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Correction: Application of QM/MM and QM methods to investigate histone deacetylase 8

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Correction for ‘Application of QM/MM and QM methods to investigate histone deacetylase 8’ by Duangkamol Gleeson *et al.*, *Med. Chem. Commun.*, 2015, 6, 477–485.

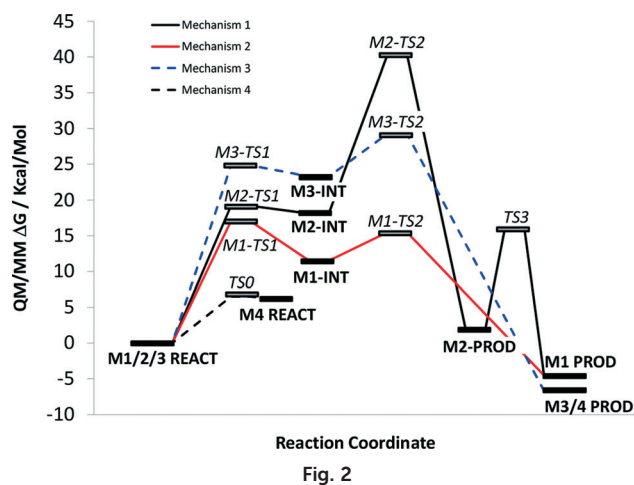
The author regrets the following errors:

Fig. 2 (top panel) was incorrectly labelled. The profiles of “Mechanism 1” and “Mechanism 2” were swapped in the centre of the figure. The corrected panel of the figure is shown below.

On page 482, column 1, line 36: 4.7 kcal mol⁻¹ should be replaced by 14.7 kcal mol⁻¹.

On page 483, column 1, line 9, the sentence should read: The rate determining barriers for mechanisms 1 and 2 are very similar at 17.9 vs. 19.7 kcal mol⁻¹, with His143 acting as the general base being lower in energy. The QM/MM results were 17.5 vs. 24.1 kcal mol⁻¹, respectively.

On page 483, column 1, line 21 the sentence should read: We find that the rate determining barrier determined from the QM calculations follows the trend: mechanism 4 < mechanism 1 < mechanism 2 < mechanism 3.



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

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