Drug Design on Quantum Computing

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Abstract

Computer aided drug design is a field that requires large computation resources, so it's easy to think of letting quantum computers play a role in it. We simulate the complexes of BACE-1 and its inhibitors, which are enzymes related to Alzheimer's disease, to see if our results gotten from quantum computer are closer to the experimental data, comparing with the one gotten from classical calculations. Meanwhile, density functional theory(DFT) based on wavelet basis is proven a fast and accurate method for calculating the value of molecular properties. In our research, we feature DFT based on wavelet basis to generate Hamiltonian, then we use that Hamiltonian to run a variational quantum eigensolver(VQE).