28707.21		
207.1225			1	34042.58		
593.2722			1	574660.31		
594.2752			1	211684.16		
595.277			1	36844.71		
685.3178	685.325	10.62	1	45358.18	C26 H48 N6 O15	(M+H)+
686.32	686.328	11.72	1	17492	C26 H48 N6 O15	(M+H)+
687.3227	687.3303	11.12	1	3927.37	C26 H48 N6 O15	(M+H)+
688.3259	688.3328	10.03	1	754.1	C26 H48 N6 O15	(M+H)+

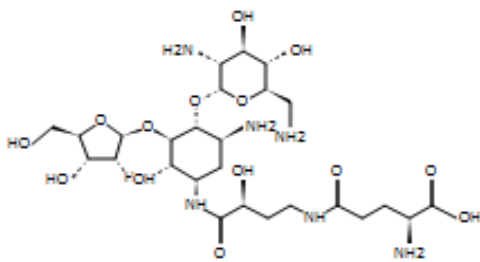
MSMS Spectrum

Qualitative Compound Report



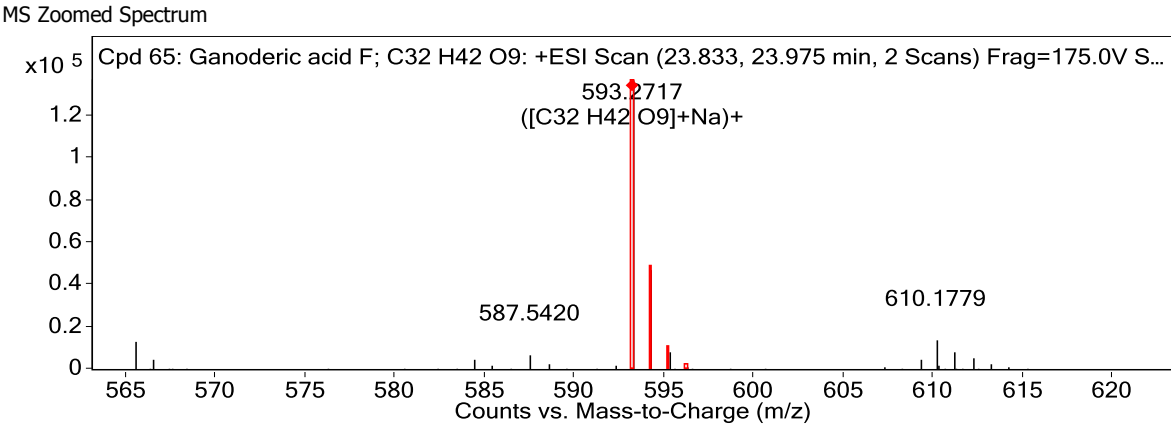
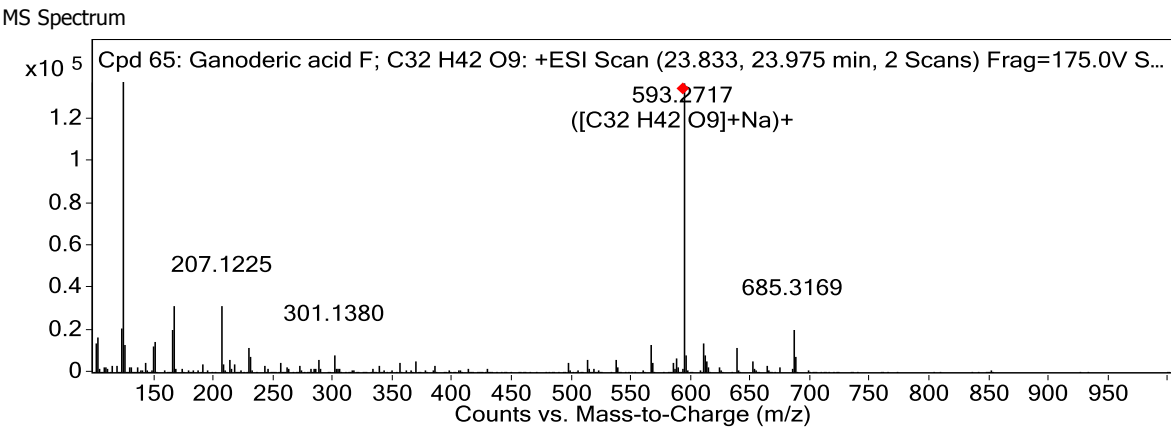
MS/MS Spectrum Peak List		
m/z	z	Abund
101.0701		354.13
102.1262		212.47
123.0915		373.64
124.0865	1	2617.67
125.0892	1	241.58
149.0221		446.57
150.0643		232.22
166.0972		416.96
593.2732	1	331.28
607.2825		205.01

Compound Structure



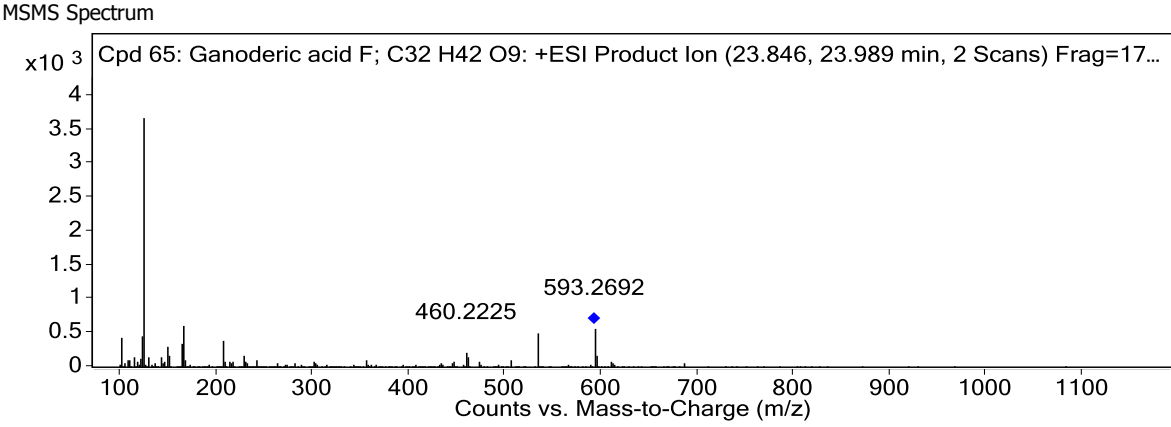
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 65: Ganoderic acid F; C32 H42 O9	Ganoderic acid F	593.2717	23.917	Auto MS/MS	570.2821

Qualitative Compound Report



MS Spectrum Peak List

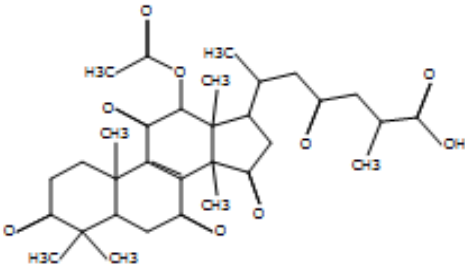
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
123.0909				21414.37		
124.0865			1	149292.75		
164.9287				20101.57		
166.0965			1	31730.93		
207.1225			1	31745.61		
593.2717	593.2721	0.75	1	136758.25	C32 H42 O9	(M+Na)+
594.2739	594.2755	2.77	1	47328.13	C32 H42 O9	(M+Na)+
595.276	595.2783	3.97	1	8436.71	C32 H42 O9	(M+Na)+
596.2786	596.2811	4.05	1	1466.59	C32 H42 O9	(M+Na)+
685.3169			1	20758.22		



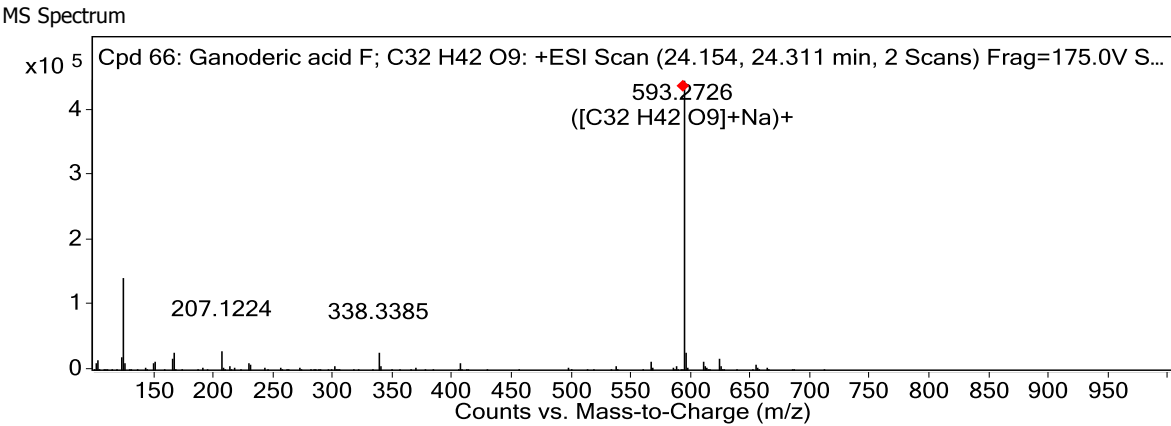
MS/MS Spectrum Peak List

m/z	z	Abund
101.0703	1	438.27
102.1273		353.31
123.0911		456.74
124.0862	1	3673.02
150.0653		306.86
164.9278		359.99
166.0966	1	614.2
207.1222	1	386.51
533.2486	1	514.43
593.2692	1	566.81

Compound Structure

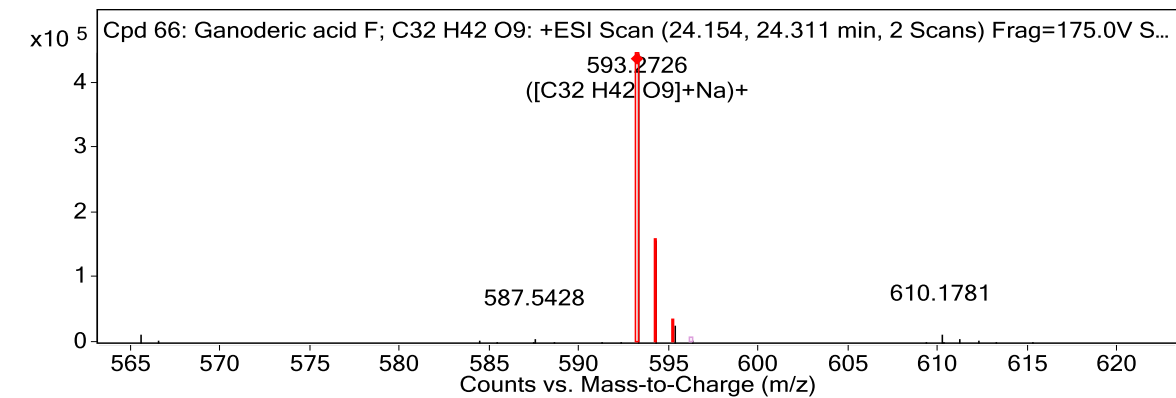


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 66: Ganoderic acid F; C32 H42 O9	Ganoderic acid F	593.2726	24.245	Auto MS/MS	570.283



MS Zoomed Spectrum

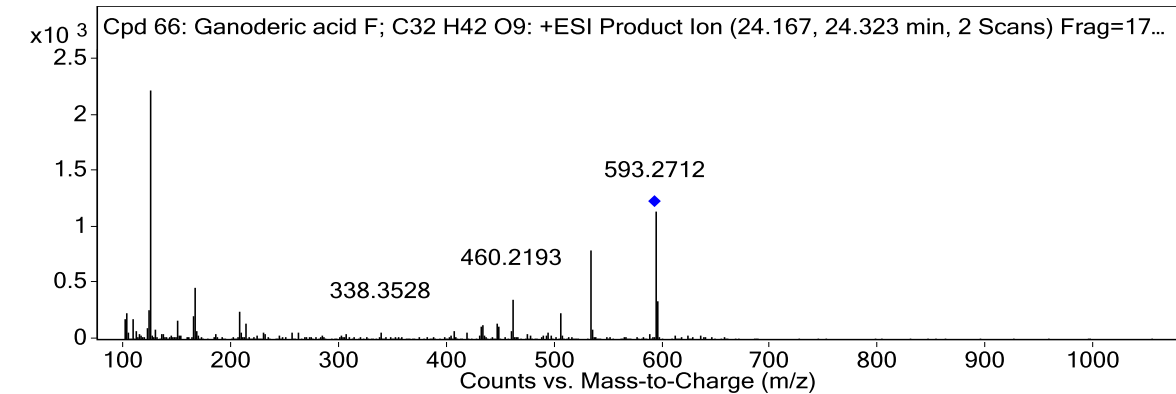
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
123.091				20728.25		
124.0864			1	141744.73		
164.9287				19054.79		
166.0965			1	27435.21		
207.1224			1	30955.84		
338.3385			1	26599.49		
593.2726	593.2721	-0.77	1	445044.38	C32 H42 O9	(M+Na)+
594.2751	594.2755	0.72	1	157561.59	C32 H42 O9	(M+Na)+
595.2765	595.2783	3.03	1	28240.34	C32 H42 O9	(M+Na)+
623.2806			1	19482.57		

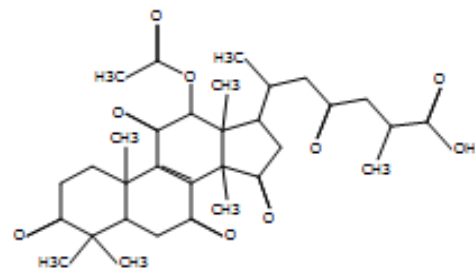
MS/MS Spectrum



MS/MS Spectrum Peak List

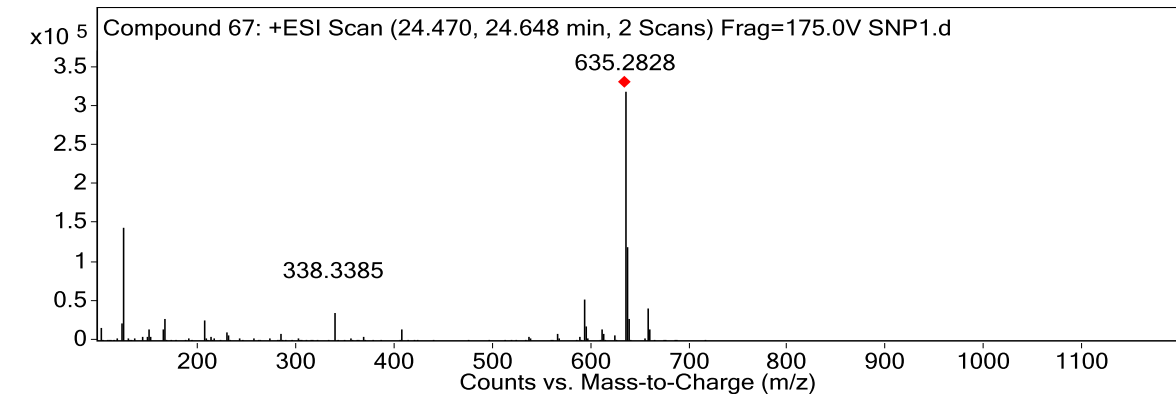
m/z	z	Abund
123.0907		263.16
124.0858	1	2228.32
125.0869	1	246.73
166.0953	1	463.11
207.1225	1	259.46
460.2193		364.97
461.2285		321.22
533.2491	1	805.1
593.2712	1	1151
594.2742	1	343.85

Compound Structure

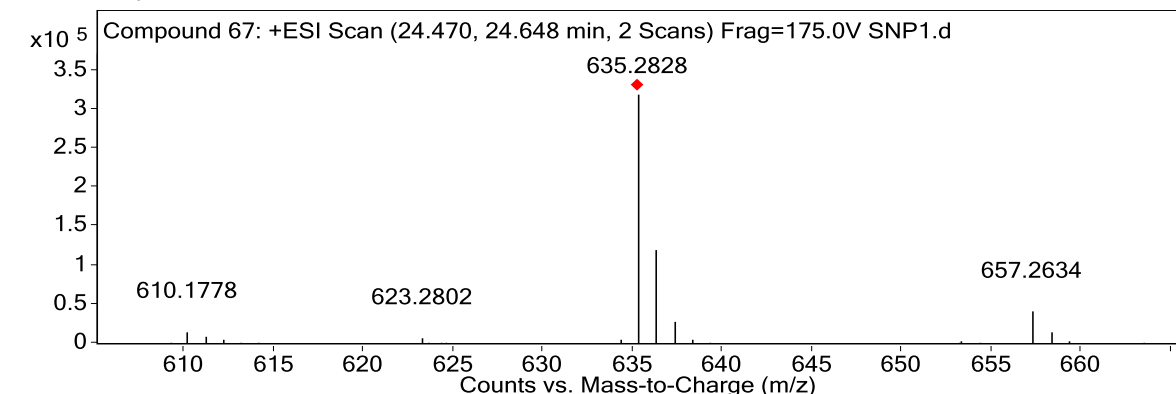


Compound Label	m/z	RT	Algorithm
Compound 67	635.2828	24.575	Auto MS/MS

MS Spectrum



MS Zoomed Spectrum



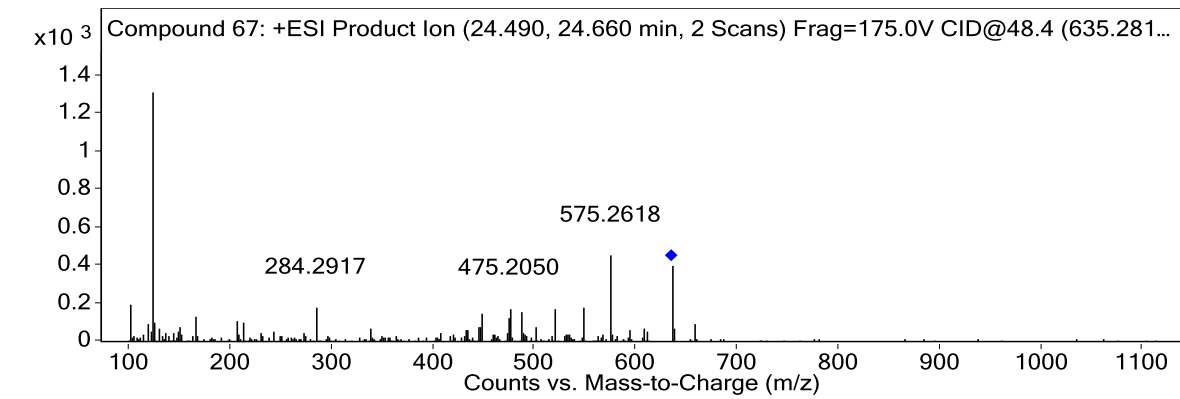
MS Spectrum Peak List

m/z	z	Abund
124.0864	1	146153.98
166.0966	1	29001.4

Qualitative Compound Report

207.1223	1	26391.07
338.3385	1	37085.94
593.2712	1	53804.14
635.2828	1	319435.84
636.2856	1	121136.47
637.2889	1	29099.47
638.292	1	5476.41
657.2634	1	41188.22

MSMS Spectrum

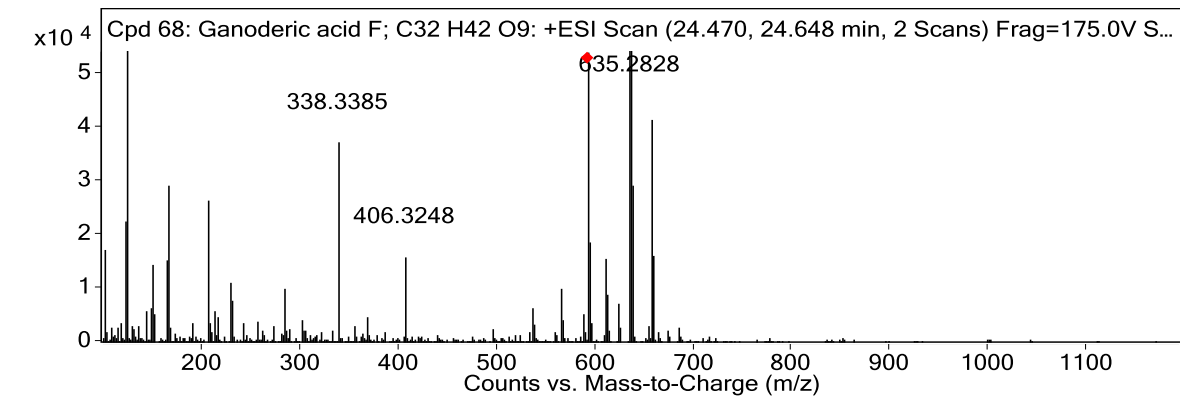


MS/MS Spectrum Peak List

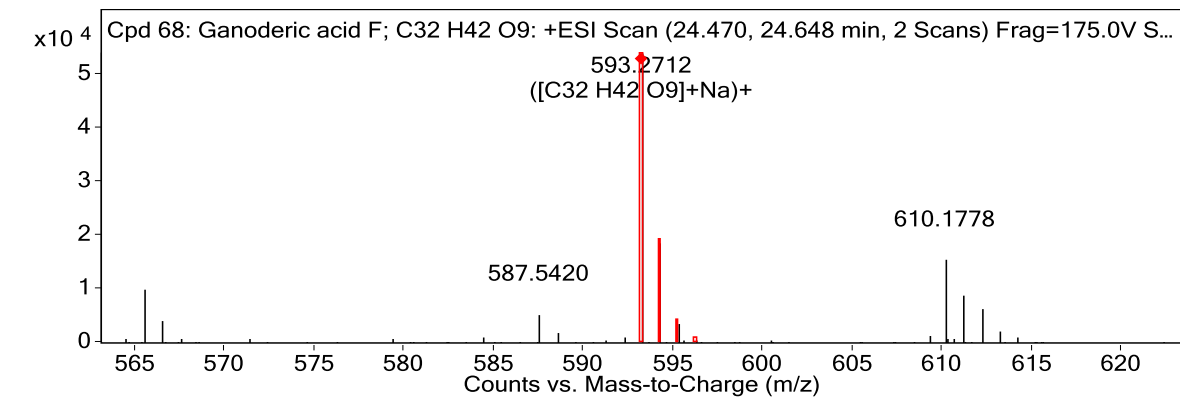
m/z	z	Abund
101.0695		193.12
102.1267		194.73
123.0907		267.96
124.0866	1	1312.86
284.2917	1	179.23
475.205	1	174.46
547.2659		181.62
575.2618	1	453.57
635.2835	1	404.22
636.2864	1	191.51

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 68: Ganoderic acid F; C32 H42 O9	Ganoderic acid F	593.2712	24.577	Auto MS/MS	570.2817

MS Spectrum



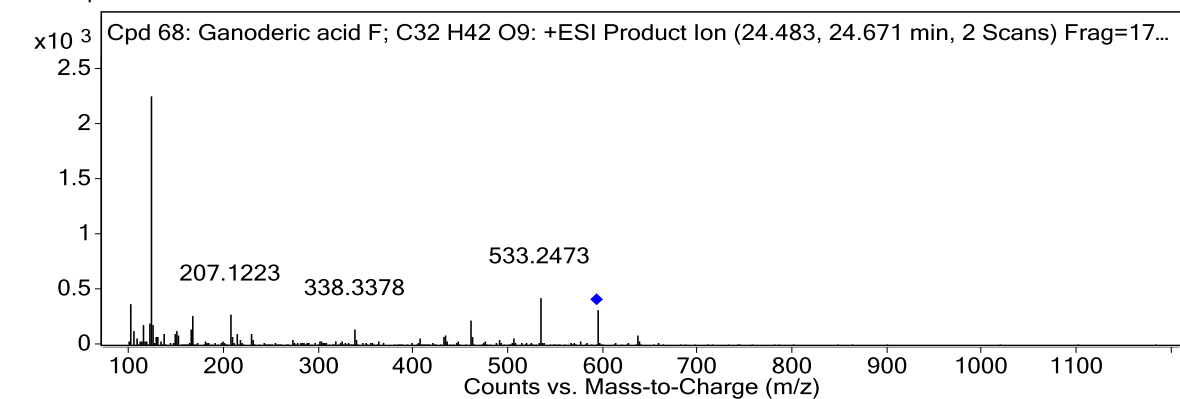
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0864			1	146153.98		
338.3385			1	37085.94		
593.2712	593.2721	1.51	1	53804.14	C32 H42 O9	(M+Na)+
594.2735	594.2755	3.35	1	18564.98	C32 H42 O9	(M+Na)+
595.2762	595.2783	3.59	1	3655.58	C32 H42 O9	(M+Na)+
596.2788	596.2811	3.76	1	632.79	C32 H42 O9	(M+Na)+
635.2828			1	319435.84		
636.2856			1	121136.47		
637.2889			1	29099.47		
657.2634			1	41188.22		

MSMS Spectrum



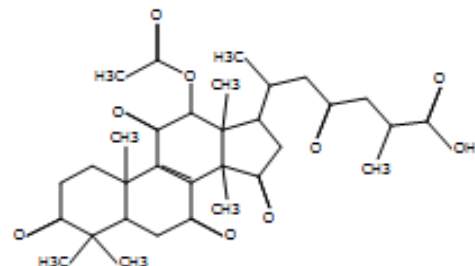
MS/MS Spectrum Peak List

m/z	z	Abund
101.0706		333.76
102.1263		379.93
122.0956		208.65
123.0906		275.97
124.0862	1	2259.02

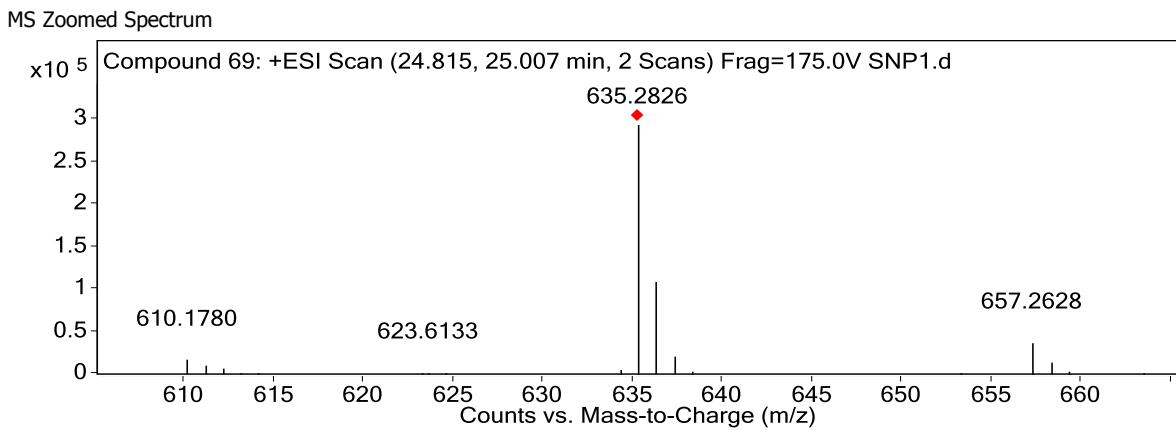
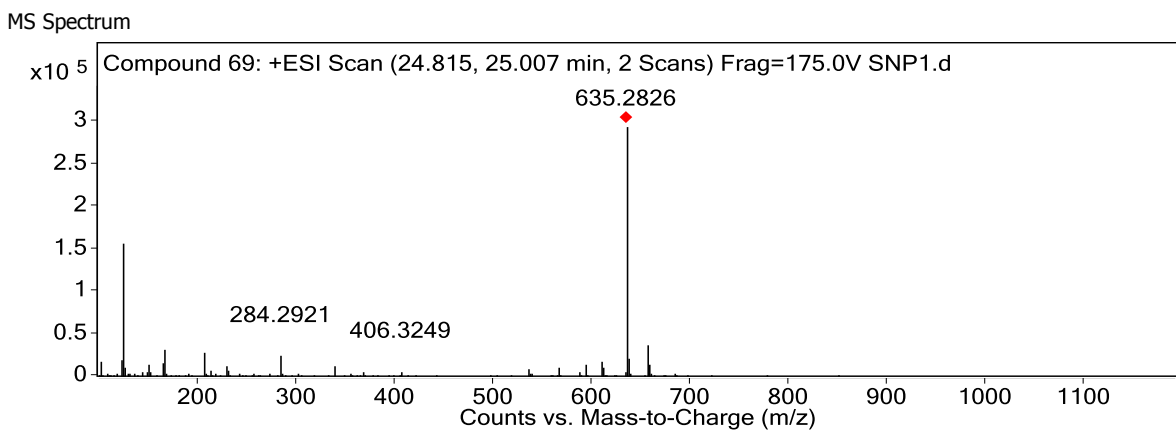
Qualitative Compound Report

166.0956	1	265.28
207.1223	1	281.14
460.2223	1	233.39
533.2473	1	437.57
593.2676	1	318.27

Compound Structure

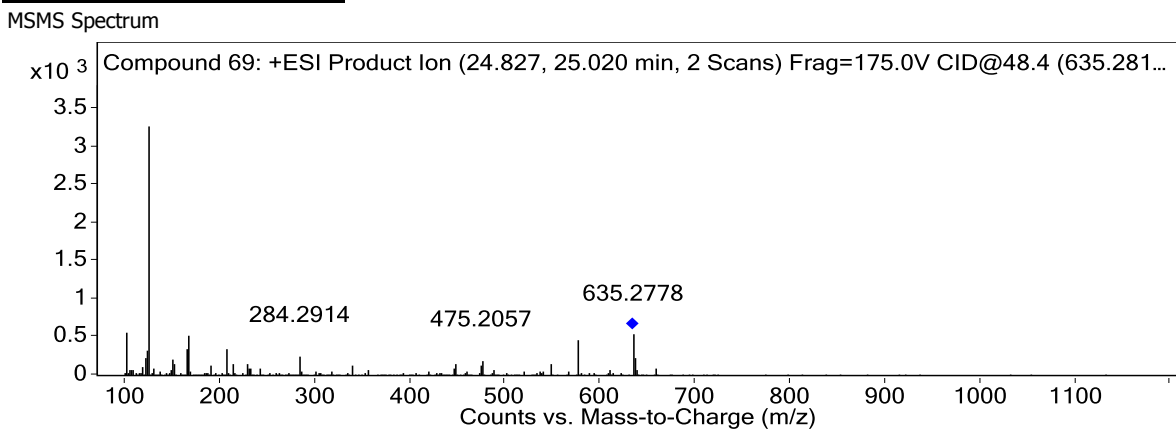


Compound Label	m/z	RT	Algorithm
Compound 69	635.2826	24.923	Auto MS/MS



MS Spectrum Peak List

m/z	z	Abund
123.091		20080.45
124.0864	1	155840.25
166.0964	1	31355.8
207.1224	1	27910.25
284.2921	1	23823.09
635.2826	1	293875.19
636.2851	1	108898.81
637.2871	1	21346.27
638.2897	1	3946.44
657.2628	1	37419.14



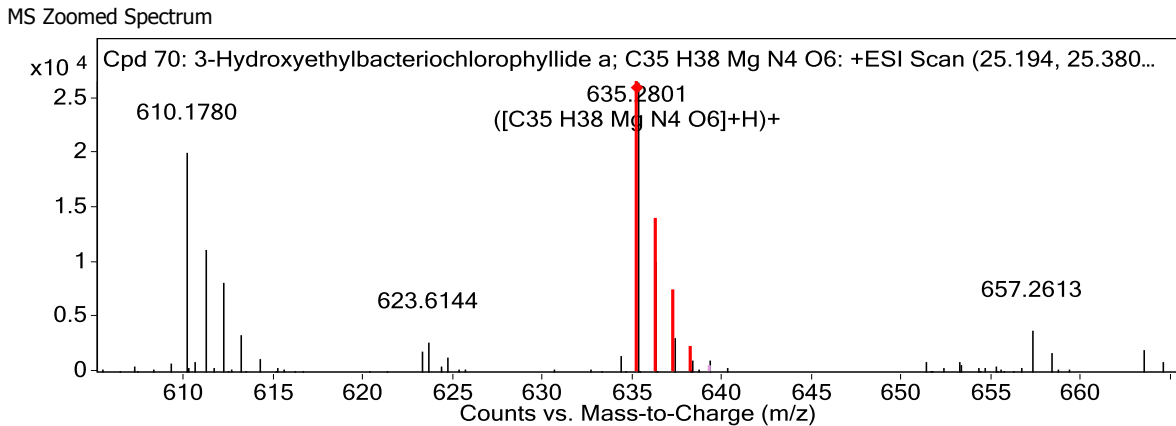
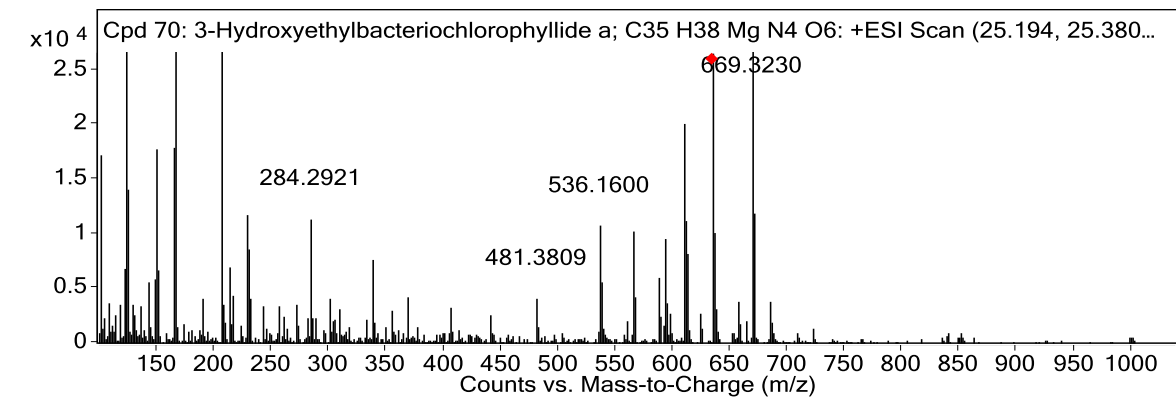
MS/MS Spectrum Peak List

m/z	z	Abund
101.0704	1	311.31
102.127		573.1
123.0907		326.49
124.0864	1	3277.75
165.1103		347.24
166.0964	1	520.84
207.1231	1	350.25
284.2914	1	258.51
575.2612		469.77
635.2778	1	539.53

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 70: 3-Hydroxyethylbacteriochlorophyllide a; C35 H38 Mg	3-Hydroxyethylbacteriochlorophyllide a	635.2801	25.306	Auto MS/MS	634.2738

MS Spectrum

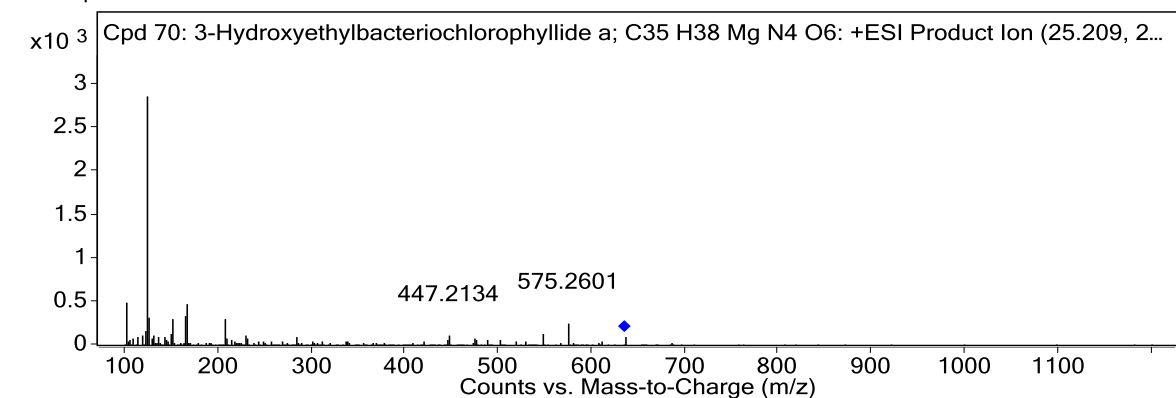
Qualitative Compound Report



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
123.091				21003.25		
124.0865			1	170118.75		
166.0965			1	35417.91		
207.1225			1	28343.83		
610.178			1	20032.69		
635.2801	635.2715	-13.59	1	26478.46	C35 H38 Mg N4 O6	(M+H)+
636.2829	636.274	-13.99	1	10070.36	C35 H38 Mg N4 O6	(M+H)+
637.2901	637.2729	-26.97	1	3154.98	C35 H38 Mg N4 O6	(M+H)+
638.2934	638.2745	-29.6	1	1131.18	C35 H38 Mg N4 O6	(M+H)+
669.323			1	28534.24		

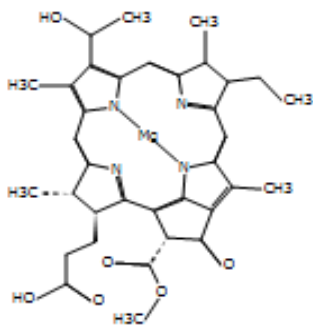
MSMS Spectrum



MS/MS Spectrum Peak List

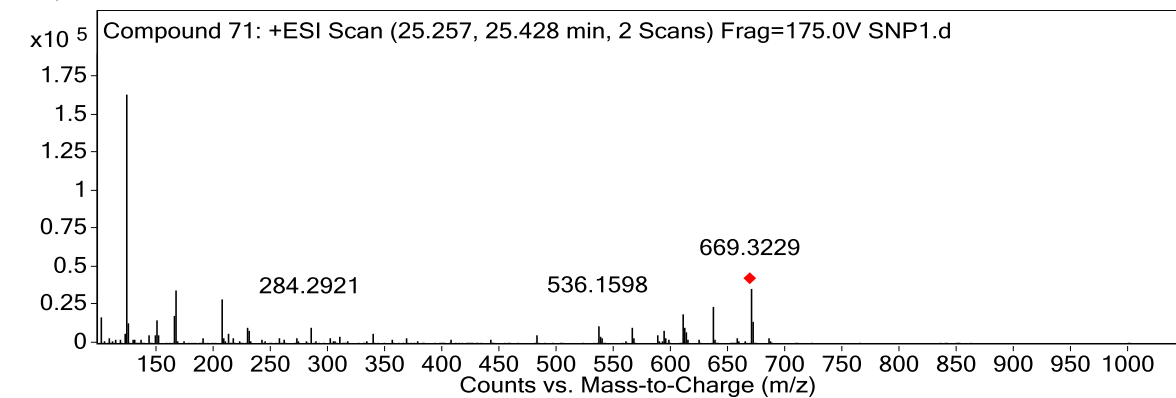
<i>m/z</i>	<i>z</i>	Abund
101.0682		416.96
102.127	1	499.07
123.0905		482.75
124.0857	1	2866.8
125.0699	1	329.1
150.0653		314.35
164.9293		343.02
166.0969		486.68
207.1225	1	305.48
575.2601		262.84

Compound Structure



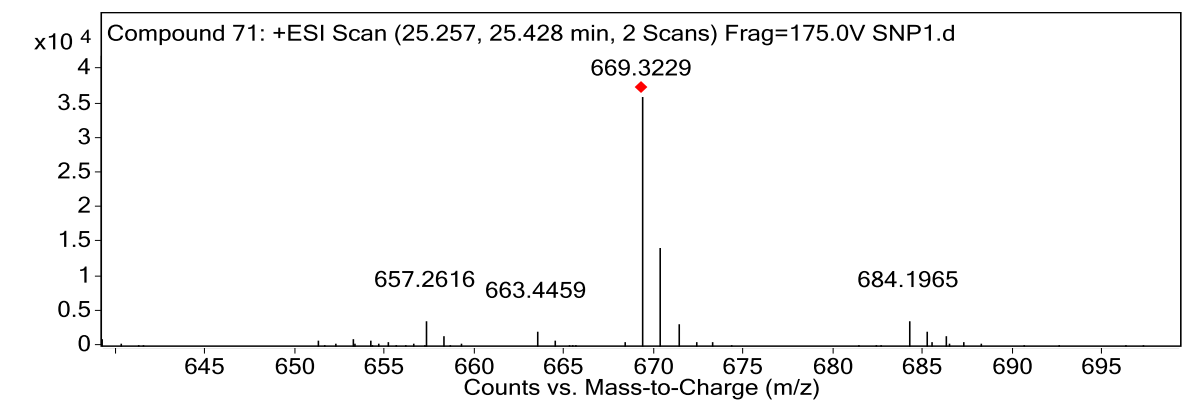
Compound Label	<i>m/z</i>	RT	Algorithm
Compound 71	669.3229	25.359	Auto MS/MS

MS Spectrum



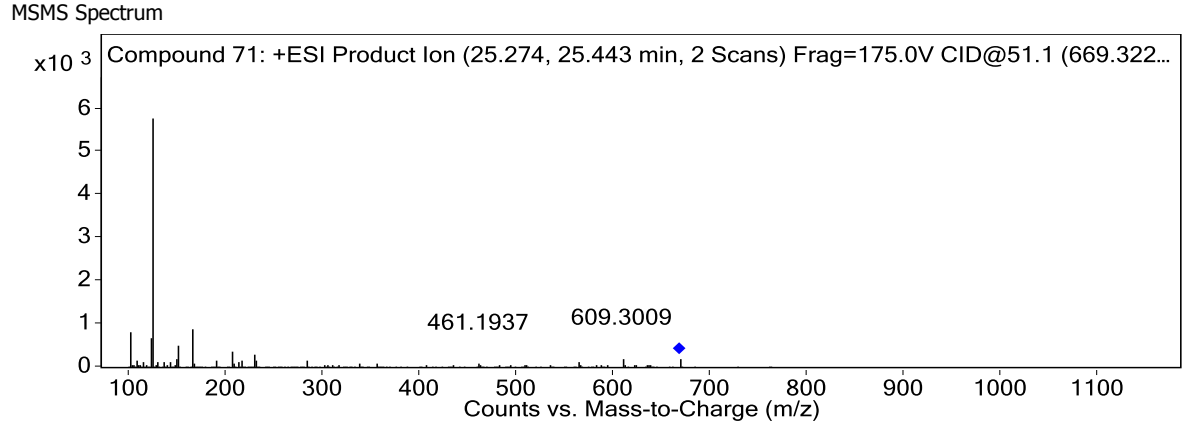
MS Zoomed Spectrum

Qualitative Compound Report



MS Spectrum Peak List

m/z	z	Abund
123.091		21362.9
124.0865	1	163839.91
166.0965	1	35164.83
207.1225	1	29617.23
610.1783	1	19602.71
635.2805	1	24694.56
669.3229	1	36050.53
670.3251	1	14224.8
671.3272	1	3190.8
672.33	1	700.4



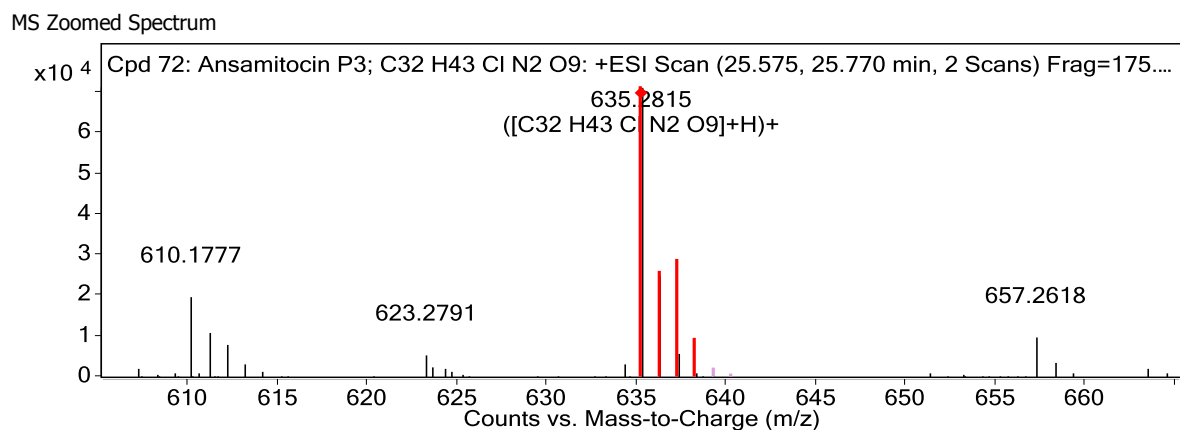
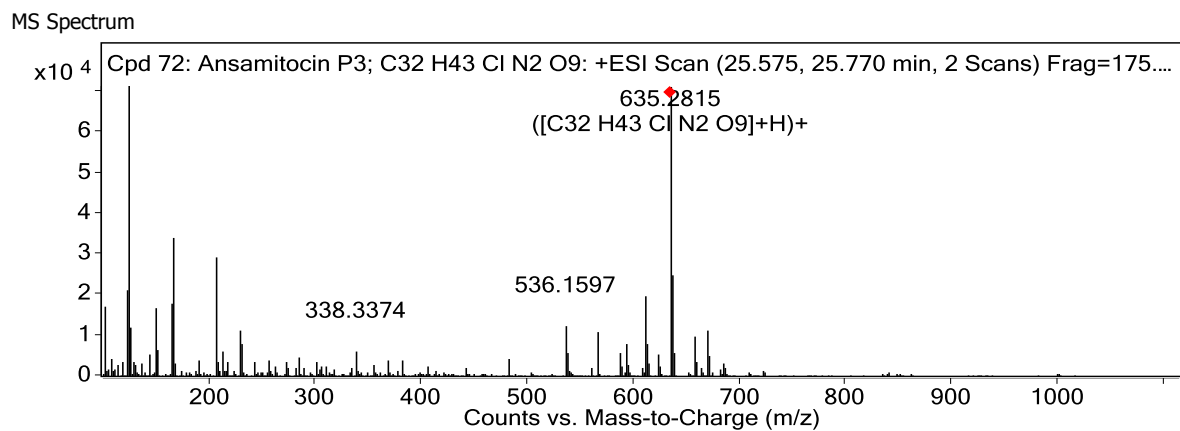
MS/MS Spectrum Peak List

m/z	z	Abund
101.0703		821.28
102.1267	1	605.55
123.0911		685.29
124.086	1	5783.32
125.0705		535.77
125.0885	1	513.53

Qualitative Compound Report

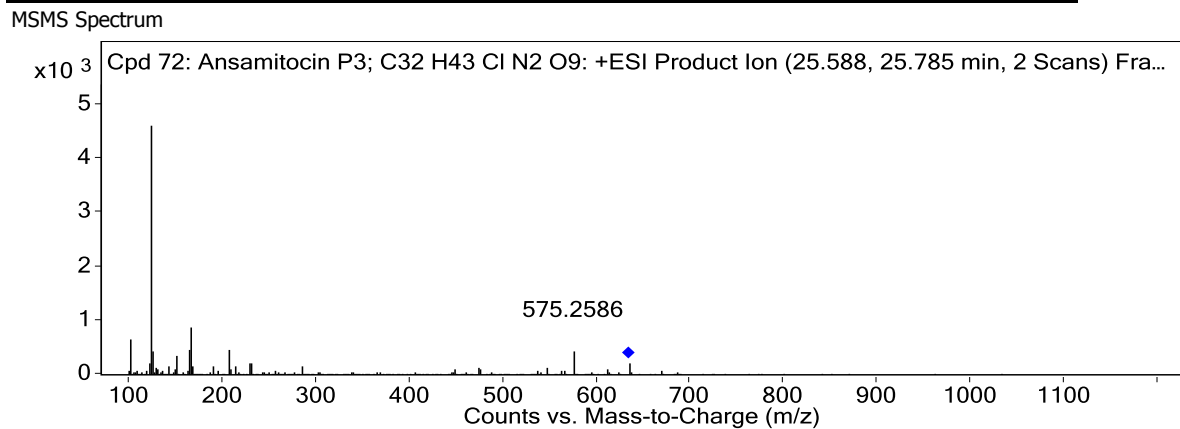
<i>m/z</i>	<i>z</i>	Abund
150.065	1	532.37
164.9287		491.74
166.0972	1	892.42
207.1221	1	388.76

Compound Label	Name	<i>m/z</i>	RT	Algorithm	Mass
Cpd 72: Ansamitocin P3; C32 H43 Cl N2 O9	Ansamitocin P3	635.2815	25.687	Auto MS/MS	634.2745



MS Spectrum Peak List

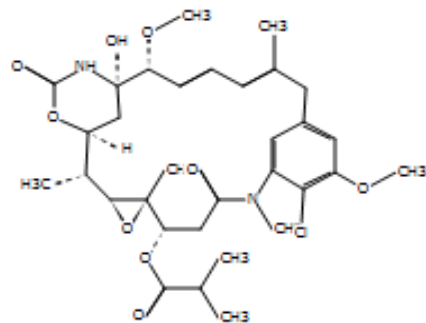
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
123.0911				21122.3		
124.0865			1	170231.2		
164.9285				18063.49		
166.0965			1	33945.91		
207.1224			1	29458.95		
610.1777			1	19905.8		
635.2815	635.273	-13.46	1	71115.91	C32 H43 Cl N2 O9	(M+H)+
636.2838	636.2763	-11.85	1	25062.29	C32 H43 Cl N2 O9	(M+H)+
637.2876	637.2719	-24.65	1	5739.59	C32 H43 Cl N2 O9	(M+H)+
638.2909	638.2742	-26.12	1	1111.18	C32 H43 Cl N2 O9	(M+H)+



MS/MS Spectrum Peak List

<i>m/z</i>	<i>z</i>	Abund
101.0702		490.02
102.1263		659.72
123.0911		719.95
124.086	1	4619.5
125.071		445.05
150.0656		370.55
164.9288		457.95
166.0963	1	871.61
207.1218	1	479.61
575.2586		445.45

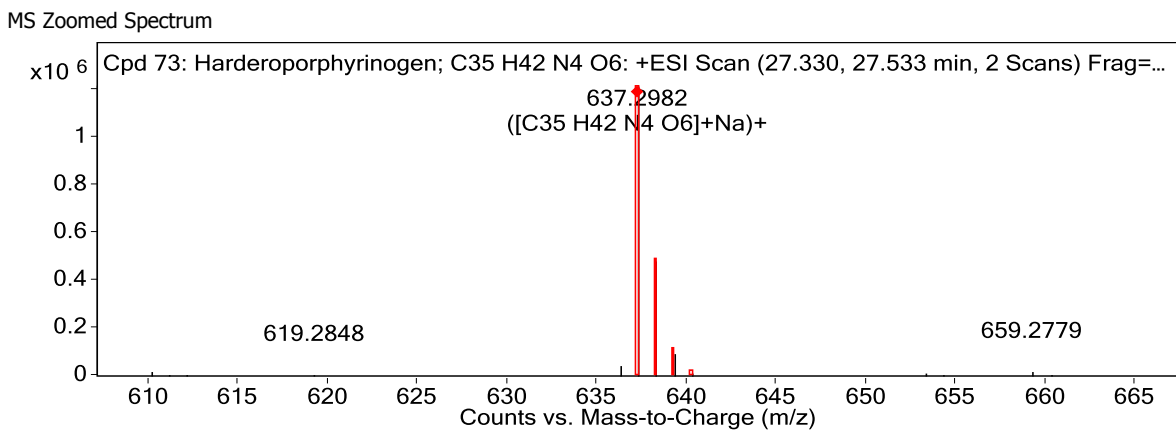
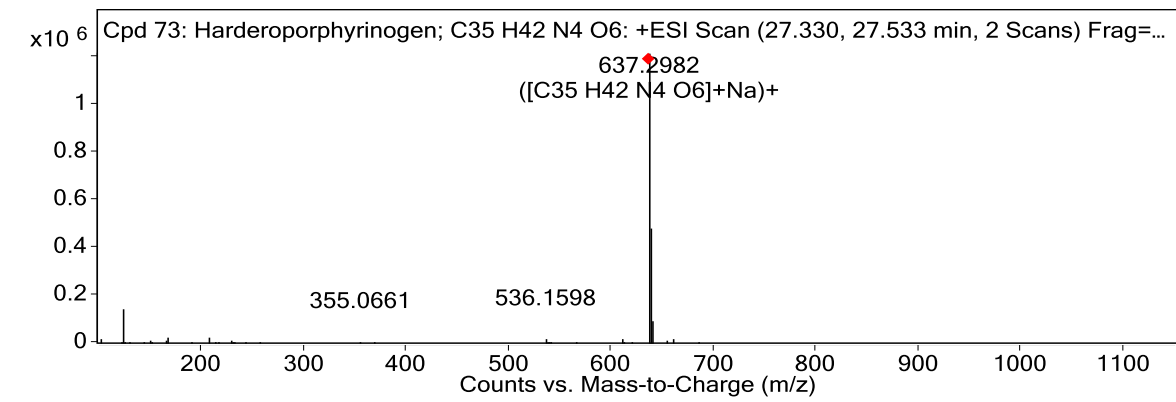
Compound Structure



Compound Label	Name	<i>m/z</i>	RT	Algorithm	Mass
Cpd 73: Harderoporphyrinogen; C35 H42 N4 O6	Harderoporphyrinogen	637.2982	27.443	Auto MS/MS	614.309

MS Spectrum

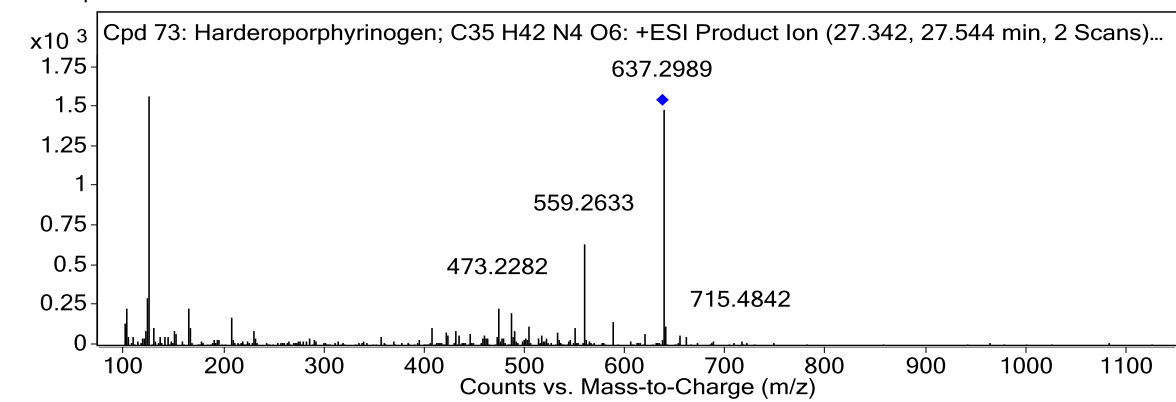
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
123.0909				18174.27		
124.0864			1	141621.86		
166.0965			1	27527.28		
207.1225			1	23645.97		
636.2891				41908.45		
637.2982	637.2997	2.28	1	1213184.75	C35 H42 N4 O6	(M+Na)+
638.3016	638.3028	1.93	1	483156.41	C35 H42 N4 O6	(M+Na)+
639.3037	639.3057	3.06	1	93006.72	C35 H42 N4 O6	(M+Na)+
640.3047	640.3084	5.8	1	12375.67	C35 H42 N4 O6	(M+Na)+
659.2779			1	17789.21		

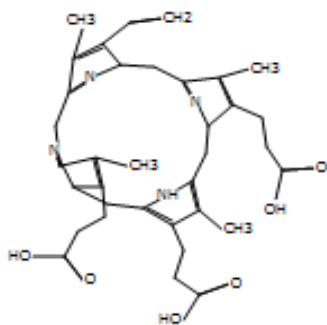
MSMS Spectrum



MS/MS Spectrum Peak List

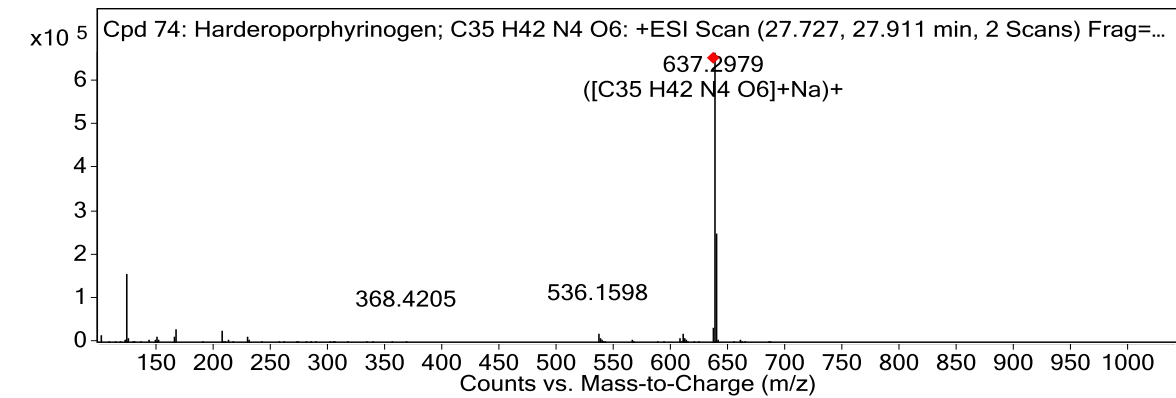
m/z	z	Abund
102.1264		230.78
123.0916		298.19
124.0861	1	1569.91
164.9288		230.66
207.1235	1	179.25
473.2282		236.13
485.2248	1	207.98
559.2633	1	637.56
637.2989	1	1481.51
638.2991	1	616.34

Compound Structure



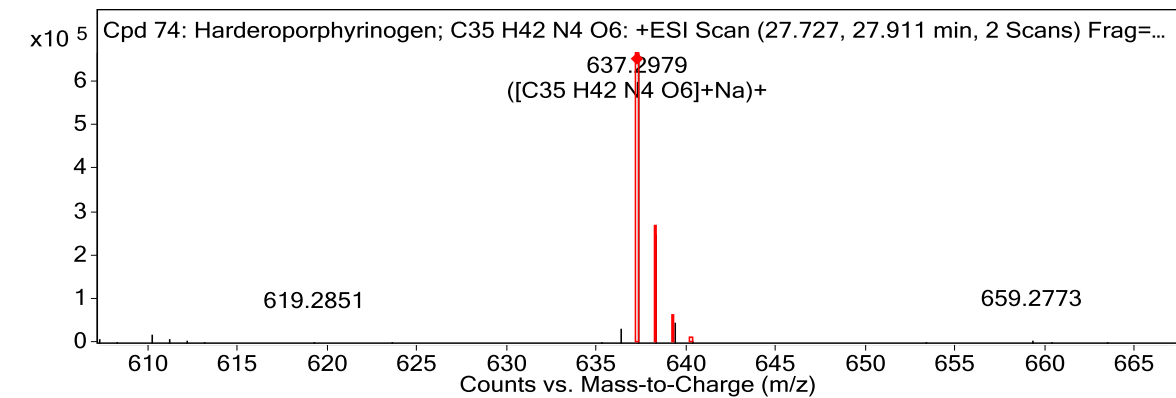
Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 74: Harderoporphyrinogen; C35 H42 N4 O6	Harderoporphyrinogen	637.2979	27.831	Auto MS/MS	614.3087

MS Spectrum



MS Zoomed Spectrum

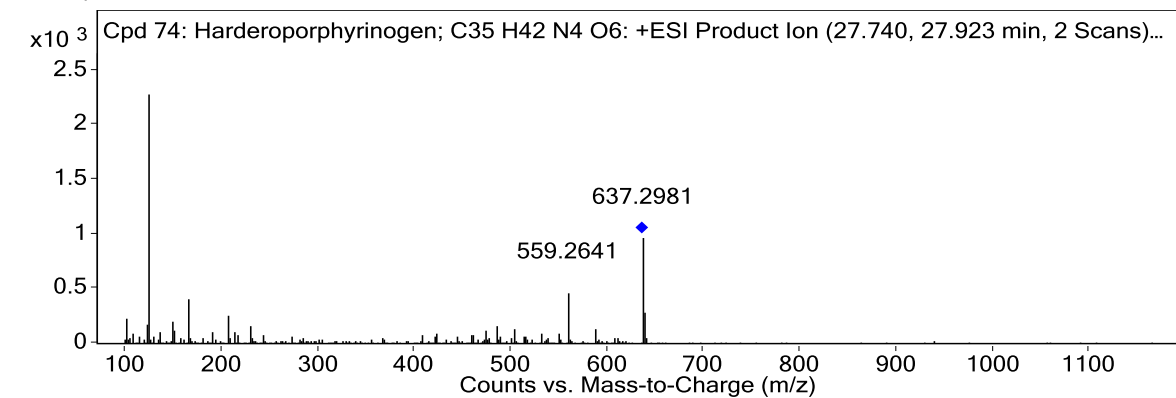
Qualitative Compound Report



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
123.0909				21546.98		
124.0864			1	157811.03		
166.0965			1	32526.23		
207.1222			1	28404.88		
610.178			1	19902.17		
636.2883				32710.82		
637.2979	637.2997	2.78	1	665532.06	C35 H42 N4 O6	(M+Na)+
638.3013	638.3028	2.44	1	250908.7	C35 H42 N4 O6	(M+Na)+
639.3031	639.3057	4.03	1	48284.89	C35 H42 N4 O6	(M+Na)+
640.3039	640.3084	7.14	1	6813.76	C35 H42 N4 O6	(M+Na)+

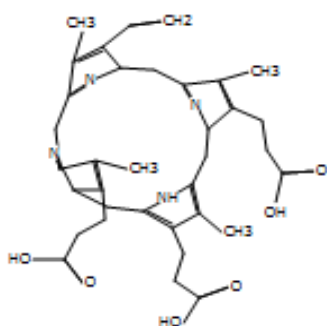
MS/MS Spectrum



MS/MS Spectrum Peak List

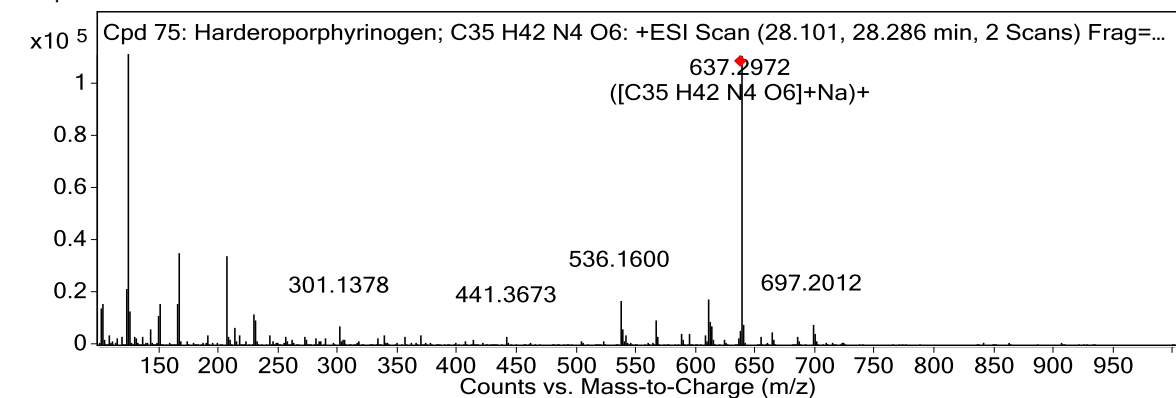
m/z	z	Abund
101.0697		234.47
123.0897		181.36
124.0863	1	2281.7
150.0638		204.15
164.9278		228.36
166.0952	1	411.44
207.122		252.87
559.2641	1	469.97
637.2981	1	970.65
638.2988	1	291.48

Compound Structure

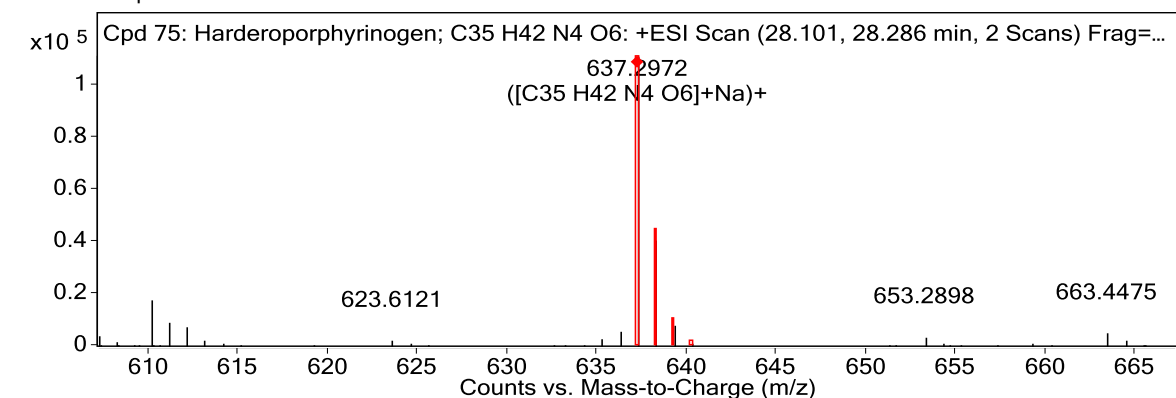


Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 75: Harderoporphyrinogen; C35 H42 N4 O6	Harderoporphyrinogen	637.2972	28.207	Auto MS/MS	614.3077

MS Spectrum

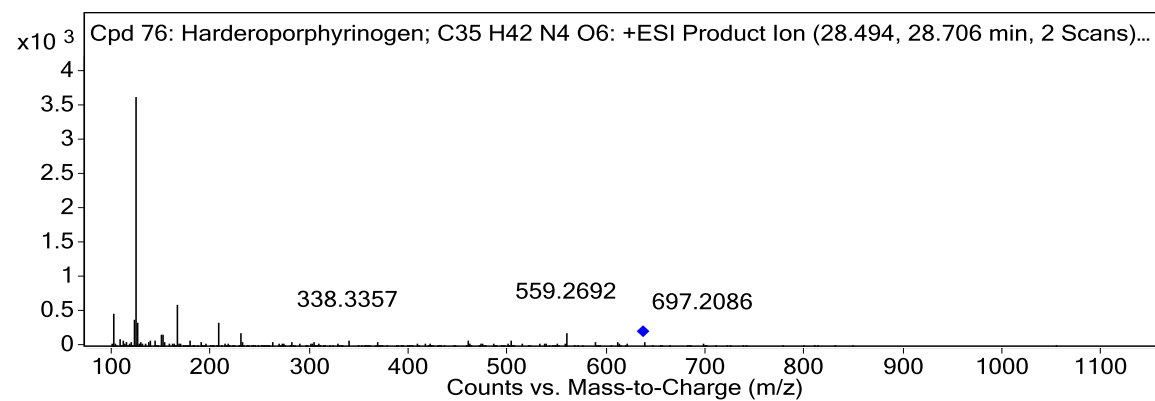


MS Zoomed Spectrum



MS Spectrum Peak List

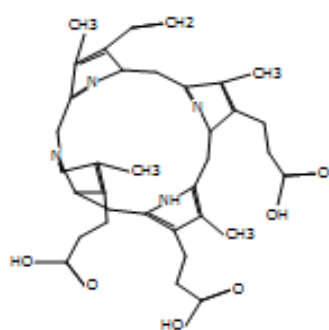
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
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MS/MS Spectrum Peak List

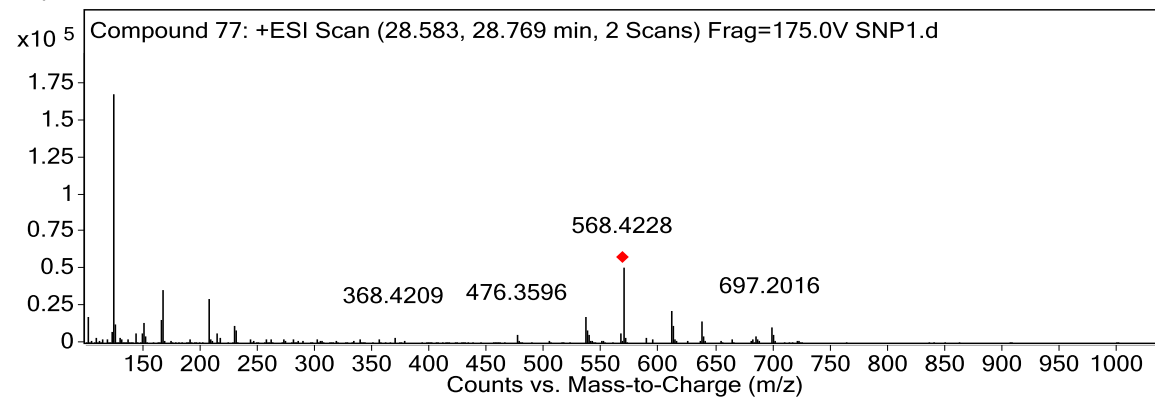
m/z	z	Abund
101.0713		364.45
102.1267	1	486.92
122.0951		197.68
123.091		393.14
124.0859	1	3638.62
125.0697	1	340.73
164.9271		270.82
166.0967	1	618.09
207.1218	1	341.86
559.2692		198.67

Compound Structure

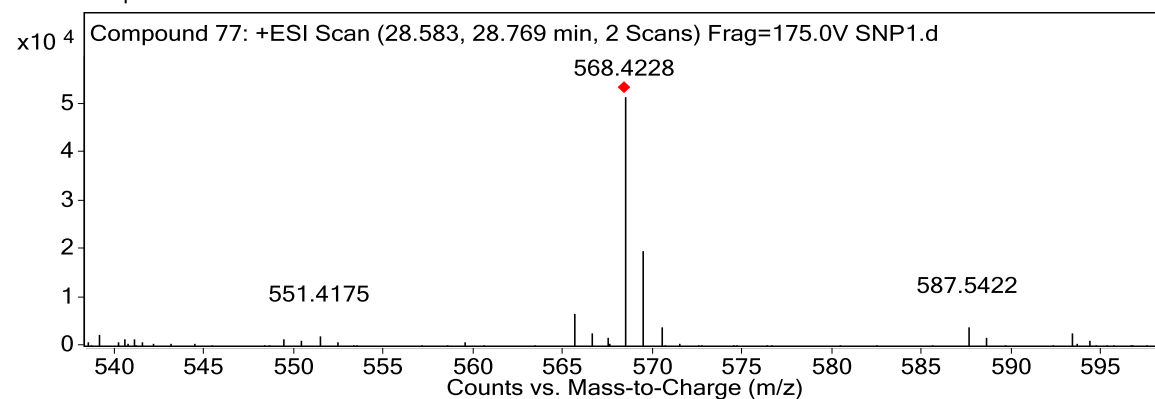


Compound Label	<i>m/z</i>	RT	Algorithm
Compound 77	568.4228	28.693	Auto MS/MS

MS Spectrum



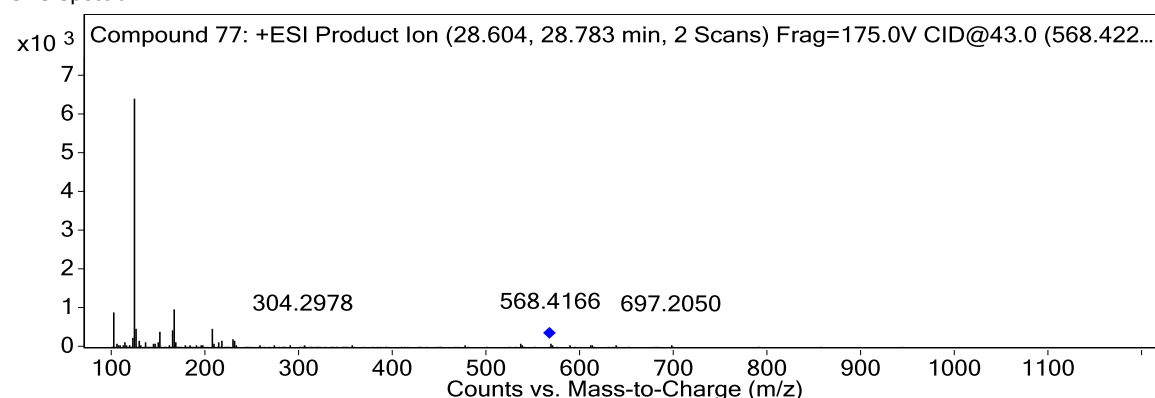
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund
123.0909		21979.25
124.0864	1	168109.63
166.0965	1	36009.98
207.1224	1	29954.42
536.1596	1	18006.25
568.4228	1	51638.37
569.4257	1	19763.35
570.4281	1	4136.18
571.4317	1	680.57
610.1782	1	21688.1

MSMS Spectrum



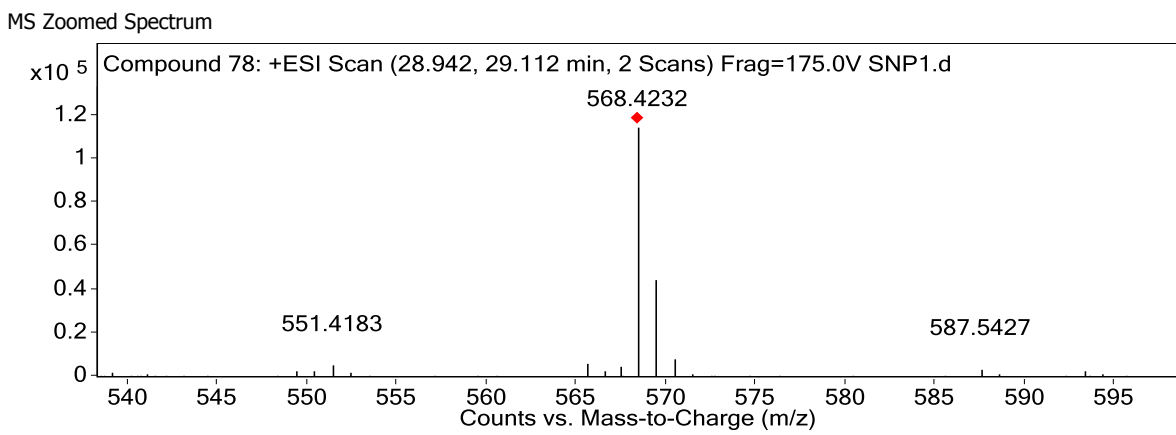
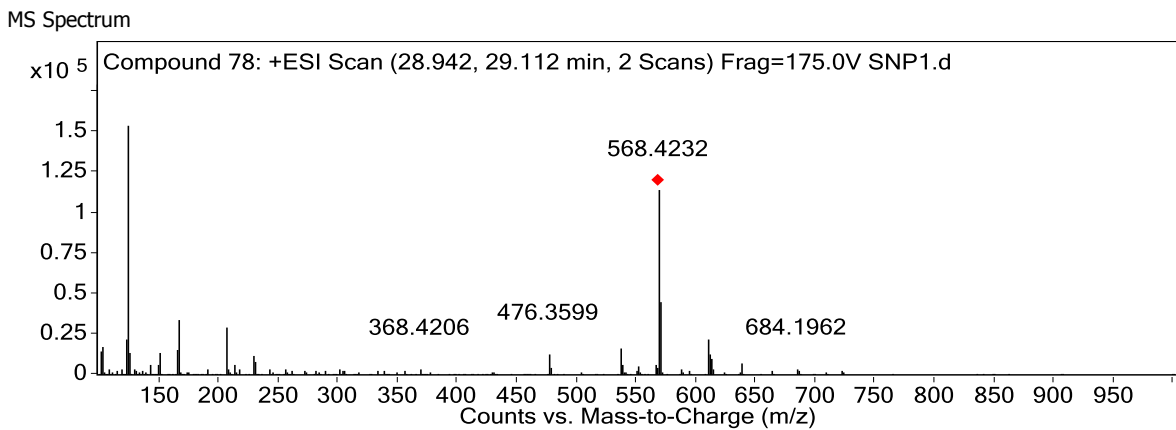
MS/MS Spectrum Peak List

m/z	z	Abund
101.0699		527.89
102.1267	1	912.22

Qualitative Compound Report

123.0905		836.48
124.0862	1	6432.72
125.0703		491.49
125.0881	1	369.03
150.0655		434.29
164.9281		450.93
166.0959	1	989.54
207.1227	1	503.41

Compound Label	m/z	RT	Algorithm
Compound 78	568.4232	29.04	Auto MS/MS

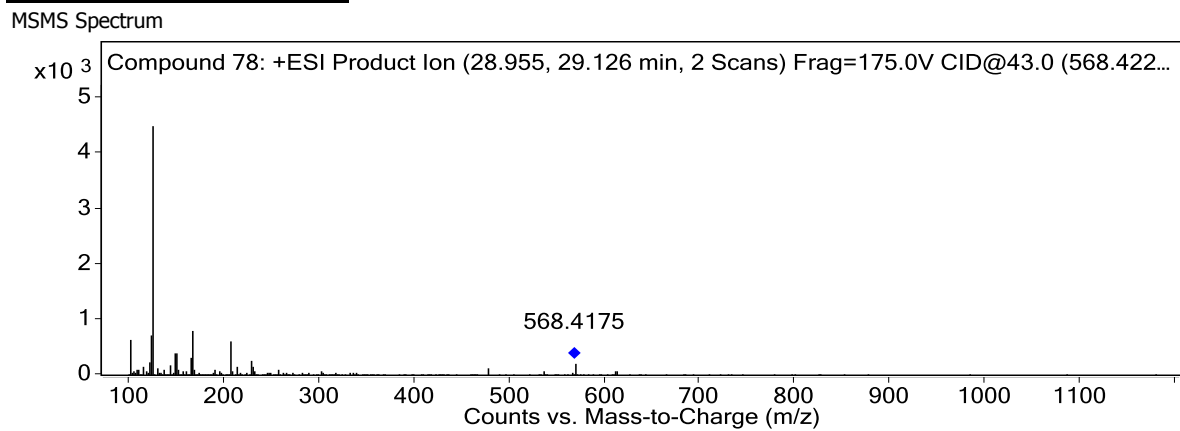


MS Spectrum Peak List

m/z	z	Abund
102.127		17339.21
123.0909		22174.99

Qualitative Compound Report

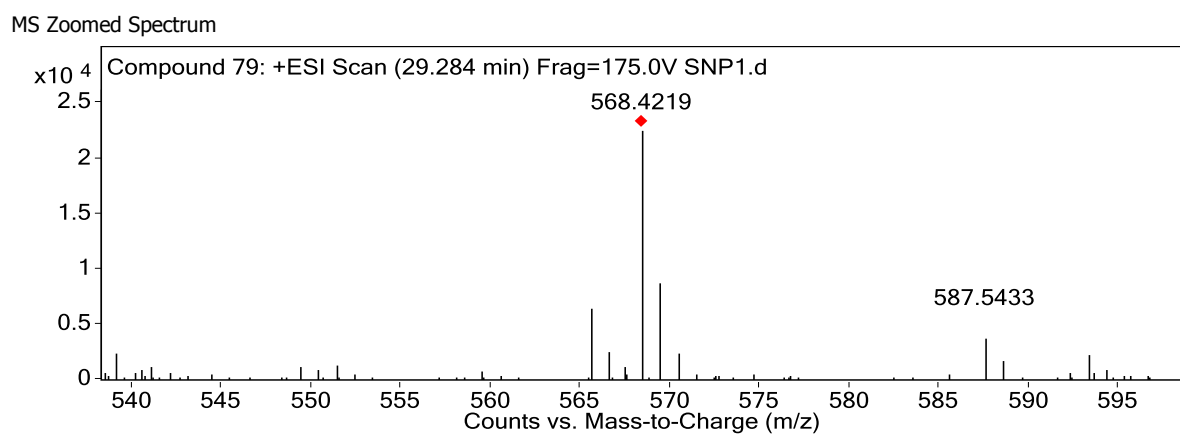
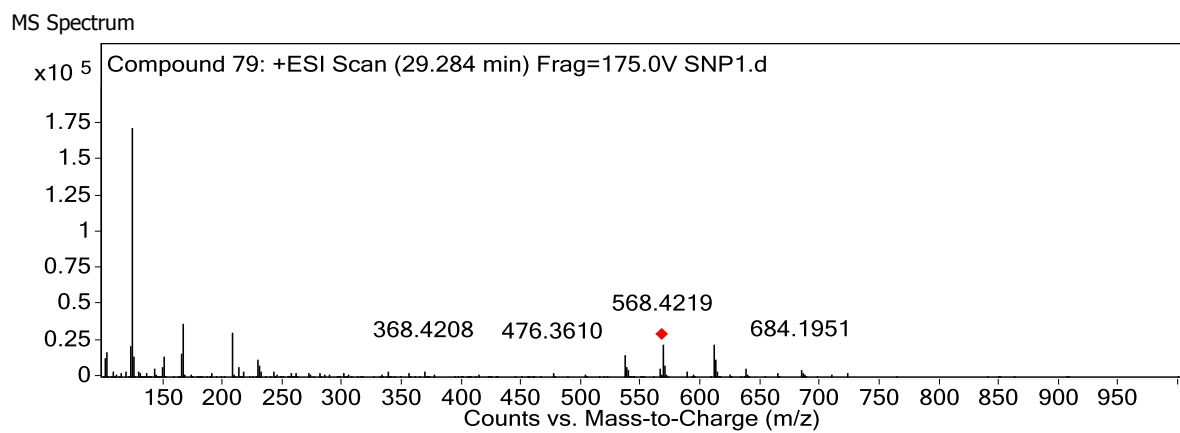
m/z	z	Abund
124.0864	1	154192.8
166.0966	1	33696.72
207.1224	1	29229.2
568.4232	1	114487.86
569.426	1	44779.63
570.4297	1	8503.24
571.4318	1	1452.57
610.1779	1	22425.62



MS/MS Spectrum Peak List

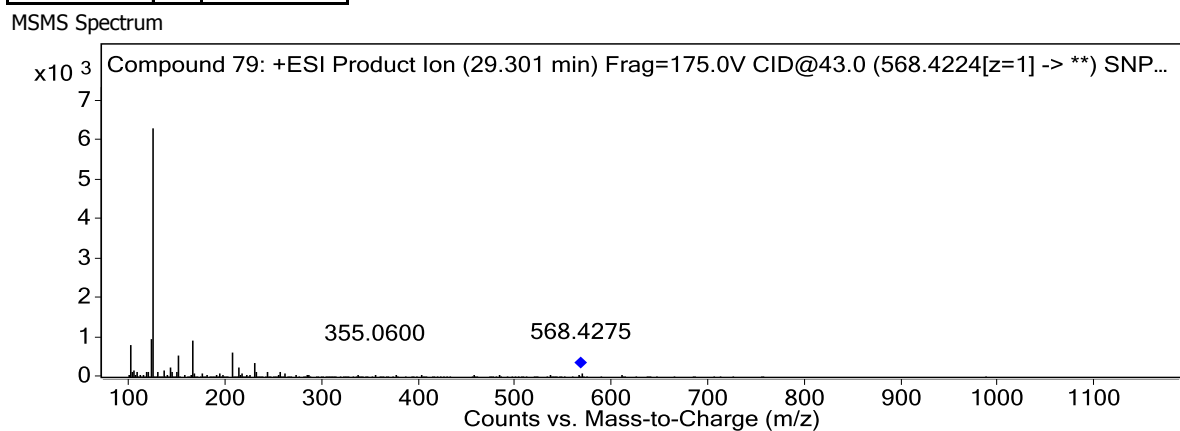
m/z	z	Abund
101.0708	1	553.79
102.1264	1	647.03
123.0908		729.91
124.0863	1	4502.68
125.0889	1	333.72
149.0225		392.15
150.0634	1	391.31
164.9281		333.49
166.0961	1	806.69
207.1223	1	613.47

Compound Label	m/z	RT	Algorithm
Compound 79	568.4219	29.301	Auto MS/MS



MS Spectrum Peak List

m/z	z	Abund
102.127		18012.53
123.091		21182.79
124.0864	1	172231.86
166.0965	1	37303.52
207.1223	1	30605.29
568.4219	1	22546.53
569.4256	1	8715.81
570.4277	1	2427.23
571.423	1	557.82
610.1789	1	22321.35



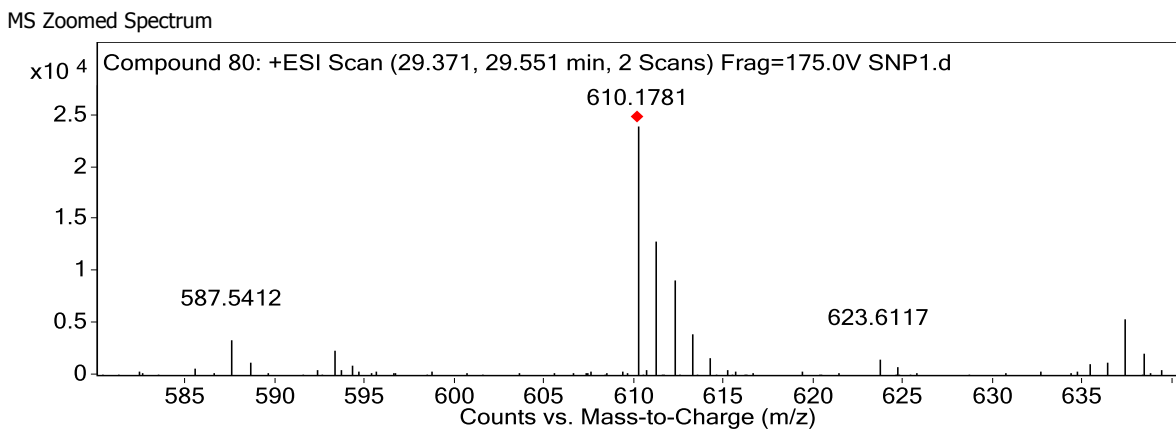
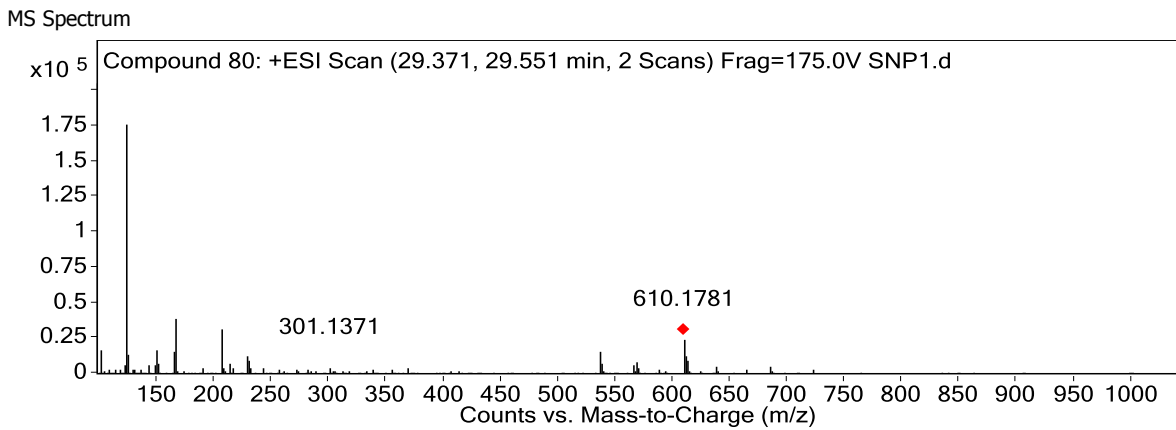
MS/MS Spectrum Peak List

m/z	z	Abund
101.0701	1	725.01
102.1271	1	830.16
123.0908		973.56
124.0859	1	6326.82
125.0705	1	471.06

Qualitative Compound Report

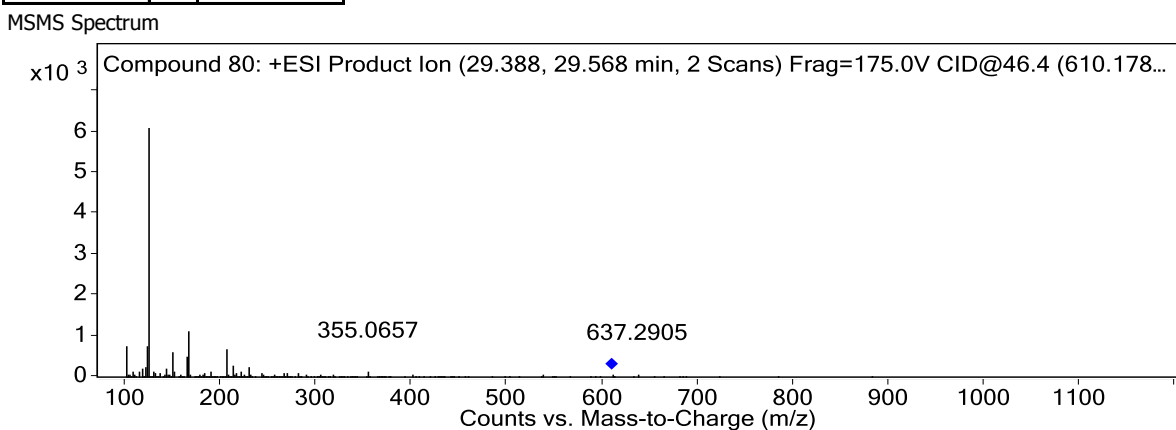
125.0871	1	627.77
150.0652	1	573.25
164.9298		514.09
166.0962	1	931
207.1223		659.66

Compound Label	m/z	RT	Algorithm
Compound 80	610.1781	29.478	Auto MS/MS



MS Spectrum Peak List

m/z	z	Abund
102.1269	1	16890.38
123.091		22447.75
124.0864	1	176231.28
150.065	1	16920.3
164.9282		15921.87
166.0964	1	39228.84
207.1224	1	31264.22
610.1781	1	24005.45
611.1781	1	12957.58
612.1767	1	9241.07



MS/MS Spectrum Peak List

m/z	z	Abund
101.0705		685.22
102.1266	1	750.32
123.0914		778.35
124.0861	1	6099.26
125.0703		642.39
125.0893	1	350.33
150.0649		611.48
164.9289		519.49
166.095	1	1137.02
207.1224	1	696.92

--- End Of Report ---