LIGAND UNBINDING VIA MULTIPLE REACTION PATHWAYS

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INTRODUCTION

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METHODOLOGY

CONCLUSIONS

References

[1] J. Rydzewski & W. Nowak. *Phys. Life Rev.* doi.org/10.1016/j.plrev.2017.03.003 (2017).
[2] W. Nowak. *Handbook of Computational Chemistry* 2nd ed. J. Leszczynski, Springer (2017).
[3] J. Rydzewski & W. Nowak. *J. Chem. Phys.* 143, 09B617_1 (2015).
[4] J. Rydzewski & W. Nowak. *J. Chem. Theory Comp.* 12, 2110 (2016).
[5] J. Rydzewski & W. Nowak. *Sci. Rep.*, submitted (2017).
[6] J. Rydzewski, R. Jakubowski, W. Nowak & H. Grubmueller, in preparation (2017).

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