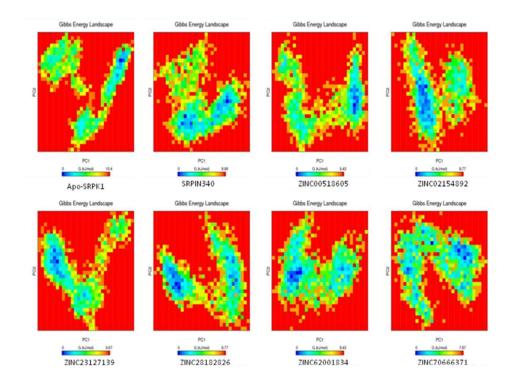


Supplementary Figure 1. Molecular dynamic simulations of apo SRPK1 and complexes. (A) RMSD of C^{α} backbone for SRPK1-Compound complexes as a function of time. (B) RMSF of residues during simulation. (C) Radius of gyration as a function of time (D) Number of hydrogen bonded interactions as a function of time. (E) Plot of eigen value vs. eigenvector index only first 50 out of 1000 are represented in the figure. (F) PCA scatter plot along first two principle components, PC1 and PC2 showing all atom fluctuations. Apo-SRPK1, SRPK1-SRPIN340, SRPK1-ZINC00518605 (C01), SRPK1-ZINC02154892 (C02), SRPK1-ZINC23127139 (C03), SRPK1-ZINC28182826 (C04), SRPK1-ZINC62001834 (C05), SRPK1-ZINC70666371 (C06) are shown in black, red, green, blue, cyan, pink, yellow, olive colors, respectively.



Supplementary Figure 2. The Gibbs energy landscape obtained during 100 ns MD simulations.