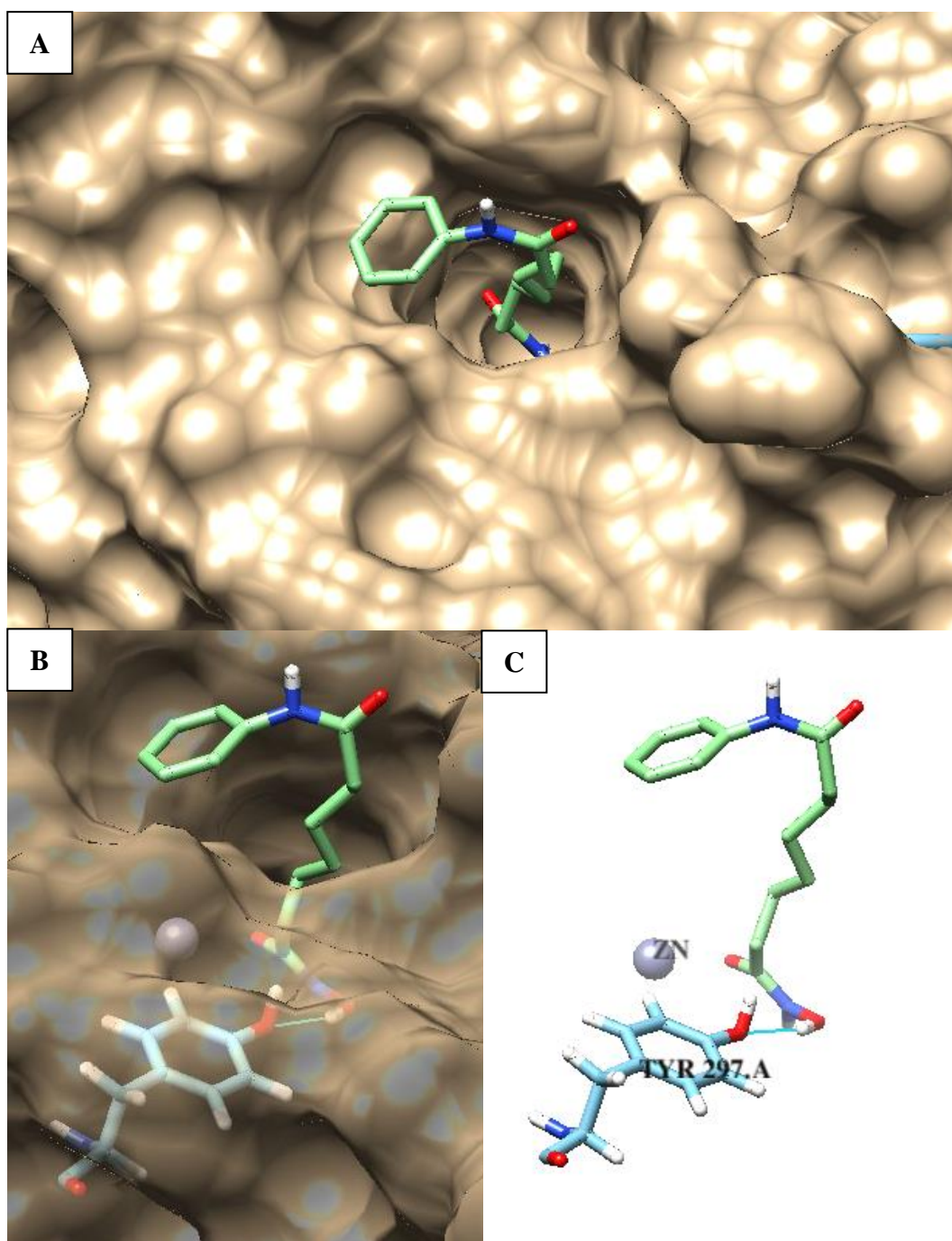


# **Supplementary File 2 for:**

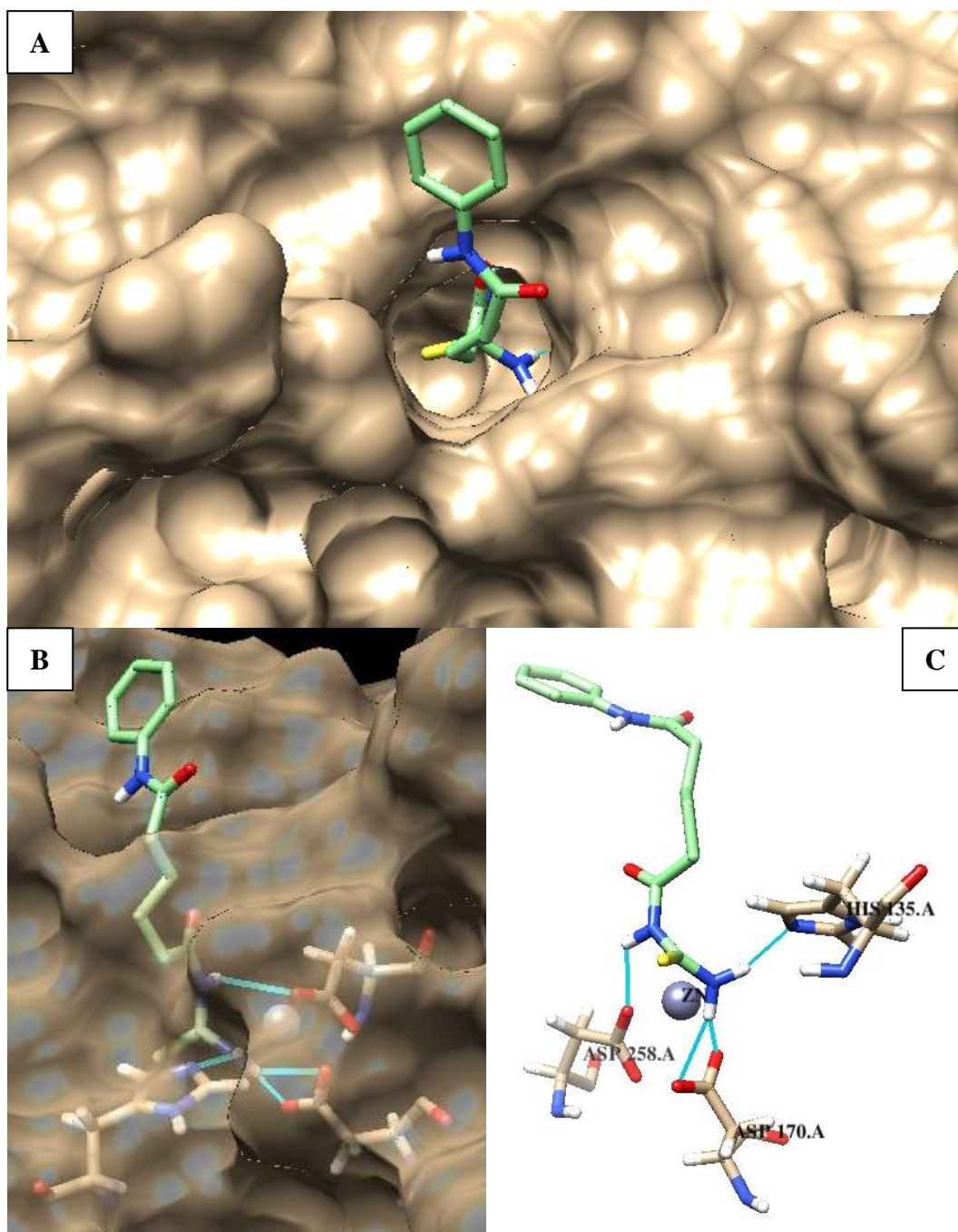
## **Design, synthesis and docking study of acyl thiourea derivatives as possible histone deacetylase inhibitors with a novel zinc binding group**

### **List of Figures**

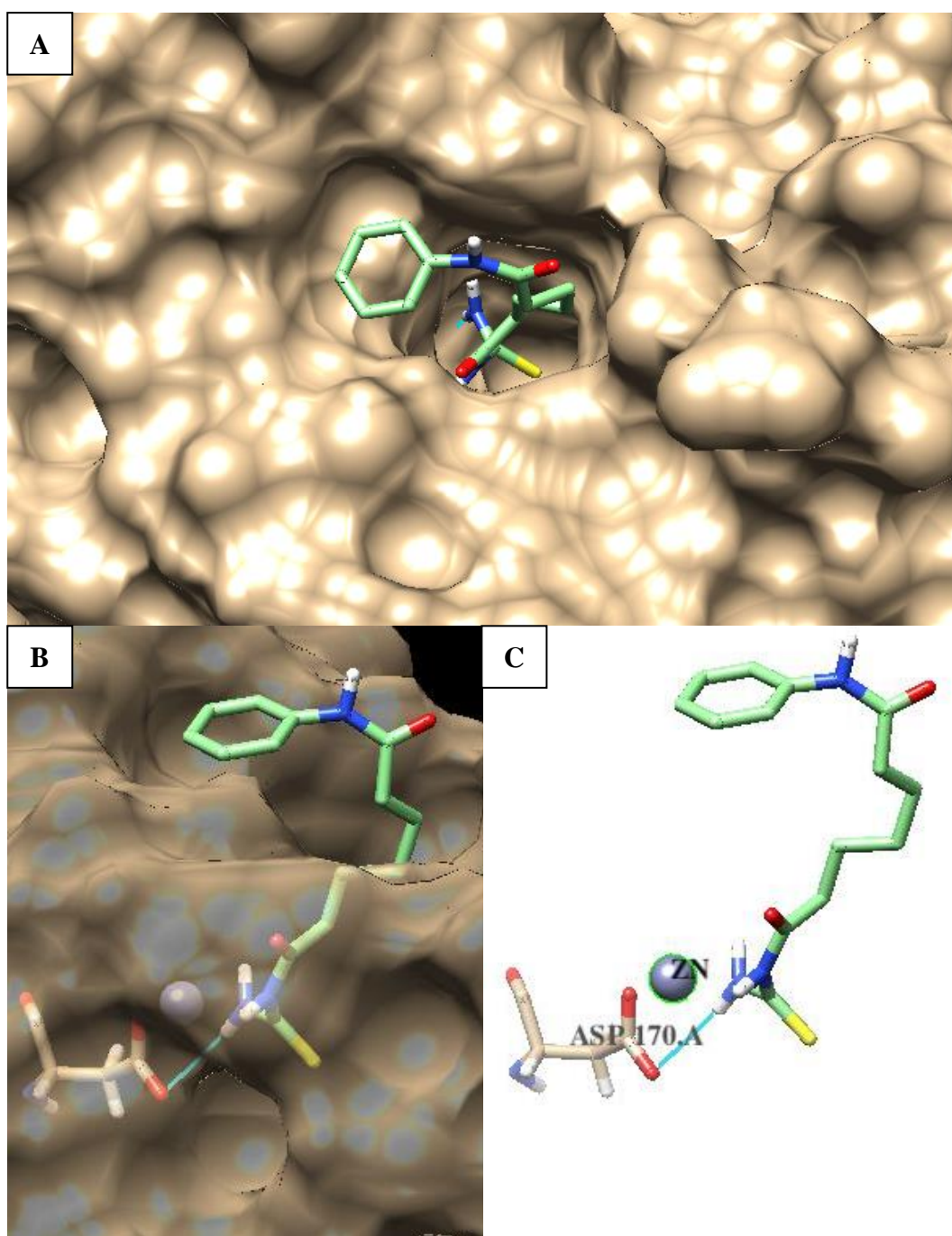
<b>Figure S1:</b> Docking of SAHA ( <b>1</b> ) into HDAC2 (4LXZ). ....	2
<b>Figure S2:</b> Docking of ( <b>4</b> ) into HDAC2 (4LXZ). ....	2
<b>Figure S3:</b> Docking of ( <b>5</b> ) into HDAC2 (4LXZ). ....	2
<b>Figure S4:</b> Docking of SAHA ( <b>1</b> ) into HDAC7 (3ZNR). ....	2
<b>Figure S5:</b> Docking of ( <b>4</b> ) into HDAC7 (3ZNR). ....	2
<b>Figure S6:</b> Docking of ( <b>5</b> ) into HDAC7 (3ZNR). ....	2



**Figure S1:** 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.

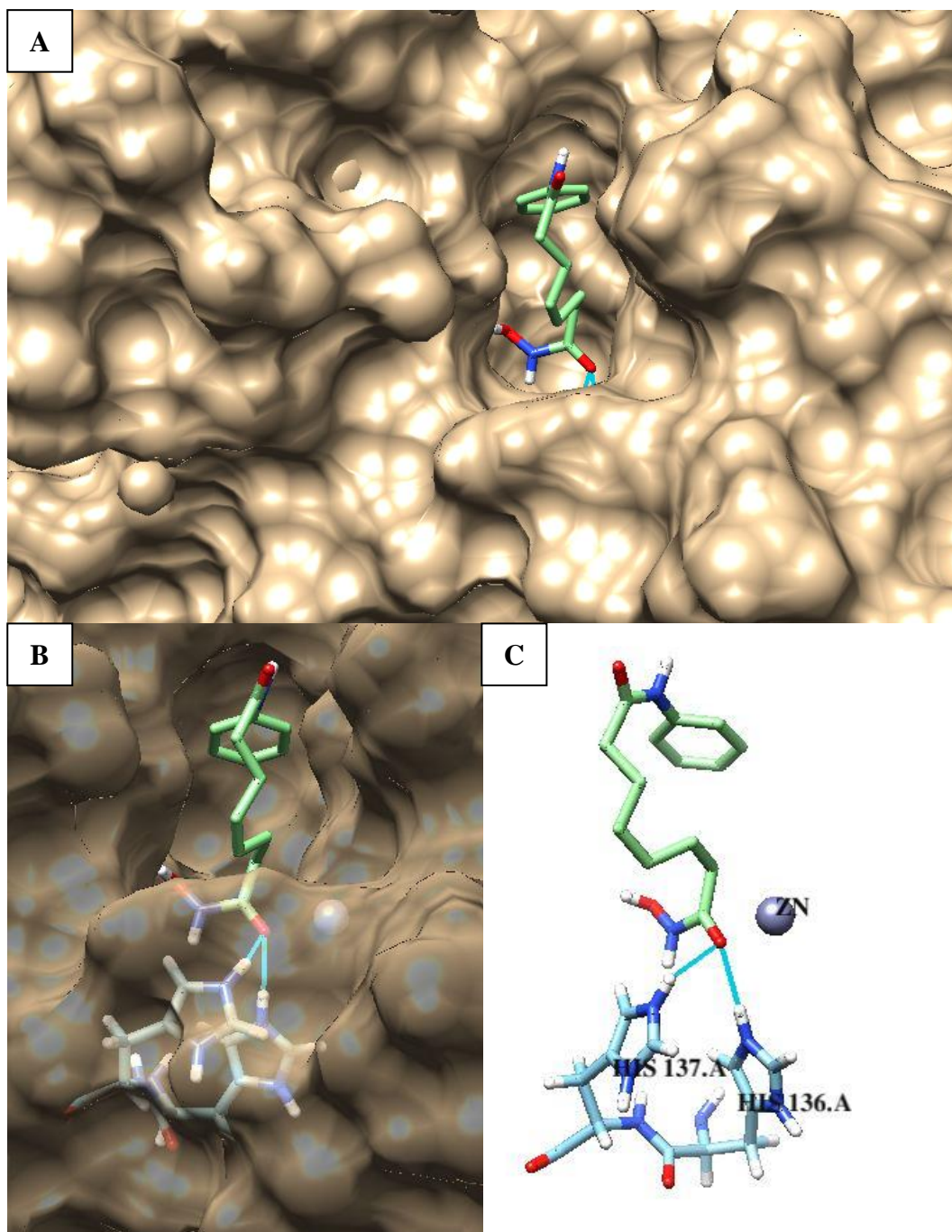


**Figure S2:** Docking of (4) into HDAC2 (4LXZ). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.

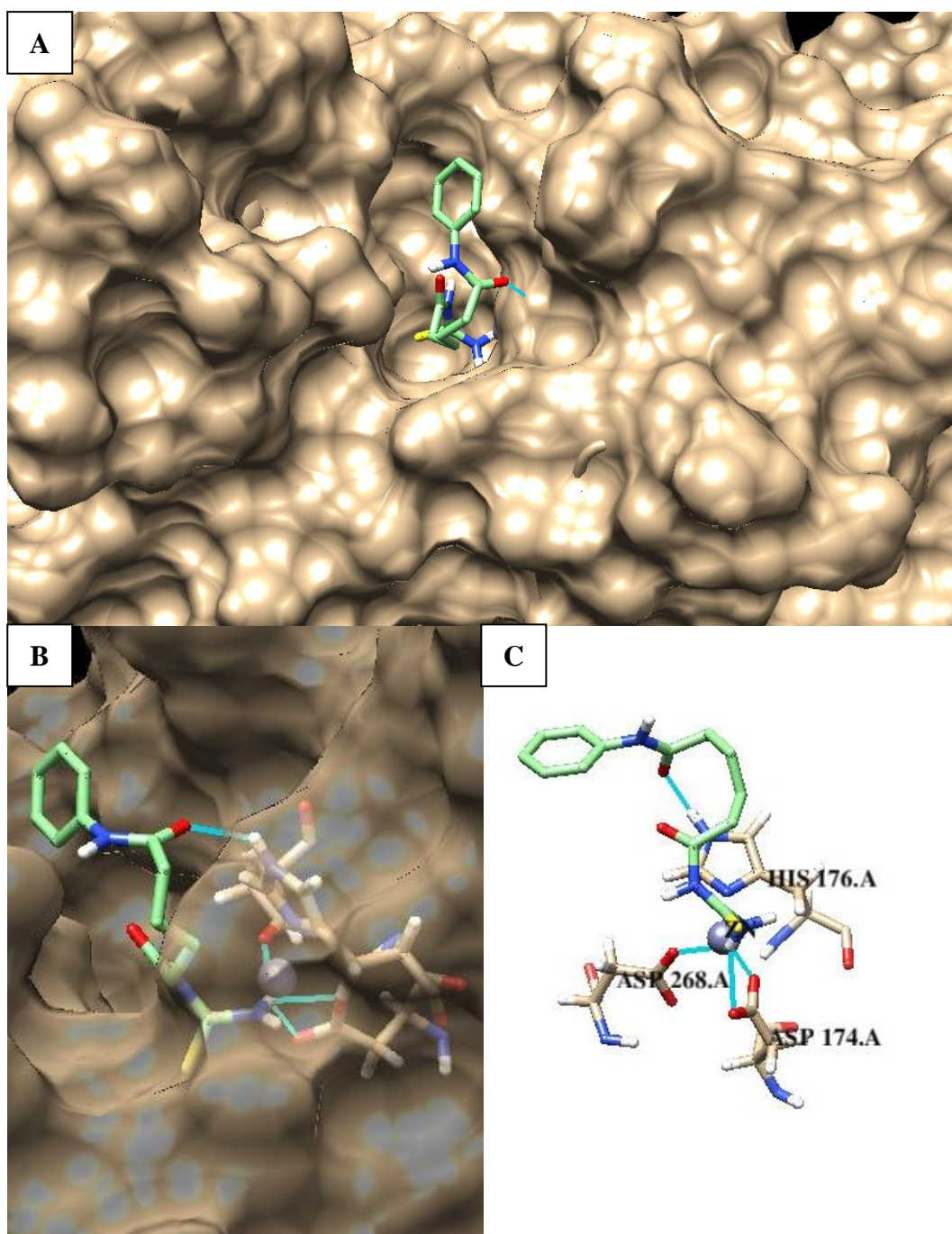


**Figure S3:** Docking of (5) into HDAC2 (4LXZ). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.



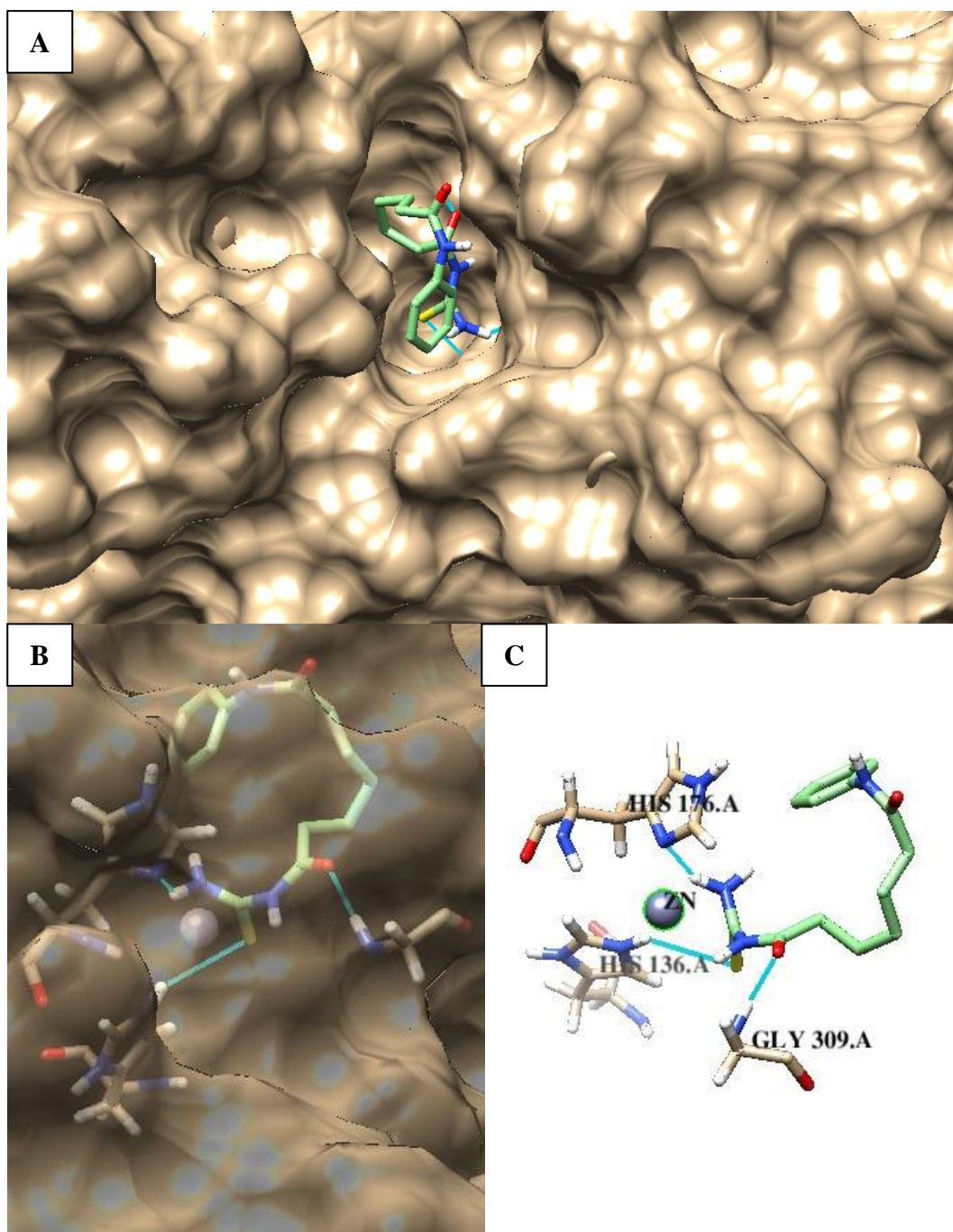


**Figure S4:** Docking of SAHA (1) into HDAC7 (3ZNR). A: Top surface view showing how it fits itself in the cavity. B: Surface view (50% transparency) showing its hydrogen bonding (blue line). C: A view showing only residues involved in hydrogen bonding together with zinc ion.



**Figure S5:** 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 S6:** 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.