Anti-HIV Cyclotides from the Chinese Medicinal Herb *Viola yedoensis*

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Supporting Information

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Table S1. Sequence Fragments from the Enzymatic Digestion of Cyclotides from *V. yedoensis*.

cyclotide	peptide sequenced			enzyme(s) used[a]	relative abundance (%)[b]	theoretical mass (Da)	experimental mass (Da)	Δm (Da)[c]
cycloviolacin	T10	-	Y17	CE	65	906.37	906.48	0.11
Y1	G31	-	E9	CE	30	1169.48	1169.60	0.12
(100)[d]	T18	-	Y30	CE	56	1370.48	1370.64	0.16
	L13	-	Y26	CE	34	1437.48	1437.66	0.18
	G31	-	F12	CE	100	1520.60	1520.76	0.16
	G27	-	E9	CE	31	1640.64	1640.75	0.11
	G27	-	F12	CE	20	1991.76	1991.92	0.16
	T10	-	E9	TE	100	3411.29	3411.62	0.33
cycloviolacin	S10	-	Y17	CE	30	892.36	892.28	0.08
Y2	G31	-	E9	CE	76	1169.48	1169.40	0.08
(100)[d]	G31	-	F12	CE	28	1506.58	1506.50	0.08
	G31	-	Y17	C	30	2043.81	2043.96	0.15
	T18	-	Y30	C	75	1333.50	1333.58	0.08
	S10	-	E9	TE	100	3360.29	3360.11	0.18
cycloviolacin	T10	-	Y17	CE	30	906.37	906.30	0.07
Y3	G31	-	E9	CE	76	1169.48	1169.40	0.08
(100)[d]	G31	-	F12	CE	28	1520.60	1520.50	0.10
	G31	-	Y17	C	30	2043.81	2043.96	0.15
	T18	-	Y30	C	75	1333.50	1333.58	0.08
cycloviolacin	S7	-	E6	TE	76	3023.31	3023.61	0.30
Y4	S7	-	Y28	CE	61	2253.97	2254.20	0.23
(100)[d]	I11	-	Y28	CE	76	1817.79	1817.98	0.19
	I11	-	E6	CE	20	2587.13	2587.40	0.27
cycloviolacin	S7	-	C13	CE	22	806.35	806.36	0.01
Y5	T14	-	Y29	CE	32	1647.74	1647.78	0.04
(100)[d]	V19	-	E6	CE	24	1846.75	1846.73	0.02
	S7	-	L18	CE	64	1291.64	1291.64	0.00
	A17	-	Y29	CE	82	1346.58	1346.56	0.02
	I11	-	L18	C	34	816.45	816.48	0.03
	V19	-	Y29	C	10	1162.46	1162.46	0.00
	N30	-	W10	C	23	1177.50	1177.50	0.00
	I11	-	Y29	C	27	1960.89	1960.62	0.27
	V19	-	W10	C	21	2321.93	2322.02	0.09
	A17	-	W10	C	15	2506.06	2506.01	0.05

[a]Enzymes used included trypsin (T), chymotrypsin (C), and endoGluC (E)
[b]The abundance relative to the most intense ion recorded in the TOF scan in the range 400-2000 Da
[c]The absolute difference between the theoretical and experimental mass
[d]Percentage (%) sequence coverage

Figure S1. A MS/MS spectrum of a peptide fragment (S7-L18) from a chymotrypsin and endoGluC digest of cycloviolacin Y5. The b- and y- ions, which are the main ions observed in a MS/MS spectrum, have been labelled.

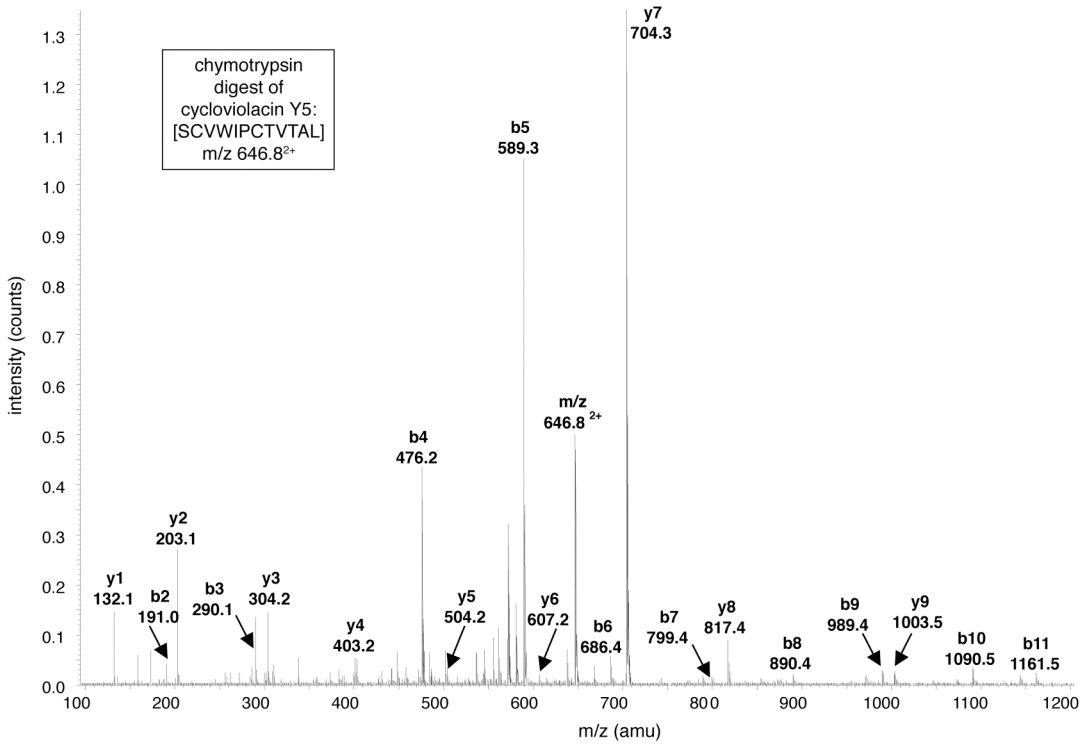

Figure S2. Hα chemical shift comparisons for selected cyclotides. Panel (A) shows the comparison of Hα chemical shifts between cycloviolacin Y1 and tricyclon A. Panel (B) shows the comparison of Hα chemical shifts between cycloviolacin Y5 and cycloviolacin O1.