

No. DCB/Admin/268/2024-25

05.02.2025

**Containing General Conditions and Schedule for the License Renewal of
Dassault Systems BIOVIA Discovery Studio Academic Teaching Suite.**

Name of Tenderer: **Professor & Head (i/c), Department of Computational Biology
and Bioinformatics.**

Address: **Head of the Department (i/c)**
Department of Computational Biology and Bioinformatics.
University of Kerala
Kariavattom Campus
Thiruvananthapuram
Kerala, PIN- 695581

Signature of Tenderer



Head of the Department (i/c)
Department of Computational
Biology & Bioinformatics
University of Kerala, Kariavattom
Thiruvananthapuram - 695 581



FORM OF TENDERER

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To

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.....

Sir,

I/We hereby tender to supply, under the annexed general conditions of contract, the whole of the articles referred to and described in the attached specification and schedule, or any portion thereof, as may be decided by the University of Kerala, Thiruvananthapuram at the rates quoted against each item. The articles will be delivered within the time and at the places specified in the schedule.

*I/We am/are remitting/have separately remitted the required amount of Rs.

.....
..... as earnest
money.

Yours faithfully (Signature)

.....

(Address)
.....
.....

Date:.....

* To be scored in cases where no earnest money deposits is furnished.

Important: This tender form may be printed on A4 size paper. Editing of the pre- printed text in the tender form in any way other than as indicated (like ticking, filling in with ink/typing, scoring off in applicable material etc.) will render the tender form invalid and liable for rejection.

GENERAL CONDITIONS

Sealed tenders are invited for the supply of the materials as specified in schedule attached below.

The tenders should be addressed to the **Head of the Department (i/c), Department of Computational Biology and Bioinformatics , University of Kerala, Kariavattom Campus, Thiruvananthapuram-695581, Kerala** in a sealed cover with the tender number and name – **“Tender for the License Renewal of Dassault Systems BIOVIA Discovery Studio Academic Teaching Suite”** duly super scribed on the cover on or before **19.02.2025, 3.00 PM**.

1. Original Equipment Manufacturer (OEM) Certificate/Undertaking: **If the bidder is not an OEM, a Certificate of authorized dealership / distributorship from the OEM for technical support to the bidder and supply of spares shall be furnished.**
2. **Compliance Statement:** Along with the technical details provide a tabular column indicating whether the item quoted by you meets the specifications by indicating 'YES' or 'NO'. If 'YES', support the claim by providing original brochures
3. Tenders which are not in the prescribed form are liable to be rejected and the cost of tender forms once paid will not be refunded. **The rates quoted should be only in Indian currency.** Tenders in any other currency are liable to rejection.
4. Intending tenderers should send their tenders so as to reach the officer mentioned in the tender notification, on or before the due date and time noted therein. No tender received after the specified date and time will be accepted on any account. The rates will be considered firm for acceptance till the date mentioned therein. Tenders not stipulating period of firmness and tenders with price variation clause and/or 'subject to prior sale' condition are liable to be rejected.
5. (a). The cost of the **tender form Rs.1,000.00** (Rupees One Thousand only) (i.e. Rs.840 + 18% GST) and the **Earnest Money Deposit of Rs. 4,200/-** (Rupees Four Thousand and Two Hundred only) should be remitted by way of **Demand Draft** issued from a nationalized/ scheduled bank, drawn in favor of , **Head of the Department (i/c), Department of Computational Biology and Bioinformatics, University of Kerala** payable at **State Bank of India, Kariavattom Branch (SBIN0070043)**. The tender documents, along with **separate DD towards the cost of the tender form and the EMD** should be submitted/ sent to **Head of the Department (i/c), Department of Computational Biology and Bioinformatics, University of Kerala, Kariavattom Campus, Thiruvananthapuram- 695581, Kerala**. **Cheque will not be accepted.** The earnest money of unsuccessful tenderers will be returned as soon as possible after the tenders are settled.
- (b). **Performance Security:** If work is awarded, a **Performance security equal to 5% of contract value shall be furnished by the bidder.** The Performance Security will be forfeited, if the firm fails to abide by the terms and conditions of the tender and subsequent execution of the work/ warranty liability. It will be released on successful completion of work and warranty period mentioned in the tender.
- (c). Tenderers whose names are registered with Government (Stores Purchase Department) are generally exempted from furnishing earnest money for such articles for which they have registered their names. If they tender for stores other than those for which they have registered their names, they will have to furnish earnest money as in the case of unregistered firms. Registered firms will have to quote invariably in every tender they

submit, the registration number assigned to them by the Stores Purchase Department.
Attested copy of registration certificate may be enclosed with the tender for reference.

- (d). Small Scale Industries and Cottage Industries within the Kerala state, which are certified as such by the Director of Industries and Commerce or by the Regional Joint Director of Industries and Commerce will be exempted from furnishing earnest money against tenders for supply of stores manufactured by them.
6. If any tenderer withdraws from his tender before the expiry of the period fixed for keeping the rates firm for acceptance, the earnest money, if any deposited by him will be forfeited to the University of Kerala or such action taken against him as the University think fit.
7. The final acceptance of the tender rests entirely with the University which do not bind itself to accept the lowest or any tender. But the tenderers on their part should be prepared to carry out such portion of the supplies included in their tender as may be allotted to them.
8. In cases where a successful tenderer, after having made partial supplies, fails to fulfill the contracts in full, all or any of the materials not supplied may at the discretion of the Registrar, be purchased by means of another tender/quotation or by negotiation or from the next higher tenderer who had offered to supply already and the loss, if any, caused to the University shall thereby, together with such sums as may be fixed by the University towards damages, be recovered from the defaulting tenderer.
9. **Payment: The University will release the payment only after inspecting the software and satisfying that the supply is as per the requirements.** The payment will be made after successful completion of the supply and installation and producing invoice in triplicate
10. The contractor shall not assign or make over the contract or the benefits or burdens thereof to any other person or body corporate. The contractor shall not underlet or sublet to any person or body corporate the execution of the contract or any part thereof without the consent in writing of the Registrar who shall have absolute power to refuse such consent or to rescind such content (if given) at any time if he is not satisfied with the manner in which the contract is being executed and no allowance or compensation shall be made to the contractor or the sub-contractor upon such recession. Provided always that is such consent is given at any time, the contractor shall not be relieved from any obligation, duty or responsibility under this contract.
11. The tenderer shall undertake to supply materials according to the standard sample and/ or specifications
12. **No representations for enhancement of rates once accepted will be considered.**
13. Any attempt on the part of the tenderers or their agents to influence the University in their favour by personal canvassing with the officers concerned will disqualify the tenderers.
14. **Installation and Commissioning:** The items shall be installed and commissioned at Department of Computational Biology and Bioinformatics, University of Kerala, Kariavattom Campus, Thiruvananthapuram. All incidental expenses should be borne by the supplier.
15. **The item should be supplied within a period of 15 days** from the date of supply order.
16. General rules relating to the purchase of materials/ equipment will also applicable to this tender.
17. **Only one model can be quoted in a tender.** If the tenderer wants to quote for more than one model, separate tenders should be submitted. If more than one model is quoted in a single tender it will be summarily rejected.
18. **Technical bid and financial bid must be placed in individual sealed envelopes and these envelopes must be placed inside a bigger envelope.** The top of cover must also contain name

and address of the tenderer, telephone number and other contact details for the further correspondence.

19. **Warranty/Guarantee:** The supplier shall guarantee to repair/replace the items or its part –if found defective within the **warranty period**. The entire expenditure for repair/ replaces of the item in this regard shall be borne by the supplier.
20. **Service facility:** Supplier should mention their details of **service setup and manpower in Kerala, especially at Trivandrum** who are responsible for after sales service. Service support undertaking should be furnished.
21. Tenderers who are black listed by State/ Central Government departments and Organizations are not eligible to participate in this tender and such tender will be summarily rejected.
22. In case of the dispute arises, the decision of University authority shall be final and binding on bidders.
23. The undersigned reserves the right to reject or accept any or all the tenders received fully or partially without assigning any reason thereof.
24. **The Validity of the Quotation will be for 180 days.**
25. The price quoted must be inclusive of GST, transportation charges, installation charges and any other charges & Government duties leviable, if any.
26. **Other special conditions:** Defective items, if any, supplied should be rectified/ replaced to the satisfaction of the University by the suppliers at their own cost.

SPECIFICATIONS FOR MOLECULAR MODELING SOFTWARE

General features:

1. The software should be compatible with windows 10/11 and Linux operating systems only 64bit.
2. Teaching Bunde -1 (30 users)
3. Technical and application support on the software.

Academic Modules:

Protein modeling and engineering

1. Protein homology models should be built and scored as probability density function scores and the corresponding loop models should display the discrete optimized protein energy score.
2. Protein verification post modeling should measure the compatibility of an amino acid sequence with 3D protein structure based on Dr. David Eisenberg algorithm (University of California)
3. In searching for side chain rotomers following all of these rotomer libraries should be available – Sutcliffe, Ponder & Richards, Lovel word & Richardson, Oldfield.
4. Protein is a measure of its tendency to aggregate via hydrophobic interactions should be calculated and scored based on paper Lauer et al., 2012

Protein-Protein docking /antigen-antibody interactions

5. Protein-Protein docking should use a simple shape complementarity method called Pairwise Shape Complementarity (PSC). The PSC method should be optionally augmented with desolvation (DE) and electrostatic (ELEC) energy terms to rank the docked poses.
6. The Side-Chain Refinement protocol optimizes the protein side-chain conformation based on systematic searching of side-chain conformation and CHARMM energy minimization using

ChiRotor algorithm.

7. The following algorithm should be used for minimization of proteins, conjugate gradient, adopted basis Newton Raphson and steepest descent

Simulations

8. Calculation of partial charge, based on momanny-rone & MMFF94 and force field should be CHARMM and its flavors allowing it to be edited.
9. Post dynamics, Trajectory analysis protocol should use Radial Distribution Function (RDF) to describe the structural correlation between atoms in a condensed phase. RDF, which is also called the pair correlation function, is commonly used in the study of the liquid state

Docking and structure-based design

10. Ability to predict active site based on receptor cavities and partition site in a protein structure
11. Use multiple copy simultaneous search to place fragments in active site
12. Link and join fragments using denovo link and denovo evolution using LUDI algorithm

Pharmacophore

13. Should include the most extensive reported ligand profiling databases for studying either off-target activity or for drug repurposing. Built from and validated using the scPDB*, the database contains approximately 140,000 receptor-ligand pharmacophore models.

ADME & Toxicity

14. ADME prediction should be
 - a. Human intestinal absorption
 - b. Aqueous solubility
 - c. Blood brain barrier penetration
 - d. Plasma protein binding
 - e. CYP2D6 binding
 - f. Hepatotoxicity
15. **Toxicity** assessment should be extensible and all models should be listed in the QMRF model data base (<https://qsardb.jrc.ec.europa.eu>) to be validated for their predictions. Below is the models that should be accessible
 - a. Ames mutagenicity
 - b. Rodent carcinogenicity (NTP and FDA data)
 - c. Weight of evidence carcinogenicity
 - d. Carcinogenic potency TD50
 - e. Developmental toxicity potential
 - f. Rat oral LD50
 - g. Rat maximum tolerated dose
 - h. Rat inhalation toxicity LC50
 - i. Rat chronic LOAEL
 - j. Skin irritancy and sensitization
 - k. Eye irritancy

- l. Aerobic biodegradability
- m. Fathead minnow LC50
- n. Daphnia magna EC50
- o. Log P

QSAR

16. Create QSAR model with genetic function approximation methods

Lead Optimization

17. Find activity cliffs and Analyze activity effects using the matched molecular pairs algorithm

Extended platform and workflow design

18. Should be able to visualize/Edit and run the workflow for each of computational drug discovery in the software with a pipeline pilot protocol

I..... (Name of Authorized Person) on behalf
of.....
(Company name) do hereby agree the terms and conditions mentioned in the tender and supply of
above item as per schedule and rate mentioned in the financial bid.

Signature and Seal of Bidder

Those who are interested should send their bid (The bid **technical and financial separately** complete in all respects) may be submitted in a sealed cover (hard copy only) superscribed with
“Tender for
.....
.....Ref. No.....
Equipment Name
..... and addressed to **Head of the Department (i/c), Department of Computational
Biology and Bioinformatics, University of Kerala, Kariavattom Campus,
Thiruvananthapuram-695581, Kerala.**

Kindly submit lowest quotes on or before 19.02.2025, 3.00 pm

05.02.2025

Kariavattom



Head of the Department(i/c)
Department of Computational Biology and Bioinformatics

Head of the Department (i/c)
Department of Computational
Biology & Bioinformatics
University of Kerala, Kariavattom
Thiruvananthapuram - 695 581