

NCR Biotech Science Cluster, 3rd Mile stone, PO Box.04,
Faridabad-Gurugram Expressway
Faridabad-121001

Ref.No. THSTI/NOC/05/21-22

08th Oct 2021

Subj: Notice For Inviting offers/Objections in respect of Procurement of Schrodinger Software Qty-01

THSTI is under process to purchase subject cited item from M/s Schrodinger on proprietary basis. The specifications of the required item are uploaded for open information to submit offers/objections, if any, from countrywide manufacturer regarding proprietary nature of the item quoting Reference No. THSTI/NOC/05/21-22. The offer should be submitted in compliance with the terms and conditions as attached herewith. Distributors are also invited to submit their best offer for the required goods. The comments/objections may be e-mailed to **equipment_purchase@thsti.res.in** or submitted by speed post/courier at the below mentioned address on or before **21st Oct 2021 up to 1500 Hrs.** In the event of non-receipt of any objections/comments with in the stipulated time, it will be presumed that vendors of prevailing market don't have any objection towards this enquiry.

The detailed specification of the equipment to be procured is given as Annexure-1 with this document.

To Be Submitted To

**Section Officer (Stores & Purchase)
Translational Health Science and Technology Institute
3rd Mile Stone, Faridabad-Gurugram Expressway, Faridabad – 121001
Phone: +91-129-2876433**

Section Officer (S&P)

Terms and Conditions: Attached on 6 & 7 | Page

Annexure-1

Software Specifications:

Sr. No.	Specifications
1.	Main License Server with floating Client Licenses to be used with multiple machines
2.	The software should be having ready compatibility with recent versions of Windows, Linux and Mac operating systems
3.	Provide a unified Modelling Environment for all the modules with Impressive Viewer, rendering capabilities, analysis tools, managing tools and an easy-to-use design with a versatile modelling tools, with visualization of non-bonded interactions (Phi-Phi, Phi-cat and hydrophobic), Movie making.
4.	Fully-fledged docking software, which uses OPLS forcefield for small molecule and peptide docking.
5.	Options for metal coordination, NOE position constraints
6.	Docking refinement with strain penalty terms
7.	Accurate favourable energy functions of Ligand for hydrophobic buried interaction and non-favourable energy functions for hydrophobically buried polar atoms and exposed hydrophobic atoms.
8.	Visualizer for important favourable and non-favourable interactions
9.	Conversion of the important ligand receptor interactions into finger-print for virtual screening
10.	Simultaneous docking of numerous ligands to numerous proteins.
11.	Automated selection of the hits from Virtual screening based on the defined interaction criteria.
12.	Facility to dock the compounds or peptides with up to 500 atoms and 100 rotatable bonds.
13.	Facility of identification of the active sites in the protein and calculates the druggability of the site.
14.	Evaluate the sites for their donor, acceptor and hydrophobic site as counters, which helps in lead optimization.
15.	Site defines the binding pocket for ligand receptor molecular docking.
16.	Identifies the shallow binding pockets on the protein for the protein-protein interactions
17.	Democratize creation and application of QSAR models through automation, following a best practices QSAR modelling workflow.

18.	Integrate on a process level into informatics platforms to facilitate the creation and application of QSAR models. As new data becomes available, QSAR models can be automatically regenerated leading to improved accuracy and applicability
19.	Embody QSAR best practices from the literature included the OECD recommendation
20.	Automated virtual screening protocol using molecular docking to prepare and screen large database compounds against multiple targets simultaneously by taking care of Toxicity, Lipinski rule of five, Herg channel blockage, membrane permeability, solubility
21.	Can be installed on Main License Server with floating Client Licenses with complete On-site training and support should be provided by the supplier/manufacturer by Technical experts to the Users Team.
22.	Predict ADMET Properties of organic molecules for Solubility, permeability, CNS activity, blood brain barrier permeability, HERG K ⁺ Channel activity, Cytochrome p450 site of metabolism and amphiphilic movement
23.	Fast, accurate, and practical binding mode identification at a given pH, with Hammett and Taft methods
24.	Accurate and efficient bioactive conformational searching for computer-aided drug design
25.	The tool should help to design rational combinatorial library and do docking program
26.	Generation of accurate 3D molecular models
27.	The tool should help to design rational combinatorial library and do docking program
28.	Reaction-based enumeration that enables the rapid exploration of synthetically tractable ligands
29.	High-performance free energy calculations for drug discovery
30.	Latest graphics processing unit (GPU) technology implemented in Desmond, MD simulation can run up to 200 times faster than on CPU, which can bring up the time scale of interest by orders of magnitude.
31.	Jaguar proceeds much faster than conventional <i>ab initio</i> programs, making it possible to carry out many more calculations within the same time frame
32.	Ligand Designer provides powerful, yet easy to use 3D visualization and ligand building capability that is scientifically proven while making it fun to design ligand modifications in 2D or 3D and see how those changes are likely to impact protein-ligand complex structures.

	Atomic-scale simulation can accelerate the development of new materials by helping identify the most promising structures and formulations before you begin synthesis and testing. Our platform is powering the design of novel materials in a wide array of industries, including aerospace, energy, semiconductors, and electronic displays
33.	Phase employs a newly developed common pharmacophore perception algorithm that flips the old paradigm by identifying ligand alignments first and then perceiving hypothesis. Using pharmacophore-based shape alignments, It quickly creates high-quality hypothesis from a handful to hundreds of known active ligands.
34.	OPLS4, builds upon the extensive coverage and high level of accuracy achieved in OPLS3e, by improving the accuracy of functional groups that have presented significant modeling challenges in the past. In particular, charged groups and sulfur containing moieties are significantly improved with OPLS4.
35.	PIPER was used to determine the top-scoring entry in the most recent CAPRI blind assessment of protein-protein docking.
36.	Workflow automation tool which can help researchers to easily assemble individual "nodes" into a complete workflow — from structure preparation and selection to a validated predictive model. Expediting a wide variety of common tasks. The tool should allow scientists to prototype, validate, automate, and deploy multi-step workflows.
37.	The software should come with free updates, onsite training and support

38. The dedicated training from scientists of Schrodinger is critically required for at least 4 weeks (twice in a year) for modules such as FEP+, water-map and biologicals. The critical training is also required for analysis and interpretation of the data generated by these modules.
39. The general hands-on training is also needed, twice in a year for all the modules.
40. The Schrodinger scientists must explain in hands-on training sessions how they did their groundbreaking discoveries using Schrodinger, starting from the scratch for those products which are in advanced research and/or in clinical trials.

41. Online webinar is mandatory from international scientists of Schrodinger so that THSTI users are well aware of global updates and can discuss their scientific and technical problems directly with them.
42. The Schrodinger team will join hand-in-hand with users in different ongoing projects of THSTI and help in technical and scientific front to develop the projects for translational point of view.
43. Full technical support, both for hardware and software are needed for proper execution of Schrodinger.
44. The User, IT team of THSTI and Schrodinger team will sit together to facilitate the regular and robust infrastructure for smooth and consistent execution.
45. For any technical problem, the users of THSTI will write their problem directly to the Schrodinger team and they will provide the solution.
46. Floating licenses for different modules (for example if glide tokens are free they can be available for piper or vice versa)
47. FEP+ licenses will be available to utilize any time till the licenses are exhausted.

1. Only manufacturers or their authorized distributors are eligible to participate in this enquiry.
2. Prices quoted /offered should be F.O.R. basis up to THSTI, Faridabad.
3. The supplies if rejected due to non-conformity with the specifications is liable to be replaced free of cost within the stipulated period at the Institution. In case of failure to do so the rejected supplies shall be disposed-off by THSTI at its own discretion and no claim shall be entertained thereof.
4. Tender shall be accompanied with Bid security declaration form as per 'Annexure-2'. Failure to provide this bid may not be considered for further process. The item to be supplied must be of genuine quality/make of authorized manufacturer.
5. Conditional offer will be liable for rejection.
6. Payment: 100% payment shall be made after successful supply, installation and commissioning (SITC) of the item at Institute site of Installation and upon receipt of PBG as per clause no.09
7. The manufacturer should send true copy of registration of the company with a copy of license of products, GST details and in the case of authorized dealers recent Authorization Certificate of the manufacturer.
8. THSTI is eligible for availing Custom Duty Exemption against DSIR Registration and in terms of Govt. Notification No. 51/96-Custom dated 23 Jul 1996, Central Excise duty exemption in terms of Govt. Notification No. 10/97-Central Excise dated 01 Mar 1997, Notfn. No. 47/2017 – Integrated Tax (Rate) dt. 14.11.2017 and Notfn. No. 45/2017 – Central Tax (Rate) dt. 14.11.2017, Notfn. No. 45/2017 – Union Territory Tax (Rate) dt. 14.11.2017, as amended from time to time.
9. Performance security equivalent to 03% of the order value, in the form of Bank Guarantee/FDR from any Nationalized Bank effective from date of Installation covering warranty of equipment plus 60 days is required to be submit immediately after successful/Satisfactory Installation.
10. Since time is the essence of the contract, delivery of the Goods and performance of the services shall be made by the supplier in accordance with the time schedule specified by the Purchaser in the Contract. If the Supplier fails to deliver any or all of the Goods or to perform services within the period(s) specified in the Contract, the Purchaser shall, without prejudice to its other remedies under the Contract, deduct from the Contract Price, a penalty, a sum equivalent to 0.5% per week and the maximum deduction is 10% of the contract price.

11. Pre installation requirements: Supplier to inform in advance pre-installation requirement to the concern lab/department and perform installation, safety and operation checks before handover the equipment at no cost.
12. Software license should remain valid for the period of 05 years from the date of successful installation.
If during the period of warranty any component or service support is needed to be imported, all associated cost for replacement shall be borne by the supplier including the cost of customs duty, customs clearance charges etc.
13. Purchase Preference to Local Suppliers: In pursuance of Government of India Order no. P-45021/2/2017-B.E.-II dated 15/06/2017 as amended by Order No.-P-45021/2/2017-B.E.-II dated 28/05/2018, P-45021/2/2017-B.E.-II dated 29/05/2019, P-45021/2/2017-B.E.-II dated 04/06/2020 and P-45021/2/2017-B.E.-II dated 16/09/2020, Eligible Supplier shall provide the certificate as per the notification on company letter head.
14. All rights are reserved with the Executive Director of THSTI who may accept or reject any or all the offers without assigning any reason thereof.

Annexure-02

BID SECURITY DECLARATION

(To be submitted by bidder on Non-Judicial Stamp Paper of Rs.100/-only duly attested by Notary)

We, (*Name of bidding firm with its address* _____) do hereby certify and declare that we are interested and genuinely participating in the Tender Enquiry No. _____ for (*tender description* _____) invited by the THSTI.

We further undertake that if we withdraw or modify the submitted bid during the period of Bid validity, or if we will be awarded the order / contract and If we fail to acknowledge the order / sign the contract, or to submit a performance security before the deadline defined in the Tender document, the order awarded / work contract issued shall be terminated at the discretion of Competent Authority, THSTI and our firm will be suspended / blacklisted for the period of 03 years from being eligible to submit Bids for tenders with the THSTI in future.

Date:

Name and Signature of Authorized
Signatory of bidding firm along with stamp