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Inviting Expression of Interest (EoI) for the supply of Single Crystal X-ray Diffractometer

Reference: Advertisement dated February 24, 2022 published in 'Times of India' and 'The Hindu'.
Contact: Stores and Purchase Department
National Institute of Pharmaceutical Education and Research (NIPER) Hyderabad, Balanagar, Hyderabad 500037
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National Institute of Pharmaceutical Education and Research (NIPER) Hyderabad is planning to procure a Single Crystal XRD (Quantity: 1) suitable for R&D activities of the institute. Interested suppliers/bidders are requested to contact the Stores and Purchase Department of the institute latest by March 7, 2022. Further details about specific R&D application needs and general requirements of the instrument are provided below:

Application Needs (representative):

1. Major applications of the Single Crystal XRD system would include structural investigations of the active pharmaceutical ingredient (API) such as structure elucidation, absolute structure determination, molecular confirmation for structure property correlation, conformational analysis of peptides and macromolecules (small to mid-sized).

2. Solid state characterization research and development: Structure determination from Single Crystal XRD, advanced structural studies involving phase transformation of APIs. quantification of solid-state impurities, etc.

3. Structure determination of API form in various formulations [Precipitate from solution, form transformation in suspension (hydrate formation, etc)] Polymorph/salt/cocrystal screening, Oral solid dosage form development projects

4. SXRD would be useful for understanding complexation/aggregation behaviour in case of lipidic formulations, microcapsules, dendrimers, etc. wherever single crystals of molecular complexes could be obtained.

5. Crystallization process development and scale up projects: Identification of solid phase of API and phase purity analysis for the bulk batches.

Single Crystal XRD-Technical requirements (general-preliminary):

A state of the art completely automated floor mounted single-crystal X-ray diffractometer (SCXRD) designed for structure determination of wide range of organic, inorganic, metal organic, MOFs and metal clusters, etc. Absolute structure determination of pharmaceutical R&D molecules and low temperature data collection facility are among critical requirements. Such an instrument should be optimally configured to achieve the best quality data from small, weakly diffracting crystals with significantly large unit cells (up to ~50 Å axes length) and/or with additional complexities in terms of twinning, disorder etc. This would ideally need a combination of a small, highest-intensity X-ray beam coupled with large area detector. The system should be fully contained within an X-ray safety enclosure as per the highest international standards and with sufficient internal working space. The exact detailed technical requirements and specifications will be finalised in discussion with expert committee, tentative basic requirements are given below:

1. **X-Ray Generator and Source:** The system should be equipped with computer controlled, automated with high stability Copper micro-focus sealed X-ray source. A source with air-cooling mechanism without any internal or external water chiller may be preferable. Should be able to achieve highly monochromatic (spectral purity >95%) stable intensity with long tube life and very minimum or no maintenance.

2. **Detector:** The system should be equipped with state of the art large **area detector** of most recent/efficient technology, preferably be **completely air-cooled** and minimal/no maintenance.

3. **Goniometer**: The diffractometer should be equipped with a fully automated high precision four circle goniometer. The goniometer must be built in such a way that the extended directions of the axes intersect at a point, with negligible error (not greater than 10 microns). The sample to the detector distance should be variable under computer control over a range of at least 35–200 mm or longer. The diffractometer system should be automatically controlled by the system software.

4. **Crystal viewing video:** Appropriate high resolution crystal viewing colour video microscope to enable mounting and centering of crystals should be included.

5. **Integrated software:** A fully integrated WINDOWS based licensed software for Data collection, processing, Data collection strategy, structure determination must be an integral part of the system with at least 1 additional license for installing in the data processing computers.

6. **Computer:** The Diffractometer Instrument should come with a PC with Factory loaded Software. Specifications of the PCs should be of the latest optimal configuration.

7. **Cryo cooling:** A low temperature (LT) device should be provided with the system, and include a temperature control device to cover the temperature range of approximately 80 – 500 K, with a good stability (+/- 0.2 K) equipped with liquid nitrogen Dewar of minimum 60 L capacity, pressure regulator, transfer line and necessary accessories.

8. **UPS:** Suitable capacity UPS with minimum 1 hour Battery backup of reputed make On-Line UPS with built-in isolation transformer and event logging facility to run the XRD system including the instrument computer.

9. **Crystal Mounting Accessories**:
    a. Goniometer Heads: 2 No's of Goniometer head with strong magnetic base
    b. Test crystals: 1 No
    c. Paratone HR2-643 cryoprotectant oil (100ml): 1 No
    d. Crystal Mounting set: Appropriate cryoloops packs of various sizes: 5 Nos

10. General requirements:

a) **Warranty:** The equipment (including all spares and accessories) and all accompanying components (cryosystem) should have **3 years warranty** from the date of handing over the fully functional unit to the Institute, against manufacturing defects of material and workmanship. Non-Comprehensive annual maintenance contract for 4^{th} and 5^{th} year should be included.

b) **Installation and Commissioning:** Installation and training should take place at NIPER Site. The expenditure involved in it will be borne by the supplier. On site application training for minimum 4 days (2 days each – 2 slots) by the company designated application Scientist for a group of technical staff/students for operating the instrument to complete structure determination/solution including software learning.

c) **Pre-Installation requirement**: Necessary pre-installation advice should be enclosed along with the technical bid.

d) **Down-time call attendance**: Supplier should clearly mention about their service set up in India (preferably in south zone) for prompt service support along with contact details of service engineers specially trained on the offered system. Service should be provided at earliest (call to be attended within 3 working days)**.**

e) **Manuals and Instruction Sheets:** All the manuals including circuit Diagrams and instruction sheets must be supplied in English for the purpose of service engineer's reference. The offered XRD system model should preferably comply with the latest machinery directive, for electrical equipment and electromagnetic compatibility under fully CE compliant guidelines (or equivalent).

f) **List of current users:** Minimum 5 users of XRD in India, for the exact quoted model, manufactured by the bidder should be provided.