

# Supplemental Information

## 5-Arylidenethioxothiazolidinones as Inhibitors of Tyrosyl-DNA

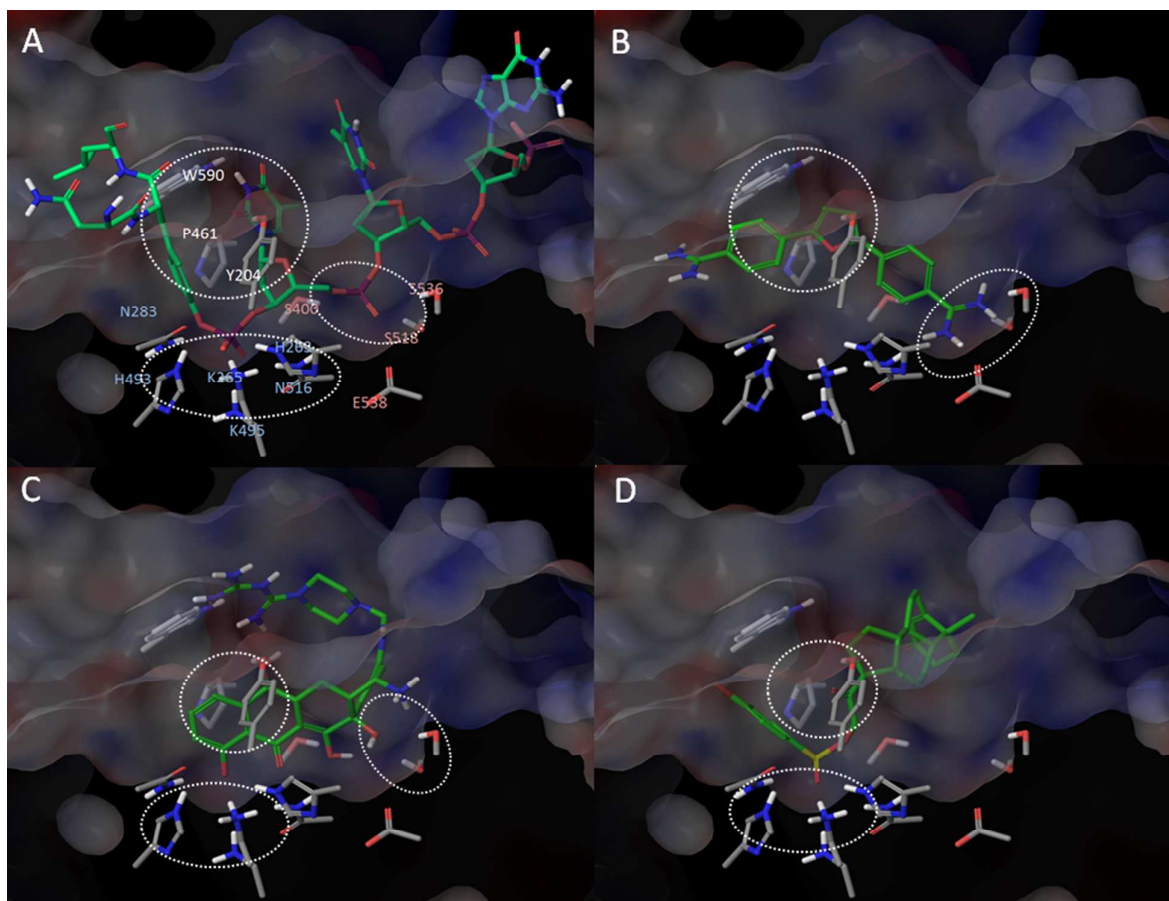
### Phosphodiesterase I (Tdp1)

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**Fig. 1S.** Modeled structure of Human Tdp1 (PDB: 1NOP) with (A) Top1-DNA substrate; (B) **1**, (C) **2**, and (D) **3**. The hydrophobic (labeled in white), the catalytic (labeled in blue), and the adjacent hydrophilic region (labeled in red) are shown. The models showed at least two of the three regions are essential for effective inhibitory binding (circled).