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ERRATUM

Erratum to: Sequence Elucidation of an Unknown Cyclic Peptide of High Doping Potential by ETD and CID Tandem Mass Spectrometry

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The sequence of the unknown peptide proposed in our published article is now found to be incorrect, though at the time of publication it was the reasonable and best candidate to the unknown peptide based on all the experimental data obtained. Recently, Dr. Rohan Steel (Racing Analytical Services Ltd, Flemington, Victoria, Australia) established that the peptide was 2′,6′-dimethyltyrosine-D-Arg-Phe-Lys-NH2 ([dmt^1]DALDA), with an elemental composition of $C_{32}H_{50}N_9O_5$. Dr. Rohan Steel initially compared and found agreement between the theoretical *m/z* values for the multiply protonated species of [dmt^1]DALDA and its predicted CID product ions and experimental *m/z* values for the unknown peptide and its product ions. He then communicated this finding to us. We did the same comparison and found the agreement too. Additionally, we compared the theoretical and experimental *m/z* values for the c- and z-product ions from ETD, and they are in agreement (see Table 1). Furthermore, [dmt^1]DALDA is reported to be a potent analgesic agent, and it is in accordance with the intelligence gathered on the unknown sample. Thus, we conclude that the unknown peptide is [dmt^1]DALDA. This peptide has a C-terminal amidation, and this amidation can be hydrolyzed by trypsin, which is in agreement with the experimental results.

Table 1. Comparison between theoretical *m/z* values for [dmt^1]DALDA, its deamidated form and their predicted product ions and experimental *m/z* values for the unknown peptide, its tryptic digest and their product ions*

2′,6′-dmt-D-Arg-Phe-Lys-NH2		**The unknown peptide**	
Species	Theoretical *m/z*	Experimental *m/z*	Error (ppm)
$[M+H]^+$	640.3929	640.3922	−1.1
$[M+2H]^{2+}$	320.7001	320.6998	−0.9
$[M+3H]^{3+}$	214.1358	214.1358	0
b_2	348.2030	348.2030	0
$[b_2\text{-}NH_3]$	331.1765	331.1764	−0.3
b_3	495.2714	495.2716	0.4
$[b_3\text{-}NH_3]$	478.2449	478.2452	0.6
y_1	146.1288	not detected	
$[y_1\text{-}NH_3]$	129.1022	129.1024	1.5
y_2	293.1972	293.1964	−2.7
$[y_2\text{-}NH_3]$	276.1707	276.1706	−0.4
y_3	449.2983	449.2977	−1.3
$[y_3\text{-}NH_3]$	432.2718	432.2720	0.5
c_1	209.1	209.1	NA
c_2	365.2	365.3	NA
c_3	512.3	512.3	NA
z_1	130.1	not detected	
z_2	277.2	277.1	NA
z_3	433.3	433.2	NA
2′,6′-dmt-D-Arg-Phe-Lys-OH		**The tryptic digest**	
$[M+H]^+$	641.3770	641.3772	0.3
$[M+2H]^{2+}$	321.1921	321.1922	0.3
$[M+3H]^{3+}$	214.4638	214.4639	0.5
b_2	348.2030	348.2027	−0.9
$[b_2\text{-}NH_3]$	331.1765	331.1762	−0.9
b_3	495.2714	495.2712	−0.4
$[b_3\text{-}NH_3]$	478.2449	478.2446	−0.6
y_1	147.1128	not detected	
$[y_1\text{-}NH_3]$	130.0863	130.0862	−0.8
y_2	294.1812	294.1804	−2.7
$[y_2\text{-}NH_3]$	277.1547	277.1540	−2.5
y_3	450.2823	450.2816	−1.6
$[y_3\text{-}NH_3]$	433.2558	433.2551	−1.6
c_1	209.1	209.1	NA
c_2	365.2	365.3	NA
c_3	512.3	512.4	NA
z_1	131.1	not detected	
z_2	278.2	278.2	NA
z_3	434.3	434.2	NA

*The conditions under which the experimental *m/z* values were obtained were presented in the published article. Most of the experimental *m/z* values listed here are from the published article, and the rest is obtained from re-examination of the initial LC-MS/MS data files.

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