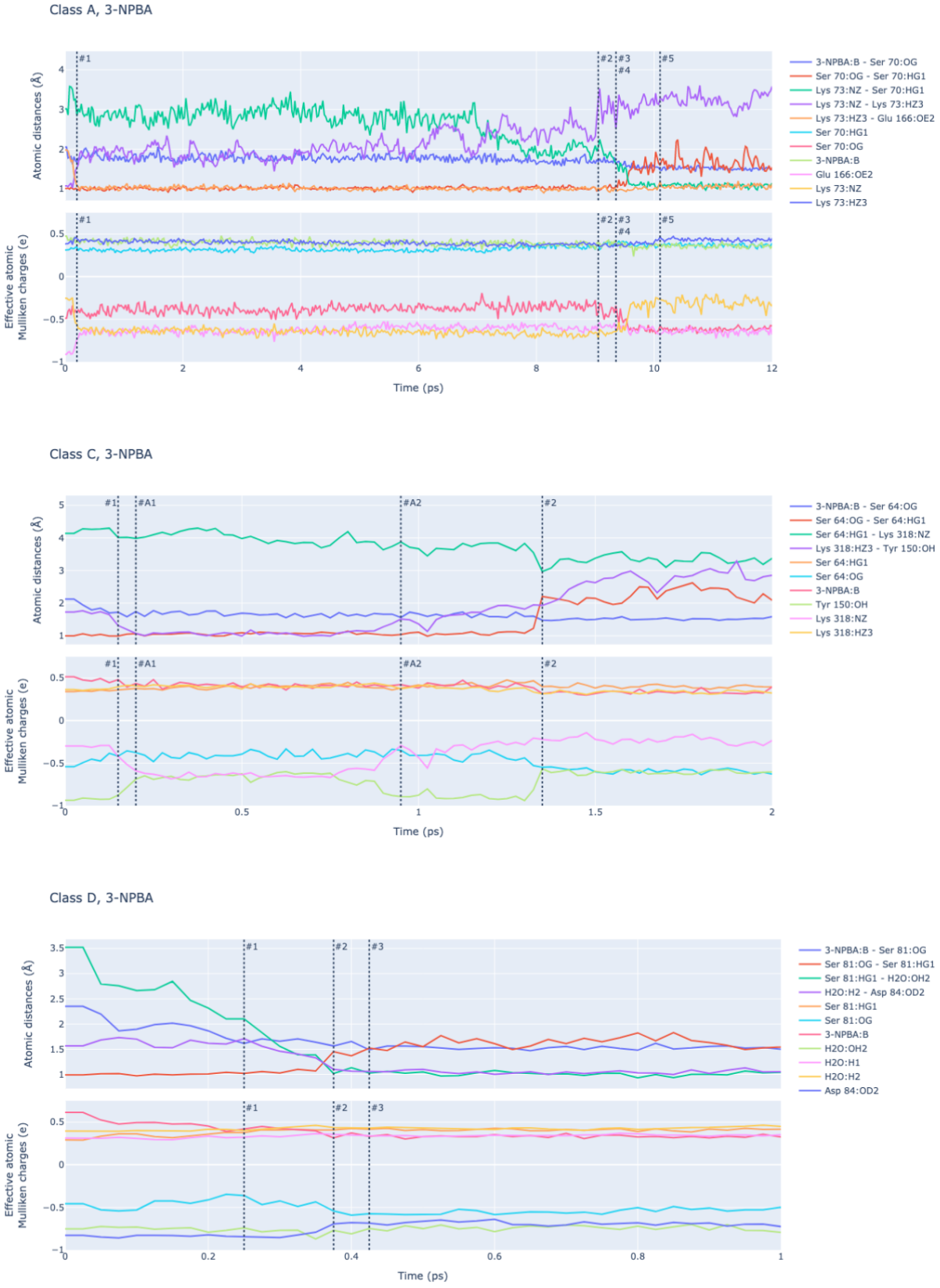

Figure S1. Atomic distances (upper subplots), and effective Mulliken atomic charges (lower subplots) of atoms directly involved in the reaction pathway, presented for 3-NPBA docked to β-lactamases which belong to the A, C, and D classes, respectively. The simulation results in the plots are based on the "first simulation" described in **Table 1**, except the class C which is represented by the "second simulation"

(due to non-productive completion of the first one). The reaction steps, marked with vertical dashed lines, correspond to denotations in **Table 1** and in **Figure 6**.