CORRECTION

Correction to: Sequence-specific backbone resonance assignments and microsecond timescale molecular dynamics simulation of human eosinophil-derived neurotoxin

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After publication of this article, the authors noticed that a ¹⁵N–¹³C dimension error was unwillingly coded in the 3D NMR spectrum “fid.com” processing script used to perform backbone assignments for this enzyme. The authors noticed that some OBS, CAR and LAB values in the “fid.com” had been switched in the y and z dimensions, probably resulting from a wrong NMRPipe selection when reading the Varian NMR experimental parameters.

They have carefully re-processed, re-analyzed, re-assigned, in addition to checking all scripts to evaluate the

extent of this processing error on the published assignments. Authors determined that the “fid.com” error resulted in a significant number of incorrect backbone resonance assignments, requiring us to issue corrections in Figs. 2, 3 and 4 of this published manuscript, in addition to Table S1. New versions of these figures and table are provided below. The corresponding BMRB entry has also been revised. The authors note that these modifications do not change the global message, conclusions, and molecular dynamics simulations presented in this article.

The authors are grateful to David N. Bernard (INRS) for help with finding and correcting these errors.

The original article can be found online at <https://doi.org/10.1007/s12104-017-9736-9>.

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Fig. 2 Two-dimensional ^1H - ^{15}N HSQC spectrum of human eosinophil-derived neurotoxin (EDN, RNase 2) acquired in 15 mM sodium acetate at pH 5.0 (90% H_2O , 10% D_2O) and 298 K. All NMR assignment experiments were acquired on a Varian Inova 500 MHz spectrometer. Assigned resonance cross peaks are labeled with sequence specific residue numbering of EDN. Panel **b** is a magnified view of the central spectral region outlined in (**a**). A total of 113 out of 122 non-proline ^1H - ^{15}N backbone amides (92.6%) were assigned. Similarly, resonances were assigned for 127 out of 134 $\text{C}\alpha$ (94.8%) and 125 out of 132 $\text{C}\beta$ (94.7%) (EDN contains two glycines, which do not have a $\text{C}\beta$). Backbone amides of residues Lys1, Thr19, His73, Ser74, Val78, Tyr98 Tyr107, Ile108 and Val109 were unassigned. 10 residues show overlapping resonances (Trp7-Lys66, Thr13-Asn32, Arg35-Ser76, Val52-Ile133 and Met105-Arg114)

Fig. 3 Linear analysis of chemical shifts (LACS) (Wang et al. 2005) for $\text{C}\alpha$ and $\text{C}\beta$ resonance assignments in human EDN (RNase 2). The difference between the chemical shift (δ) of each amino acid with the BMRB average random coil chemical shift were used to produce the plots and to detect outliers. The two blue lines represent the best fitted data using lines of pre-calculated slopes. The fitted lines intersect at 0, indicating that the data are properly referenced. The outliers identified in this analysis (Table S1) include: $\text{C}\alpha$ -Tyr123 (58.10 ppm, mean of 51.98 ppm), $\text{C}\beta$ -Asn41 (38.64 ppm, mean of 44.26 ppm), $\text{C}\beta$ -Asp112 (40.81 ppm, mean of 45.81 ppm), H-Ala8 (8.18 ppm, mean of 10.05 ppm), H-Asp115 (8.32 ppm, mean of 10.35 ppm), N-His15 (119.47 ppm, mean of 105.92 ppm), N-Val128 (121.06 ppm, mean of 106.56)

Fig. 4 Conformational dynamics of EDN (RNase 2) on the ps-ns timescale. Comparison of order parameters (S^2) calculated for the NMR (red) and MD ensemble (black). S^2 was calculated from backbone chemical shifts using TALOS+ (Shen et al. 2009). Residues 57–60 and 65–70 (loop 4), 74–77 (loop 5) and 85–94 (loop 6) were observed to be most flexible on this timescale in both MD and NMR