Supplementary Information

Observing the Invisible through Imaging Mass Spectrometry, a Window into the Metabolic Exchange Capacity of Microbes

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Contents

Supplementary Table 1 Growth conditions and MALDI signals of the strains used in this study. Column definitions: (i) Strains. Indicates the specific name of the organism used in the study. (ii) Medium. Indicates the specific medium used to grow the organism. (iii) Growth time. Indicates the growth time in days (d) of the organism before analysis. (iv) MALD-I mass range. Indicates the mass-to-charge (m/z) range monitored during data collection. (v) Mass-to-charge signals observed. Ions with spatial distributions either colony bound or released into the agar and had distinct patterns to the matrix peaks were recorded as ion candidates. (vi) Identified ions. Indicates ions that were structurally verified by tandem mass spectrometry including parent masses [M] and salt adducts [Na or K]. (vii) References. List of publications with information either on the specific strain used or the resolved molecules.

Strains	**Medium**	**Growth time**	**MALDI-I (m/z range)**	**m/z signals observed**	**The ions identified (SI-4) annotated m/z signals**	**References**
Beauveria bassiana ATCC 7159	ISP-2	6d	(200-3700)	204, 217, 222, 231, 236, 242, 246, 258, 260, 274, 281, 370, 296, 397, 412, 428, 461, 477, 520, 522, 575, 577, 579, 591, 593, 597, 600, 613, 615,617, 629, 631, 654, 656, 804, 807, 823, 932, 948	Beauvericin ([M+Na]$^+$, 807; [M+K]$^+$,823), Bassianolide ([M+Na]$^+$, 932; [M+K]$^+$, 948)	Xu, 2009
	PDA	6d	(200-3400)	231, 393, 397, 412, 520, 577, 600, 656, 688, 767, 789, 807, 823, 932, 948		
Chaetomium chiversii CS-36-62	ISP-2	5d	(200-1600)	404, 409, 490, 492, 505, 507, 530, 542, 546, 557, 562, 611, 633, 649, 667, 689, 705		Wang, 2009
	PDA	5d	(200-1600)	404, 409, 412, 486, 520, 542, 546, 404, 409, 490, 492, 505, 507, 530, 542, 546, 557, 562, 611, 633, 649, 667, 689, 705611, 633, 649, 667, 689, 705		
Fusarium verticillioides 5777	ISP-2	5d	(300-3600)	664, 1311, 1327, 655, 677, 693		Zhu, 2008
	PDA	5d	(300-3600)	751, 760, 766, 893 1311, 1327, 655, 677, 693		
Fusarium sp.CNL 292	ISP-2	5d	(350-3000)	412, 645, 647, 663, 673, 675, 691, 802, 609, 625		Belofsky, 1999
	A1	5d	(350-1600)	412, 496, 562, 581, 595, 587, 609, 625		
Acremonium sp. CNC890	ISP-2	5d	(300-3600)	515, 520, 531, 764, 780, 796		This study
	A1	5d	(300-3600)	476, 750, 764, 766, 780, 796, 876		

Fusarium sp.CNC 477	ISP-2	5d	(200-3600)	258, 296, 493, 515, 531, 547		Renner 1998
	A1	7d	(350-1600)	493, 515, 531, 547, 747		
Thermofungus C030813_30	PDA		(350-1600)	460, 476, 546,688, 739, 767, 842, 863, 881		This study
Thermofungus C030813_40	PDA		(350-1600)	445, 460, 589, 656, 672, 751, 767, 771, 786, 881		
Salinispora arenicola CNS205	A1	15d	(350-1600)	354, 365, 447, 458, 497, 527, 540, 556, 655, 672, 729, 751, 767, 940		Schultz 2008
Salinispora pacifica CNS 143	A1	11d	(250-1600)	None		Jensen 2006
Salinispora pacifica CNT 133	A1	11d	(250-1600)	495		This study
Salinispora arenicola CNH 643	A1	11d	(250-1600)	457, 467, 489, 556		This study
Salinispora arenicola CNT 088	A1	11d	(250-1600)	354, 557		Asolkar 2009
Actinomycete CNS 575	ISP-2	16d	(250-1600)	879, 901, 917	Etamycin of [M+H] +, 879; [M+Na]+, 901; and [M+K]+, 917.	Haste 2010
	A1	11d	(250-1600)	623, 901, 917		
Streptomyces sp. SPB74	ISP-2	10d	(300-3600)	637, 682, 857, 877, 909, 1044, 1046, 1105		Oh 2009
Streptomyces sp. AA#4	ISP-2	7d	(300-3600)	655, 666, 682, 693, 720, 777, 877, 1059, 1073, 1089, 1102, 1111, 1182, 1354.		This study
Streptomyces sp. Mg1	ISP-2	8d	(300-3600)	668, 973, 1007, 1988, 1904, 1969, 1985, 2003		This study
Streptomyces sp. WASP	ISP-2	7d	(300-3600)	582, 618, 634, 656, 672, 705		This study
S.coelicolor A3(2)	ISP-2	8d	(300-3600)	424, 392, 394, 1536, 2027, 2065	Prodiginines(392, 394), CDA(1536), sapB(2027, 2065)	Yang 2009
S. roseosporus NRRL15998	ISP-2	8d	(300-3600)	799, 815, 831, 845, 848, 862, 864, 878, 893, 972, 2237, 2253		Debono 1987
S. hygroscopicus ATCC53653	ISP-2	10d	(300-3600)	1038, 1060, 1076, 1102, 1118, 1136, 1462, 1476, 1490, 1548, 1562, 1573, 1587, 1601, 1615, 1629, 1639, 1653, 1667		Lam 1990
S. albus J1074	ISP-2	9d	(300-3600)	486, 655, 732, 950, 1061, 1077, 1093, 1109, 2266, 2282, 2304. 1320		Lombó 2006
S. ghanaensis 14672	ISP-2	7d	(300-3600)	666, 739, 809, 823, 841, 2014, 2052		Endler 1998

S. clavuligerus ATCC 53653	ISP-2	9d	(300-3600)	2181, 2197, 2219, 2235		
S. roseosporus NRRL11379	ISP-2	11d	(300-3600)	1207, 1209, 1221, 1223, 1237, 1673, 1687, 1701, 1705, 1719, 1733, 1747, 1749, 2236, 2252		Huber 2005
S. pristinispiralis ATCC25486	ISP-2	8d	(300-3600)	641, 645, 650, 673, 711, 2014, 1036, 2052, 2074, 2090		This study
S.viridochromogenes 40736	ISP-2	7d	(300-3600)	992, 1689. 1711, 1727, 2068, 2169		Blodgett 2005
Streptomyces sviceus 29083	ISP-2	7d	(300-3600)	1698, 1812, 1826, 1954, 1870, 1888, 1910, 1926, 1948, 1968, 1984, 2084, 2106, 2122, 2138, 2154		This study
Streptomyces sp. SPB 78	ISP-2	7d	(300-3600)	509, 540, 553, 587, 589, 2251, 2267, 2289, 2305		This study
Kutzneria sp. 744	ISP-2	7d	(300-3600)	867, 883, 888, 905, 907, 921, 923, 942, 944, 958, 960, 983, 998, 1065, 1073, 1087, 1089, 1103, 1131, 1133,		Broberg 2006
Actinoplanes teichomyceticus PSK0532	ISP-2	7d	(300-3600)	666, 682, 684, 893, 1189		This study
Streptoverticillium griseoverticillatum ATCC 31499	ISP-2	8d	(300-3600)	693, 709, 809, 1728, 1750, 1766, 2025, 2041, 2057, 2063, 2079, 2101, 2117, 2139, 2155	Cinnamycin ([M+H] +, 2041), [M+Na]+, 2063; [M+K]+,2079)	Kaletta 1991
Pseudomonas aeruginosa PAO	ISP-2	2d	(500-2000)	577, 591, 616, 625, 651, 740, 746, 756, 760, 770, 778, 794, 798, 808, 830, 714, 1334	Polyglutamate (714),	Meyer 1996
Staphylococcus aureus USA300	ISP-2	2d	(300-3600)	537, 551, 565,594, 748, 762, 775, 785, 797, 799, 804, 814, 841, 886, 904, 916, 931, 941, 946, 957, 970, 974,	δ-toxin (3006)	Schlievert 2010
Nostoc sp. PCC 7120	BG-11	12d	(300-3600)	775, 871, 1013, 1338, 1500	Pheophytin A ([M+H]+, 871)	Dembitsky 2005
Lysobacter enzymogenes C3	ISP-2	4d	(300-3600)	571, 573, 587, 589, 1106, 1108, 1275, 1277, 1484, 1500, 1516, 1536, 1549, 1563, 1571, 1577, 1581, 1585, 1601, 1615, 1633, 1649, 1715, 1729, 1743, 1757, 1771, 1785, 1799, 1813, 511, 533, 549, 513, 535, 551	Maltophilin ([M+H] +, 511), [M+Na]+, 533; [M+K]+,549). Dihydromaltophilin ([M+H] +, 513), [M+Na]+, 535; [M+K]+,551)	Yu 2007
Bacillus subtilis 3610	ISP-2	2d	(300-3600)	655, 714, 1031, 1045, 1047, 1059, 1061, 1075, 1517, 1531, 1545	Polyglutamate (714), Surfactin(1075), Plipastatin (1545)	Yang 2009
Bacillus pumilus CNJ762	ISP-2	3d	(200-3800)	551, 616, 655, 844, 1051, 1059, 1073, 1087, 714, 1075, 1089, 1103, 1117	Polyglutamate (714), Surfactin (1075)	This study
	A1	5d	(300-3600)	1059, 1073, 1081, 1087, 1095, 1101, 1123, 1133, 1089, 1103, 1117		

Rhizobium leguminosarum S36	ISP-2	6d	(300-3600)	415, 563, 814, 843	This study
Pseudomonas fluorescens PFO-1	ISP-2	3d	(300-3600)	395, 428, 563, 575, 578, 585, 590, 592, 604, 616, 626, 648, 652, 664, 678, 680, 700, 715, 733, 743, 747, 761	This study
Mycobacterium smegmatis MC2 155 ISP-2	ISP-2	6d	(300-3600)	715, 1275, 1287, 1301	Billman-Jacobe 2002

References to accompany Supplementary Table 1

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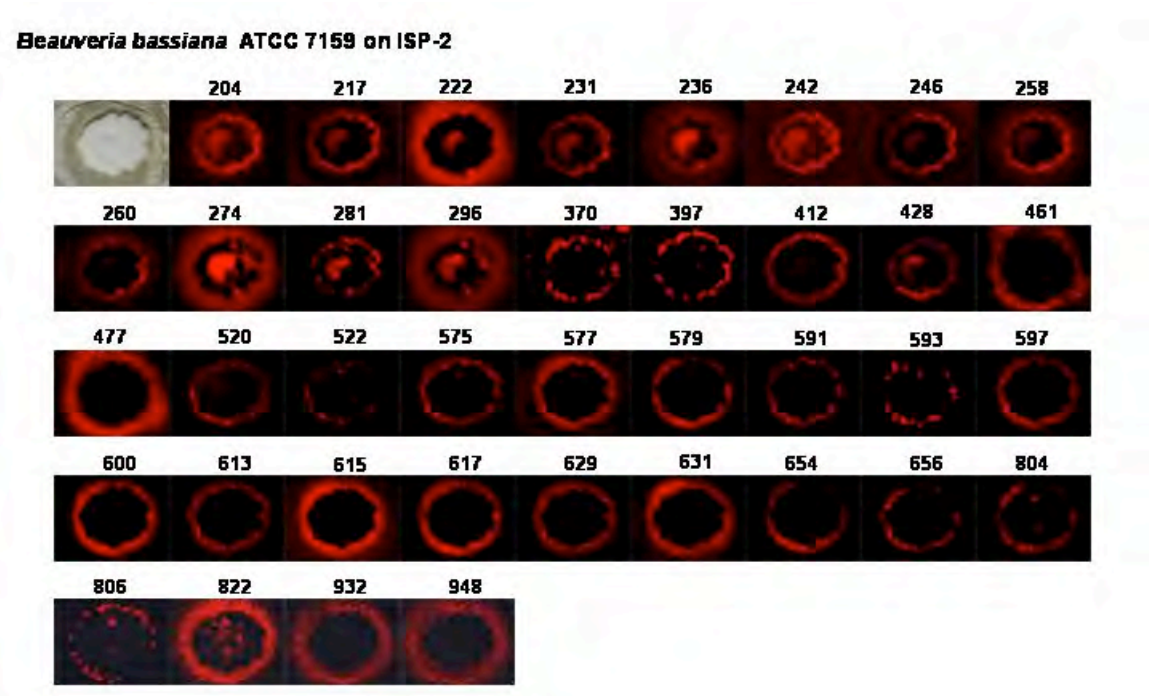
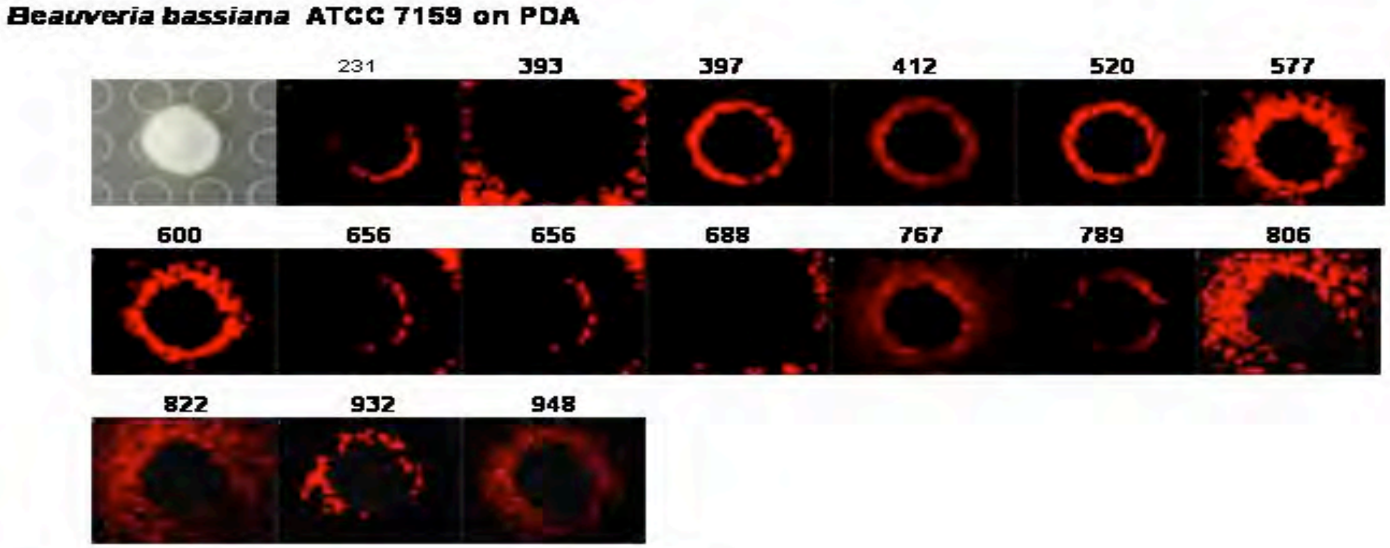
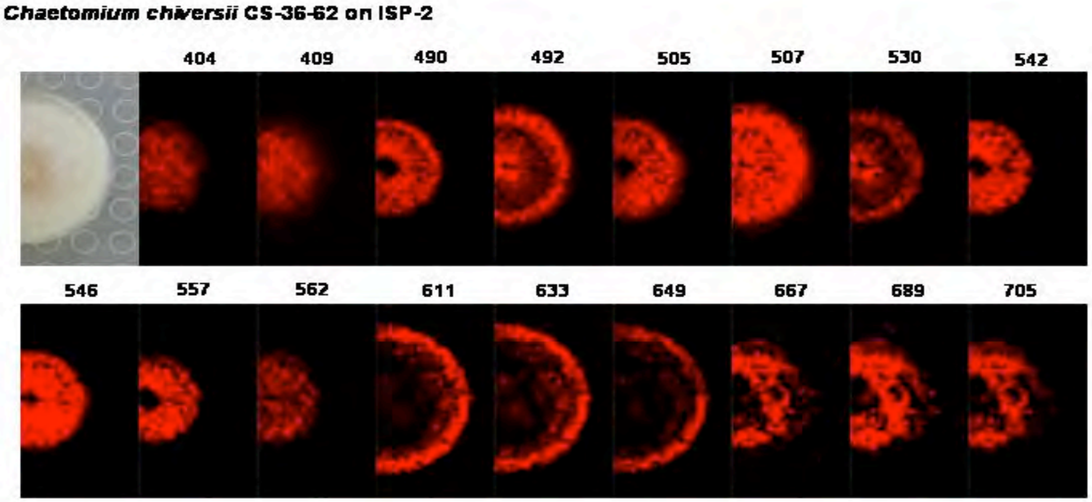
Supplementary Figure 1. The IMS images of strains indicated in Supplementary Table 1.



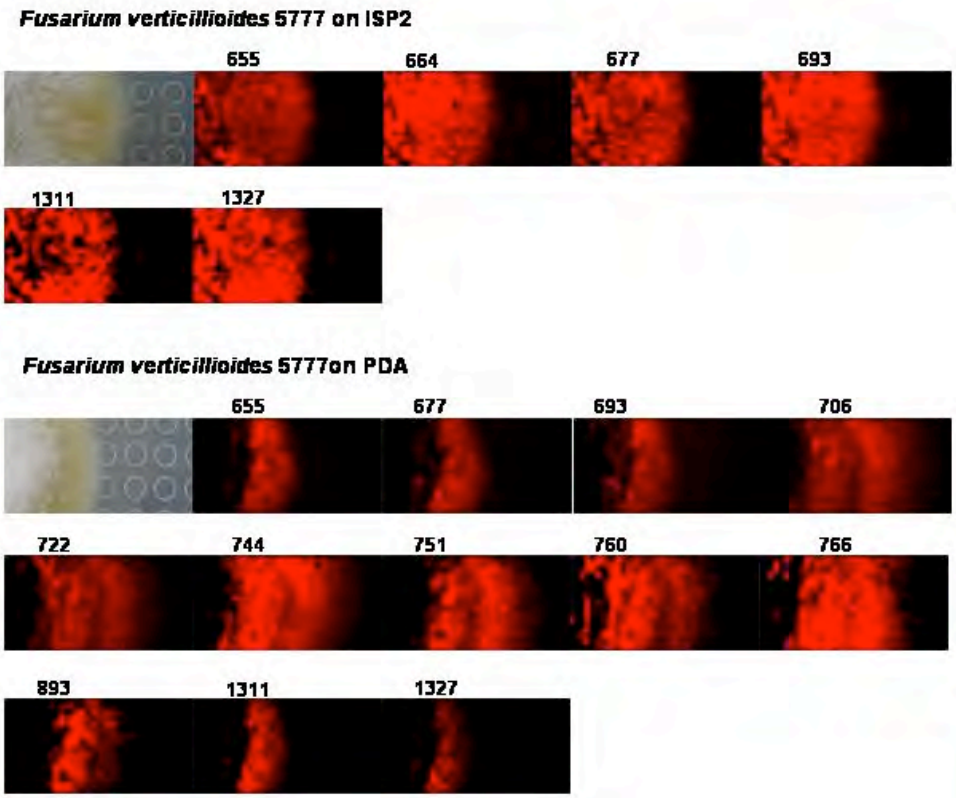
IMS 1. Beauveria bassiana grown on ISP-2 media. The ion at 806 Da was identified to be the [M+Na] of Beauvericin by tandem mass spectrometry (Supplemental Figure 2). IMS did not detect the [M+H] ion corresponding to Beauvericin. Liquid-liquid extraction of the organism showed the presence of the [M+H] that was resolved at 3.8 ppm mass error by FTICR-MS. Liquid-liquid extraction showed the presence of the [M+K] at 7.8 ppm mass error. The ion at 932 Da was identified to be the [M+Na] of Bassianolide by tandem mass spectrometry (Supplemental Figure 2).



IMS 2. Beauveria bassiana grown on ISP-2 media. The ion at 806 Da was identified to be the [M+Na] of Beauvericin by tandem mass spectrometry (Supplemental Figure 2). IMS did not detect the [M+H] ion corresponding to Beauvericin. Liquid-liquid extraction of the organism showed the presence of the [M+H] that was resolved at 3.8 ppm mass error by FTICR-MS. Additionally, the liquid-liquid extraction showed the presence of the [M+K] at 7.8 ppm mass error. The ion at 932 Da was identified to be the [M+Na] of Bassianolide by tandem mass spectrometry (Supplemental Figure 2).



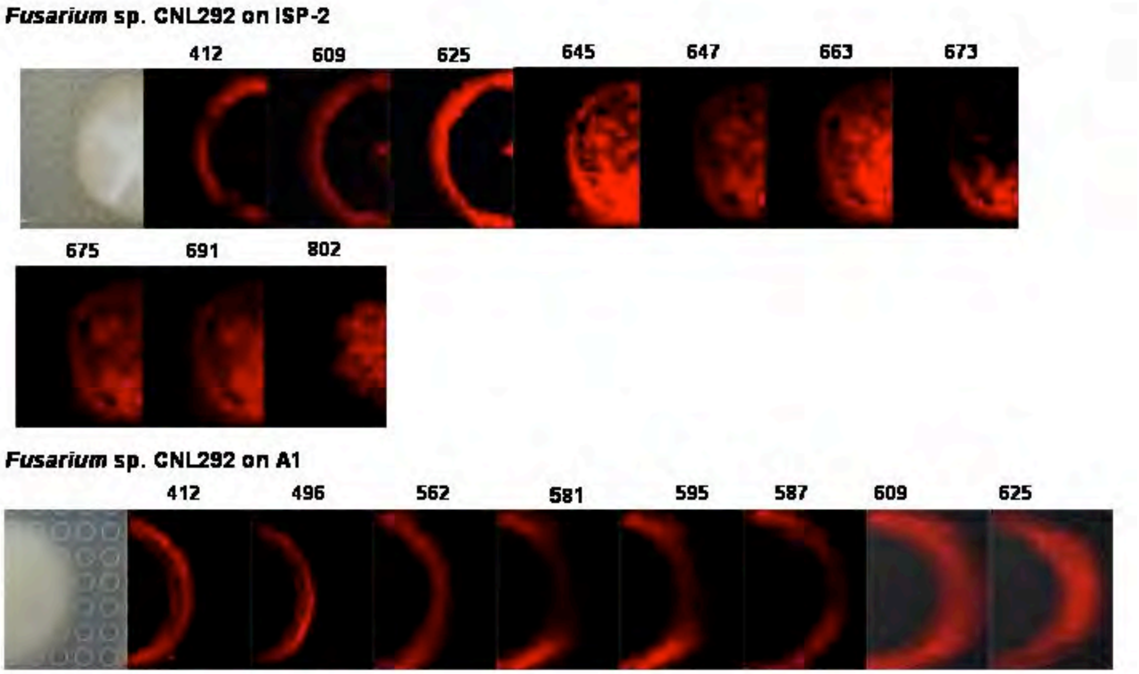
IMS 3. Chaetomium chiversii grown on ISP-2 media.



Fusarium verticillioides 5777 on ISP2

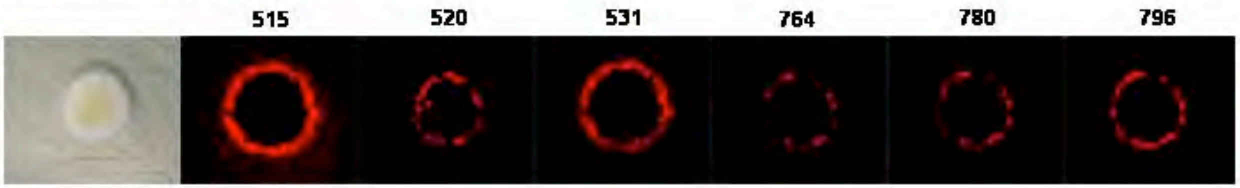
Fusarium verticillioides 5777on PDA

IMS 4. Fusarium verticillioides grown on ISP-2 media (top) and PDA media (bottom).

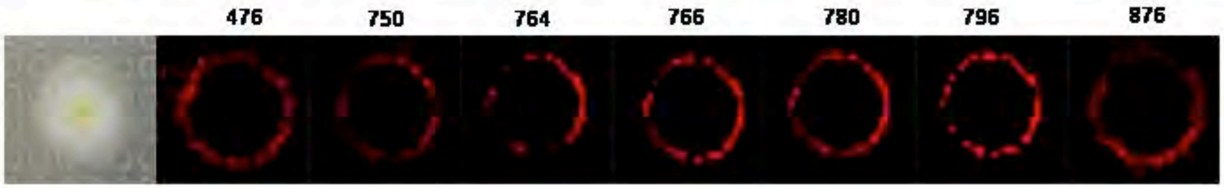


IMS 5. Fusarium sp. CNL292 grown on ISP-2 media (top) and A1 media (bottom).

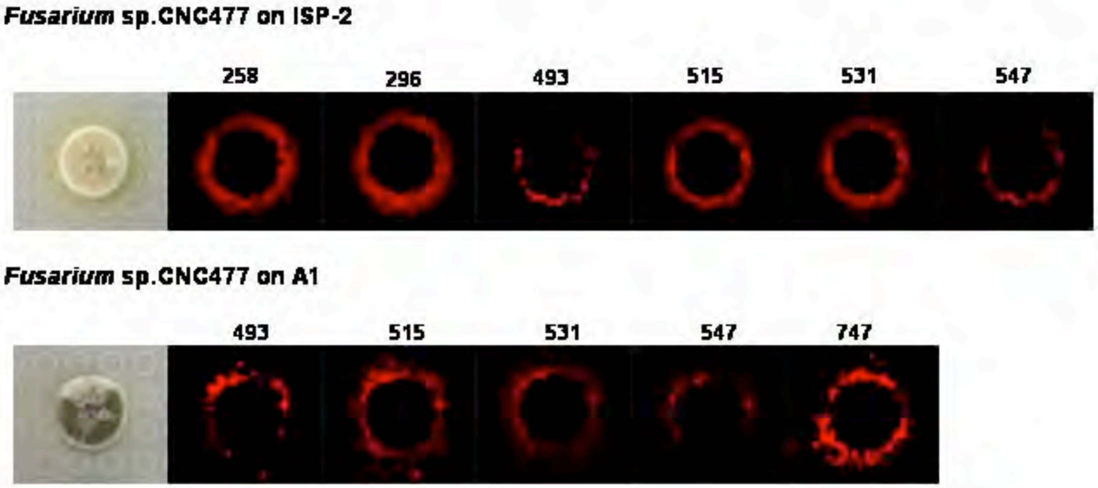
***Acremonium* sp. CNC890 on ISP-2**



***Acremonium* sp. CNC890 on A1**



IMS 6. Acremonium sp. CNC890 grown on ISP-2 media (top) and A1 media (bottom).

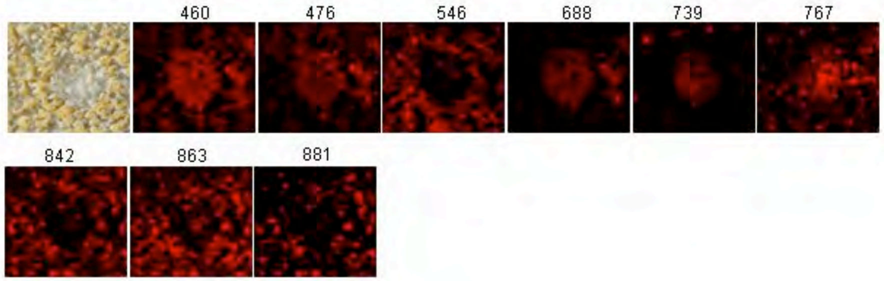


Fusarium sp.CNC477 on ISP-2

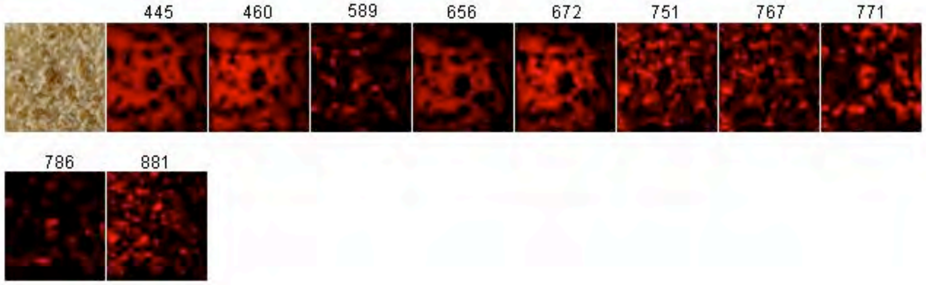
Fusarium sp.CNC477 on A1

IMS 7. Fusarium sp. CNC477 grown on ISP-2 media (top) and A1 media (bottom).

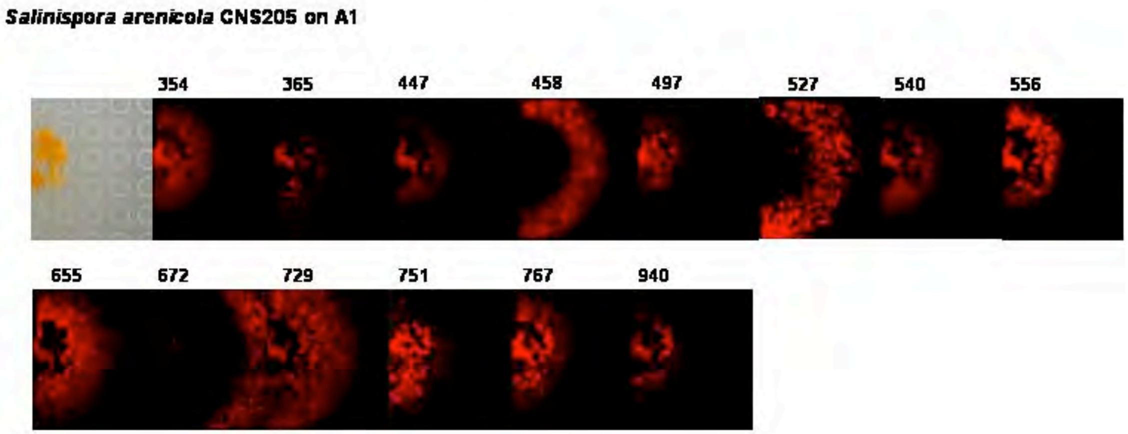
Thermo-fungus C030813-30



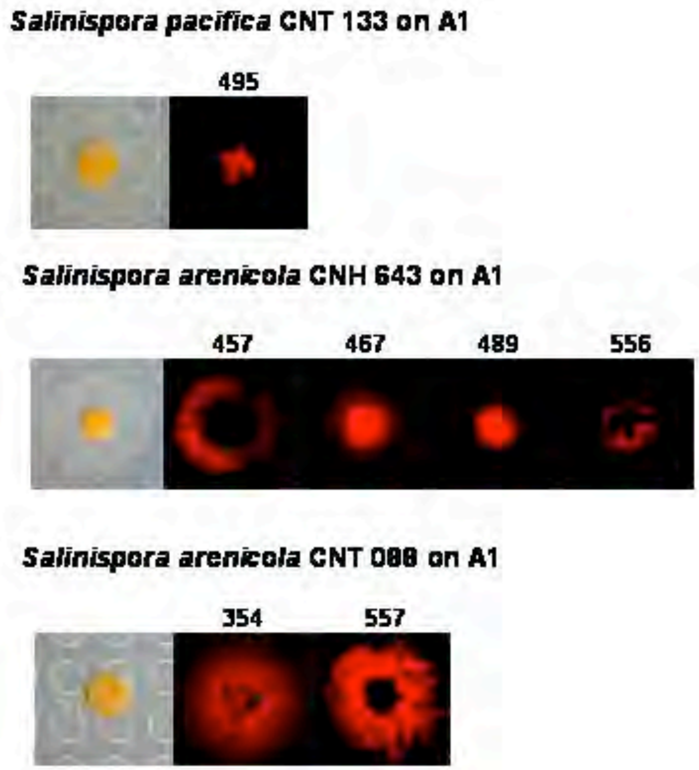
Thermo-fungus C030813-34



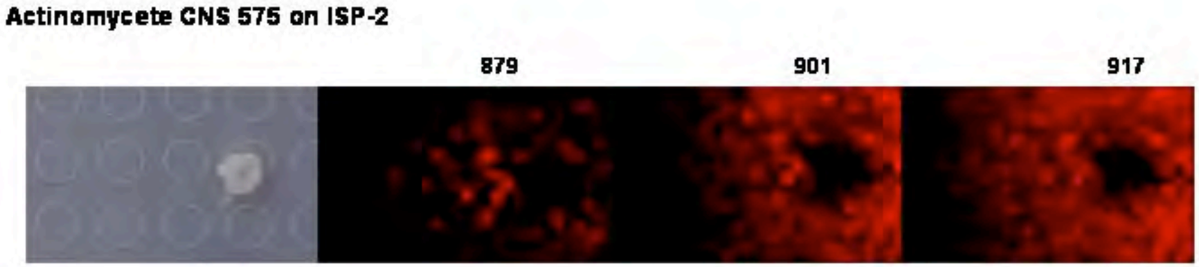
IMS 8. Thermo-fungus grown on PDA media.



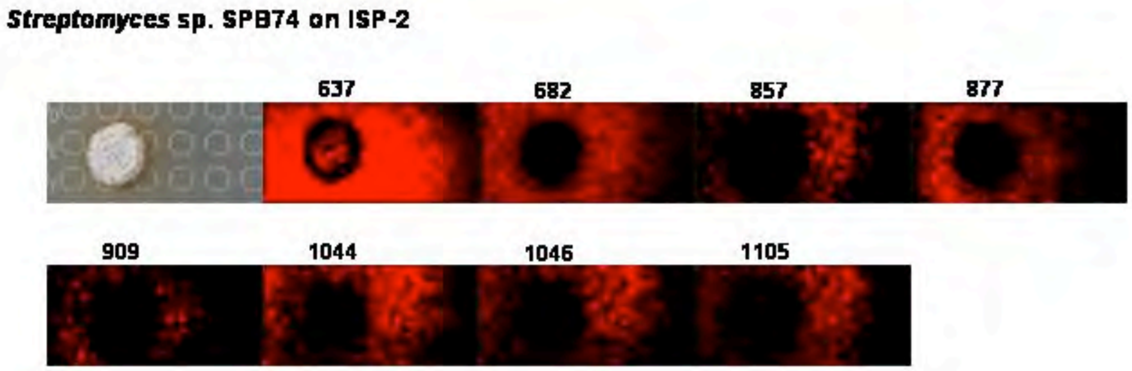
IMS 9. Salinispora arenicola CNS205 grown on A1 media.



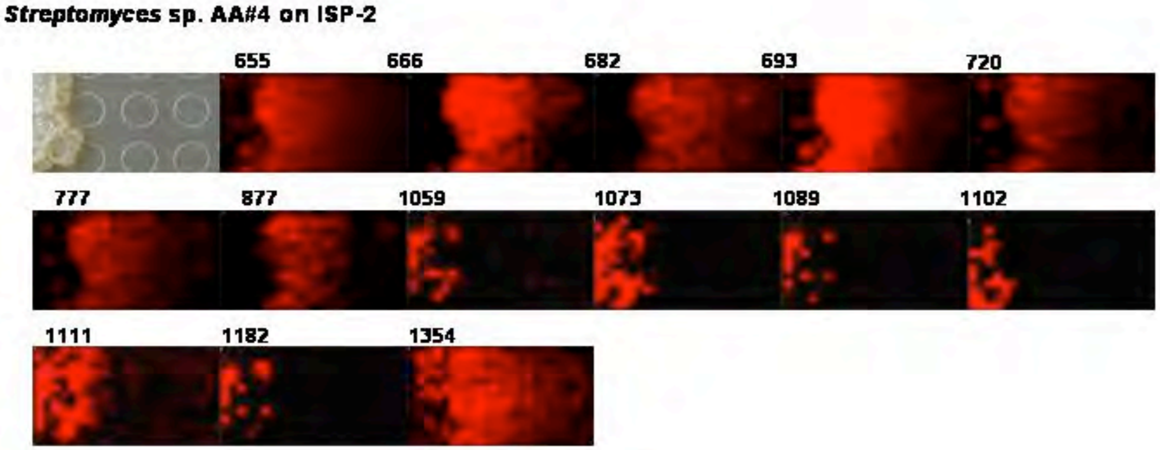
IMS 10. Salinispora pacifica CNT 133 grown on A1 media (top). Salinispora arenicola CNH 643 grown on A1 media (middle). Salinispora arenicola CNT 088 grown on A1 media.



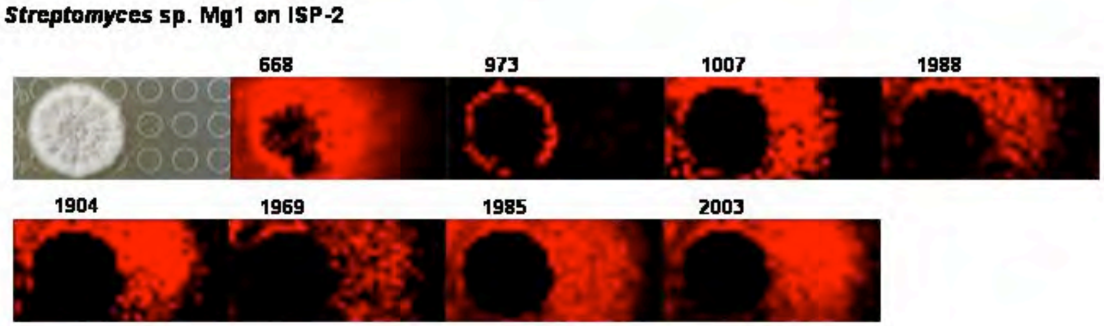
IMS 11. Actinomycete CNS 575 grown on ISP-2 media. The ion at 879 Da was identified to be the [M+H] of Etamycin by tandem mass spectrometry and FTICR-MS analysis of the intact mass (Supplemental Figure 2).



IMS 12. Streptomyces sp. SPB74 grown on ISP-2 media.

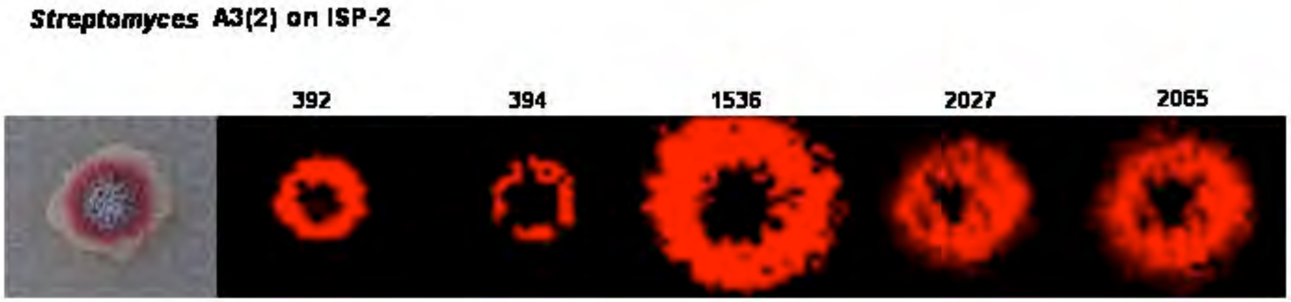


IMS 13. Streptomyces sp. AA#4 grown on ISP-2 media.

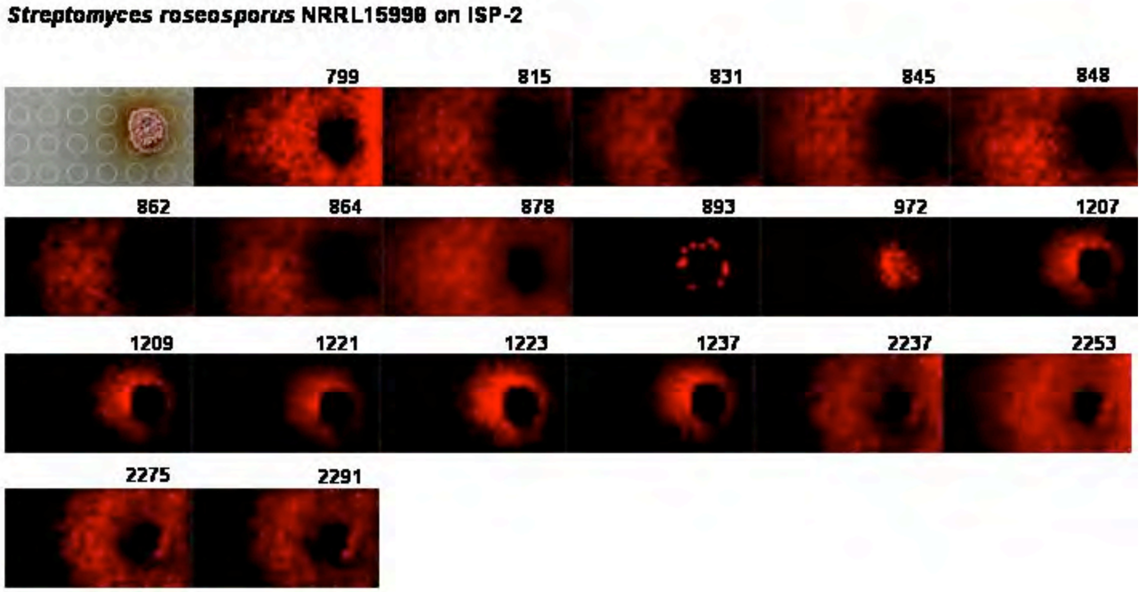


IMS 14. Streptomyces sp. Mg1 grown on ISP-2 media.

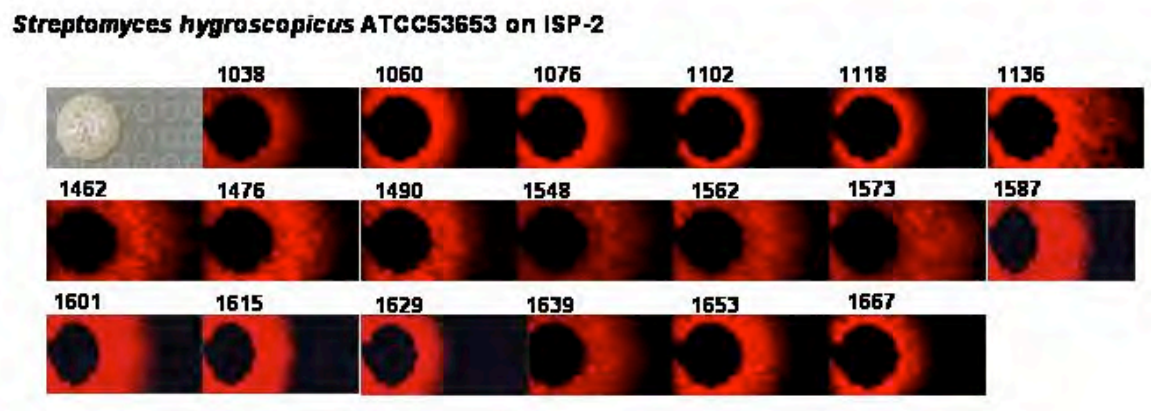
IMS 15. Streptomyces sp. WASP grown on ISP-2 media.



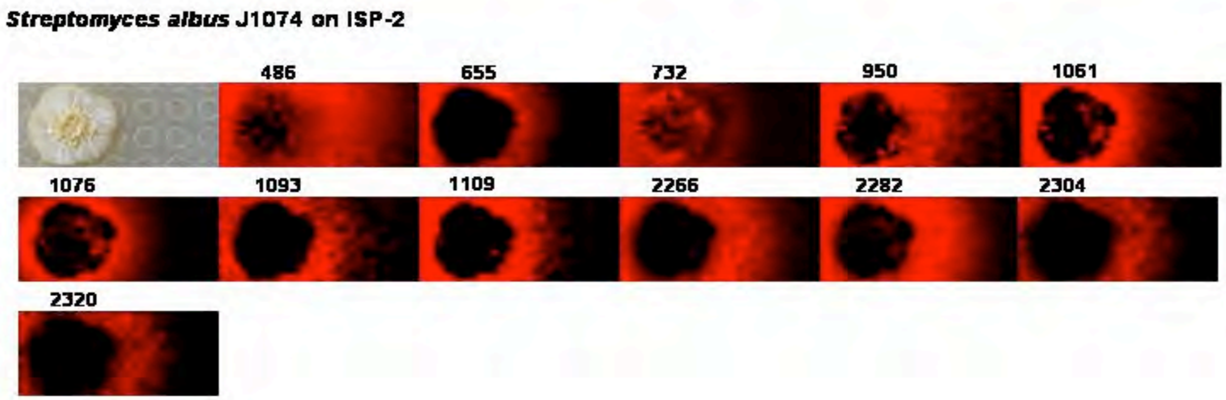
IMS 16. Streptomyces coelicolor grown on ISP-2 media. The ion at 392 Da was identified to be the [M+H] of Streptorubin B by tandem mass spectrometry (Supplemental Figure 2). The ion at 1536 Da was identified to be the [M+K] of CDA (Supplemental Figure 2). IMS did not detect the [M+H] ion corresponding to CDA. Liquid-liquid extraction of the organism showed the presence of the [M+H] CDA ion that was resolved at 17.5 ppm mass error by MALDI-MS. Additionally, the liquid-liquid extraction showed the presence of the [M+K] at 6.5 ppm mass error.



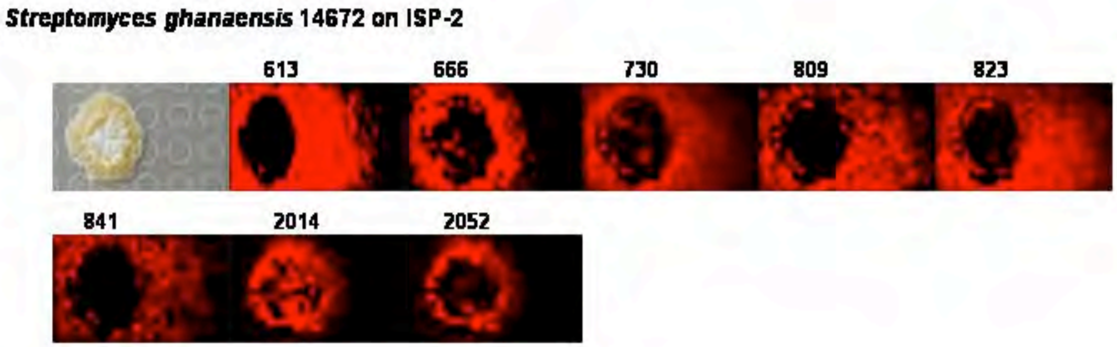
IMS 17. Streptomyces roseosporus grown on ISP-2 media.



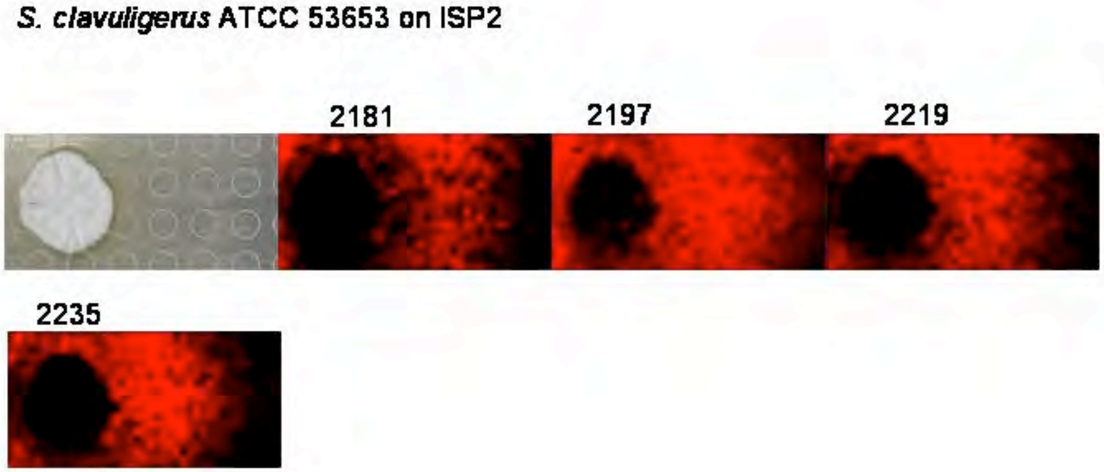
IMS 18. Streptomyces hygroscopicus grown on ISP-2 media.



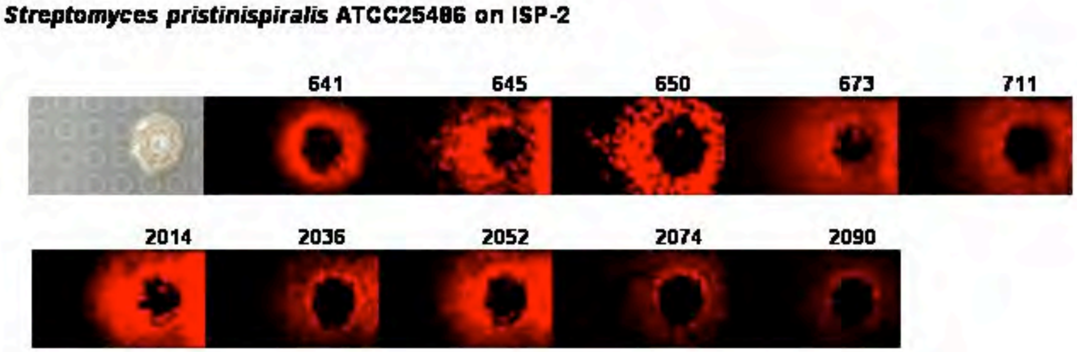
IMS 19. Streptomyces albus grown on ISP-2 media.



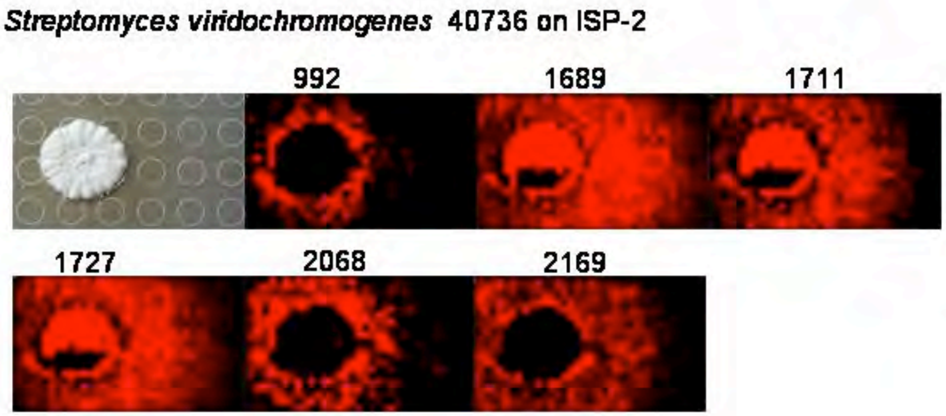
IMS 20. Streptomyces ghanaensis grown on ISP-2 media.



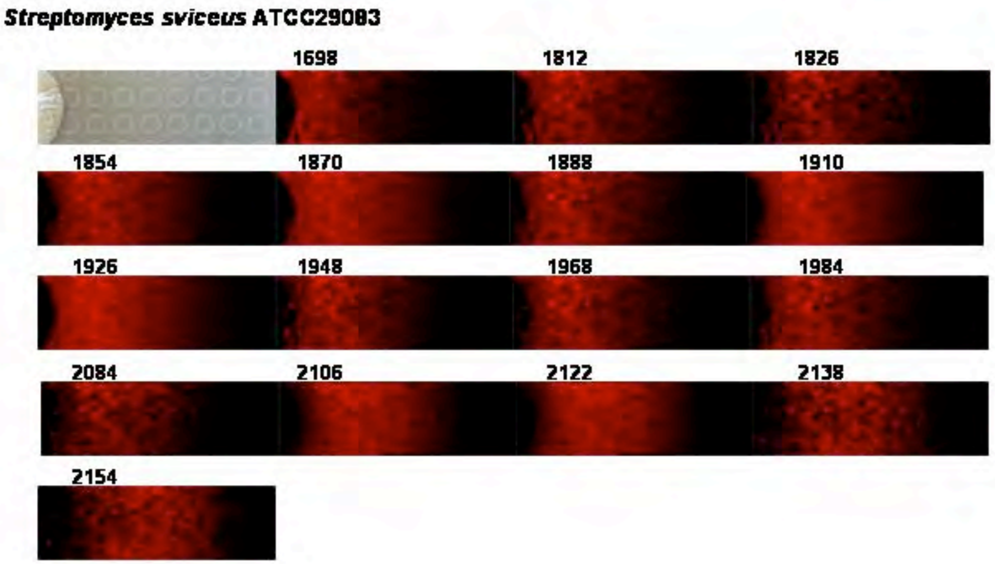
IMS 21. Streptomyces clavuligerus grown on ISP-2 media.



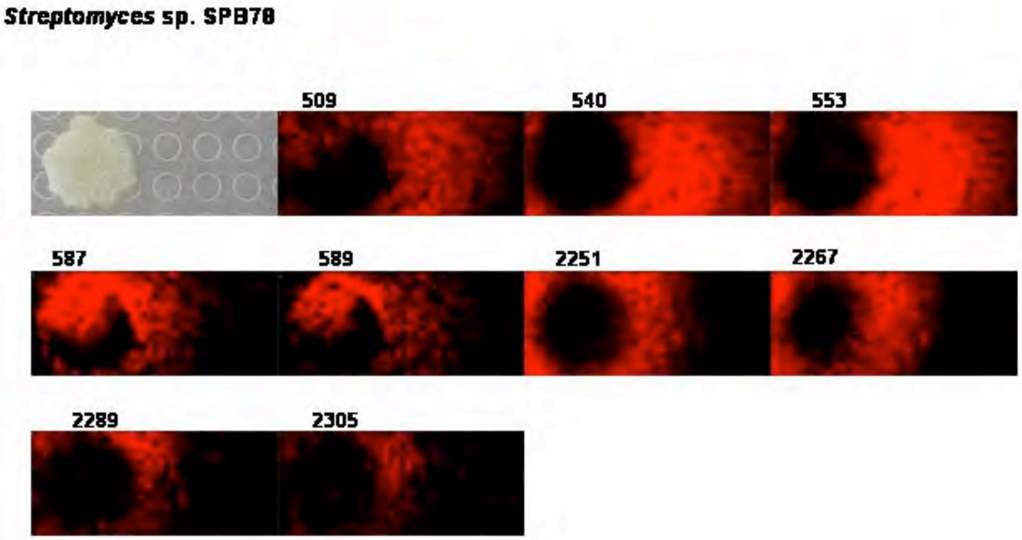
IMS 22. Streptomyces pristinispiralis grown on ISP-2 media.



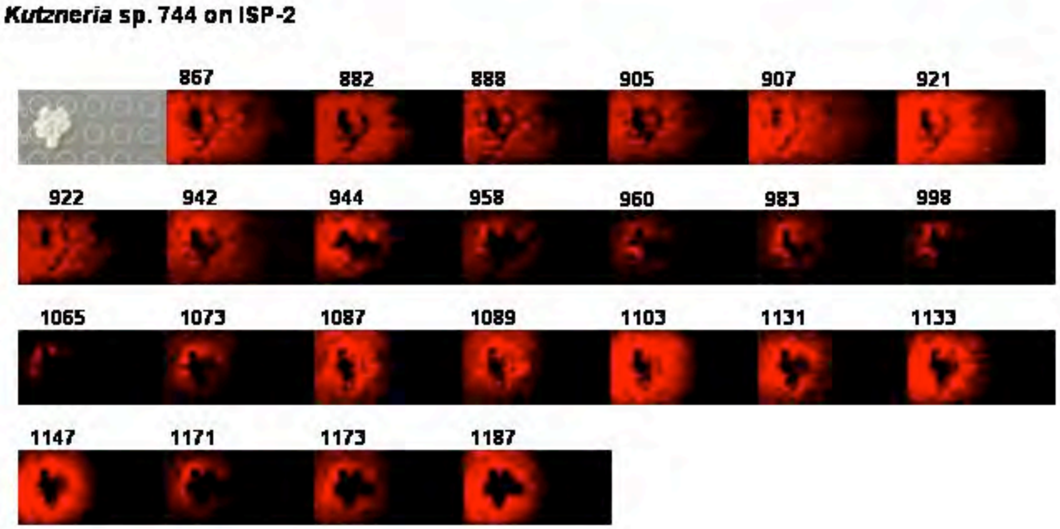
IMS 23. Streptomyces viridochromogenes grown on ISP-2 media.



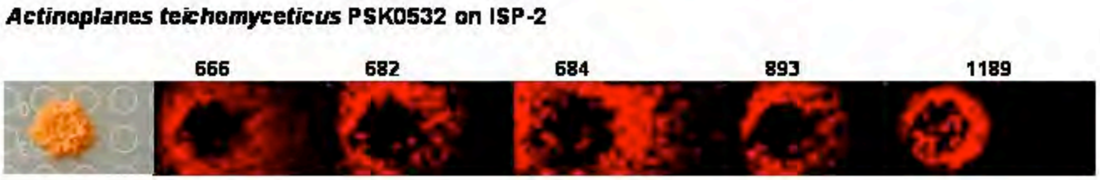
IMS 24. Streptomyces sviceus grown on ISP-2 media.



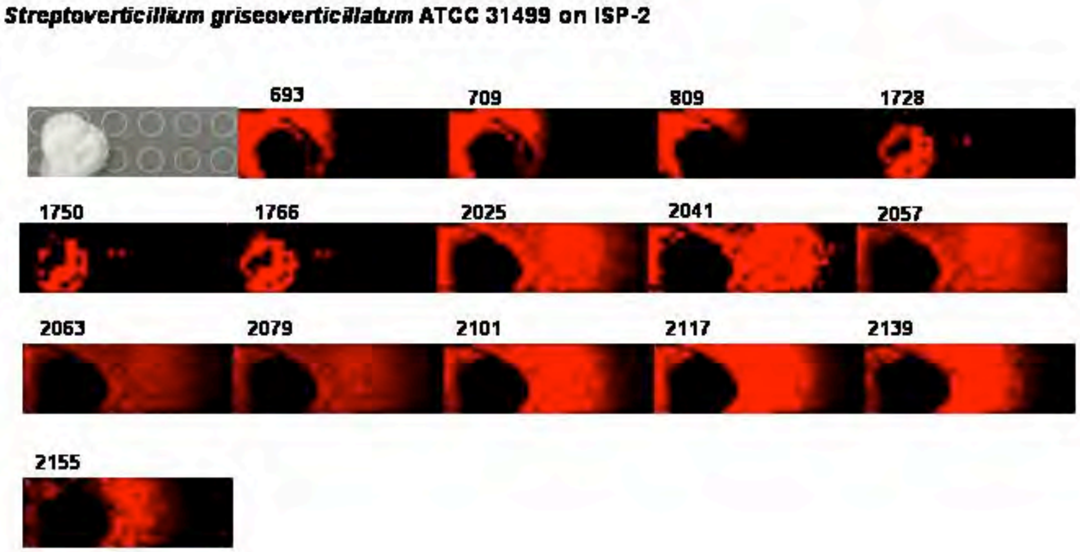
IMS 25. Streptomyces sp. SPB78 grown on ISP-2 media.



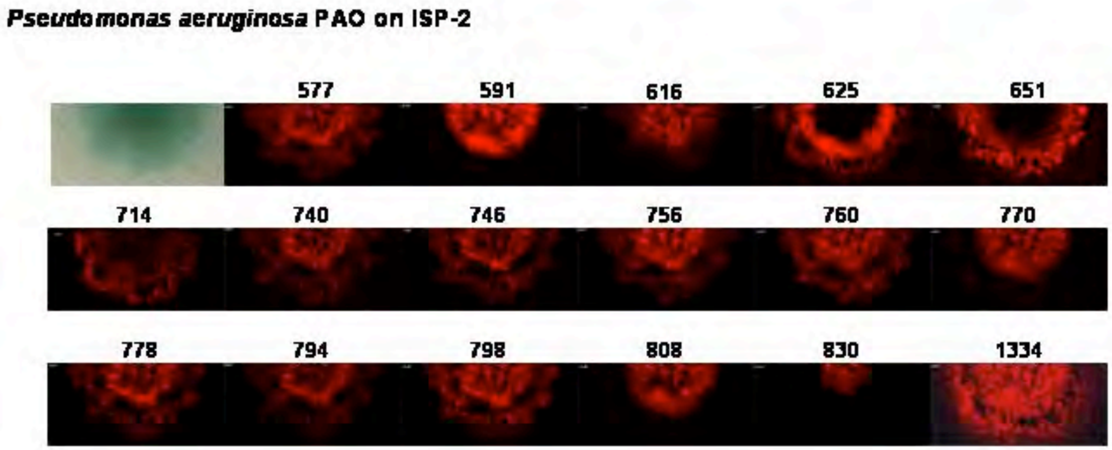
IMS 26. Kutzneria sp. 744 grown on ISP-2 media.



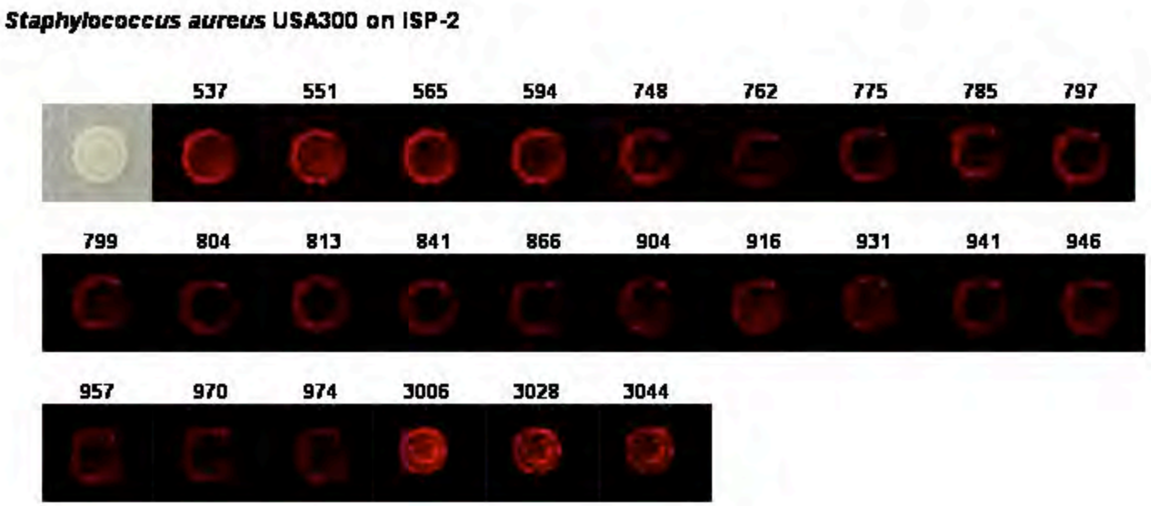
IMS 27. Actinoplanes teichomyceticus grown on ISP-2 media.



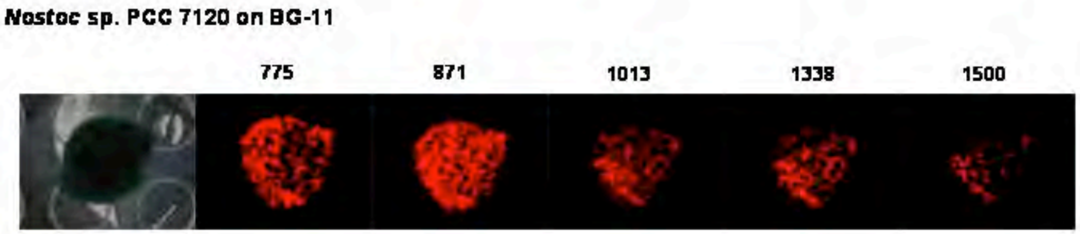
IMS 28. Streptoverticillium griseoverticillatum on ISP-2 media. The ion at 2041 Da was identified to be the [M+H] of Cinnamycin by tandem mass spectrometry (Supplemental Figure 2).



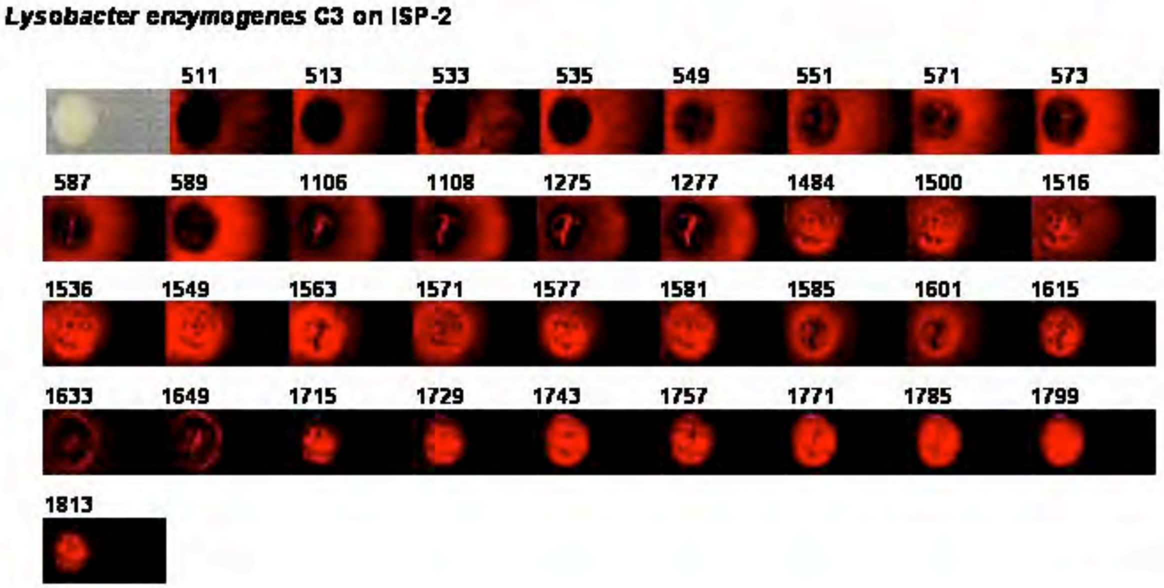
IMS 29. Pseudomonas aeruginosa grown on ISP-2 media.



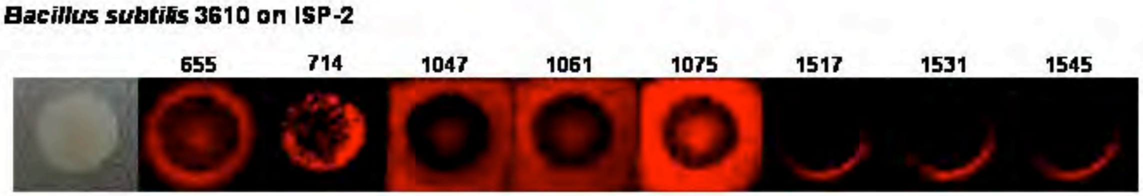
IMS 30. Staphylococcus aureus USA300 grown on ISP-2 media. The ion at 3006 was indentified to be δ -toxin (PSMλ) by tandem mass spectrometry.



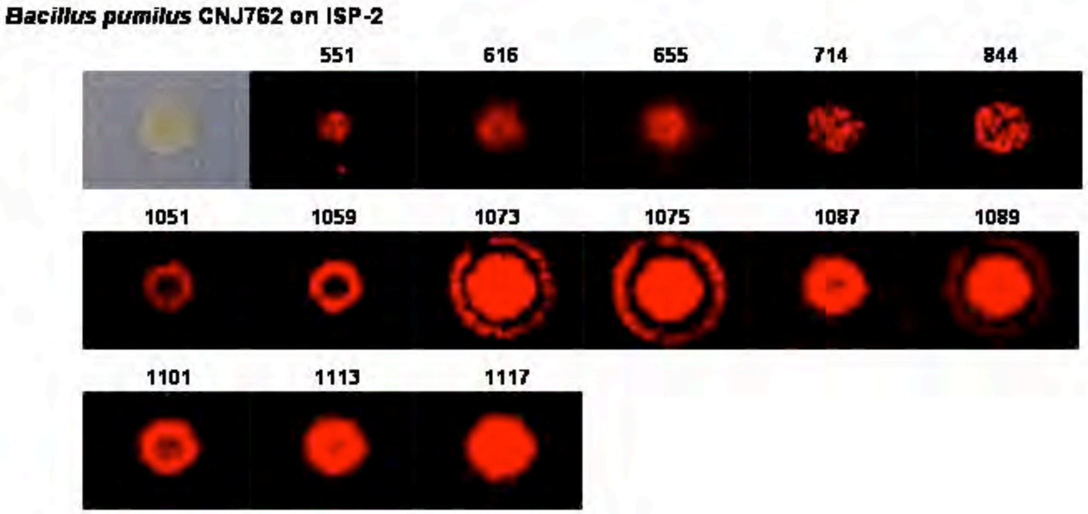
IMS 31. Nostoc sp. grown on BG-11 media.



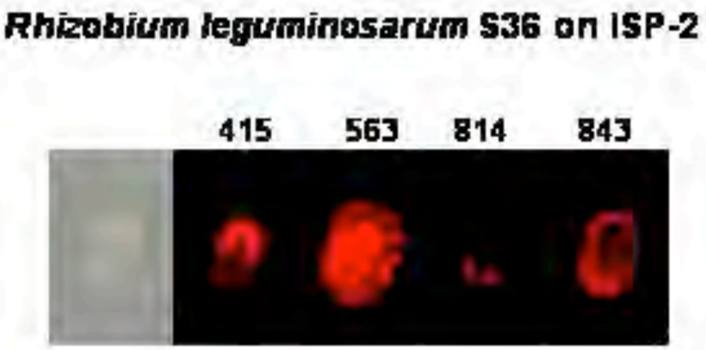
IMS 32. Lysobacter enzymogenes grown on ISP-2 media.



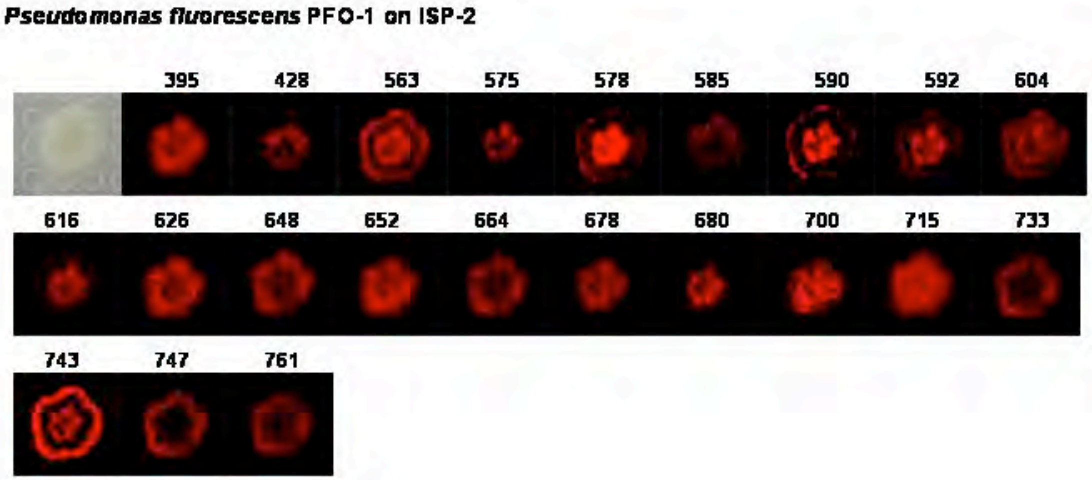
IMS 33. Bacillus subtilis grown on ISP-2 media. The ion at 1075 Da was identified to be the [M+K] of Surfactin by tandem mass spectrometry. IMS did not detect the [M+H] (Supplemental Figure 2). The ion at 1545 Da was identified to be the [M+K] of Plipastatin by tandem mass spectrometry. IMS did not detect the [M+H] (Supplemental Figure 2).



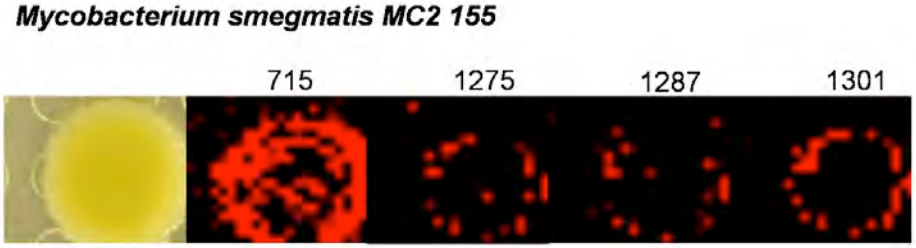
IMS 34. Bacillus pumilus grown on ISP-2 media. The ion at 1075 Da was identified to be the [M+K] of Surfactin by tandem mass spectrometry. IMS did not detect the [M+H] (Supplemental Figure 2).



IMS 35. Rhizobium leguminosarum grown on ISP-2 media.



IMS 36. Pseudomonas fluorescens grown on ISP-2 media.



IMS 37. Mycobacterium smegmatis grown on ISP-2 media.

Supplementary Table 2 Characterization of named ions in this study.

	Streptorubin B*	**error ppm**	**Surfactin-C_{15}***	**error ppm**	**CDA***	**error ppm**	**Plipastatin-C_{17}-Val***	**error ppm**	**SapB***	**error ppm**	**Beauvericin**	**error ppm**
Molecular formula	$C_{25}H_{33}N_3O$		$C_{53}H_{93}N_7O_{13}$		$C_{67}H_{78}N_{14}O_{26}$		$C_{75}H_{116}N_{12}O_{20}$		$C_{84}H_{139}N_{25}O_{29}S_2$		$C_{45}H_{57}N_3O_9$	
Calcd. [M+H]$^+$	392.2702		1036.6910		1497.5290		1505.8507		2026.9690		784.4173	
Calcd. [M+K]$^+$	430.2261		1074.6468		1536.4849		1543.8066		2064.9249		822.3732	
Calcd. [M+Na]$^+$	414.2521		1058.6729		1519.5109		1527.8327		2048.9510		806.3993	
Found w/ MALDI [M+H]$^+$	392.2720	4.6	ND		1497.5029	17.5	ND		2026.9706	0.8	ND	
Found w/ MALDI [M+K]$^+$			1074.6710	22.5	1536.4749	6.5	1543.8571	32.7	2064.9165	4.1		
Found w/ MALDI [M+Na]$^+$			1058.6765	3.4	1519.4967	9.4	1527.8605	18.2				
Found w/ FTMS [M+H]$^+$	392.2698	1.0			1497.5316	1.7	1505.8563	3.7			784.4203	3.8
Found w/ FTMS [M+K]$^+$			1074.6469	0.1							822.3754	2.7
Found w/ FTMS [M+Na]$^+$											806.4056	7.8
MS2	TOFTOF		TOFTOF		TOFTOF		TOFTOF		TOFTOF		ITMS2	
Representive in imaging	392		1075		1536		1545		2027		806	

Supplementary Table 2. Characterization of named ions in this study (continued)

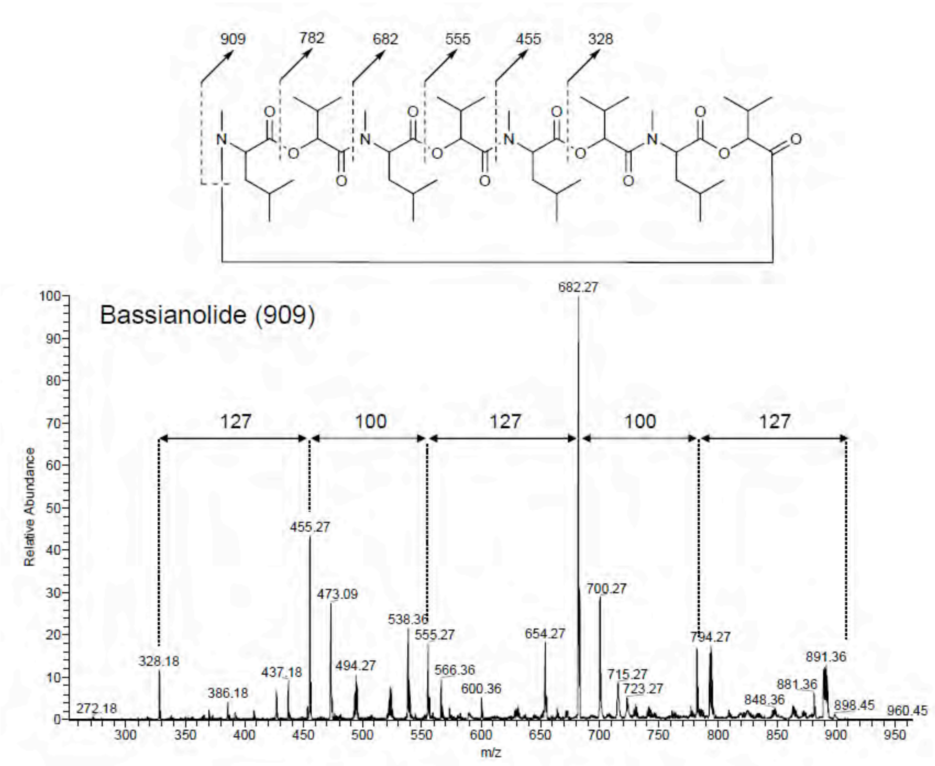
	Bassianolide	**error ppm**	**Etamycin**	**error ppm**	**Cinnamycin**	**error ppm**	**Maltophytin**	**error ppm**	**Dihydromaltophytin**	**error ppm**	**Pheophytin A**	**error ppm**
Molecular formula	$C_{48}H_{84}N_4O_{12}$		$C_{44}H_{62}N_8O_{11}$		$C_{89}H_{125}N_{25}O_{25}S_3$		C29H38N2O6		C29H40N2O6		$C_{55}H_{74}N_4O_5$	
Calcd. $[M+H]^+$	909.6164		879.4616		2040.8519		511.2808		513.2965		871.5737	
Calcd. $[M+K]^+$	947.5723		917.4175		2078.8078		549.2367		551.2523		909.5296	
Calcd. $[M+Na]^+$	931.5983		901.4436		2062.8338		533.2628		535.2784		893.5557	
Found w/ MALDI $[M+H]^+$											871.5559	20.4
Found w/ MALDI $[M+K]^+$												
Found w/ MALDI $[M+Na]^+$												
Found w/ FTMS $[M+H]^+$	909.6212	5.3	879.4642	3.0	2040.8566	2.3	511.2819	2.2	513.2971	1.2		
Found w/ FTMS $[M+K]^+$	947.5770	5.0	917.4245	7.6	2078.8156	3.8						
Found w/ FTMS $[M+Na]^+$	931.6022	4.2	901.4495	6.5			533.2651	4.3	535.2804	3.7		
MS2	ITMS2		ITMS2		ITMS2		ITMS2		ITMS2		TOFTOF	
Representive in imaging	932		879		2041		511		513		871	

* Described in Yang Y.L., Xu Y., Straight P., Dorrestein P.C. Translating metabolic exchange with imaging mass spectrometry. Nature Chemical Biology. 5, 885-887. 2009

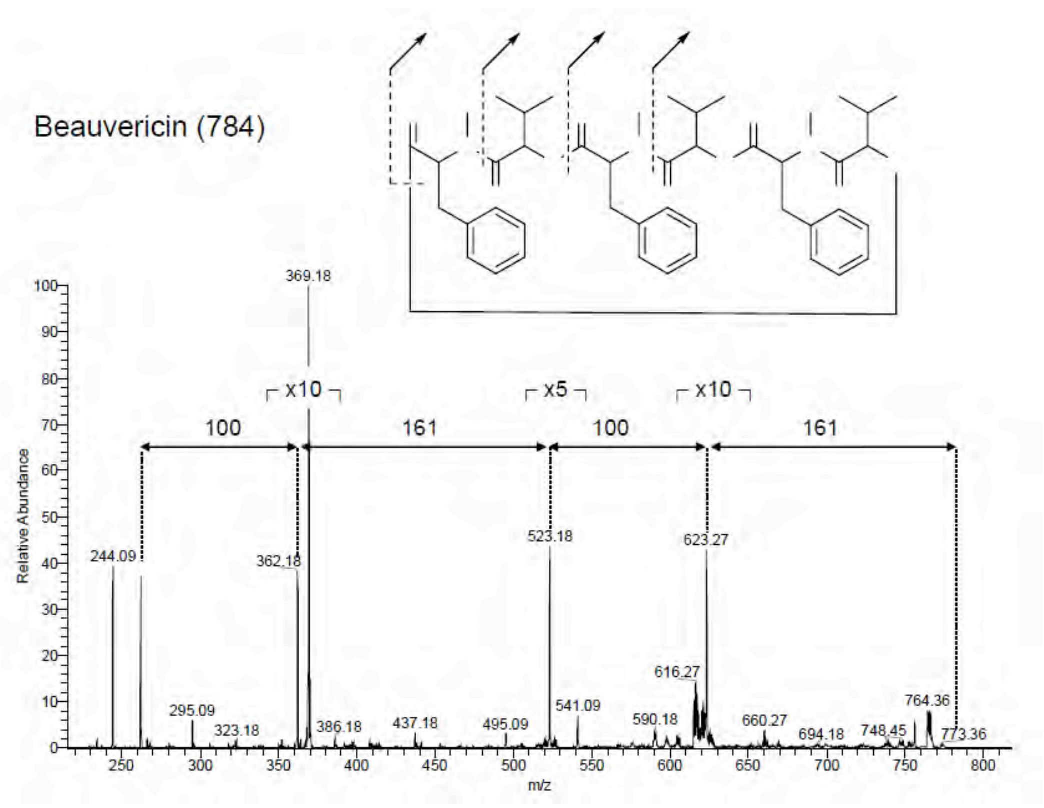
Supplementary Table-2. Characterization of named ions in this study (continued)

	δ-toxin	**error ppm**										
Molecular formula	$C_{137}H_{225}N_{33}O_{40}S$											
Calcd. $[M+H]^+$	3005.6379											
Calcd. $[M+K]^+$	3043.5938											
Calcd. $[M+Na]^+$	3027.6199											
Found in MALDI $[M+H]^+$	3005.5007	45.6										
Found in MALDI $[M+K]^+$	3043.4419	49.9										
Found in MALDI $[M+Na]^+$	3027.4771	47.2										
Found in FTMS $[M+H]^+$												
Found in FTMS $[M+K]^+$												
Found in FTMS $[M+Na]^+$												
MS2	TOFTOF											
Representive in imaging	3005											

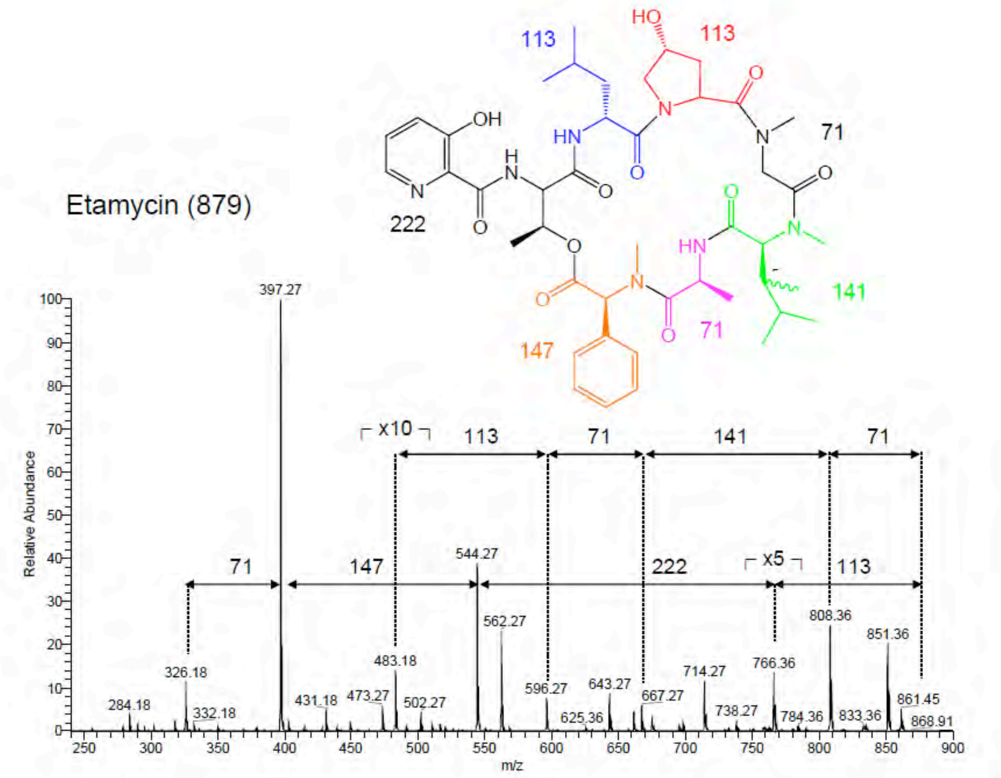
Supplementary Figure 2. The annotated known compounds observed by TLA-IMS



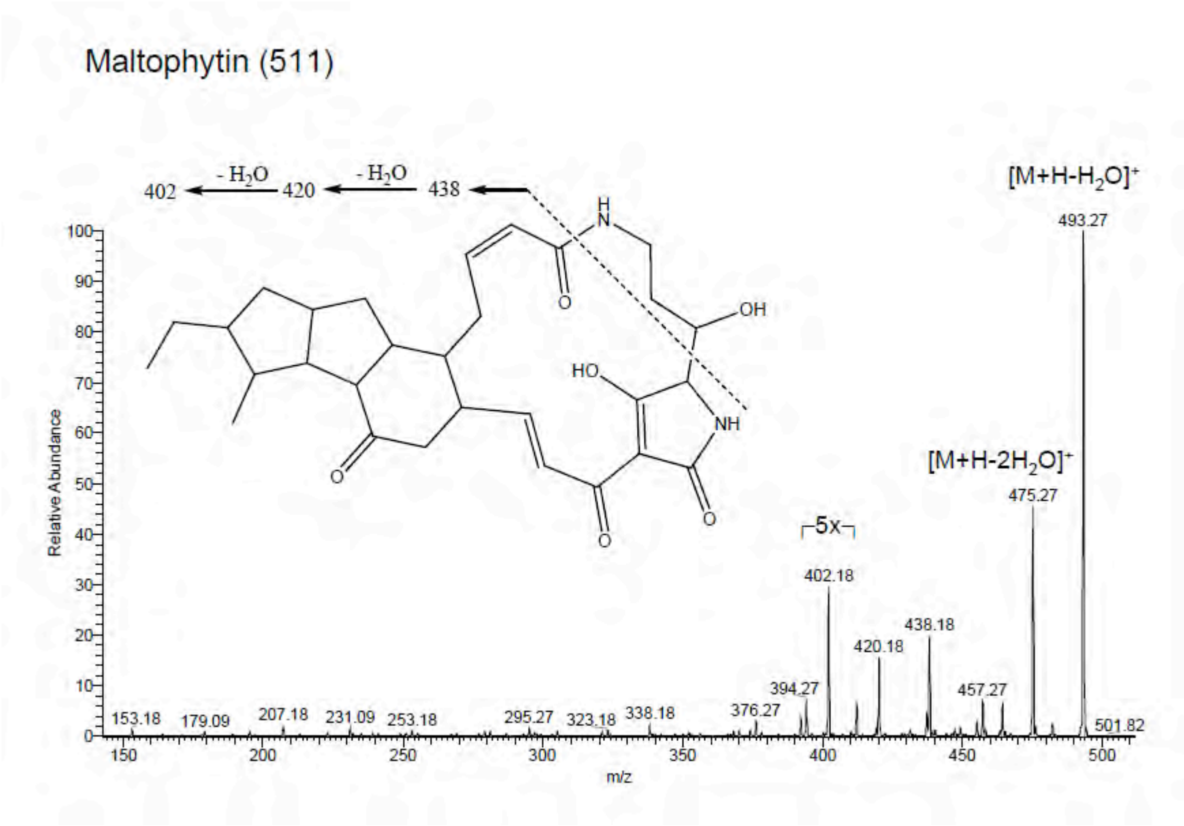
Spectrum 1. Bassianolide. FTICR-MS was used to identify the [M+H] ion at 5.3 ppm mass error. Thereafter, tandem mass spectrometry using a LTQ-MS was performed to identify fragment ions. The number in brackets within the figures is the molecular mass of the compound.



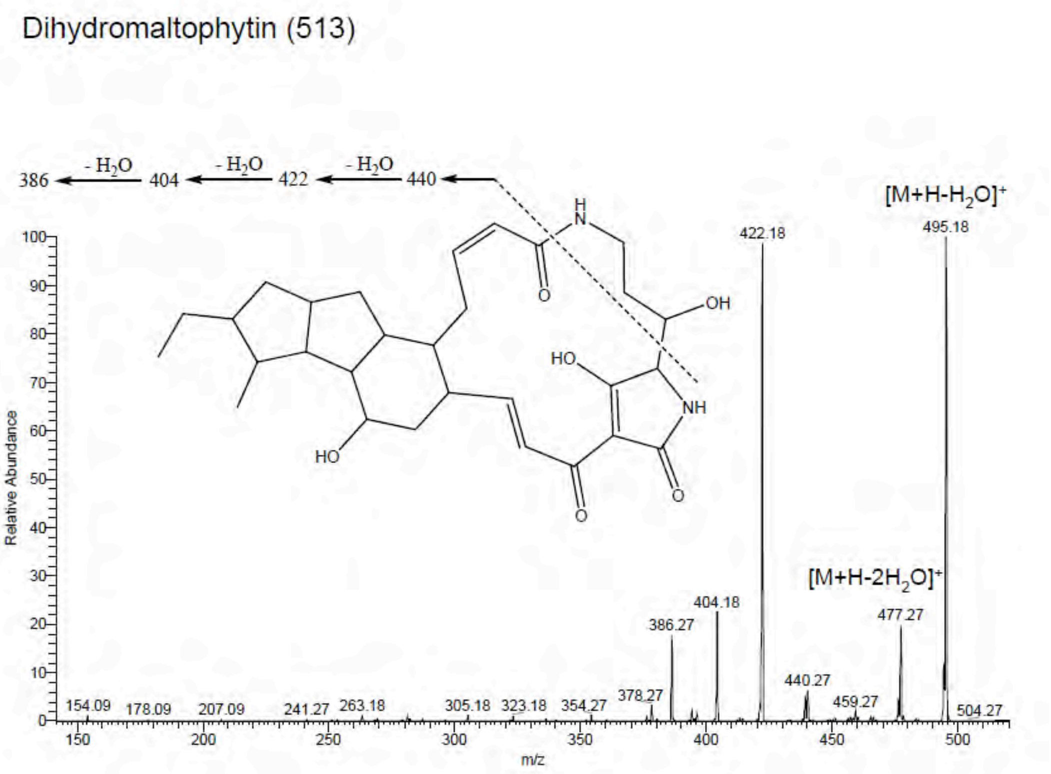
Spectrum 2. Beauvericin. FTICR-MS was used to identify the [M+H] ion at 3.8 ppm mass error. Thereafter, tandem mass spectrometry using a LTQ-MS was performed to identify fragment ions. The number in brackets within the figures is the molecular mass of the compound.



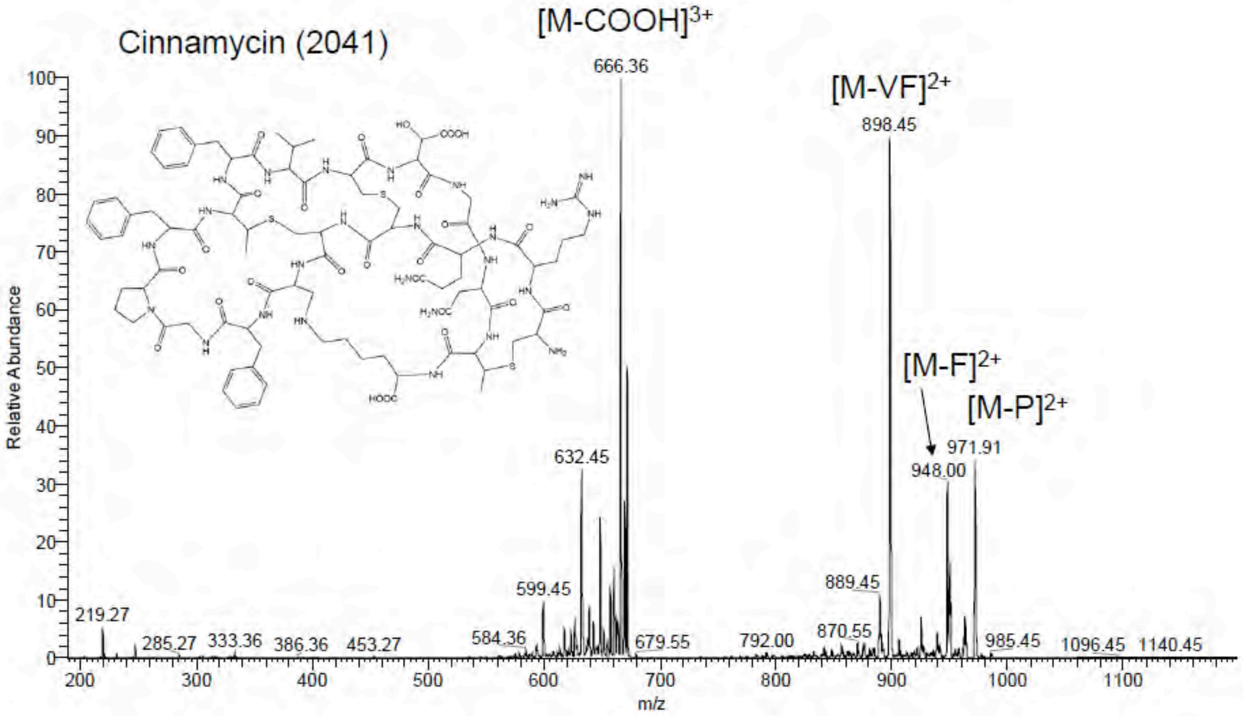
Spectrum 3. Etamycin. FTICR-MS was used to identify the [M+H] ion at 3 ppm mass error. Thereafter, tandem mass spectrometry using a LTQ-MS was performed to identify fragment ions. Identified fragments are depicted in the structure insert. The number in brackets within the figures is the molecular mass of the compound.



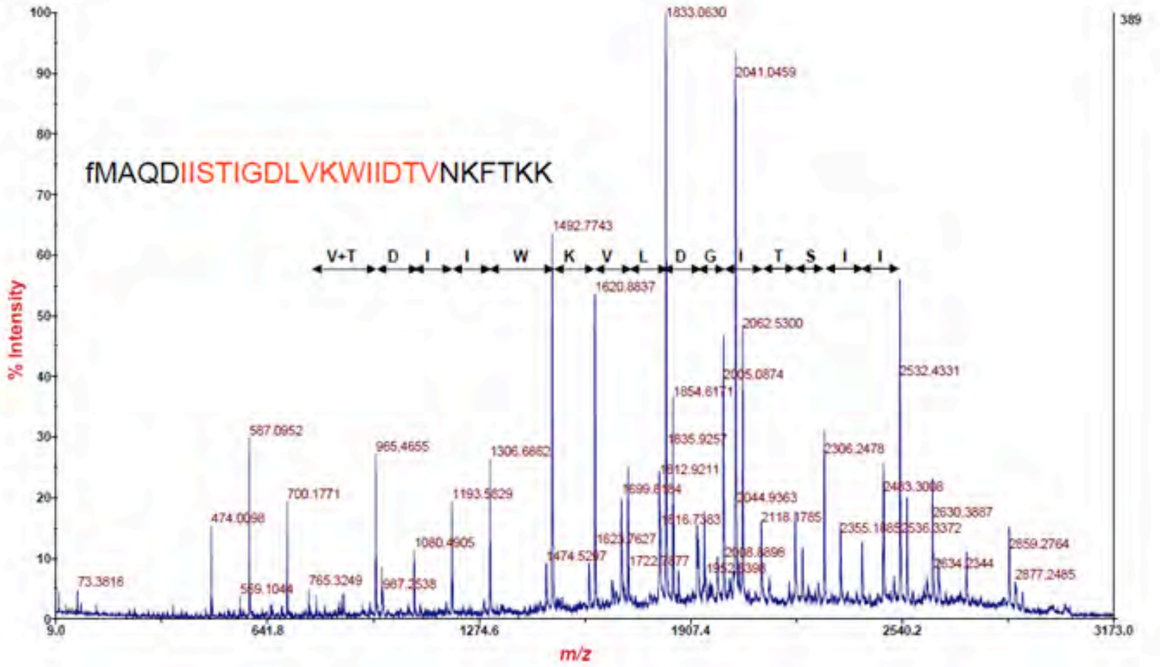
Spectrum 4. Maltophytin. FTICR-MS was used to identify the [M+H] ion at 2.2 ppm mass error. Thereafter, tandem mass spectrometry using a LTQ-MS was performed to identify fragment ions. Structure insert depicts identified fragment ions. The number in brackets within the figures is the molecular mass of the compound.



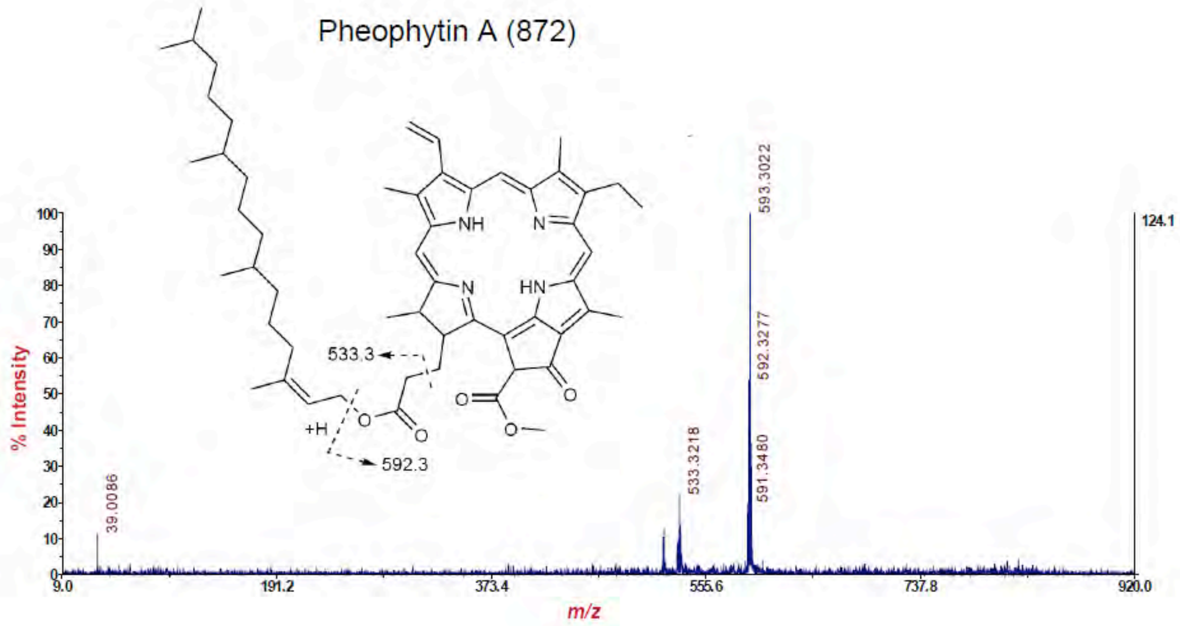
Spectrum 5. Dihydromaltophytin. FTICR-MS was used to identify the [M+H] ion at 1.2 ppm mass error. Thereafter, tandem mass spectrometry using a LTQ-MS was performed to identify fragment ions. Structure insert depicts identified fragment ions. The number in brackets within the figures is the molecular mass of the compound.



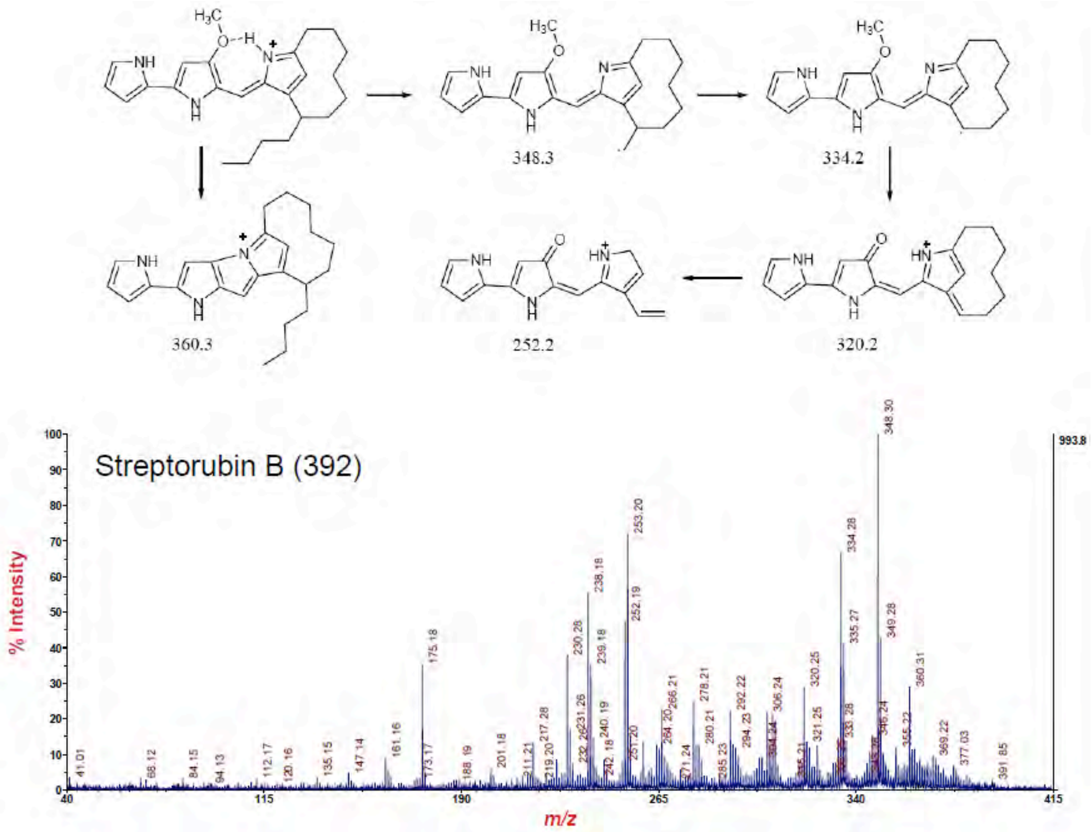
Spectrum 6. Cinnamycin. FTICR-MS was used to identify the ion corresponding to Cinnamycin at 2.3 ppm mass error. Thereafter, tandem mass spectrometry using a LTQ-MS was performed to identify fragment ions as indicated on the spectrum. The number in brackets within the figures is the molecular mass of the compound.



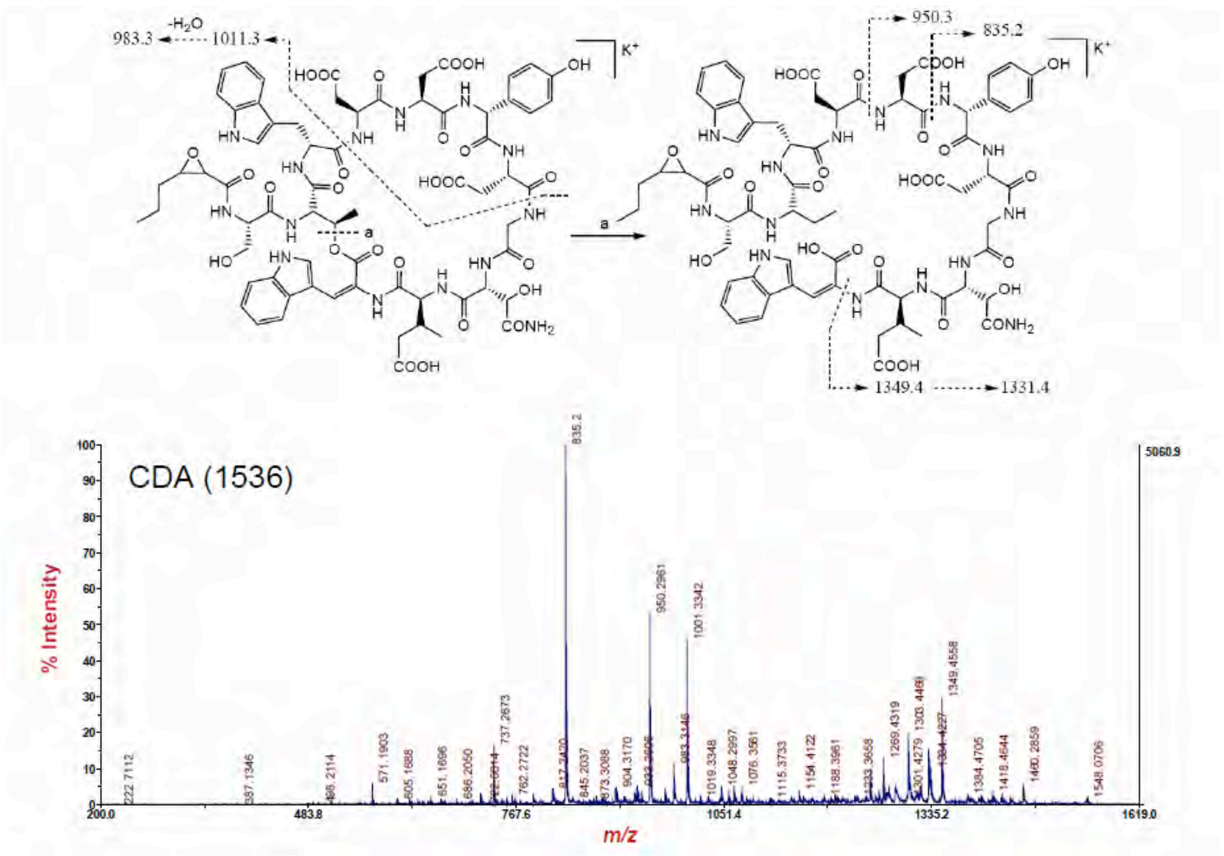
Spectrum 7. δ-toxin. The ABI 4800 MALDI-TOF/TOF was used to identify the [M+H] ion at 45.6 ppm mass error. Thereafter, tandem mass spectrometry was performed to fragment the target ion. A sequence tag was generated as indicated within the spectrum and BLAST analysis was used to identify the ion as δ-toxin.



Spectrum 8. Pheophytin A. The ABI 4800 MALDI-TOF/TOF was used to identify the [M+H] ion at 20.4 ppm mass error. Thereafter, tandem mass spectrometry was performed to fragment the target ion. Ion fragments were identified and are indicated on the structure insert. The number in brackets within the figures is the molecular mass of the compound.



Spectrum 9. Streptorubin B. The ABI 4800 MALDI-TOF/TOF was used to identify the [M+H] ion at 4.6 ppm mass error and further verified with FTICR-MS at 1.0 ppm mass error. Thereafter, tandem mass spectrometry was performed to fragment the target ion. Ion fragments were identified and are indicated on the structure insert. The number in brackets within the figures is the molecular mass of the compound.



Spectrum 10. CDA. The ABI 4800 MALDI-TOF/TOF was used to identify the [M+H] ion at 17.5 ppm mass error and further verified with FTICR-MS at 1.7 ppm mass error. Thereafter, tandem mass spectrometry was performed to fragment the target ion. Ion fragments were identified and are indicated on the structure insert. The number in brackets within the figures is the molecular mass of the compound.