Supporting information

Computational study on the unbinding pathways of B−RAF inhibitors and its implication for the difference of residence time: insight from random acceleration and steered molecular dynamics simulations

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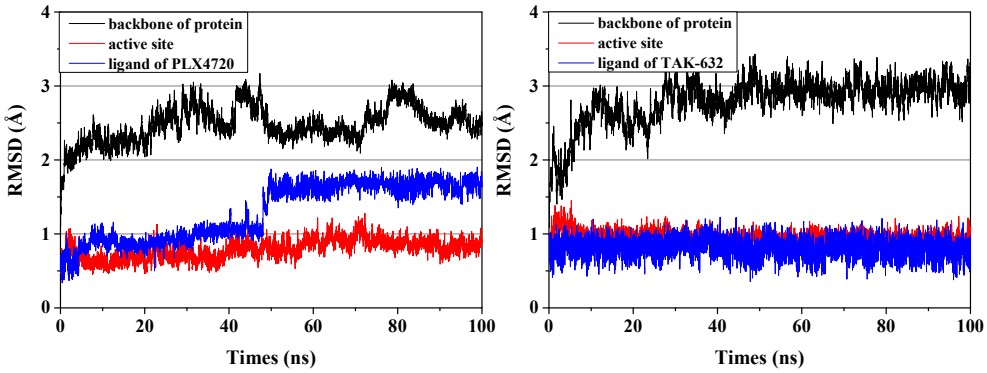

Figure S1. Monitoring the fluctuations of the RMSD of protein. Left : PLX4720.

Right : TAK-632

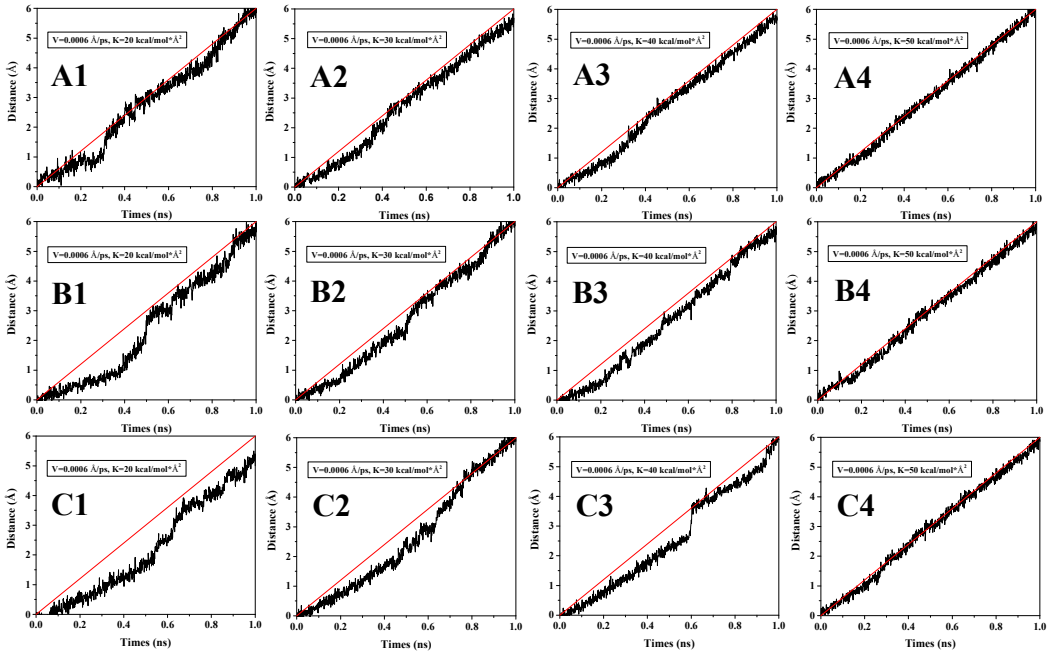

Figure S2. Calibration of SMD parameters. Various k and keeping a V=0.0006 Å/ps. First row is the ATP-channel of PLX4720, while the second row is the ATP-channel of TAK-632 and the third row is the allosteric-channel of TAK-632.

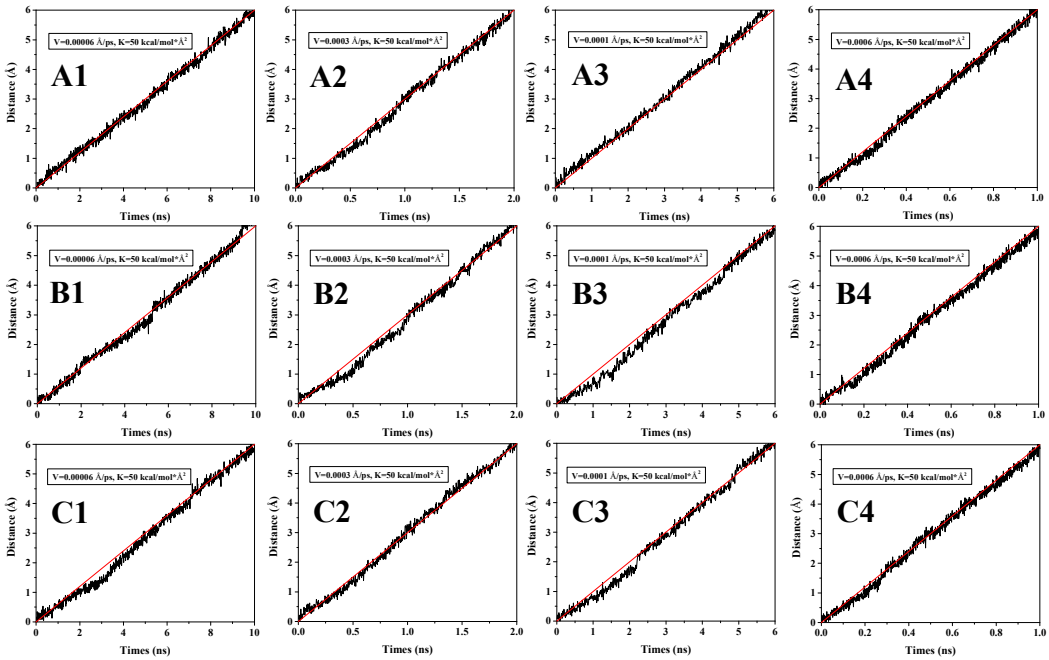

Figure S3. Calibration of SMD parameters. Various V and keeping a K=50 kcal/mol • A^2. First row is the ATP-channel of PLX4720, while the second row is the ATP-channel of TAK-632 and the third row is the allosteric-channel of TAK-632.