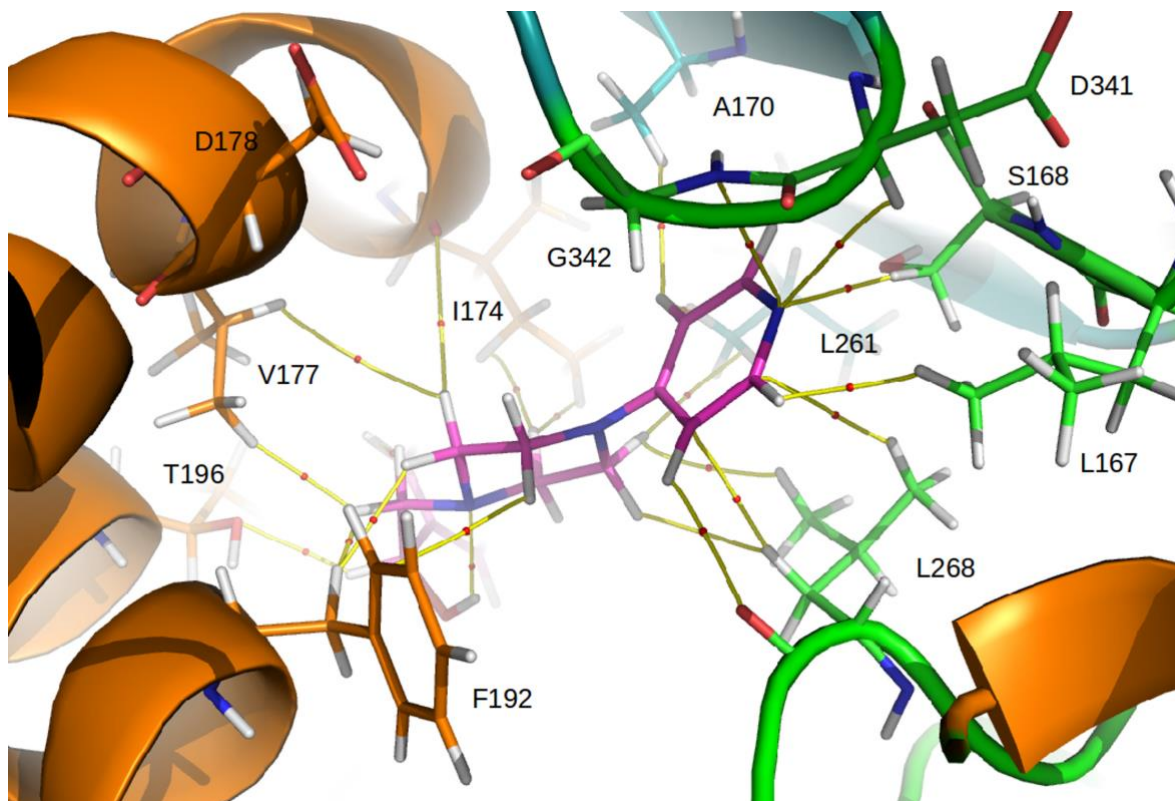


S1: Charge density molecular graph for the complex of SphK1 with compound **4** (in cyan). Yellow lines connecting the nuclei are the bond paths, and the small red spheres on them are the bond critical points (BCPs).



S2: Charge density molecular graph for the complex of SphK1 with compound **3** (in magenta). Yellow lines connecting the nuclei are the bond paths, and the small red spheres on them are the bond critical points (BCPs).