MedChemComm



View Article Online

CORRECTION



2015, 6, 1699

Cite this: Med. Chem. Commun.,

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

Duangkamol Gleeson^a and M. Paul Gleeson^{*b}

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.

www.rsc.org/medchemcomm

DOI: 10.1039/c5md90040a

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 3.



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

^a Department of Chemistry, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok 10520, Thailand

^b Department of Chemistry, Faculty of Science, Kasetsart University, 50 Phaholyothin Rd, Chatuchak, Bangkok 10900, Thailand. E-mail: paul.gleeson@ku.ac.th; Fax: +66 2 5793955; Tel: +66 2 562 5555 extn 2210