Attachment no 1 Technical Specification

Name:	Software for drug designing process
Term of license:	12 months
Number of licences:	1
Technical Specification	

Integrated software package with the remote access possibility and following instruments:

1. The system should have the ability to calculate and visualize ΔG using at least two forces: desolvation and H-Bond interactions

2. The system for **s**caffold hopping should have at least the following functions, replacing the central part of the ligand and generating suitable 3D replacement.

3. The system should provide pharmacophore constraints (3D) and be able to use the fragments from PDB or ZINC database.

4. System for the hit optimization should be able to provide growing the fragments inside the binding pocket and linking fragments in 3D.

5. Visual torsions system provides a statistical assessment of the likelihood of dihedrals.

6. System for pocket detection should be able to detect the binding pocket, assess the quality of binding pocket and visualize it.

7. A Molecular docking system should be able to perform a docking (places a ligand into a binding site), including a template-based docking, by determining the Maximum Common Substructure (MCS) or similar scoring.