UTKAL UNIVERSITY
NAAC ACCREDITED A+

CENTRE OF EXCELLENCE IN INTEGRATED OMICS AND COMPUTATIONAL BIOLOGY

(Supported by the Govt. of Odisha and WB-OHEPEE)

UTKAL UNIVERSITY, VANI VIHAR, BHUBANESWAR-751 004, ODISHA

ADDENDUM

To Notification No. UCoE/Tend/01/2022, Date: 18.02.2022

Sealed tenders are also invited for Software for Computational Analysis (Item no. 38).

Coordinator

CoE-IOCB

Co ordinator
COE-Integrated Omics
& Computational Biology,
Utkal University

Item no. 38

Software for Computational Analysis

Dated: ..... **Tender Form No: .....**

FORMAT

From:

M/S----------

To,
The Coordinator,
Centre of Excellence in Integrated Omics & Computational Biology,
Utkal University, Vani Vihar, Bhubaneswar-751 004

Sub: Procurement of Software for Computational Analysis for the financial year 2021-2022.

Ref. Advertisement (Name of the Newspaper) ....., Dated: .....
Amount: Rs.1,000.00 (Rupees one thousand) only (D.D. No....., Dated: .....
Bank.....

Sl. No.	Software for Computational Analysis	Unit Price + Tax FOR Destination
A	Computational Simulation Software Applications should provide - 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). Holds options for server floating based license policy. Compatible with windows, Linux and Mac operating systems. Fast, accurate, and practical binding mode identification at a given pH. Predict accurate protein structure prediction model where an experimental structure is unavailable, and with capability to refine experimental structures obtained through X-ray crystallography or NMR, providing an even more accurate and detailed starting point for subsequent simulations and computational analyses. Facility to study molecular dynamics of materials and life science systems motions at the molecular and atomistic level with full fledged qualitative and quantitative analysis outputs as pdfs, Images and data. Small molecule and Peptide virtual screening via multiple mode docking with OPLS force field Optimizations with Accurate favourable energy functions of Ligand for hydrophobic buried interaction and non-favourable energy functions for hydrophobically buried polar atoms and exposed hydrophobic atoms It should handle induced fit docking, Covalent docking, blind docking etc. Toxicity prediction by Lipinski rule of five, Herg channel blockage, membrane permeability, Solubility, permeability, CNS activity, blood brain barrier permeability, HERG K+ Channel activity, Cytochrome p450 site of metabolism and amphiphilic movement Capable of created custome Machine learning & Deep Learning models through automation, workflow options includes descriptor generation,	

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	feature selection, creation of a large number of QSAR models from several methods including kernel-based partial least squares, naive bayes, and ensemble-based recursive partitioning with different training/test set splits, and ranking of QSAR models by performance. Predictions capability of consensus of the best models or from a particular model. Software to execute Quantum mechanical code which proceeds much faster than conventional programs, its important solvent effects should be applying a self-consistent reaction field (SCRF), it should generate comprehensive array of molecular properties including NMR, IR, UV-vis, VCD, pKa, partial charges, multipole moments, polarizabilities, molecular orbitals, electron density, electrostatic potential, Fukui functions, Mulliken population, and NBO analysis. Potential energy surface to maps reaction coordinates between reactants, products, and transition states together with potential energy surfaces. Generates Energetics based pharmacophore generation from protein ligand complex and from Apo Protein or from multiple or single ligands. Single Lead optimization interface to do molecule optimization considering key pharmacophore, residue interactions, extending cavity space and water thermodynamics. The software should come with free updates, onsite training and support.	

Dated: .....

Signature of the
Manufacturer / Authorized Dealer
Seal

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