I/3125/2022

अखिल भारतीय आयुर्वेद संस्थान

All INDIA INSTITUTE OF AYURVEDA (AIIA)

(आयुष मंत्रालय , भारत सरकार के अंतर्गत स्वयात्त संस्थान)

(An Autonomous Organization under the Ministry of AYUSH, Govt. of India)

F.No S-11/21/2021-AIIA

Call for objection for procurement of Proprietary items

Subject : Purchase of schrodinger software i.e Glide software, Prime software and desmond/Jaguar from M/s Schodinger, Inc 101 SW Main Street, Suite 1300 Portland, OR 97204 .

The Notice is being uploaded for general information of prospective manufacturer/Authorized Distributor/Dealers to submit their objection/proposal/comments, if any, on proprietorship of the item.

In case the product of any manufacturer/Authorized distributor/Dealer conforms to the enclosed specifications, they may submit their proposal for the supply of the same along with the brochures, point by point compliance of the enclosed specifications along with all documentary evidence.

The objections/comments/proposal should be sent in through email with all relevant supporting documents to I/c IT email ID -shivakumar.harti@aiia.gov.in with CC to the director AIIA director@aiia.gov.in, hod-kaumarabhritya@aiia.gov.in by mentioning above subject in subject line of email on or **before 15 Nov 2022**. failing which it will be presumed that no other firm is interested to offer comments/protest/object and case will be decided on its merits.

Enclosure:

1. Proprietary Article Certificate of AIIA **as Annexure-1**
2. Proprietary Article Certificate Signed By M/S M/s Schodinger **as Annexure-2**
3. Sole Source certificate Signed By M/S M/s Schodinger **as Annexure-2**
4- Single source product undertaking by By M/S M/s Schodinger **as Annexure-3**
5- Exclusively distruster under taking by By M/S M/s Schodinger **as Annexure-4**
6 .Price quotes for By M/S M/s Schodinger **as Annexure-5**
7- schrodinger software i.e i.e Glide software, Prime software and desmond/Jaguar functionality and features **as Annexure-6**

Yours faithfully

(Dr Umesh Tagade)
Joint Director

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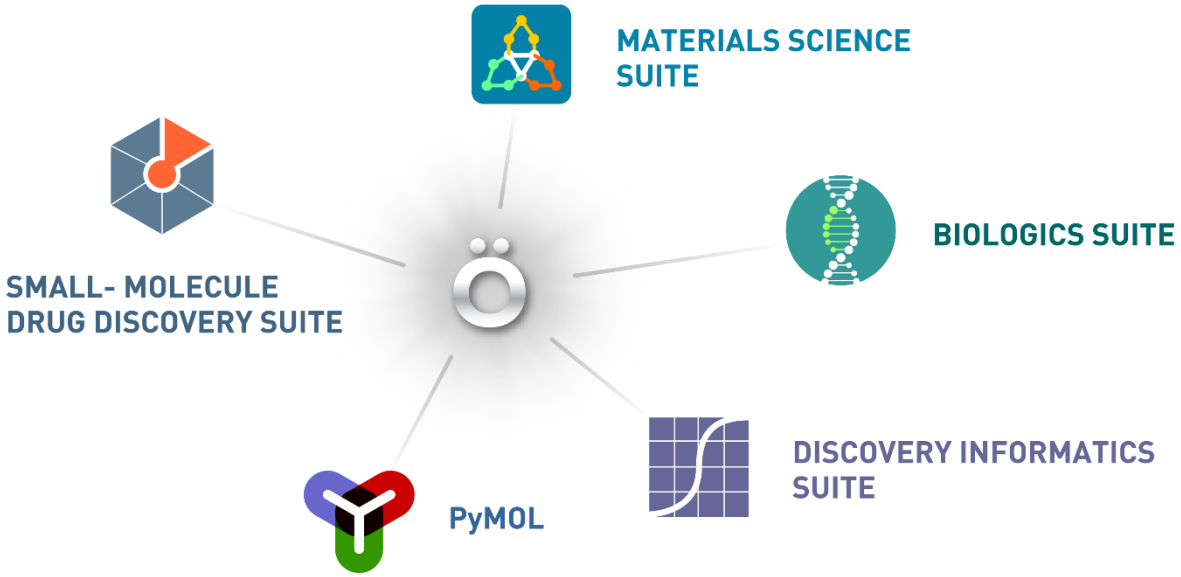
Schrödinger software profile and price details



SMALL-MOLECULE DRUG DISCOVERY SUITE

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Schrödinger software profile and price details

Premium Products Description	
Glide:*A complete solution for ligand-receptor docking*	Glide offers the full spectrum of speed and accuracy from high-throughput virtual screening of millions of compounds to extremely accurate binding mode predictions, providing consistently high enrichment at every level.
Prime:*A powerful and innovative package for accurate protein structure predictions*	Prime is a fully-integrated protein structure prediction program. It provides an easy-to-use interface that takes a novice user intuitively from sequence to alignment to refined structure. Prime also provides expert users complete control over calculational settings to maximize accuracy of predictions. Prime is a powerful and complete tool for generating accurate receptor models for structure-based drug design.
Phase :*An easy-to-use pharmacophore modeling solution for ligand- and structure-based drug design*	Phase is a complete, user-friendly pharmacophore modeling solution designed to maximize performance in virtual screening and lead optimization. Fast, accurate, and easy-to-use, Phase includes a novel, scientifically validated common pharmacophore perception algorithm.
Field-Based QSAR:*Discover and optimize new lead compounds using quantitative predictions of binding-site chemistry*	Field-Based QSAR opens up new possibilities in ligand-based drug discovery projects. Supplied with an aligned training set of active and inactive compounds, Field-Based QSAR predicts drug activity on the basis of either force fields or Gaussian fields that describe ligand chemistry.
Canvas: *A comprehensive cheminformatics computing environment*	Complete cheminformatics package for fingerprinting, similarity based screening, clustering and regression analysis etc.
Core hopping : Comprehensive ligand- and receptor-based scaffold exploration for lead optimization	In addition to more conventional ligand-based methods, Core Hopping offers receptor-based scaffold hopping, exploiting information about the active site and known binding poses to guide the search for novel cores.
QSite : A high-performance QM/MM program	QSite applies quantum mechanics to the reactive center of a protein active site and molecular mechanics to the rest of the system. Its accuracy allows detailed understanding of reactions involving proteins, making it a powerful tool for lead optimization.
Jaguar : Rapid ab initio electronic structure package	Jaguar is a high-performance ab initio package for both gas and solution phase simulations, with particular strength in treating metal containing systems, making it the most practical quantum mechanical tool for solving real-world problems.
BioLuminate: *Providing a comprehensive modeling solution for biologic***s**	BioLuminate is a brand-new, intuitive user interface that is specifically designed for examining biologics and protein systems with seamless access to superior scientific modeling algorithms.

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PIPER: *A state of the art protein-protein docking program*	PIPER is a state-of-the-art protein-protein docking program based on a multi-staged approach and advanced numerical methods that reliably generates accurate structures of protein-protein complexes.
OPLS3: *A revolutionary advance in modern force fields.*	OPLS3 is the culmination of a significant, large-scale effort to create the most accurate force field with the most comprehensive coverage of chemical space.
Desmond: *High-performance molecular dynamics simulations.*	Desmond's combined speed and accuracy make possible long time scale molecular dynamics simulations, allowing users to examine events of great biological and pharmaceutical importance. Seamlessly integrated with Maestro, Desmond provides comprehensive setup, simulation, and analysis tools.
Membrane Permeability: *Physics-based, accurate predictions of passive membrane permeability.*	The Prime physics-based membrane predictor combines conformational sampling with Schrödinger's advanced force field and solvent models within a physics-based framework to produce more accurate predictions of passive membrane permeability.
PrimeX: *A comprehensive package for accurate protein crystal structure refinement*	PrimeX uses state-of-the-art technologies to refine protein crystal structures for computational drug discovery.
Seurat	Seurat streamlines data access and analysis from a broad mixture of in-house and in□licensed databases, reports, literature, and computational results.
P450 Site of Metabolism	P450 Site of Metabolism workflow combines induced-fit docking (IFD) for the determination of accessibility of small molecules to the reactive center of p450 for metabolism.
Essential Products (All the following Modules comes free if you buy any single premium product)	
Maestro 11 GUI: *The completely reimagined all-purpose molecular modeling environment*	LigPrep goes far beyond simple 2D to 3D structure conversions by including tautomeric, stereochemical, and ionization variations, as well as energy minimization and flexible filters to generate fully customized ligand libraries for further computational analyses.
LigPrep: Versatile generation of accurate 3D molecular models.	LigPrep goes far beyond simple 2D to 3D structure conversions by including tautomeric, stereochemical, and ionization variations, as well as energy minimization and flexible filters to generate fully customized ligand libraries for further computational analyses.
Protein Preparation Wizard: *An easy-to-use tool for correcting common structural problems and creating reliable, all-atom protein models.*	Protein Preparation Wizard is designed to help researchers ensure structural correctness at the outset of a project, equipping them with a high-confidence structure ideal for use with a wide variety of modeling applications.
MacroModel: *Versatile, full-featured program for molecular modeling.*	MacroModel combines leading force fields, accurate effective solvation models, and advanced conformational searching methods to provide the most complete molecular modeling package suitable for a wide array of research.

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QikProp : Rapid ADME predictions of drug candidates	QikProp efficiently evaluates pharmaceutically relevant properties for over half a million compounds per hour, making it an indispensable lead generation and lead optimization tool.
Strike	Powerful software for statistical modeling and 2D- QSAR
Epik: Rapid and robust pKa predictions	Combining the proven reliability of Hammett and Taft methods with powerful tautomerization tools, Epik is the program of choice for accurate enumeration of ligand protonation states in biological conditions.
SiteMap: Fast, accurate, and practical binding site identification	Combining a novel algorithm for rapid binding site identification and evaluation with easy-to-use property visualization tools, SiteMap provides researchers with an efficient means to find and better exploit the characteristics of ligand binding sites.
ConfGen: Accurate and efficient bioactive conformational searching	Reproducing bioactive ligand geometries in minimally sized conformer sets, accurate results from high-performance ConfGen calculations save time and effort in downstream applications.
KNIME extensions	A modular, highly configurable framework for easy workflow automation and data analysis
Solutions and Work-Flows	
Induced fit docking: *A novel method for fast and accurate prediction of ligand induced conformational changes in receptor active sites*	A novel method for fast and accurate prediction of ligand induced conformational changes in receptor active sites. ***Require Prime and Glide license***
QPLD: *A novel research solution that combines the power of Glide with the accuracy of QSite.*	The first such algorithm of its kind, QM-Polarized Ligand Docking uses ab initio methodology to calculate ligand charges within the protein environment. Innovative and practical, QM-Polarized Ligand Docking offers substantially enhanced accuracy over pure MM docking algorithms. ***Require Glide and QSite license***
E-Pharmacopore: *Energetically optimized structure-based pharmacophores*	A novel approach for generating structure-based pharmacophores that unites the speed of pharmacophore screening with the energetic binding terms from Glide XP. (***Require Glide and Phase license)***
CovDock: *An all-in-one workflow for pose prediction and scoring of covalently bound ligands*	Combining the power and accuracy of Glide with the advanced protein refinement capabilities of Prime, CovDock provides an all-in-one workflow for accurate prediction and scoring of covalently bound ligands. ***Require Prime and Glide license***
Advanced Work-Flows	
FEP+ :*High-performance free energy calculations for drug discovery.*	FEP+ combines an exceptionally accurate force field (OPLS3) with improved sampling algorithms that exploit the high performance of GPUs to deliver binding free energies with unprecedented accuracy, providing

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	significant value to structure-enabled drug discovery projects. Note :(GPU cards are mandatory for FEP+ please get in touch with us for hardware requirements)
WaterMap: A new paradigm in ligand optimization	WaterMap offers a new paradigm for designing optimal ligands based upon their ability to differentially displace and retain specific water molecules in protein binding sites.
PLDB: *An active knowledge base of structural data and protein-ligand interactions*	PLDB is an active structural data store that can be pipelined in any custom workflow, while flexibly allowing searches using advanced structure motifs and protein-ligand interaction patterns.

+

The price depends upon the number of premium products and the number of years etc. The base price starts with $ 100,000 for 1 premium product with all essential products. **If you are an academic Institute you will get 95% discount from the commercial price and your base price starts with just $ 6,000 for 1 premium product and all essential products comes free.**

If you wish to add any additional premium software the price would increase by $ 1,500 for every software.

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Schrödinger, Inc
101 SW Main Street, Suite 1300
Portland, OR 97204
Phone: +1 503 299-1150
Fax: +1 503 299-4532

Price Quotation: 59423
Date: 10-July-2022
Offer Expires: 31-August-2022
Payment Terms: Upon Receipt

Licensee: The Director, All India Institute of Ayurveda
Sarita Vihar, New Delhi
Dr.Prashant Gupta
assoprof-kb@govcontractor.in

Account Manager: Shelvia Malik
Phone: +91 9900090082
shelvia.malik@schrodinger.com

Quantity	Item	Term	Amount
26	Tokens for interchangeable library including ConfGen, Epik, Glide, Impact, Jaguar, LigPrep, MacroModel, Prime, QikProp, SiteMap	3 years from date of delivery	
1	Desmond GPU Floating License	3 years from date of delivery	
1	OPLS Access License	3 years from date of delivery	
	Subtotal		31,500.00
1	Maestro Access License	3 years from date of delivery	0.00
1	KNIME Access License	3 years from date of delivery	0.00
	Special Discount		-1,575.00
	Total		**USD 29,925.00**

- An on-site training and workshop once the purchase is done. The technical and scientific support will be provided for the entire duration of license term (three years).
- Software shall be installed solely on machines located at Licensee's facilities in All India Institute of Ayurveda, Delhi Mathura Rd, Gautam Puri, Sarita Vihar, New Delhi, Delhi 110076 or installed solely on Licensee's cloud accounts.
- Software shall be used solely by Licensee's End Users affiliated with Licensee's facilities in All India Institute of Ayurveda, Delhi Mathura Rd, Gautam Puri, Sarita Vihar, New Delhi, Delhi 110076.
- To accept this Price Quotation, please e-mail or fax a Purchase Order to your Account Manager no later than the expiration date above. For details on payment methods and order processing, please see schrodinger.com/salespolicies.
- **Please include our Price Quotation number (59423) on your Purchase Order.**
- Payment Methods: Bank Wire Transfer or Demand Draft.
- Payment information for wire transfer:

  Bank: US Bank, 555 SW Oak Street, Suite 400 Portland, OR 97204
  Account name: Schrodinger, Inc.
  Account number: 153695189131
  Bank routing number: 123000220
  SWIFT Code: USBKUS44IMT
- Payment Information for Demand Draft:

  US$ Demand Draft in the name of Schrodinger, Inc., payable to Portland, OR, USA
  Send Demand Draft to: 101 SW Main Street, Suite 1300, Portland, OR 97204 USA
- Licensee's use of the Software above is governed by the terms and conditions of the Schrödinger End User License Agreement available online at schrodinger.com/EULA and which is incorporated by reference (the 'Agreement').

- This Price Quotation, together with the Statement of Work ("SOW") (if any), and the Agreement, constitutes the entire agreement between the parties and supersedes all prior agreements, whether written or oral, concerning its subject matter. In the event of any inconsistency among this Price Quotation, the SOW (if any), and the Agreement, the controlling provisions shall be determined by reference to the following order: (i) SOW (if any), (ii) Price Quotation and (iii) Agreement.
- Pre-printed terms of any Purchase Order or similar document that is provided by Licensee to Schrödinger will have no effect and Schrödinger does not agree to any of its terms.
- PAN# ABCCS3216L

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To whom it may concern

Proprietary certificate

This is to certify that Schrödinger, Inc. is the sole manufacturer and distributor of the following molecular modeling software products in India:

AutoQSAR, AutoTS, AxPyMOL, BioLuminate, Canvas, ConfGen, CoreHopping, Covalent Docking, e-Pharmacophore, Epik, FEP+, FFBuilder, Field-based QSAR, GA Optoelectronics, Glide, Glide XP Visualizer, Impact, Induced Fit Docking, Jaguar, Jaguar pKa, KNIME, LigPrep, LiveDesign, MacroModel, Maestro, MCPRO+, Membrane Permeability, MS CG, MS Combi, MS Jaguar, MS Maestro, MS Transfusion, OPLS, OPLSe, PSOM 450, Phase, Prime, PrimeX, PLDB, Protein Preparation Wizard, PyMOL, QikProp, QSite, QM Polarized Ligand Docking, Quantum Espresso Interface, R Group Analysis, Seurat, Shape Screening, SiteMap, Strike, Virtual Screening Work Flow, and WaterMap.

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

Regards,

Cony R. D'Cruz
Executive Vice President and Chief Business Officer
Schrödinger, Inc.

अखिल भारतीय आयुर्वेद संस्थान
ALL INDIA INSTITUTE OF AYURVEDA (AIIA)

(आयुष मन्त्रालय, भारत सरकार के अन्तर्गत स्वायत्त संस्थान)
(An Autonomous Organization under the Ministry of AYUSH, Govt. of India)

Subject: Schrodinger software for AyuInformatics Lab, Dept. of KB,AIIA

As per direction of the competent authority, AIIA regarding establishment of Ayuinformatics lab, the requirement and technical specifications of Required Schrodinger software was assessed by departmental committee consisting of following members: -

1. Dr. Rajagopala S, Head, Dept of KB, AIIA (Chairman)
2. Dr. Prashant Gupta, Associate Professor, Dept of KB, AIIA (Member)
3. Dr. Mahapatra Arun Kumar, Assistant Professor, Dept. of KB, AIIA (Member)

The committee observed that, Schrodinger computational platform evaluate compounds in silico, with experimental accuracy on properties such as binding affinity and solubility. As per AIIA requirement, Schrodinger computational platform is unique in term of its usefulness in molecular docking of metallic preparations which are used in Ayurvedic formulations. This feature is presently not available in any other Computational software. The computational results are accurate and widely used globally for conducting computational Research. The committee evaluated the following modules of software which were found to useful for Ayurveda Research :-

I. Docking tools like GLIDE and PRIME
II. Dynamics tools like DESMOND
III. Metalloorganic in-silico research through JAGUR module and other modules like LIGPREP, MAESTRO and KNIWE etc.

This, Committee recommends to proceed for submitting a requirement proposal of Schrodinger software for AyuInformatics Lab, Department of Kaumarabhritya, AIIA.

Dr. Rajagopala S

Dr. Prashant Gupta

Dr. Mahapatra Arun Kumar

Proprietary Article Certificate

(Rule 166 of GFR 2017)

1. The indented goods are manufactured by **M/s SCHRODINGER INC PORTLAND USA**
2. No other make or model is acceptable for the following reasons: -
   a. **Modules for molecular docking of metallic formulations is not available with any other available software**
   b. **Computational results obtained with Schrodinger software are worldwide accepted, interpretable and reliable.**
3. Concurrence of finance wing to the proposal vide: **AIIA eOffice File No: S-11/21/2021-AIIA dated 07.07.2022 (Note No. 85)**
4. Approval of the competent authority vide: **AIIA eOffice File No: S-11/21/2021-AIIA dated 07.07.2022 (Note No. 85)**

Signature with date and designation of the indenting officers

(DR PRASHANT K GUPTA)

(Dr. N. Ailin Lunn)

विभागाध्यक्ष कौमारभृत्य विभाग
Head, Dept. of Kaumarbhritya
अखिल भारतीय आयुर्वेद संस्थान
All India Institute of Ayurveda
(भारत सरकार, आयुष मंत्रालय)
(Govt. of India, Ministry of AYUSH)
गौतमपुरी, सरिता विहार / Gautampuri, Sarita Vihar,
नई दिल्ली-110076 / New Delhi-110076
(MON/TUE/WED/THU/FRI/SAT)

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Schrödinger

101 SW Main Street, Suite
1300
Portland, OR 97204

January 11, 2022

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: Canvas, Epik, Jaguar, Jaguar pKa, LigPrep, MacroModel, MS CG, MS Transport, QikProp, Quantum Espresso Interface, StrikeGlide, GlideXP Visualizer, Prime, Phase, PrimeX, MCPRO+, CombiGlide, QSite, Field-based QSAR, Bioluminate, Confgen, Epik, SiteMap, Impact, LigPrep, PyMOL, AxPyMOL, 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,

DocuSigned by:
B396FA8F9580436...

Jenny Herman

January 11, 2022

SVP Controller