



■ Van der Waals ■ Carbon Hydrogen Bond ■ Alkyl
■ Conventional Hydrogen Bond ■ Unfavorable Acceptor-Acceptor

Figure S2. Molecular docking interactions of LC, PS, and STR ligands. (1-6) Illustrates the interactions of ligand molecules with p53 protein in 3D and 2D images. (7-12) Illustrates the interactions of ligand molecules with CCNK protein in 3D and 2D images. (13-18) Illustrates the interactions of ligand molecules with CASP9 protein in 3D and 2D images. (19-24) Illustrates the interactions of ligand molecules with BCL2L1 protein in 3D and 2D images. (25-30) Illustrates the interactions of ligand molecules with CDK7 protein in 3D and 2D images. (31-36) Illustrates the interactions of ligand molecules with CDK2 protein in 3D and 2D images. (37-42) Illustrates the interactions of ligand molecules with CDK2AP1 protein in 3D and 2D images. (43-48) Illustrates the interactions of ligand molecules with CDKN1A protein in 3D and 2D images.