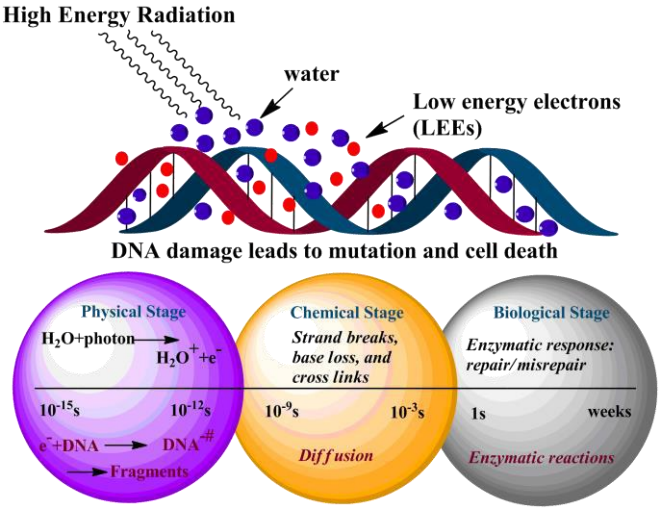
Modelling Potential Radiosensitizer Molecules for Chemotherapy

It has now been well understood that low energy electrons play a crucial role in rupturing DNA double helix as these electrons on attachment to biomolecules leads to the formation of highly unstable transient negative ion states. Interaction of ionizing radiations (for e.g., UV, X-rays, and Gamma rays) generates low energy electrons (LEEs) in jillion when they are in contact with living cells. These sub-ionization particles exhibit high efficiency to disrupt the cell metabolism by inducing chemical bond cleavage to life sustaining molecules like amino acids, proteins, DNA double helix and so forth, which further develops to mutation and cell death.

Cancer patients may undergo radiotherapy at some stages of their treatment followed by chemotherapy. At present, effective drug molecules available for chemotherapy is less.

To address this issue, we are aiming to develop an algorithm for simulating the suitability of molecules that can serve as potential radiosensitizer molecules in chemotherapy. This will eventually help us in setting up a database for clinical researchers who can refer our database for their clinical trials. Our objective is to help people who are under the treatment (say, radiotherapy/chemotherapy) for cancer disease.



La-Fondation is constantly supporting researchers in our institute to sprawl their expertise through rigorous research activities while addressing a socially challenging problem. The project titled above is immensely supported by La-Fondation to procure a high-performance compute cluster for running the simulation work and BIOVIA program package for modelling the target drug molecules at higher accuracy level.