toxins

MDPI

Article

Characterizing the Influence of a Heterotrophic Bicosoecid Flagellate *Pseudobodo* sp. on the Dinoflagellate *Gambierdiscus balechii*

Table S1. Total algal cell number in each group.

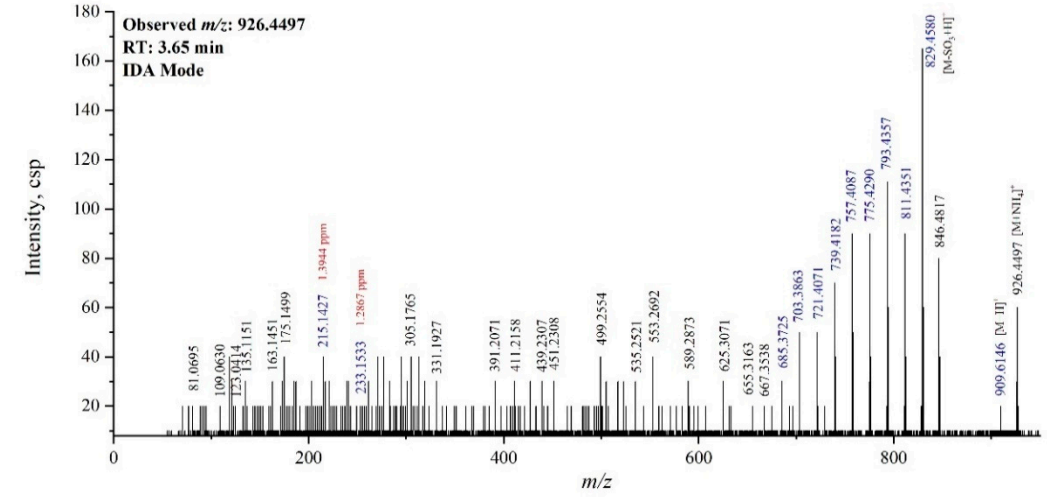
Groups	Control groups			Infected groups		
	A1	A2	A3	B1	B2	B3
Cell Number	6.52×10^5	6.00×10^5	5.93×10^5	3.08×10^5	2.38×10^5	2.42×10^5

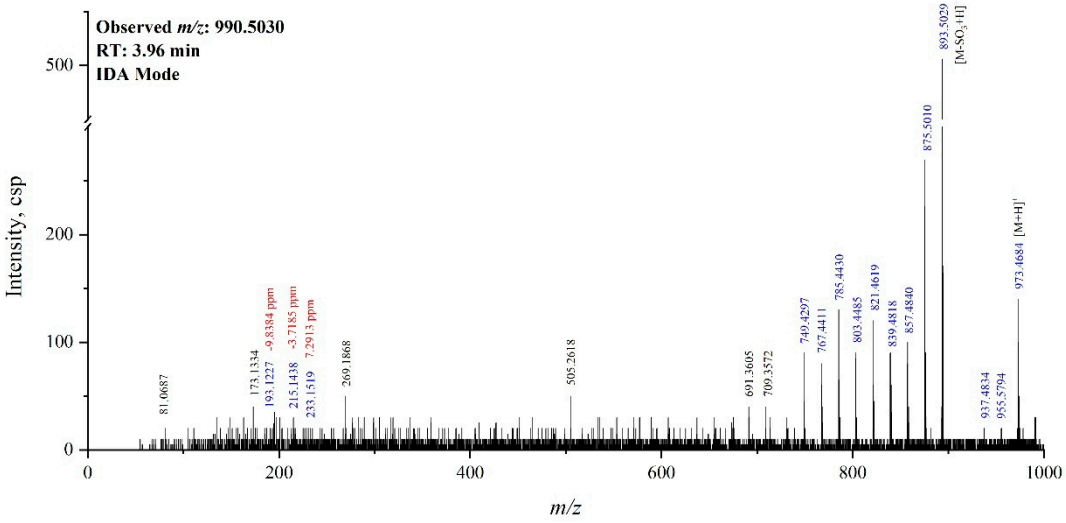
Table S2. Cellular production of individual toxins in the control and infected group.

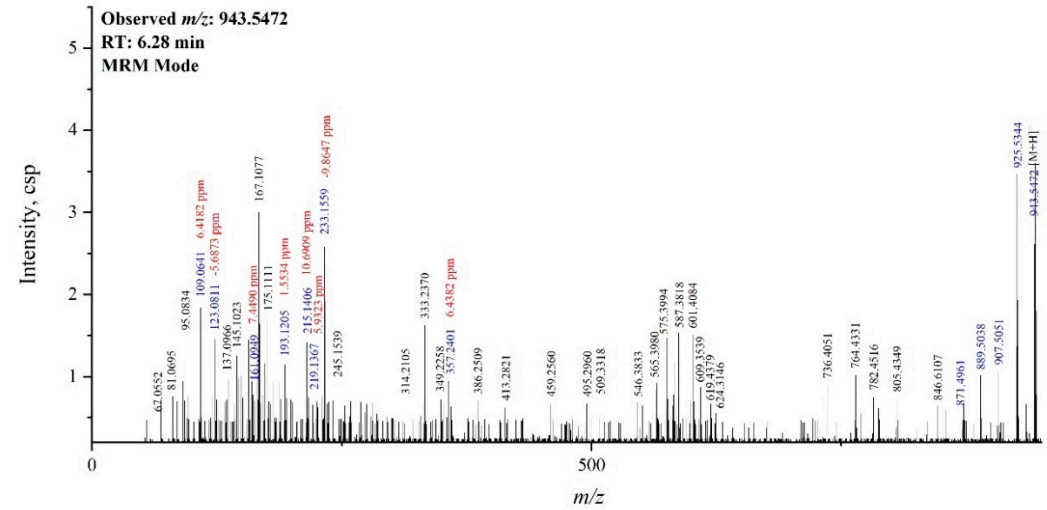
Observed *m/z*	Retention time (min)	Peak area (mean ± SD)		Significant difference
		Control group	Infected group	
1039.5041	**6.55**	278.19 ± 33.50	172.54 ± 10.00	$p < 0.05$
1041.5166	6.28	214.02 ± 30.77	145.17 ± 8.89	$p < 0.05$
1021.4921	6.57	47.52 ± 3.71	24.76 ± 2.38	$p < 0.05$
1023.5066	6.28	48.74 ± 5.29	29.57 ± 3.99	$p < 0.05$
926.4497	3.65	57.37 ± 3.94	35.37 ± 2.03	$p < 0.05$
980.5669	5.61	61.09 ± 9.15	38.71 ± 0.80	$p < 0.05$
990.5030	3.96	30.09 ± 4.06	19.10 ± 1.89	$p < 0.05$
943.5472	6.28	34.40 ± 2.78	20.79 ± 1.39	$p < 0.05$
944.4608	3.67	23.97 ± 2.57	15.07 ± 1.06	$p < 0.05$
958.4905	5.20	96.47 ± 27.09	52.00 ± 0.26	$p > 0.05$
1154.5658	6.21	65.80 ± 23.04	26.30 ± 0.35	$p > 0.05$
1060.5256	4.86	19.52 ± 3.40	13.99 ± 2.48	$p > 0.05$
1042.5164	5.47	14.99 ± 2.43	11.20 ± 0.03	$p > 0.05$
1171.5919	6.21	18.51 ± 7.09	8.23 ± 0.64	$p > 0.05$
1001.7577	6.42	50.74 ± 13.13	76.03 ± 3.87	$p < 0.05$
1019.7697	6.40	86.27 ± 22.50	135.74 ± 5.80	$p < 0.05$
1036.7966	6.42	12.48 ± 3.17	20.94 ± 0.79	$p < 0.05$
1063.5001	6.25	15.78 ± 1.96	11.60 ± 1.16	$p < 0.05$
983.7480	6.41	40.41 ± 10.42	61.28 ± 3.58	$p < 0.05$

947.7255	21.67	13.80 ± 3.52	0.22 ± 0.38	$p < 0.05$
996.7793	21.70	9.48 ± 2.21	ND	$p < 0.05$
1415.0502	28.11	59.21 ± 3.64	37.78 ± 10.55	$p < 0.05$
939.7218	30.41	81.46 ± 8.07	117.89 ± 12.10	$p < 0.05$
1072.7972	31.76	602.14 ± 126.88	834.62 ± 69.50	$p < 0.05$
1092.8602	7.77	11.59 ± 2.57	9.26 ± 0.75	$p > 0.05$
1076.8276	6.88	67.25 ± 17.12	51.62 ± 12.01	$p > 0.05$
1075.8319	7.81	49.51 ± 11.33	40.81 ± 2.43	$p > 0.05$
1080.8220	6.15	26.47 ± 3.99	32.70 ± 3.28	$p > 0.05$
1057.8229	7.72	51.63 ± 12.74	39.56 ± 2.35	$p > 0.05$
1027.7753	6.72	322.48 ± 82.79	311.38 ± 29.06	$p > 0.05$
1041.7906	6.95	173.89 ± 42.88	128.86 ± 15.02	$p > 0.05$
1059.8024	6.90	54.38 ± 14.35	38.77 ± 5.10	$p > 0.05$
1045.7870	6.07	181.25 ± 41.68	187.34 ± 13.76	$p > 0.05$
1029.7904	7.20	278.78 ± 78.96	316.37 ± 20.35	$p > 0.05$
1047.8019	7.22	163.27 ± 49.55	198.66 ± 17.04	$p > 0.05$
1064.8277	7.29	143.25 ± 44.94	177.59 ± 15.86	$p > 0.05$
895.6585	26.38	63.86 ± 5.34	58.64 ± 10.08	$p > 0.05$
953.6993	25.09	13.26 ± 2.55	17.43 ± 2.37	$p > 0.05$
1055.7699	31.75	585.22 ± 95.01	703.84 ± 80.58	$p > 0.05$
1069.7499	26.39	91.60 ± 4.04	86.80 ± 20.55	$p > 0.05$
1086.7762	26.30	94.97 ± 6.53	98.63 ± 24.83	$p > 0.05$
543.8892	26.36	308.10 ± 20.12	287.73 ± 48.96	$p > 0.05$

Note: ND = not detected.


Observed m/z: 926.4497
RT: 3.65 min
IDA Mode
Intensity, csp
m/z
829.4580 [M-SO3+H]+
926.4497 [M+NH4]+
909.6146 [M+H]+
846.4817
811.4351
793.4357
775.4290
757.4087
739.4182
721.4071
703.3863
685.3725
667.3538
655.3163
625.3071
589.2873
553.2692
535.2521
499.2554
451.2308
439.2307
411.2158
391.2071
331.1927
305.1765
233.1533 1.2867 ppm
215.1427 1.3944 ppm
175.1499
163.1451
135.1151
123.0414
109.0630
81.0695


Observed m/z: 990.5030
RT: 3.96 min
IDA Mode
Intensity, csp
m/z
893.5029 [M-SO3+H]+
973.4684 [M+H]+
875.5010
955.5794
937.4834
857.4840
839.4818
821.4619
803.4485
785.4430
767.4411
749.4297
691.3605
709.3572
505.2618
269.1868
233.1519 7.2913 ppm
215.1438 -3.7185 ppm
193.1227 -9.8384 ppm
173.1334
81.0687


Observed m/z: 943.5472
RT: 6.28 min
MRM Mode
Intensity, csp
m/z
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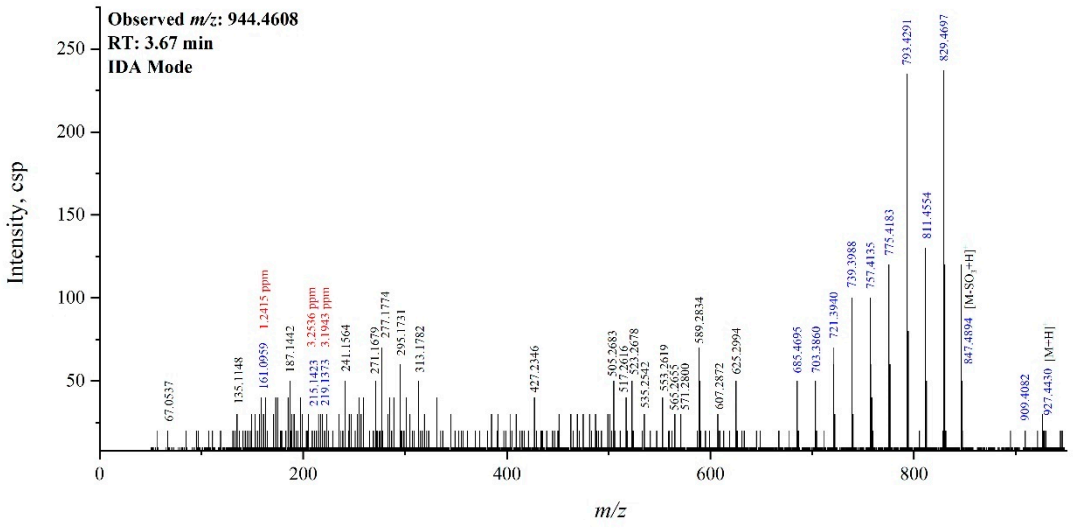
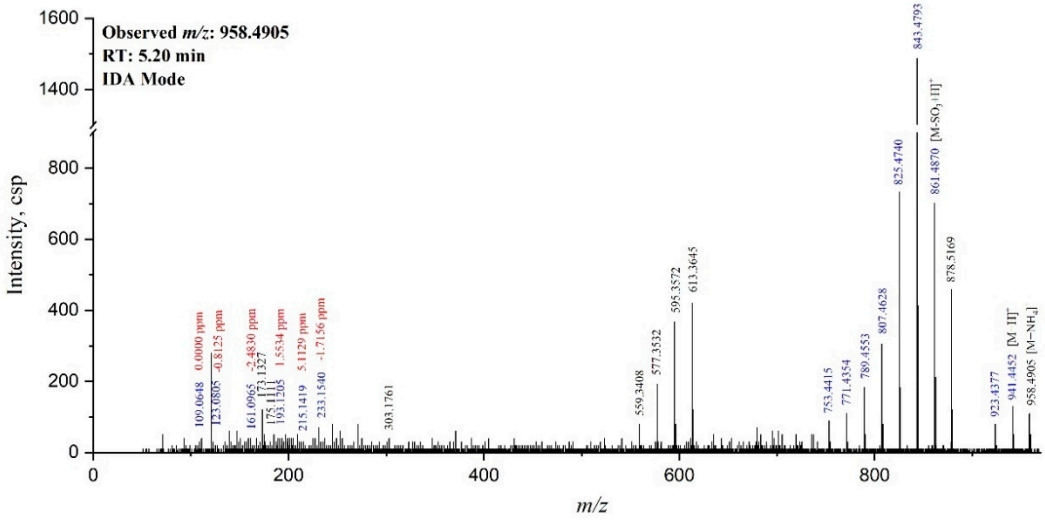
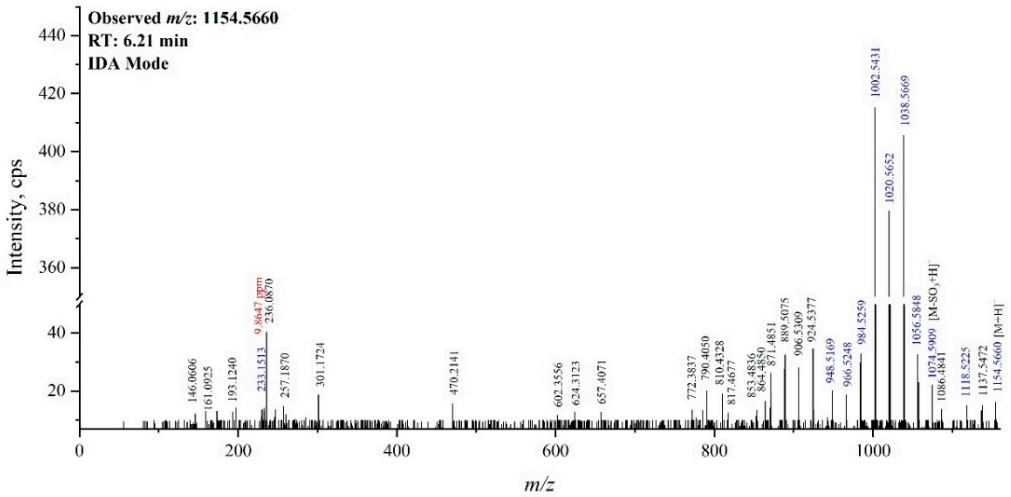
943.5472 [M+H]+
907.5051
889.5038
871.4961
846.6107
805.4349
782.4516
764.4331
736.4051
624.3146
619.4379
609.3539
601.4084
587.3818
575.3994
565.3980
546.3833
509.3318
495.2960
459.2560
413.2821
386.2509
357.2401 6.4382 ppm
349.2258
333.2370
314.2105
245.1539
233.1559 -9.8647 ppm
219.1367 5.9323 ppm
215.1406 10.6909 ppm
193.1205 1.5534 ppm
175.1111
167.1077
160.0939 7.4490 ppm
145.1023
137.0966
123.0811 -5.6873 ppm
109.0641 6.4182 ppm
95.0834
81.0695
62.0552


Observed m/z: 944.4608
RT: 3.67 min
IDA Mode
Intensity, csp
m/z
67.0537
135.1148
161.0959
1.2415 ppm
187.1442
215.1423
3.2536 ppm
219.1373
3.1943 ppm
241.1564
271.1672
277.1774
295.1731
313.1782
427.2346
505.2683
517.2676
523.2678
535.2542
553.2619
565.2655
571.2800
589.2834
607.2872
625.2994
685.4695
703.3860
721.3940
739.3988
757.4135
775.4183
793.4291
811.4554
829.4697
847.4894 [M-SO3+H]
909.4082
927.4430 [M-H]


Observed m/z: 958.4905
RT: 5.20 min
IDA Mode
Intensity, csp
m/z
109.0648
0.0000 ppm
123.0805
-0.8125 ppm
161.0966
-2.4830 ppm
173.1327
175.1111
1.5534 ppm
193.1205
215.1419
5.1129 ppm
233.1540
-1.7156 ppm
303.1761
559.3408
577.3532
595.3572
613.3645
753.4415
771.4354
789.4553
807.4628
825.4740
843.4793
861.4870 [M-SO3-H]-
878.5169
923.4377
941.4452 [M H]-
958.4905 [M-NH4]-


Observed m/z: 1154.5660
RT: 6.21 min
IDA Mode
Intensity, cps
m/z
146.0606
161.0925
193.1240
233.1513
9.8647 ppm
236.0870
257.1870
301.1724
470.2141
602.3556
624.3123
657.4071
772.3837
790.4050
810.4328
817.4677
853.4836
864.4851
871.4851
889.5075
906.5309
924.5377
948.5169
966.5248
981.5259
1002.5431
1020.5652
1038.5669
1056.5848
1074.5909 [M-SO3+H]
1086.6841
1118.5225
1137.5472
1154.5660 [M-H]

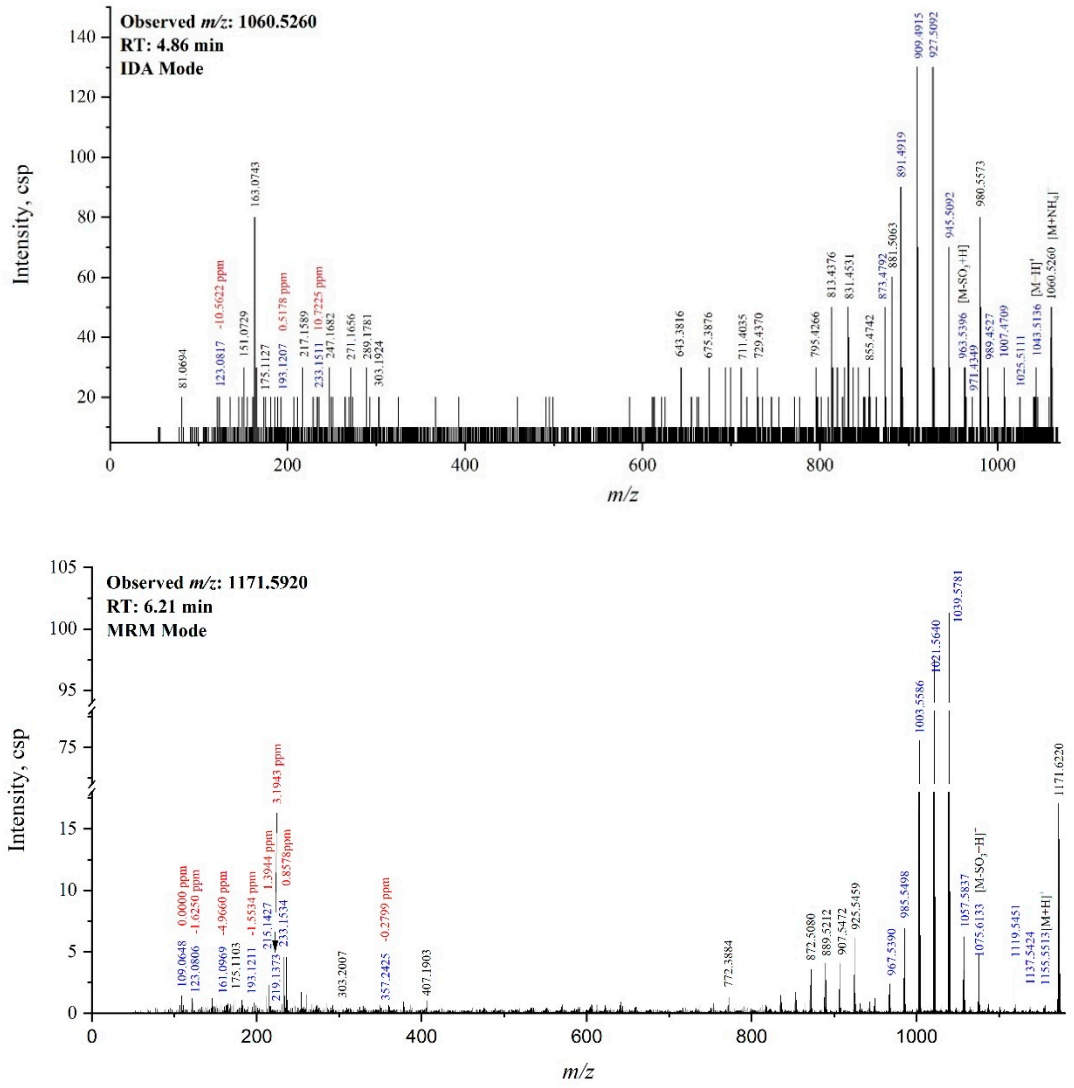
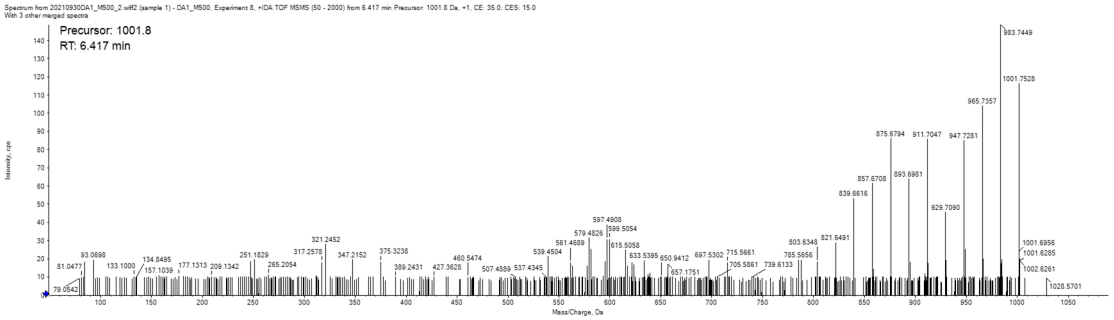
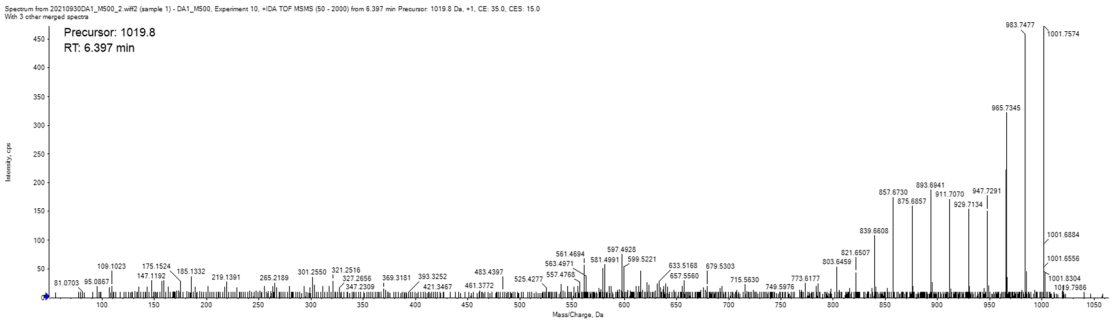
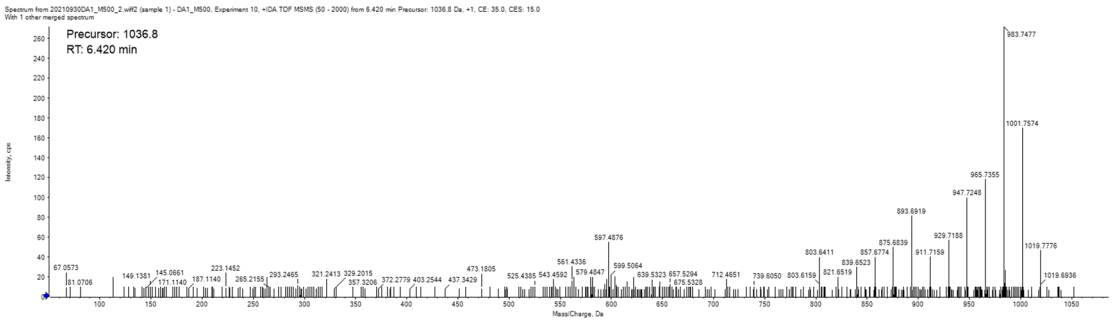
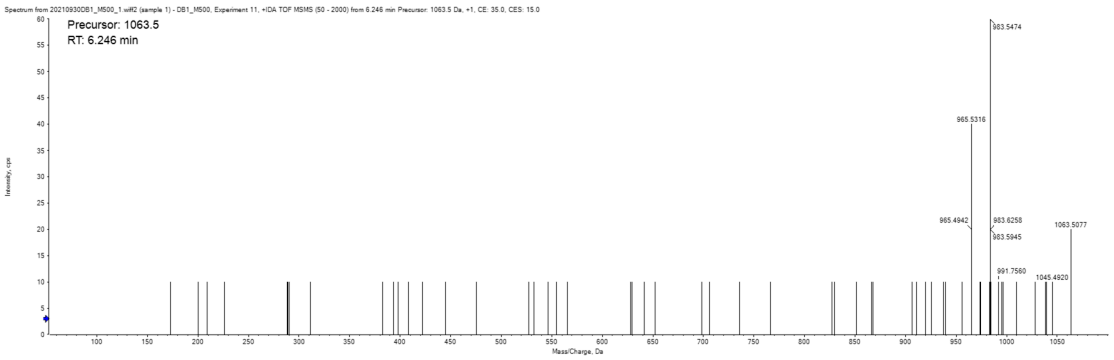


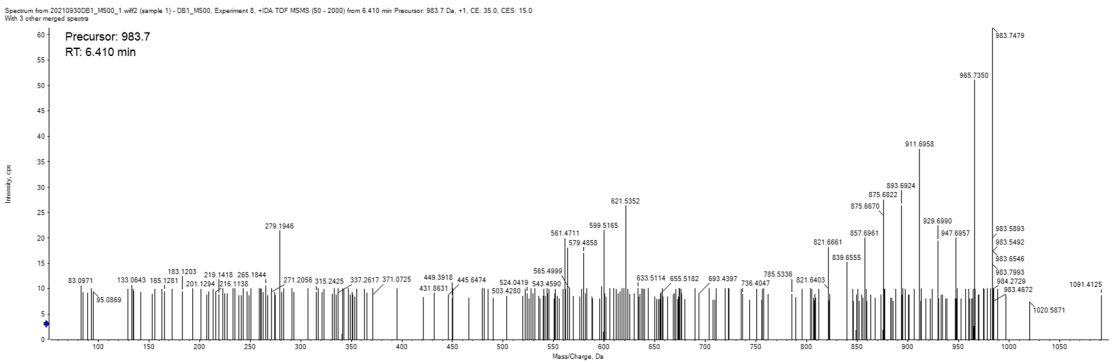
Figure S1. MS/MS spectra of gambierone analogues. The specific neutral losses and fragments of gambirones were shown in blue, and mass errors of specific fragments were shown in red.

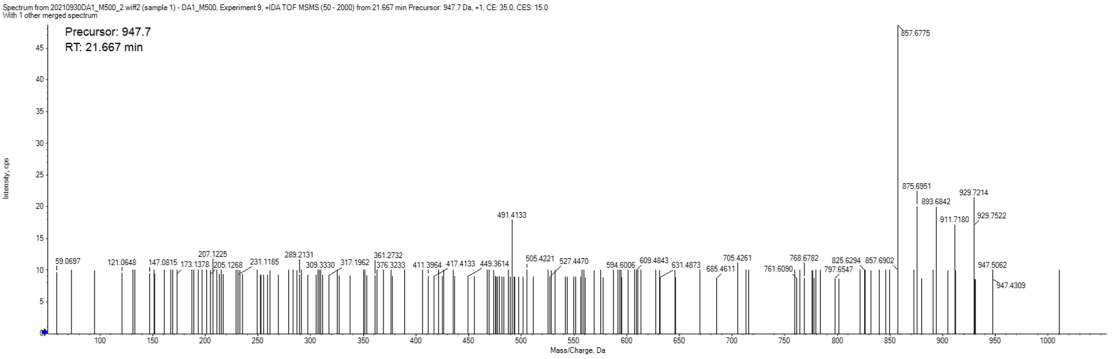

Precursor: 1001.8
RT: 6.417 min
Intensity, cps
Mass/Charge, Da

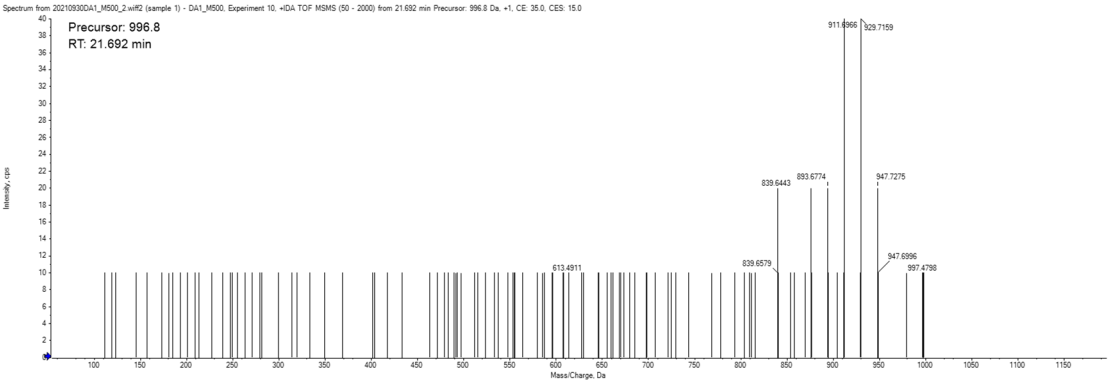

Precursor: 1019.8
RT: 6.397 min
Intensity, cps
Mass/Charge, Da

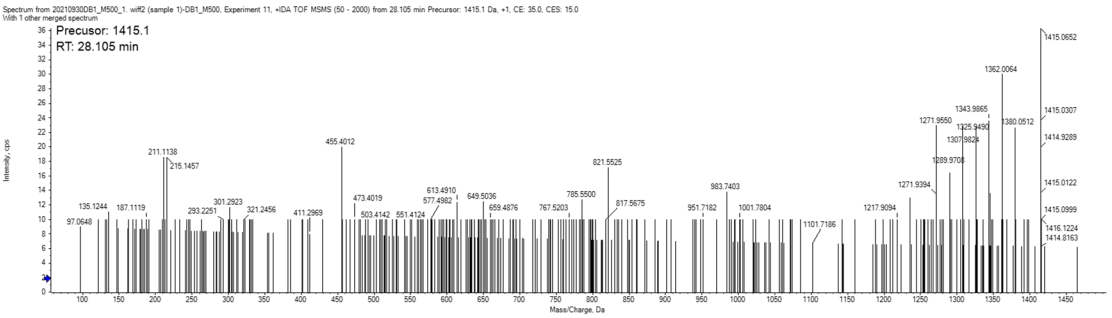

Precursor: 1036.8
RT: 6.420 min
Intensity, cps
Mass/Charge, Da

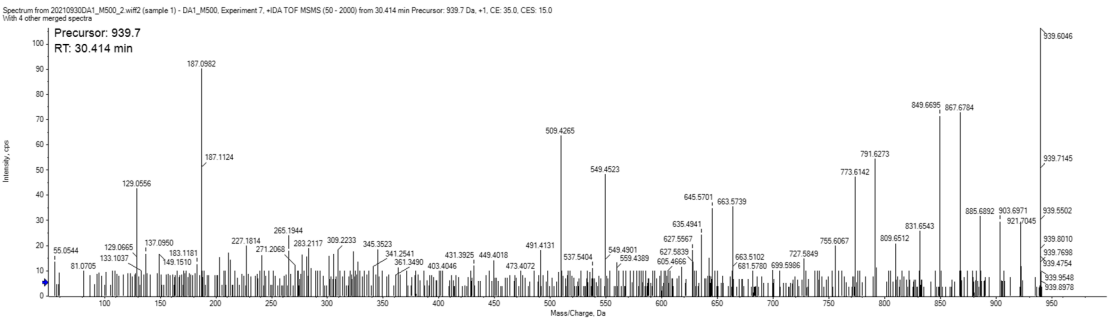

Precursor: 1063.5
RT: 6.246 min
Intensity, cps
Mass/Charge, Da

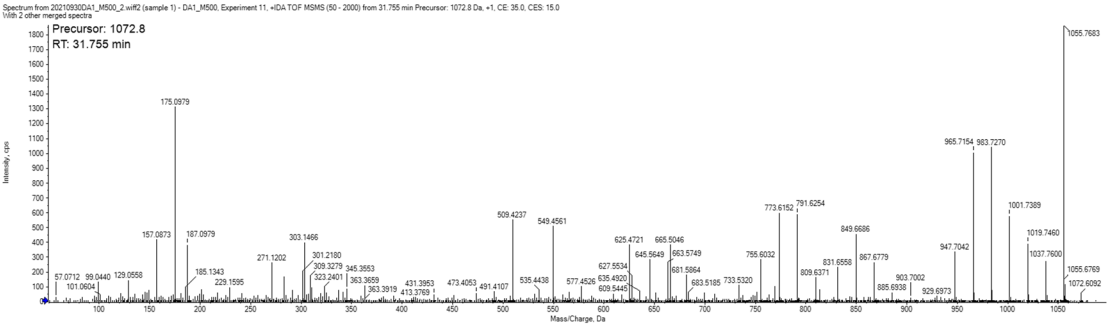

Precursor: 983.7
RT: 6.410 min
Intensity, cps
Mass/Charge, Da

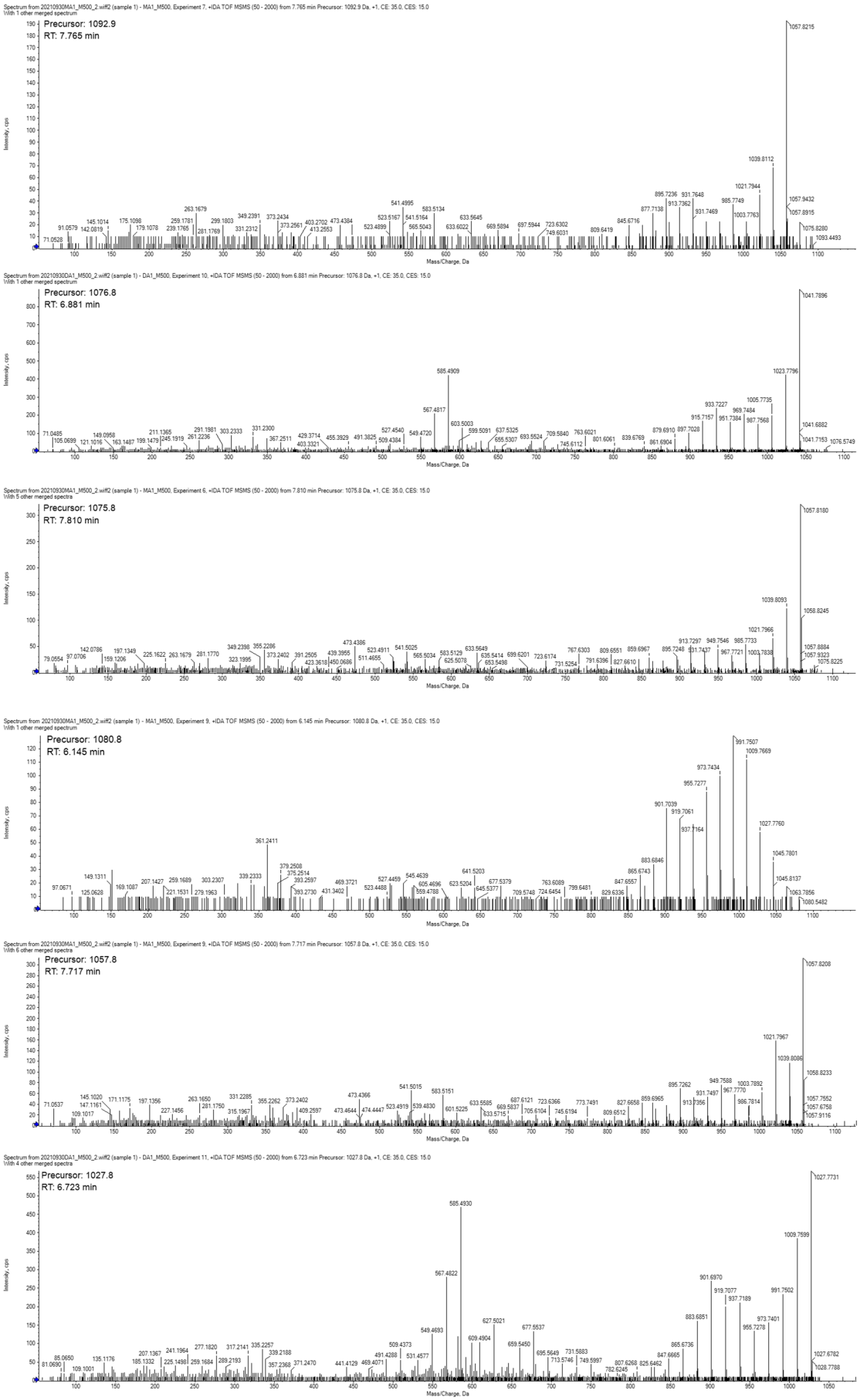

Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 9, +IDA TOF MSMS (50 - 2000) from 21.667 min Precursor: 947.7 Da, +1, CE: 35.0, CES: 15.0
With 1 other merged spectrum
Precursor: 947.7
RT: 21.667 min
Intensity, cps
Mass/Charge, Da

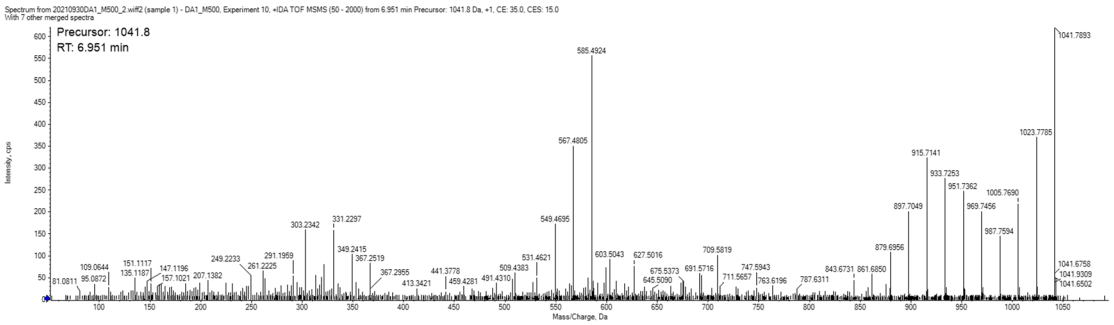

Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 10, +IDA TOF MSMS (50 - 2000) from 21.692 min Precursor: 996.8 Da, +1, CE: 35.0, CES: 15.0
Precursor: 996.8
RT: 21.692 min
Intensity, cps
Mass/Charge, Da

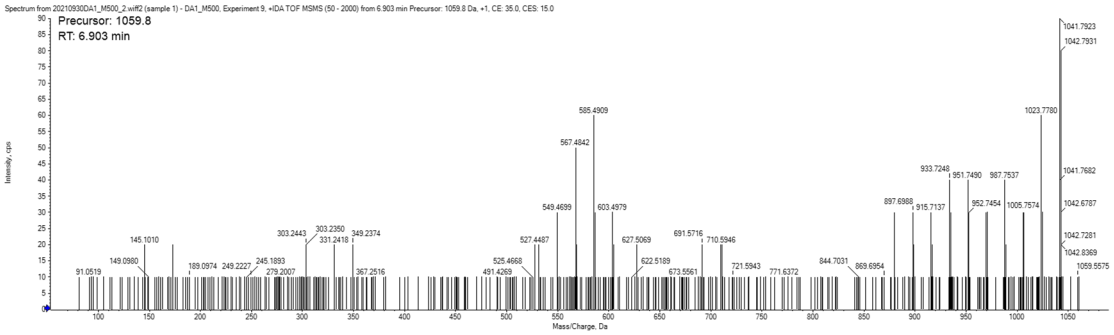

Spectrum from 20210930DB1_M500_1.wiff2 (sample 1)-DB1_M500, Experiment 11, +IDA TOF MSMS (50 - 2000) from 28.105 min Precursor: 1415.1 Da, +1, CE: 35.0, CES: 15.0
With 1 other merged spectrum
Precusor: 1415.1
RT: 28.105 min
Intensity, cps
Mass/Charge, Da

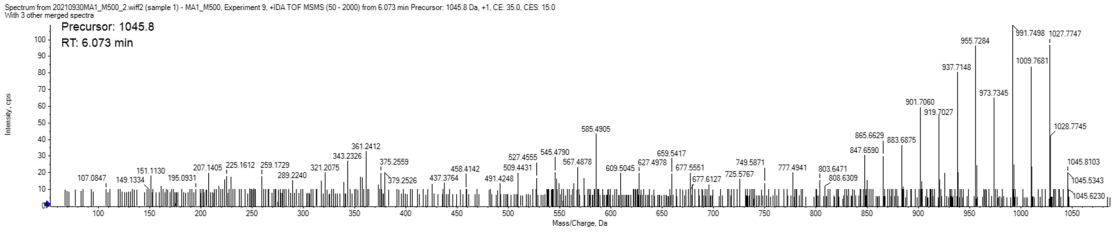

Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 7, +IDA TOF MSMS (50 - 2000) from 30.414 min Precursor: 939.7 Da, +1, CE: 35.0, CES: 15.0
With 4 other merged spectra
Precursor: 939.7
RT: 30.414 min
Intensity, cps
Mass/Charge, Da

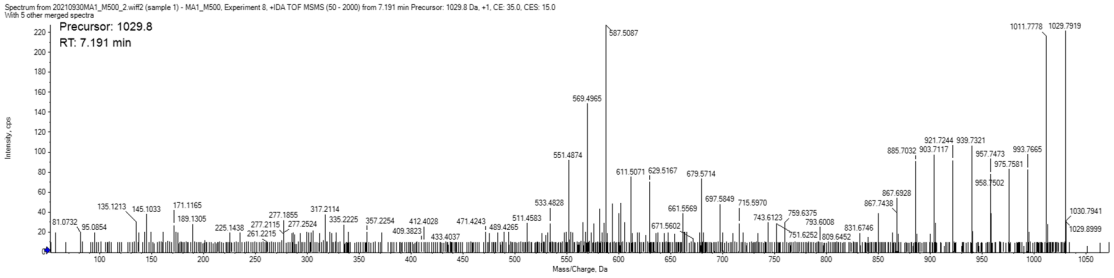

Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 11, +IDA TOF MSMS (50 - 2000) from 31.755 min Precursor: 1072.8 Da, +1, CE: 35.0, CES: 15.0
With 2 other merged spectra
Precursor: 1072.8
RT: 31.755 min
Intensity, cps
Mass/Charge, Da

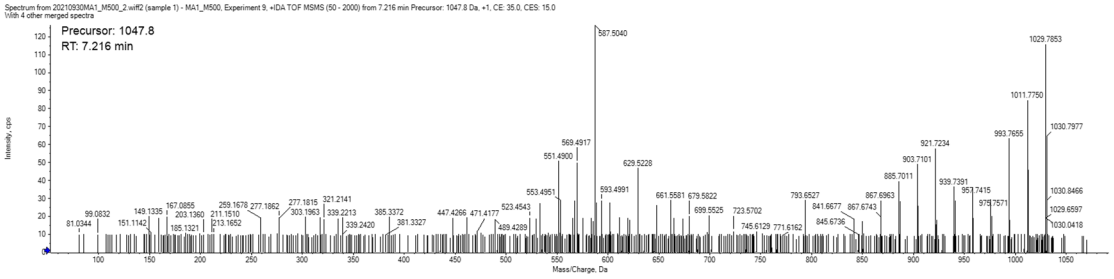

Spectrum from 20210930MA1_M500_2.wiff2 (sample 1) - MA1_M500, Experiment 7, +IDA TOF MSMS (50 - 2000) from 7.765 min Precursor: 1092.9 Da, +1, CE: 35.0, CES: 15.0
With 1 other merged spectrum
Precursor: 1092.9
RT: 7.765 min
Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 10, +IDA TOF MSMS (50 - 2000) from 6.881 min Precursor: 1076.8 Da, +1, CE: 35.0, CES: 15.0
With 1 other merged spectrum
Precursor: 1076.8
RT: 6.881 min
Spectrum from 20210930MA1_M500_2.wiff2 (sample 1) - MA1_M500, Experiment 6, +IDA TOF MSMS (50 - 2000) from 7.810 min Precursor: 1075.8 Da, +1, CE: 35.0, CES: 15.0
With 5 other merged spectra
Precursor: 1075.8
RT: 7.810 min
Spectrum from 20210930MA1_M500_2.wiff2 (sample 1) - MA1_M500, Experiment 9, +IDA TOF MSMS (50 - 2000) from 6.145 min Precursor: 1080.8 Da, +1, CE: 35.0, CES: 15.0
With 1 other merged spectrum
Precursor: 1080.8
RT: 6.145 min
Spectrum from 20210930MA1_M500_2.wiff2 (sample 1) - MA1_M500, Experiment 9, +IDA TOF MSMS (50 - 2000) from 7.717 min Precursor: 1057.8 Da, +1, CE: 35.0, CES: 15.0
With 6 other merged spectra
Precursor: 1057.8
RT: 7.717 min
Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 11, +IDA TOF MSMS (50 - 2000) from 6.723 min Precursor: 1027.8 Da, +1, CE: 35.0, CES: 15.0
With 4 other merged spectra
Precursor: 1027.8
RT: 6.723 min
Intensity, cps
Mass/Charge, Da

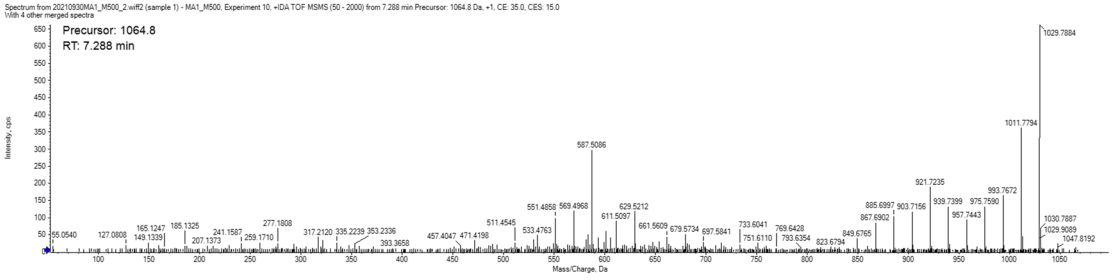

Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 10, +IDA TOF MSMS (50 - 2000) from 6.951 min Precursor: 1041.8 Da, +1, CE: 35.0, CES: 15.0
With 7 other merged spectra
Precursor: 1041.8
RT: 6.951 min
Intensity, cps
Mass/Charge, Da

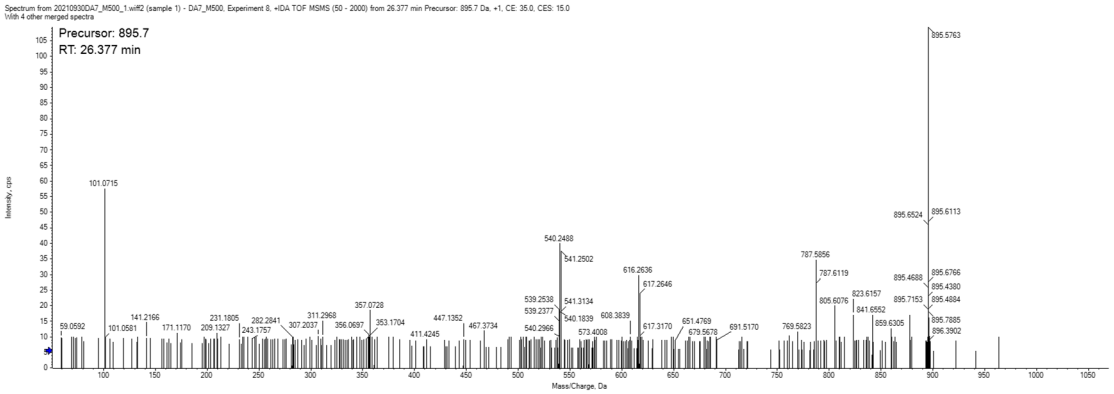

Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 9, +IDA TOF MSMS (50 - 2000) from 6.903 min Precursor: 1059.8 Da, +1, CE: 35.0, CES: 15.0
Precursor: 1059.8
RT: 6.903 min
Intensity, cps
Mass/Charge, Da

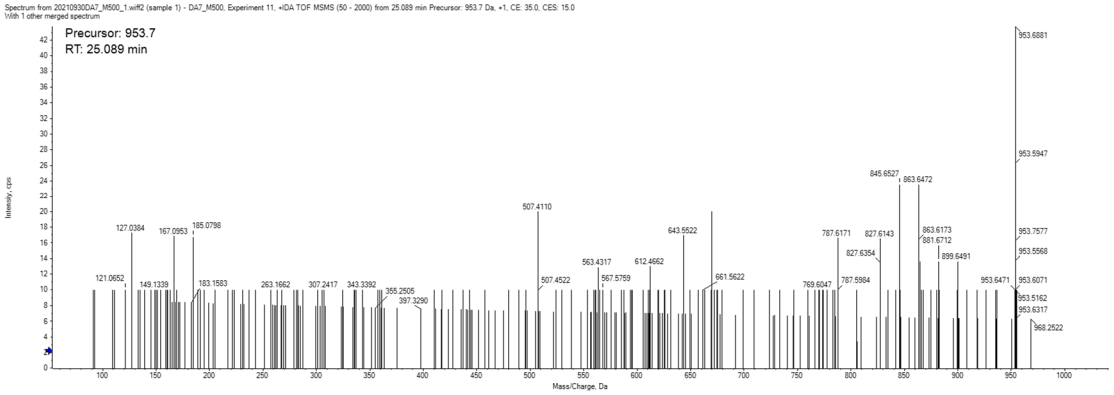

Spectrum from 20210930MA1_M500_2.wiff2 (sample 1) - MA1_M500, Experiment 9, +IDA TOF MSMS (50 - 2000) from 6.073 min Precursor: 1045.8 Da, +1, CE: 35.0, CES: 15.0
With 3 other merged spectra
Precursor: 1045.8
RT: 6.073 min
Intensity, cps
Mass/Charge, Da

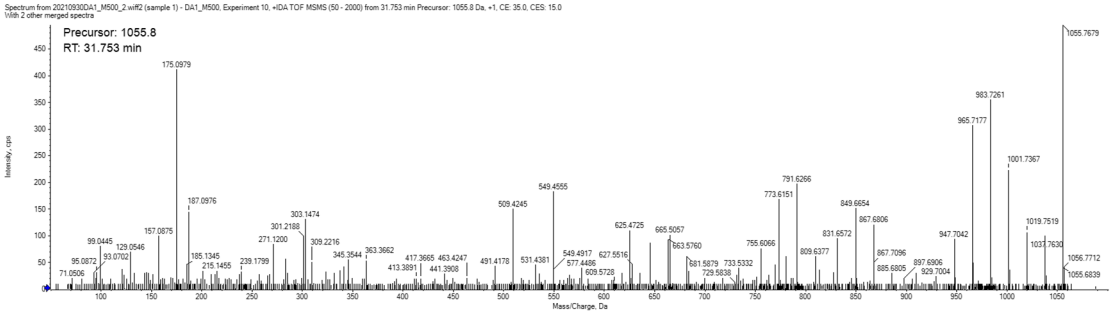

Spectrum from 20210930MA1_M500_2.wiff2 (sample 1) - MA1_M500, Experiment 8, +IDA TOF MSMS (50 - 2000) from 7.191 min Precursor: 1029.8 Da, +1, CE: 35.0, CES: 15.0
With 5 other merged spectra
Precursor: 1029.8
RT: 7.191 min
Intensity, cps
Mass/Charge, Da

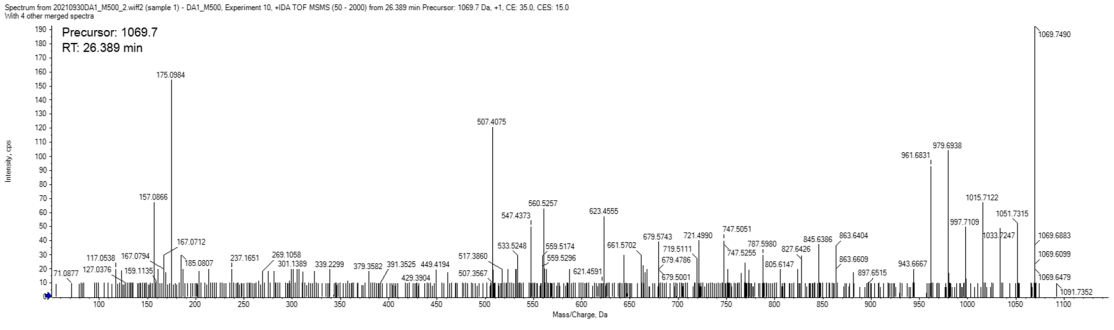

Spectrum from 20210930MA1_M500_2.wiff2 (sample 1) - MA1_M500, Experiment 9, +IDA TOF MSMS (50 - 2000) from 7.216 min Precursor: 1047.8 Da, +1, CE: 35.0, CES: 15.0
With 4 other merged spectra
Precursor: 1047.8
RT: 7.216 min
Intensity, cps
Mass/Charge, Da

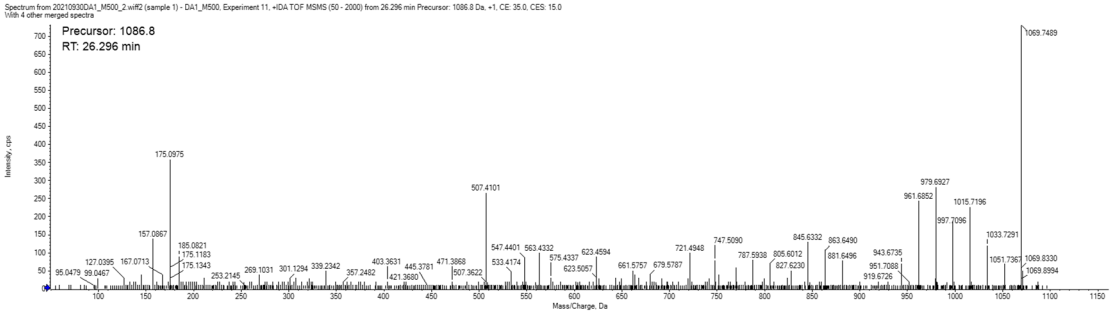

Spectrum from 20210930MA1_M500_2.wiff2 (sample 1) - MA1_M500, Experiment 10, +IDA TOF MSMS (50 - 2000) from 7.288 min Precursor: 1064.8 Da, +1, CE: 35.0, CES: 15.0
With 4 other merged spectra
Precursor: 1064.8
RT: 7.288 min
Intensity, cps
Mass/Charge, Da


Spectrum from 20210930DA7_M500_1.wiff2 (sample 1) - DA7_M500, Experiment 8, +IDA TOF MSMS (50 - 2000) from 26.377 min Precursor: 895.7 Da, +1, CE: 35.0, CES: 15.0
With 4 other merged spectra
Precursor: 895.7
RT: 26.377 min
Intensity, cps
Mass/Charge, Da


Spectrum from 20210930DA7_M500_1.wiff2 (sample 1) - DA7_M500, Experiment 11, +IDA TOF MSMS (50 - 2000) from 25.089 min Precursor: 953.7 Da, +1, CE: 35.0, CES: 15.0
With 1 other merged spectrum
Precursor: 953.7
RT: 25.089 min
Intensity, cps
Mass/Charge, Da


Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 10, +IDA TOF MSMS (50 - 2000) from 31.753 min Precursor: 1055.8 Da, +1, CE: 35.0, CES: 15.0
With 2 other merged spectra
Precursor: 1055.8
RT: 31.753 min
Intensity, cps
Mass/Charge, Da


Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 10, +IDA TOF MSMS (50 - 2000) from 26.389 min Precursor: 1069.7 Da, +1, CE: 35.0, CES: 15.0
With 4 other merged spectra
Precursor: 1069.7
RT: 26.389 min
Intensity, cps
Mass/Charge, Da


Spectrum from 20210930DA1_M500_2.wiff2 (sample 1) - DA1_M500, Experiment 11, +IDA TOF MSMS (50 - 2000) from 26.296 min Precursor: 1086.8 Da, +1, CE: 35.0, CES: 15.0
With 4 other merged spectra
Precursor: 1086.8
RT: 26.296 min
Intensity, cps
Mass/Charge, Da

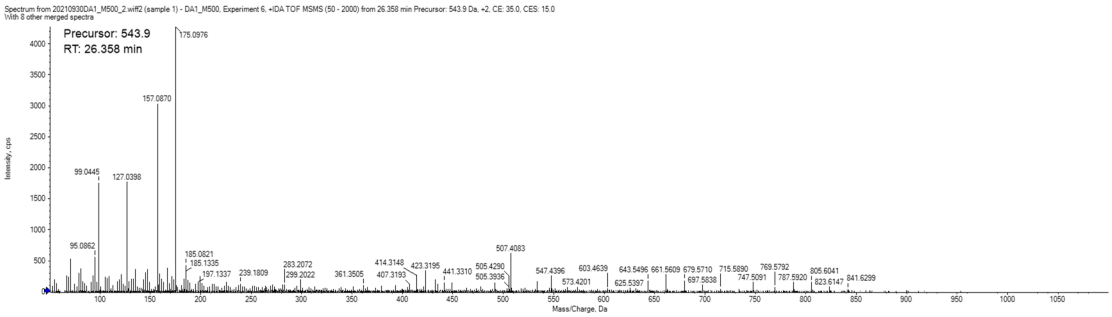


Figure S2. MS/MS spectra of polyol-polyene super-carbon-chain compounds.