



## Computational Chemistry – Group Leader

**Department:** Computational Chemistry

**Location:** Bengaluru

**Desirable Qualification:** Ph.D (Computational Chemistry or Molecular Biophysics or related area) with post-doc and experience in computational chemistry with knowledge on AI & ML with minimum 5-7 years of experience in a drug discovery industry/ CRO with good interpersonal & communication skills.

### Experience required:

- Good knowledge of chemistry and sufficient knowledge of biology and biophysics.
- Enthusiasm to learn new skills and software relevant to the work
- Should be able to prepare good presentations
- Should be able to work in a multi-functional team towards project goals

### Key responsibilities:

- Collaborate with colleagues in medicinal chemistry and other teams for providing scientific knowledge obtained through molecular modelling, supporting small molecule drug discovery.
- Provide leadership to associates in computational chemistry to deliver modelling results.
- Responsible for optimal utilization of resources in his organization through monitoring, measuring and reporting on scientific issues, opportunities and developmental plans and achievements within agreed formats & timescales.
- Posses experience in most Compchem methodologies (structure- and ligand-based approaches & virtual screening)
- Knowledge on AI & ML usage in drug discovery space
- Publish scientific articles in reputed scientific journals
- Propose and support new drug discovery therapeutic targets
- Allocate departmental resources to project requirements based on skills matching the requirements and work loads
- Resolve any conflicts arising within the department and in collaborations with internal interfaces
- Support business developmental activities to attract, acquire and retain customers.
- Continuously monitor the group members, appraise/assess their progress and learning to improve departmental and individual performance levels and impact on project deliverables
- Initiate development of new models, algorithms and methodologies to align with the latest developments in the field.

- Assess software requirements and accordingly procure & license
- Possess good judgmental and decision making capabilities.
- Strong networking skills with experts in academia & industry
- Active participation in departmental seminars
- Ensure a safe work environment
- Provide training for less experienced teammates