

A

	1	17	21 23	37 38 40	45			
Cal12.1.1a	DVCD	SLVGGH	CIHNGC	WCDQEAP	HGNCCD	TDGCTAA	WWCPG	TKWD
cal12a	DVCD	SLVGGH	CIHNGC	<u>W</u> CDQ	γ AOH	GNC	CDTDGCTAA	<u>W</u> <u>W</u> COG <u>T</u> <u>K</u> <u>W</u> <u>D</u>

unmodified average mass	4869.4	
disulfide bonds (4)	-8.0	
gamma-carboxyglutamate (1)	+44.0	(E21)
hydroxyproline residues (2)	+32.0	(P23, P40)
6-bromotryptophan (4)	<u>+315.6</u>	(W17, W37, W38, W44)
Predicted final mass	5253	
Observed mass	5253	

B

	1	17	23	37 38 40	45			
Cal12.1.1b	DVCD	SLVGGH	CIHNGC	WCDQDAP	HGNCCD	TDGCTAA	WWCPG	TKWD
cal12b	DVCD	SLVGGH	CIHNGC	<u>W</u> CDQ	DAOH	GNC	CDTDGCTAA	<u>W</u> <u>W</u> COG <u>T</u> <u>K</u> <u>W</u> <u>D</u>

unmodified average mass	4855.4	
disulfide bonds (4)	-8.0	
hydroxyproline residues (2)	+32.0	(P23, P40)
6-bromotryptophan (4)	<u>+315.6</u>	(W17, W37, W38, W44)
Predicted final mass	5195	
Observed mass	5194	

S2. Matching of the primary structure of peptides predicted by cDNAs Cal12.1.1a (panel A) and B (panel B) to the actual masses of the mature, processed toxins cal12a and cal12b as observed with MS analysis. This was accomplished by informative addition/subtraction of masses associated with specific PTMs. W = bromotryptophan; O = hydroxyproline; C = non-specifically disulfide-bonded cysteine; γ = Gla (gamma-carboxyglutamic acid).