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Commentary

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# Noncovalent Interactions Structural Analysis In cyclin-dependent kinase complex

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In the present work we have analyzed these interactions in the cyclin-dependent kinase complex 2ATP complexes as well as CDK2 inhibitor complexes. Based on these interactions we have developed multiple regression models to account for the experimentally observed IC50 values. We have made extensive analysis of the amino acids ATP contacts amino acids inhibitor contacts. Also the extend of similarity between the various ligands has been quantified using 2D and 3D analysis methods.

Kinases are become one of the most important classes of drug target with around 30 different kinase are being developed and investigated for cancer treatment[1]. Cyclin-dependent kinases (CDKs) are protein kinases with a cyclin subunit and it is essential for enzymatic activity [2]. It is present in all type of eukaryotes, and is having crucial roles in signaling pathways to control normal human cell functions and active merely when linked with a regulatory partner. Eukaryotic cells contain at most nine CDKs, and those are, CDK1, 2, 3, and 4, are openly involved in regulation of cell cycle .CDKs are dependable for regulating cell division cycle, helping to make sure that the genome is replicated once per cell cycle and it is required for timing and order of cell division [3,4].CDK2 is a major constituent of the CDK complex, and it is responsible for the transition of G1/S phase and it is a monomer comprised of a polypeptide chain consisting of 298 amino acid residues with mainly α-helix elements as well as a β-sheet terminus.

The activation CDK involves two-step process and that requires phosphorylation and cycline binding in the T loop . Over-activity or insufficient activity of CDKs or is linked with several tumors, for this reason it became an important target in anticancer and antiviral drug discovery. CDK2 inhibitors show exciting potential activity as tumor suppressors. The inhibitors of kinases interact with the backbone motif and are the part of bindingsite. Finn et al in their article provides the most recent approaches of targeting this essential cell cycle regulatory mechanism in the perspective of breast cancer therapy.

Nonbonding interactions among proteins and ligands play essential roles in important biological processes mainly signal transduction and enzymatic reaction. Understanding these interactions is important for designingsynthetic inhibitors. In this work, we focus on non-covalent interactions of 6 CDK2 ATP complexes and 50.

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CDK2 inhibitor complexes and discussed structural analysis of these interactions in 56 CDK complexes. Analyzing Structural information can be helpful for understanding these complexes at the molecular level. CDK2 small molecule inhibitor complexes that have IC50 values out of 50 CDK2 inhibitor complexes are also taken for various types of analysis. As binding to the ATP site and biological activity may be dependent on the different non-covalent interactions such as hydrogen bonds, hydrophobic bonds hydrophilic bonds and electrostatic vander-waals such as other interactions. Further from various noncovalent interactions we have developed multiple regression models to accounts for the experimentally observed IC50 values and to predict biological activity based on the different non covalent interactions.

## References

1. Zhang J, Yang PL, Gray NS (2009) Targeting cancer with small molecule kinase inhibitors. Nature Reviews Cancer 9: 28.
2. Malumbres, M. (2014) Cyclin-dependent kinases. Genomebiology 15: 122.
3. Card GL, Knowles P, Laman, NH (2000) Crystal structure of γ-herpesvirus cyclin-CDK complex. The EMBO Journal 19: 2877-2888.
4. Honda R, Lowe ED, Dubinina E, Skamnaki V (2005) The structure of cyclin E1/CDK2: implications for CDK2 activation and CDK2-independent roles. The EMBO Journal 24: 452-263.

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