

Marine Sediment-derived *Streptomyces* strain Produces Angucycline Antibiotics against Multidrug Resistant *Staphylococcus aureus* harboring *SCCmec* type 1 gene

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Supplementary Files

Supplemental Table S1. Primers for Multilocus Sequence Analysis [50].

Gene		Primer Sequence (5' to 3')	Amplicon Size
<i>atpD</i>	<i>atpDF</i>	GTCGGCGACTTCACCAAGGGCAAGGTGTTCAACACC	998
	<i>atpDR</i>	GTGAACTGCTTGGCGACGTGGGTGTTCTGGGACAGGAA	
<i>recA</i>	<i>recAF</i>	CCGCRCTCGCACAGATTGAACGSCAATTC	913
	<i>recAR</i>	GCSAGGTCGGGGTTGTCCTTSAGGAAGTTGCG	
<i>rpoB</i>	<i>rpoBF</i>	GAGCGCATGACCACCCAGGACGTCGAGGC	994
	<i>rpoBR</i>	CCTCGTAGTTGTGACCCTCCCACGGCATGA	
<i>trpB</i>	<i>trpBF</i>	GCGCGAGGACCTGAACCACACCGGCTCACACAAGATCAACA	822
	<i>trpBR</i>	TCGATGGCCGGGATGATGCCCTCGGTGCGCGACAGCAGGC	

Supplemental Table S2. Degenerate Primers for PCR Screening of Polyketide Synthase and Non-Ribosomal Synthase

Target Gene for Amplification	Length (bp)	Primer Name	Primer Sequence (5' to 3')	Reference
PKS-I β -ketoacyl synthase (KS) domains fragments	670	KS-F	CCS CAG SAG CGC STS YTS CTS GA	51
		KS-R	GTS CCS GTS CCG TGS GYS TCS A	
PKS-I KS Domain Fragments	700	KSMAF KSMBR	TSG CSA TGG ACC CSC AGC AG CCS GTS CCG TGS GCC TCS AC	52
PKS-II KS α and KS β domain fragments	800-900	KS α	TSG RCT ACR TCA ACG GSC ACG G	53
		KS β	TAC SAG TCS WTC GCC TGG TTC	
PKS-II KS α domain fragments	613	KS1-F	TSG CST GCT TGG AYG CSA TC	54
		KS1-R	TGG AAN CCG CCG AAB CCT CT	
PKS-II at 5' portion of KS α genes	554	540F 1100R	GGI TGC ACS TCI GGI MTS GAC CCG ATS GCI CCS AGI GAG TG	55
NRPS Adenylation domain (AD) fragments	700	A3F	GCS TAC SYS ATS TAC ACS TCS GG	56
		A7R	SAS GTC VCC SGT SCG GTA S	

Supplemental Table S3. Growth Characteristics of *Streptomyces* sp. strain DSD011 in various NaCl concentration (% w/v) after 7 days of incubation.

Strain	Morphological Characteristics	0	3	5	7	10	12	15	20
DSD011	Diffusible Pigment	-	-	-	-	-	-	-	-
	Aerial Substratum	white	-	-	-	-	-	-	-
	Substrate Mycelium	brown	white	white	white	-	-	-	-

Nil= -.

Supplemental Table S4. Growth Characteristics of *Streptomyces* sp. strain DSD011 in various carbon source (% w/v) after 7 days of incubation.

Strain	Morphological Characteristics	Starch (1.0%)	Mannitol (0.05%)	Glucose (0.05%)	Trehalose (0.05%)	Raffinose (0.05%)
DSD011	Diffusible Pigment	-	-	-	Light brown	
	Aerial Substratum	grey	white	grey	white	-
	Substrate Mycelium	yellowish brown	white	light brown	light brown	white

Nil= -.

Supplemental Table S5. Antibacterial Activity of strain DSD011 crude fermented extract.

Test Pathogen	Zone of Inhibition (mm)	
	Strain DSD011 (5 mg/disk)	Tetracycline (0.50 mg/disk)
<i>Enterococcus faecium</i> ATCC 700221	9.0 ± 1.1	14
<i>Staphylococcus aureus</i> ATCC BAA-44	17.0 ± 0.5	19
<i>Klebsiella pneumoniae</i> ATCC BAA-1705	--	20
<i>Acinetobacter baumannii</i> ATCC BAA-1605	--	8
<i>Pseudomonas aeruginosa</i> ATCC BAA-1744	--	16
<i>Pseudomonas aeruginosa</i> ATCC 27853	--	15
<i>Enterobacter cloacae</i> ATCC BAA-2341	--	25
<i>Klebsiella aerogenes</i> ATCC 13048	--	14
<i>Escherichia coli</i> ATCC 25922	*17.0 ± 0.5	17
<i>Escherichia coli</i> ATCC BAA-2469	--	10
<i>Salmonella typhimurium</i> ATCC 25241	--	8

*growth was observed within the zone of inhibition; -- No antibacterial Activity

Supplemental Table S6. Latest Library Spectrum Information on GNPS match for fridamycin A, **1** (*m/z* 487 [M+H]⁺).

Spectrum ID	CCMSLIB00000846275
Compound Name	NCGC00380629-01!(3R)-4-[6-[(2R,4R,5S,6R)-4,5-dihydroxy-6-methyloxan-2-yl]-1,5-dihydroxy-9,10-dioxoanthracen-2-yl]-3-hydroxy-3-methylbutanoic acid
PI	Jadhav/Dorrestein
Data Collector	lfnothias
Pubmed	n/a
CAS Number	n/a
Original Submitter	mwang87
Original Submitter Email	miw023@ucsd.edu
Most Recent Revisor	mwang87
Most Recent Revisor Email	miw023@ucsd.edu
Library Quality	Gold Spectrum
Smiles	<chem>C[C@H]1O[C@H](C[C@@H](O)[C@@H]1O)C2=CC=C3C(=O)C4=C(C=CC(C[C@@](C)(O)CC(O)=O)=C4O)C(=O)C3=C2O</chem>
InChI	InChI=1S/C25H26O10/c1-10-20(29)15(26)7-16(35-10)12-5-6-14-19(22(12)31)24(33)13-4-3-11(21(30)18(13)23(14)32)8-25(2,34)9-17(27)28/h3-6,10,15-16,20,26,29-31,34H,7-9H2,1-2H3,(H,27,28)/t10-,15-,16-,20-,25-/m1/s1
Metabolomics Spectrum Resolver	mzspec:GNPSLIBRARY:CCMSLIB00000846275
Precursor M/Z	487.16
Exact Mass	486.153
Charge	1
Adduct	M+H
Ion Source	LC-ESI
Instrument	Maxis II HD Q-TOF Bruker
Ion Mode	positive
Library Membership	GNPS-NIH-NATURALPRODUCTSLIBRARY_ROUND2_POSITIVE
SPLASH Key	null-null-null-null

Supplemental Table S7. Waters UNIFI Scientific Information System Report for fridamycin A, **1** (m/z 487 [M+H]⁺).



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Created by: Administrator, UNIFI

Created on: Sep 15, 2020

Created time: 10:40:06 Malay Peninsula
Standard Time

Item name: Sample 7A

Item name: Sample 7A, Sample position: 1:E,6, Replicate number: 1

	Component name	Neutral mass (Da)	Observed neutral mass (Da)	Observed m/z	Observed RT (min)	Mass error (ppm)	Detector counts	Response	Adducts
1	Fridamycin A	486.15260	486.1527	487.1600	8.19	0.2	578134	430161	+H



Item name: sample 7A and 8A for report

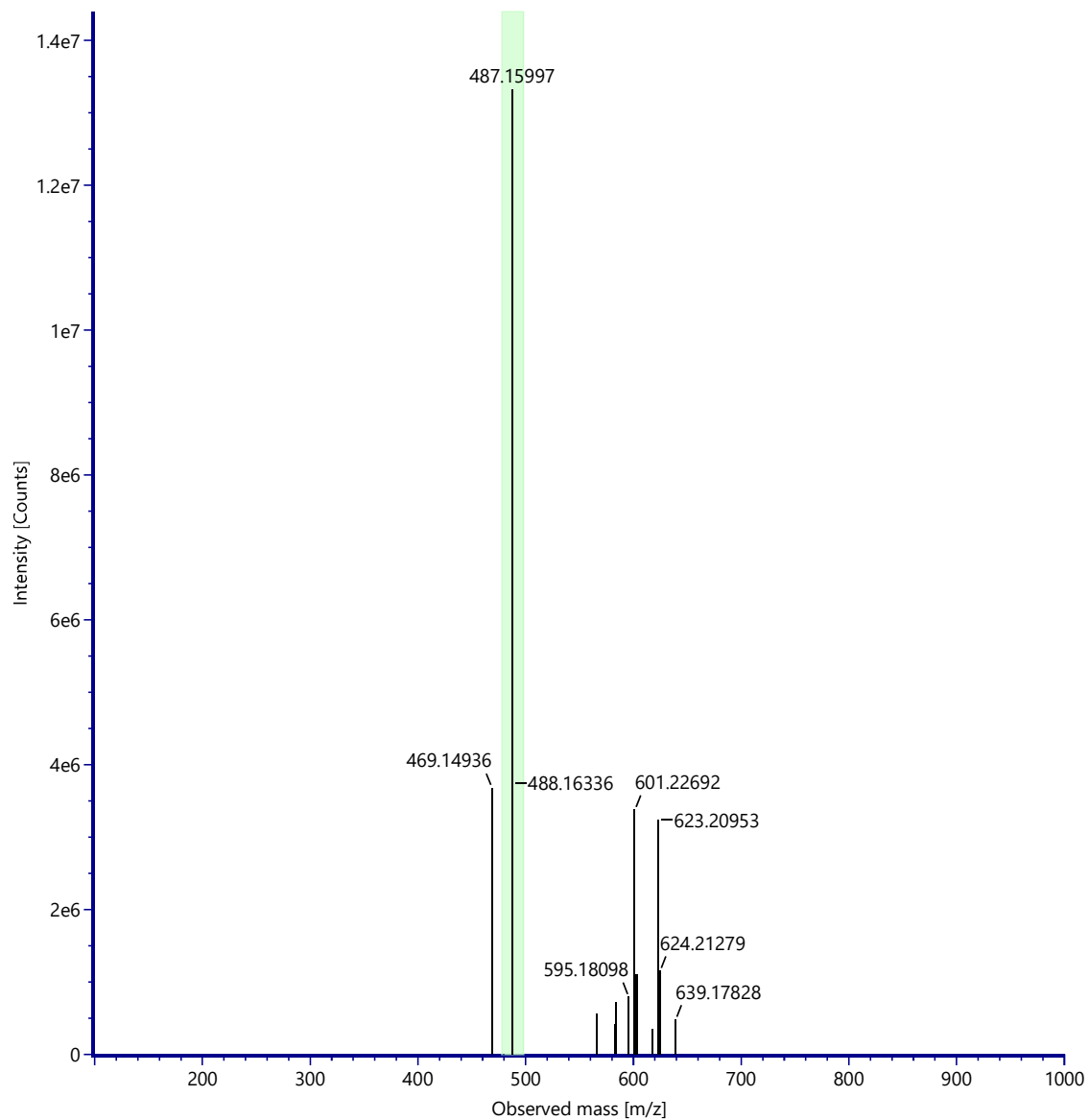
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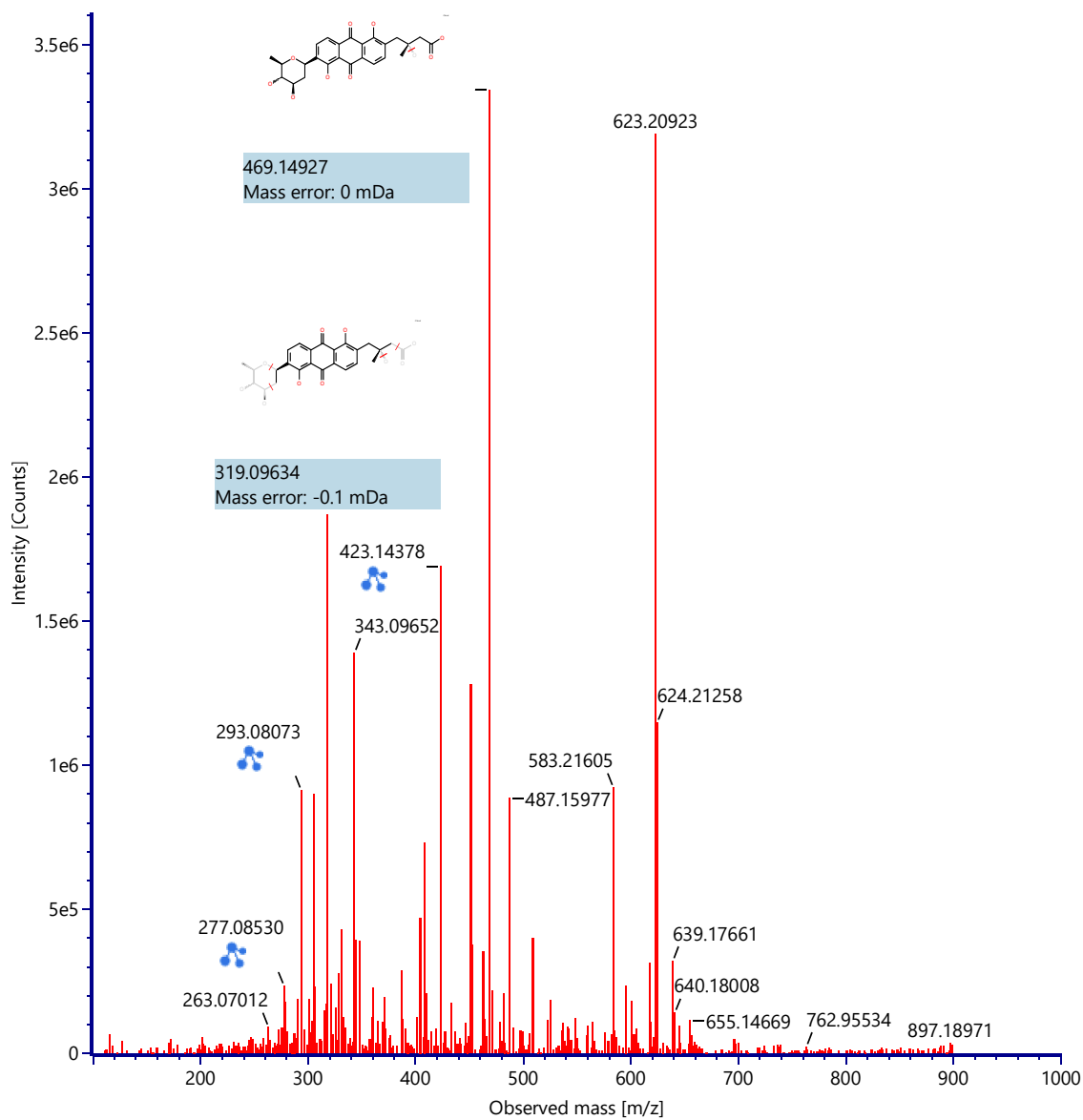
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Component name: Fridamycin A





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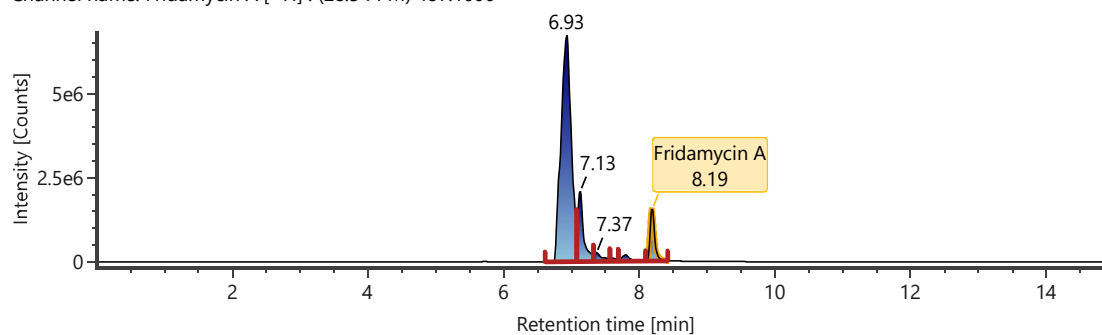
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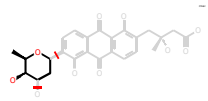
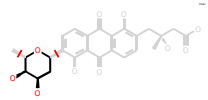
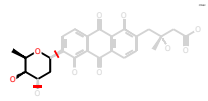
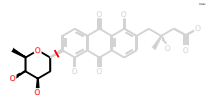
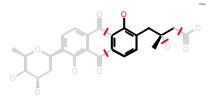
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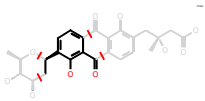
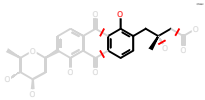
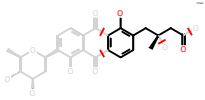
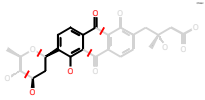
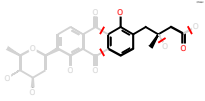
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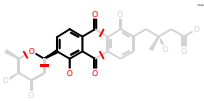
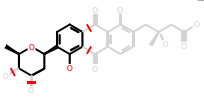
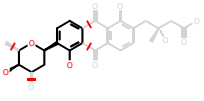
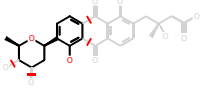
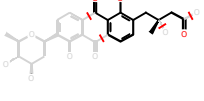


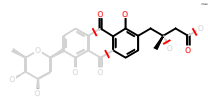
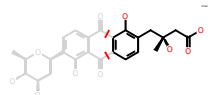
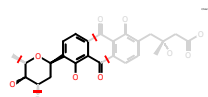
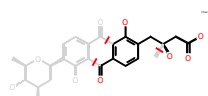
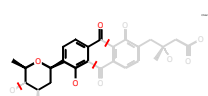
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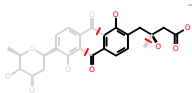
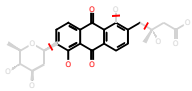
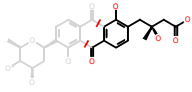
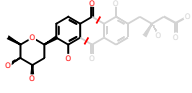
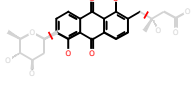
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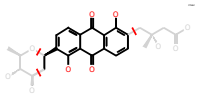
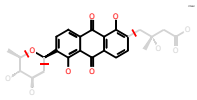
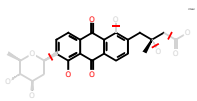
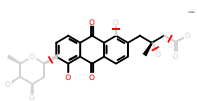
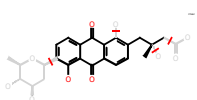
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3	115.0390	Theoretical	115.0386	-0.3	-2.875	88	8.19205	C ₅ H ₇ O ₃	
4	115.0754	Theoretical	115.0755	0.2	1.597	1044	8.19420	C ₆ H ₁₁ O ₂	
5	131.0703	Theoretical	131.0703	0.0	0.054	132	8.17174	C ₆ H ₁₁ O ₃	
6	143.0491	Theoretical	143.0496	0.4	2.971	132	8.19530	C ₁₀ H ₇ O	

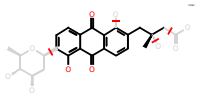
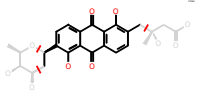
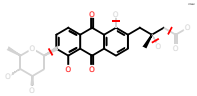
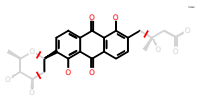
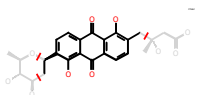
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8	145.0648	Theoretical	145.0650	0.2	1.545	295	8.19334	C ₁₀ H ₉ O	
9	171.0441	Theoretical	171.0434	-0.7	-4.114	702	8.19050	C ₁₁ H ₇ O ₂	
10	173.0233	Theoretical	173.0230	-0.4	-2.026	408	8.19253	C ₁₀ H ₅ O ₃	
11	173.0597	Theoretical	173.0589	-0.8	-4.716	999	8.18980	C ₁₁ H ₉ O ₂	

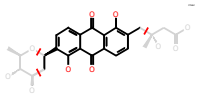
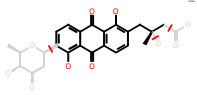
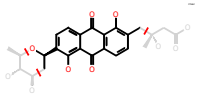
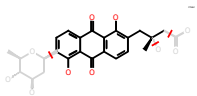
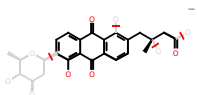
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13	185.0597	Theoretical	185.0598	0.1	0.761	85	8.19095	C ₁₂ H ₉ O ₂	
14	187.0390	Theoretical	187.0388	-0.2	-1.021	275	8.19187	C ₁₁ H ₇ O ₃	
15	187.0754	Theoretical	187.0726	-2.8	-14.86 5	177	8.20341	C ₁₂ H ₁₁ O ₂	
16	199.0390	Theoretical	199.0351	-3.9	-19.37 7	629	8.19179	C ₁₂ H ₇ O ₃	

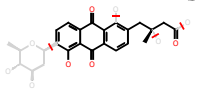
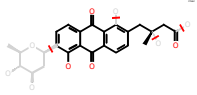
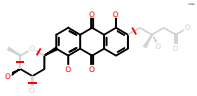
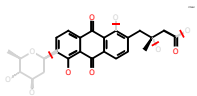
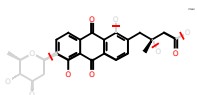
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18	211.0965	Theoretical	211.0951	-1.4	-6.736	161	8.21589	C ₁₁ H ₁₅ O ₄	
19	215.0339	Theoretical	215.0343	0.4	2.036	253	8.19166	C ₁₂ H ₇ O ₄	
20	219.0288	Theoretical	219.0296	0.8	3.473	193	8.16170	C ₁₁ H ₇ O ₅	
21	221.1172	Theoretical	221.1134	-3.8	-17.339	77	8.19156	C ₁₃ H ₁₇ O ₃	

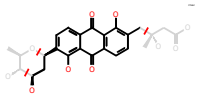
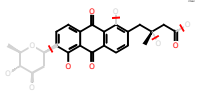
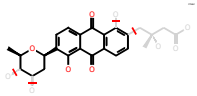
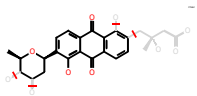
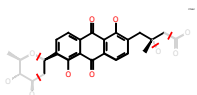
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
22	222.0523	Theoretical	222.0424	-9.8	-44.320	63	8.18457	C11H10O5	
23	237.0546	Theoretical	237.0541	-0.5	-2.203	637	8.19460	C15H9O3	
24	239.0914	Theoretical	239.0883	-3.1	-12.870	715	8.18819	C12H15O5	
25	253.1071	Theoretical	253.1037	-3.3	-13.153	414	8.18904	C13H17O5	
26	254.0574	Theoretical	254.0529	-4.5	-17.532	233	8.19350	C15H10O4	

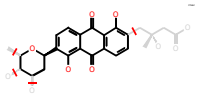
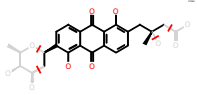
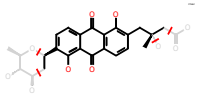
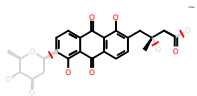
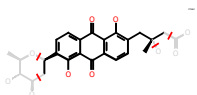
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
27	265.0495	Theoretical	265.0495	0.0	-0.104	315	8.18006	C ₁₆ H ₉ O ₄	
28	267.0288	Theoretical	267.0285	-0.3	-1.185	419	8.17223	C ₁₅ H ₇ O ₅	
29	274.0624	Theoretical	274.0613	-1.1	-4.095	347	8.19255	C ₁₈ H ₁ O ₃	
30	275.0703	Theoretical	275.0698	-0.5	-1.810	1885	8.19257	C ₁₈ H ₁ O ₃	
31	276.0781	Theoretical	276.0772	-0.9	-3.196	2155	8.19182	C ₁₈ H ₁ O ₃	

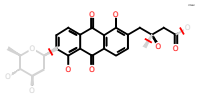
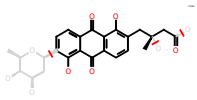
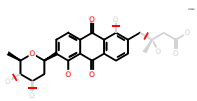
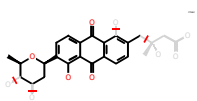
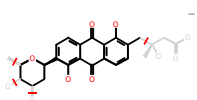
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
32	277.0859	Theoretical	277.0853	-0.6	-2.256	5681	8.19247	C18H13O3	
33	278.0574	Theoretical	278.0568	-0.6	-2.157	715	8.19125	C17H10O4	
34	278.0937	Theoretical	278.0896	-4.2	-14.951	2287	8.19407	C18H14O3	
35	279.0652	Theoretical	279.0653	0.1	0.515	4319	8.19167	C17H11O4	
36	280.0730	Theoretical	280.0708	-2.2	-7.832	3201	8.19606	C17H12O4	

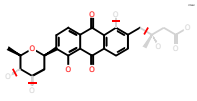
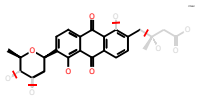
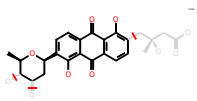
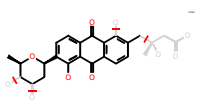
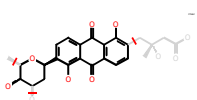
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
37	282.0887	Theoretical	282.0836	-5.1	-17.940	431	8.19697	C17H14O4	
38	291.0652	Theoretical	291.0651	-0.1	-0.220	6257	8.19580	C18H11O4	
39	293.0444	Theoretical	293.0420	-2.5	-8.477	257	8.16208	C17H9O5	
40	293.0808	Theoretical	293.0807	-0.1	-0.370	36815	8.19177	C18H13O4	
41	301.0495	Theoretical	301.0469	-2.6	-8.659	401	8.19296	C19H9O4	

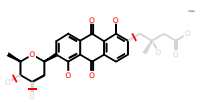
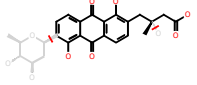
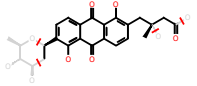
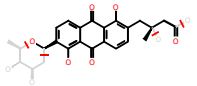
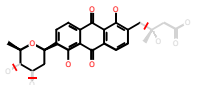
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
42	303.0652	Theoretical	303.0650	-0.2	-0.754	1839	8.18952	C ₁₉ H ₁₀ O ₄	
43	304.0730	Theoretical	304.0723	-0.7	-2.369	2825	8.19129	C ₁₉ H ₁₂ O ₄	
44	305.0444	Theoretical	305.0410	-3.5	-11.316	488	8.18600	C ₁₈ H ₉ O ₅	
45	305.0808	Theoretical	305.0807	-0.1	-0.487	22931	8.19116	C ₁₉ H ₁₃ O ₄	
46	306.0887	Theoretical	306.0845	-4.1	-13.528	5887	8.19088	C ₁₉ H ₁₄ O ₄	

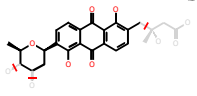
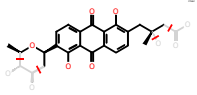
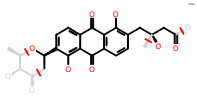
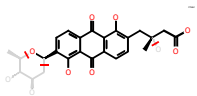
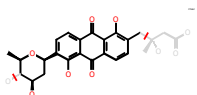
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
47	307.0601	Theoretical	307.0592	0.9	2.943	2557	8.17531	C ₁₈ H ₁₀ O ₅	
48	307.0965	Theoretical	307.0944	2.1	6.923	2964	8.19182	C ₁₉ H ₁₅ O ₄	
49	314.0574	Theoretical	314.0569	0.5	1.492	249	8.19419	C ₂₀ H ₁₀ O ₄	
50	315.0652	Theoretical	315.0634	1.8	5.627	1051	8.19239	C ₂₀ H ₁₀ O ₄	
51	316.0730	Theoretical	316.0717	1.3	4.109	1269	8.19075	C ₂₀ H ₁₂ O ₄	

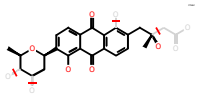
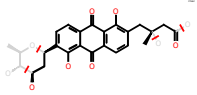
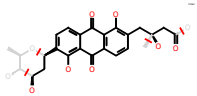
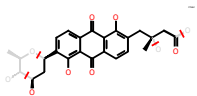
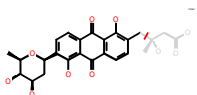
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
52	317.0444	Theoretical	317.0438	-0.6	-2.001	287	8.16838	C ₁₉ H ₉ O ₅	
53	317.0808	Theoretical	317.0802	-0.6	-1.909	4431	8.19184	C ₂₀ H ₁₃ O ₄	
54	318.0887	Theoretical	318.0865	-2.1	-6.680	2482	8.19133	C ₂₀ H ₁₃ O ₄	
55	319.0601	Theoretical	319.0566	-3.5	-10.957	2507	8.19011	C ₁₉ H ₁₁ O ₅	
56	319.0965	Theoretical	319.0963	-0.1	-0.447	63445	8.19176	C ₂₀ H ₁₃ O ₄	

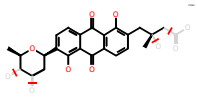
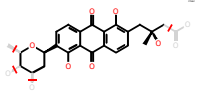
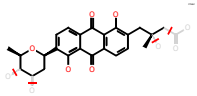
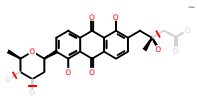
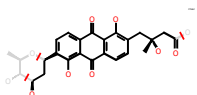
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
57	321.0394	Theoretical	321.0379	-1.4	-4.457	521	8.16368	C ₁₈ H ₉ O ₆	
58	321.0757	Theoretical	321.0758	0.1	0.204	9440	8.19202	C ₁₉ H ₁ 3O ₅	
59	328.0730	Theoretical	328.0727	-0.3	-1.054	1545	8.19049	C ₂₁ H ₁ 2O ₄	
60	329.0808	Theoretical	329.0805	-0.4	-1.117	11411	8.19091	C ₂₁ H ₁ 3O ₄	
61	331.0601	Theoretical	331.0577	-2.4	-7.102	749	8.18495	C ₂₀ H ₁ 1O ₅	

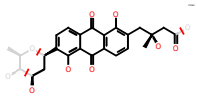
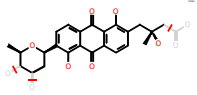
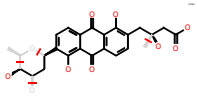
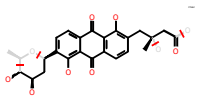
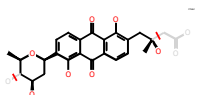
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
62	331.0965	Theoretical	331.0961	-0.4	-1.293	11426	8.19183	C ₂₁ H ₁₅ O ₄	
63	332.1043	Theoretical	332.1003	-4.0	-11.991	3271	8.19164	C ₂₁ H ₁₆ O ₄	
64	333.0757	Theoretical	333.0751	-0.6	-1.807	2693	8.18801	C ₂₀ H ₁₃ O ₅	
65	333.1121	Theoretical	333.1108	-1.3	-3.861	4128	8.19161	C ₂₁ H ₁₇ O ₄	
66	335.0550	Theoretical	335.0529	-2.1	-6.170	673	8.18977	C ₁₉ H ₁₁ O ₆	

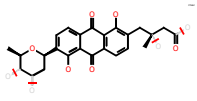
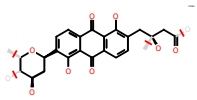
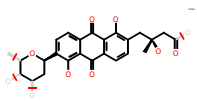
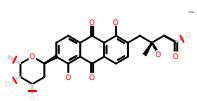
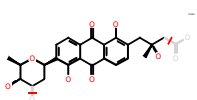
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
67	335.0914	Theoretical	335.0907	-0.7	-2.045	2856	8.19183	C20H15O5	
68	339.0863	Theoretical	339.0857	-0.6	-1.672	2928	8.19258	C19H15O6	
69	345.0757	Theoretical	345.0722	-3.5	-10.203	1217	8.18051	C21H13O5	
70	347.0550	Theoretical	347.0525	-2.6	-7.384	549	8.18266	C20H11O6	
71	347.0914	Theoretical	347.0912	-0.2	-0.575	13491	8.19149	C21H15O5	

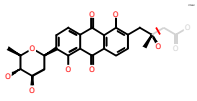
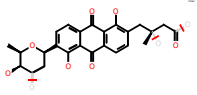
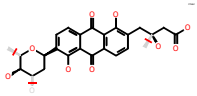
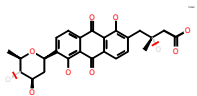
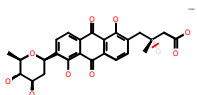
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
72	349.1071	Theoretical	349.1060	-1.0	-2.936	3650	8.19312	C ₂₁ H ₁₇ O ₅	
73	361.1071	Theoretical	361.1068	-0.2	-0.678	9337	8.19198	C ₂₂ H ₁₇ O ₅	
74	363.0499	Theoretical	363.0513	1.4	3.792	310	8.18190	C ₂₀ H ₁₁ O ₇	
75	365.0656	Theoretical	365.0641	-1.5	-4.110	282	8.19040	C ₂₀ H ₁₃ O ₇	
76	365.1020	Theoretical	365.1014	-0.5	-1.438	4017	8.19308	C ₂₁ H ₁₇ O ₆	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
77	373.1071	Theoretical	373.1058	-1.2	-3.260	3181	8.19179	C23H17O5	
78	375.0863	Theoretical	375.0860	-0.3	-0.803	1489	8.18349	C22H15O6	
79	377.0656	Theoretical	377.0686	3.0	8.073	2234	8.19173	C21H13O7	
80	377.1020	Theoretical	377.1032	1.3	3.378	1068	8.19074	C22H17O6	
81	383.1125	Theoretical	383.1122	-0.3	-0.745	1104	8.19573	C21H15O7	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
82	387.1227	Theoretical	387.1226	-0.1	-0.343	10541	8.19299	C ₂₄ H ₁₉ O ₅	
83	389.1020	Theoretical	389.1022	0.2	0.619	4395	8.18675	C ₂₃ H ₁₇ O ₆	
84	389.1384	Theoretical	389.1383	-0.1	-0.132	415	8.19437	C ₂₄ H ₂₁ O ₅	
85	391.1176	Theoretical	391.1168	-0.8	-2.124	3222	8.19061	C ₂₃ H ₁₉ O ₆	
86	393.0969	Theoretical	393.0973	0.5	1.194	743	8.19432	C ₂₂ H ₁₇ O ₇	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
87	395.1125	Theoretical	395.1151	2.6	6.605	2179	8.19223	C22H19O7	
88	405.1333	Theoretical	405.1331	-0.2	-0.383	18514	8.19249	C24H21O6	
89	407.0761	Theoretical	407.0773	1.1	2.800	1044	8.19107	C22H15O8	
90	407.1125	Theoretical	407.1118	-0.8	-1.863	1657	8.18563	C23H19O7	
91	409.1282	Theoretical	409.1280	-0.1	-0.320	29557	8.19308	C23H21O7	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
92	415.1176	Theoretical	415.1173	-0.4	-0.874	2951	8.19270	C25H19O6	
93	419.0761	Theoretical	419.0793	3.2	7.549	3492	8.19086	C23H15O8	
94	419.1125	Theoretical	419.1157	3.2	7.649	317	8.16385	C24H19O7	
95	421.1282	Theoretical	421.1277	-0.5	-1.188	581	8.16903	C24H21O7	
96	423.1438	Theoretical	423.1438	0.0	-0.117	70400	8.19287	C24H23O7	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
97	427.1387	Theoretical	427.1383	-0.5	-1.151	3739	8.19153	C23H2 3O8	
98	433.1282	Theoretical	433.1278	-0.4	-0.908	7533	8.19305	C25H2 1O7	
99	437.0867	Theoretical	437.0872	0.5	1.052	862	8.19771	C23H1 7O9	
100	451.1387	Theoretical	451.1388	0.1	0.171	55351	8.19326	C25H2 3O8	
101	469.1493	Theoretical	469.1493	0.0	-0.083	144402	8.19373	C25H2 5O9	



Item name: sample 7A and 8A for report

Created by: Administrator, UNIFI

Created on: Sep 15, 2020

Created time: 10:40:06 Malay Peninsula
Standard Time

Report Log

Template Report

Body Objects

Deleted report objects:

Report Object [5]: Untitled

Chapter: Analysis results

Untitled

Report Object [4]: Sample results

Object saved in the Report Template was modified

Report Object [13]: PLG spectrum

Object saved in the Report Template was modified

Report Object [20]: Autoscaled chromatogram

Object saved in the Report Template was modified

Report Object [17]: Fragments

Object saved in the Report Template was modified

Supplemental Table S8. Latest Library Spectrum Information on GNPS match for fridamycin D, **2** (*m/z* 597 [M+H]⁺).

Spectrum ID	CCMSLIB00000846420
Compound Name	NCGC00384755-01!(3R)-4-[6-[(2S,4aS,5aR,9R,9aR,10aR)-2,9-dimethyl-3-oxo-4,4a,5a,6,7,9,9a,10a-octahydrodipyran-4,2-a:4',3'-e][1,4]dioxin-7-yl]-1,5-dihydroxy-9,10-dioxoanthracen-2-yl]-3-hydroxy-3-methylbutanoic acid
PI	Jadhav/Dorrestein
Data Collector	lfnothias
Pubmed	n/a
CAS Number	n/a
Original Submitter	mwang87
Original Submitter Email	miw023@ucsd.edu
Most Recent Revisor	mwang87
Most Recent Revisor Email	miw023@ucsd.edu
Library Quality	Gold Spectrum
Smiles	<chem>C[C@H]1OC(C[C@H]2O[C@H]3CC(=O)[C@H](C)O[C@H]3O[C@H]12)C4=C(O)C5=C(C=C4)C(=O)C6=C(C=CC(C[C@@](C)(O)CC(O)=O)=C6O)C5=O</chem>
InChI	InChI=1S/C31H32O12/c1-12-18(32)8-21-30(41-12)43-29-13(2)40-19(9-20(29)42-21)15-6-7-17-24(26(15)36)28(38)16-5-4-14(25(35)23(16)27(17)37)10-31(3,39)11-22(33)34/h4-7,12-13,19-21,29-30,35-36,39H,8-11H2,1-3H3,(H,33,34)/t12-,13+,19?,20+,21-,29+,30-,31+/m0/s1
Metabolomics Spectrum Resolver	mzspec:GNPSLIBRARY:CCMSLIB00000846420
Precursor M/Z	597.196
Exact Mass	596.189
Charge	1
Adduct	M+H
Ion Source	LC-ESI
Instrument	Maxis II HD Q-TOF Bruker
Ion Mode	positive
Library Membership	GNPS-NIH-NATURALPRODUCTSLIBRARY_ROUND2_POSITIVE
SPLASH Key	null-null-null-null

Supplemental Table S9. Waters UNIFI Scientific Information System Report for fridamycin D, **2** (m/z 597 [M+H]⁺).



Item name: sample 7A and 8A for report

Created by: Administrator, UNIFI

Created on: Sep 15, 2020

Created time: 10:48:17 Malay Peninsula
Standard Time

Item name: Sample 8A

Item name: Sample 8A, Sample position: 1:E,7, Replicate number: 1

	Component name	Neutral mass (Da)	Observed neutral mass (Da)	Observed m/z	Observed RT (min)	Mass error (ppm)	Detector counts	Response	Adducts
1	Fridamycin D	596.18938	596.1898	597.1971	9.11	0.8	3894530	2337770	+H, +Na



Item name: sample 7A and 8A for report

Created by: Administrator, UNIFI

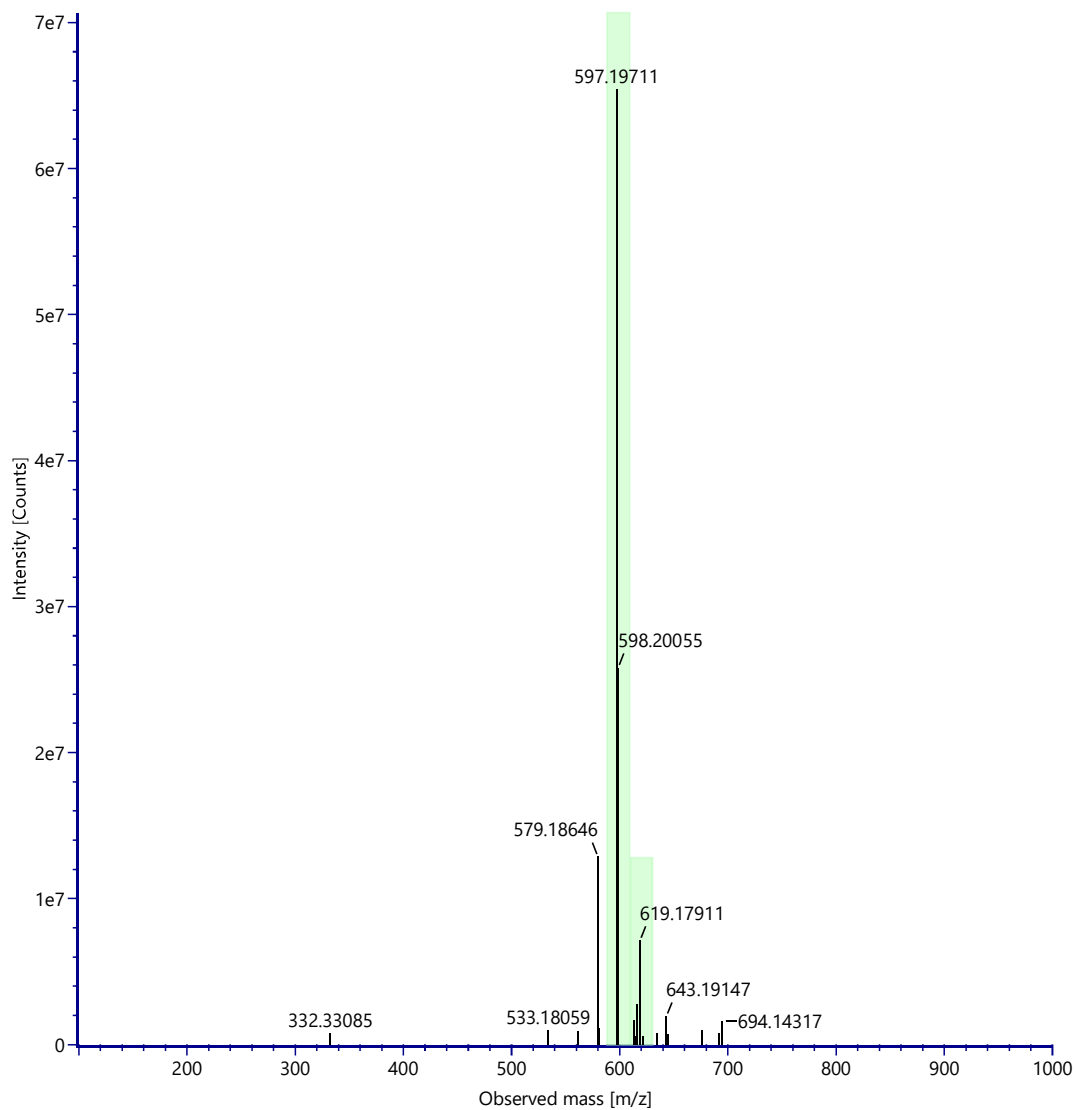
Created on: Sep 15, 2020

Created time: 10:48:17 Malay Peninsula
Standard Time

Item name: Sample 8A

Item description:

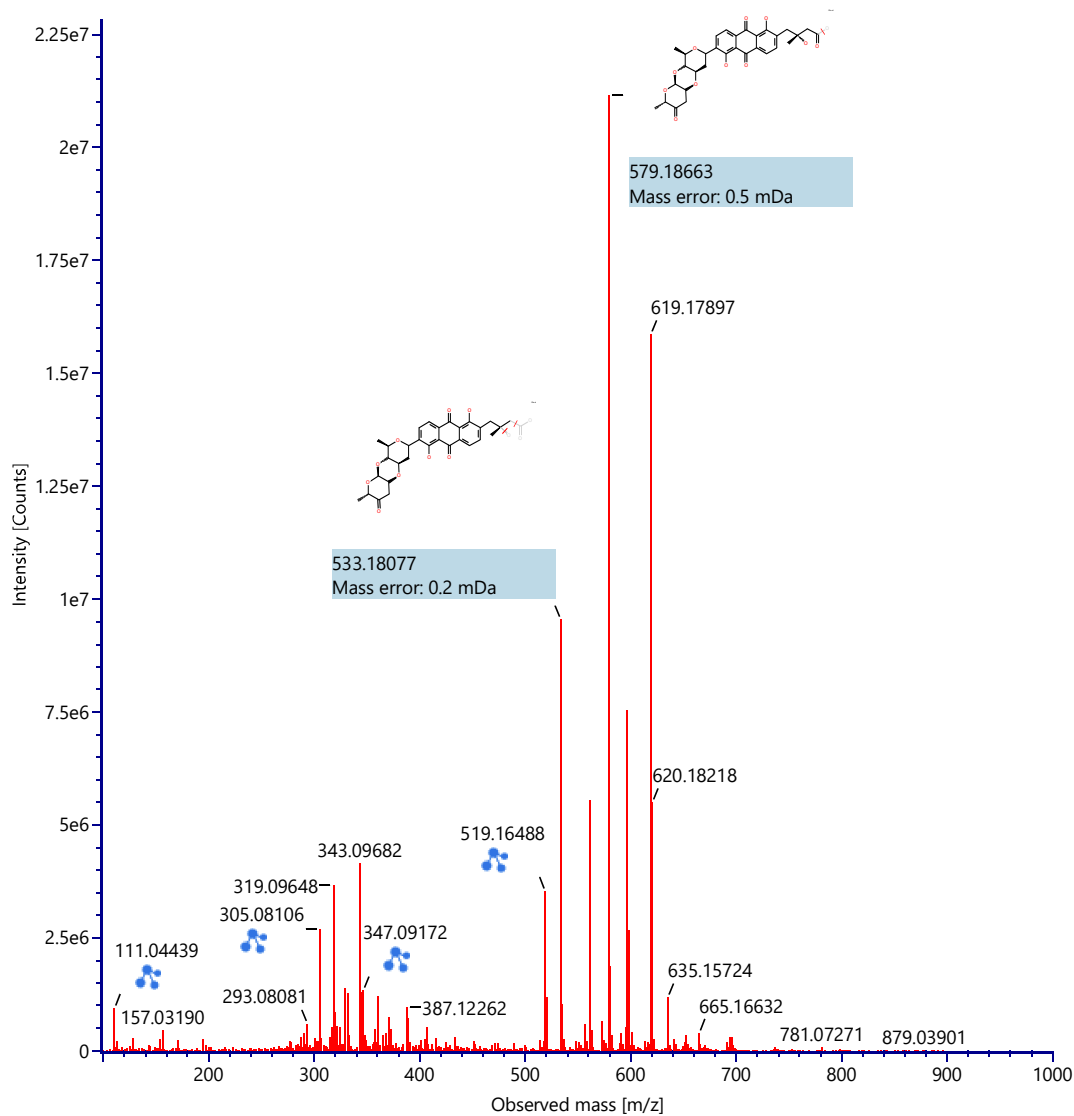
Component name: Fridamycin D



Item name: Sample 8A

Item description:

Component name: Fridamycin D

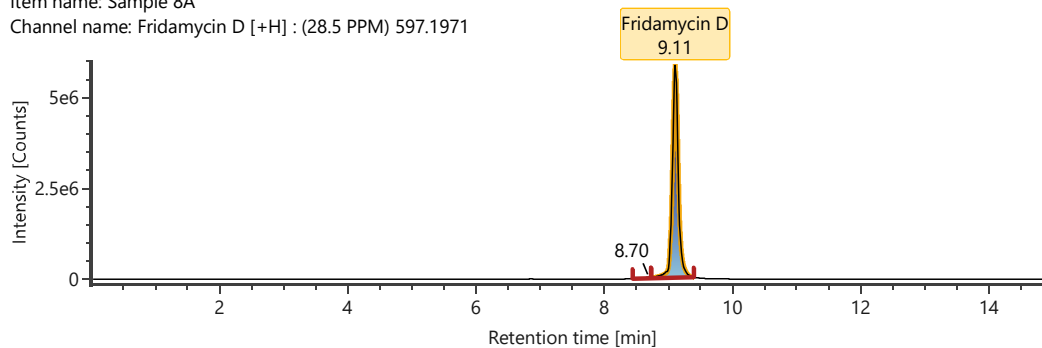


Item name: sample 7A and 8A for report

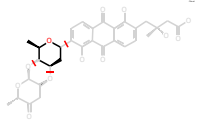
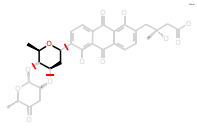
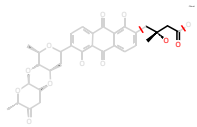
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Standard Time

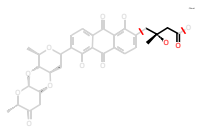
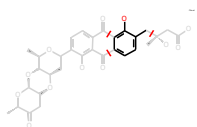
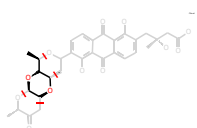
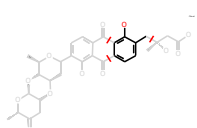
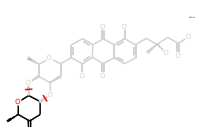
Item name: Sample 8A

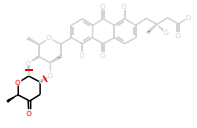
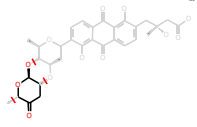
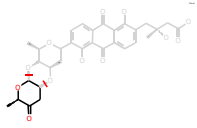
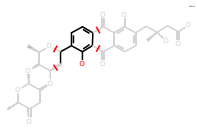
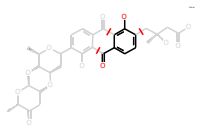
Channel name: Fridamycin D [+H] : (28.5 PPM) 597.1971

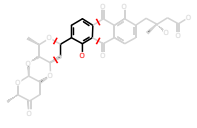
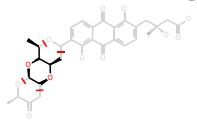
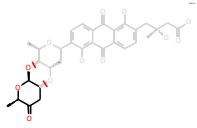
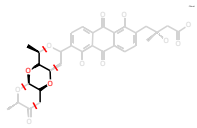
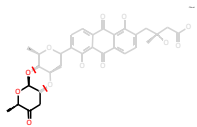


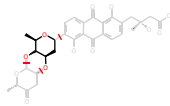
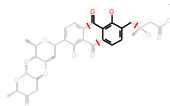
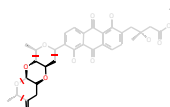
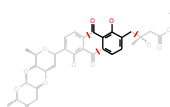
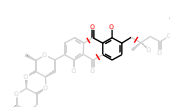
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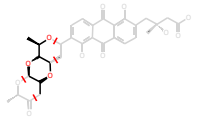
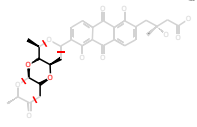
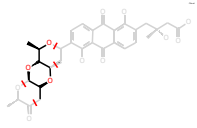
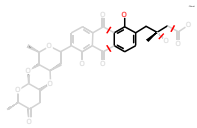
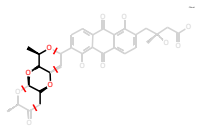
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1	95.0491	Theoretical	95.0496	0.4	4.729	31	9.12363	C ₆ H ₇ O	
2	97.0648	Theoretical	97.0650	0.2	1.838	106	9.11560	C ₆ H ₉ O	
3	99.0441	Theoretical	99.0444	0.4	3.829	206	9.10507	C ₅ H ₇ O ₂	

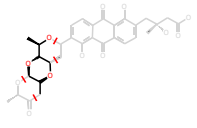
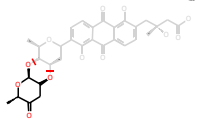
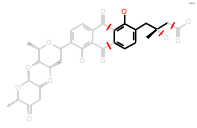
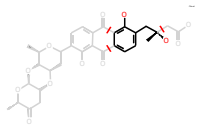
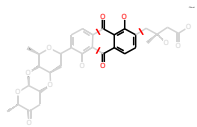
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
4	101.0597	Theoretical	101.0594	-0.3	-3.047	112	9.10468	C ₅ H ₉ O ₂	
5	107.0491	Theoretical	107.0496	0.5	4.274	658	9.10998	C ₇ H ₇ O	
6	109.0284	Theoretical	109.0288	0.4	3.719	247	9.13532	C ₆ H ₅ O ₂	
7	109.0648	Theoretical	109.0650	0.2	1.674	369	9.10592	C ₇ H ₉ O	
8	111.0441	Theoretical	111.0444	0.3	3.019	15683	9.11027	C ₆ H ₇ O ₂	

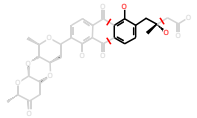
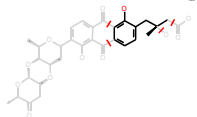
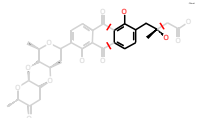
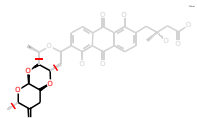
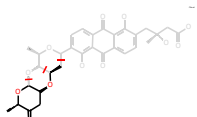
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
9	113.0597	Theoretical	113.0597	0.0	0.207	509	9.11035	C ₆ H ₉ O ₂	
10	115.0390	Theoretical	115.0393	0.3	2.984	153	9.20377	C ₅ H ₇ O ₃	
11	115.0754	Theoretical	115.0757	0.4	3.195	98	9.09990	C ₆ H ₁₁ O ₂	
12	121.0648	Theoretical	121.0646	-0.2	-1.717	478	9.10556	C ₈ H ₉ O	
13	123.0441	Theoretical	123.0424	-1.7	-13.847	1108	9.11403	C ₇ H ₇ O ₂	

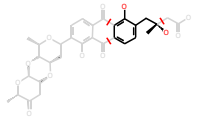
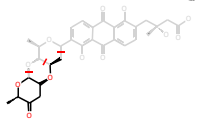
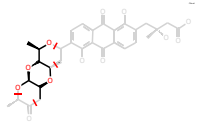
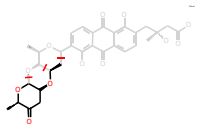
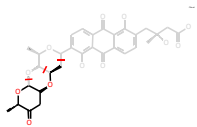
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
14	123.0804	Theoretical	123.0804	0.0	0.010	993	9.10723	C ₈ H ₁₁ O	
15	125.0597	Theoretical	125.0599	0.2	1.733	2269	9.10911	C ₇ H ₉ O ₂	
16	127.0390	Theoretical	127.0392	0.2	1.771	712	9.11155	C ₆ H ₇ O ₃	
17	127.0754	Theoretical	127.0750	-0.3	-2.692	206	9.10873	C ₇ H ₁₁ O ₂	
18	129.0546	Theoretical	129.0549	0.3	2.297	5096	9.10924	C ₆ H ₉ O ₃	

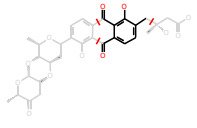
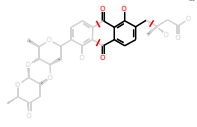
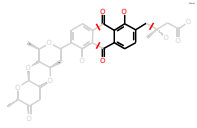
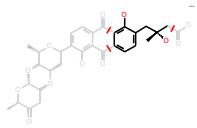
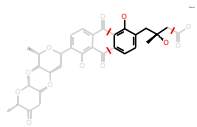
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
19	133.0859	Theoretical	133.0862	0.2	1.780	140	9.06551	C ₆ H ₁₃ O ₃	
20	135.0441	Theoretical	135.0441	0.0	0.293	1121	9.11246	C ₈ H ₇ O ₂	
21	136.0155	Theoretical	136.0068	-8.7	-64.029	112	9.10228	C ₇ H ₄ O ₃	
22	136.0519	Theoretical	136.0615	9.7	70.987	92	9.10575	C ₈ H ₈ O ₂	
23	137.0597	Theoretical	137.0591	-0.6	-4.586	1150	9.10924	C ₈ H ₉ O ₂	

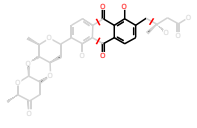
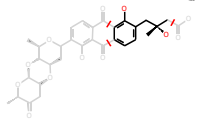
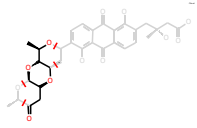
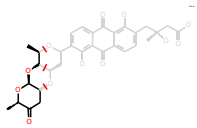
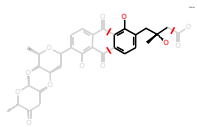
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
24	139.0390	Theoretical	139.0382	-0.8	-5.551	69	9.12057	C ₇ H ₇ O ₃	
25	139.0754	Theoretical	139.0752	-0.2	-1.394	550	9.11088	C ₈ H ₁₁ O ₂	
26	141.0546	Theoretical	141.0545	-0.1	-0.807	227	9.11380	C ₇ H ₉ O ₃	
27	143.0491	Theoretical	143.0489	-0.2	-1.446	92	9.10633	C ₁₀ H ₇ O	
28	143.0703	Theoretical	143.0706	0.4	2.572	2121	9.10799	C ₇ H ₁₁ O ₃	

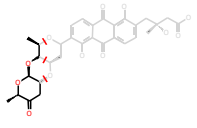
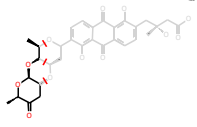
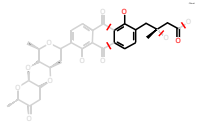
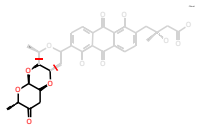
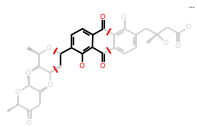
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
29	144.0781	Theoretical	144.0773	-0.8	-5.517	349	9.09823	C ₇ H ₁₂ O ₃	
30	145.0495	Theoretical	145.0498	0.3	1.940	1762	9.10454	C ₆ H ₉ O ₄	
31	145.0648	Theoretical	145.0667	1.9	13.114	205	9.10436	C ₁₀ H ₉ O	
32	147.0441	Theoretical	147.0454	1.4	9.224	208	9.10925	C ₉ H ₇ O ₂	
33	148.0155	Theoretical	148.0246	9.1	61.216	138	9.18335	C ₈ H ₄ O ₃	

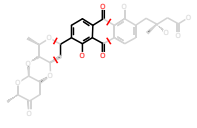
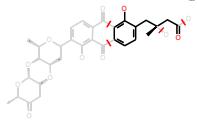
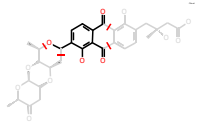
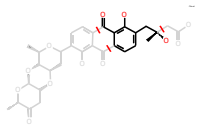
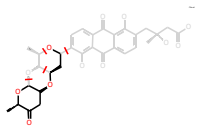
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
34	149.0597	Theoretical	149.0592	-0.5	-3.102	79	9.09750	C ₉ H ₉ O ₂	
35	149.0961	Theoretical	149.0961	0.0	0.181	1516	9.10894	C ₁₀ H ₁₃ O	
36	151.0754	Theoretical	151.0753	0.0	-0.256	923	9.10968	C ₉ H ₁₁ O ₂	
37	153.0182	Theoretical	153.0090	-9.2	-60.361	317	9.11678	C ₇ H ₅ O ₄	
38	153.0546	Theoretical	153.0548	0.2	1.357	5134	9.10747	C ₈ H ₉ O ₃	

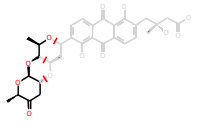
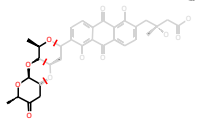
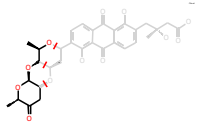
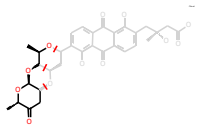
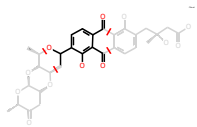
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
39	153.0910	Theoretical	153.0911	0.1	0.595	310	9.11116	C ₉ H ₁₃ O ₂	
40	155.0703	Theoretical	155.0700	-0.3	-1.826	638	9.10767	C ₈ H ₁₁ O ₃	
41	157.0495	Theoretical	157.0501	0.6	3.556	167	9.10343	C ₇ H ₉ O 4	
42	157.0859	Theoretical	157.0862	0.3	1.598	594	9.10683	C ₈ H ₁₃ O ₃	
43	158.0937	Theoretical	158.0959	2.2	13.772	96	9.05380	C ₈ H ₁₄ O ₃	

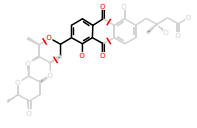
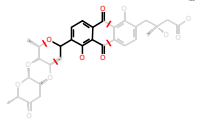
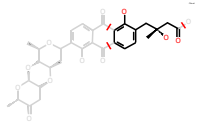
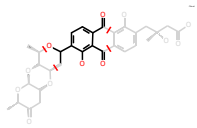
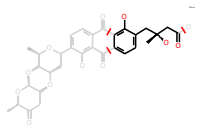
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
44	159.0077	Theoretical	159.0086	0.9	5.948	181	9.11082	C ₉ H ₃ O ₃	
45	160.0155	Theoretical	160.0162	0.7	4.326	50	9.10476	C ₉ H ₄ O ₃	
46	161.0233	Theoretical	161.0140	-9.3	-57.870	153	9.09697	C ₉ H ₅ O ₃	
47	161.0597	Theoretical	161.0602	0.5	2.924	151	9.10809	C ₁₀ H ₉ O ₂	
48	163.0754	Theoretical	163.0744	-1.0	-6.140	215	9.11512	C ₁₀ H ₁₁ O ₂	

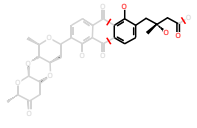
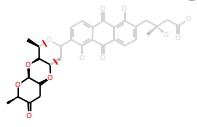
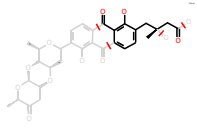
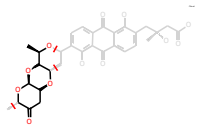
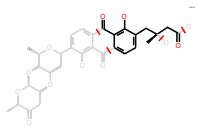
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
49	165.0546	Theoretical	165.0523	-2.3	-14.206	342	9.10324	C ₉ H ₉ O ₃	
50	165.0910	Theoretical	165.0914	0.4	2.269	231	9.11426	C ₁₀ H ₁₃ O ₂	
51	166.0261	Theoretical	166.0163	-9.7	-58.564	379	9.09982	C ₈ H ₆ O ₄	
52	167.0703	Theoretical	167.0706	0.3	2.068	1052	9.10605	C ₉ H ₁₁ O ₃	
53	167.1067	Theoretical	167.1066	0.0	-0.191	260	9.11137	C ₁₀ H ₁₅ O ₂	

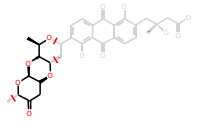
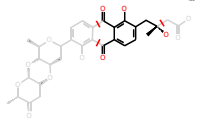
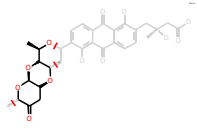
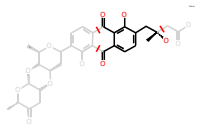
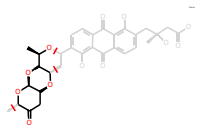
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
54	169.0859	Theoretical	169.0861	0.2	1.067	1208	9.10338	C ₉ H ₁₃ O ₃	
55	170.0937	Theoretical	170.0936	-0.2	-0.882	148	9.11203	C ₉ H ₁₄ O ₃	
56	171.0441	Theoretical	171.0430	-1.1	-6.195	794	9.10719	C ₁₁ H ₇ O ₂	
57	171.0652	Theoretical	171.0652	0.0	-0.010	6112	9.10933	C ₈ H ₁₁ O ₄	
58	172.0155	Theoretical	172.0164	0.9	5.159	396	9.10551	C ₁₀ H ₄ O ₃	

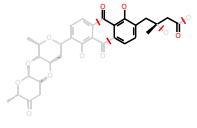
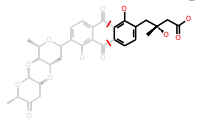
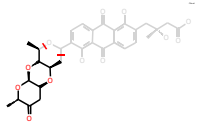
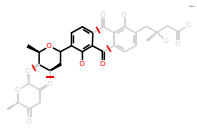
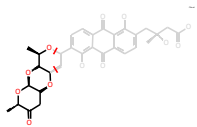
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
59	173.0233	Theoretical	173.0242	0.9	5.014	992	9.10525	C ₁₀ H ₅ O ₃	
60	177.0910	Theoretical	177.0906	-0.4	-2.518	876	9.10683	C ₁₁ H ₁ 3O ₂	
61	179.0339	Theoretical	179.0246	-9.3	-52.01 6	574	9.11225	C ₉ H ₇ O 4	
62	179.0703	Theoretical	179.0682	-2.1	-11.69 4	790	9.10833	C ₁₀ H ₁ 1O ₃	
63	181.0495	Theoretical	181.0496	0.1	0.317	204	9.08596	C ₉ H ₉ O 4	

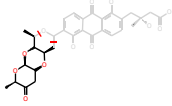
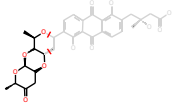
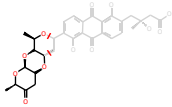
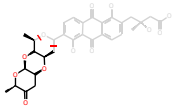
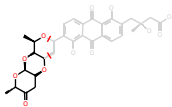
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
64	183.0652	Theoretical	183.0636	-1.5	-8.402	153	9.11372	C ₉ H ₁₁ O ₄	
65	184.0730	Theoretical	184.0733	0.3	1.844	76	9.11288	C ₉ H ₁₂ O ₄	
66	185.0808	Theoretical	185.0805	-0.3	-1.615	145	9.10955	C ₉ H ₁₃ O ₄	
67	187.0965	Theoretical	187.0975	1.1	5.667	142	9.10855	C ₉ H ₁₅ O ₄	
68	189.0182	Theoretical	189.0196	1.3	6.999	272	9.11683	C ₁₀ H ₅ O ₄	

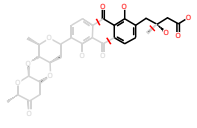
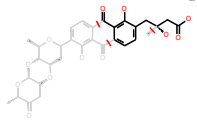
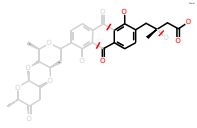
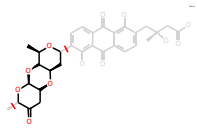
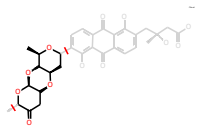
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
69	190.0261	Theoretical	190.0283	2.3	11.875	31	9.16597	C10H6 O4	
70	191.0339	Theoretical	191.0348	0.9	4.843	65	9.10613	C10H7 O4	
71	191.0703	Theoretical	191.0683	-2.0	-10.21 2	352	9.10592	C11H1 IO3	
72	192.0417	Theoretical	192.0321	-9.6	-50.19 6	494	9.09384	C10H8 O4	
73	193.0859	Theoretical	193.0836	-2.3	-11.92 2	591	9.11828	C11H1 3O3	

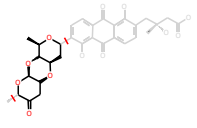
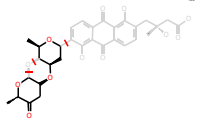
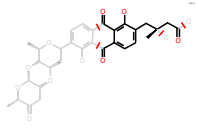
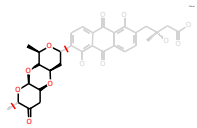
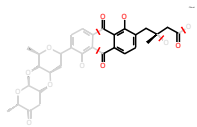
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
74	195.1016	Theoretical	195.1012	-0.4	-2.036	6234	9.10916	C ₁₁ H ₁₅ O ₃	
75	197.0808	Theoretical	197.0803	-0.5	-2.508	3059	9.11009	C ₁₀ H ₁₃ O ₄	
76	199.0390	Theoretical	199.0390	0.1	0.270	572	9.11103	C ₁₂ H ₇ O ₃	
77	200.0679	Theoretical	200.0626	-5.3	-26.708	353	9.11179	C ₉ H ₁₂ O ₅	
78	201.0546	Theoretical	201.0474	-7.3	-36.068	1346	9.11228	C ₁₂ H ₉ O ₃	

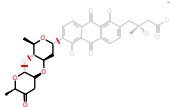
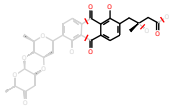
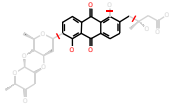
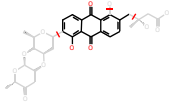
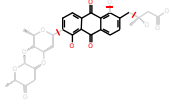
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
79	201.0757	Theoretical	201.0714	-4.3	-21.449	343	9.09950	C ₉ H ₁₃ O ₅	
80	202.0261	Theoretical	202.0268	0.8	3.726	580	9.10019	C ₁₁ H ₆ O ₄	
81	202.0836	Theoretical	202.0775	-6.1	-30.057	1967	9.10613	C ₉ H ₁₄ O ₅	
82	203.0339	Theoretical	203.0349	1.0	4.764	923	9.09641	C ₁₁ H ₇ O ₄	
83	203.0914	Theoretical	203.0834	-8.0	-39.545	1413	9.11330	C ₉ H ₁₅ O ₅	

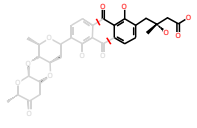
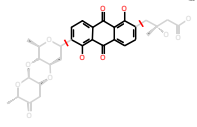
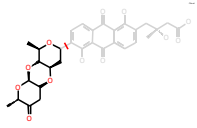
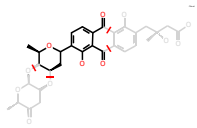
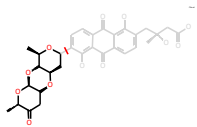
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
84	207.1016	Theoretical	207.1001	-1.4	-6.924	156	9.05329	C ₁₂ H ₁₅ O ₃	
85	209.0808	Theoretical	209.0788	-2.0	-9.622	1046	9.12236	C ₁₁ H ₁₃ O ₄	
86	211.0965	Theoretical	211.0946	-1.9	-8.841	426	9.10947	C ₁₁ H ₁₅ O ₄	
87	212.0468	Theoretical	212.0406	-6.2	-29.232	309	9.11054	C ₁₃ H ₁₈ O ₃	
88	213.0757	Theoretical	213.0701	-5.7	-26.574	480	9.10582	C ₁₀ H ₁₃ O ₅	

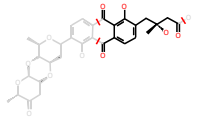
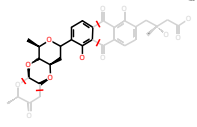
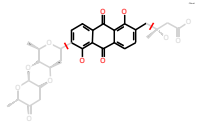
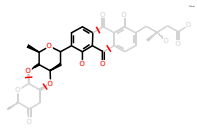
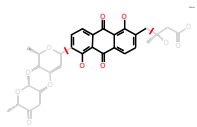
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
89	213.1121	Theoretical	213.1121	-0.1	-0.328	784	9.10749	C ₁₁ H ₁ 7O ₄	
90	214.0836	Theoretical	214.0782	-5.4	-25.250	122	9.10423	C ₁₀ H ₁ 4O ₅	
91	215.0914	Theoretical	215.0883	-3.1	-14.556	2427	9.10927	C ₁₀ H ₁ 5O ₅	
92	215.1278	Theoretical	215.1247	-3.1	-14.445	254	9.20014	C ₁₁ H ₁ 9O ₄	
93	217.1071	Theoretical	217.1038	-3.2	-14.896	793	9.11190	C ₁₀ H ₁ 7O ₅	

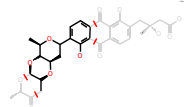
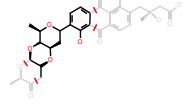
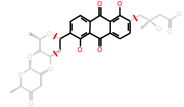
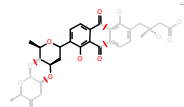
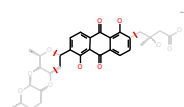
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
94	222.0523	Theoretical	222.0424	-9.8	-44.338	711	9.10381	C ₁₁ H ₁₀ O ₅	
95	223.0601	Theoretical	223.0505	-9.6	-42.935	1743	9.09908	C ₁₁ H ₁₀ O ₅	
96	223.0965	Theoretical	223.0947	-1.7	-7.842	523	9.11517	C ₁₂ H ₁₅ O ₄	
97	224.0679	Theoretical	224.0584	-9.5	-42.369	241	9.09709	C ₁₁ H ₁₂ O ₅	
98	225.0757	Theoretical	225.0750	-0.8	-3.364	256	9.11866	C ₁₁ H ₁₃ O ₅	

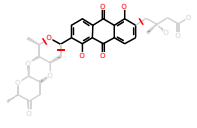
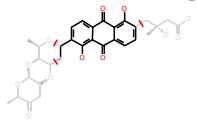
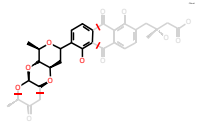
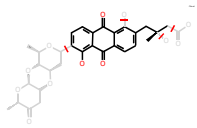
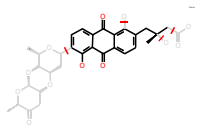
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
99	226.0836	Theoretical	226.0777	-5.9	-26.024	1583	9.10741	C11H14O5	
100	227.1278	Theoretical	227.1277	-0.1	-0.491	35	9.14753	C12H19O4	
101	228.0417	Theoretical	228.0426	0.9	3.924	32	9.10203	C13H8O4	
102	228.0992	Theoretical	228.0926	-6.7	-29.232	791	9.11201	C11H16O5	
103	229.0495	Theoretical	229.0487	-0.9	-3.862	365	9.08748	C13H9O4	

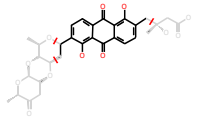
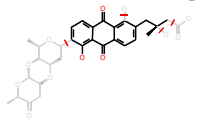
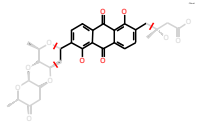
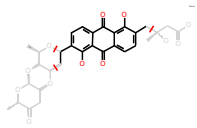
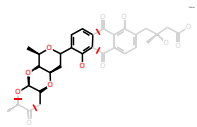
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
104	229.1434	Theoretical	229.1407	-2.7	-11.858	177	9.18577	C ₁₂ H ₂₁ O ₄	
105	235.0965	Theoretical	235.0962	-0.3	-1.189	338	9.07679	C ₁₃ H ₁₅ O ₄	
106	236.0468	Theoretical	236.0409	-5.9	-24.850	47	9.10221	C ₁₅ H ₈ O ₃	
107	237.0546	Theoretical	237.0533	-1.3	-5.518	836	9.10439	C ₁₅ H ₉ O ₃	
108	239.0703	Theoretical	239.0665	-3.8	-15.801	271	9.11158	C ₁₅ H ₁₁ O ₃	

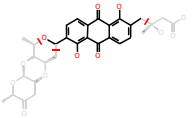
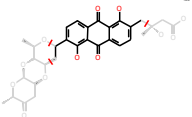
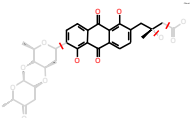
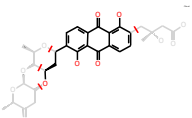
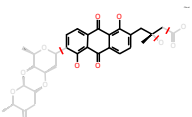
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
109	239.0914	Theoretical	239.0878	-3.6	-15.067	1796	9.10849	C ₁₂ H ₁₅ O ₅	
110	241.0495	Theoretical	241.0493	-0.2	-0.932	411	9.10174	C ₁₄ H ₉ O ₄	
111	241.1071	Theoretical	241.1013	-5.7	-23.685	563	9.10614	C ₁₂ H ₁₇ O ₅	
112	242.0574	Theoretical	242.0583	1.0	4.037	268	9.09606	C ₁₄ H ₁₁ O ₄	
113	243.1227	Theoretical	243.1157	-7.0	-28.988	55	9.11774	C ₁₂ H ₁₉ O ₅	

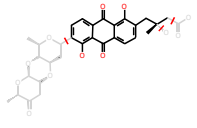
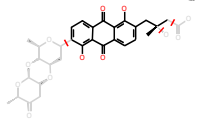
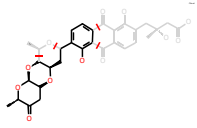
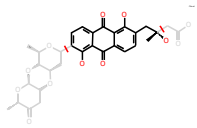
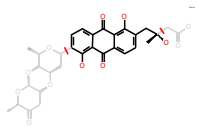
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
114	245.0444	Theoretical	245.0428	-1.6	-6.626	239	9.12572	C13H9 O5	
115	251.1278	Theoretical	251.1255	-2.2	-8.916	523	9.12016	C14H1 9O4	
116	253.0495	Theoretical	253.0495	0.0	0.012	1263	9.10642	C15H9 O4	
117	253.1071	Theoretical	253.1027	-4.4	-17.36 3	1375	9.10991	C13H1 7O5	
118	255.0652	Theoretical	255.0614	-3.8	-14.99 3	409	9.11738	C15H1 10O4	

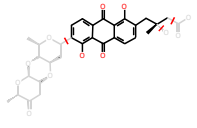
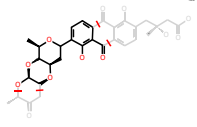
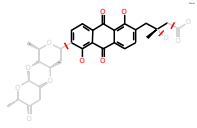
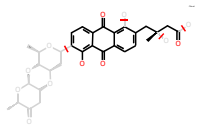
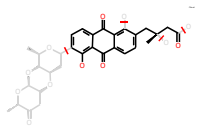
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
119	260.1043	Theoretical	260.1054	1.1	4.299	188	9.01191	C ₁₅ H ₁₆ O ₄	
120	263.1278	Theoretical	263.1270	-0.8	-2.951	391	9.14352	C ₁₅ H ₁₉ O ₄	
121	264.0417	Theoretical	264.0511	9.4	35.679	166	9.09910	C ₁₆ H ₁₈ O ₄	
122	265.1071	Theoretical	265.1059	-1.2	-4.366	349	9.10258	C ₁₄ H ₁₇ O ₅	
123	266.0574	Theoretical	266.0548	-2.6	-9.762	443	9.10998	C ₁₆ H ₁₈ O ₅	

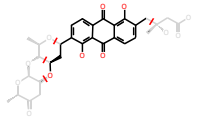
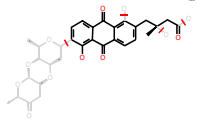
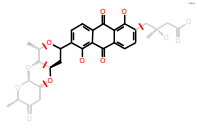
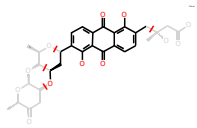
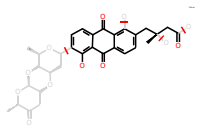
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
124	267.0288	Theoretical	267.0335	4.7	17.515	82	9.12010	C15H7 O5	
125	267.0652	Theoretical	267.0643	-0.9	-3.399	3516	9.10905	C16H1 104	
126	267.1227	Theoretical	267.1202	-2.5	-9.294	1166	9.10851	C14H1 905	
127	273.0546	Theoretical	273.0558	1.2	4.461	1050	9.10551	C18H9 O3	
128	275.0703	Theoretical	275.0700	-0.2	-0.869	4586	9.10836	C18H1 103	

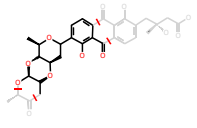
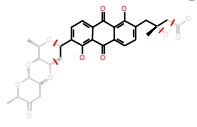
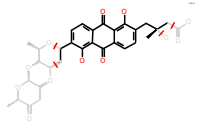
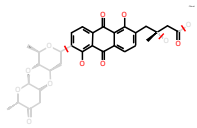
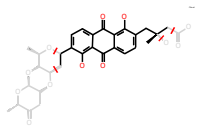
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
129	277.0495	Theoretical	277.0491	-0.5	-1.658	454	9.10726	C17H9 O4	
130	277.0859	Theoretical	277.0856	-0.3	-1.212	9380	9.10010	C18H1 3O3	
131	278.0574	Theoretical	278.0516	-5.8	-20.87 6	1048	9.11510	C17H1 0O4	
132	279.0652	Theoretical	279.0640	-1.2	-4.186	6661	9.10669	C17H1 1O4	
133	279.1227	Theoretical	279.1222	-0.5	-1.776	510	9.12396	C15H1 9O5	

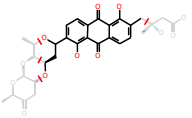
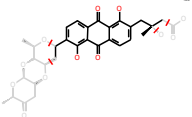
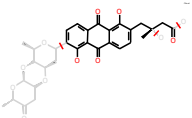
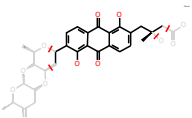
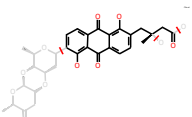
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
134	281.0444	Theoretical	281.0458	1.4	4.836	1177	9.10161	C16H9 O5	
135	281.0808	Theoretical	281.0787	-2.1	-7.507	1209	9.11210	C17H1 3O4	
136	290.0574	Theoretical	290.0571	-0.3	-0.907	765	9.10581	C18H1 0O4	
137	291.0288	Theoretical	291.0317	2.9	9.834	44	9.13252	C17H7 O5	
138	291.0652	Theoretical	291.0653	0.1	0.508	9820	9.10952	C18H1 1O4	

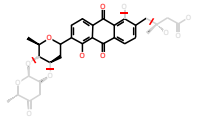
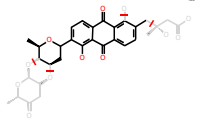
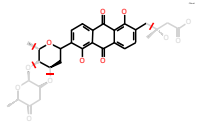
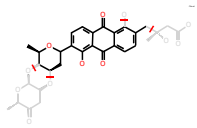
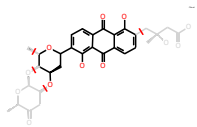
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
139	292.0730	Theoretical	292.0706	-2.4	-8.297	3630	9.10891	C18H1 2O4	
140	293.0808	Theoretical	293.0808	0.0	-0.085	23151	9.10709	C18H1 3O4	
141	293.1384	Theoretical	293.1358	-2.5	-8.544	635	9.11595	C16H2 1O5	
142	294.0523	Theoretical	294.0524	0.1	0.289	65	9.10881	C17H1 0O5	
143	295.0601	Theoretical	295.0694	9.3	31.656	891	9.11713	C17H1 1O5	

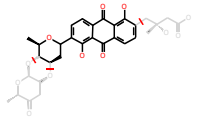
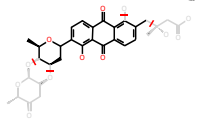
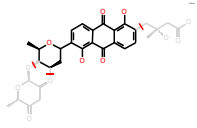
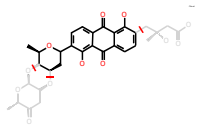
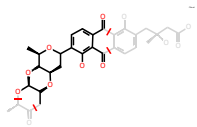
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
144	295.0965	Theoretical	295.0934	-3.1	-10.473	2287	9.10544	C ₁₈ H ₁₅ O ₄	
145	295.1176	Theoretical	295.1181	0.5	1.571	380	9.12160	C ₁₅ H ₁₉ O ₆	
146	296.1043	Theoretical	296.1039	-0.4	-1.463	561	9.10939	C ₁₈ H ₁₆ O ₄	
147	302.0574	Theoretical	302.0559	-1.5	-4.879	383	9.11032	C ₁₉ H ₁₀ O ₄	
148	303.0652	Theoretical	303.0651	-0.1	-0.196	11041	9.10638	C ₁₉ H ₁₀ O ₄	

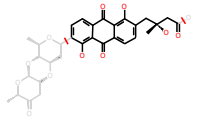
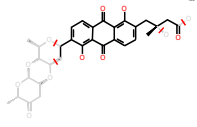
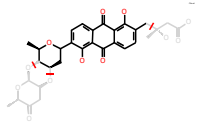
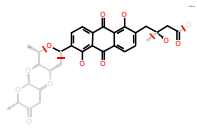
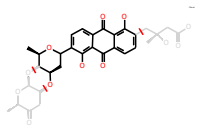
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
149	305.0444	Theoretical	305.0410	-3.5	-11.312	781	9.10576	C18H9O5	
150	305.0808	Theoretical	305.0811	0.2	0.748	94945	9.10855	C19H13O4	
151	307.0237	Theoretical	307.0269	3.2	10.400	174	9.14149	C17H7O6	
152	307.0601	Theoretical	307.0585	-1.6	-5.296	6543	9.10537	C18H11O5	
153	308.1043	Theoretical	308.0987	-5.6	-18.151	2007	9.10532	C19H16O4	

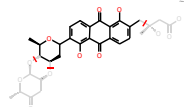
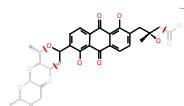
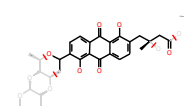
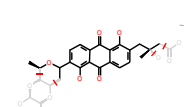
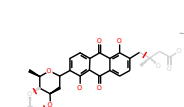
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
154	309.1333	Theoretical	309.1311	-2.2	-7.039	429	9.12181	C ₁₆ H ₂ O ₆	
155	316.0730	Theoretical	316.0716	-1.4	-4.494	2306	9.10941	C ₂₀ H ₁ O ₄	
156	317.0808	Theoretical	317.0809	0.1	0.273	27448	9.10714	C ₂₀ H ₁ O ₄	
157	319.0601	Theoretical	319.0560	-4.1	-12.848	3824	9.10984	C ₁₉ H ₁ O ₅	
158	319.0965	Theoretical	319.0965	0.0	-0.013	95558	9.10899	C ₂₀ H ₁ O ₄	

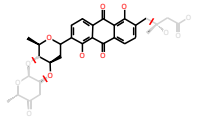
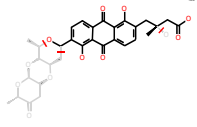
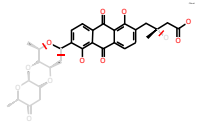
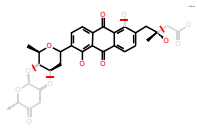
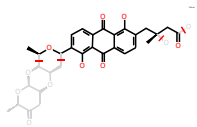
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
159	320.0315	Theoretical	320.0317	0.1	0.367	217	9.11482	C ₁₈ H ₈ O ₆	
160	320.1043	Theoretical	320.1000	-4.3	-13.567	22652	9.10886	C ₂₀ H ₁₆ O ₄	
161	321.0757	Theoretical	321.0764	0.7	2.104	18207	9.10739	C ₁₉ H ₁₃ O ₅	
162	321.1121	Theoretical	321.1100	-2.1	-6.677	4095	9.11077	C ₂₀ H ₁₇ O ₄	
163	323.0914	Theoretical	323.0905	-0.9	-2.641	3792	9.10860	C ₁₉ H ₁₅ O ₅	

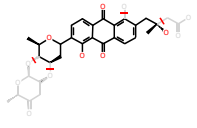
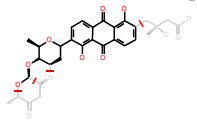
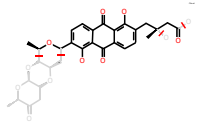
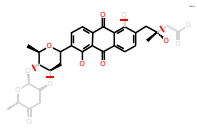
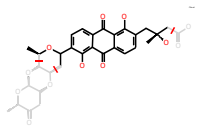
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
164	328.0730	Theoretical	328.0729	-0.1	-0.218	2187	9.10810	C ₂₁ H ₁ 2O ₄	
165	329.0808	Theoretical	329.0811	0.2	0.691	49601	9.10820	C ₂₁ H ₁ 3O ₄	
166	331.0601	Theoretical	331.0572	-2.9	-8.848	822	9.10982	C ₂₀ H ₁ 1O ₅	
167	331.0965	Theoretical	331.0962	-0.3	-0.810	43807	9.10805	C ₂₁ H ₁ 5O ₄	
168	333.0394	Theoretical	333.0410	1.6	4.835	518	9.08964	C ₁₉ H ₉ O ₆	

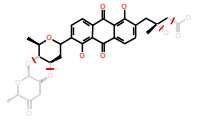
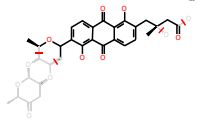
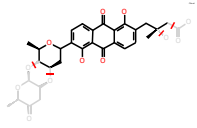
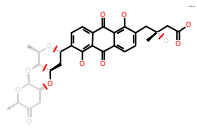
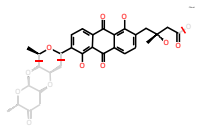
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
169	333.0757	Theoretical	333.0758	0.1	0.243	11874	9.10922	C ₂₀ H ₁₃ O ₅	
170	333.1121	Theoretical	333.1114	-0.7	-2.097	8647	9.10740	C ₂₁ H ₁₇ O ₄	
171	335.0914	Theoretical	335.0908	-0.6	-1.940	3487	9.11245	C ₂₀ H ₁₅ O ₅	
172	337.1071	Theoretical	337.1137	6.6	19.580	704	9.17081	C ₂₀ H ₁₇ O ₅	
173	337.1282	Theoretical	337.1264	-1.8	-5.329	436	9.11897	C ₁₇ H ₂₁ O ₇	

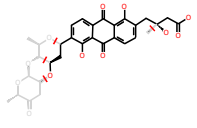
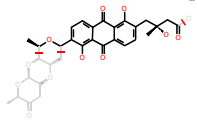
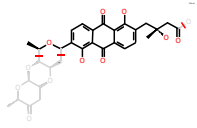
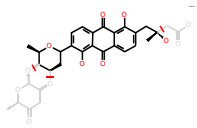
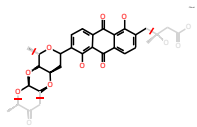
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
174	339.0863	Theoretical	339.0950	8.7	25.522	1545	9.10999	C19H15O6	
175	345.0757	Theoretical	345.0716	-4.1	-11.901	4670	9.10956	C21H13O5	
176	347.0914	Theoretical	347.0917	0.3	0.918	45645	9.10958	C21H15O5	
177	349.0343	Theoretical	349.0365	2.3	6.479	579	9.10506	C19H9O7	
178	349.0707	Theoretical	349.0693	-1.4	-4.028	3502	9.10561	C20H13O6	

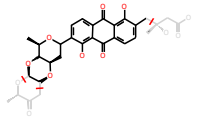
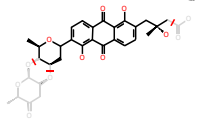
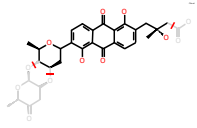
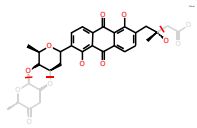
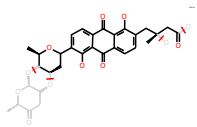
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observ ed RT	Formu la	Structure
179	349.1071	Theoretical	349.1055	-1.5	-4.302	8076	9.11120	C ₂₁ H ₁₇ O ₅	
180	351.0863	Theoretical	351.0864	0.1	0.175	7316	9.10957	C ₂₀ H ₁₅ O ₆	
181	360.0628	Theoretical	360.0605	-2.4	-6.557	895	9.11781	C ₂₁ H ₁₇ O ₆	
182	361.1071	Theoretical	361.1071	0.0	0.092	46827	9.10861	C ₂₂ H ₁₇ O ₅	
183	363.0863	Theoretical	363.0837	-2.6	-7.272	1821	9.11139	C ₂₁ H ₁₅ O ₆	

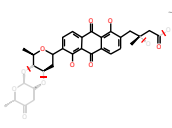
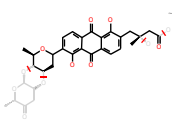
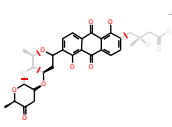
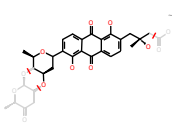
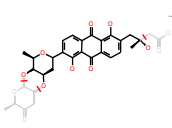
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
184	365.1020	Theoretical	365.1019	0.0	-0.059	12402	9.11427	C ₂₁ H ₁₇ O ₆	
185	367.0812	Theoretical	367.0811	-0.2	-0.448	2841	9.11045	C ₂₀ H ₁₅ O ₇	
186	368.0891	Theoretical	368.0970	7.9	21.503	1013	9.10899	C ₂₀ H ₁₆ O ₇	
187	373.1071	Theoretical	373.1067	-0.3	-0.818	17548	9.10866	C ₂₃ H ₁₇ O ₅	
188	375.0863	Theoretical	375.0858	-0.5	-1.367	3369	9.11618	C ₂₂ H ₁₅ O ₆	

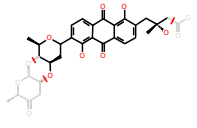
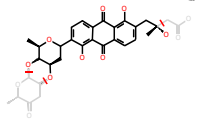
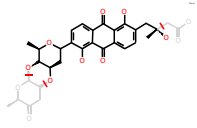
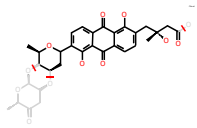
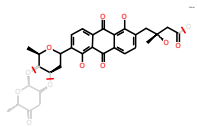
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
189	375.1227	Theoretical	375.1218	-0.9	-2.452	2368	9.10926	C23H19O5	
190	377.0656	Theoretical	377.0664	0.8	2.049	3113	9.11246	C21H13O7	
191	377.1020	Theoretical	377.1018	-0.1	-0.395	10417	9.11072	C22H17O6	
192	379.1540	Theoretical	379.1624	8.4	22.195	1397	9.01995	C23H23O5	
193	384.1567	Theoretical	384.1595	2.8	7.196	887	9.01528	C22H24O6	

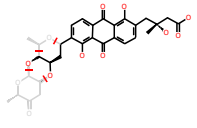
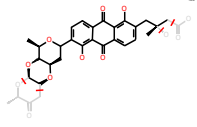
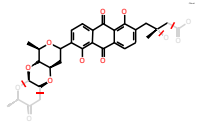
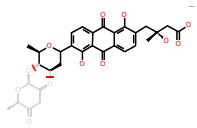
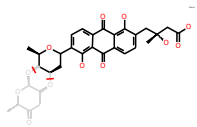
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
194	387.1227	Theoretical	387.1226	-0.1	-0.198	35448	9.10853	C ₂₄ H ₁₉ O ₅	
195	389.1020	Theoretical	389.1026	0.6	1.644	36410	9.11071	C ₂₃ H ₁₇ O ₆	
196	389.1384	Theoretical	389.1410	2.6	6.769	2401	9.10800	C ₂₄ H ₂₁ O ₅	
197	391.0812	Theoretical	391.0796	-1.6	-4.077	406	9.12230	C ₂₂ H ₁₅ O ₇	
198	394.1047	Theoretical	394.1109	6.2	15.624	940	9.10839	C ₂₂ H ₁₇ O ₇	

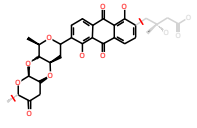
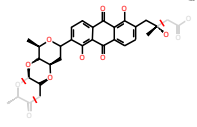
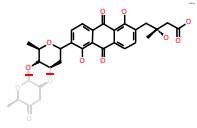
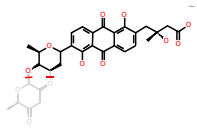
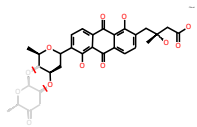
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
199	395.0761	Theoretical	395.0799	3.7	9.479	840	9.10759	C21H15O8	
200	395.1125	Theoretical	395.1173	4.8	12.083	3522	9.10997	C22H19O7	
201	396.1204	Theoretical	396.1150	-5.4	-13.635	563	9.09908	C22H20O7	
202	397.1646	Theoretical	397.1740	9.5	23.799	836	9.01774	C23H25O6	
203	405.0605	Theoretical	405.0643	3.8	9.400	1243	9.09463	C22H13O8	

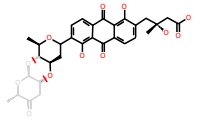
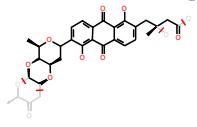
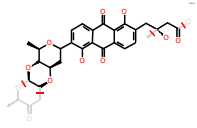
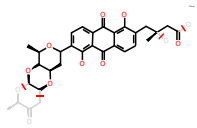
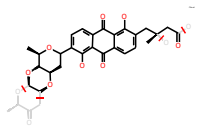
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
204	405.0969	Theoretical	405.0952	-1.7	-4.187	3220	9.13646	C23H17O7	
205	405.1333	Theoretical	405.1331	-0.2	-0.522	7832	9.10934	C24H21O6	
206	406.1411	Theoretical	406.1364	-4.7	-11.643	2134	9.10986	C24H22O6	
207	407.1125	Theoretical	407.1133	0.8	1.849	28305	9.11057	C23H19O7	
208	415.1176	Theoretical	415.1172	-0.4	-0.982	8680	9.11076	C25H19O6	

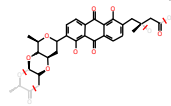
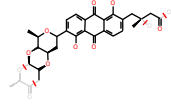
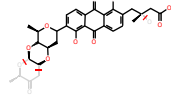
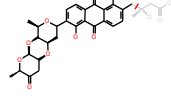
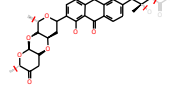
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
209	416.1254	Theoretical	416.1209	-4.5	-10.890	5093	9.11135	C ₂₅ H ₂₀ O ₆	
210	418.1411	Theoretical	418.1365	-4.6	-11.030	673	9.11160	C ₂₅ H ₂₀ O ₆	
211	419.0761	Theoretical	419.0796	3.5	8.279	4123	9.10616	C ₂₃ H ₁₅ O ₈	
212	422.1360	Theoretical	422.1424	6.4	15.177	615	9.18382	C ₂₄ H ₂₀ O ₇	
213	423.1074	Theoretical	423.1073	-0.1	-0.251	1874	9.11248	C ₂₃ H ₁₉ O ₈	

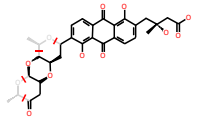
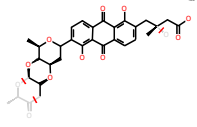
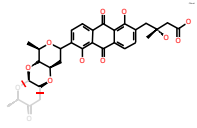
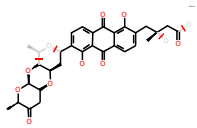
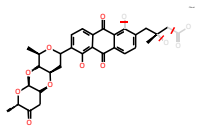
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
214	423.1438	Theoretical	423.1469	3.1	7.281	579	9.12655	C ₂₄ H ₂ 307	
215	424.1153	Theoretical	424.1088	-6.5	-15.34 6	376	9.15413	C ₂₃ H ₂ 008	
216	425.1231	Theoretical	425.1268	3.7	8.637	14965	9.10830	C ₂₃ H ₂ 108	
217	432.1204	Theoretical	432.1194	-0.9	-2.196	632	9.10232	C ₂₅ H ₂ 007	
218	433.1282	Theoretical	433.1281	-0.1	-0.169	15103	9.11324	C ₂₅ H ₂ 107	

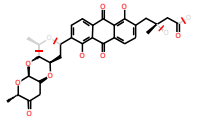
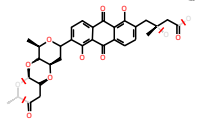
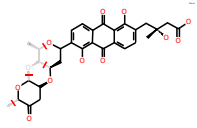
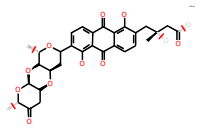
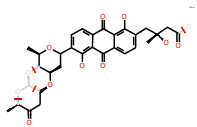
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
219	437.0867	Theoretical	437.0928	6.1	14.013	1080	9.10667	C23H17O9	
220	445.1282	Theoretical	445.1295	1.3	3.017	3127	9.11174	C26H21O7	
221	447.1438	Theoretical	447.1461	2.3	5.174	1168	9.10804	C26H23O7	
222	450.1309	Theoretical	450.1284	-2.5	-5.575	423	9.11345	C25H22O8	
223	451.1387	Theoretical	451.1392	0.5	1.019	13229	9.11527	C25H24O8	

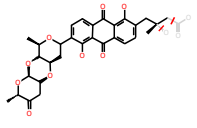
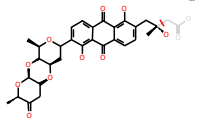
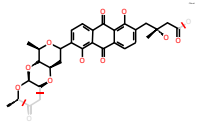
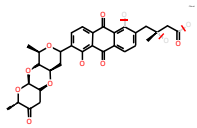
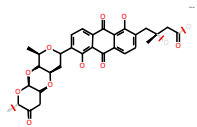
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
224	463.1024	Theoretical	463.1074	5.0	10.813	2555	9.12072	C25H19O9	
225	463.1387	Theoretical	463.1427	4.0	8.620	993	9.10839	C26H23O8	
226	466.1258	Theoretical	466.1239	-1.9	-4.084	330	9.11423	C25H22O9	
227	467.1337	Theoretical	467.1332	-0.5	-1.023	1071	9.14318	C25H23O9	
228	468.1415	Theoretical	468.1408	-0.6	-1.385	438	9.13522	C25H24O9	

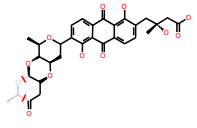
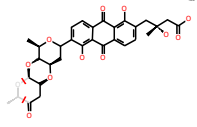
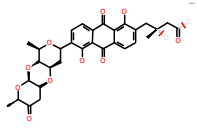
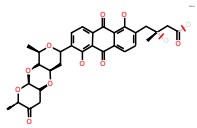
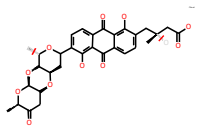
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
229	469.1493	Theoretical	469.1486	-0.7	-1.473	11282	9.11948	C25H2 5O9	
230	473.1231	Theoretical	473.1197	-3.4	-7.120	1355	9.10868	C27H2 1O8	
231	475.1024	Theoretical	475.0991	-3.2	-6.765	379	9.08403	C26H1 9O9	
232	475.1387	Theoretical	475.1382	-0.6	-1.168	7039	9.10951	C27H2 3O8	
233	477.1544	Theoretical	477.1550	0.6	1.296	624	9.11123	C27H2 5O8	

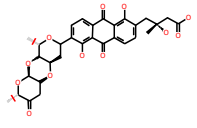
	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
234	488.1466	Theoretical	488.1387	-7.9	-16.135	501	9.10883	C28H24O8	
235	489.1544	Theoretical	489.1540	-0.4	-0.736	7732	9.10981	C28H25O8	
236	491.1337	Theoretical	491.1307	-3.0	-6.028	1143	9.11799	C27H23O9	
237	493.1493	Theoretical	493.1489	-0.4	-0.728	7066	9.10923	C27H25O9	
238	501.1180	Theoretical	501.1201	2.1	4.159	3879	9.10567	C28H21O9	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
239	505.1129	Theoretical	505.1147	1.8	3.492	300	9.10106	C27H2 1010	
240	505.1493	Theoretical	505.1498	0.5	1.060	792	9.11569	C28H2 509	
241	511.1599	Theoretical	511.1574	-2.5	-4.864	135	9.18608	C27H2 7010	
242	515.1337	Theoretical	515.1254	-8.2	-15.94 7	586	9.16222	C29H2 309	
243	515.1700	Theoretical	515.1694	-0.7	-1.338	10700	9.10768	C30H2 708	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
244	517.1493	Theoretical	517.1494	0.1	0.225	9951	9.11175	C ₂₉ H ₂ 5O ₉	
245	519.1650	Theoretical	519.1649	-0.1	-0.154	166183	9.10803	C ₂₉ H ₂ 7O ₉	
246	520.1000	Theoretical	520.0975	-2.6	-4.922	689	9.10688	C ₂₇ H ₂ 0O ₁₁	
247	529.1129	Theoretical	529.1164	3.4	6.491	1715	9.10748	C ₂₉ H ₂ 1O ₁₀	
248	531.1650	Theoretical	531.1645	-0.5	-0.958	927	9.18372	C ₃₀ H ₂ 7O ₉	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
249	533.1806	Theoretical	533.1808	0.2	0.304	465316	9.10749	C30H2 9O9	
250	537.1755	Theoretical	537.1760	0.5	0.875	12191	9.10625	C29H2 9O10	
251	541.2068	Theoretical	541.2015	-5.4	-9.915	399	9.10832	C29H3 3O10	
252	543.1650	Theoretical	543.1645	-0.5	-0.891	4627	9.11085	C31H2 7O9	
253	549.1755	Theoretical	549.1753	-0.3	-0.476	9617	9.18256	C30H2 9O10	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
254	551.1548	Theoretical	551.1512	-3.6	-6.545	2075	9.18817	C ₂₉ H ₂₇ O ₁₁	
255	553.1704	Theoretical	553.1696	-0.9	-1.598	6742	9.10796	C ₂₉ H ₂₉ O ₁₁	
256	560.1677	Theoretical	560.1615	-6.2	-11.127	1123	9.10742	C ₃₁ H ₂₈ O ₁₀	
257	561.1755	Theoretical	561.1757	0.2	0.365	278636	9.10860	C ₃₁ H ₂₉ O ₁₀	
258	565.1704	Theoretical	565.1698	-0.6	-1.087	851	9.20533	C ₃₀ H ₂₉ O ₁₁	

	Expected m/z	Status	Observed m/z	Mass error (Da)	Mass error (ppm)	Detector counts	Observed RT	Formula	Structure
259	569.1654	Theoretical	569.1653	0.0	-0.017	852	9.18988	C ₂₉ H ₂ 9O ₁₂	
260	579.1861	Theoretical	579.1866	0.5	0.930	1100130	9.10959	C ₃₁ H ₃ 10O ₁₁	