Attachment no 1 Technical Specification

Name:	Software for molecular designing
Term of license:	12 months
Number of licences:	1

Technical Specification

The integrated software package and at least the following instruments:

1. The instrument for binding pocket detection. It should visualize the molecular surfaces, electron density, and interactions. It should be able to create and export images and videos.
2. The instrument for structure-based design. It should have functions for interactive ligand modification in the pocket, creating protein-ligand interaction diagrams, predicting water sites, induced-fit docking, linking, growing, and replacing the fragments.
3. The instrument for SAR exploration should have the following functions: 1) SPR visualization 2) Free-Wilson analysis 3) MMP3) R-Group analysis. The instrument should also provide a substructure and similarity search.
4. The instrument for ligand-based drug discovery should generate conformations for small molecules, align and superpose small molecules. The instrument should have functions for pharmacophore screening, QSAR analysis, combinatorial library enumeration.
5. The instrument for protein modeling should contain functions for visualizing proteins and interfaces, prediction of 3D structure from sequence, and protein-protein docking.
6. The instrument for fragment-based discovery should have functions for 3D pharmacophore screening, small molecule docking, 2D and 3D fingerprint screening, scaffold, and fragment replacement.
7. The instrument for structural bioinformatics should contain functions for multiple sequences and structure alignment, creating and searching protein family databases, analyzing conserved residues, and generating clustered phylogenetic trees.
8. The instrument for molecular simulation should be able to perform for molecular dynamics simulations (including structure preparation). It
9. should have functions for free energy calculations, flexible alignment of multiple molecules, torsion scan, and analysis.
10. The instrument for peptide modeling should have functions for modeling macrocyclic and linear peptides, identification of peptide-protein contacts, conformational searching, enumeration of non–natural peptide libraries, and peptide docking.
11. The instrument for structural biology should have functions for plotting electron densities, displaying crystal lattices and contacts, prediction of water positions, electron density-guided docking, creating aligned protein family databases, and homology modeling.
12. The instrument for chemoinformatics should have functions for a generation of at least 300 2D and 3D molecular descriptors, pKa prediction, linear QSAR/QSPR, bayesian classification chemical similarity, diversity, and clustering.