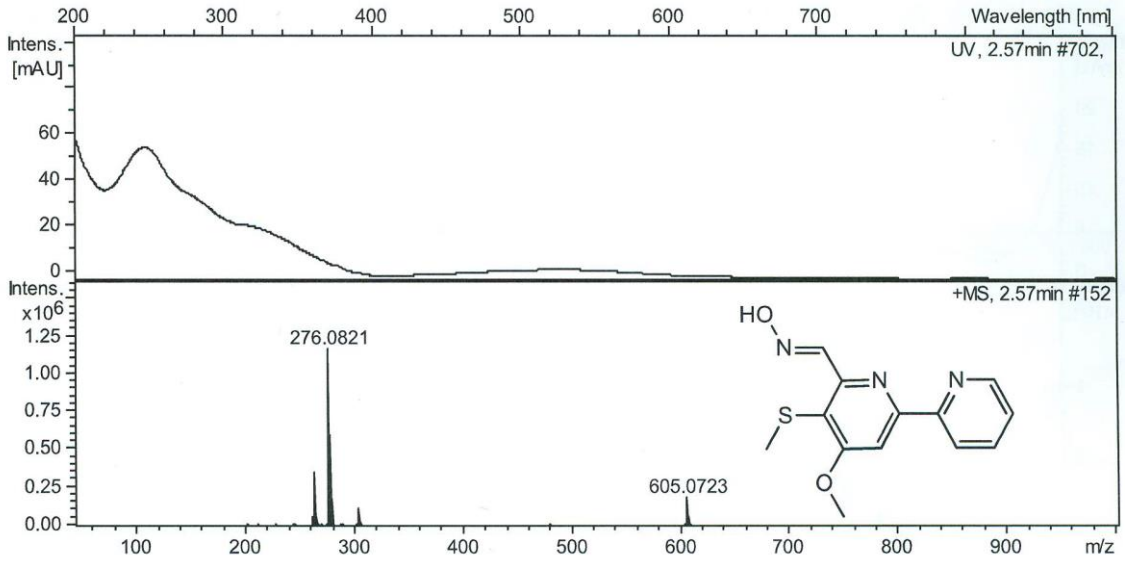
LC-MS dereplication.

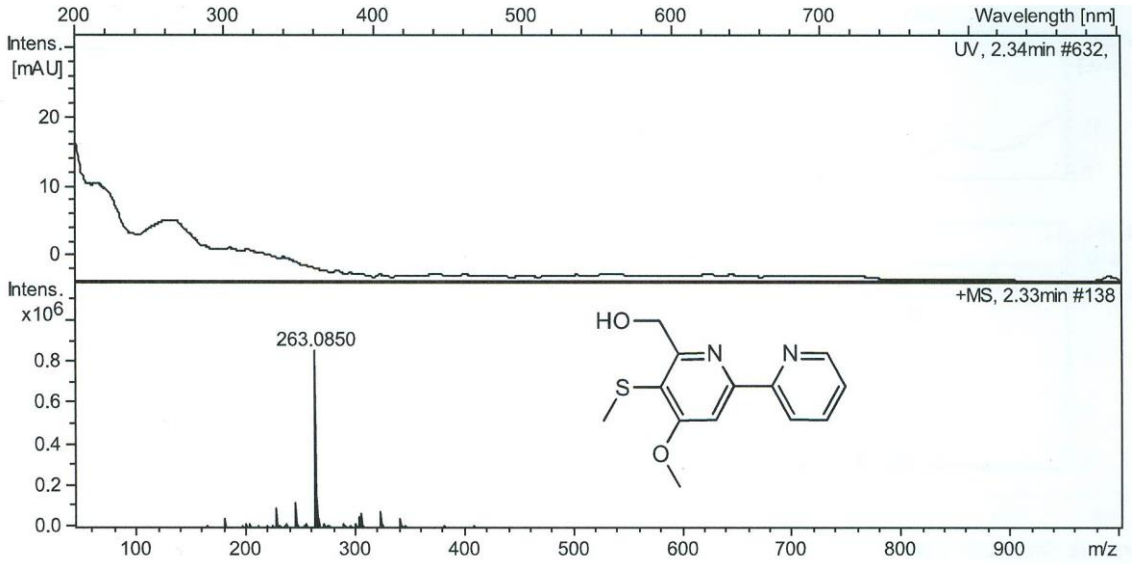
Section 3.2. New or incremented antibiotic production in VOC chambers

CS014:

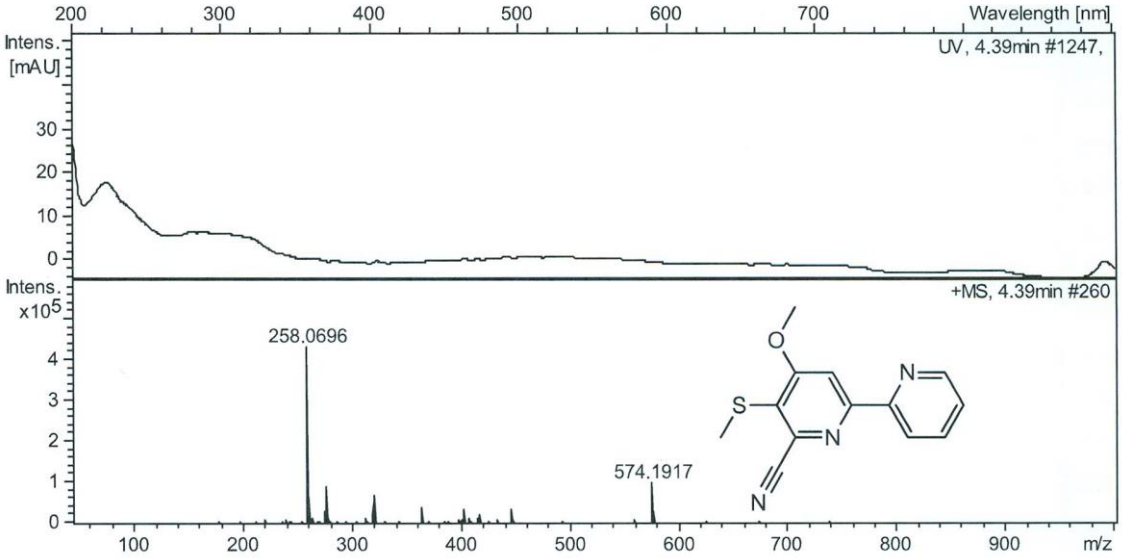
Collismycin A-B, $C_{13}H_{13}N_3O_2S$:



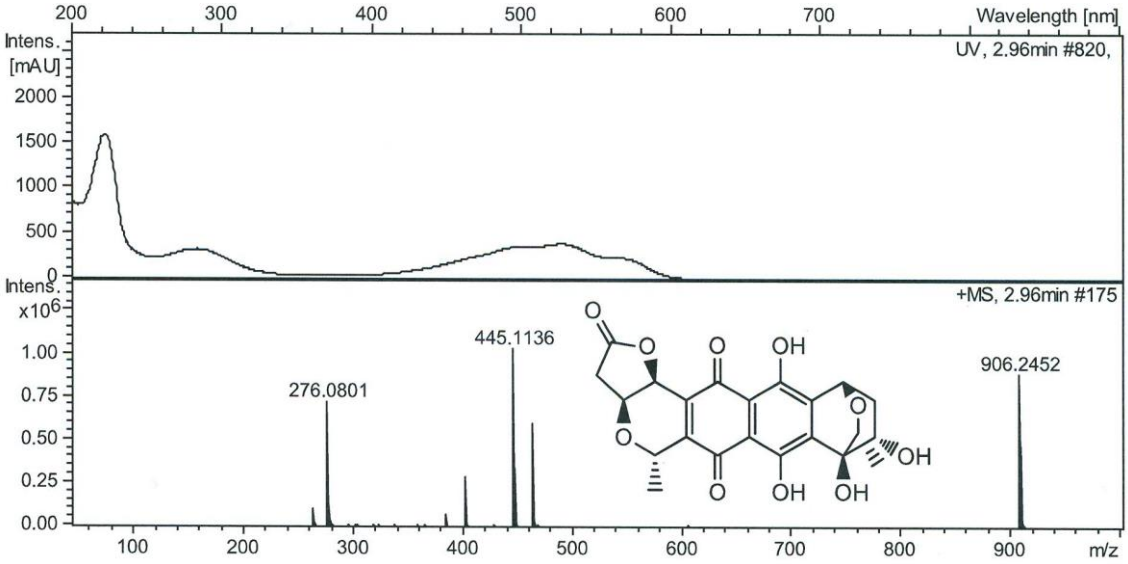
Collismycin C, $C_{13}H_{14}N_2O_2S$:



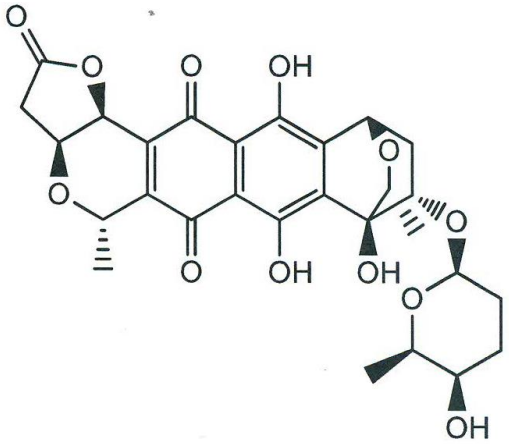
Collismycin D, $C_{13}H_{11}N_3OS$:

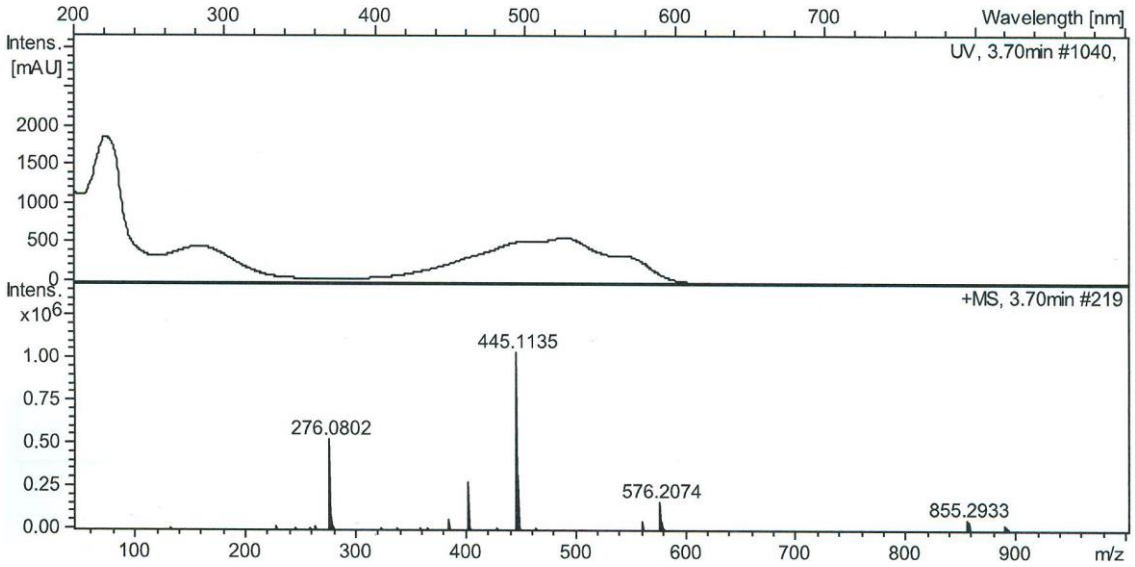


Granaticin A, $C_{22}H_{20}O_{10}$:



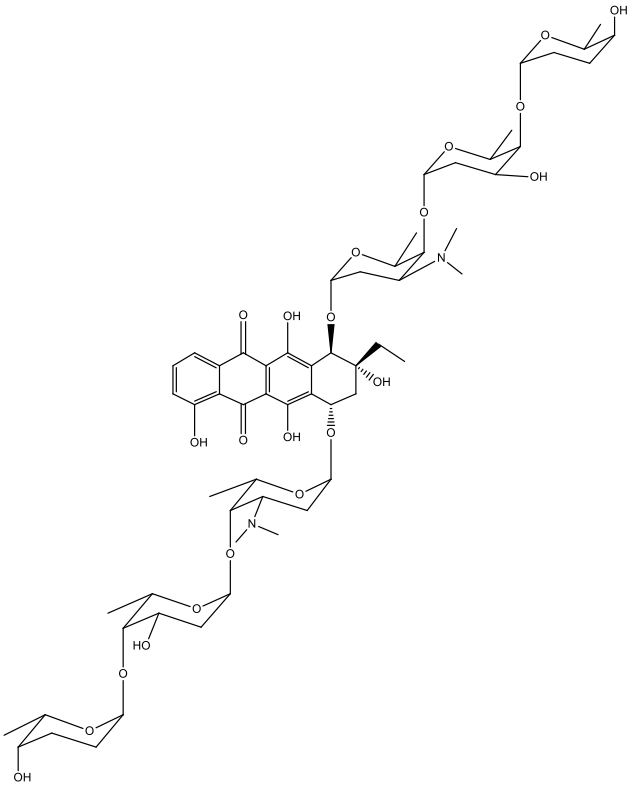
Granaticin C, $C_{28}H_{30}O_{12}$:

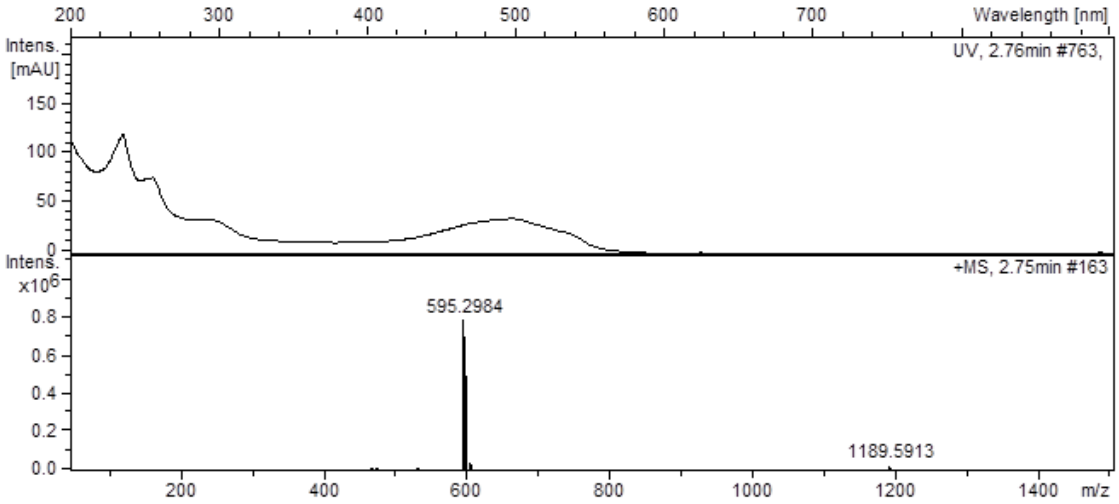




CS081a:

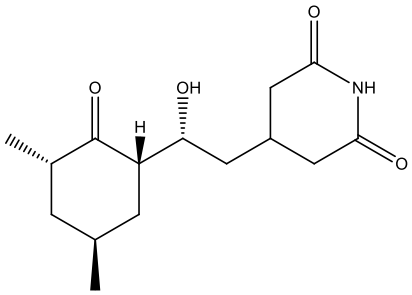
Cosmomycin D, $C_{60}H_{88}N_2O_{22}$:

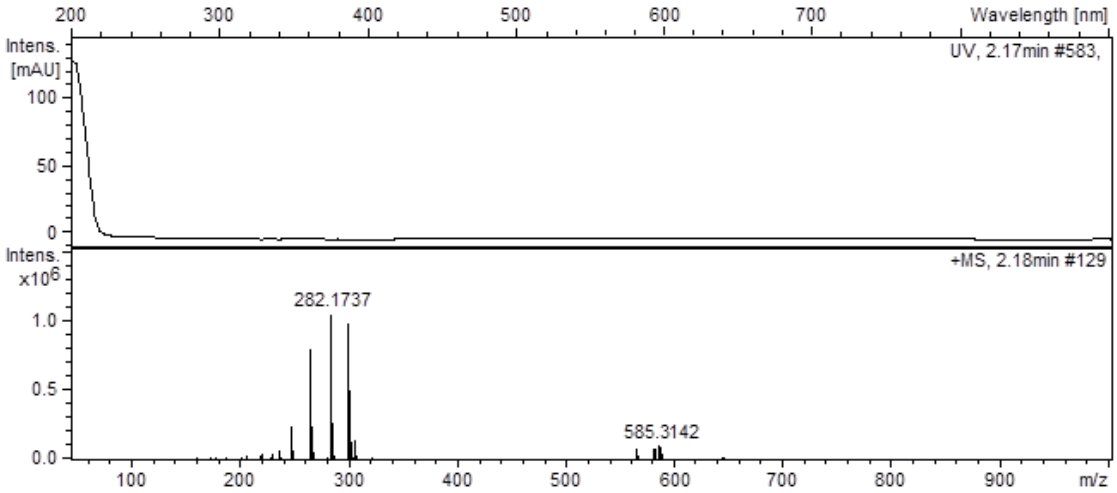




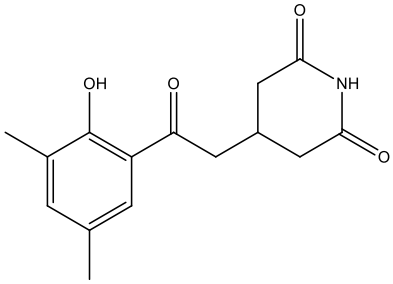
CS057:

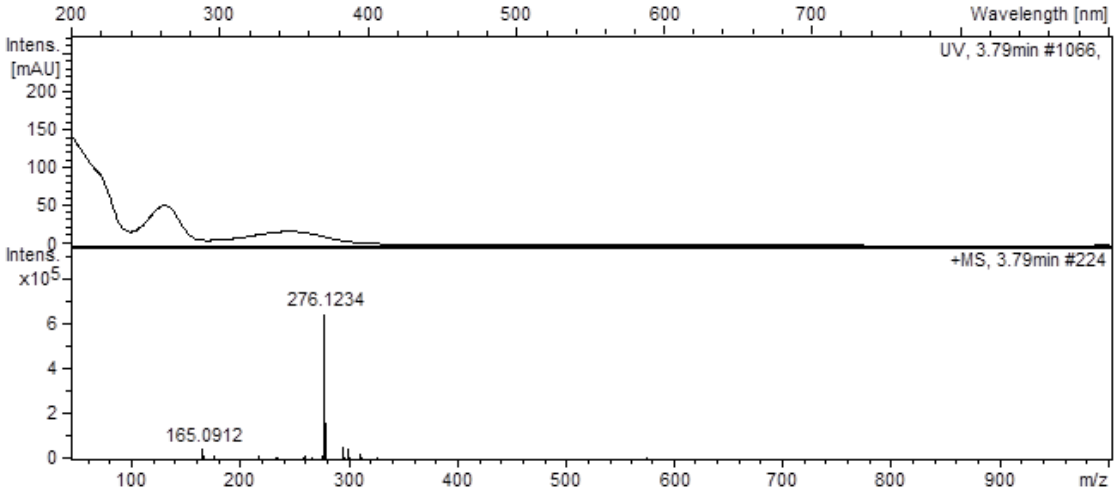
Cycloheximide, $C_{15}H_{23}NO_4$:





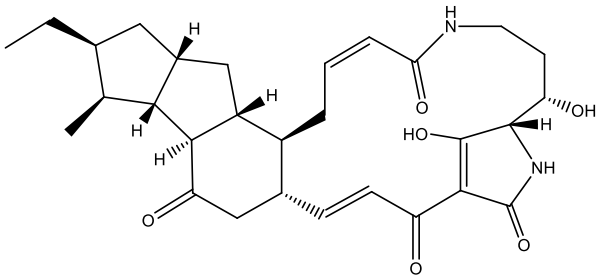
Actiphenol, $C_{15}H_{17}NO_4$:

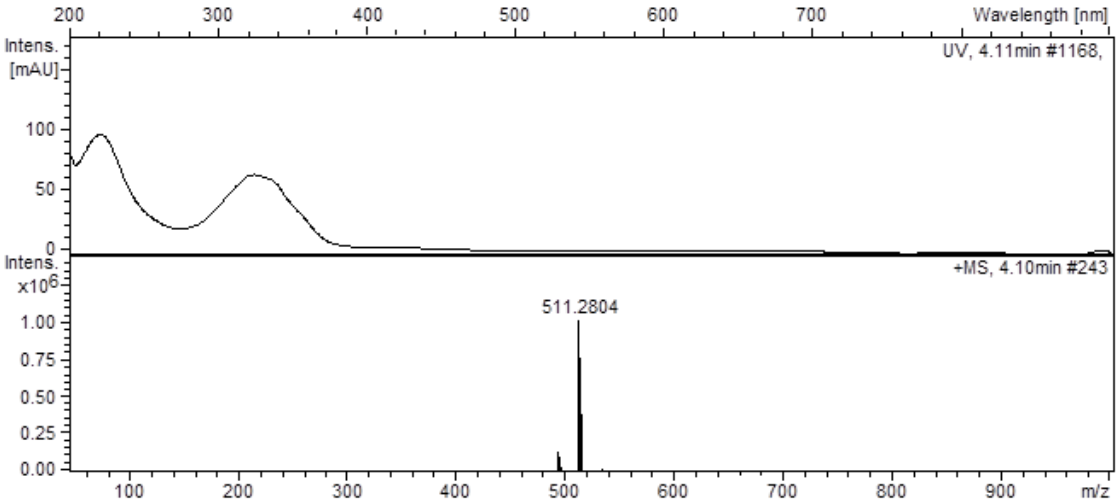




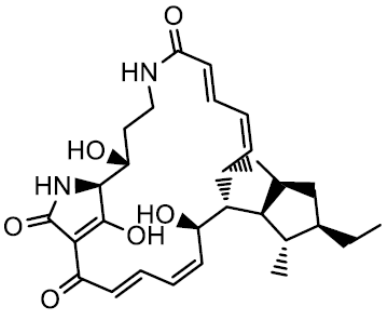
CS090a:

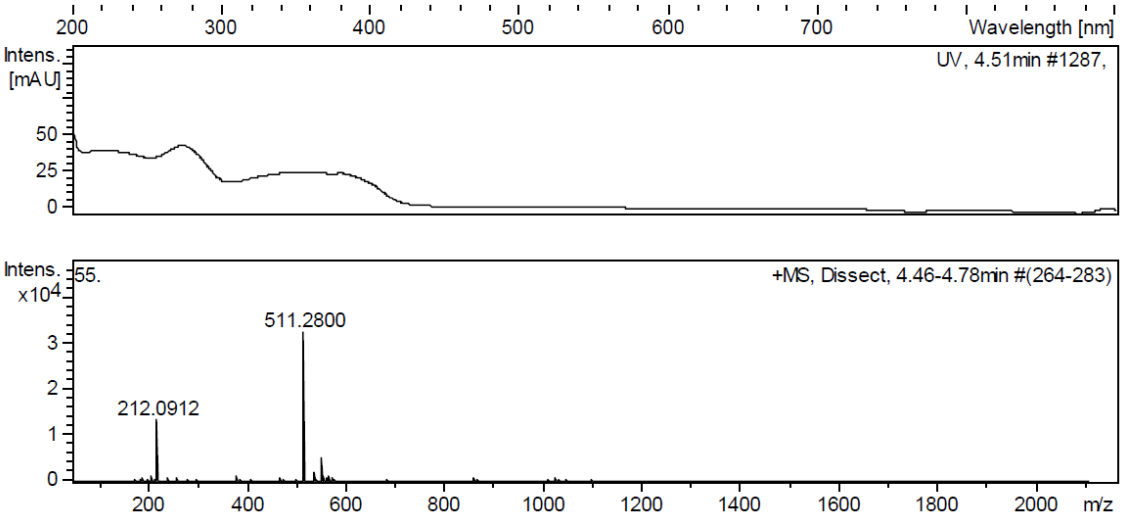
Maltophilin, $C_{29}H_{38}N_2O_6$:





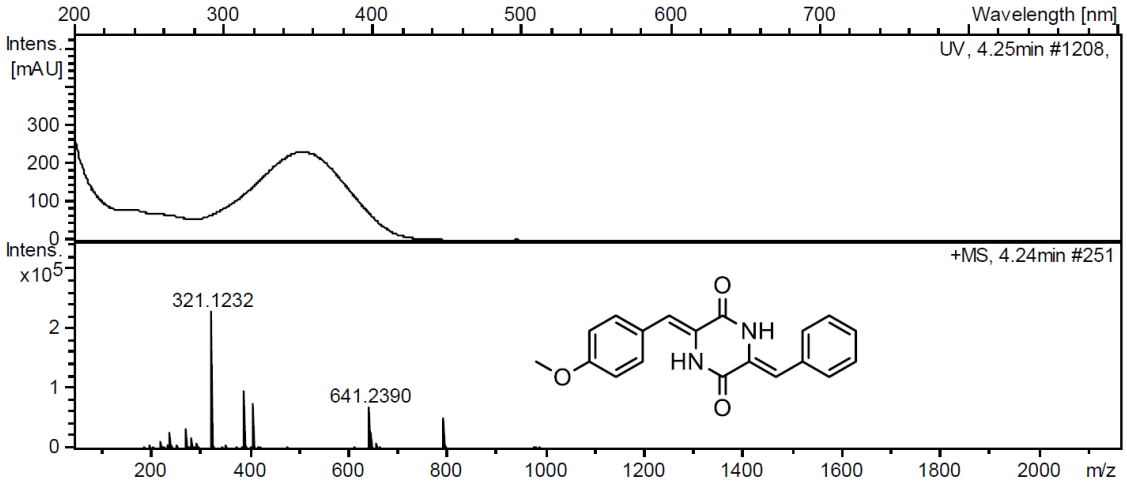
Alteramide A, $C_{29}H_{38}N_2O_6$:



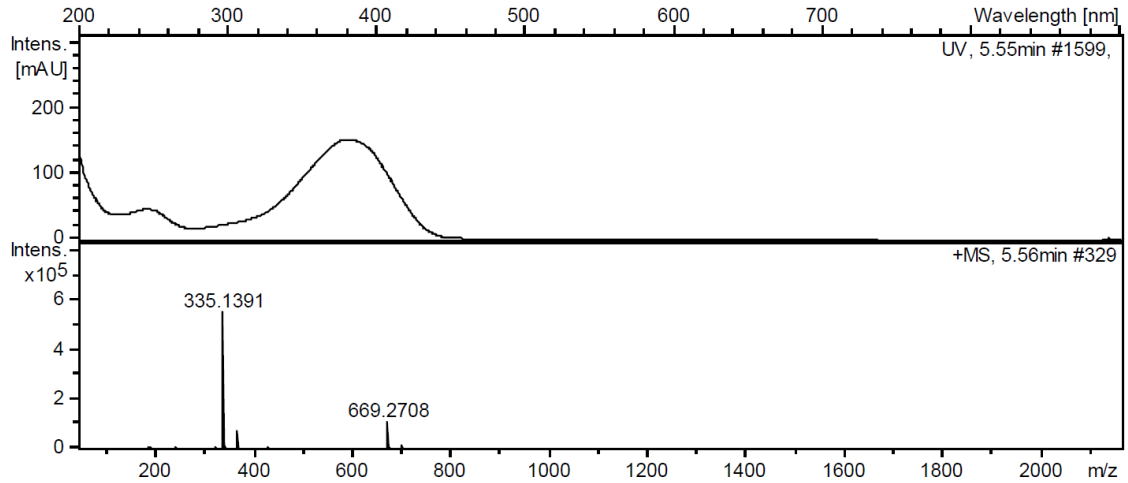


CS194:

Piperazinedione XR 334, $C_{19}H_{16}N_2O_3$:

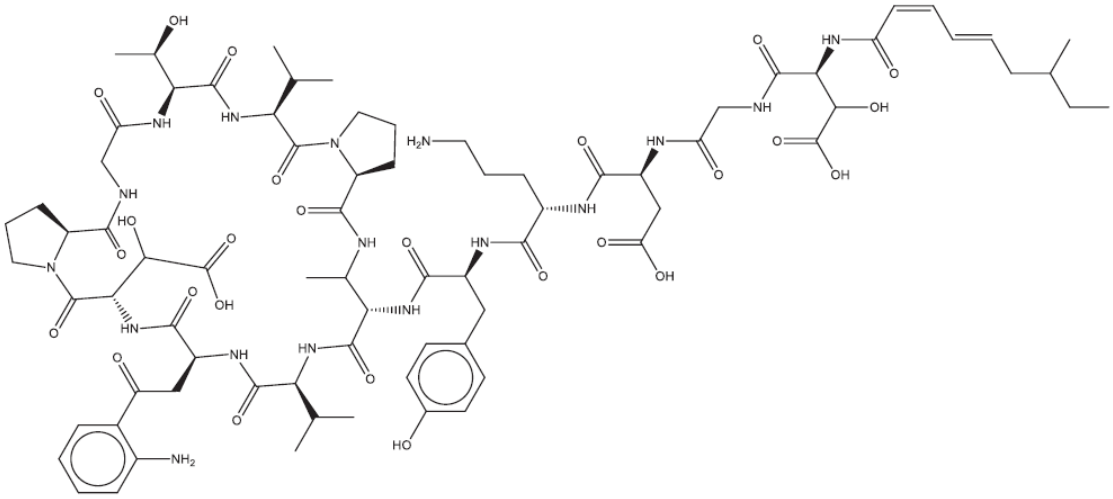


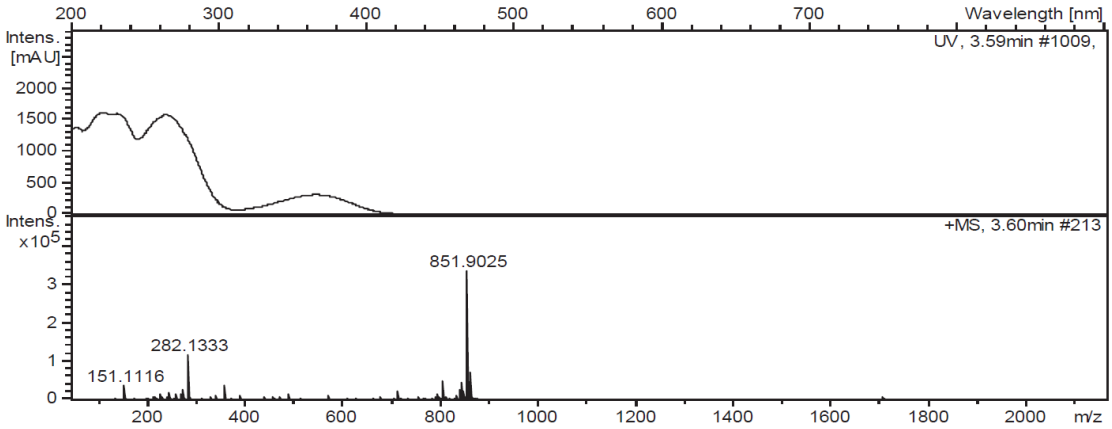
Piperazinedione XR 330, $C_{20}H_{18}N_2O_3$:



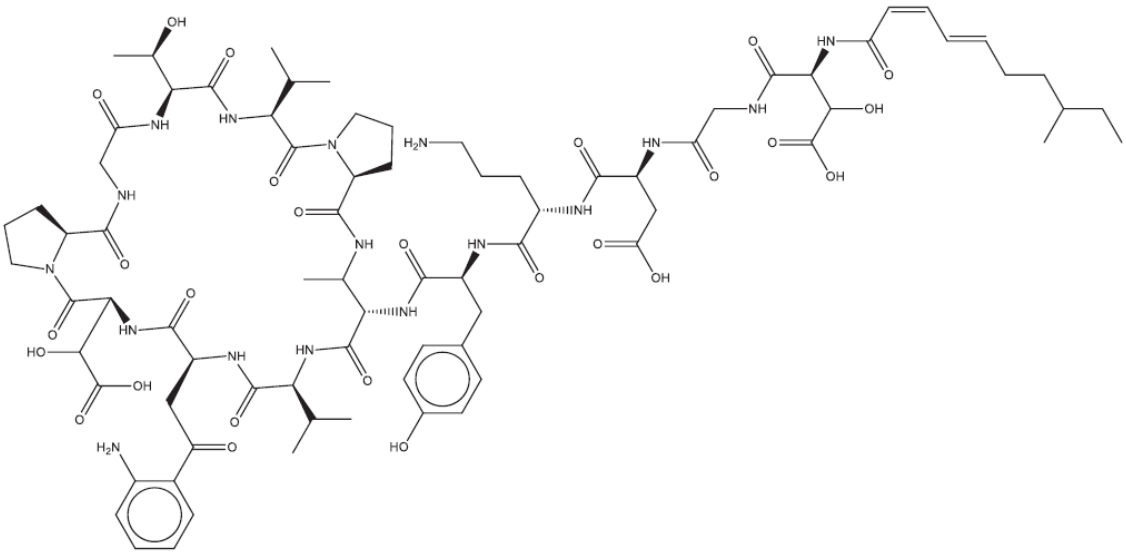
CS149:

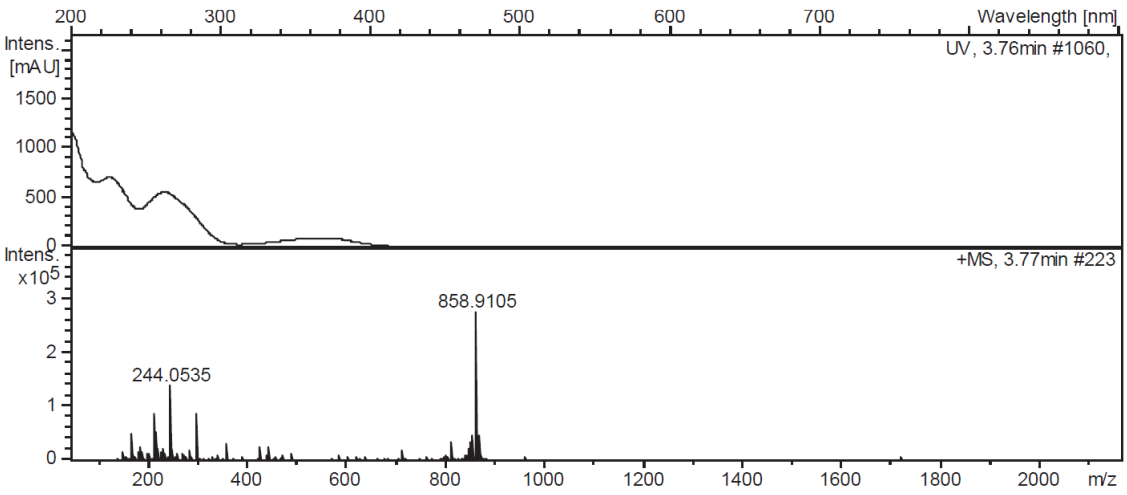
Rumycin 1, $C_{78}H_{111}N_{17}O_{26}$:





Rumycin 2, $C_{79}H_{113}N_{17}O_{26}$:

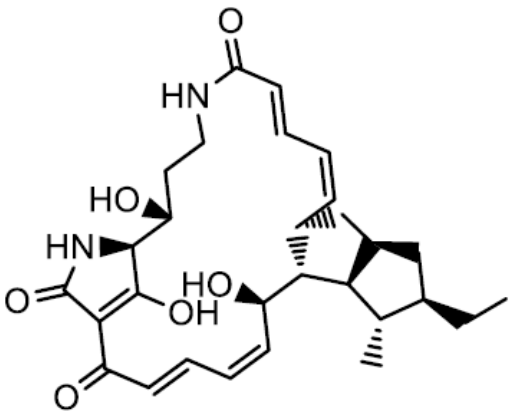


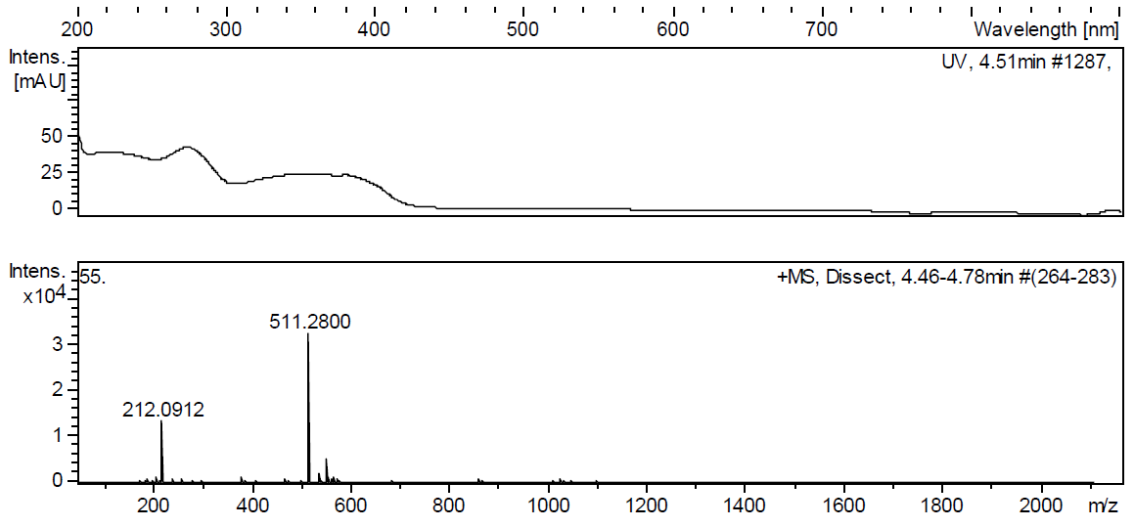


Section 3.3. Effect of VOCs in multiple co-culture

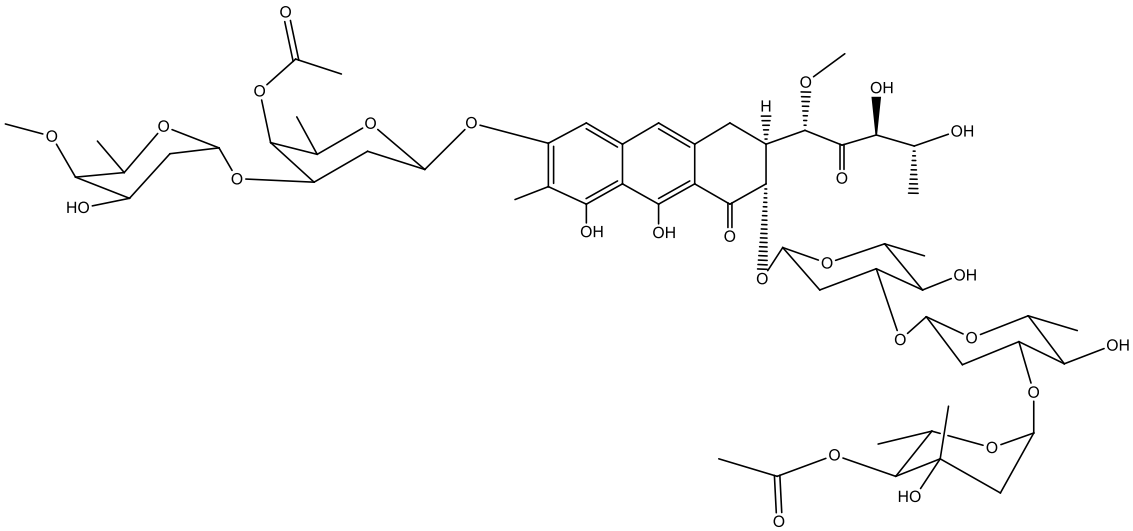
CS065a:

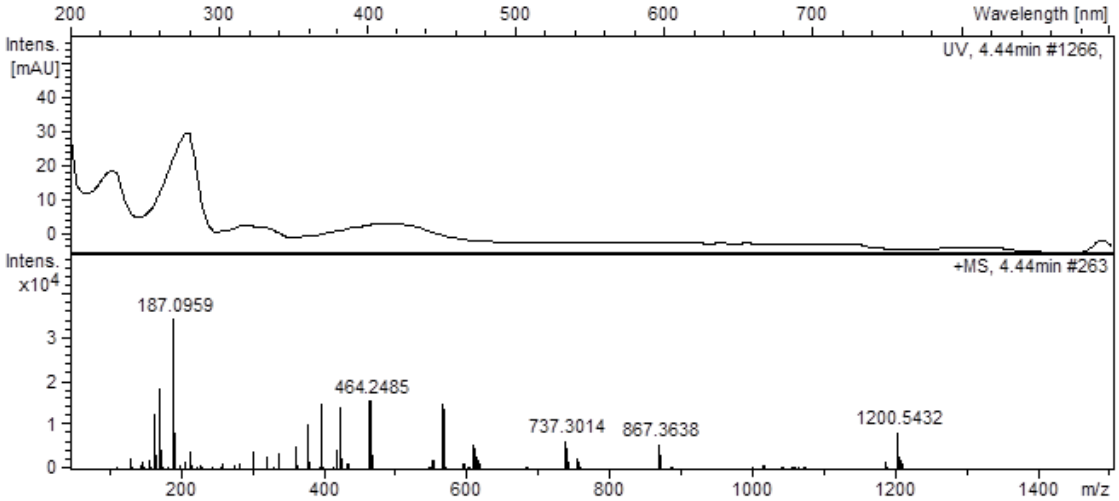
Alteramide A, $C_{29}H_{38}N_2O_6$:





Chromomycin A3, $C_{57}H_{82}O_{26}$:





Overview of the dereplication analysis.

Compound	**Molecular formula**	**Measured mass**	**Calculated mass**	**Most prominent ions**	**UV max (nm)**
Collismycin A-B	$C_{13}H_{13}N_3O_2S$	276.0821	275.33	276.0821 605.0723	249,5 332,7 469,8
Collismycin C	$C_{13}H_{14}N_2O_2S$	263.0850	262.33	263.0850	225,0 249,5 332,7 469,8

Collismycin D	$C_{13}H_{11}N_3OS$	258.0696	257.32	258.0696 574.1917	225,0 332,7 469,8
Granaticin A	$C_{22}H_{20}O_{10}$	445.1136	444.39	276.0801 445.1136 906.2452	215,3 280,9 494,2
Granaticin C	$C_{28}H_{30}O_{12}$	576.2074	558.54	276.0802 445.1135 576.2074 855.2933	215,3 280,9 494,2
Cosmomycin D	$C_{60}H_{88}N_2O_{22}$	1189.5913	1189.36	595.2984 1189.5913	235,4 255,0 295,0 493,5
Cycloheximide	$C_{15}H_{23}NO_4$	282.1737	281.35	282.1737 585.3142	200,0
Actiphenol	$C_{15}H_{17}NO_4$	276.1234	275.30	165.0912 276.1234	216,5 262, 4 345,2
Maltophilin	$C_{29}H_{38}N_2O_6$	511.2804	510.63	511.2804	222,6 322,8
Alteramide A	$C_{29}H_{38}N_2O_6$	511.2800	510.63	212.0912 511.2800	273,5 360,1
Piperazinedione XR 334	$C_{19}H_{16}N_2O_3$	321.1232	320.35	321.1232 641.2390	241,0 334,6
Piperazinedione XR 330	$C_{20}H_{18}N_2O_3$	335.1391	334.38	335.1391 669.2708	241,0 334,6
Rumycin 1	$C_{78}H_{111}N_{17}O_{26}$	851.9025	1702.84	151.1116 282.1333 851.9025	231,2 264,4 365,1
Rumycin 2	$C_{79}H_{113}N_{17}O_{26}$	858.9105	1716.87	244.0535 858.9105	226,9 261.8 365,7
Chromomycin A3	$C_{57}H_{82}O_{26}$	1200.5432	1183.26	187.0959 464.2485 737.3014 867.3638 1200.5432	229,3 277,8 317,3 403.7