Qualitative Compound Report

Data File Litchnill_r1.d **Sample Name** Litchnill
Sample Type Sample **Position** P1-B5
Instrument Name QTOF **User Name**
Acq Method 50min_+ESI_11012021_MSMS.m **Acquired Time** 8/7/2021 1:02:15 PM
IRM Calibration Status Success **DA Method** Default.m
Comment

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

Compound Table

Compound Label	RT	Mass	Abund	Name	Formula	MFG Formula	DB Formula	DB Diff (ppm)	Hits (DB)
Cpd 1: 1.082	1.082								
Cpd 2: 1.147	1.147								
Cpd 3: 1.420	1.42								
Cpd 4: 1.526	1.526								
Cpd 5: 1.771	1.771								
Cpd 6: 2.145	2.145								
Cpd 7: Actinidine	3.134	147.1038		Actinidine	C10 H13 N	C10 H13 N	C10 H13 N	6.53	3
Cpd 8: Pirimicarb	3.419	238.1399		Pirimicarb	C11 H18 N4 O2	C11 H18 N4 O2	C11 H18 N4 O2	13.04	3
Cpd 9: Actinidine	3.497	147.1038		Actinidine	C10 H13 N	C10 H13 N	C10 H13 N	7.08	3
Cpd 10: Pirimicarb	3.797	238.1399		Pirimicarb	C11 H18 N4 O2	C11 H18 N4 O2	C11 H18 N4 O2	12.82	1
Cpd 11: Oxymetazoline	4.902	260.1845		Oxymetazoline	C16 H24 N2 O	C16 H24 N2 O	C16 H24 N2 O	16.91	8
Cpd 12: Diethylstilbestrol monomethyl ether	5.31	282.1661		Diethylstilbestrol monomethyl ether	C19 H22 O2	C19 H22 O2	C19 H22 O2	-14.52	7
Cpd 13: Istamycin AP	6.314	304.2101		Istamycin AP	C13 H28 N4 O4	C13 H28 N4 O4	C13 H28 N4 O4	3.24	10
Cpd 14: Piperolein B	6.316	343.2183		Piperolein B	C21 H29 N O3	C21 H29 N O3	C21 H29 N O3	-10.31	4
Cpd 15: Istamycin AP	6.648	304.21		Istamycin AP	C13 H28 N4 O4	C13 H28 N4 O4	C13 H28 N4 O4	3.35	10
Cpd 16: Piperolein B	6.649	343.2185		Piperolein B	C21 H29 N O3	C21 H29 N O3	C21 H29 N O3	-10.83	4
Cpd 17: 7.407	7.407								
Cpd 18: 1-epi-Fortimicin B	7.412	348.2357		1-epi-Fortimicin B	C15 H32 N4 O5	C15 H32 N4 O5	C15 H32 N4 O5	4.37	10
Cpd 19: 9alpha-Fluoro 11beta,17alpha,21-trihydroxy 6alpha-methylpregna-1,4-diene-3,20-dione	7.452	392.1996		9alpha-Fluoro 11beta,17alpha,21-trihydroxy 6alpha-methylpregna-1,4-diene-3,20-dione	C22 H29 F O5	C22 H29 F O5	C22 H29 F O5	0.81	10
Cpd 20: Coronatine	7.635	319.1782		Coronatine	C18 H25 N O4	C18 H25 N O4	C18 H25 N O4	0.36	8
Cpd 21: 7.757	7.757								
Cpd 22: Coronatine	8.01	319.1783	114652	Coronatine	C18 H25 N O4	C18 H25 N O4	C18 H25 N O4	0.17	8
Cpd 23: Istamycin C1	8.331	431.2701		Istamycin C1	C19 H37 N5 O6	C19 H37 N5 O6	C19 H37 N5 O6	9.87	2
Cpd 24: 8.347	8.347								
Cpd 25: Istamycin C1	8.696	431.2703		Istamycin C1	C19 H37 N5 O6	C19 H37 N5 O6	C19 H37 N5 O6	9.54	2
Cpd 26: Taurohyocholic acid	8.877	515.2905		Taurohyocholic acid	C26 H45 N O7 S	C26 H45 N O7 S	C26 H45 N O7 S	2.2	7
Cpd 27: Progeldanamycin	9.079	475.2959		Progeldanamycin	C27 H41 N O6	C27 H41 N O6	C27 H41 N O6	-5.27	4
Cpd 28: Prednisolone tebutate	9.136	458.2691		Prednisolone tebutate	C27 H38 O6	C27 H38 O6	C27 H38 O6	-4.95	3
Cpd 29: Progeldanamycin	9.421	475.2958		Progeldanamycin	C27 H41 N O6	C27 H41 N O6	C27 H41 N O6	-5.01	4
Cpd 30: Prednisolone tebutate	9.465	458.2693		Prednisolone tebutate	C27 H38 O6	C27 H38 O6	C27 H38 O6	-5.39	3
Cpd 31: Auriculine	9.578	559.3166		Auriculine	C31 H45 N O8	C31 H45 N O8	C31 H45 N O8	-3.67	1
Cpd 32: 9.813	9.813								
Cpd 33: 20-hydroxyecdysone	9.848	480.3134		20-hydroxyecdysone	C27 H44 O7	C27 H44 O7	C27 H44 O7	-9.85	7
Cpd 34: 10.180	10.18								
Cpd 35: Janthitrem E	10.233	603.3428		Janthitrem E	C37 H49 N O6	C37 H49 N O6	C37 H49 N O6	21.79	1
Cpd 36: 10.437	10.437								
Cpd 37: Westiellamide	10.488	546.3217		Westiellamide	C27 H42 N6 O6	C27 H42 N6 O6	C27 H42 N6 O6	-9.45	1
Cpd 38: 10.790	10.79								
Cpd 39: 10.796	10.796								
Cpd 40: 11.042	11.042								

Cpd 41: Chivosazole F	11.3	691.395		Chivosazole F	C41 H57 N O8	C41 H57 N O8	C41 H57 N O8	19.38	1
Cpd 42: 11.379	11.379								
Cpd 43: 11.532	11.532								
Cpd 44: Chivosazole F	11.599	691.395		Chivosazole F	C41 H57 N O8	C41 H57 N O8	C41 H57 N O8	19.34	1
Cpd 45: 11.767	11.767								
Cpd 46: 11.822	11.822								
Cpd 47: Mycinamicin IV	12.069	695.4263		Mycinamicin IV	C37 H61 N O11	C37 H61 N O11	C37 H61 N O11	-2.62	1
Cpd 48: Lycoperoside D	12.48	739.4525		Lycoperoside D	C39 H65 N O12	C39 H65 N O12	C39 H65 N O12	-2.48	2
Cpd 49: PE(P 16:0/18:4(6Z,9Z,12Z,15Z))	12.487	695.4891	301409	PE(P 16:0/18:4(6Z,9Z,12Z,15Z))	C39 H70 N O7 P	C39 H70 N O7 P	C39 H70 N O7 P	-0.21	3
Cpd 50: Ophiopogonin B	12.581	722.4265	189942	Ophiopogonin B	C39 H62 O12	C39 H62 O12	C39 H62 O12	-3.23	6
Cpd 51: 12.586	12.586								
Cpd 52: PE(20:3(8Z,11Z,14Z)/18:4(6Z, 9Z,12Z,15Z))	12.912	761.4963		PE(20:3(8Z,11Z,14Z)/18:4(6Z, 9Z,12Z,15Z))	C43 H72 N O8 P	C43 H72 N O8 P	C43 H72 N O8 P	4.24	10
Cpd 53: Pitheduloside A	13.014	766.4522	148990	Pitheduloside A	C41 H66 O13	C41 H66 O13	C41 H66 O13	-2.48	6
Cpd 54: Spiramycin 2	13.13	884.526		Spiramycin 2	C45 H76 N2 O15	C45 H76 N2 O15	C45 H76 N2 O15	-1.65	10
Cpd 55: 13.197	13.197		63279						
Cpd 56: beta-Solamarine	13.213	867.4998		beta-Solamarine	C45 H73 N O15	C45 H73 N O15	C45 H73 N O15	-2.04	3
Cpd 57: Mycobactin S	13.344	827.5045	251043	Mycobactin S	C44 H69 N5 O10	C44 H69 N5 O10	C44 H69 N5 O10	-0.06	1
Cpd 58: Halstoctacosanolide A	13.345	844.5311	214932	Halstoctacosanolide A	C48 H76 O12	C48 H76 O12	C48 H76 O12	3.1	3
Cpd 59: 13.489	13.489								

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Cpd 60: PI(20:3(5Z,8Z,11Z)/18:0)	13.694	888.5569	171896	PI(20:3(5Z,8Z,11Z)/18:0)	C47 H85 O13 P	C47 H85 O13 P	C47 H85 O13 P	17.89	8
Cpd 61: 13.908	13.908								
Cpd 62: 14.232	14.232								
Cpd 63: 14.236	14.236								
Cpd 64: 14.242	14.242		91509						
Cpd 65: Ganglioside GM3 (d18:0/20:0)	14.381	1210.7803		Ganglioside GM3 (d18:0/20:0)	C61 H114 N2 O21	C61 H114 N2 O21	C61 H114 N2 O21	9.15	1
Cpd 66: T-kinin	14.479	1259.6992	103121	T-kinin	C59 H89 N17 O14	C59 H89 N17 O14	C59 H89 N17 O14	-17.21	1
Cpd 67: 14.646	14.646		85366						
Cpd 68: Tetrahexosylceramide (d18:1/18:0)	14.797	1254.8061		Tetrahexosylceramide (d18:1/18:0)	C62 H114 N2 O23	C62 H114 N2 O23	C62 H114 N2 O23	-19.79	3
Cpd 69: 15.008	15.008		98250						
Cpd 70: 15.091	15.091		52878						
Cpd 71: 15.123	15.123								
Cpd 72: 15.421	15.421		96445						
Cpd 73: 15.614	15.614		80838						
Cpd 74: Dihydrodeoxystreptomycin	19.194	567.2855		Dihydrodeoxystreptomycin	C21 H41 N7 O11	C21 H41 N7 O11	C21 H41 N7 O11	1.64	2
Cpd 75: Manumycin A	19.226	550.2587	164983	Manumycin A	C31 H38 N2 O7	C31 H38 N2 O7	C31 H38 N2 O7	16.7	1
Cpd 76: Decursinol	19.921	246.09		Decursinol	C14 H14 O4	C14 H14 O4	C14 H14 O4	-3.21	10
Cpd 77: Schleicherastatin 6	23.298	430.3439		Schleicherastatin 6	C28 H46 O3	C28 H46 O3	C28 H46 O3	1.79	10
Cpd 78: C16 Sphinganine	24.095	273.265		C16 Sphinganine	C16 H35 N O2	C16 H35 N O2	C16 H35 N O2	6.64	1
Cpd 79: Teasterone	33.654	448.3544		Teasterone	C28 H48 O4	C28 H48 O4	C28 H48 O4	2.01	10
Cpd 80: N Hexadecanoylpyrrolidine	41.17	309.3009		N-Hexadecanoylpyrrolidine	C20 H39 N O	C20 H39 N O	C20 H39 N O	7.25	1

Compound Label	m/z	RT	Algorithm
Cpd 1: 1.082	148.132	1.082	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
148.132	1	610799.06
149.1353	1	43541.3
162.1113	1	48645.55
192.1576	1	74985.57
193.1611	1	6939.41
215.0148	1	16404.14
236.9961	1	7550.72
243.1812	1	14525
252.9704	1	7918.96
270.2002	1	5743.35

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0476		770.34
60.0795		677.97
104.1066	1	5155.95
105.1089	1	266.99
112.8952		103.02
148.132	1	4878.98
149.1358	1	473.27
162.1103		219.29
243.1812		142.53
831.5972		113.54

Qualitative Compound Report

Compound Label	m/z	RT	Algorithm
Cpd 2: 1.147	192.1577	1.147	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
148.132	1	922381.69
149.1353	1	67150.43
162.1113	1	55535.7
192.1577	1	103778.62
193.1615	1	10660.23
215.0146	1	40729.98
236.9964	1	15814.05
243.1813	1	12505.69
252.9705	1	13172.07
287.2071	1	7729.3

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0475		355.25
59.2902		97.27
60.0797		241.94
104.1063	1	1748.84
105.109	1	257.82
112.8958		106.96
133.084		114.97
148.1318	1	4805.69
149.1341	1	404.71
192.1571	1	1828.04

Compound Label	m/z	RT	Algorithm
Cpd 3: 1.420	148.132	1.42	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

m/z	z	Abund
148.132	1	951923.63
149.1352	1	69191.95
162.1113	1	75392.97
192.1578	1	469557.44
193.1614	1	48184.21
215.0148	1	272636.41
216.0179	1	20471.29
236.1837	1	14990.42
236.9964	1	38641.26
252.9702	1	36083.92

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0487	1	511.76
59.0716		103.86
60.0803		273.26
104.1046	1	543.39
148.1321	1	1814.57
149.1356	1	206.67
192.1572	1	456.28
215.0139		375.3
236.1826		101.09
289.023		100.66

Compound Label	m/z	RT	Algorithm
Cpd 4: 1.526	192.1578	1.526	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
148.132	1	854075.75
149.1352	1	60098.46
162.1113	1	70436.99
192.1578	1	188442.47
193.1614	1	19021.71
215.0146	1	118436.36
236.1836	1	67890.42
236.9964	1	27240.02
252.9701	1	26025.08
268.944	1	9259.69

MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0478	1	979.42
104.1068	1	1822.54
105.1085	1	152.84
148.1319	2	2855.69
149.1345	2	183.15
162.1112		299.51
173.0688		116.2
192.1572	1	1233.65
215.014		245.82
236.1825	1	191.26

Compound Label	m/z	RT	Algorithm
Cpd 5: 1.771	148.132	1.771	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
120.0803	1	30391.95
148.132	1	725018.25
149.1355	1	49133.2
162.1114	1	61344.95
192.1578	1	120731.89
193.1615	1	12690.56
215.0146	1	54615.68
217.1031	1	24805.94
236.9966	1	15085.89
252.9701	1	10987.2

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484		905.46
104.1064		528.98
105.1088		216.18
111.0428		209.95
120.0806		89.52
148.132	1	2934.29
149.1339	1	195.56
150.1383	1	84.5
192.1574	1	383.16
217.1047		248.9

Compound Label	m/z	RT	Algorithm
Cpd 6: 2.145	148.1321	2.145	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
120.08	1	62634.95
136.0497	1	10995.68
148.1321	1	462005.5
149.1353	1	33995.88
162.1114	1	32091.42
166.0849	1	14203.12
192.1578	1	64996.13
195.1213	1	8965.12
215.0145	1	14504.19
217.1031	1	63849.92

MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.048		1234.1
60.0798		348.64
104.1056		749.13
109.0223		128.98
110.0588		137.15
111.0441		266.67
111.0791	1	236.76
120.0806	1	268.21
148.1319	1	2467.83
217.1023		172.25

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 7: Actinidine	**Actinidine**	148.1111	3.134	Auto MS/MS	147.1038

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
133.0854			1	20082.93		
136.0496			1	53953.36		
148.1111	148.1121	6.47	1	152690.25	C10 H13 N	(M+H)+
148.1317			1	24972.8		
149.1143	149.1153	6.42	1	15795.39	C10 H13 N	(M+H)+
162.1112			1	20036.42		
166.1213			1	27379.37		
239.1471			1	101489.37		
261.129			1	116989.5		
262.1322			1	14289.39		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483		1855.66
60.0794		271.05
104.108		302.86
111.0422	2	380.8
133.0863	1	253.11
136.0497		275.05
148.1108	1	1903.24
148.1312	1	305.1
239.1462	1	329.86
261.1298	1	317.28

Compound Structure

Compound Label	Name	m/z	RT	Algorithm	Mass

Qualitative Compound Report

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 8: Pirimicarb	**Pirimicarb**	261.1291	3.419	Auto MS/MS	238.1399

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

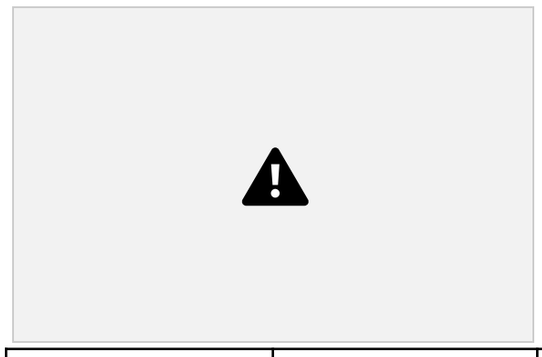
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
133.0851			1	35028.64		
136.0497			1	94707.33		
148.1111			1	184339.72		
149.114			1	18220.5		
166.1214			1	27916.95		
239.1471			1	176339.64		
240.1504			1	18735.88		
261.1291	261.1322	11.97	1	183177.84	C11 H18 N4 O2	(M+Na)+
262.1321	262.1349	10.65	1	21398.32	C11 H18 N4 O2	(M+Na)+
263.1339	263.1372	12.76	1	3199.4	C11 H18 N4 O2	(M+Na)+

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483		1336.45
99.0785		153.23
111.0431	1	380.55
111.0786		202.74
133.0859		168.05
136.0491		403.35
148.1116	2	256.2
166.12	1	268.11
239.1466	1	585.23
261.1295	1	1609.87

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 9: Actinidine	**Actinidine**	148.1111	3.497	Auto MS/MS	147.1038

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

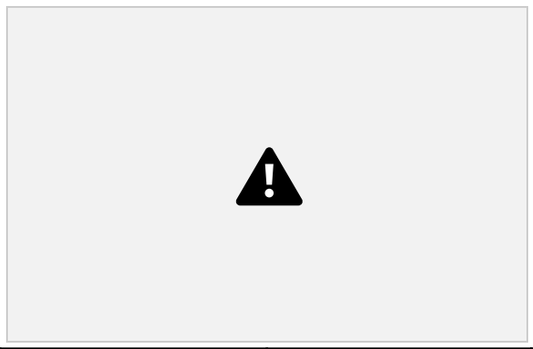
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
133.0851			1	33638.46		
136.0498			1	81432.09		
148.1111	148.1121	6.89	1	137836.47	C10 H13 N	(M+H)+
149.1141	149.1153	8.16	1	15723.91	C10 H13 N	(M+H)+
162.1116			1	16428.89		
166.1214			1	17709.79		
239.1472			1	187533.98		
240.1505			1	22551.11		
261.1291			1	184858.97		
262.1324			1	22496.13		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
59.0479			1	1954.49		
89.0592				366.83		
104.1064				261.37		
111.0429				485.45		
133.0873			1	229.79		
136.0497				415.27		
148.1111	148.1121	6.48	1	426.5	C10 H13 N	(M+H)+
148.1317				341.25		
239.1465			1	763.84		
261.1284				491.61		

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 10: Pirimicarb	**Pirimicarb**	239.1472	3.797	Auto MS/MS	238.1399

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
133.0849				15333.96		
136.0497			1	33157.08		

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148.1107			1	37838.52		
148.1314			1	23948.1		
162.1116			1	15623.98		
188.0694			1	25977.52		
239.1472	239.1503	12.97	1	82062.3	C11 H18 N4 O2	(M+H)+
240.1505	240.153	10.4	1	9296.21	C11 H18 N4 O2	(M+H)+
241.1509	241.1553	17.99	1	1246.48	C11 H18 N4 O2	(M+H)+
261.1291			1	78172.47		

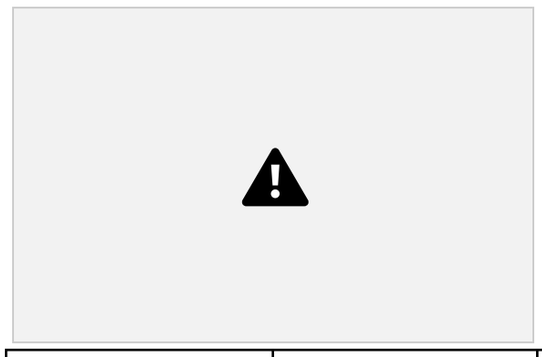
MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.048	1	1826.48
59.0711		132.5
104.1061		141.05
110.0588		143.24
111.043		624.83
117.0568		168.85
136.0489	1	334.15
148.1105	1	146.04

148.1303		126.22
261.1285	1	529.3

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 11: Oxymetazoline	**Oxymetazoline**	283.1737	4.902	Auto MS/MS	260.1845

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
136.0499			1	20675.82		
148.1319				11957.76		
190.0485			1	47418.35		
250.1421			1	20099.88		
283.1737	283.1781	15.57	1	266812.13	C16 H24 N2 O	(M+Na)+
284.177	284.1812	15	1	37143.76	C16 H24 N2 O	(M+Na)+
285.1792	285.1841	17.22	1	5612.88	C16 H24 N2 O	(M+Na)+
300.1999			1	76031.66		
305.1552			1	101665.59		
306.1587			1	13375.52		

MSMS Spectrum

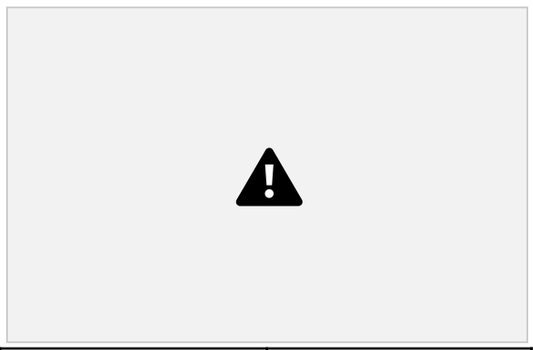
Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	2949.35

89.0592		274.16
99.0805		259.02
111.0439	1	961.62
111.0787		353.01
112.0453	1	197.46
136.0482		240.73
283.1732	1	339.51
305.1542		235.73
421.0468		213.61

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 12: Diethylstilbestrol monomethyl ether	**Diethylstilbestrol monomethyl ether**	283.1734	5.31	Auto MS/MS	282.1661

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
133.0851			1	28117.57		
190.0483			1	83267.06		
283.1734	283.1693	-14.57	1	631611.38	C19 H22 O2	(M+H)+
284.1768	284.1727	-14.67	1	82455.34	C19 H22 O2	(M+H)+
285.1784	285.1756	-9.66	1	12331.85	C19 H22 O2	(M+H)+
295.1266			1	46611.32		
300.1998			1	165868.28		
301.2029			1	22892.93		
305.1552			1	223560.59		
306.1584			1	30972.63		

MSMS Spectrum

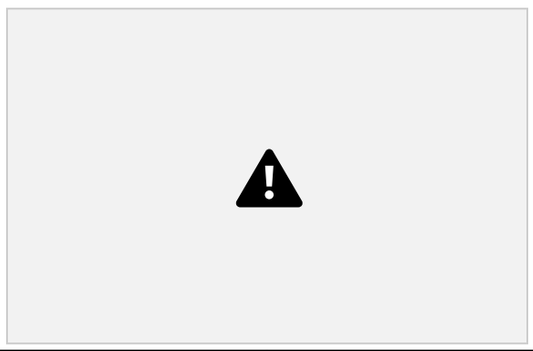
MS/MS Spectrum Peak List

m/z	z	A

Qualitative Compound Report

59.0489		1365.29
89.0597		322.88
111.0427		584.5
190.047	1	238.05
283.1743	1	875.03
284.1758	1	314.51
300.0881		133.19
300.1988	1	307.82
305.1556		262.87
333.4422		133.56

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 13: Istamycin AP	**Istamycin AP**	327.1993	6.314	Auto MS/MS	304.2101

MS Spectrum

Qualitative Compound Report

MS Zoomed Spectrum

MS Spectrum Peak List

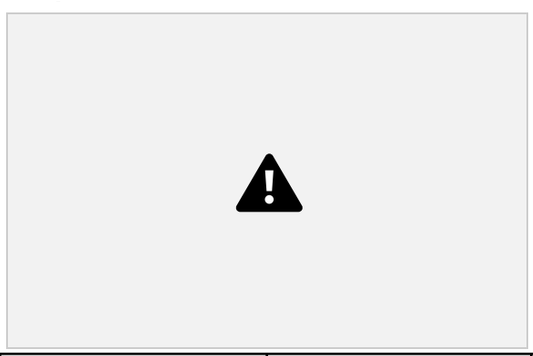
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
120.0544			1	17837.34		
136.0496			1	16574.8		
268.1527			1	16510.9		
327.1993	327.2003	3.1	1	618160.63	C13 H28 N4 O4	(M+Na)+
328.2024	328.2031	2.35	1	96330.84	C13 H28 N4 O4	(M+Na)+
329.2046	329.2054	2.25	1	15753.21	C13 H28 N4 O4	(M+Na)+
344.2255			1	505600.97		
345.229			1	82241.07		
349.1811			1	156390.7		
350.1844			1	25150.48		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0481	1	2291.59
89.0591		245.29
111.0432		299.82
111.0787		213.21
136.0481		117.24
272.0882		116.47
327.1994	1	804.03
328.2011	1	180.26
344.2263	1	483.28
349.1786		177.62

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 14: Piperolein B	**Piperolein B**	344.2255	6.316	Auto MS/MS	343.2183

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(	Abund	Ion	z Formula

Qualitative Compound Report

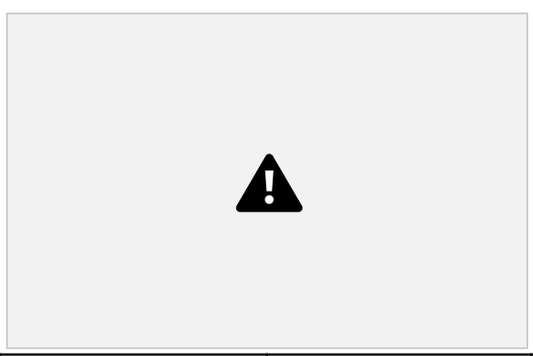
120.0544			1	17837.34		
136.0496			1	16574.8		
268.1527			1	16510.9		
327.1993			1	618160.63		
328.2024			1	96330.84		
344.2255	344.222	-10.23	1	505600.97	C21 H29 N O3	(M+H)+
345.229	345.2253	-10.72	1	82241.07	C21 H29 N O3	(M+H)+
346.2308	346.2282	-7.45	1		8 C21 H29 N O3	(M+H)+
349.1811			1	156390.7		
350.1844			1	25150.48		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	1713.28
60.0523		117.2
69.0303		65.53
81.0698		128.09
89.059		868.71
111.0423	1	396.34
133.0848	1	351.77
267.0996		67.61
283.1758		73.94
327.197		199.84

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 15: Istamycin AP	**Istamycin AP**	327.1992	6.648	Auto MS/MS	304.21

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
133.0852			1	16218.07		
327.1992	327.2003	3.29	1	928507.13	C13 H28 N4 O4	(M+Na)+
328.2026	328.2031	1.71	1	136645.91	C13 H28 N4 O4	(M+Na)+
329.2044	329.2054	2.83	1	24680.33	C13 H28 N4 O4	(M+Na)+
344.2258			1	746190.56		
345.2291			1	123149.86		
346.2306			1	19681.78		
349.1812			1	230486.08		
350.1844			1	35775.44		
365.154			1	18618.09		

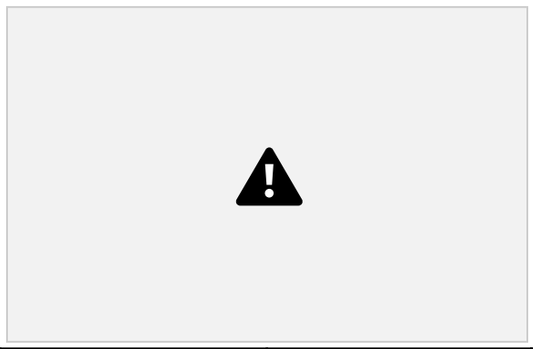
MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0479		1440.71
107.0234		127.98
111.0444		329.68
111.0785		170.15
123.0793		113.51
327.1994	1	814.93
328.201	1	154.4
344.2268	1	596.96
345.2426	1	143.29
349.1794	1	164.21

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 16: Piperolein B	**Piperolein B**	344.2258	6.649	Auto MS/MS	343.2185

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
133.0852			1	16218.07		
327.1992			1	928507.13		
328.2026			1	136645.91		
329.2044			1	24680.33		
344.2258	344.222	-10.87	1	746190.56	C21 H29 N O3	(M+H)+
345.2291	345.2253	-10.87	1	123149.86	C21 H29 N O3	(M+H)+
346.2306	346.2282	-6.99	1	19681.78	C21 H29 N O3	(M+H)+
349.1812			1	230486.08		
350.1844			1	35775.44		
365.154			1	18618.09		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0479		1668.92
87.0408		101.73
89.059	2	516.6
111.0418		201.27
131.0676		123.1
133.0842		226.42
134.0866		103.18
327.197		267.12

Qualitative Compound Report

344.2331		74.52
1030.033		80.74

Compound Structure

Compound Label	m/z	RT	Algorithm
Cpd 17: 7.407	388.2511	7.407	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
371.2248	1	913443.69
372.2287	1	158968.61
373.2303	1	27105.54
388.2511	1	1216398.63
389.2549	1	204654.39
390.2566	1	40041.84
393.2068	1	201126.98
394.2098	1	35429.77
411.2196	1	25529.32
428.2459	1	20060.53

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0485	1	2845.14
60.0429	1	117.78
89.058		414.27
111.0433		671.14
133.0862		175.04
371.227		559.51
388.2495	1	505.8
389.2514	1	247.77
393.2057		129.32
411.2162		149.12

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 18: 1-epi-Fortimicin B	**1-epi-Fortimicin B**	371.2248	7.412	Auto MS/MS	348.2357

Qualitative Compound Report

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
371.2248	371.2265	4.51	1	913443.69	C15 H32 N4 O5	(M+Na)+
372.2287	372.2294	1.93	1	158968.61	C15 H32 N4 O5	(M+Na)+
373.2303	373.2317	3.73	1	27105.54	C15 H32 N4 O5	(M+Na)+
388.2511			1	1216398.63		
389.2549			1	204654.39		
390.2566			1	40041.84		
393.2068			1	201126.98		
394.2098			1	35429.77		
411.2196			1	25529.32		
428.2459			1	20060.53		

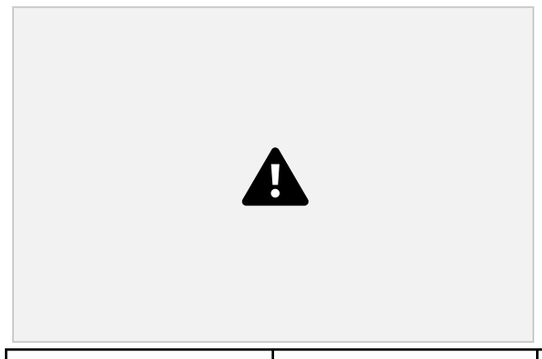
MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund

59.0484	1	996.43
89.0589		600.17
99.0785		150.08
111.0424		180.86
111.0804		42.64
126.0888		51.83
134.0862		80.3
137.0585		50.52
151.0361		57.69
393.2099		72.04

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 19: 9alpha-Fluoro 11beta,17alpha,21-trihydroxy-6alpha methylpregna-1,4-diene 3,20-dione	**9alpha-Fluoro 11beta,17alpha,21-trihydroxy-6alpha methylpregna-1,4-diene-3,20-dione**	393.207	7.452	Auto MS/MS	392.1996

MS Spectrum

Qualitative Compound Report

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
371.225			1	1057639.25		
372.2287			1	181792.48		
373.2307			1	30647.2		
388.2514			1	1339573.75		
389.2552			1	231991.97		
390.257			1	43170.48		
393.207	393.2072	0.51	1	225638	C22 H29 F O5	(M+H)+

394.2099	394.2106	1.71	1	39369.5	C22 H29 F O5	(M+H)+
395.2115	395.2133	4.45	1	6975.92	C22 H29 F O5	(M+H)+
411.2196			1	23609.34		

MSMS Spectrum

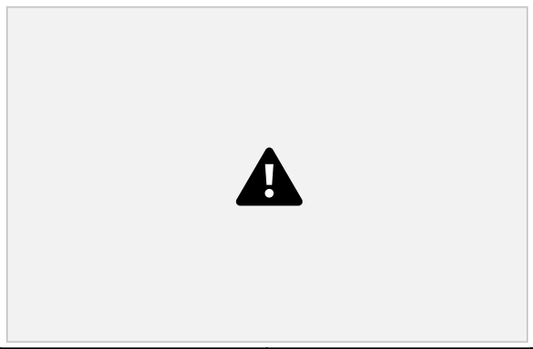
MS/MS Spectrum Peak List

m/z	z	Abund
59.0484		1687.09

Qualitative Compound Report

m/z	z	Abund
130.0055		123.12
202.1221		96.18
220.0604		97.2
237.8341		117.47
371.2239	1	532.9
372.2281	1	207.51
388.2503	2	458.92
393.2077	1	2418.05
394.207	1	700.61

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 20: Coronatine	**Coronatine**	342.1675	7.635	Auto MS/MS	319.1782

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
342.1675	342.1676	0.23	1	115704.53	C18 H25 N O4	(M+Na)+
343.1705	343.1709	1.02	1	25640.41	C18 H25 N O4	(M+Na)+
344.1734	344.1735	0.31	1	4493.73	C18 H25 N O4	(M+Na)+
371.2249			1	1279629.13		
372.2286			1	222615.47		
388.2514			1	1664051.5		
389.2551			1	285790.63		
390.257			1	53530.79		
393.207			1	280908.41		
394.21			1	47810.18		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
58.0641	1	253.25
59.0485	1	2195.62
111.0426	1	322.17
237.0863	1	163.28
265.0827	1	506
297.1092	1	480.04
342.1677		240.78
371.2239	1	540.73
372.2274	1	170.12
388.2493	1	797.78

Compound Structure

Qualitative Compound Report

Compound Label	m/z	RT	Algorithm
Cpd 21: 7.757	388.2512	7.757	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
220.059	1	24077.19
342.1674	1	181148
343.1705	1	40263.04
371.2249	1	541365.56
372.2284	1	91066.45
388.2512	1	757153.56

389.2545	1	129575.91
390.2565	1	26741.41
393.2065	1	129237.94
394.2099	1	22404.41

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0488	1	1687.77
89.0594		342.95
111.0433	1	327.81
111.0778		114.12
342.1664		273.33
343.1687		136.14
371.2256		246.11
372.2274		203.73
388.2515	1	861.03
402.2354		213.83

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 22: Coronatine	**Coronatine**	342.1676	8.01	Auto MS/MS	319.1783

MS Spectrum

Qualitative Compound Report

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
136.0497				19334.62		
342.1676	342.1676	0.05	1	114651.73	C18 H25 N O4	(M+Na)+
343.1706	343.1709	0.76	1	28732.44	C18 H25 N O4	(M+Na)+

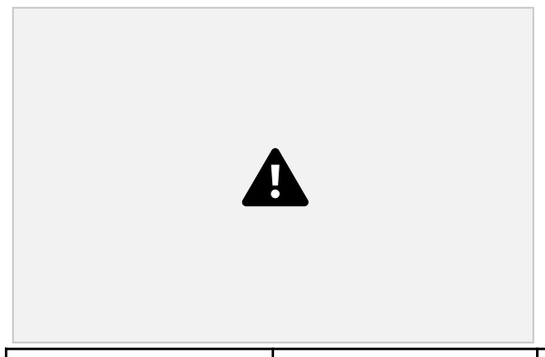
344.1736	344.1735	-0.53	1	4148.3	C18 H25 N O4	(M+Na)+
371.2246			1	80534.3		
372.2277			1	16685.68		
388.2512			1	113328.48		
389.2545			1	20312.27		
393.2068			1	17635.94		
472.2714			1	27021.91		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
58.0645		240.17
59.0485	1	2333.54
111.0426		557.22
111.0804	1	172.92
237.0896		321.01
265.0866		237.44
297.1068		203.75
342.1666	1	664.86
388.254	1	180.51
472.2724	1	201.18

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 23: Istamycin C1	**Istamycin C1**	432.2773	8.331	Auto MS/MS	431.2701

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

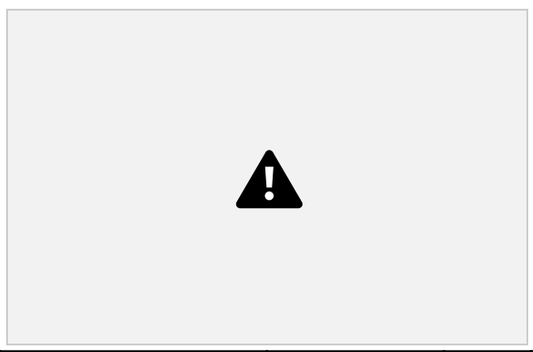
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
342.1674			1	34678.38		
415.2509			1	933455.69		
416.2544			1	180295.33		
432.2773	432.2817	10	1	1736002.38	C19 H37 N5 O6	(M+H)+
433.2807	433.2846	8.95	1	320722.97	C19 H37 N5 O6	(M+H)+
434.2825	434.287	10.25	1	62701.04	C19 H37 N5 O6	(M+H)+
437.2329			1	188865.77		
438.236			1	43440.06		
455.2455			1	44886.78		
472.2719			1	70476.09		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0482	1	2097.55
87.0437		233.98
89.0592		810.99
111.042		180.75
111.078		176.51
133.0851		603.12
207.0819		129.31
415.2506	1	669.76
432.2781	1	612.47
433.2791	1	189.82

Compound Structure



Compound Label	m/z	RT	Algorithm
Cpd 24: 8.347	415.2509	8.347	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
415.2509	1	962439.75
416.2544	1	186382.47

Qualitative Compound Report

417.256	1	32932.36
432.2773	1	1797798.25
433.2807	1	333240.09
434.2825	1	65595.33
437.2328	1	195529.88
438.236	1	44771.05
455.2451	1	46895.52
472.2715	1	65673.04

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0486	1	1607.28
71.0473		128.67
75.08		127.57
89.0589		233.08
111.042		197.74
112.0823		128.91
119.03		128.12
123.0406		127.51
415.2504	1	193.73
432.279	1	347.65

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 25: Istamycin C1	**Istamycin C1**	432.2775	8.696	Auto MS/MS	431.2703

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
136.05			1	15889.38		
342.1673			1	18308.57		
415.251			1	300409.38		
416.2539			1	60942.16		
432.2775	432.2817	9.51	1	665904.81	C19 H37 N5 O6	(M+H)+
433.2804	433.2846	9.53	1	127987.59	C19 H37 N5 O6	(M+H)+
434.2826	434.287	10.12	1	24113.03	C19 H37 N5 O6	(M+H)+
437.2325			1	78879.8		
438.2357			1	17844.13		
446.2564			1	14836.42		

MSMS Spectrum

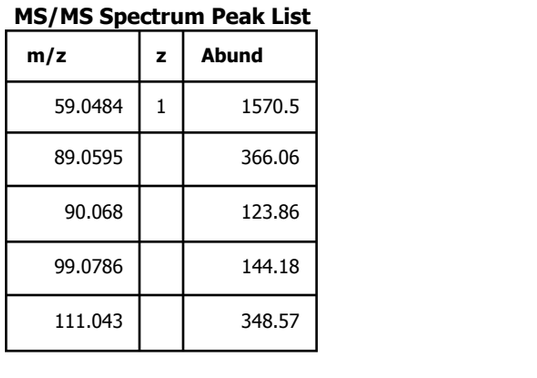
MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	1570.5
89.0595		366.06
90.068		123.86
99.0786		144.18
111.043		348.57

Qualitative Compound Report

111.0807		272.66
136.0496		158.63
415.2486	1	441.37
416.2556	1	182.85
432.2768	1	522.93

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 26: Taurohyocholic acid	**Taurohyocholic acid**	516.2977	8.877	Auto MS/MS	515.2905

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
136.05			1	18626.14		
415.2506			1	78255.41		

432.2772 1157542.53

Qualitative Compound Report

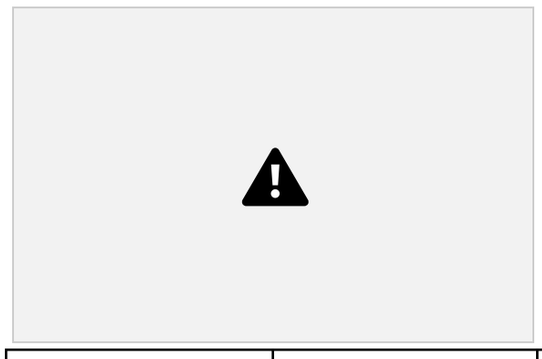
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
433.28			1	29720.27		
437.2323			1	17583.89		
499.2705			1	35786.15		
516.2977	516.2989	2.38	1	145328.75	C26 H45 N O7 S	(M+H)+
517.3006	517.3022	3.07	1	36502.57	C26 H45 N O7 S	(M+H)+
518.3031	518.3005	-5.03	1	7876.78	C26 H45 N O7 S	(M+H)+
521.253			1	33612.24		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0482	1	1622.15
87.0427		170.25
89.0581		336.8
97.0051		127.68
99.0812		218.17
111.043	1	608.47
111.0802		130.17
133.0574		130.92
133.0828		124.25
516.2942	1	305.73

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 27: Progeldanamycin	**Progeldanamycin**	476.3031	9.079	Auto MS/MS	475.2959

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
459.2764			1	692788.81		
460.2801			1	146987.98		
476.3031	476.3007	-5.19	1	1804223	C27 H41 N O6	(M+H)+
477.3068	477.304	-5.83	1	406979.16	C27 H41 N O6	(M+H)+
478.3086	478.3068	-3.71	1	72802.48	C27 H41 N O6	(M+H)+
481.2586			1	177535.09		
499.2707			1	61301		
516.2976			1	195368.61		
517.3008			1	47960.93		
521.2526			1	62363.45		

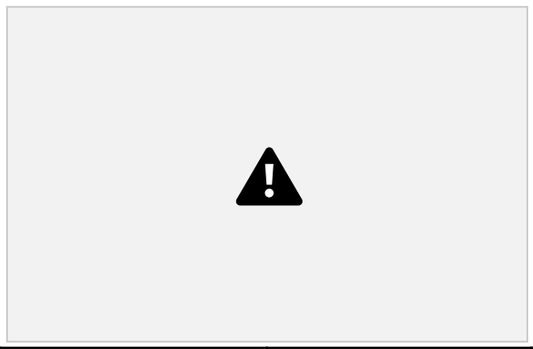
MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0486	1	3431.34
60.052	1	193.08
89.0589		868.73
111.0438		588.77
111.0796	1	642.06
133.0835		286.87
459.2758	1	247.64
476.3033	1	634.47
477.3082	1	223.96
516.2959	2	234.6

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 28: Prednisolone tebutate	**Prednisolone tebutate**	459.2763	9.136	Auto MS/MS	458.2691

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
459.2763	459.2741	-4.81	1	711919.31	C27 H38 O6	(M+H)+
460.2801	460.2775	-5.59	1	155212.91	C27 H38 O6	(M+H)+
461.2822	461.2804	-4.01	1	29906.99	C27 H38 O6	(M+H)+
476.303			1	1824315		

477.3066			1	405758.53		
478.3084			1	74564.66		
481.2584			1	184901.03		
499.2709			1	57179.49		
516.2978			1	183749.66		
521.2531			1	67149.62		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
59.0485			2	2784.12		

Qualitative Compound Report

89.0595				240.79		
99.0774				107.39		
111.044				520.01		
130.0486				118.09		
180.1423				133.86		
459.2749			1	480.26		
460.2802	460.2775	-5.79	1	133.76	C27 H38 O6	(M+H)+
476.3005			1	940.35		
516.2994				210.83		

Compound Structure

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 29: Progeldanamycin	**Progeldanamycin**	476.303	9.421	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
136.0499			1	15121.63		
459.2766			1	361633.06		
460.2798			1	83700.42		
461.2823			1	18275.84		
476.303	476.3007	-4.95	1		3 C27 H41 N O6	(M+H)+
477.3066	477.304	-5.53	1	228980.61	C27 H41 N O6	(M+H)+
478.3087	478.3068	-4.03	1	45047.61	C27 H41 N O6	(M+H)+
481.2582			1	117410.65		
482.2618			1	24225.47		
516.297			1	28469.21		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0487	1	974.3
89.0588		600.82
111.0432	1	218.87
136.0535		120.9
140.9926		126.81
220.0598		135.06
459.2757	1	219.79
476.3009	1	525.67
477.307	1	104.46
482.2582		108.24

Compound Structure

Qualitative Compound Report

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 30: Prednisolone tebutate	**Prednisolone tebutate**	459.2768	9.465	Auto MS/MS	458.2693

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
459.2768	459.2741	-5.75	1	242709.33	C27 H38 O6	(M+H)+
460.2795	460.2775	-4.32	1	60519.91	C27 H38 O6	(M+H)+
461.2818	461.2804	-3.1	1	13215.68	C27 H38 O6	(M+H)+
476.3031			1	751394.75		
477.3067			1	163613.98		
478.3087			1	31481.89		
481.2582			1	85962.79		
482.2617			1	19110.95		
516.2976			1	33369.47		
560.3235			1	33660.71		

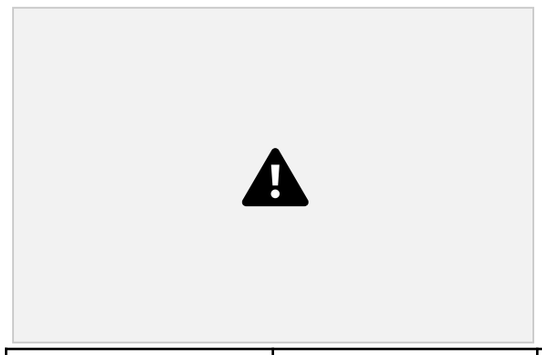
MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0482	1	2403.8
89.0589		165.55

99.0797		210.14
111.0428	1	536.05
111.0786	1	242.09
182.1863		204.73
459.2781	2	142.54
476.3023	1	454.76
477.3048	1	140.22
481.2582	1	140.48

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass

Qualitative Compound Report

Cpd 31: Auriculine	**Auriculine**	560.3239	9.578	Auto MS/MS	559.3166

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
459.2766			1	92114.42		
476.3034			1	274670.63		
477.3063			1	63661.73		
481.2582			1	31530.81		
516.2975			1	24662.01		
543.2972			1	65400.8		
560.3239	560.3218	-3.83	1	316458.44	C31 H45 N O8	(M+H)+
561.327	561.3251	-3.29	1	79407.5	C31 H45 N O8	(M+H)+
562.3298	562.3279	-3.36	1	18343.1	C31 H45 N O8	(M+H)+
565.2792			1	70823.08		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	2943.91
87.0435		145.33
89.0591		305.86
99.0441		156.25
104.0735		122.78
111.0446		906.12
111.0798		194.36
182.1894		168.13
476.3002	2	430.8
560.3227	1	342.01

Compound Structure

Compound Label	m/z	RT	Algorithm
Cpd 32: 9.813	520.3291	9.813	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

m/z	z	Abund
503.3025	1	618694.06
504.3062	1	151310.58
520.3291	1	1701952.38
521.3325	1	444386.28
522.3345	1	89986.66
525.2846	1	171345.95
543.2969	1	82653.88
560.3239	1	365692.88

561.3271	1	93296.75
565.2786	1	93241.86

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0485	2	1624.98
69.0322		192.37
87.0425		424.55
89.0594		1248.28
97.027		119.98
111.042	1	592.11
133.0848	1	770.03
182.1885	1	201.15
520.3279	1	605.09
521.33	1	111.27

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 33: 20-hydroxyecdysone	**20-hydroxyecdysone**	503.3027	9.848	Auto MS/MS	480.3134

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
503.3027	503.2979	-9.39	1	579093.31	C27 H44 O7	(M+Na)+
504.3062	504.3013	-9.64	1	142635.09	C27 H44 O7	(M+Na)+
505.3083	505.3041	-8.36	1	28286.33	C27 H44 O7	(M+Na)+
520.3292			1	1702182.13		
521.3331			1	436929.69		
522.3347			1	89592.98		
525.2848			1	185505.08		
560.324			1	271213.66		
561.3273			1	71741.16		
565.279			1	78474.79		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	2105.92
89.0591		377.23
111.0437		342.56
111.0788		285.4
503.3014	1	307.65
520.3277	1	770.02
521.33	1	260.95
525.2839	1	214.69
560.3215	1	373.02
561.3308	1	138.04

Compound Structure

Compound Label	m/z	RT	Algorithm
Cpd 34: 10.180	520.329	10.18	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
503.3027	1	150930.98
520.329	1	521004.84
521.3324	1	132113.14
522.3343	1	27752.22
525.2841	1	57417.65
560.3236	1	52122.77
587.3231	1	44921.82
604.3503	1	278672.13
605.3534	1	84088.82
609.3052	1	39566.07

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0485		1951.48
74.9294		127.5

Qualitative Compound Report

87.0421		135.87
89.0586		218.36
111.0432		445.02
175.0737		129.83
249.1087	1	131.39
503.2976		123.1
520.3266	1	273.36
604.3527	1	461.93

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 35: Janthitrem E	**Janthitrem E**	604.3502	10.233	Auto MS/MS	603.3428

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

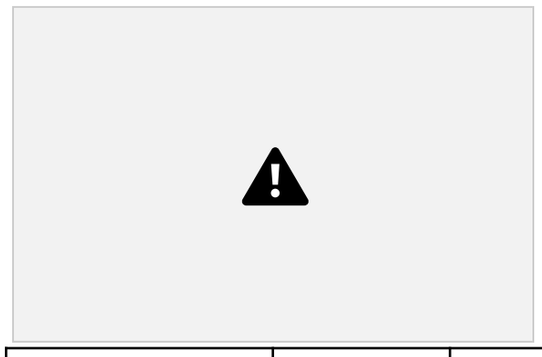
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
503.3026			1	96751.77		
520.3297			1	340059.69		
521.3326			1	83173.58		
525.2842			1	38844.64		
587.3236			1	80570.98		
604.3502	604.3633	21.65	1	517671.66	C37 H49 N O6	(M+H)+
605.3536	605.3666	21.57	1	147545.23	C37 H49 N O6	(M+H)+
606.3556	606.3696	23.09	1	36492.79	C37 H49 N O6	(M+H)+
607.358	607.3725	23.91	1	6079.9	C37 H49 N O6	(M+H)+
609.3052			1	90000.4		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0479	1	989.63
69.0332		141.04
89.0594		440.99
99.0436		194.98
111.0428		269.59
249.1133		116.72
327.0719		108.02
345.0549		122.47
525.2804		128.45
604.3511	1	202.02

Compound Structure



Compound Label	m/z	RT	Algorithm
Cpd 36: 10.437	564.3557	10.437	Auto MS/MS

MS Spectrum

Qualitative Compound Report

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
547.3291	1	303573.22
548.3324	1	79264.61
564.3557	1	1763730.38
565.3589	1	453483.31
566.3614	1	99986.23
569.3111	1	154025.53
587.3235	1	90501.27
604.3502	1	560715.94

605.3536	1	159852.84
609.3052	1	95989.53

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	1555.36
89.0591		458.06
111.0428	1	185.53
111.0785		196.72
129.993		127.58
133.0845		309.33
178.998		119.81
564.353	1	641.65
565.2798		180.31
565.3543	1	287.34

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 37: Westiellamide	**Westiellamide**	547.3291	10.488	Auto MS/MS	546.3217

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(	Abund	Ion	z	Formula

Qualitative Compound Report

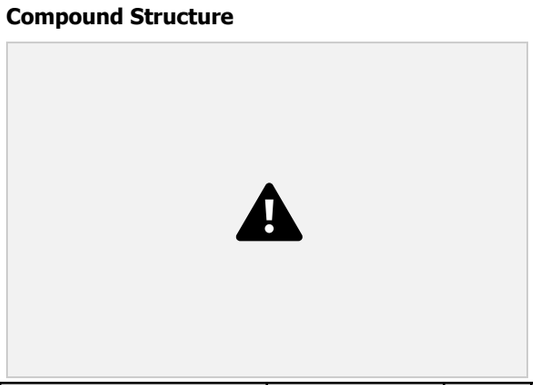
547.3291	547.3239	-9.52	1	244165.09	C27 H42 N6 O6	(M+H)+
548.332	548.3268	-9.49	1	64495.38	C27 H42 N6 O6	(M+H)+
549.3343	549.3295	-8.73	1	14763.8	C27 H42 N6 O6	(M+H)+
550.337	550.332	-9.11	1	2864.87	C27 H42 N6 O6	(M+H)+
564.3552			1	1457170		
565.3586			1	387103.63		
569.3106			1	125415.32		
604.3499			1	487638.03		
605.3535			1	145564.48		
609.3049			1	87797.04		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
55.0539		104.88
59.049	1	1624.07
89.0592		213.25
111.0431		139.73
152.0659		94.25
547.3224		89.55
548.3288		178.97
564.3553	1	607.15
569.3072	1	137.99
604.3454		91.64

Compound Structure



Compound Label	m/z	RT	Algorithm
Cpd 38: 10.790	564.3554	10.79	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
547.3285	1	111740.69
564.3554	1	541738.81
565.3585	1	136689.28
566.3603	1	31607.82
567.3629	1	5686.19
604.3497	1	73396.73
631.3493	1	66572.46
648.3759	1	531591.81
649.3798	1	168688.77
653.3312	1	78063.16

MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0493	1	1413.62
83.0482		88.12
89.0593		367.33
111.0425	1	231.75
111.0784		88.93
122.0961		102.01
186.0872		107.09
224.0848		92.5
312.2656		95.56
564.3527	1	120.97

Compound Label	m/z	RT	Algorithm
Cpd 39: 10.796	648.3759	10.796	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
547.3285	1	111740.69
564.3554	1	541738.81
565.3585	1	136689.28
604.3497	1	73396.73
631.3493	1	66572.46
648.3759	1	531591.81
649.3798	1	168688.77
650.3817	1	39776.73
651.3846	1	7038.7
653.3312	1	78063.16

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0486	1	647.33
69.0332		128.61
87.0438		196.72
89.0586		382.56
99.0405		132.33
99.0795		94.95
111.0427		452.46
136.109		103.36
165.0876		126.76
648.3761	2	187.31

Compound Label	m/z	RT	Algorithm
Cpd 40: 11.042	608.3813	11.042	Auto MS/MS

Qualitative Compound Report

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
296.1815	2	91967.15
591.3549	1	190263.97
608.3813	1	1235471.63
609.385	1	343692.59
610.3871	1	84806.79
611.3893	1	13164.91
613.3366	1	103553.34
648.376	1	588767
649.3797	1	183178.97
653.3313	1	92092.51

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0481		1144.17
74.0971		105.53
87.0435		248.84
89.0592		507.64
111.044		134.81
133.0858		267.51
177.1114		125.19
591.3498	1	247.15
608.3822	1	447.12
609.3817	1	255.92

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 41: Chivosazole F	**Chivosazole F**	692.4025	11.3	Auto MS/MS	691.395

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
338.1916			2	65045.47		
591.3549			1	107743.66		
608.3813			1	771549.69		
609.3848			1	213898		
613.3364			1	67294.88		
648.3758			1	90759.55		
692.4025	692.4157	19.09	1	386112.28	C41 H57 N O8	(M+H)+
693.4053	693.419	19.87	1	126394.56	C41 H57 N O8	(M+H)+
694.4081	694.4221	20.14	1	31594.13	C41 H57 N O8	(M+H)+
695.4115	695.4249	19.33	1	7292.68	C41 H57 N O8	(M+H)+

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	Abund
59.0485	519.61
87.0431	114.52
89.0585	260.16
107.0753	133.9
133.0849	201.74
136.0493	99.04
147.0408	123
324.6962	125.14
345.1286	104.14
692.3991	182.6

Compound Structure

Compound Label	m/z	RT	Algorithm
Cpd 42: 11.379	608.3816	11.379	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
338.1917	2	100973.37
346.7051	2	83274.23
608.3816	1	285262.84
609.3842	1	83148.64
610.3862	1	20255.86
611.3883	1	3591.85
648.3758	1	74076.61
692.4019	1	588572.69
693.4056	1	180170.7
697.3575	1	96803.69

MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	1150.35
89.0587		99.74
111.0418		167.18
111.0825		205.56
193.0074		115.52
206.0667		95
324.6885		97.77
373.1235		95.23
608.378	1	214.98
648.4014		92.52

Compound Label	m/z	RT	Algorithm
Cpd 43: 11.532	652.4071	11.532	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
318.1947	2	210300.53
326.7079	2	148477.94
338.1917	2	117140.48
635.3809	1	128945.75
652.4071	1	909531.25
653.4107	1	276553.47
654.413	1	67409.63
655.4159	1	11577.71
692.4018	1	640204.5
693.4056	1	195864.53

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0481		645.11
83.0483		75.57
89.0591	2	827.85
111.0427	1	190.88
133.084		122.8
179.1656		86.51
318.195		151.45
358.0679		76.62
652.4044	1	261.58
693.3971		76.9

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 44: Chivosazole F	**Chivosazole F**	692.4025	11.599	Auto MS/MS	691.395

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

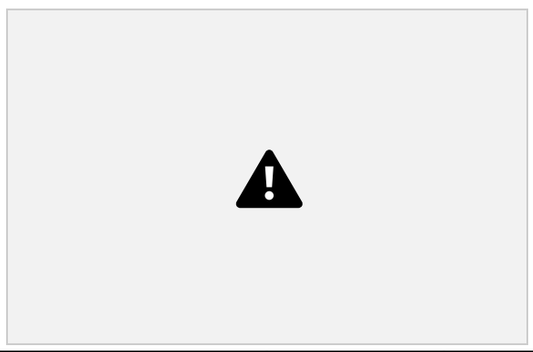
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
318.1947			2	301318.5		
326.7079			2	220335.78		
635.381			1	159308.13		
652.4075			1	1222270.75		
653.411			1	364698.81		
657.3625			1	126331		
692.4025	692.4157	19.05	1	262718.44	C41 H57 N O8	(M+H)+
693.4054	693.419	19.72	1	85621.86	C41 H57 N O8	(M+H)+
694.4077	694.4221	20.67	1	22710.62	C41 H57 N O8	(M+H)+
695.4094	695.4249	22.3	1	4017.71	C41 H57 N O8	(M+H)+

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0487	1	590.49
111.0443	1	100.4
133.0854		83.7
136.0497		123.16
318.2001		77.12
343.3112		91.88
652.4098	1	272.49
654.4049	1	75.3
657.3602	2	71.83
692.3989	1	83.41

Compound Structure



Compound Label	m/z	RT	Algorithm
Cpd 45: 11.767	652.4076	11.767	Auto MS/MS

MS Spectrum

Qualitative Compound Report

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
318.1947	2	133728.83
318.696	2	44812.56
326.708	2	105092.92
635.3809	1	58492.02
652.4076	1	428214.47
653.4103	1	136016.34
654.4127	1	34859.97
655.4162	1	5655.79
657.3626	1	44041.31
692.4019	1	88476.74

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	1394.81
60.0506	1	165.42
89.0596		350.32
111.0417	1	342.98
125.058		198.07
128.0604		223.73
132.0499		218
233.15		218.44
298.2506		176.92
652.408		183.13

Compound Label	m/z	RT	Algorithm
Cpd 46: 11.822	736.4281	11.822	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
318.1944	2	117359.75
326.7078	2	88092.93
360.205	2	130748.3
368.7183	2	145688.03
652.4075	1	437114.47
653.4106	1	125698.03
736.4281	1	455703.81
737.4317	1	158500.94
738.4343	1	40280.45
739.4367	1	10184.94

MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0485	1	1969.01
89.0001		107.11
89.0595		172.56
90.0613		114.03
99.0778		115.24
111.042	1	249.54
113.9659		128.9
136.0499		138.67
136.0988		126.19
167.0827		123.85

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 47: Mycinamicin IV	**Mycinamicin IV**	696.4336	12.069	Auto MS/MS	695.4263

MS Spectrum

Qualitative Compound Report

MS Zoomed Spectrum

MS Spectrum Peak List

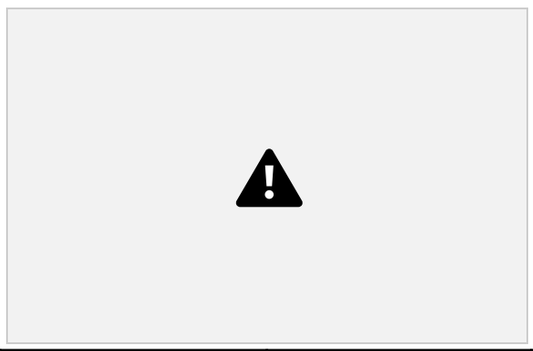
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
340.2079			2	308377.59		
340.7093			2	115225.48		
348.721			2	326050.63		
349.2223			2	112150.08		
357.234			2	145225.59		
696.4336	696.4317	-2.66	1	765394.25	C37 H61 N O11	(M+H)+
697.437	697.4351	-2.76	1	242970.34	C37 H61 N O11	(M+H)+
698.439	698.4379	-1.59	1	64655.16	C37 H61 N O11	(M+H)+
699.4425	699.4407	-2.62	1	11795.18	C37 H61 N O11	(M+H)+
736.4286			1	259250.66		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	1170.85
60.051	1	120.28
89.0608		315.39
100.0898		116.06
111.0423	1	221.39
117.0892		160.05
133.0841		115.5
340.2113	2	143.79
696.4295	1	284.91
736.4305	1	181.65

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 48: Lycoperoside D	**Lycoperoside D**	740.4598	12.48	Auto MS/MS	739.4525

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(	Abund	Ion	z Formula

Qualitative Compound Report

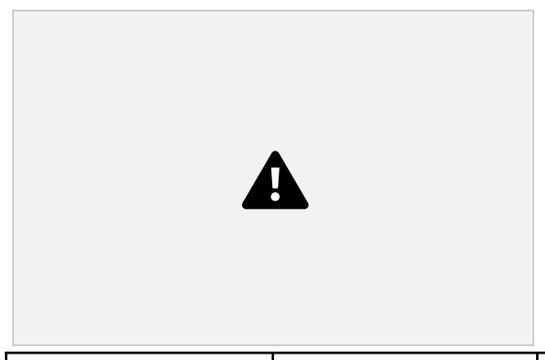
362.221			2	206349.8		
370.7338			2	301408.72		
382.2184			2	152747.17		
390.7313			2	208321.39		
740.4598	740.458	-2.52	1	413917.03	C39 H65 N O12	(M+H)+
741.4632	741.4613	-2.54	1	149452.41	C39 H65 N O12	(M+H)+
742.4655	742.4642	-1.81	1	39817.66	C39 H65 N O12	(M+H)+
743.4674	743.4669	-0.64	1	7502.19	C39 H65 N O12	(M+H)+
780.4546			1	372356.97		
781.4576			1	137731.13		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	625.77
87.0431		225.01
89.0592		421.13
111.0419		157.12
133.0865		139.47
199.126		124.03
362.2226	2	166.97
362.7223	2	138.64
399.2436		118.64
740.4523	1	112.2

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 49: PE(P 16:0/18:4(6Z,9Z,12Z,15Z))	**PE(P 16:0/18:4(6Z,9Z,12Z,1 5Z))**	370.7338	12.487	Auto MS/MS	695.4891

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
362.221			2	206349.8		
370.7338	370.7337	-0.1	2	301408.72	C39 H70 N O7 P	(M+2Na)+2
371.2357	371.2354	-0.71	2	104068.22	C39 H70 N O7 P	(M+2Na)+2
371.7369	371.7369	0.14	2	26025.26	C39 H70 N O7 P	(M+2Na)+2
372.2371	372.2384	3.45	2	6218	C39 H70 N O7 P	(M+2Na)+2
382.2184			2	152747.17		
390.7313			2	208321.39		
740.4598			1	413917.03		
741.4632			1	149452.41		
780.4546			1	372356.97		

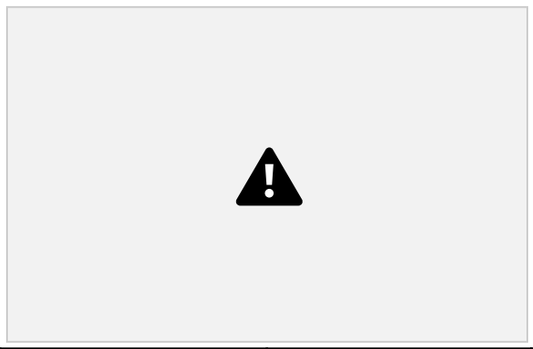
MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.048	1	1465.41
69.0333		324.93
73.0274		524.85
83.0491		243.25
87.0435	1	506.19
89.0593	1	1939.05
90.0619	1	410.78
111.0425		355.63
133.0849	1	631.73
177.1119		350.78

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 50: Ophiopogonin B	**Ophiopogonin B**	362.2205	12.581	Auto MS/MS	722.4265

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
362.2205	362.2193	-3.27	2	189941.64	C39 H62 O12	(M+2H)+2
362.7222	362.721	-3.28	2	71135.78	C39 H62 O12	(M+2H)+2
363.2236	363.2225	-3.12	2	18077.21	C39 H62 O12	(M+2H)+2
363.7244	363.7239	-1.41	2	3671.51	C39 H62 O12	(M+2H)+2
370.734			2	255259.86		
379.2468			2	132103.86		
390.7311			2	105239.03		
740.46			1	318676.03		
741.4628			1	126494.77		
780.4545			1	170607.2		

MSMS Spectrum

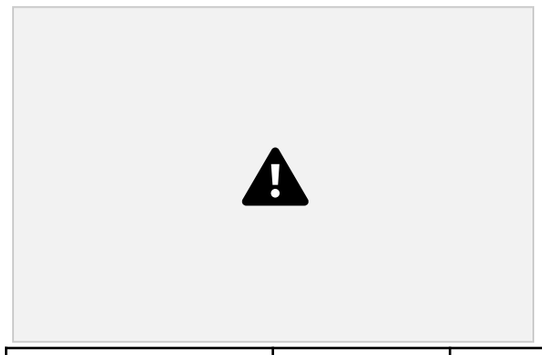
MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	1675.05
89.0586		334.41
99.0783		115.03
111.0438	1	149.91
112.0823		125.37
133.0842		211
136.05		165.51
370.7265	2	199.92

Qualitative Compound Report

379.2649	1	103.78
740.4627	1	235.72

Compound Structure



Compound Label	m/z	RT	Algorithm
Cpd 51: 12.586	379.2468	12.586	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
362.2205	2	189941.64
370.734	2	255259.86
379.2468	2	132103.86
379.7485	2	45363.92
380.2498	2	13259.26
380.7507	2	2859.2
390.7311	2	105239.03
740.46	1	318676.03
741.4628	1	126494.77
780.4545	1	170607.2

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.048	1	1898.4
73.0289		110.7
83.0486		100.4
87.0429		98.27
89.0599		1005.29
115.0751		84.34
133.0849	1	556.57
362.2254		128.12
362.2527		88.5
370.7384		84.12

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 52: PE(20:3(8Z,11Z,14Z)/18:4 (6Z,9Z,12Z,15Z))	**PE(20:3(8Z,11Z,14Z)/ 18:4(6Z,9Z,12Z,15Z))**	784.4857	12.912	Auto MS/MS	761.4963

Qualitative Compound Report

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
384.2334			2	152054.91		
392.7469			2	243534.13		
401.26			2	160033.66		
412.7442			2	193568.19		
421.2572			2	145267.58		
784.4857	784.4888	3.95	1	246821.83	C43 H72 N O8 P	(M+Na)+
785.4889	785.4921	4.08	1	92787.88	C43 H72 N O8 P	(M+Na)+
786.4911	786.4952	5.25	1	24015.66	C43 H72 N O8 P	(M+Na)+
787.4933	787.4981	6.09	1	5838.46	C43 H72 N O8 P	(M+Na)+
824.4805			1	207005.47		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0487		260.21
87.043		99.11
111.0448		121.51
111.0791		129.78
167.0312		85.01
221.1344		98.89
401.7629	2	117.84
402.2597	2	87.03
784.4847	1	180.72
825.532		105.14

Compound Structure

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 53: Pitheduloside A	**Pitheduloside A**	384.2333	13.014	Auto MS/MS	766.4522

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
384.2333	384.2324	-2.24	2	148990.47	C41 H66 O13	(M+2H)+2
384.7354	384.7342	-3.13	2	60367.7	C41 H66 O13	(M+2H)+2
385.2362	385.2356	-1.7	2	17612.24	C41 H66 O13	(M+2H)+2
385.739	385.737	-5.18	2	3614.21	C41 H66 O13	(M+2H)+2
392.747			2	228962.84		
401.2599			2	146453.19		
434.7571			2	156799.22		
443.2702			2	143786.28		

784.4856			1	239635.09		
868.506			1	127862.01		

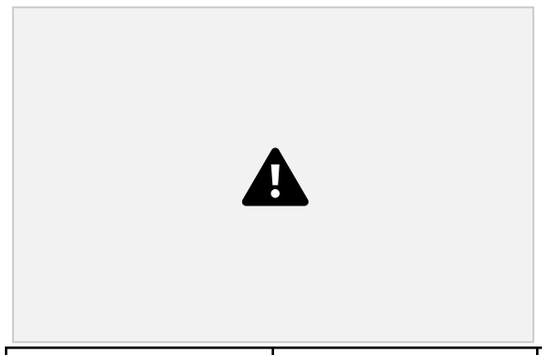
MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0485	1	1051.44
89.0595		442.32
99.0814		95.02
111.0427		222.75
111.0794		165.2
125.0658		119.32
133.0866		106.3
253.1816		102.52
404.7313		110.4
784.4699	1	110.41

Qualitative Compound Report

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 54: Spiramycin 2	**Spiramycin 2**	443.2704	13.13	Auto MS/MS	884.526

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
392.7469			2	164253.52		
401.2599			2	107678.76		
434.7575			2	188244.73		
443.2704	443.2696	-1.88	2	183421.03	C45 H76 N2 O15	(M+2H)+2
443.772	443.7712	-1.64	2	81878.21	C45 H76 N2 O15	(M+2H)+2
444.2728	444.2727	-0.24	2	25966.45	C45 H76 N2 O15	(M+2H)+2
444.7743	444.774	-0.63	2	5958.75	C45 H76 N2 O15	(M+2H)+2
445.2773	445.2754	-4.26	2	2204.43	C45 H76 N2 O15	(M+2H)+2
784.4856			1	150430.67		
868.5066			1	161769.66		

MSMS Spectrum

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484		1479.18
69.0335		653.08
85.0639		155.67
87.0435		753.97

Qualitative Compound Report

89.0598		1452.27
113.0588		185.33
133.0842	1	232
137.0562		155.78
287.1366		166.06
518.3211		169.01
59.0484	1	1646.8
83.0483		222.33
87.0436		492.94
89.059		805.55
111.0432		213.34
133.0846	1	919.67
134.0876	1	219.69
177.113		311.5
437.2326		253.63
443.2779	2	485.42

Compound Structure

Compound Label	m/z	RT	Algorithm
Cpd 55: 13.197	445.7475	13.197	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
426.2439	2	166179.3
434.7575	2	361167.63
435.2587	2	162887.52
443.2705	2	344896.13
443.7721	2	153617.08
445.7475	2	63278.8
446.2495	2	31174.19
446.7511	2	9205.26
447.2503	2	2459.15
868.5066	1	310914.28

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0487		2258.99
69.0336		427.31
87.0434		1685.88
89.0593	1	4246.3
99.043		1274.06
111.042		467.73
129.0587		299.7
133.0849	1	1382.34
347.163		290.45
653.3402		272.4

Qualitative Compound Report

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 56: beta-Solamarine	**beta-Solamarine**	434.7574	13.213	Auto MS/MS	867.4998

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
392.7469			2	114614.55		
414.7598			2	124222.63		
423.2731			2	103502.74		
434.7574	434.7563	-2.55	2	153940.86	C45 H73 N O15	(M+2H)+2
435.2586	435.258	-1.37	2	70427.71	C45 H73 N O15	(M+2H)+2
435.76	435.7594	-1.44	2	23330.56	C45 H73 N O15	(M+2H)+2
436.2604	436.2608	0.8	2	5760.85	C45 H73 N O15	(M+2H)+2
443.2703			2	150646.92		
784.4856			1	104955.71		
868.5063			1	131629.2		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	1004.83
69.0339		418.04
83.0482		168.9
87.0432	1	459.76
89.0597	1	1748.64
99.0434	1	295.86
111.0436		609.23
111.0547		137.83
133.0854	1	752.22
137.0578		227.26

Compound Structure

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 57: Mycobactin S	**Mycobactin S**	414.7596	13.344	Auto MS/MS	827.5045

MS Spectrum

Qualitative Compound Report

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
406.2463			2	132331.25		
414.7596	414.7595	-0.34	2	251042.75	C44 H69 N5 O10	(M+2H)+2
415.2609	415.2611	0.35	2	120044.72	C44 H69 N5 O10	(M+2H)+2
415.7624	415.7625	0.41	2	33799.75	C44 H69 N5 O10	(M+2H)+2

416.2634	416.2639	1.27	2	8107.41	C44 H69 N5 O10	(M+2H)+2
423.273			2	214932.27		
423.7743			2	93624.81		
434.7569			2	104837.52		
443.2702			2	101443.13		
828.5114			1	173585.97		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484		1762.18
89.0595		404.55
99.0803		216.25
111.0435		324.14
133.0843		393.62
136.0474		139.15
414.7564	2	228.08
415.2639	2	217.62
423.2719	2	236.24
443.2711		128.16

Compound Structure

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 58: Halstoctacosanolide A	**Halstoctacosanolide A**	423.273	13.345	Auto MS/MS	844.5311

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

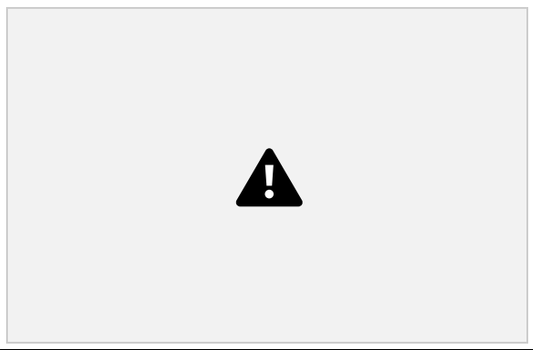
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
406.2463			2	132331.25		
414.7596			2	251042.75		
415.2609			2	120044.72		
423.273	423.2741	2.7	2	214932.27	C48 H76 O12	(M+2H)+2
423.7743	423.7758	3.48	2	93624.81	C48 H76 O12	(M+2H)+2
424.2756	424.2773	4.11	2	27770.36	C48 H76 O12	(M+2H)+2
424.7758	424.7788	6.93	2	6593.19	C48 H76 O12	(M+2H)+2
434.7569			2	104837.52		
443.2702			2	101443.13		
828.5114			1	173585.97		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0487	1	1231.57
60.0522	1	137.36
73.0278	1	132.31
89.0592	1	1409.18
111.0427		154.97
117.0899		132.6
133.085	1	1025.43
177.1124		182.44
414.7599	2	140.03
435.2503		132.1

Compound Structure



Compound Label	m/z	RT	Algorithm
Cpd 59: 13.489	465.2829	13.489	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
414.7595	2	138265.2

423.2728	2	122745.91

Qualitative Compound Report

456.7699	2	159272.97
465.2829	2	184518.19
465.7844	2	96525.71
466.2862	2	31152.19
466.7868	2	7507.46
467.2876	2	2356.1
828.5112	1	92995.03
912.5314	1	96814.23

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0481	1	2147.34
60.0501	1	192.01
69.0323		207.59
87.0438		555.44
89.0593	1	1111.2
90.0626	1	153.95
99.0433		249.34
111.0445	1	510.19
133.0845	1	1123.42
465.2899	1	205.81

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 60: PI(20:3(5Z,8Z,11Z)/18:0)	**PI(20:3(5Z,8Z,11Z)/18 :0)**	445.2859	13.694	Auto MS/MS	888.5569

Qualitative Compound Report

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

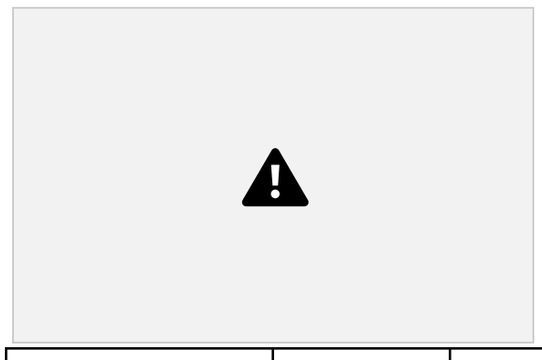
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
436.7726			2	167036.47		
437.274			2	77492.38		
445.2859	445.2937	17.44	2	171895.88	C47 H85 O13 P	(M+2H)+2
445.787	445.7954	18.7	2	70402.84	C47 H85 O13 P	(M+2H)+2
446.2889	446.2969	17.96	2	24163.53	C47 H85 O13 P	(M+2H)+2
446.7901	446.7983	18.33	2		8 C47 H85 O13 P	(M+2H)+2
456.77			2	105215.34		
465.2829			2	121166.17		
562.3401			2	102129.46		
872.537			1	84402.97		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	2638.08
84.9588		232.75
89.0592		1408.53
99.0787		224.86
111.0424	1	342.73
111.0812		178.13
133.0858		469.97
437.273	2	191.27
448.7626		164.21
565.3176	2	145.08

Compound Structure



Compound Label	m/z	RT	Algorithm
Cpd 61: 13.908	487.2961	13.908	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

m/z	z	Abund
436.7726	2	82075.69
445.2859	2	83851.73
467.2988	2	75240.87
478.7829	2	92812.84
487.2961	2	148946.98
487.7976	2	72071.77
488.2995	2	23784.85
488.8005	2	6369.5
489.3041	2	1611.12
584.3533	2	121205.69

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0493	1	1358.22
69.0326		133.62
87.0431	1	353.6
89.0592	1	1331.22
90.0614	1	124.32
99.0417		109.87
111.0426		217.5
133.086	1	681.17
177.1128		93.02
371.2332		135.74

Compound Label	m/z	RT	Algorithm
Cpd 62: 14.232	509.3095	14.232	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
500.7962	2	119940.56
509.3095	2	227236.97
509.8109	2	109026.74
510.3124	2	37501.58
510.8151	2	9426.5
511.3157	2	3535.86
597.8532	2	122542.39
606.3667	2	290346.13
606.8683	2	169214.63
608.8442	2	91509.38

MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	1908.55
87.0434		229.04
89.0593		429.05
99.0467		165.24
111.0429		839.51
111.0786		339.06
133.0836		290.61
509.3076	2	196.02
510.3424		176.45
611.8385		172.09

Compound Label	m/z	RT	Algorithm
Cpd 63: 14.236	606.3667	14.236	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
500.7958	2	92156.96
509.3092	2	170427.03
509.8107	2	82192.38
597.8531	2	107138.3
606.3667	2	257572.31
606.8678	2	146762.19
607.3694	2	60985.5
607.8701	2	19785.45
608.3743	2	5449.27
628.379	2	80534.16

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	2	1430.54
89.0584		180.29
99.0798		184.53
111.043		306.6
133.0856		305.31
186.2224		132.06
500.7981	1	134.86
597.8543		171.61
606.3674	2	180.72
606.867	2	174.1

Compound Label	m/z	RT	Algorithm
Cpd 64: 14.242	608.8442	14.242	Auto MS/MS

Qualitative Compound Report

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
500.7962	2	119940.56
509.3095	2	227236.97
597.8532	2	122542.39
606.3667	2	290346.13
606.8683	2	169214.63
608.8442	2	91509.38
609.3457	2	55249.22
609.8458	2	27309.65
610.348	2	8994.67
610.8491	2	2445.09

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0481	1	1909.42
87.0434		390.48
89.0584	1	2025.53

111.0447		221
133.0851	1	1363.42
134.0862	1	258.79
135.0938		233.02
414.2672		238.86
507.2817		239.07
608.3095	1	246.24

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 65: Ganglioside GM3 (d18:0/20:0)	**Ganglioside GM3 (d18:0/20:0)**	628.3795	14.381	Auto MS/MS	1210.7803

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

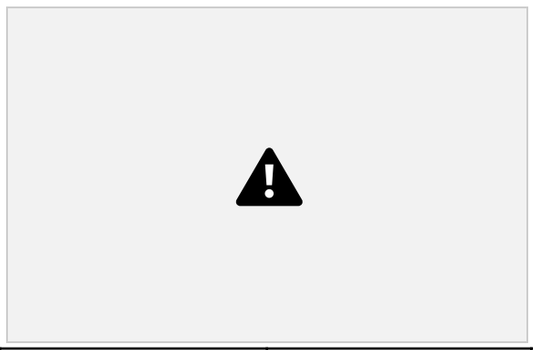
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
489.3118			2	83839.73		
606.3665			2	166471.17		
606.8678			2	94421.2		
619.8657			2	86855.68		
628.3795	628.3849	8.58	2	225963.47	C61 H114 N2 O21	(M+2Na)+2
628.8811	628.8866	8.76	2	139881.61	C61 H114 N2 O21	(M+2Na)+2
629.3822	629.3881	9.29	2	58685.03	C61 H114 N2 O21	(M+2Na)+2
629.8831	629.8895	10.15	2	17631.3	C61 H114 N2 O21	(M+2Na)+2
630.3846	630.3909	9.96	2	4864.77	C61 H114 N2 O21	(M+2Na)+2
650.3919			2	98526.25		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	Abund
59.0486	1181.58
71.0117	286.21
73.0277	110.99
87.0417	148.55
89.0591	431.7
111.0431	225.52
111.0781	166.51
133.0941	112.41
609.3424	113.72
650.886	112.47

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 66: T-kinin	**T-kinin**	630.8567	14.479	Auto MS/MS	1259.6992

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
531.3217			2	101432.64		
619.8657			2	145675.09		

Qualitative Compound Report

628.3798			2	371694.38		
628.8813			2	229807.31		
630.8567	630.846	-16.96	2	103121.11	C59 H89 N17 O14	(M+2H)+2
631.3586	631.3474	-17.59	2	72178.09	C59 H89 N17 O14	(M+2H)+2
631.8601	631.8488	-17.84	2	32178.91	C59 H89 N17 O14	(M+2H)+2
632.3595	632.3501	-14.88	2	10458.92	C59 H89 N17 O14	(M+2H)+2
632.8598	632.8514	-13.34	2	2962.84	C59 H89 N17 O14	(M+2H)+2
650.3918			2	102109.73		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.048		1668.35
69.0331		368.28
87.0433		980.06
89.0592	1	4718.72
90.0626	1	491.58
99.0437		386.71
111.0423		742
133.0852	1	3014.12
134.0879	1	398.52
630.3273	2	443.52

Compound Structure

Compound Label	m/z	RT	Algorithm
Cpd 67: 14.646	652.8706	14.646	Auto MS/MS

Qualitative Compound Report

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
628.3797	2	189260.81
641.8793	2	129480.43
650.393	2	296591.22
650.8944	2	188644.02
652.8706	2	85366.41
653.3718	2	59548.82
653.8723	2	24975.9
654.3738	2	6816.67
654.8714	2	2618.1
672.4058	2	139645.48

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	2	2392.49
87.0441		1277.01
89.0594	1	4774.72
95.0475		392.37
99.0433		690.94
111.0443		808.67
133.0851		2274.55
137.0593		477.17
155.0695	1	488.59
239.1466		312.41

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 68: Tetrahexosylceramide (d18:1/18:0)	**Tetrahexosylceramide (d18:1/18:0)**	650.3923	14.797	Auto MS/MS	1254.8061

MS Spectrum

MS Zoomed Spectrum

Qualitative Compound Report

MS Spectrum Peak List

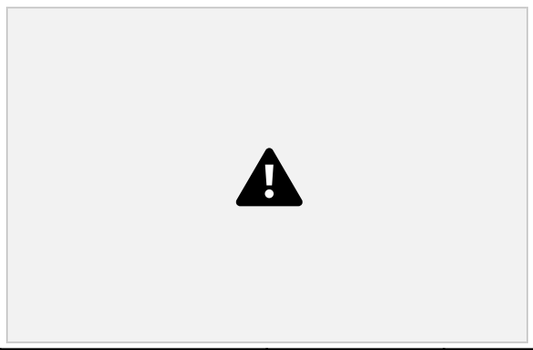
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
641.8789			2	152289.27		
642.3807			2	98018.14		
650.3923	650.3798	-19.22	2	398464.56	C62 H114 N2 O23	(M+2Na)+2
650.894	650.8815	-19.1	2	245749.16	C62 H114 N2 O23	(M+2Na)+2
651.3953	651.383	-18.91	2	103789	C62 H114 N2 O23	(M+2Na)+2
651.8959	651.8844	-17.66	2	34167.18	C62 H114 N2 O23	(M+2Na)+2
652.398	652.3858	-18.77	2	8888.43	C62 H114 N2 O23	(M+2Na)+2
672.4054			2	222033.25		
672.9066			2	151984.23		
694.4177			2	122277.77		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	1273.4
87.0432		211.73
89.059		154.29
111.045		285.92
133.0858		182.01
271.0923		104.13
439.6002		94.23
512.8284		91.98
650.3988	2	178.49
672.9066	2	183.03

Compound Structure



Compound Label	m/z	RT	Algorithm
Cpd 69: 15.008	674.8829	15.008	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
663.8918	2	153041.81
672.4055	2	389791.75
672.907	2	267765.09
674.8829	2	98250.22
675.3843	2	66243.11
675.8856	2	29848.07
676.3866	2	10299.36
676.8877	2	3074.14
694.4183	2	180838.63
694.9197	2	123910.36

MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	z	Abund
59.0485	1	3433.88
73.0273		206.62
87.044		1069.09
89.0593	1	4843.08
99.0428		260.99
111.043		760.54
113.0578		349.02
133.086	1	1767.32
137.0563		380.08
177.1101		529.75

Compound Label	m/z	RT	Algorithm
Cpd 70: 15.091	696.8955	15.091	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
672.4055	2	312487.09
672.9071	2	207290.05
694.4182	2	234084.19
694.9197	2	159109.97
696.8955	2	52878.49
697.3968	2	41278.21
697.8987	2	18185.68
698.3982	2	9200.05
698.8971	2	2242.91
716.4314	2	154774.67

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483		3052.04
87.0433	1	2780.06
88.0471	1	544.63
89.0596	1	10113.03
99.0432		441.37
111.0423		1259.21
113.0582		696.48
129.0514		394.41
133.0853	1	4488.36
137.0573		474.43

Compound Label	m/z	RT	Algorithm
Cpd 71: 15.123	694.4185	15.123	Auto MS/MS

Qualitative Compound Report

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
663.8916	2	104621.2
672.4053	2	273826.78
672.907	2	191191.3
685.9048	2	99241.1
694.4185	2	274980.44
694.9199	2	189671.41
695.4211	2	91015.08
695.9224	2	28514.75
696.4239	2	8484.31
716.4308	2	111141.05

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0485		920.58
73.0273		195.04
89.0593		250.05

137.0582		98.77
283.1721		75.94
415.2435		80.77
525.7784		81.86
694.4117	2	117.2
694.9234	2	147.2
893.8209		72.9

Compound Label	m/z	RT	Algorithm
Cpd 72: 15.421	718.9091	15.421	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

Qualitative Compound Report

m/z	z	Abund
694.4188	2	132402.11
707.9177	2	135852.55
716.4317	2	408831.94
716.9331	2	288615.91
717.4342	2	140123.69
718.9091	2	96445.38
719.4104	2	71330.41
719.9113	2	31682.73
720.4118	2	11652.63
720.9157	2	3644.05

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0487	1	4110.82
69.0331		412.12
87.0438		1667.81
89.0593	1	5008.94
90.0622	1	738.4
111.0428		639.33
113.0581	1	780.43
133.0851	1	4090.12

155.0712	1	456.43
177.109	1	906.92

Compound Label	m/z	RT	Algorithm
Cpd 73: 15.614	740.9221	15.614	Auto MS/MS

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund
486.9564	1	153725.72
492.6319	1	142319.91
716.431	2	141724.78
738.4439	2	314865.41
738.9459	2	245648.41
740.9221	2	80837.7
741.4231	2	62726
741.9235	2	32062.89
742.425	2	11479.7
742.9252	2	3145.69

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	3211.41
69.0338		298.81
73.0283		324.3

Qualitative Compound Report

79.0544		250.62
87.0435	1	1907.2
88.047	1	421.03
89.0595	1	8709.5
111.0421		472.24
133.0852	1	3007.3
177.1104		873.46

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 74: Dihydrodeoxystreptomycin	**Dihydrodeoxystreptom ycin**	568.2927	19.194	Auto MS/MS	567.2855

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(	Formula	Ion
136.0499	1	9855.81		

Qualitative Compound Report

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
242.2825			1	19859.02		

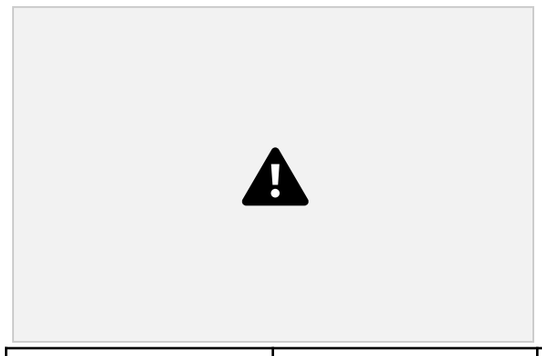
259.0952			1	5883.27		
551.2656			1	12991.54		
568.2927	568.2937	1.78	1	381722.88	C21 H41 N7 O11	(M+H)+
569.2958	569.2965	1.24	1	99101.51	C21 H41 N7 O11	(M+H)+
570.2984	570.2987	0.61	1	19943.47	C21 H41 N7 O11	(M+H)+
573.2482			1	175774.66		
574.2509			1	48610.84		
575.2531			1	13018.74		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	3077.88
71.0121		186.07
99.0437	1	1064.77
99.0793		244.5
111.0432		805.03
111.0522		150.01
111.0767		218.1
118.0844		159.71
125.0574		199.59
568.2908		187.24

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 75: Manumycin A	**Manumycin A**	573.248	19.226	Auto MS/MS	550.2587

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
136.0502			1	11079.74		
242.2823			1	18763.33		
259.0951			1	6400.51		

551.2654			1	11781.32		
568.2925			1	349569.44		
569.2958			1	97883.94		
570.2978			1	22051.62		
573.248	573.2571	15.91	1	164983.11	C31 H38 N2 O7	(M+Na)+
574.2511	574.2604	16.15	1	44806.41	C31 H38 N2 O7	(M+Na)+
575.2536	575.2632	16.71	1	10794.34	C31 H38 N2 O7	(M+Na)+

MSMS Spectrum

Qualitative Compound Report

MS/MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
59.0485			2	1921.1		
60.0526			2	149.03		
99.0803				124.22		
111.0427				480.49		
111.0786				166.07		
118.0855				113.38		
132.9715				149.78		
343.1309			2	267.17		
568.2897			1	368.03		
573.2481	573.2571	15.78	1	1095.41	C31 H38 N2 O7	(M+Na)+

Compound Structure

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 76: Decursinol	**Decursinol**	269.0792	19.921	Auto MS/MS	246.09

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
120.0546				4560.73		
136.05			1	13100.59		
242.2822			1	11836.78		
249.1214			1	4807.38		
269.0792	269.0784	-3.03	1		8 C14 H14 O4	(M+Na)+
270.0823	270.0818	-1.86	1	22364.77	C14 H14 O4	(M+Na)+
271.0855	271.0841	-4.99	1	2609.47	C14 H14 O4	(M+Na)+
568.2924			1	24240.08		
569.2953			1	7429.88		
573.2477			1	9830.96		

MSMS Spectrum

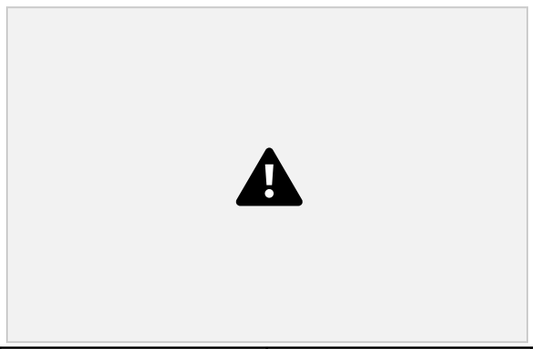
MS/MS Spectrum Peak List

m/z	z	Abund
59.0487	1	3091.65
60.0525	1	175.2

Qualitative Compound Report

99.0803	1	300.82
111.0425		551.95
136.05		218.87
213.089		353.1
226.0599	1	176.57
237.0508		382.46
254.0551		475.46
269.0796	1	2527.33

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 77: Schleicherastatin 6	**Schleicherastatin 6**	453.3331	23.298	Auto MS/MS	430.3439

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
136.0499			1	12039.29		
298.2719			1	19816.46		
412.3182			1	9749.48		
453.3331	453.3339	1.78	1	92201.08	C28 H46 O3	(M+Na)+
454.3367	454.3373	1.29	1	31979.87	C28 H46 O3	(M+Na)+
455.3394	455.3404	2.28	1		6 C28 H46 O3	(M+Na)+
647.3748			1	20643.09		
823.4061			1	27585.36		
824.4094			1	12203.64		
845.3876			1	19420.72		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0484	1	2429.79
60.0429	1	202.34
60.0513		148.46
99.0801		240.09
111.0443		343.05
111.0781		143.66
189.1621		152.88
295.2276		165.98
453.3343	1	501.57
454.3381	1	157.09

Compound Structure

Qualitative Compound Report

Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 78: C16 Sphinganine	**C16 Sphinganine**	274.2723	24.095	Auto MS/MS	273.265

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
120.0548				3608.65		
136.0498			1	10794.9		
209.1524			1	5944.43		
219.0935			1	19708.93		
242.2817			1	5322.52		
274.2723	274.2741	6.23	1	87079.25	C16 H35 N O2	(M+H)+
275.275	275.2774	8.41	1	13778.49	C16 H35 N O2	(M+H)+
276.2773	276.2802	10.19	1	1537.27	C16 H35 N O2	(M+H)+
298.2713				3584.79		
312.2514			1	4057.49		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0483	1	3651.35
60.0518	1	288.2
99.0798		336.34
111.0428		874.29
111.0792		308.58
118.085		170.68
136.0497		134.4
256.2618		384.48
274.2721	1	2626
275.2755	1	177.77

Compound Structure

Compound Label	Name	m/z	RT	Algorithm	Mass

Qualitative Compound Report

Cpd 79: Teasterone	**Teasterone**	471.3437	33.654	Auto MS/MS	448.3544

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
269.2453			1	16853.44		
284.3293			1	77805.82		
285.3326			1	15692.14		
315.251			1	9872.24		
332.3282			1	16181.68		
444.3286			1	10921.79		
471.3437	471.3445	1.72	1	113008.23	C28 H48 O4	(M+Na)+

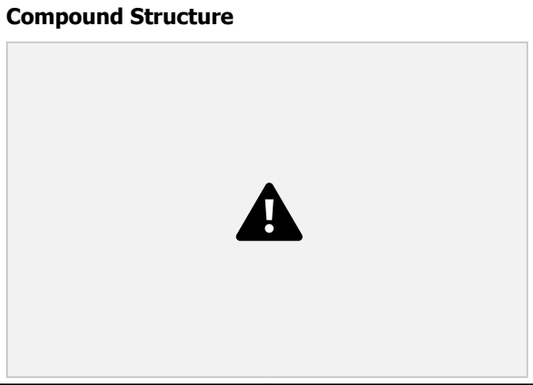
472.3467	472.3479	2.5	1	34792.79	C28 H48 O4	(M+Na)+
473.3501	473.3509	1.64	1	7078.34	C28 H48 O4	(M+Na)+
488.3547			1	10762.89		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
59.0485			1	1729.78		
95.0849				220.95		
149.0945				230.87		
161.1299				172.22		
189.1613				313.71		
207.1728				212.74		
217.1591				280.42		
284.3287			1	477.15		
317.2076			1	309.82		
471.3436	471.3445	1.94	1	570.58	C28 H48 O4	(M+Na)+

Compound Structure



Compound Label	Name	m/z	RT	Algorithm	Mass
Cpd 80: N Hexadecanoylpyrrolidine	**N Hexadecanoylpyrrolidi**	310.3082	41.17	Auto MS/MS	309.3009

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MS Spectrum

Qualitative Compound Report

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
124.0861				8914.42		
242.2819			1	9234.26		
284.2928			1	7861.01		
310.3082	310.3104	7.36	1	142502.66	C20 H39 N O	(M+H)+
311.3115	311.3138	7.31	1		1 C20 H39 N O	(M+H)+
312.3159	312.3169	3.22	1	4038.94	C20 H39 N O	(M+H)+
338.3391			1	59523.42		
339.3422			1	16157.8		
512.4997			1	17319.49		
513.5025			1	6824.66		

MSMS Spectrum

MS/MS Spectrum Peak List

m/z	z	Abund
59.0481	1	2085.58
60.0433	1	226.72
69.069		180.08
111.0411	1	185.69
124.0854		234.08
256.2604		143.05
283.2631		186.76

310.3076 2459.63

Qualitative Compound Report

m/z	z	Abund
311.3084	2	313.88
338.3379	1	163.76

Compound Structure

--- End Of Report ---