## **Binding Mode and Induced Fit Predictions for Prospective**

## **Computational Drug Design**

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## Supporting Information

ANM/PCA modes for c-Src and Abl	SI2
ANM/PCA modes for ER and HNE	SI3
ANM/PCA modes for Syk	SI4
LRMSD and backbone RMSD from MD simulations: HNE	SI5
Covered phase space MD/PELE: HNE	SI5
LRMSD and backbone RMSD from MD simulations: ER (1U3Q)	SI6
Covered phase space MD/PELE: ER (1U3Q)	SI6
LRMSD and backbone RMSD from MD simulations: ER (1U3S)	SI7
Covered phase space MD/PELE: ER (1U3S)	SI7
LRMSD and backbone RMSD from MD simulations: Syk (4IOS)	SI8
Covered phase space MD/PELE: Syk (4IOS)	SI8
LRMSD and backbone RMSD from MD simulations: Syk (4XR8)	SI9
Covered phase space MD/PELE: Syk (4XR8)	SI9
LRMSD and backbone RMSD from MD simulations: Abl (2HYY)	SI10
Covered phase space MD/PELE: Abl (2HYY)	SI10
LRMSD and backbone RMSD from MD simulations: Abl (2F4J)	SI11
Covered phase space MD/PELE: Abl (2F4J)	SI11
LRMSD and backbone RMSD from MD simulations: c-Src (1Y57)	SI12
Covered phase space MD/PELE: c-Src (1Y57)	SI12
LRMSD and backbone RMSD from MD simulations: c-Src (1YOM)	SI13
Covered phase space MD/PELE: c-Src (1YOM)	SI13



Figure S1 First six normal modes from ANM and the first six principal components from PCA of the MD simulations for c-Src and Abl kinase.



Figure S2 First six normal modes from ANM and the first six principal components from PCA of the MD simulations for ER and HNE.



Figure S3 First six normal modes from ANM and the first six principal components from PCA of the MD simulations for the SYK kinase.



Figure S4 LRMSD and backbone RMSD of 3Q77 during MD simulation.



Figure S5 Ligand positions during the MD (left) and the PELE (right) simulation for 3Q77. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).





Figure S6 LRMSD and backbone RMSD of 1U3Q during MD simulation.



Figure S7 Ligand positions during the MD (left) and the PELE (right) simulation for 1U3Q. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).



Figure S8 LRMSD and backbone RMSD of 1U3S during MD simulation.



Figure S9 Ligand positions during the MD (left) and the PELE (right) simulation for 1U3S. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).



Figure S10 LRMSD and backbone RMSD of 4IOS during MD simulation.



Figure S11 Ligand positions during the MD (left) and the PELE (right) simulation for 4IOS. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).



Figure S12 LRMSD and backbone RMSD of 4XR8 during MD simulation.



Figure S13 Ligand positions during the MD (left) and the PELE (right) simulation for 4XR8. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).



Figure S14 LRMSD and backbone RMSD of 2HYY during MD simulation.



Figure S15 Ligand positions during the MD (left) and the PELE (right) simulation for 2HYY. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).



Figure S16 LRMSD (for 60ns and 200ns) and backbone RMSD of 2F4J during MD simulation.



Figure S17 Ligand positions during the MD (left) and the PELE (right) simulation for 2F4J. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).



Figure S18 LRMSD (for 60ns and 200ns) and backbone RMSD of 1Y57 during MD simulation.



Figure S19 Ligand positions during the MD (left) and the PELE (right) simulation for 1Y57. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).



Figure S20 LRMSD and backbone RMSD of 1YOM during MD simulation.



Figure S21 Ligand positions during the MD (left) and the PELE (right) simulation for 1YOM. The central atom of the ligand is indicated by a sphere colored due to its simulation step (red to blue).