

Eli Lilly Services India, Bengaluru

Solid Form Structure and Modelling Scientist

Crystallographer

- Process and manipulate data from various sources (SC-XRD, XRPD, synchrotron, Cryo-EM) for small molecule structure determination
- Collaborate with interdisciplinary teams to inform solid form, particle, crystallization and drug product design and optimization efforts based on crystal structure analysis and computational results (structure-property relationships)
- Develop novel computational chemistry techniques and tools to investigate surface, physical and mechanical properties of materials
- Document experimental procedures, results and conclusions in laboratory notebooks and/or technical reports to support regulatory submissions and patent filing

Additional Responsibilities:

- Apply structural informatics tools, i.e. hydrogen-bond propensity, conformational and intermolecular interaction analyses to assess solid form development risk
- Model crystal morphology and facet surfaces to assess effect of solvent, impurities, additives or excipients on morphology and/or solid state stability
- Develop crystal structure and/or molecular modelling approaches for mechanical property prediction and/or structure-property correlation

Maintain in-house, searchable database of high-fidelity crystal structures

Position Requirements

- Up-to-date knowledge of relevant programs for optimal crystal structure data acquisition, processing, structure solution, refinement and validation, including advanced applications for the study of disordered systems
- Strong understanding of computational chemistry techniques to investigate surface and mechanical properties
- Knowledge of intermolecular interactions and their role in stabilization of crystal structure and properties
- Coding (C/C++, Python, Fortran, Perl)
- Experience in Small molecule crystallography, computational chemistry, solid state structure-property modelling

Excellent oral and written communication skills.

Candidates can apply by sending email with resume directly to Kishore_gaurav@lilly.com