Electronic Supplementary Material (ESI) for RSC Advances.

A Molecular Dynamics Simulation Study for Variant Drug Responses Due to FMS-Like Tyrosine Kinase 3 G697R Mutation

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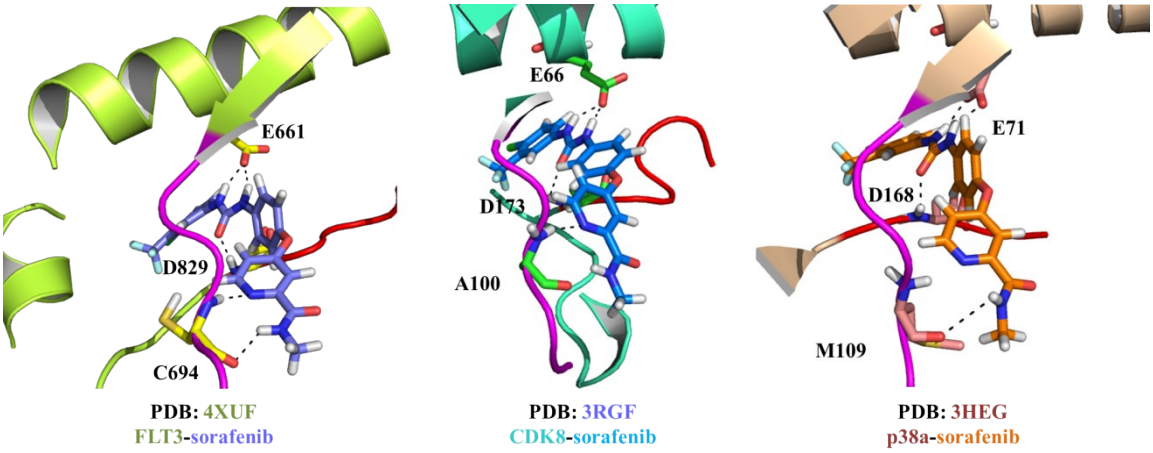

Fig. S1 A structural comparison is made among sorafenib-bound FLT3, CDK8, and p38α kinases to support our modeled FLT3^{ITD}:sorafenib complex.

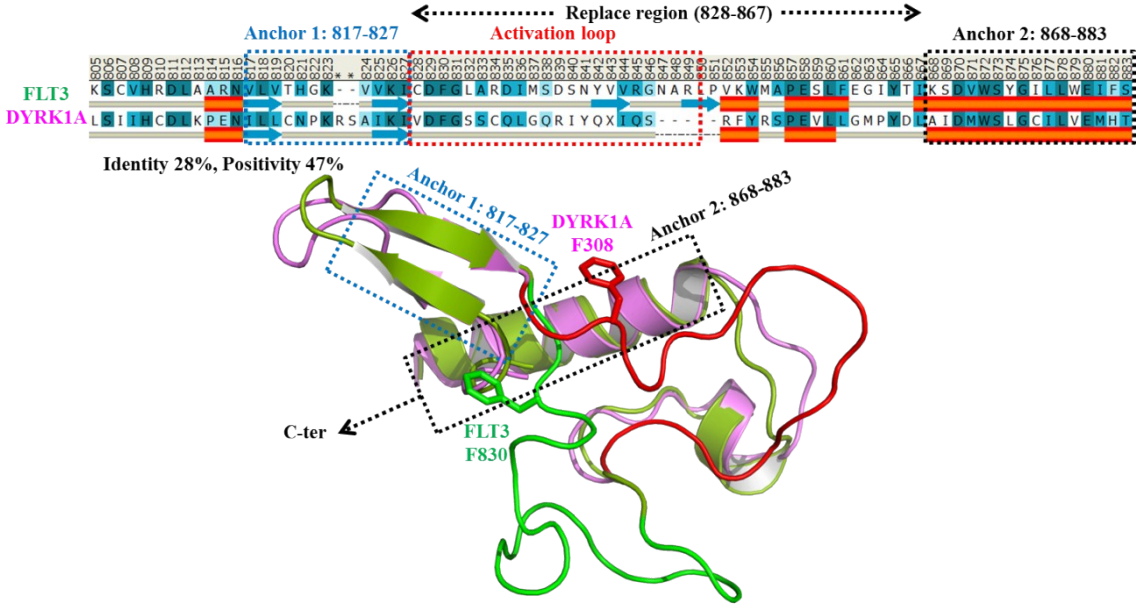

Fig. S2 A structural comparison is made between PKC412-bound FLT3 and PKC412-bound DYRK1A with parallel ligand-receptor interaction to support our modeled FLT3^{ITD}:PKC412 complex structure.