

ALL INDIA INSTITUTE OF MEDICAL SCIENCES  
ANSARI NAGAR, NEW DELHI-29  
STORES SECTION (DO)

Ref. No. 42/Stores(DO)/Biophy/PAC/2019-20/FSC      Dated-14/01/2020

Sub:- Purchase of "Software for Computational Modeling and Docking – 01 No." for the Department of Biophysics at AIIMS, New Delhi-110029, on proprietary basis inviting comments thereon.

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The Institute is in the process to purchase "Software for Computational Modeling and Docking – 01 No. at AIIMS, New Delhi from M/s. Schrodinger, Inc, USA. The PAC Certifications by M/s. Schrodinger, Inc, USA as well as the user department are attached.

The above documents are being uploaded for open information to submit objections, comments, if any, from any manufacturer regarding proprietary nature of the equipment/item within 15 day from the date of issue/uploading of the notification giving reference No. 42/Stores(DO)/Biophy/PAC/2019-20/FSC. The comments should be received in office of Stores Officer (FSC), Store Section (DO), Animal House Building, Near Biotechnology Building at AIIMS on or before 03/02/2020 upto 12.30 p.m. failing which it will be presumed that any other vendor is having no comment to offer and case will be decided on merits.

Yours faithfully,

  
SR. STORES OFFICER (DO)

Encl: Related documents enclosed.

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**Specifications (approx 40 lakhs)**

**Software for Computational Molecular Modeling and Docking (Proprietary)**

**Must include**

1. Structural Viewer and Modeling Environment
2. *Ab initio* Modeling calculations
3. Molecular Dynamic Simulations including required force field
4. Ligand-Receptor Docking Drug-Protein/DNA interaction including Flexible and Induced Fit Docking
5. Structure prediction of proteins including GPCR
6. Drug-metalloprotease docking including Quantum mechanics polarized docking
7. Automatic Pharmacophore based and QSAR modeling including predictive modelling
8. Combinatorial technology for lead discovery including scaffold hopping and exploration
9. Chemoinformatics with similarity based screening and fingerprinting with required statistical analysis
10. Integrated Multi-stage approach for Program for protein-protein docking

**User License for three years with upgrades as and when released by OEM**

Shivendra Singh

Puneet Kam

05/09/2019

SS

Renu Dhingra

Anil

Golao

ALL INDIA INSTITUTE OF MEDICAL SCIENCES  
ANSARI NAGAR, NEW DELHI-110029

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RESEARCH SECTION

PROPRIETARY/SPECIFIC BRAND GOODS CERTIFICATE

1. Item/Type/Model No. required alongwith specification. *Software for Computational Molecular Modeling and Docking*
2. Is the item a spare parts attachment or accessory for an existing equipment. *Renewal of Expired License.*
3. Name of the manufacturers/supplier of the item proposed by the Indentor. *Schrodinger Inc., Portland*
4. Are they sole manufacturers/sole distributors of the item. *Yes.*
5. Is there any other item with similar/ equivalent specification available in the market to meet the job requirement envisaged. If the answer is yes, why the same can't be procured. Demanding officer should bring out comparative functional advantages/cost effectiveness of the recommended item from these offered by other. *No This is the only software which offers flexible docking and the force fields required for our work.*
6. What were the efforts made to locate alternative source of supply or use other substitutes. *Yes through a web-based search.*
7. Why open/limited tender can't be resorted to, for locating alternative source. *This is the only software for the specific methodology.*
8. Are the proprietary items certifying that the rates are reasonable or not. *Yes.*
9. Any other justification for procuring item from single source. *The software was procured in Feb 2014. The licence has expired and this is renewal of the same.*

Signature of Indentor  
(Demanding Officer)

डॉ० पुनीत कौर  
Dr. PUNIT KAUR  
आचार्य एवं अध्यक्ष/Professor & Head  
जैवभौतिकी विभाग/Dept. of Biophysics  
आर्यभट्ट जी स्मृति संस्थान/ARIYBHATTA JI SMRITI SANSTHAN  
आर्यभट्ट जी स्मृति संस्थान, नई दिल्ली-29  
ARIYBHATTA JI SMRITI SANSTHAN, NEW DELHI-29

COUNTERSIGNED  
(Head of the Department)

डॉ० पुनीत कौर  
Dr. PUNIT KAUR  
आचार्य एवं अध्यक्ष/Professor & Head  
जैवभौतिकी विभाग/Dept. of Biophysics  
आर्यभट्ट जी स्मृति संस्थान/ARIYBHATTA JI SMRITI SANSTHAN  
आर्यभट्ट जी स्मृति संस्थान, नई दिल्ली-29  
ARIYBHATTA JI SMRITI SANSTHAN, NEW DELHI-29

I certify that the item at Sl. No. *1* above is required to be procured on single tender basis as the source of supply is definitely known/the specified brand proposed was advantages in meeting our functional requirements and limited tender system could be dispensed with as they would serve no useful purpose in this particular case.

(Strike out whichever is not applicable)

SCHRÖDINGER®

January 05, 2019

Proprietary Certificate and Authorization Certificate

To whom it may concern,

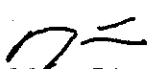
This is to certify that Schrödinger, Inc. is the sole manufacturer of the molecular modeling software products listed below, and is the sole distributor of the products in India. You would be placing your order directly to Schrödinger, Inc, located in Portland, Oregon, USA, and transferring payment directly to Schrodinger Inc. in the USA.

Products include: Glide, GlideXP Visualizer, Prime, Phase, PrimeX, MCPRO+, CombiGlide, QSite, Canvas, Field-based QSAR, Bioluminate, Confgen, Jaguar, Jaguar pKa, MacroModel, Epik, SiteMap, Impact, LigPrep, QikProp, Strike, Mint, PyMOL, AxPyMOL, Seurat, P450 SOM, Shape Screening, and Maestro.


We have authorized Mr. Raghu, Vice President, Schrödinger GmbH, to deliver the Quote on our behalf and to attend to any administrative details as necessary.

Please do not hesitate to contact us if you need any further information.

Regards,

  
Murco Ringnalda  
Chief Financial Officer



  
जेवभातिकी विभाग/Dept. of Biophysics  
अखिल भारतीय आयुर्विज्ञान संस्थान/A.I.I.M.S.  
अंसारी नगर, नई दिल्ली/Ansari Nagar, New Delhi-29