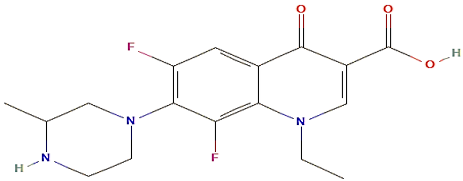
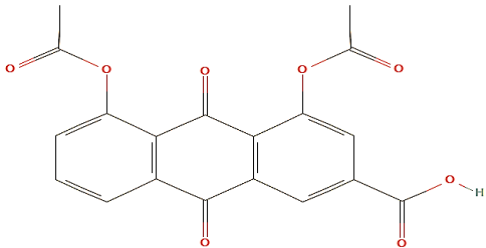
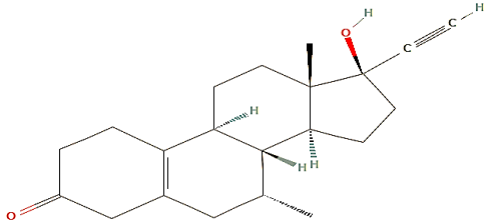
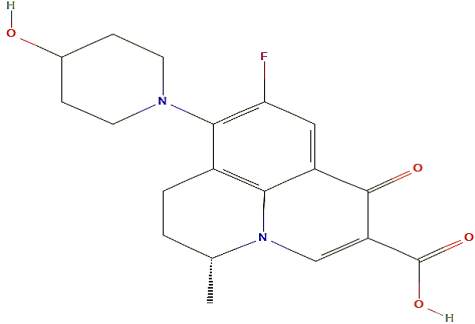
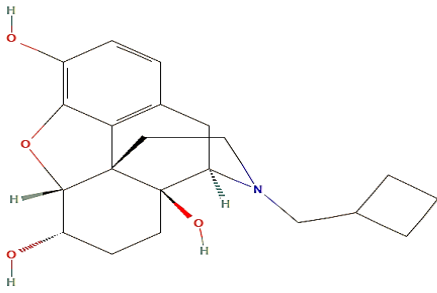
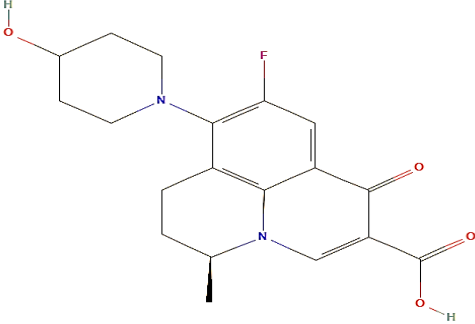
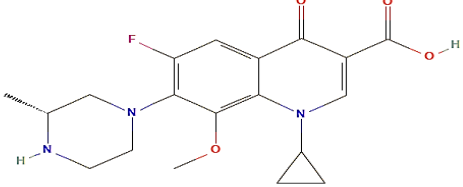
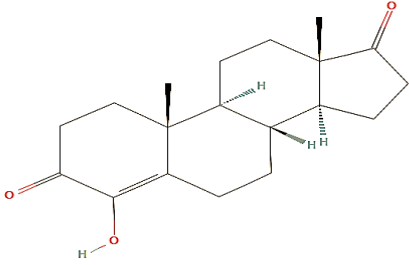
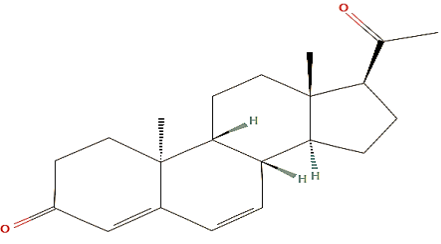
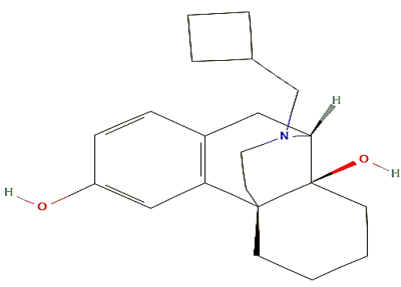
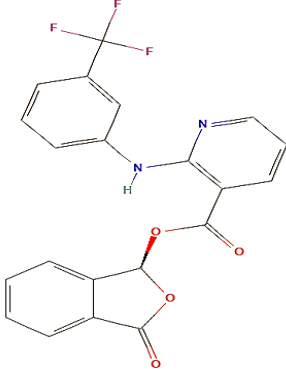
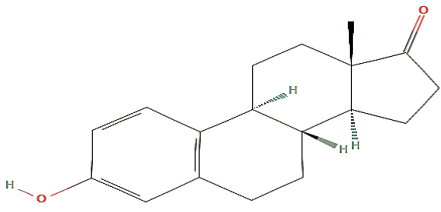
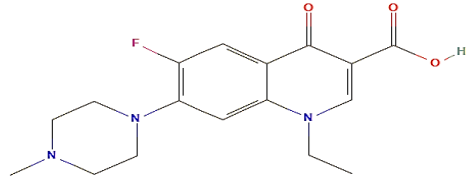
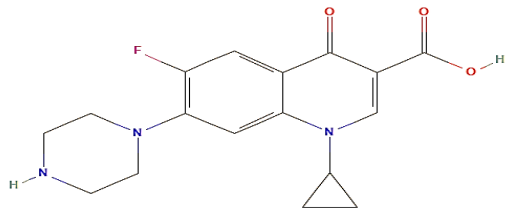
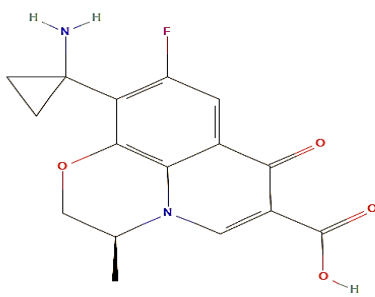


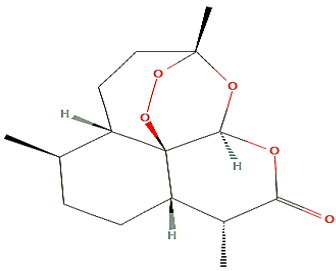
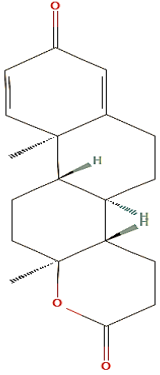
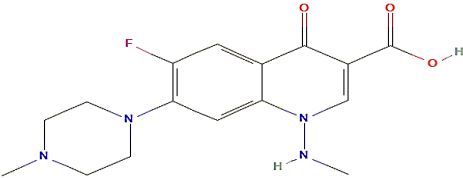
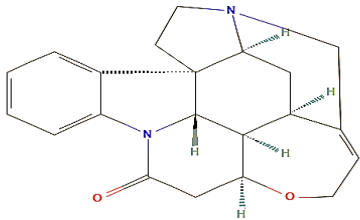
**S1 Table. Structure and binding affinity values of top 20 molecules after VS.**

Ligand	2D Structure	Binding Affinity
ZINC000003873157 (Lomefloxacin)	 <p>The structure of Lomefloxacin is a fluoroquinolone. It features a central pyridone ring system with two fluorine atoms at the 6 and 8 positions. The 7-position is substituted with a piperazine ring, which has a methyl group on one nitrogen and a hydrogen atom on the other. The 4-position is substituted with an ethyl group, and the 3-position is substituted with a propionic acid group.</p>	-9.6
ZINC000003812842 (Diacerein)	 <p>The structure of Diacerein is a tricyclic compound consisting of a central naphthalene ring system with two fused benzene rings. It has two acetoxy groups at the 1 and 8 positions and a propionic acid group at the 3 position. There are also two carbonyl groups on the central ring.</p>	-9.5
ZINC000003812889 (Tibolone)	 <p>The structure of Tibolone is a complex polycyclic steroid-like molecule. It features a fused ring system with a ketone group, a hydroxyl group, and an ethynyl group. The structure is shown with stereochemistry, including wedged and dashed bonds for the hydroxyl and ethynyl groups.</p>	-9.5

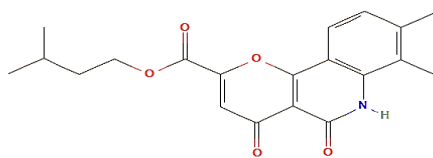
<p>ZINC000003794622 (Nadifloxacin)</p>	 <p>The chemical structure of Nadifloxacin features a central quinolone ring system. It is substituted with a piperidine ring at the 7-position, which has a hydroxyl group at the 4-position. At the 8-position, there is a methyl group shown with a dashed bond. At the 6-position, there is a fluorine atom. At the 2-position, there is a cyclopropane ring. At the 3-position, there is a carboxylic acid group.</p>	<p>-9.4</p>
<p>ZINC000003812989 (Nalbuphine)</p>	 <p>The chemical structure of Nalbuphine is a complex pentacyclic system. It consists of a benzene ring fused to a six-membered ring, which is further fused to a five-membered ring containing an oxygen atom. This is fused to another six-membered ring, which is finally fused to a five-membered ring containing a nitrogen atom. The nitrogen atom is substituted with a propyl chain that ends in a cyclobutane ring. There are several hydroxyl groups attached to the structure, with one shown in red.</p>	<p>-9.4</p>
<p>ZINC00000603195 (Levonadifloxacin)</p>	 <p>The chemical structure of Levonadifloxacin is similar to Nadifloxacin, featuring a central quinolone ring system. It has a piperidine ring at the 7-position with a hydroxyl group at the 4-position. At the 8-position, there is a methyl group shown with a solid wedge bond. At the 6-position, there is a fluorine atom. At the 2-position, there is a cyclopropane ring. At the 3-position, there is a carboxylic acid group.</p>	<p>-9.3</p>
<p>ZINC000003607120 (Gatifloxacin)</p>	 <p>The chemical structure of Gatifloxacin features a central quinolone ring system. It is substituted with a piperazine ring at the 7-position, which has a methyl group at the 3-position. At the 8-position, there is a methyl group shown with a dashed bond. At the 6-position, there is a fluorine atom. At the 2-position, there is a cyclopropylidene group. At the 3-position, there is a carboxylic acid group. There is also a methoxy group at the 5-position.</p>	<p>-9.3</p>

<p>ZINC000003919580 (Formestane)</p>	 <p>The structure of Formestane is a steroid derivative. It features a four-ring steroid nucleus with a ketone group at C-3, a double bond between C-4 and C-5, and a hydroxyl group at C-14. There are methyl groups at C-10 and C-13, and an acetyl group at C-17. Stereochemistry is indicated with wedges and dashes.</p>	<p>-9.3</p>
<p>ZINC000003875998 (Isopregnenone)</p>	 <p>The structure of Isopregnenone is a steroid derivative. It features a four-ring steroid nucleus with a ketone group at C-3, a double bond between C-4 and C-5, and a double bond between C-14 and C-15. There are methyl groups at C-10 and C-13, and an acetyl group at C-17. Stereochemistry is indicated with wedges and dashes.</p>	<p>-9.2</p>
<p>ZINC000003812988 (Butorphanol)</p>	 <p>The structure of Butorphanol is a complex molecule. It features a morphine-like pentacyclic core with a cyclopropylmethyl group at the N-4 position, a hydroxyl group at C-3, and a hydroxyl group at C-17. Stereochemistry is indicated with wedges and dashes.</p>	<p>-9.1</p>
<p>ZINC000000601275 (Talniflumate)</p>	 <p>The structure of Talniflumate consists of two parts. The first part is a pyridine ring substituted with a trifluoromethyl group and a 2-(4-hydroxyphenyl)amino group. The second part is a benzofuranone ring system. The two parts are connected via an ester linkage between the carbonyl oxygen of the pyridine derivative and the 2-position of the benzofuranone ring.</p>	<p>-9.0</p>

<p>ZINC000013509425 (Estrone)</p>	 <p>The structure of Estrone is a steroid nucleus consisting of four fused rings: a six-membered aromatic A ring with a hydroxyl group at the 3-position, a six-membered B ring, a five-membered C ring, and a five-membered D ring with a ketone group at the 17-position. Stereochemistry is indicated with a dashed bond for the hydrogen at C-13 and a wedged bond for the hydrogen at C-14.</p>	<p>-9.0</p>
<p>ZINC000000001894 (Pefloxacin)</p>	 <p>The structure of Pefloxacin is a quinolone derivative. It features a central quinolone core with a fluorine atom at the 6-position, a piperazine ring at the 7-position, an ethyl group at the 8-position, and a carboxylic acid group at the 3-position.</p>	<p>-8.9</p>
<p>ZINC000000020220 (Ciprofloxacin)</p>	 <p>The structure of Ciprofloxacin is a quinolone derivative. It features a central quinolone core with a fluorine atom at the 6-position, a piperazine ring at the 7-position, a cyclopropyl group at the 8-position, and a carboxylic acid group at the 3-position.</p>	<p>-8.9</p>
<p>ZINC000003779726 (Pazufloxacin)</p>	 <p>The structure of Pazufloxacin is a quinolone derivative. It features a central quinolone core with a fluorine atom at the 6-position, a piperazine ring at the 7-position, a cyclopropyl group at the 8-position, a methyl group at the 9-position, and a carboxylic acid group at the 3-position.</p>	<p>-8.9</p>

<p>ZINC000008143788 (Artemisinin)</p>		<p>-8.9</p>
<p>ZINC000004081771 (Testolactone)</p>		<p>-8.9</p>
<p>ZINC00000000917 (Amifloxacin)</p>		<p>-8.8</p>
<p>ZINC000000119434 (Strychnine)</p>		<p>-8.8</p>

ZINC000000538285  
(Repirinast)



-8.8