# Designing peptides on a quantum computer

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We investigated the use of quantum hardware as a potential alternative for solving conformational search problems in protein design. We developed an algorithm, the qPacker, to frame the side-chain rotamer search as a constrained binary optimization problem and solve it on two types of quantum devices: quantum annealers (e.g. D-Wave), and gate-based quantum computers (e.g. Rigetti). The qPacker algorithm was successful in finding low energy solutions for side-chain conformational optimization problems of varying sizes, and in many cases yielding results superior to Rosetta's Monte Carlo/simulated annealing methods. These promising results foreshadow an exciting new route for emerging quantum computing technologies in synthetic biology and biochemistry with a wide range of applications in the pharmaceutical and chemical industries.

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