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Reply to Comment on "Another look at the molecular mechanism of the resistance of H5N1 influenza A virus neuraminidase (NA) to oseltamivir (OTV)"

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The comment of Rungrotmongkol et al. [1], observed as a whole, on our previous publication [2] is scientifically incorrect. Rungrotmongkol et al. have noted the discrepancies between the theoretical and experimental structures of NA:OTV protein:ligand complexes used in this work, and have questioned the relevance of such modelling. We would like to point out that these discrepancies were known to us at the time and, indeed, were commented upon in the original publication (pp. 156–158, Fig. 5) [2]. The interest here is that, despite these discrepancies, the binding free energies reported agree with the experimental values of K_i. It is for this reason that we chose to entitle our paper "*Another look at* the molecular mechanism…".

We have extensively (220 docking experiments using all NA subtypes) verified the applicability of the docking algorithms [3] and have also included protein flexibility to account for any incorrect choice of starting structure [4]. This has allowed us to confirm that the correct ligand orientations are obtained in these docking procedures.

References

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[2] M.L. Mihajlovic, P.M. Mitrasinovic, Another look at the molecular mechanism of the resistance of H5N1 influenza A virus neuraminidase (NA) to oseltamivir (OTV), Biophysical Chemistry 136 (2008) 152–158.

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