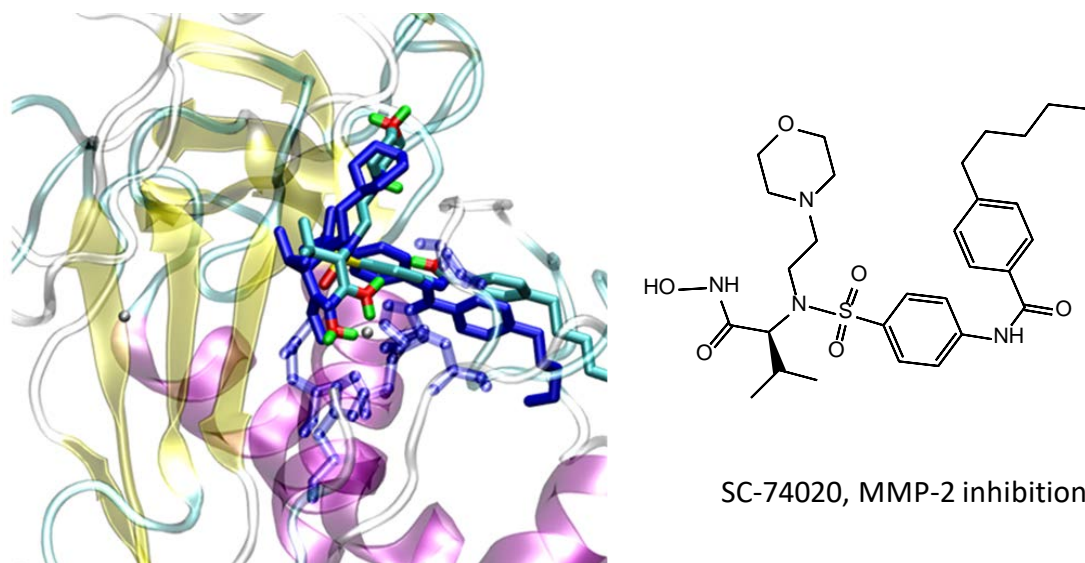


**Supplementary Figure 2:**



SC-74020 docked into the 1EAK 3D structure (the blue structure is the conformation of SC-74020 based on the NMR structure of the 1HOV – SC-74020 complex for comparison). Gold docking (fitness) scores for ABT-518 was 95.55 and for PD-166793, 83.51. Gold docking score characterizes the level of fitness of the docking and correlates with the binding strength (and activity).