Supporting Information 3

Design, synthesis and docking study of acyl thiourea derivatives as possible histone deacetylase inhibitors with novel zinc binding group

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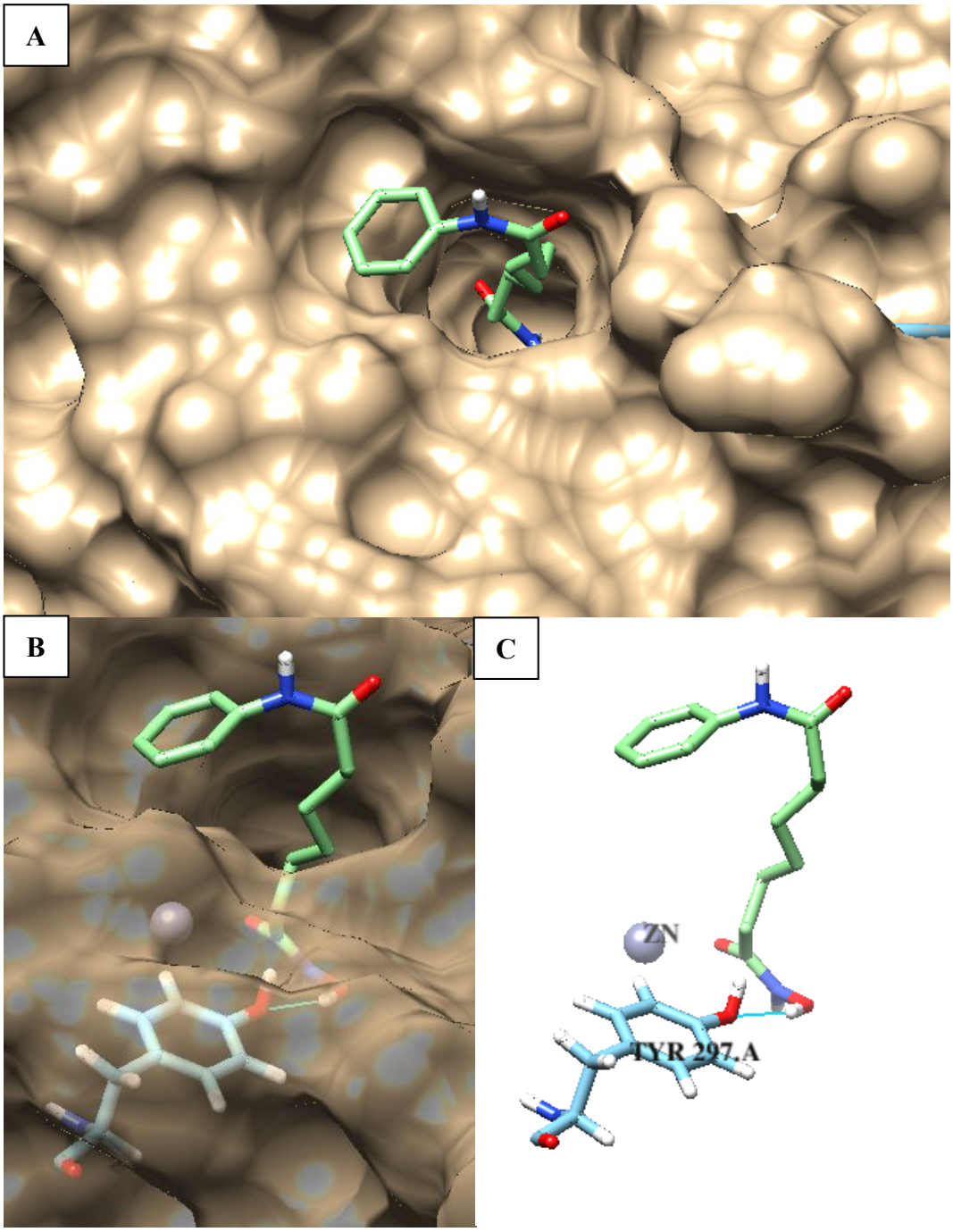

Figure 1: Docking of SAHA (**1**) into HDAC2 (4LXZ). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.

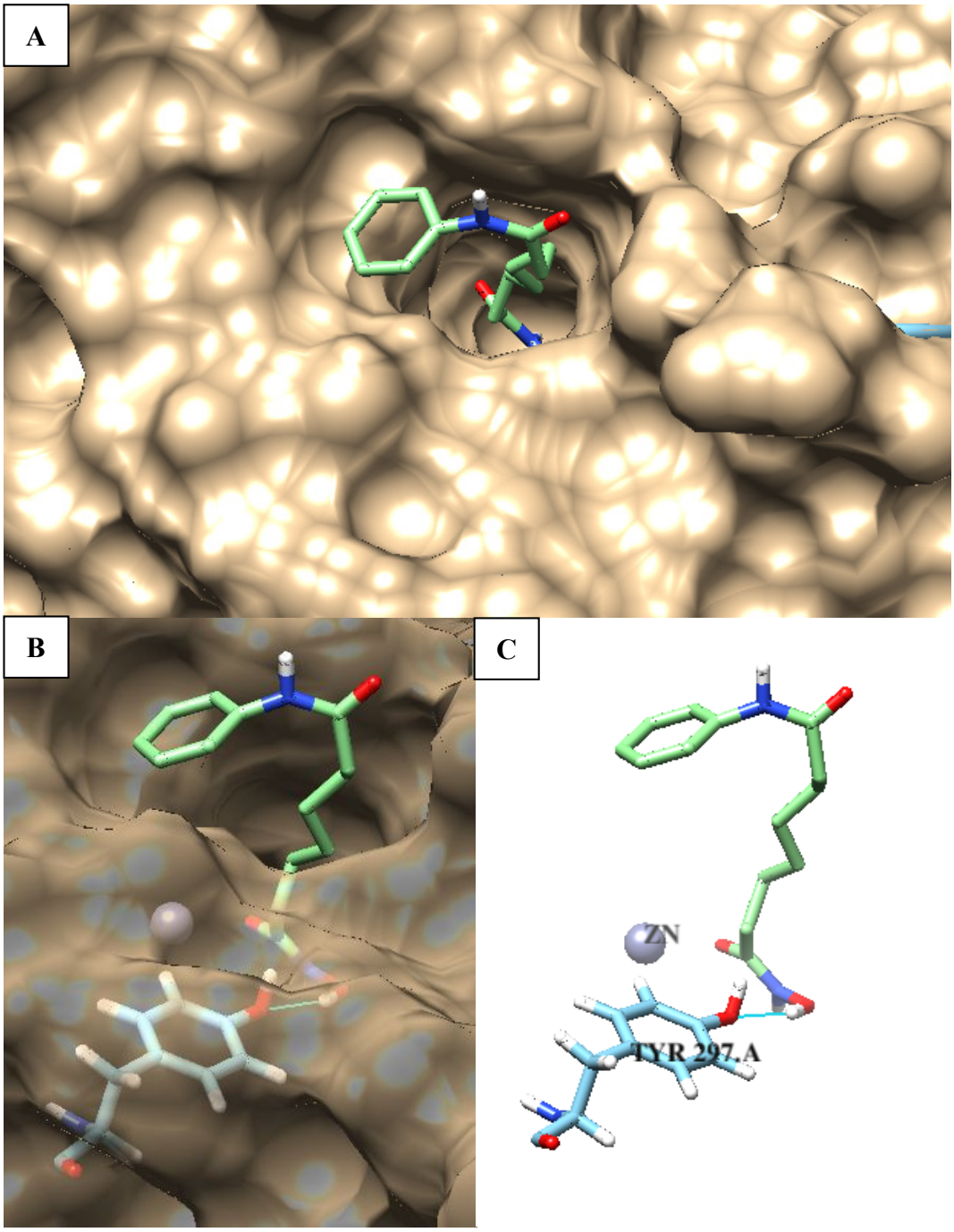

Figure 2: Docking of (**4**) into HDAC2 (4LXZ). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.

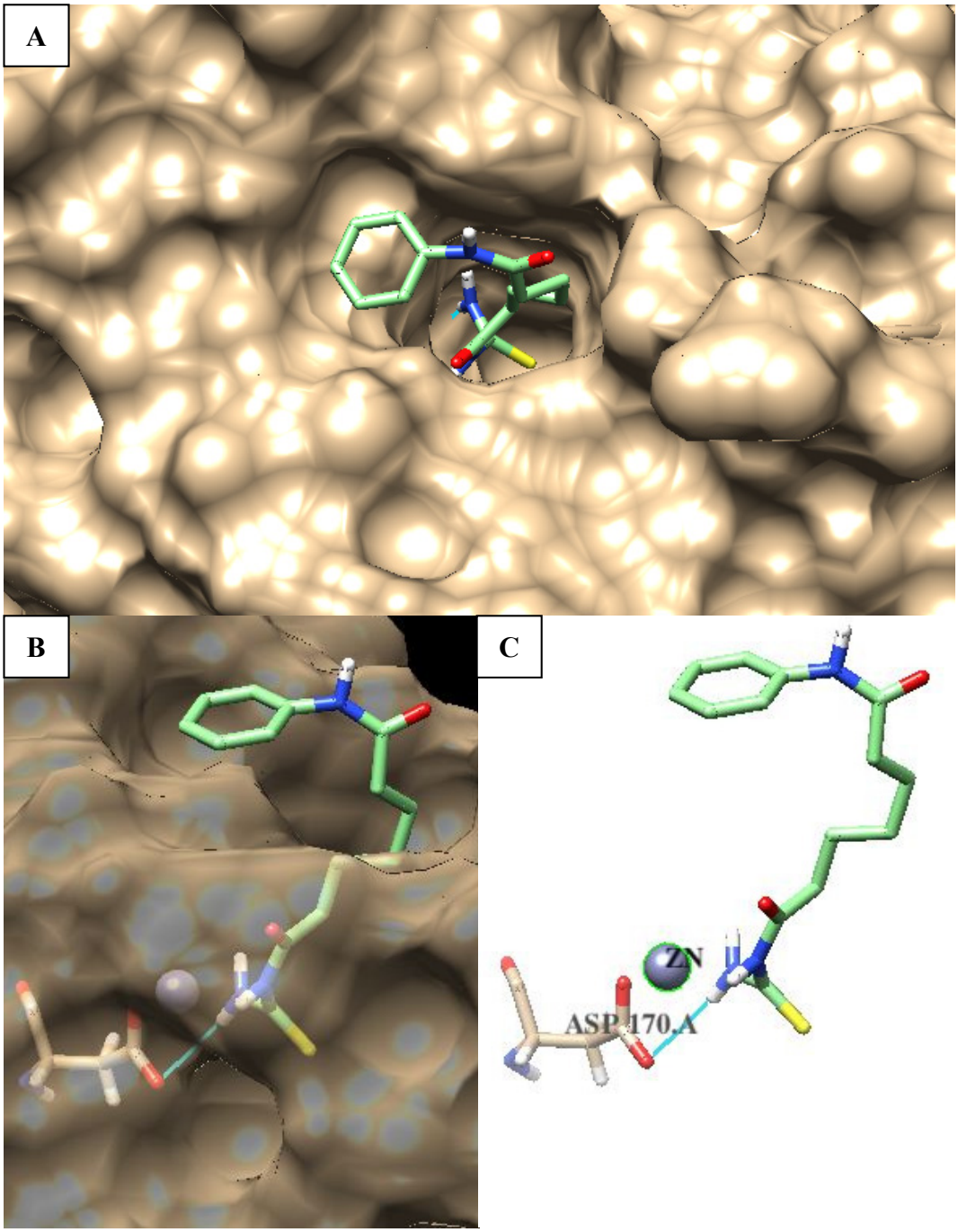

Figure 3: Docking of (**5**) into HDAC2 (4LXZ). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.

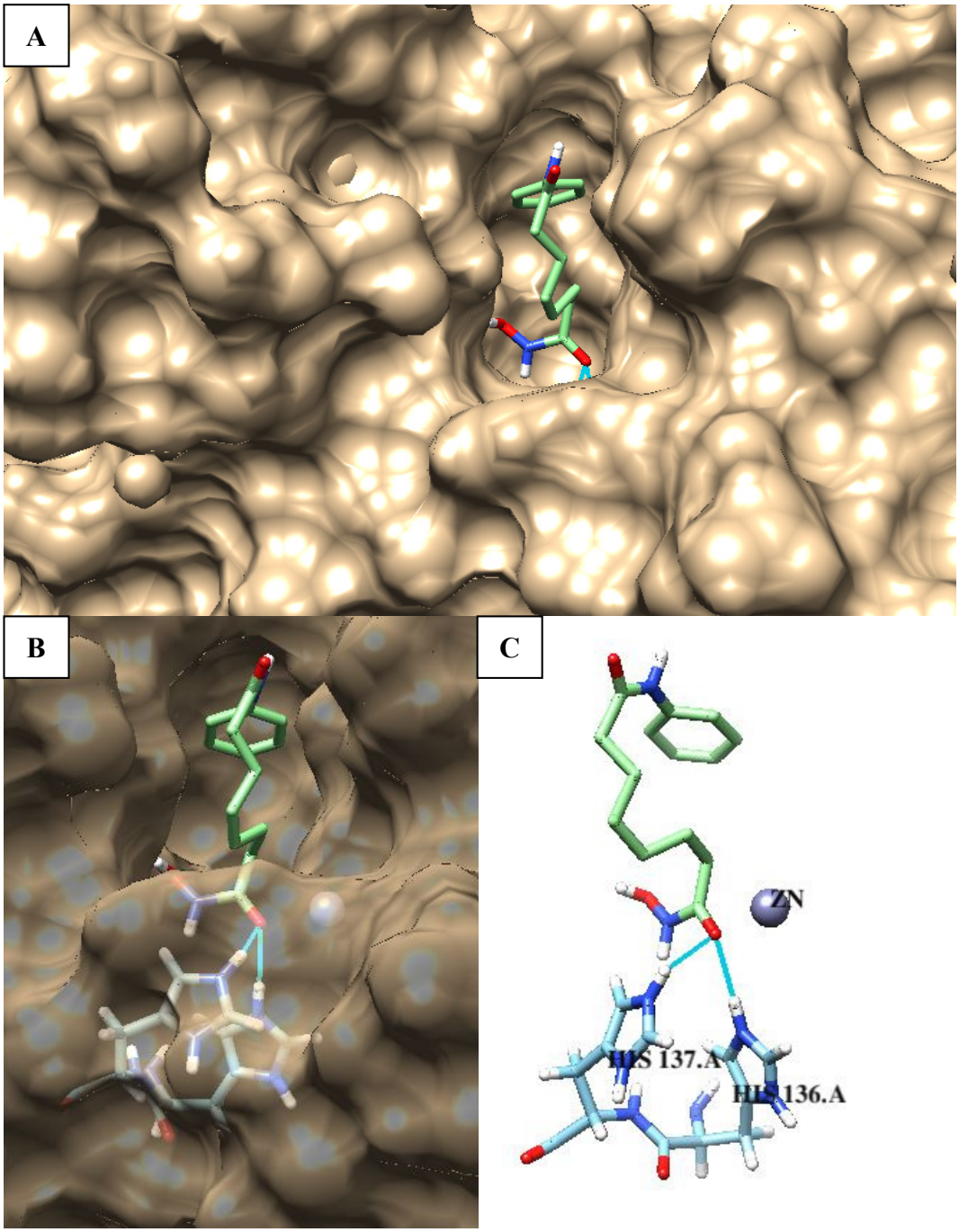

Figure 4: Docking of SAHA (**1**) into HDAC7 (3ZNR). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.

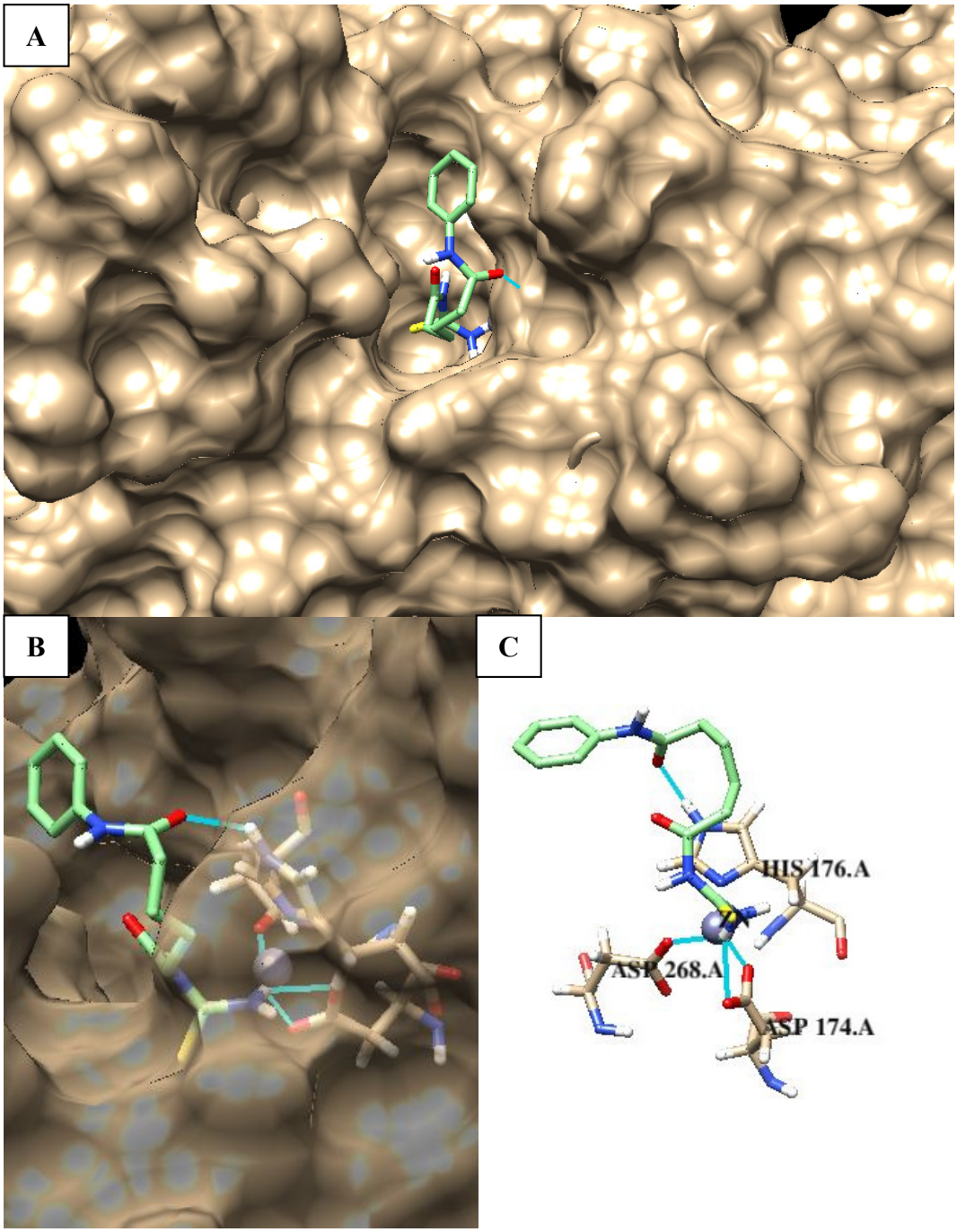

Figure 5: Docking of (**4**) into HDAC7 (3ZNR). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.

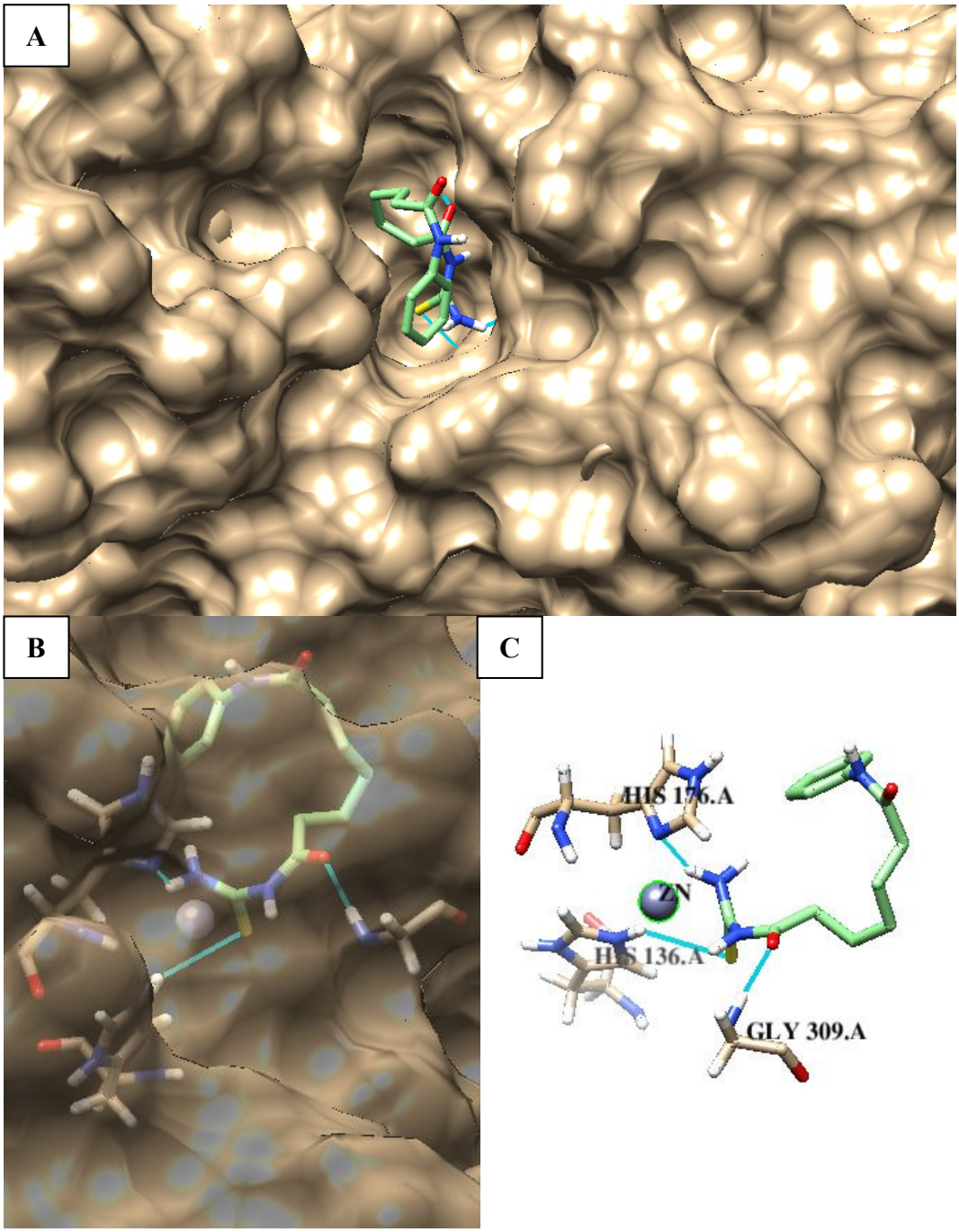

Figure 6: Docking of (**5**) into HDAC7 (3ZNR). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.