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(54) **Title:** PREDICTING JOINT THREE-DIMENSIONAL (3D) STRUCTURES OF PROTEINS AND LIGANDS BY COFOLDING

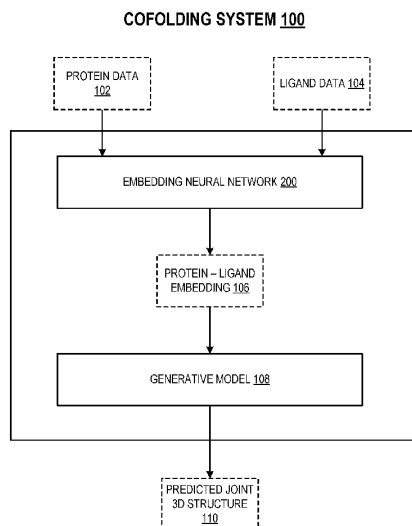


FIG. 1

(57) **Abstract:** Methods, systems, and apparatus, including computer programs encoded on a computer storage medium, for generating a predicted joint 3D structure of a protein and one or more ligands. In one aspect, a method comprises: obtaining a network input that characterizes the protein and the one or more ligands; processing the network input using an embedding neural network to generate a protein - ligand embedding of the protein and the one or more ligands; and generating, using a generative model and while the generative model is conditioned on the protein - ligand embedding, the predicted joint three-dimensional (3D) structure of the protein and the one or more ligands.

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