ProteinQure empowers protein drug discovery teams through the use of cutting-edge computational methods. We create novel therapeutics for challenging drug targets such as GPCRs. We achieve this by combining state-of-the-art structure-based algorithms, including molecular dynamics simulations and machine learning. Our design platform allows us to explore vast regions of sequence space and predict functional properties of therapeutics to rapidly deliver new insights to our partners in pharmaceutical R&D.

Protein Folding / Structure Determination

ProteinQure can obtain structures for protein therapeutics and drug targets (up to ~100 amino acids). Our integrative models can use external data (sequence, structure, and functional measurements) to increase the speed and accuracy of our predictions. This approach has shown strong agreement to experimental structures in blind protein folding challenges (CASP).

ProteinQure is applying these methods to develop a novel class of peptide-mimetic polymers with SRI International. These molecules have shown high binding affinity to well-established drug targets involved in cell signalling (cytokines, nucleotide-binding proteins). By modelling the combinatorial space containing non-natural amino acids, we support rational drug design and optimization of these peptides for stability and binding affinity.

Protein Drug Discovery and Optimization

We specialize in the design of novel protein scaffolds and libraries suitable for modern protein engineering display technologies. Combining high-accuracy biophysical models (homology, simulation) and high-throughput sequence search (machine learning), we have generated massive libraries of protein binders enriched for desired structural and functional characteristics (sequence diversity of $10^7-10^{10}$).

Upon identifying hits, we provide computational models of protein-protein interactions suitable for optimizing affinity and selectivity. We have validated structural properties for novel protein scaffolds through CROs. Our computationally-designed libraries enable high-throughput hit identification across a broad range of targets, and we’re working with an undisclosed industry partner on a large-scale validation of these methods.

Quantum Computing for Drug Discovery

We are world-leaders in quantum computing algorithms for structural biology. Our biomolecular models can integrate outputs from quantum computers to accelerate CPU or GPU-based methods routinely used in structure-based drug discovery, such as molecular similarity and conformational search.

We have published three quantum computing algorithms in the areas of protein folding and molecular docking, with results that match the accuracy of classical solvers. Within 2-3 years, our algorithms will scale with hardware improvements to enable the design of larger proteins modalities outside the reach of modern supercomputers. We have partnerships with Microsoft, D-Wave, IBM, Rigetti, Xanadu and Fujitsu.