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CORRECTION

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Correction: Dynamic properties of dipeptidyl peptidase III from *Bacteroides thetaiotaomicron* and the structural basis for its substrate specificity – a computational study

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Correction for 'Dynamic properties of dipeptidyl peptidase III from *Bacteroides thetaiotaomicron* and the structural basis for its substrate specificity – a computational study' by M. Tomin *et al.*, *Mol. BioSyst.*, 2017, **13**, 2407–2417.

Regrettably, in the original manuscript, several amino acid residues were misnumbered throughout the paper.

D208 should be D209; Asp208 should be Asp209; Ser340 should be Ser363; His458 should be His448; His463 should be His453; Glu432 should be Glu442; Ser473 should be Ser472; Ala619 should be Ala617.

In addition, on page 2412, section 3.2, paragraph 1, 'six-coordinated zinc ion' should read 'hexacoordinated zinc ion'.

The paper should read as follows:

Page 2410, Table 2

Geometric parameters	oXR	cXR	WT_{MD}	WT–RRNA	WT–KANA
R_g/Å	27	25	26	26	26
d_1 (D193–K468)/Å	41	24	34	31	32
d_2 (D209–K468)/Å	33	21	25	27	23
d_3 (A394–K468)/Å	26	23	8	17	17

Page 2411, section 3.1. Protein flexibility, paragraph 1

However, distances between Cα atoms of D193–K468, D209–K468 and A394–K468, d_1, d_2 and d_3, respectively, are more appropriate than R_g to describe the mutual orientation of domains, and therefore represent good parameters for structure differentiation, see Table 2 and Fig. 1. D193, D209 and A394 belong to sheet 1 and helices 9 and 16 from the lower domain while K468 belongs to the helix 20 from the upper domain (Fig. 1).

Page 2411, section 3.1. Protein flexibility, paragraph 2

However, the other four geometric parameters, R_g, and the Cα distances D193–K468 (d_1), D209–K468 (d_2) and A394–K468 (d_3) (Fig. 1), are more appropriate to quantify differences among the sampled conformations.

Page 2412, section 3.1. Protein flexibility, the last paragraph

RMSF values calculated for the individual residues of the APO form revealed that the residues from the upper (Leu328–Lys365; Ser455–Ala477; Val521–Ala617) and lower (Val175–Val235) domain, which constitute the outer rim of the inter-domain cleft, correspond to the most flexible regions (Fig. S8–S11, ESI†) indicating that the long range protein closure is indeed the dominant structural change noticed during MD simulations.

Page 2412, section 3.2. Zinc ion coordination, paragraph 1

The crystal structure of the ligand free *Bt*DPP III revealed the hexacoordinated zinc ion coordinated by two histidines (His448 and His453), two glutamates (Glu449 and Glu476) and two water molecules (Fig. 5) wherein both glutamates coordinate Zn^{2+} monodentately.

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Page 2412, section 3.2. Zinc ion coordination, paragraph 2

During MD simulations His453, His448, Glu449 and Glu476 remained in the Zn^{2+} coordination sphere, and furthermore, differently from the initial structure, glutamates occasionally coordinated the metal ion bidentately.

Page 2413, section 3.3. The role of Ser363 and Tyr287, paragraph 1

The computational studies revealed the important role of Ser363 for the protein closure. Namely the Ser363–Asp446 hydrogen bond formed at the early stage of MD simulations (5th–10th ns) facilitates the inter-domain motion through the Ser363–Asp446–Arg333–Glu442 chain of interactions.

Page 2413, section 3.4. MD simulations of the DPP III–RRNA complex, paragraph 3

Apparently, during aMD simulations of the *Bt*DPP III–RRNA complex, a sudden drop in the radius of gyration was noticed accompanied by the decrease of the Asp209–Lys468 distance.

Page 2414, section 3.4. MD simulations of the DPP III–RRNA complex, paragraph 6

In the case of cMD simulations, Arg residues are orientated towards the lower domain, forming hydrogen bonds with Glu320, Gly383, Glu307 and Glu476. aMD simulations resulted in a binding mode where Arg sidechains of RRNA interact with Ser472, Glu476 and Asp465 of the upper domain (Fig. 10).

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

