

## Role of CADD in rational drug discovery and development

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The science of computer aided drug design has seen an exponential growth in recent past owing to more and more research being carried out in this field. This has furthered our understanding of protein-ligand and drug-receptor interaction. Not only a lot of time and effort have been saved, but also a number of new moieties have come out of high throughput screening thus facilitating an impetus by regulatory agencies as well as pharmaceutical industry. The resources thus saved can be used elsewhere for the betterment of mankind. The ability of CADD to predict with reasonable accuracy, the ADME and activity of yet to be synthesized molecules through the use of rationally derived molecular descriptors has brought laurels to it with many successful examples. This ability to work at high resolution with both proteins and drug compounds makes CADD one of the most powerful methods in drug design. After a number of lead compounds have been identified, structure based drug design techniques effectively refine their 3D structures to improve their binding to protein active sites through lead optimization. This is followed by biological screening and, if need be, synthesis of some new derivatives. The promising candidates are subjected to clinical trials and subsequent NDA review process. Researchers and stake holders are actively involved in development of computational tools that will improve effectiveness and efficiency of drug discovery and development process, decrease use of animals, and increase predictability.

### Biography

Pooja Chawla holds B.Pharm. and M.Pharm. (Medicinal Chemistry) degree. She completed her Ph.D. from Shobhit University Meerut, India. She is working as Associate Professor and Head, Department of Pharmaceutical Chemistry, Gyani Inder Singh Institute of Professional Studies, Dehradun, India. She has published 3 books and more than 25 papers in national/international journals and is serving as a reviewer for international journals of repute. She also presented a poster at FIP 2011 and CTDDR 2013. She has guided 25 post graduate projects and her research team consists of 13 master and 2 doctoral research scholars.

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