Annex No. 1. – The object of purchase specification

1) Integrated software platform for chemical informatics

The required product is a software platform that would facilitate close collaboration between computational and pharmacological chemists. To that end, we need an integrated solution that would allow us to import, sanitize, visualize (both 2D and 3D) and manipulate small molecules, as well as large biomacromolecules. The platform should be able to compute 3D structures of the small molecules, and to detect and visualize potential binding regions within the biomacromolecules. The platform should also allow us to perform standard virtual screening-related techniques without the need for third-party products: conformer calculation, docking, pharmacophore and scaffold analysis, etc. Additional needs of note are some form of a license server or other such licensing scheme that would allow for off-site work, good overall performance and support for distributed computing.

Characteristic of the software – the software must	**Desirable value YES/NO**
• **allow for construction of customized workflows**. A single self-contained unified interface is needed for quick prototyping and evaluating of custom workflows. Within this unified interface all standard procedures and techniques must be accessible via a flexible domain-specific programming language.	XXX
• **allow for import, sanitization, visualization, manipulation and export of both 2D and 3D structures.** The necessities are: o The import and export functionality needed to interface the software with the rest of our workflow. The functionality has to include the current standard file formats for small molecules and biomolecules (SMILES, InChI, FASTA, PDB, mol2, etc.) o The visualization of 2D and 3D chemical structures of both small molecules and biomacromolecules o 3D structure calculation for both small molecules and biomolecules, including automated detection of potential binding regions (hydrophilic cavities, etc.) o Structure manipulation functionality necessary for workflow preparation and continual monitoring and adjustment (solvent removal, manual structure correction, protonation, etc.)	XXX
• **contain advanced chemical informatics functionality.** To reduce the workflow complexity and dependence on other software, the requested software must have the following functionality: o Structure based design and scaffold replacement o Fragment based design and pharmacophore discovery o Ligand based virtual screening o Molecular descriptors and QSAR modelling o Molecular dynamics and docking	XXX

• **be able to interface with external databases and software well.** To best integrate with the in-house software and infrastructure, the requested software should be able to interface with external database servers (preferably SQL-based) and with web servers over some of the standard web services.	XXX
• **be able to handle large datasets well.** The early phases of our workflows often involve extensive virtual chemical libraries of hundreds of millions of small molecules. The software should be able to access and process such datasets directly.	XXX
• **support basic web-based services.** Browser-based access to the basic software features, especially the visualization-related ones, is ideal for project collaborators who do not require the full software feature set that comes with local installation.	XXX
• **support remote work.** Due to the distance between NUDZ and UCT, where expertise related to this software is housed, remote access needs to be supported to allow for smooth cooperation. This form of access should also be allowed by the software license.	XXX
• **be multiplatform.** The software is intended to be deployed on a multitude of machines with various operating systems. Therefore, it has to be compatible with Windows (7, 8, 10) and Linux (Debian- and RHEL-based) operating systems.	XXX

Offer price in EUR excluding VAT	**XXXXXXXXX**
VAT	**XXXXXXXXX**
Offer price in EUR including VAT	**XXXXXXXXX**