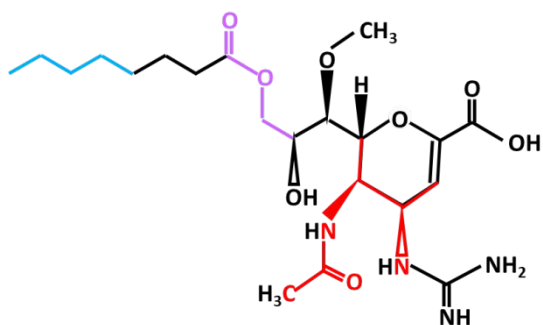Finding Maximum Common Subgraph from Molecular Structural Formulas through Maximum Clique Approach Combined with Ising Model
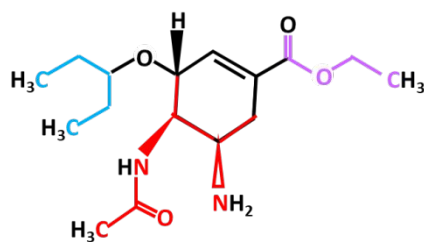
Yasuharu Okamoto

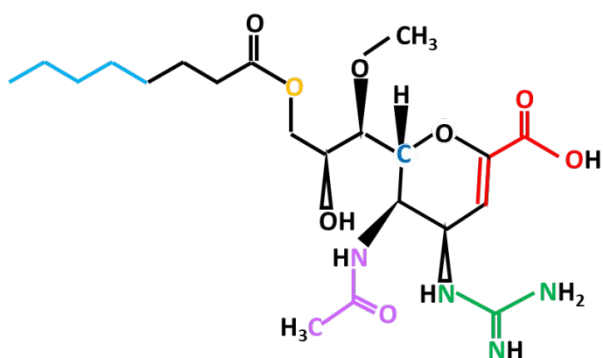Supporting Information

Figure S1: Structural formula of laninamivir octanoate and oseltamivir (top panel), laninamivir octanoate and peramivir (middle panel), and oseltamivir and peramivir (bottom panel). In each panel, the corresponding substructures in the MCS are distinguished by different colors.
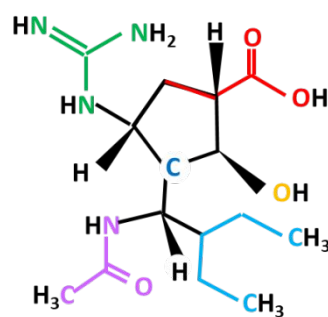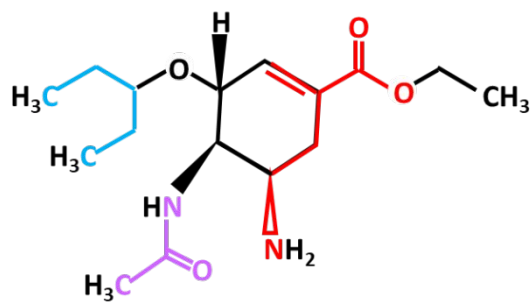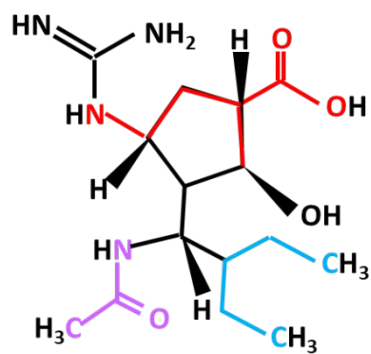
laninamivir octanoate

oseltamivir

laninamivir octanoate

peramivir

oseltamivir

peramivir