

## Designing of small molecule inhibitors for NMPRTase as Anticancer leads using insilico approach

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Nicotinamide Phospho ribosyltransferase (NMPRTase) is an enzyme catalyses the biosynthesis of NAD<sup>+</sup>. It is generally expressed more in cancerous cell lines. The inhibitors targeted to NMPRTase reduce the cellular NAD<sup>+</sup> concentration which results in apoptosis and cell death, hence can be used to treat cancer. These inhibitors could also target the NAD<sup>+</sup> dependent enzymes like sirtuins indirectly, which were implicated in many diseases like diabetes, neurodegeneration and inflammation. Thus designing inhibitors to NMPRTase would be a good strategy to treat various disorders. In the present work, crystal structure of NMPRTase (2GVJ) with 2.1 Å resolution, was employed for the energy based pharmacophore model generation for the crystal ligand (FK866) and virtual screening was carried out using Glide docking (Schrodinger). Commercial databases were used for virtual screening. Top30 potential hits were shortlisted by comparing pharmacophore fitness, docking score and hydrogen bonds with crystal ligand. These top hits are the potential lead compounds for treating cancer and other disorders.

### Biography

Venkat Koushik Pulla has completed his MSc from Sheffield Hallam University, UK. Currently he is doing PhD in Bits Pilani, Hyderabad campus. His area of interest is to design and screen the lead compounds targeted to cancer.

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## To study the mechanism of the formation of controlled Ag nanoparticles using E.coli

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Our work, demonstrates the microbial synthesis of controlled silver nanoparticles along with the growth mechanism of formation of desired silver nanoparticles. However, the partially known mechanism says that the formation of nanoparticles is due to the reduction of ions into silver metal. The bacterial machinery consists of ions and enzymes that help in reduction of silver ions into the silver metal. In natural environment also this technique is followed where microbes involve their systems to convert the reactive metal ions called radicals into the stable metal. Hence, this helps in decreasing the toxicity from the environment. The experiment on lab scale consists of the study of controlled nanoparticles with respect to the change in their environment. This involved the change in their temperature, duration, pH, concentration of the enzyme as well as the substrate. The proper combination of these parameters can help a lot in optimizing the growth of the nanoparticles in the desired range. The analysis has been done with the help of UV-Visible Spectrophotometer and SEM, where the existence of Ag nanoparticles is confirmed within the desired range. We are also trying to keep the size dispersion as low as possible. The interaction, formation and the results will be discussed accordingly.

### Biography

Vibha Saklani has completed her M.Tech in Biotechnology from Faridabad. Her six months internship was on "Bioequivalence and Bioavailability studies". She also undertook various trainings in the field of Clinical research, Agribiotechnology (Plant Quarantine Division), Water purification through Nanobiotechnology, Diagnostic oncology, Instrumentation and Wet lab analysis. Currently, she is working as a Research Scholar at Amity Institute of Advanced Research and Studies at Amity University, Noida. She is also an author of a book chapter to be published on: "Piriformospora indica- A multifunctional symbiotic fungus" written for a new book entitled: "Symbiotic Endophytes" finalized under Soil biology series. She has also been awarded as best speaker in a lecture competition at International year of physics, 2005 organized by B.H.E.L Gurgaon and MNRE.

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