

Identification of fosaprepitant as a novel GSTP1 inhibitor through structure-based virtual screening, molecular dynamics simulation, and biological evaluation

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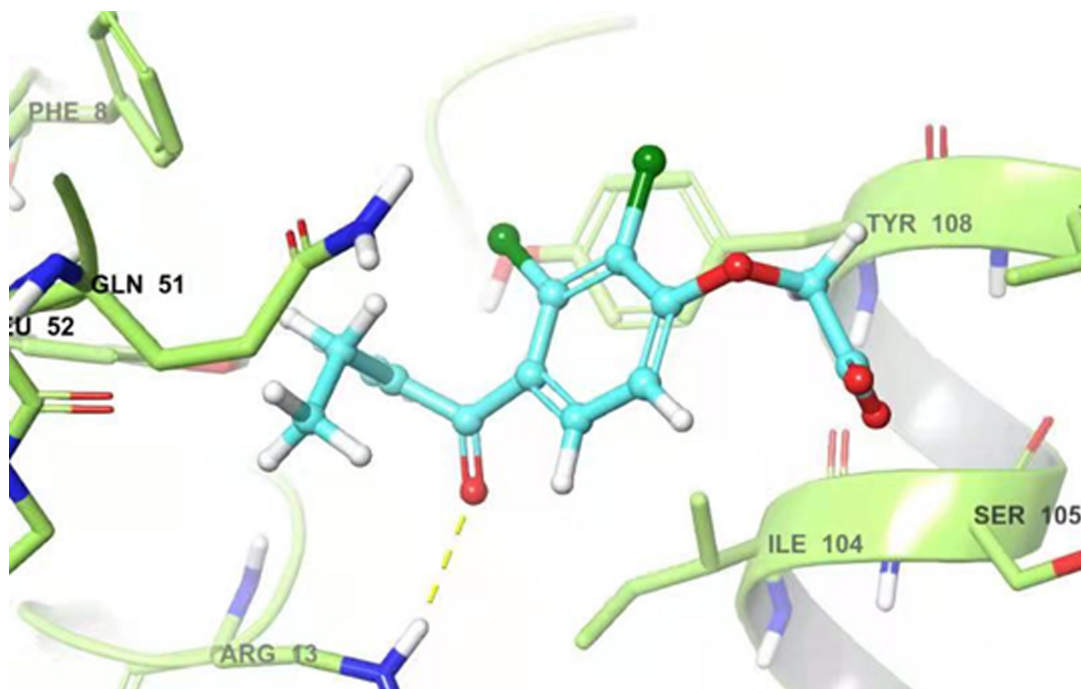
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Supplementary Fig. 1

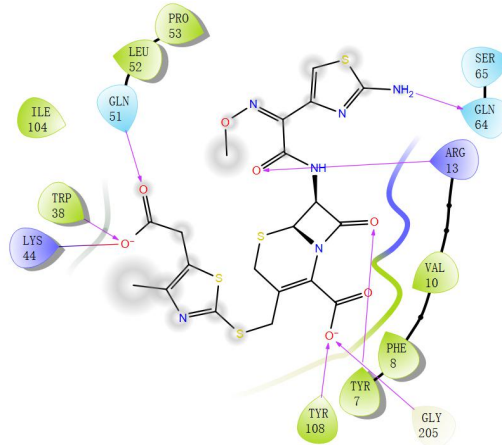


Supplementary Fig1. Binding modes of co-crystal compound ethacrynic acid(EA) with GSTP1.

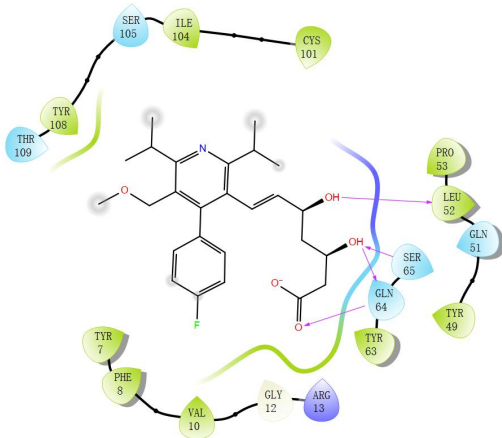
Supplementary Table1: Receptor-ligand interactions of the virtual screening hits

Title	Receptor-ligand interactions
ZINC000003939013	<p>Diagram illustrating the receptor-ligand interactions for ZINC000003939013. The ligand is shown in stick representation, and the interacting residues are highlighted in colored circles. Key interactions include hydrogen bonds (red dashed lines) and hydrophobic contacts (green dashed lines) involving residues such as GLN 51, GLN 64, SER 65, ASN 66, GLU 91, CYS 101, ARG 13, ILE 104, GLY 12, SER 105, TYR 108, THR 109, TYR 7, PHE 8, ASN 204, and GLY 205.</p>
ZINC000003830431	<p>Diagram illustrating the receptor-ligand interactions for ZINC000003830431. The ligand is shown in stick representation, and the interacting residues are highlighted in colored circles. Key interactions include hydrogen bonds (red dashed lines) and hydrophobic contacts (green dashed lines) involving residues such as ILE 104, CYS 101, SER 105, ARG 13, VAL 10, PRO 9, PHE 8, TYR 7, VAL 35, ASN 206, GLY 205, TRP 38, TYR 108, THR 109, LYS 44, and GLN 51.</p>
ZINC000100004233	<p>Diagram illustrating the receptor-ligand interactions for ZINC000100004233. The ligand is shown in stick representation, and the interacting residues are highlighted in colored circles. Key interactions include hydrogen bonds (red dashed lines) and hydrophobic contacts (green dashed lines) involving residues such as ILE 104, ARG 13, GLN 51, LEU 52, PRO 53, GLY 205, VAL 10, TYR 108, PHE 8, TYR 7, VAL 35, TRP 38, and GLN 39.</p>

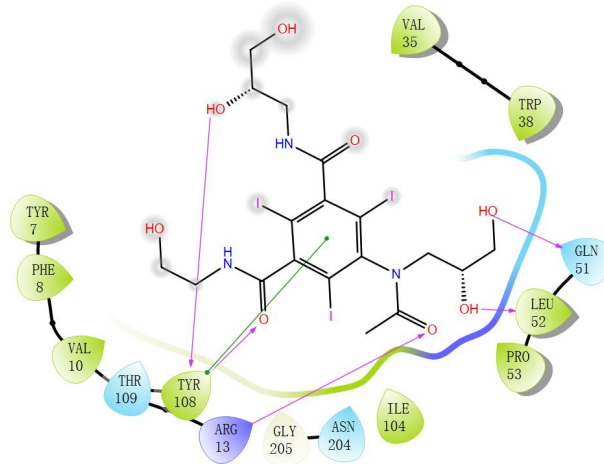
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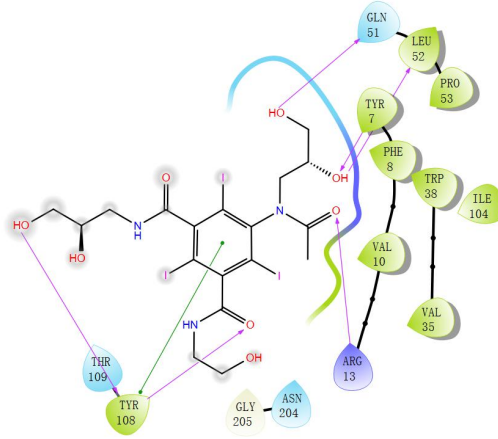
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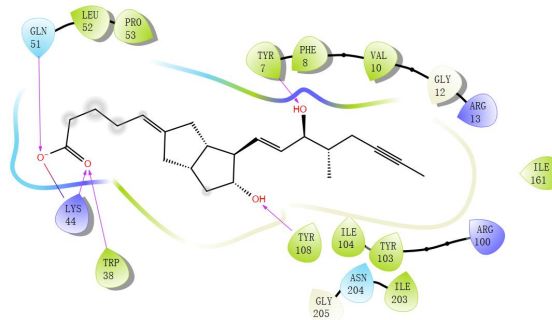
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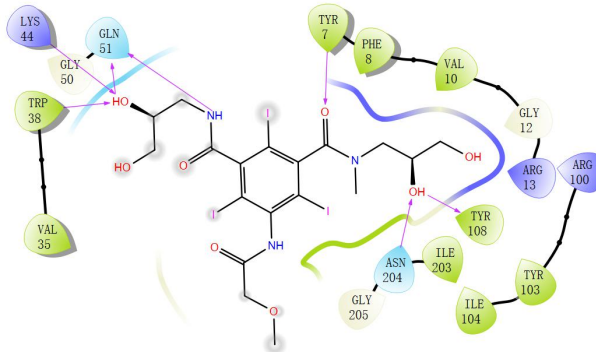
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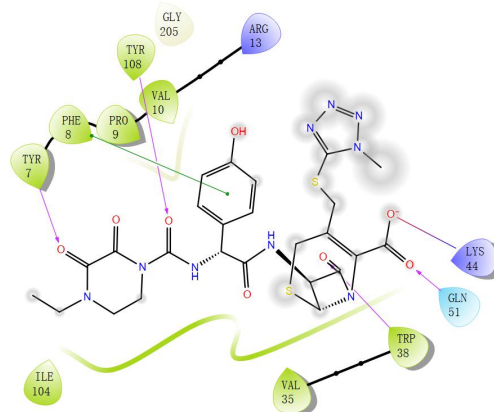
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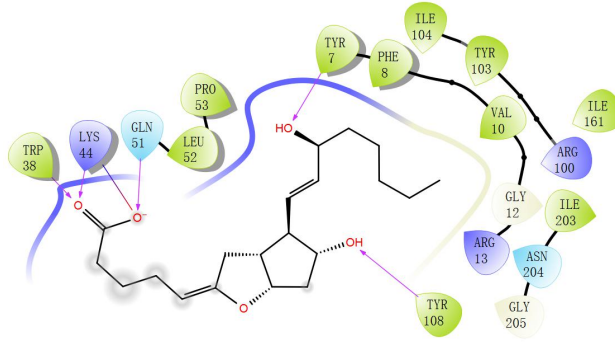
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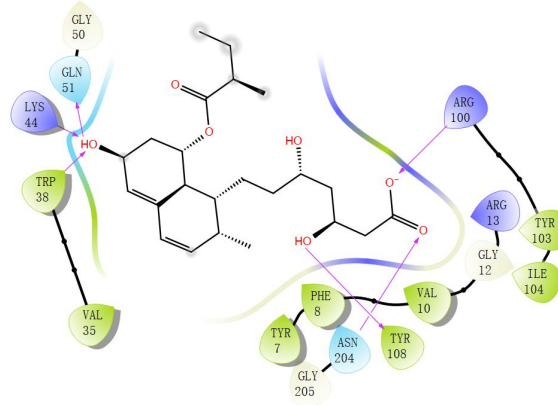
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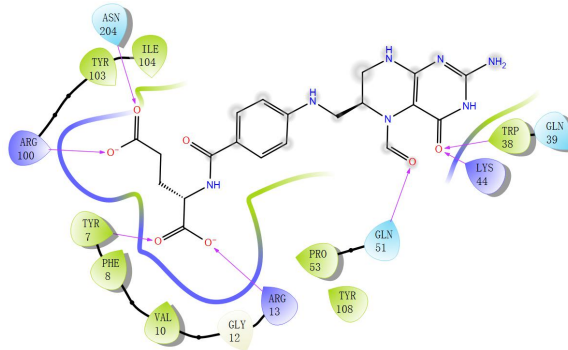
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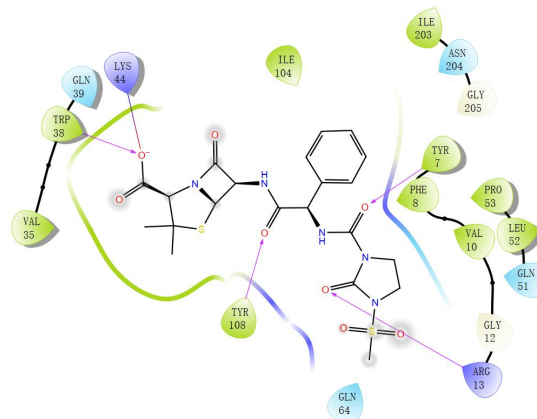
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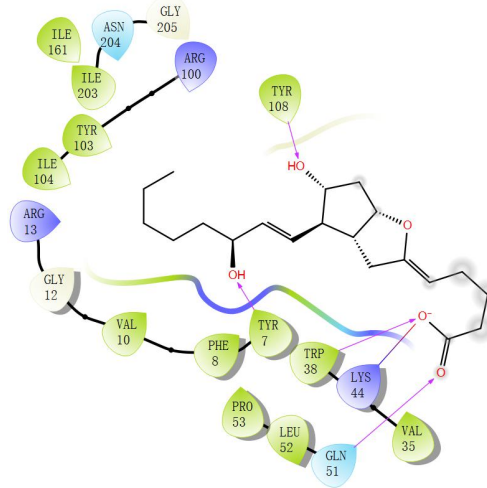
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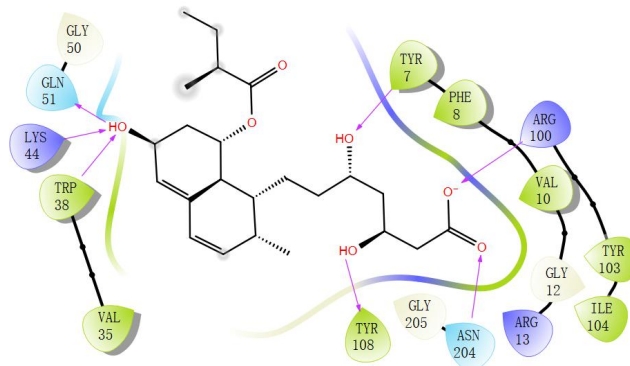
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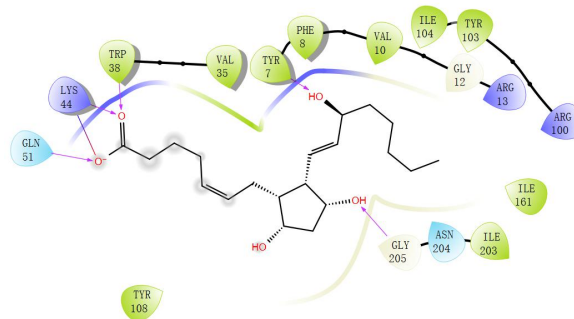
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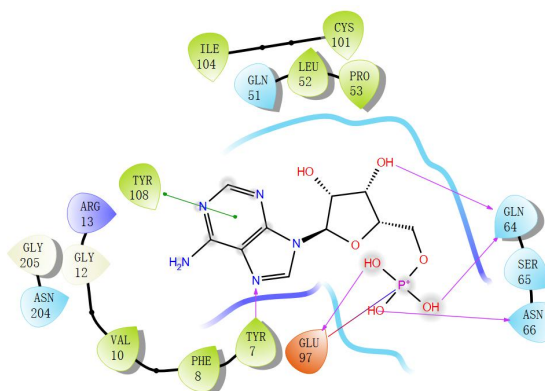
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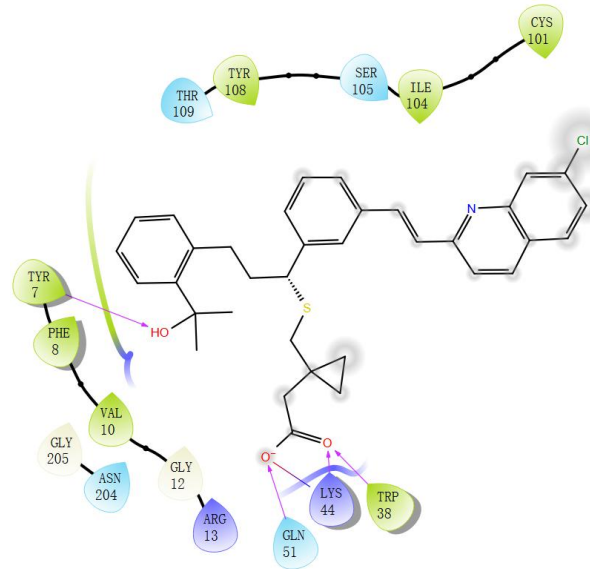
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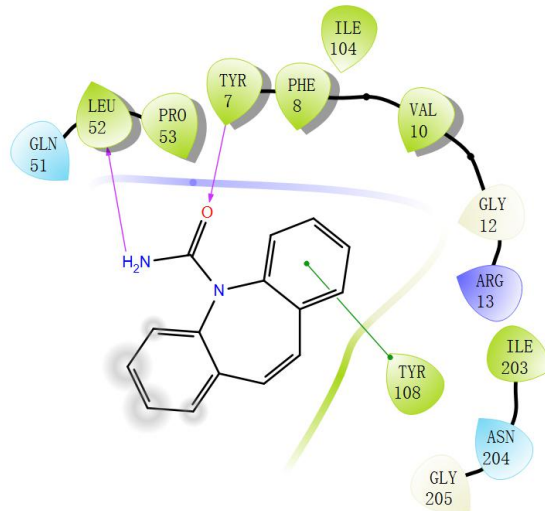
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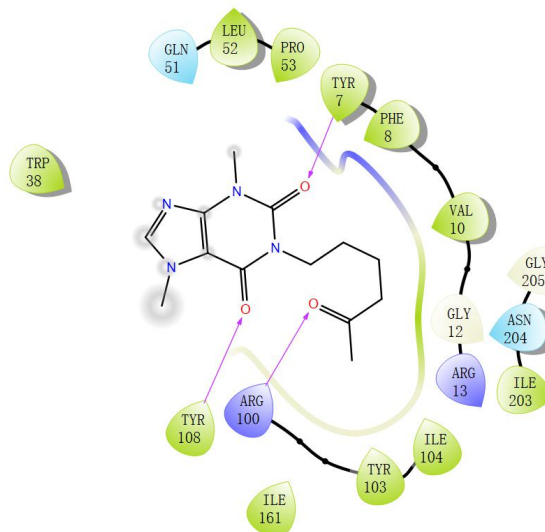
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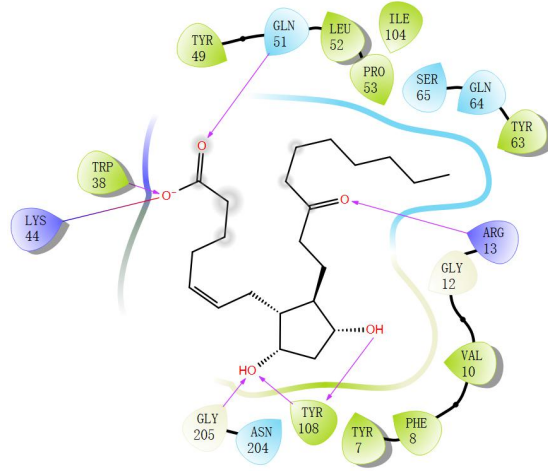
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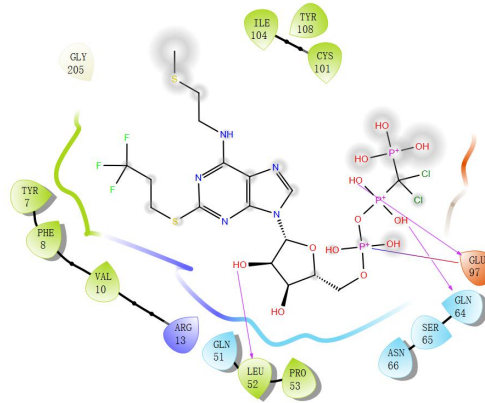
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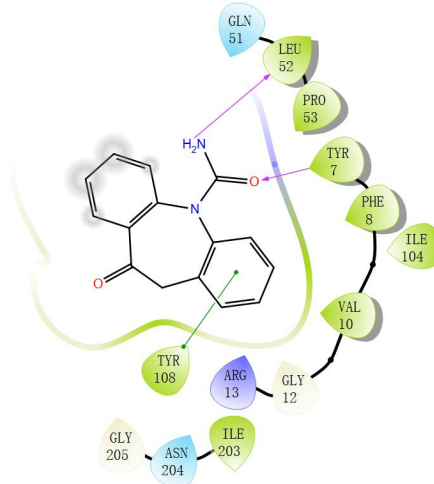
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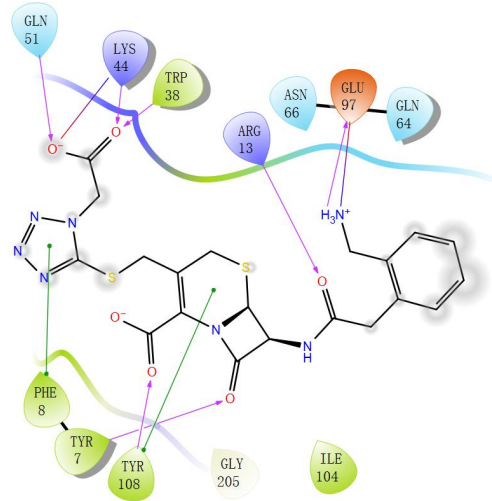
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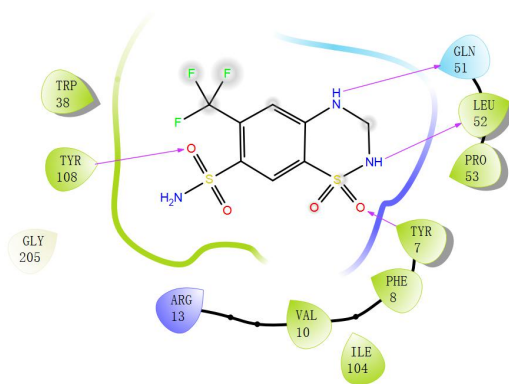
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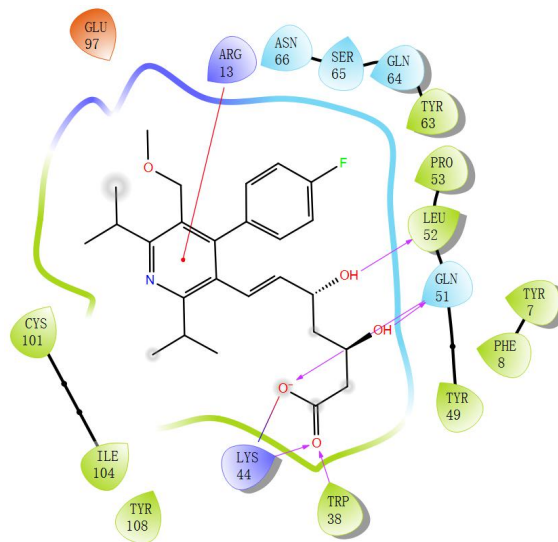
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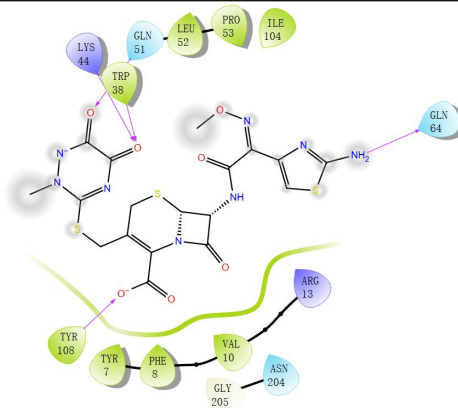
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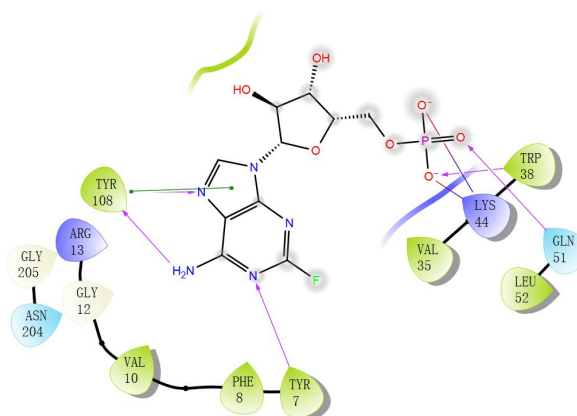
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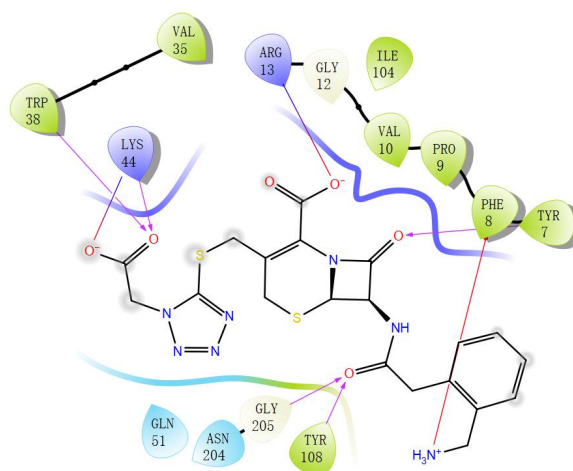
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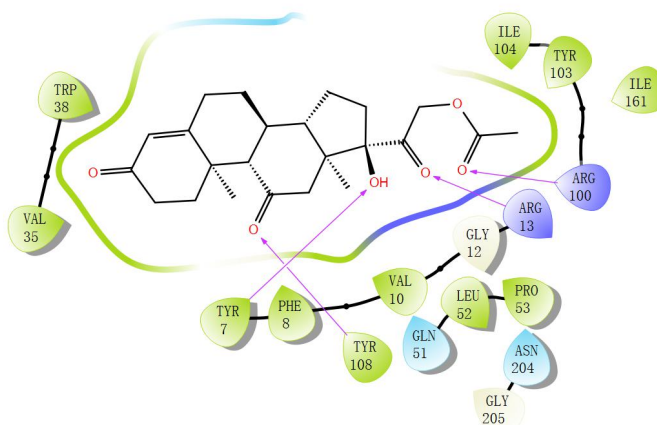
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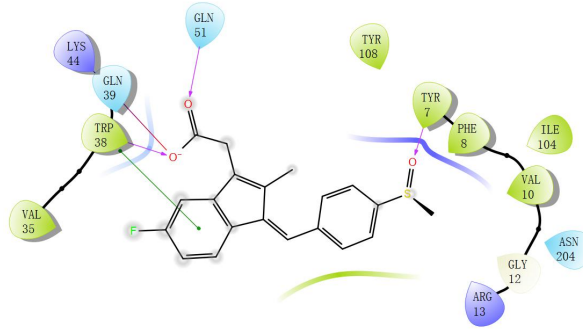
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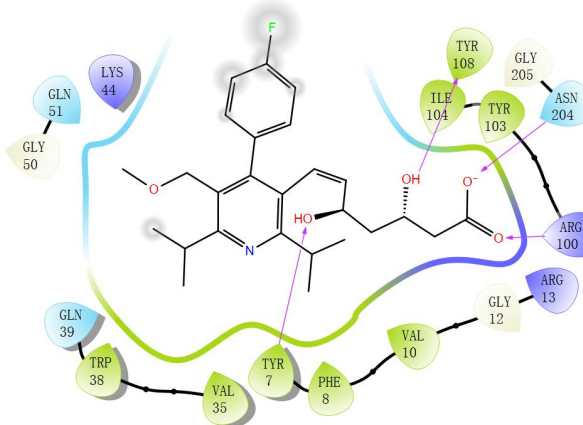
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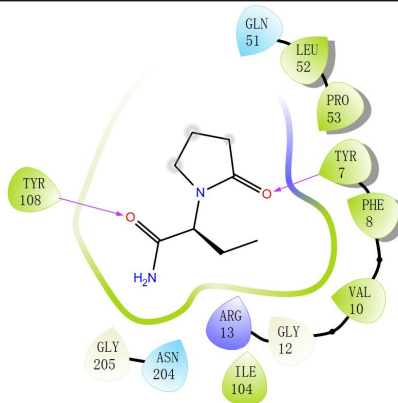
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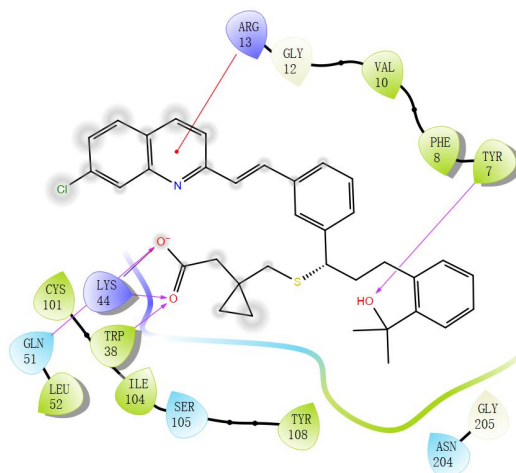
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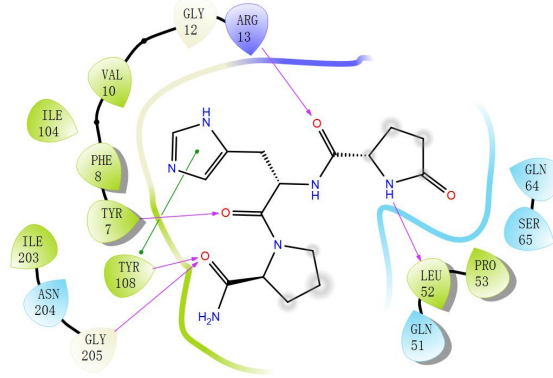
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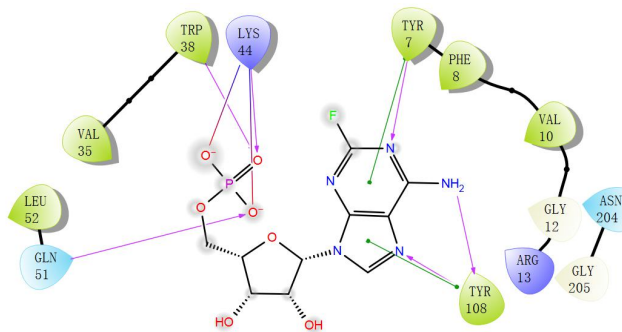
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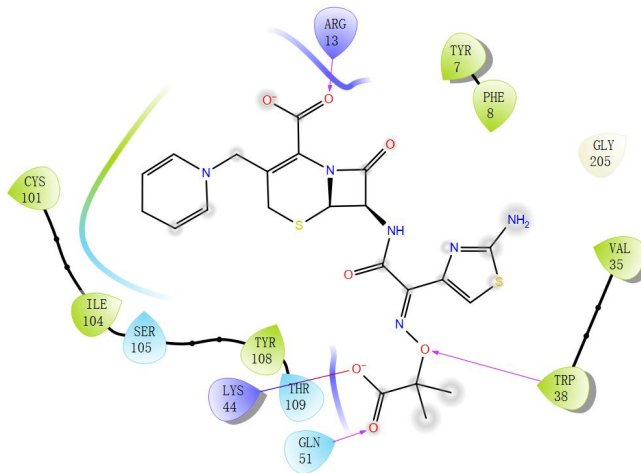
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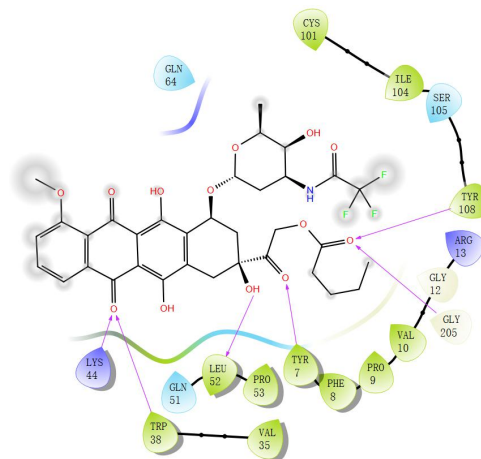
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