

Sample	m/z (detected, peak apex)	RT (min, peak apex)	Peak height (apex scan, raw)	Putative composition (m-NHMe, c-OH)	Theoretical m/z	Mass error (ppm)	MSMS isolation (m/z)	MSMS spectral RT	Putative C-terminal residue	Peptide species	Putative Sequence ID Note, C=ClBht, X=CTyr, H=Hpg, D=Dpg, Y=Tyr	Sequence within NRPS Pathway - (red sequences excluded)	Proposed Module Pathway - (red sequences excluded)	Notes (main sequence ions detected with losses as # = -CO, * = -NH3, ^ = -CH5 (MA), * = -H2O)
												unusual communication; anticipated; N-term extension	(Z) = unusual communication; anticipated	
M5-6 + M7a	559.15997	23.19	2.16E+06	1Hpg1Dpg1ClBht-m	559.15901	1.72	559.158996	23.18	D		HCD		56-7	v1, b2*, y2*, M^#*, M^#*, M^#*, M^#* - however noisy with many abundant unexplained ions
	559.16022	24.1	1.00E+06	1Hpg1Dpg1ClBht-m	559.15901	2.16	559.158996	24.09	D		HCD		56-7	v1, b2*, y2*, M^#*, M^#*, M^#*, M^#* - however noisy with many abundant unexplained ions
	559.15985	25.54	1.68E+06	1Hpg1Dpg1ClBht-m	559.15901	1.50	559.158996	25.53	D		HCD		56-7	v1, b2*, y2*, M^#*, M^#*, M^#*, M^#* - however noisy with many abundant unexplained ions
	559.15973	26.1	9.37E+05	1Hpg1Dpg1ClBht-m	559.15901	1.29	559.158996	26.09	D		HCD		56-7	v1, b2*, y2*, M^#*, M^#*, M^#*, M^#* - however noisy with many abundant unexplained ions
M5-6a + M3	559.15967	24.01	1.28E+06	1Hpg1Dpg1ClBht-m	559.15901	1.18	559.158996	24.01	D	3a	HCD?	HCD	56a-3	y1, b2*, y2*, M^#*, M^#*, M^#*, M^#* - however noisy with many abundant unexplained ions
	559.15948	24.7	1.29E+06	1Hpg1Dpg1ClBht-m	559.15901	0.84	559.158996	24.69	D		HCD?		56a-3	y1, b2*, y2*, M^#*, M^#*, M^#*, M^#* - however noisy with many abundant unexplained ions
M5-6a + M3 + M4	708.20709	21.76	3.04E+07	2Hpg1Dpg1ClBht-m	708.20669	0.56	708.206726	21.79	H	13a	HCDH	H-C-D-H-H-C-D-H	56a-3-4-56a-3-4	y1*, y1, y2, y2*, CDH**, CDH**, CDH*, CDH*
	708.20721	22.51	1.97E+06	2Hpg1Dpg1ClBht-m	708.20669	0.73	708.206726	22.53	H/C	13a/15a	HCDH/DHHC/CDH/HDC (combination spectrum)	H-C-D-H-H-C-D-H/H-C-D-H-H-C-D-H	56a-3-4-56a-3-4/56a-3-4-56a-3-4	combination of neighbouring peak spectra
	708.20734	22.78	4.77E+06	2Hpg1Dpg1ClBht-m	708.20669	0.92	708.206726	22.78	C	15a	DHHC/HDC	H-C-D-H-H-C-D-H	56a-3-4-56a-3-4	y1*, y2**, y2*, y2**, DH#, DH#*
	708.20728	22.91	1.04E+07	2Hpg1Dpg1ClBht-m	708.20669	0.83	708.207164	22.91	H		CDHH	H-C-D-H-H-C-D-H	56a-3-4-56a-3-4	y1*, b2*, y2*, y2**#, a2*, y1, DH#, y2**, DH#, a3*, b3*, y3, a3**, a3#**, a3
	708.20764	23.37	6.23E+06	2Hpg1Dpg1ClBht-m	708.20669	1.34	708.206726	23.37	H	18a	CDHH	H-C-D-H-H-C-D-H	56a-3-4-56a-3-4	y1*, y2*, b2*, y2**#, a2*, y1, DH#, y2**, DH#, a3#**, a3*, a3
	873.24927	22.76	5.40E+07	2Hpg2Dpg1ClBht-m	873.24928	0.01	873.249103	22.83	D	20a	HCDHD	H-C-D-H-D-C-D-H	56a-3-4-(Z)-56a-3-4	y1, y2*, y1*, y2**#, y2**#, a3**, a3#**, b3**, b2**, y2**, a2**, a4**, a4*, y2, a3*, M^#**#, a2*, y4**#, a2*
	873.24951	23.09	1.22E+08	2Hpg2Dpg1ClBht-m	873.24928	0.26	NA	NA	NA	NA	NA	NA	NA	peak without MSMS spectrum
	873.24945	23.2	2.22E+08	2Hpg2Dpg1ClBht-m	873.24928	0.19	873.249767	23.18	D		HCDHD	H-C-D-H-D-C-D-H	56a-3-4-(Z)-56a-3-4	y1, y1*, y2*, y2**#, y2**#, a3**, b2*, b3**, b2**, a3#**, y2**, a2**, b3*, a4**, a2**, y2, M^#**#, a2*, a4*, a2*, a2#**, a3*, y4**#, y3, b2, a2#**, a4
	873.24957	23.44	1.38E+07	2Hpg2Dpg1ClBht-m	873.24928	0.33	873.24932	23.35	D	20a	HCDHD	H-C-D-H-D-C-D-H	56a-3-4-(Z)-56a-3-4	highly similar to above
	873.24963	23.55	8.53E+06	2Hpg2Dpg1ClBht-m	873.24928	0.40	873.24995	23.53	H		HCDHD??			similar fragment masses but different abundances
	1070.27502	26.89	5.74E+06	3Hpg1Dpg2ClBht-m	1070.27364	1.29	NA	NA	NA	NA	NA	NA	NA	peak without MSMS spectrum
	1070.27502	27.06	1.93E+07	3Hpg1Dpg2ClBht-m	1070.27364	1.29	NA	NA	NA	NA	NA	NA	NA	peak without MSMS spectrum
	1070.27490	27.28	3.42E+07	3Hpg1Dpg2ClBht-m	1070.27364	1.18	1070.27563	27.26	C	19a	??HHC	H-C-D-H-H-C-D-H	56a-3-4-56a-3-4	y1*, y1^0, HH#, CH*, DH#, CD*, DH#, HCD*, HH, y2, HCD*, CHC**#, HH#, y2*, y1, y1**
	M5-6 + M3a + M4	708.20685	27.13	1.67E+06	2Hpg1Dpg1ClBht-m	708.20669	0.23	708.206726	27.13	H	13a	HCDH	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4
708.20685		27.32	2.09E+06	2Hpg1Dpg1ClBht-m	708.20669	0.23	708.206726	27.35	H		HCDH	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4	y1*, y1, y2, y2*, CDH**, CDH**, CDH*, CDH*
708.20770		28.53	2.92E+06	2Hpg1Dpg1ClBht-m	708.20669	1.43	708.206726	28.44	C	15a	DHHC/HDC	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4	y1*, y2**, y2*, y2*, y2**, DH#, DH
708.20734		28.99	8.60E+06	2Hpg1Dpg1ClBht-m	708.20669	0.92	708.206726	28.99	H		HCDH	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4	y1*, y1, y2, y2*, CDH**, CDH**, CDH*, CDH*
708.20721		29.12	1.31E+07	2Hpg1Dpg1ClBht-m	708.20669	0.73	708.206726	29.12	H	13a	HCDH	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4	y1*, y1, y2, y2*, CDH**, CDH**, CDH*, CDH*
708.20746		29.52	2.23E+06	2Hpg1Dpg1ClBht-m	708.20669	1.09	708.206726	29.52	D	7a	HHC	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4	y2** y1, b3**, a3**, y1*, y2**#, y2*, y3**#, y3**#, M^#**
857.25488		29.77	1.18E+08	3Hpg1Dpg1ClBht-m	857.25437	0.59	857.254846	29.83	H	14a	?HHC	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4	v1, y2 - but presence of HH#, HD, HC, HH, DC related ions
857.25494		30.2	1.64E+08	3Hpg1Dpg1ClBht-m	857.25437	0.66	857.255645	30.39	H		?HHC			v1, y2 - but presence of HH#, HD, HC, HH, DC related ions
857.25507		30.51	1.01E+08	3Hpg1Dpg1ClBht-m	857.25437	0.82	857.255267	30.57	D/C	17a	HHHC	H-C-H-H-H-C-D-H/H-C-H-H-H-C-D-H	56-(Z)-56-3a-4/56-(Z)-4-56-3a-4	a3*, y1, y2**, b3*, y2**#, y2* - but also presence of HD related ions
857.25500		30.88	1.22E+08	3Hpg1Dpg1ClBht-m	857.25437	0.73	857.255318	30.95	D/C		HHHC			a3*, y1, y2**, b3*, y2**#, y2* - but also presence of HD related ions
857.25507		31.31	1.43E+08	3Hpg1Dpg1ClBht-m	857.25437	0.82	NA	NA	NA	NA	NA	NA	NA	peak without MSMS spectrum
857.25543		31.56	7.80E+07	3Hpg1Dpg1ClBht-m	857.25437	1.24	857.255448	31.50	H	14a	?HHC	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4	y1, y2 - but presence of HH#, HD, HC, HH, DC related ions
873.24957		29.83	3.00E+07	2Hpg2Dpg1ClBht-m	873.24928	0.33	873.249182	29.77	D	16a	DHHC	H-C-D-H-H-C-D-H	56-3a-4-56-3a-4	a2, b2, y1, y2**, y2*, HHC**, y3**#, y3**#, y3**#, y3**
873.24921		30.17	3.10E+07	2Hpg2Dpg1ClBht-m	873.24928	0.08	873.249218	30.14	D		DHHC			a2, b2, y1, y2**, y2*, HHC**, y3**#, y3**#, y3**#, y3**
M6a + M3 + M4 + M5 + M6 + M7	527.17047	26.62	2.63E+05	2Hpg1CTYr-m	527.16919	2.43	527.169799	26.60	H		XHH			y1*, a2, y2**#, y2*, y1
	527.16937	27.19	3.07E+05	2Hpg1CTYr-m	527.16919	0.34	527.169433	27.17	H		XHH			y1*, a2, y2**#, y2*, y1
	527.16974	27.58	8.05E+04	2Hpg1CTYr-m	527.16919	1.04	527.169305	27.60	H		XHH			y1*, a2, y2**#, y2*, y1
	530.13354	27.7	2.41E+05	1Hpg1Dpg1CTYr-c	530.13247	2.02	530.132507	27.69	D	24b	HXD	X-D-H-H-X-D	6a-3-4-5-6-7	y1 - noisy, as coeluting with 529.757 2+ ion
	530.13330	29.77	3.77E+06	1Hpg1Dpg1CTYr-c	530.13247	1.57	530.132507	29.77	D		XHD?			y1, b2*, a2*, b2, y2*(very low)
	692.21259	27.41	1.49E+06	2Hpg1Dpg1CTYr-m	692.21178	1.17	692.211791	27.42	H		XDHH			y1*, y2*, y1, HH#, a2, b2, y2, a3, b3
	692.21283	27.58	7.37E+05	2Hpg1Dpg1CTYr-m	692.21178	1.52	692.211791	27.57	H		XDHH	X-D-H-H-X-D	6a-3-4-5-6-7	y1*, y2*, y1, HH#, a2, b2, y2, a3, b3
	692.21448	28.05	3.68E+06	2Hpg1Dpg1CTYr-m	692.21178	3.90	692.211791	28.03	H		XDHH			y1*, y2*, y1, HH#, a2, b2, y2, a3, b3
	692.21344	28.59	2.16E+06	2Hpg1Dpg1CTYr-m	692.21178	2.40	692.211791	28.57	H		XDHH			y1*, y2*, y1, HH#, a2, b2, y2, a3, b3
	841.26202	30.49	1.92E+06	3Hpg1Dpg1CTYr-m	841.25946	3.04	841.26062	30.41	H	23a	XDHHH	X-D-H-H-H-D	6a-3-4-5-(Z)-7, Z=5 in this case	a3*, a3#*, y1*, b3*, DH#, y2**#, a2#*, y2*, a4*, DH#, y2, y3**#
	841.26154	30.83	7.24E+05	3Hpg1Dpg1CTYr-m	841.261474	2.47	841.261474	30.81	H		XDHHH			a3*, a3#*, y1*, b3*, DH#, y2**#, a2#*, y2*, a4*, DH#, y2, y3**#, b3
	844.22510	33.99	4.55E+05	2Hpg2Dpg1CTYr-c	844.22274	2.80	844.224792	33.95	?	25a	Uncertain (weak)	X-D-H-H-X-D	6a-3-4-5-6-7	DH#, XHH#, XDHH#, XDH#, HH#, CH#, CH*
	1041.24878	37.8	4.38E+04	2Hpg2Dpg2CTYr-c	1041.2471	1.61	1041.24707	37.80	?		Uncertain (weak, coeluting 6+ species)	X-D-H-H-X-D		HH#*
	1041.24890	38.39	5.48E+04	2Hpg2Dpg2CTYr-c	1041.2471	1.73	1041.24707	38.42	?	26b	Uncertain (weak)	X-D-H-H-X-D	6a-3-4-5-6-7	DH#*, DX#
M3 + M5	509.20352	24.79	4.21E+06	1Hpg1Dpg1TYr-m	509.20307	0.88	509.203094	24.79	D	10a	HYD	(HYD)	(HYD)-3 (synthetic tripeptide)	y1, y2, b2*, y1*, M^#*, M^#*, M^#**
	509.20364	25	4.88E+06	1Hpg1Dpg1TYr-m	509.20307	1.12	509.203094	25.00	D		HYD		(HYD)-3 (synthetic tripeptide)	y1, y2, b2*, y1*, M^#*, M^#*, M^#**
	509.20380	27.05	3.92E+05	1Hpg1Dpg1TYr-m	509.20307	1.43	509.203094	26.98	D		HYD?		(HYD)-3 (synthetic tripeptide)	y1, b2*, y1*, M^#*, M^#*, M^#**
	658.25134	28.23	2.83E+07	2Hpg1Dpg1TYr-m	658.25075	0.90	658.250732	28.23	D	28a	HHYD	H-(HYD)	5-(HYD)-3	a3*, b3*, y1, y2, b2, b3, y3*, M^#*
	658.25128	28.33	1.90E+08	2Hpg1Dpg1TYr-m	658.25075	0.81	658.250732	28.35	D		HHYD		5-(HYD)-3	a3*, b3*, y1, y2, b2, b3, y3*, M^#*
	658.25122	28.49	2.63E+08	2Hpg1Dpg1TYr-m	658.25075	0.71	658.250732	28.49	D		HHYD		5-(HYD)-3	a3*, b3*, y1, y2, b2, b3, y3*, M^#*
	807.29907	30.23	4.40E+07	3Hpg1Dpg1TYr-m	807.29843	0.79	807.298539	30.32	D		HHHYD	H+-(HYD)	5-5-(HYD)-3	a3*, b3*, y1, b2, b2*, y2, y2^, a4*
	807.29919	30.42	4.22E+07	3Hpg1Dpg1TYr-m	807.29843	0.94	807.299178	30.51	D	29a	HHHYD	H+-(HYD)	5-5-(HYD)-3	a3*, b3*, y1, b2, b2*, y2, y2^, a4*
807.29895	31.09	2.38E+06	3Hpg1Dpg1TYr-m	807.29843	0.64	807.298553	31.07	D		HHHYD		5-5-(HYD)-3	a3*, b3*, y1, b2, b2*, y2, y2^, a4*	
M3 + M5c	658.25134	27.69	8.50E+08	2Hpg1Dpg1TYr-m	658.25075	0.90	658.250732	27.70	H	11a	HYDH	(HYD)-H	(HYD)-3-4a	a3*, b3*, a3#*, y1*, y2**#, y2, y1, b3, y3, M^#*
	807.29877	30.11	3.37E+08	3Hpg1Dpg1TYr-m	807.29843	0.42	807.299177	30.07	H	12a	?[D]HH, most probably HYDHH	(HYD)-H-H	(HYD)-3-4a-4a	a3*, a3#*, b3*, y1*, y2*, y1, y2, b3, a4*
	807.29913	30.24	2.89E+08	3Hpg1Dpg1TYr-m	807.29843	0.87	807.299114	30.26	H		?[D]HH, most probably HYDHH		(HYD)-3-4a-4a	a3*, a3#*, b3*, y1*, y2*, y1, y2, b3, a4*
	807.29938	31.03	4.63E+08	3Hpg1Dpg1TYr-m	807.29843	1.18	807.299481	31.01	H	27a	HHYDH	H-(HYD)-H	4-(HYD)-3-4a	a3*, y1*, b3*, y2**#, y1, a2*, y2**#, y2^, y2, b3, a4*
M3 + M5c + M6	658.25116	27.72	1.80E+08	2Hpg1Dpg1TYr-m	658.25075	0.62	658.250732	27.73	H	11a	HYDH	(HYD)-H	(HYD)-3-4a	a3*, b3*, a3#*, y2, y2**#, y1, y2^, y2**#, b3, y3, M^#*
	858.23938	32.87	6.60E+08	2Hpg1Dpg1TYr1ClBht-c	858.23839	1.15	858.238403	32.89	C	21b	HYDHC (OH)	(HYD)-H-C	(HYD)-3-4a-6	a3*, a3*, a3#*, y1*, DH#, DH#, DH, b2*, y2**, b3,