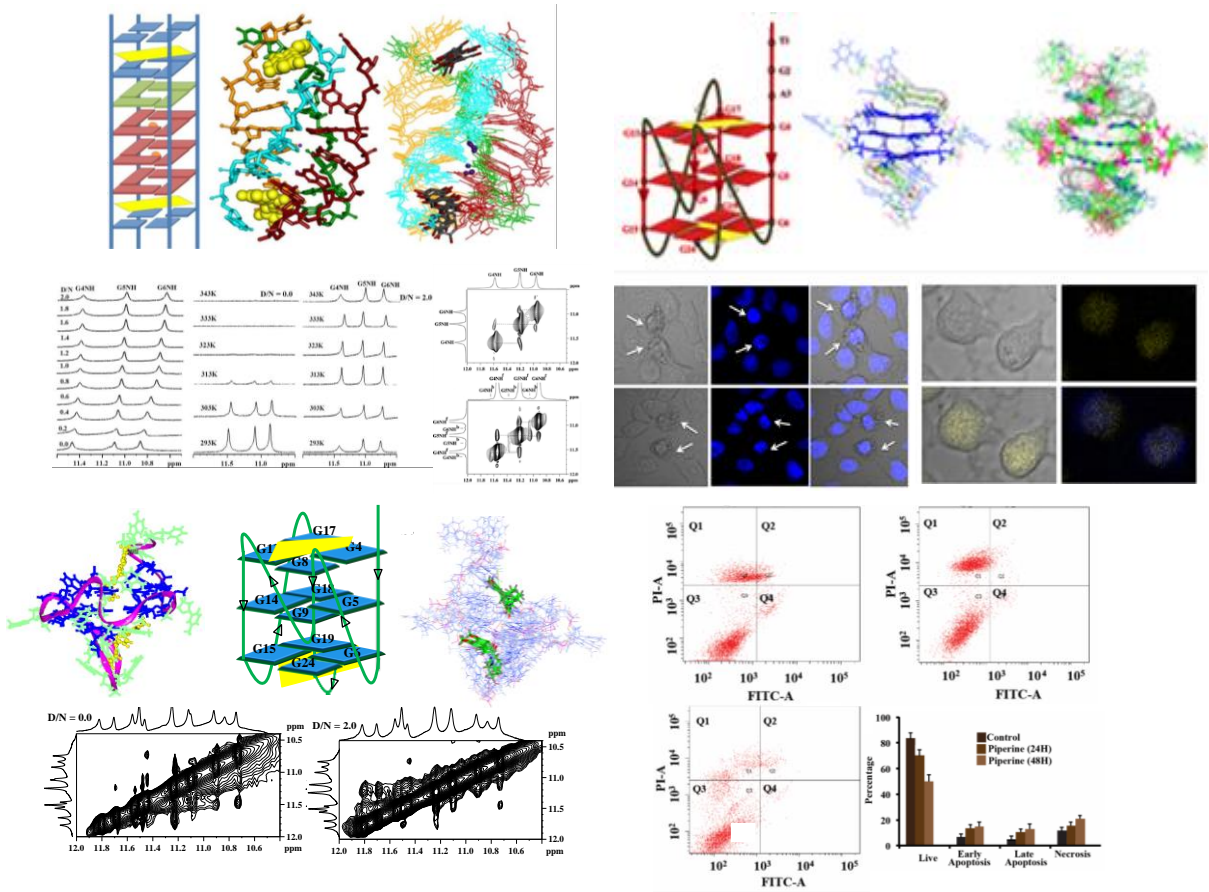


Research Highlights from Dr. Amit Kumar's Research Group

In structural biology lab, we have been working on elucidation of structural and molecular basis of Drug-Nucleic acid interactions. In this context we have studied the interaction of small molecules of natural origin readily available in human diets with G-quadruplex DNA formed at various regions of human genome like telomeric DNA, promoter region of various proto-oncogenes such as c-myc, c-kit21, bcl2, etc. These genes are known to be involved in development and progression of various cancers. First of all, we have studied the interaction of flavonoids with G-quadruplex DNA formed by human telomeric DNA sequence. By employing detailed biophysical techniques like Circular Dichroism (CD), UV-Visible, steady state, and time resolved fluorescence spectroscopy, we have probed these interactions. Further, the structural basis of this interaction and we have reported the first solution structure of the complex formed by Quercetin and G-quadruplex DNA formed by human telomeric DNA sequence. Furthermore, we have explored the mechanism for anticancer activity of flavonoids. It inhibits the cell growth by inducing apoptosis and it also down-regulates the gene expression in cancer cells upon binding. Our study highlights the potential of flavonoids as useful candidates for anti-cancer therapeutics by regulating DNA secondary structures.



Following this idea we have also explored the interaction of an alkaloid, Piperine, to various G-quadruplex DNA sequences formed in human genome. We have reported for the first time the binding of Piperine to with highest affinity for G-quadruplex structure formed at c-myc promoter region. We have proposed the model of this complex that showed Piperine stacks at both of terminal G-tetrads via π - π interactions and stabilizes G-quadruplex structure. Moreover, in-vitro studies show that Piperine is cytotoxic to various cancer cells and causes apoptosis-mediated cell death. Our study highlights the molecular aspects of its anti-cancer mechanism emphasizing its potential to down-regulate c-myc gene expression.

Nucleic Acid - Ligand Database (NALDB)
 Indian Institute of Technology Indore (भारतीय प्रौद्योगिकी संस्थान इन्दौर)

G4IPDB: G-Quadruplex DNA/RNA Interacting Protein Database
 Indian Institute of Technology Indore

Discover the Healthy Life in Faster Way

Traditional way for Drug Discovery

0.5-1 Year: Target identification
 0.5-1 Year: Target Validation
 0.5-1 Year: Lead Identification
 1-2 Year: Lead Optimization
 1-2 Year: Pre-Clinical
 4-6 Year: Clinical

Virtual screening Approach for Drug Discovery

0.5-1 Year: Virtual Screening
 0.5-1 Year: Clinical Proof of Screened Ligands

About

- G-quadruplex DNA
- G-quadruplex RNA
- Double stranded DNA
- Double stranded RNA
- Nucleic acid aptamer
- Special structure nucleic acid

Latest Entries

NALDB ID: G4DB0898

G4IPDB is a unique and interactive database of proteins which interacting with G-quadruplex forming nucleic acid sequences and have the detailed information about their nucleic acid target name, target sequences, ΔT_m values, binding constant, dissociation constant, gene name, gene ID, techniques which were used to detect their interactions with target, FASTA sequence, Gene ID of protein, nucleic acid interacting residue, their related PDB id's, interaction id's, and link of Protein graphical view available in the NCBI database. We connect the each interacting protein entry with their related Gene ID available in the GENE database. We also included the link of Protein Graphical view with their associated proteins. This database also allows provides an efficient and robust tool to predict the putative G-quadruplex forming sequences in the given sequences. Database users have both options to enter the query sequence manually or browse and upload the query sequence directly from the local disk space in either FASTA or Text file format. This web based tool predicted the putative G quadruplex forming sequence in both direction (sense and antisense strands) and gives a confidence score of cG/cC. These assembled information's at single platform makes this database unique and user friendly. G4IPDB database is freely available database which can be efficiently browse and search by different protein names and nucleic acid target name. To the best of our knowledge, G4IPDB is first database which is specifically focused on the any type of G-quadruplex DNA and RNA interacting protein and includes their interaction data available in the literature. We believe that the entries reported in this database would be useful for larger scientific community targeting the G-quadruplex nucleic acid and their binding protein as potential drug targets.

Our lab is also involved in providing scientific community with various databases for ease of drug discovery and development of novel therapeutics for various diseases. **We have developed NALDB** which is the first ligand database that contains ligand information for all type of nucleic acid. NALDB contains more than 3500 ligand entries with detailed pharmacokinetic and pharmaco-dynamic informations. All these details at single platform would be helpful for the development and betterment of novel ligands targeting nucleic acids that could serve as a potential target in different diseases including cancers and neurological disorders. Further, **we have developed G4IPDB** which is the first database that provides detailed information for various proteins that binds to G-quadruplex structures forming DNA and/or RNA. Development of G4IPDB database provides assistance to the scientific community in further improving the efficiency of small molecule therapeutics for nucleic acid based diseases.