Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2020

Fig. S1 a. Three times SMD for PRH from T3, b. Three times SMD for PRH from T2, c. Three times SMD for PRH from T1 d. Three times SMD for FRK from T3, e. Three times SMD for FRK from T2, f. Three times SMD for FRK from T1

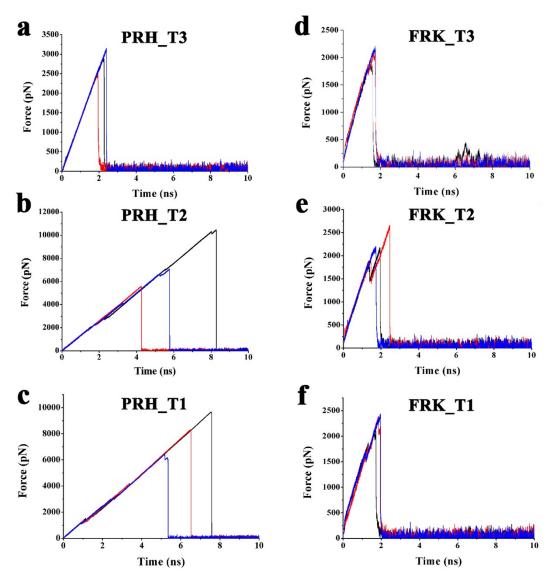
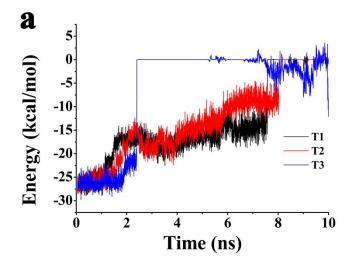


Fig. S2 a Total energy for PRK from T1(black), T2(red), T3 (blue), b Total energy for FRK from T1(black), T2(red), T3 (blue)



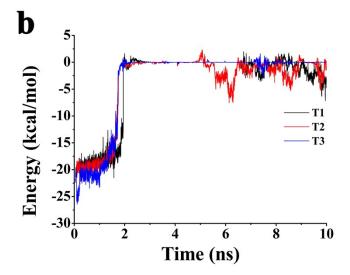


Fig. S3 the active residues for PRH binding.

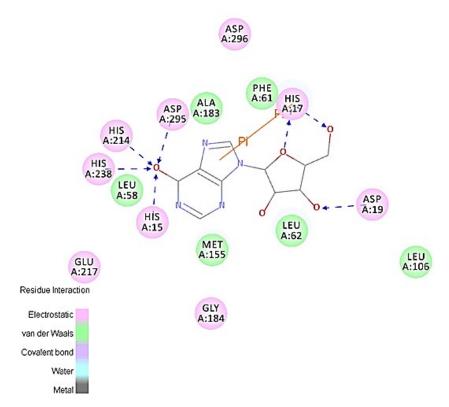


Fig. S4 the residues located at the peak of PRH via T3.

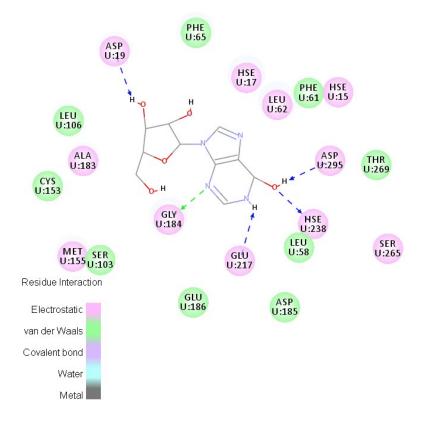


Fig. S5 the residues located at the peak of PRH via T2.

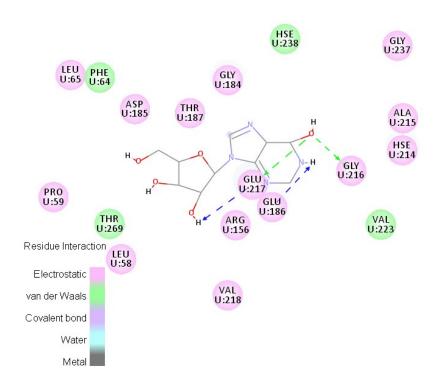


Fig. S6 the residues located at the peak of PRH via T1.

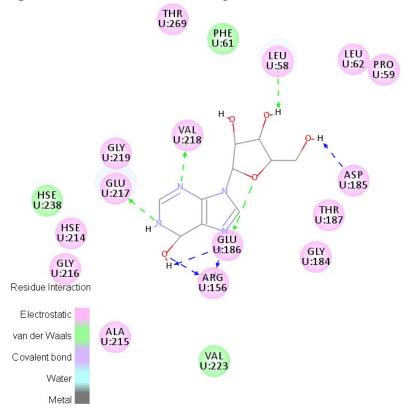


Fig. S7 the active residues for FRK binding.

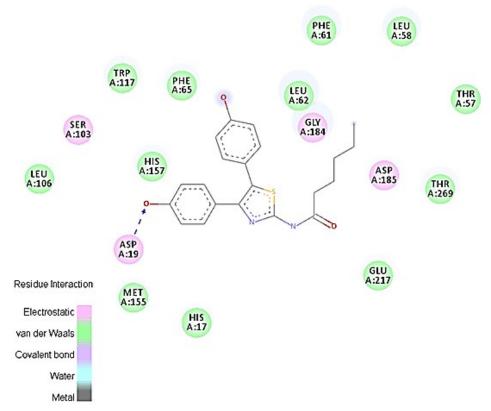


Fig. S8 the residues located at the peak of FRK via T3.

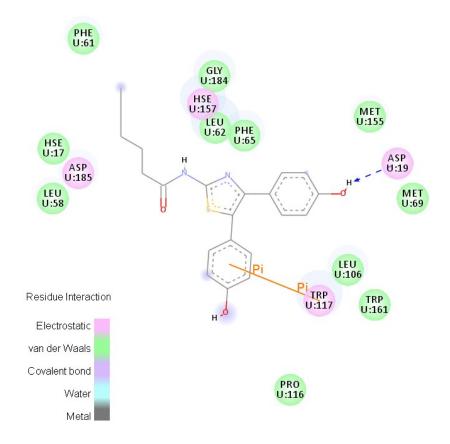


Fig. S9 the residues located at the peak of FRK via T2.

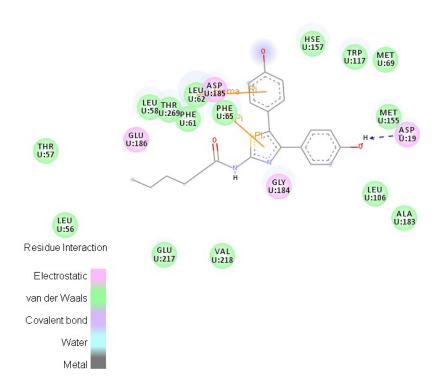


Fig. S10 the residues located at the peak of FRK via T1.

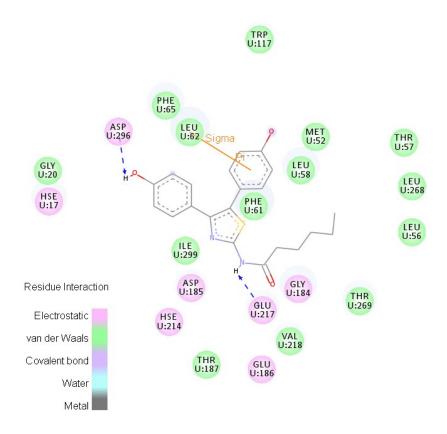


Fig. S11 Sequence alignment of the ADA, ADA2, ADAL, AMPD1, AMPD2, AMPD3, the unique and stable entry identifiers are P56658, F1N144, Q0VC13, F1MLX6, A0A3Q1M723, E1BA23. (the blue boxes are the fragments we selected)

