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Correction: Simultaneous engineering of an enzyme's entrance tunnel and active site: the case of monoamine oxidase MAO-N

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www.rsc.org/chemicalscienceCorrection for 'Simultaneous engineering of an enzyme's entrance tunnel and active site: the case of monoamine oxidase MAO-N' by Guangyue Li *et al.*, *Chem. Sci.*, 2017, 8, 4093–4099.

The authors regret that there are instances in the work where the mutants and one compound are mislabelled. These are described correctly below:

On page 4095, in the text discussing the single, double and triple mutants, the double mutant is mislabelled as LG-F-B5 and should instead read:

Single mutant LG-F-B5 (T354S) shows no activity, but in concert with the double mutant LG-F-B6 (W230I/W430R) having a specific activity of 0.22 U mg⁻¹, the respective triple mutant W230I/T354S/W430R displays a notable improvement (0.3 U mg⁻¹). Thus, a strong cooperative effect is operating.¹⁹

On page 4095, in the text discussing the deracemization of the compounds 1–5, the racemic compound 1 is mislabelled as *rac*-2 and should instead read:

Compounds *rac*-4 and *rac*-5 have not been previously subjected to MAO-N-catalyzed deracemization, in contrast to *rac*-1 (providing (*R*)-1 during deracemization).^{9,20}

On pages 4096–4097, in the paragraph discussing the catalytic activity when moving from LG-F-B6 to LG-J-B4, the terms LG-F-B6 and LG-J-B4 are incorrectly displayed. The corrected text is included below:

In order to shed light on the further enhanced catalyst activity upon going from LG-F-B6 to LG-J-B4, MD simulations were performed in the absence of 2. This allowed the visualization of representative conformations of variants LG-J-B4 and LG-F-B6 without any bias arising from interactions with the substrate. A representative conformation was selected after clustering of the phase space sampled from the 50 ns MD trajectory. The conformational change of tunnels of LG-J-B4 and LG-F-B6 is described in Fig. 4. The side-chain of M242R forms a hydrogen bond with the oxygen atom of residue D146 which reduces the polarity of the tunnel. The mutation Y365V results in a similar effect at the tunnel entrance and exit (Fig. 4A). In contrast, residues D146 and Y365 do not undergo similar interactions and consequently do not contribute to a reduction of the polarity in the tunnel (see Fig. 4B). Overall, a decrease in polarity makes it easier for hydrophobic substrates and products to enter and exit the enzyme, thereby increasing the catalytic activity of LG-J-B4.²³ The respective engineered tunnels of LG-J-B4 and LG-F-B6 are shown in Fig. S32 (ESI[†]). It should be pointed out that in the present case the tunnel volume has not increased significantly upon mutagenesis, which means that the polarity change upon going from LG-F-B6 to LG-J-B4 constitutes the determining factor.

In the caption of Fig. 4, the terms LG-J-B4 and LG-F-B6 are displayed incorrectly and should read:

Fig. 4. Comparison of the tunnel surface potential of LG-J-B4 (A) and LG-F-B6 (B). Different colors denote different levels of polarity, deeper red coloring denoting increasing polarity.

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

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