Quantum computer assisted drug design

Project Description

ABSTRACT A key target protein to develop drugs, diagnostics and vaccines against SARS-CoV-2 is spike, a trimeric glycoprotein that decorates the surface of the virus and promotes the fusion of the viral and host membranes after binding the angiotensin converting enzyme 2 from the host cells. In silico virtual screening approaches represent a first fundamental step for drug discovery, however they are extremely computationally demanding. In this proposal we aim at a step change in drug discovery in silico by developing quantum computation algorithms with unprecedented efficiency. We will apply these approaches to target the activation mechanism of spike and trap it in an inactive state.

IMPORTANCE
A novel betacoronavirus, SARS-CoV-2, was identified in early December 2019, causing a global pandemic in 2020. A detailed molecular understanding of SARS-CoV-2 infection is necessary to identify effective drugs to stop the pandemic. Early phase drug discovery approaches resort to in silico virtual screening (VS): computer simulations that enable the identification of potential candidate molecules from large databases. One of the key steps in VS is measuring similarity between molecules. The most widely used methods employ molecular fingerprints to encode structural information (e.g. Extended Connectivity Fingerprinting method). These methods are computationally inexpensive; however, they do not consider all the relevant aspects of the molecular structure and lead to a high failure rate of potential drug candidates. To improve the drug discovery in silico, it is necessary to develop novel accurate methods of VS that properly describe the three-dimensional structure of the molecule and of its pharmacophore features. State of the art approaches are based on graph matching algorithms. Graphs encode any molecular information perceived as relevant. Each molecule is modelled in terms of graphs and graph similarity methods are exploited to identify candidate molecules within large databases.

GOAL
We propose to transform the key step of VS using quantum computers (QC). Graph similarity problems fall in the class of NP-hard problems with an exponential time required to solve the number of entries. Quantum superposition and quantum entanglement cooperate in QC exploiting massively quantum parallelism and allow solving certain classes of computationally hard problems in ultra-fast and accurate manner. Besides the very celebrated quantum search, quantum factoring and the other pioneering quantum algorithms , nowadays experimental proofs of quantum speedup have been observed on real quantum hardware such as, for instance, the efficient molecular variational eigensolver by IBM and the quantum supremacy experiment by Google. We will develop new protocols specifically designed to run on currently available quantum hardware, capable of exploiting the quantum speedup, allowing for large scale screening of molecular databases in less than exponential time. QC will give a boost to this critical step of drug designing with respect to all other possible classical approaches.

PROSPECTIVE STUDENTS

Possible candidates are expected to have a background in computational chemistry/biology (e.g. molecular dynamics) and basic knowledge of quantum mechanics.

Supervisor(s), Lab/Group details, other additional info.

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