Annex No. 1. – The object of purchase specification

1) Computer aided drug design (CADD) software suite

The required product is a full-featured Computer-Aided Drug Design (CADD) suite to complement our toolset for psychopharmacological research. The intended use cases for the suite include, among others, QSAR, docking and pharmacophore modelling. In addition, extensive customizability is required in order to chain the individual methods into a cohesive workflow that can be easily integrated into our current cheminformatic infrastructure. The suite should also allow for off-site work and for distributed computing.

Characteristic of the software – the software must	Desirable value YES/NO
• **include a complete pipeline of the standard Computer-Aided Drug Design (CADD) and the related Molecular Modelling procedures.** Several parallel approaches will be used in the design and modelling of new ligands for this project, so all the standard procedures and techniques must be available. The required functionality consists of at least: molecular mechanics, quantum mechanics (including DFT) and mixed QM/MM calculations, homology and pharmacophore modelling, (3D)-QSAR, and a full-featured molecular docking toolkit: tools for conformation search, scoring, quantitative assessment, etc.	XXX
• **be easily customizable for advanced applications.** Extensive customization is a must so the maximum potential of the modelling software can be achieved and so it can be used in workflows involving our own in-house developed software. Because the majority of the in-house software is developed in the Python programming language, the software should be able to expose its functionality through a Python application programming interface (API).	XXX
• **have state-of-the-art performance in the native modules for computationally intensive tasks (docking, pharmacophore modelling, molecular dynamics, etc.).** Because the calculations will result in predictions that decide which chemical and biological steps to prioritize, a subpar tool performance will result in a significant time loss or low-precision results. For particularly computationally intensive tasks, GPU computation support is preferred.	XXX
• **support remote execution of internal computational tasks on a remote machine or cluster.** To perform the intended computationally intensive tasks, the use of remote dedicated machines will be necessary. The software must allow us to leverage our off-site computational resources, such as those of the Czech national grid infrastructure and our own remote servers.	XXX
• **must 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. The software license must also permit the use of this functionality.	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 operating systems (Ubuntu and RHEL).	XXX

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