

COFOLDING SYSTEM 100

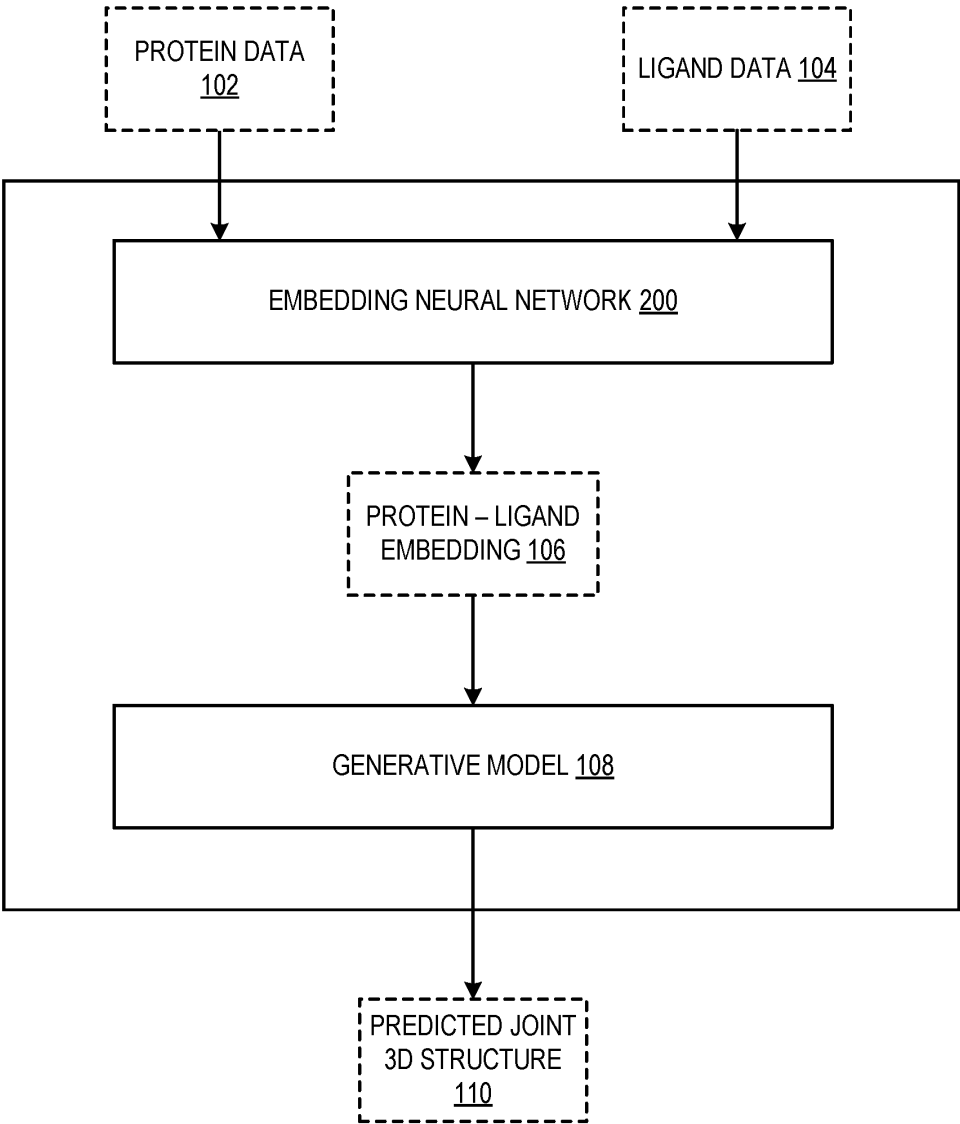


FIG. 1

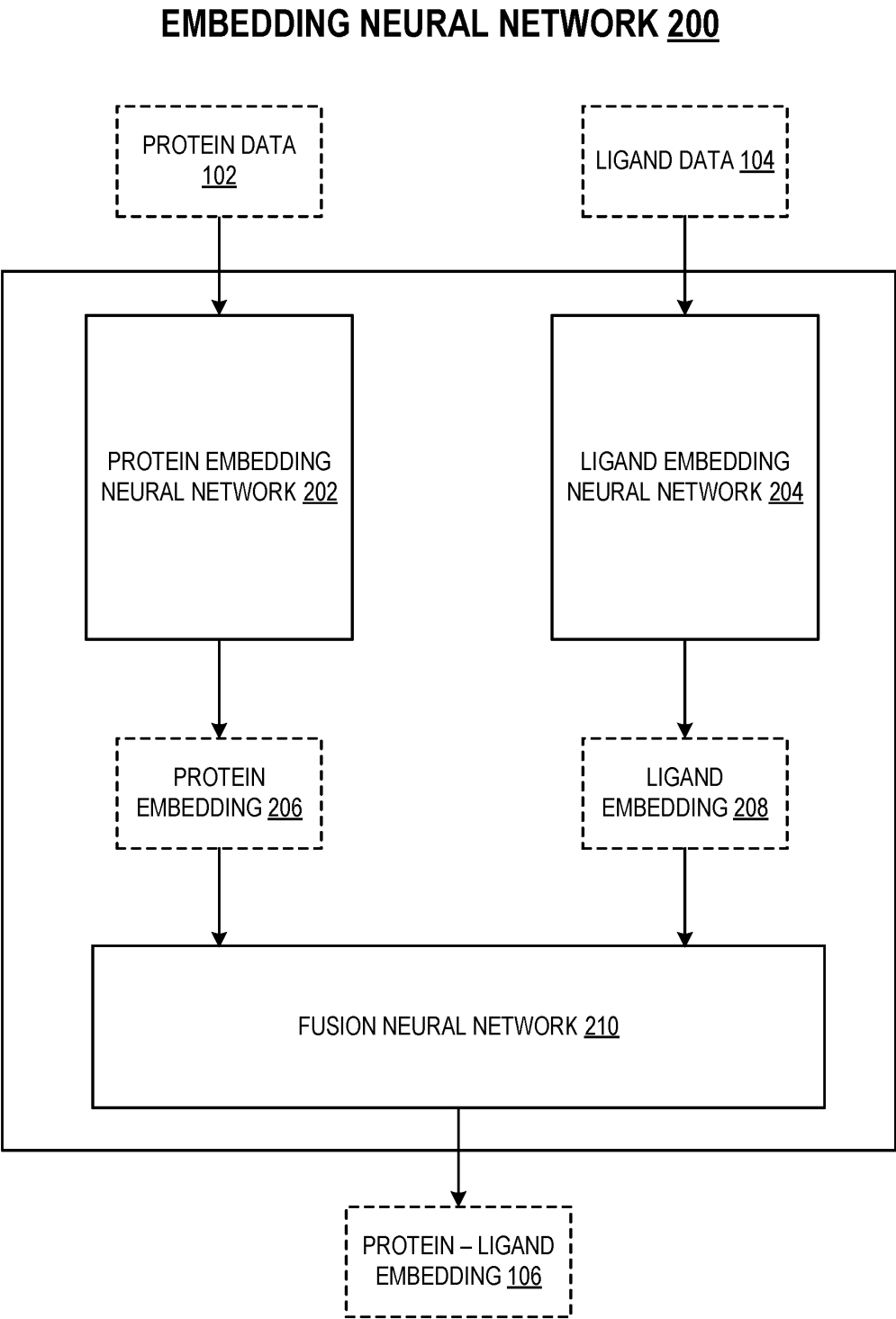


FIG. 2

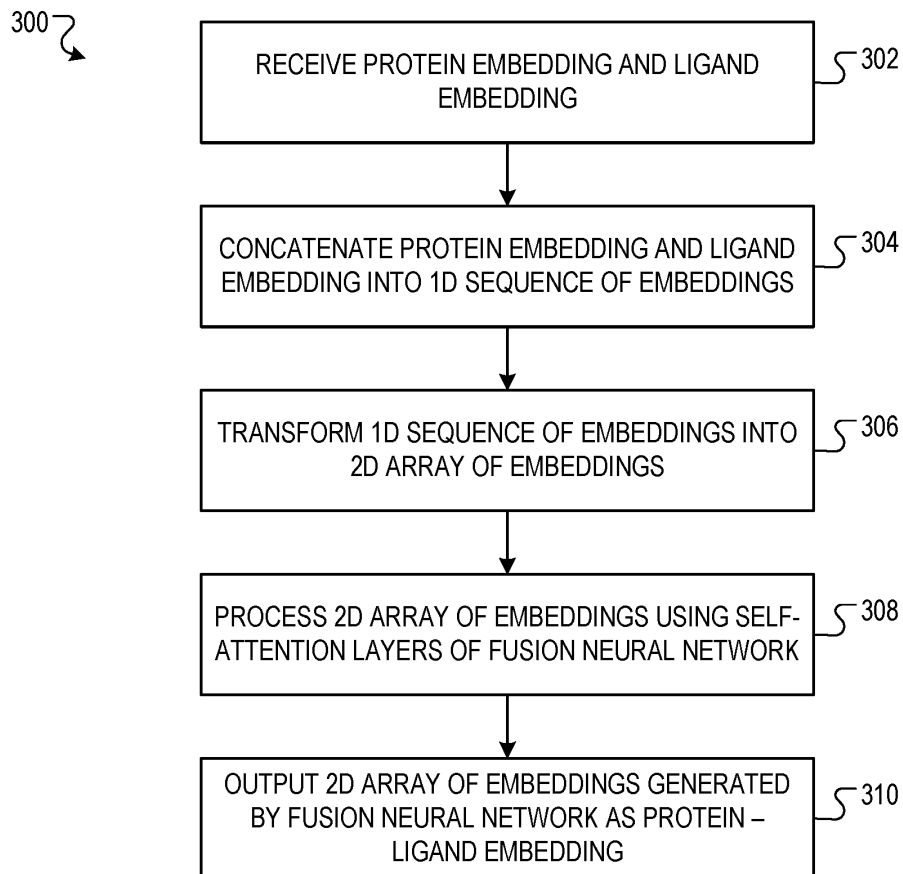
GENERATING JOINT EMBEDDING OF PROTEIN AND LIGAND(S)

FIG. 3A

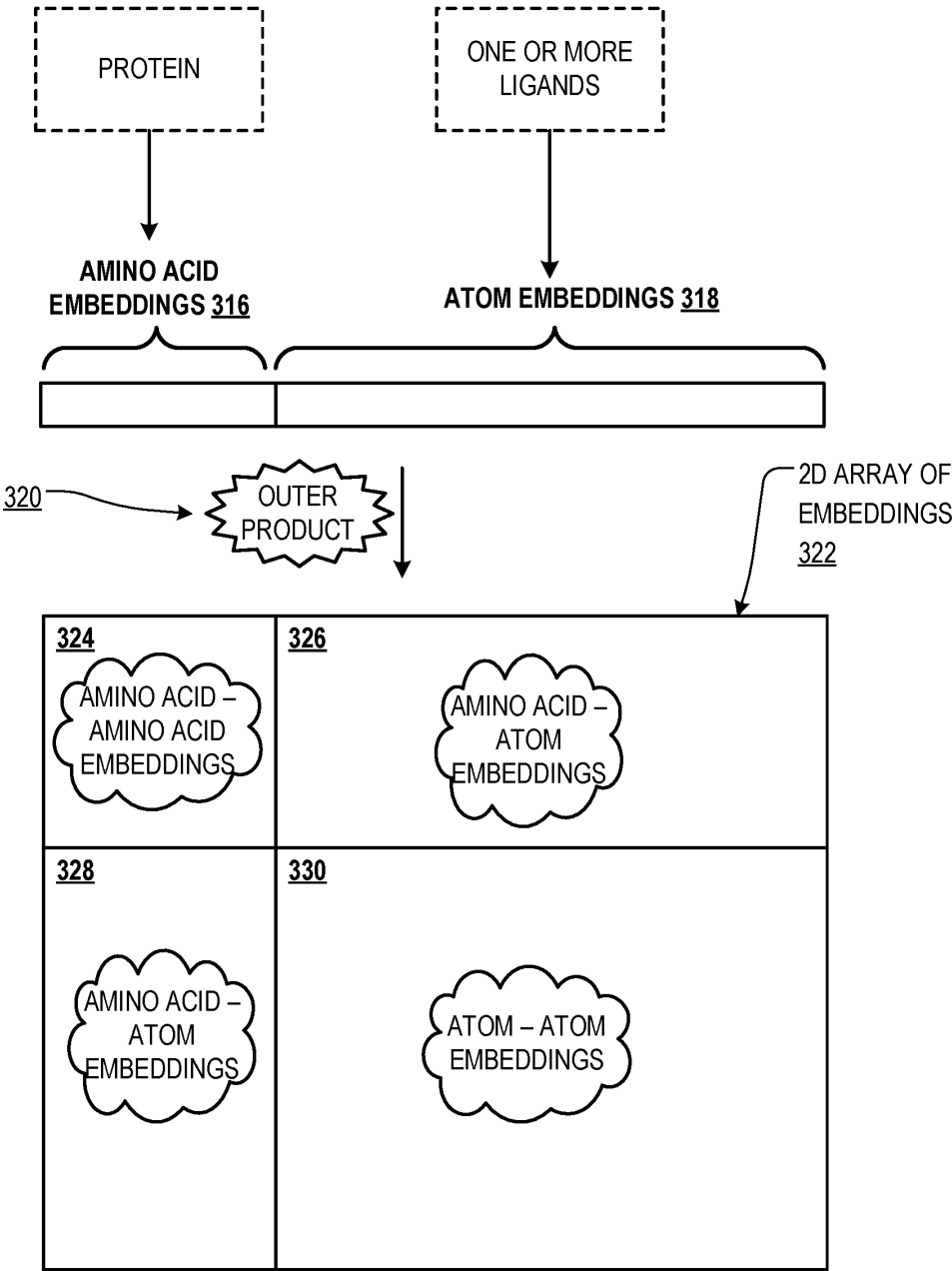


FIG. 3B

OPERATIONS OF A GENERATIVE DIFFUSION MODEL
CONDITIONED ON A PROTEIN – LIGAND EMBEDDING

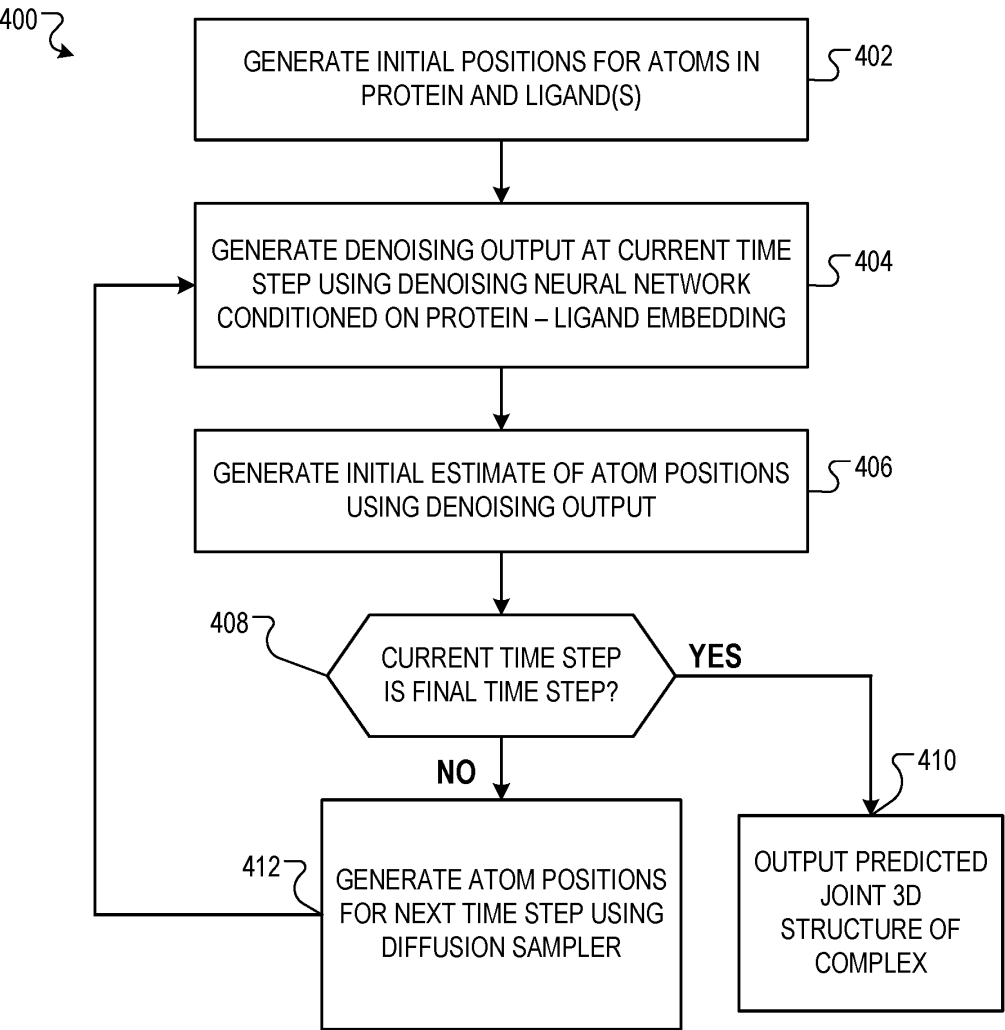


FIG. 4

GENERATING DENOISING OUTPUT USING DENOISING NEURAL NETWORK

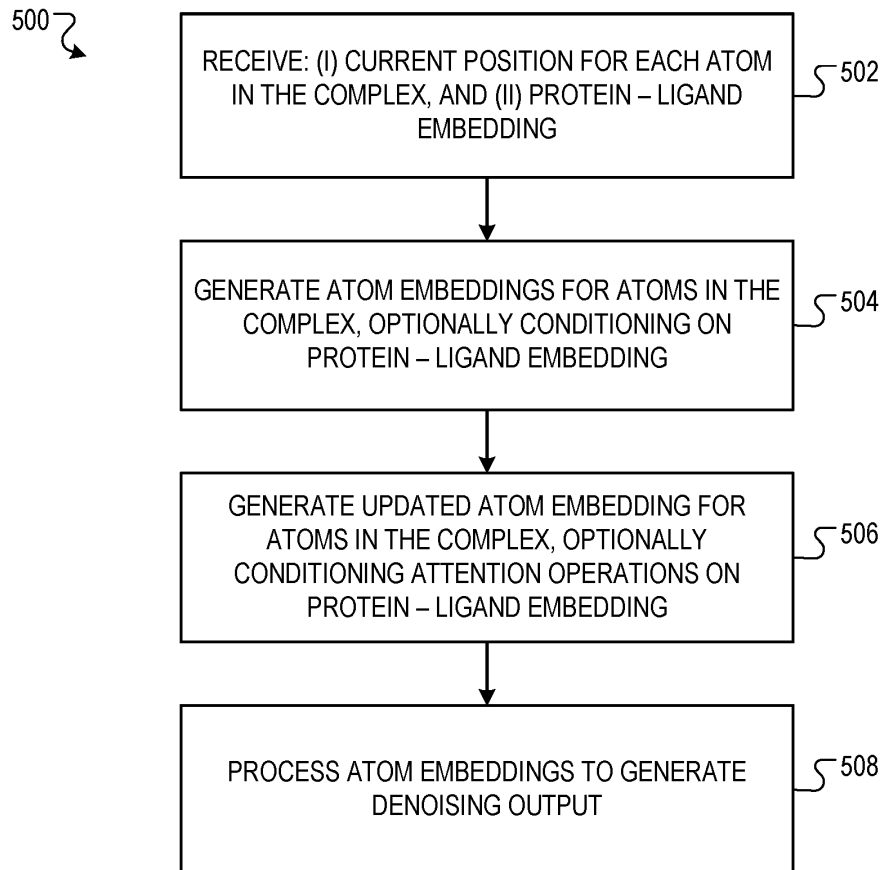


FIG. 5

CONDITIONING A SELF-ATTENTION OPERATION ON A PROTEIN – LIGAND EMBEDDING

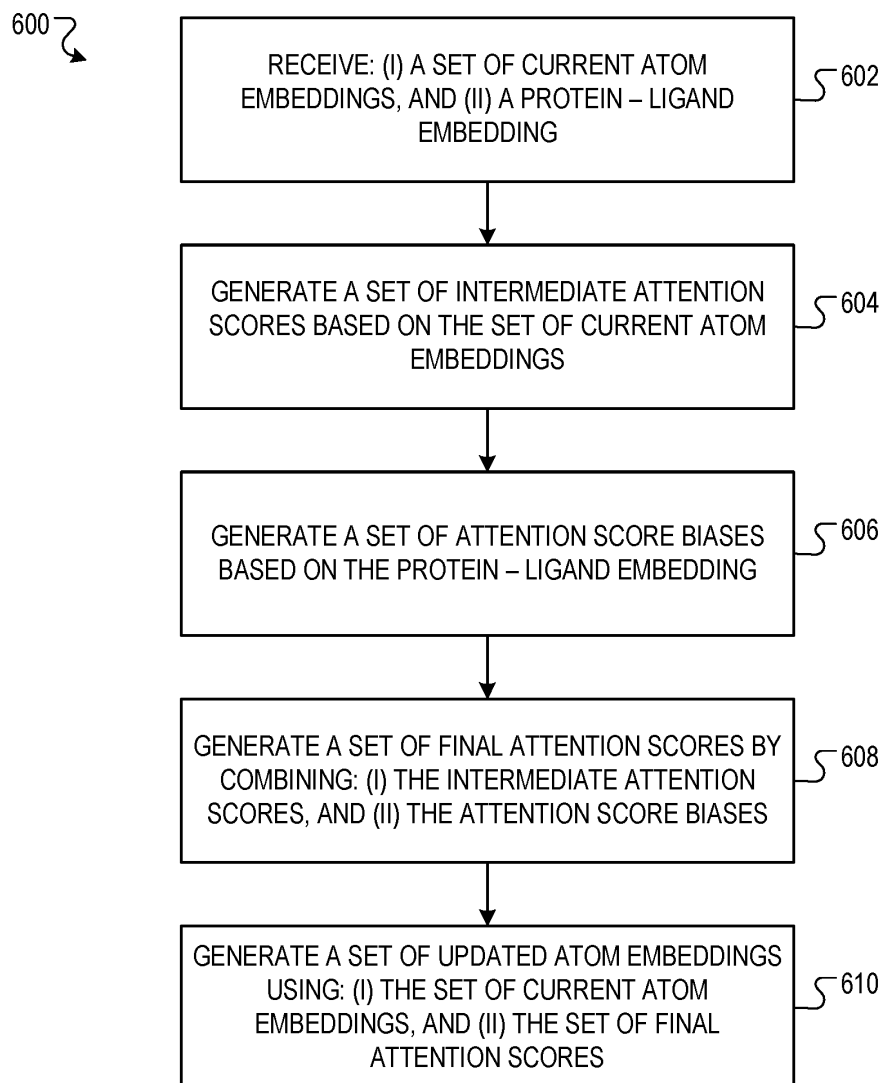


FIG. 6

TRAINING THE EMBEDDING NEURAL NETWORK AND THE GENERATIVE MODEL

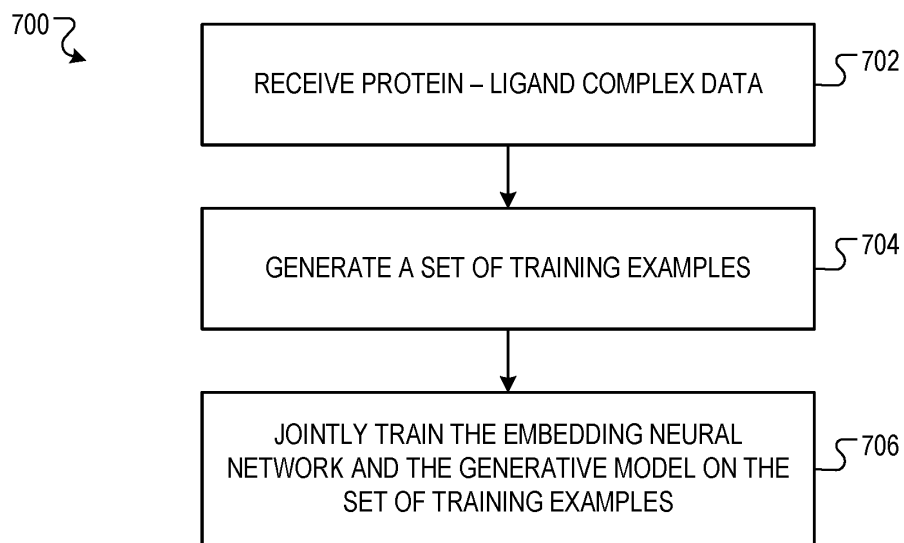


FIG. 7

JOINT TRAINING EMBEDDING NEURAL NETWORK AND GENERATIVE DIFFUSION MODEL ON TRAINING EXAMPLE

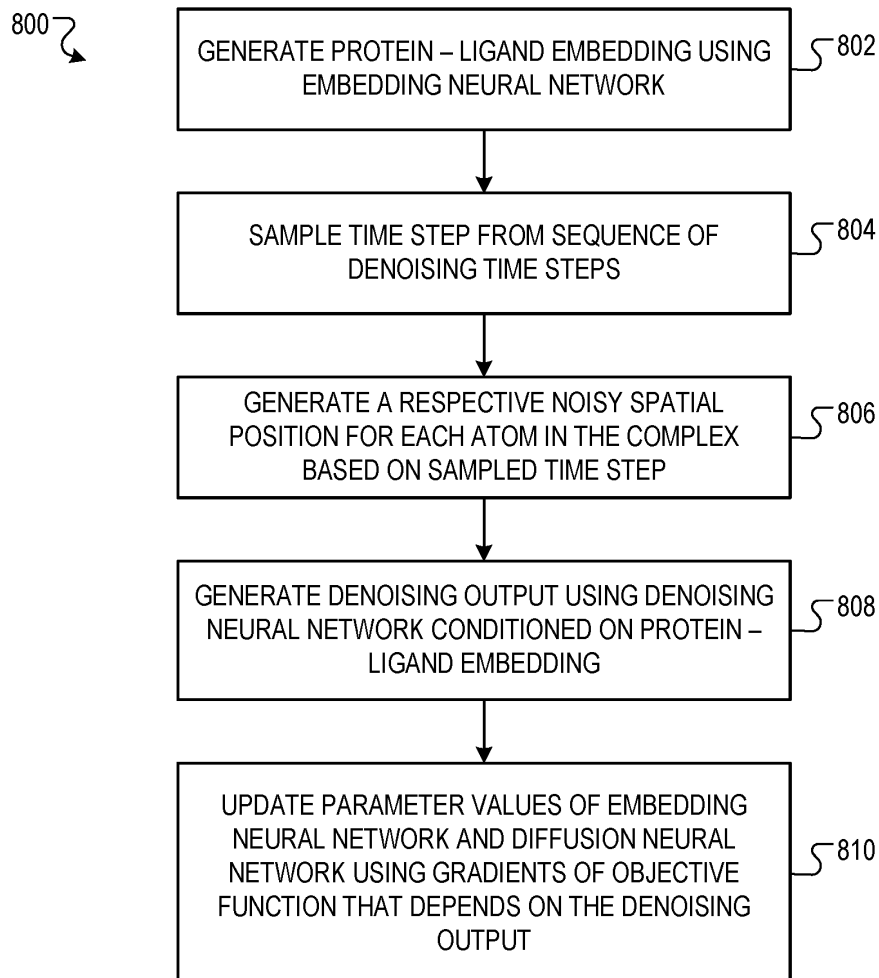


FIG. 8

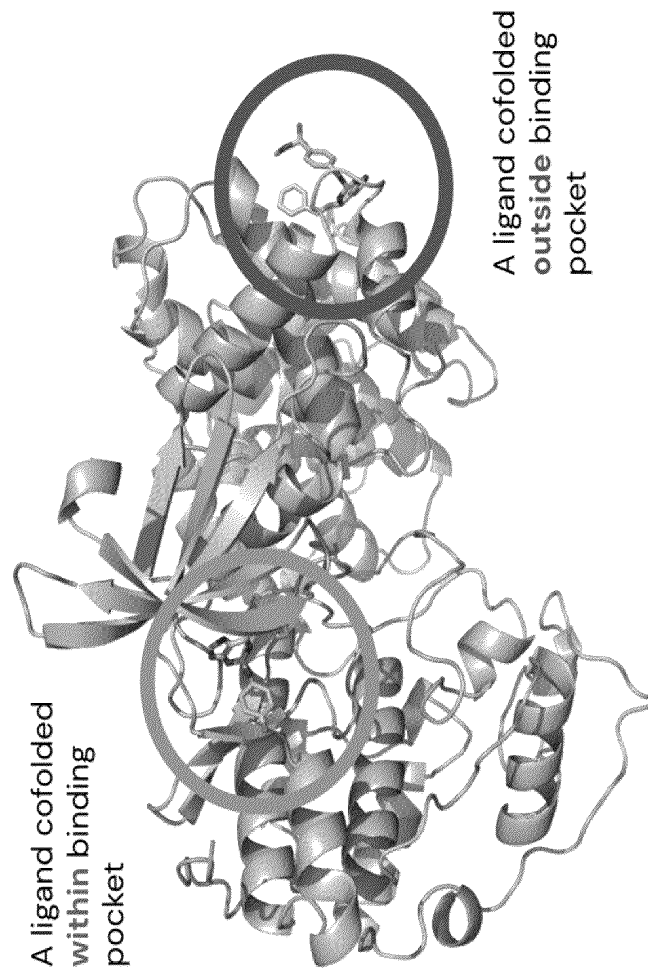


FIG. 9