

Research Plan – Bioinformatics and Genomics

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Bioinformatics and Chemoinformatics:

- Proteins (computational proteomics) analysis (including, 2°, 3°, and 4° structures) and *in silico* modelling of protein which yet not been structured either by X-ray or NMR spectroscopy, i.e., Comparative Protein modeling;
- Genomic (computational genomics) analysis through computational approaches;
- Small and organic molecular modeling;
- Studies of protein-protein, protein-nucleotide, protein-ligand, nucleotide-ligand, etc., macromolecular interactions;
- Structure- and ligand- based Drug-design
- Bio-molecular dynamics (MD) simulations, Monte Carlo (MC) simulations, etc.

Etc.

Molecular biology:

- Protein-transcription factor interactions, Protein-nucleotide interactions, etc., *in vitro* to confirm the *in silico* results, using different molecular biology and biochemical approaches.
- Study of transcription factor-small drug-like molecule interactions *in vitro*, again to confirm the *in silico* results.