

Discovery of new dual binding TNKS inhibitors of Wnt Signaling Inhibition by pharmacophore modeling, molecular docking and bioassay

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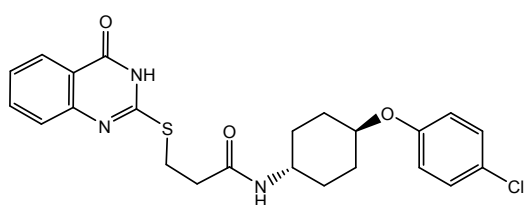
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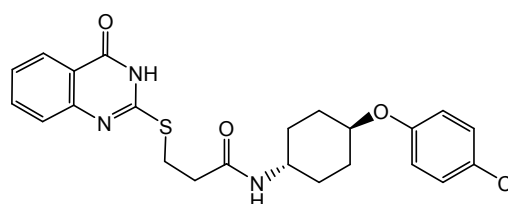
Supporting Information

The Structures and Active Information of Test Set Molecules

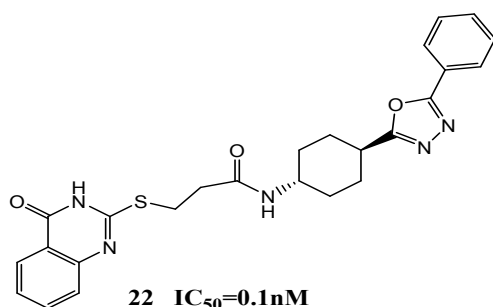
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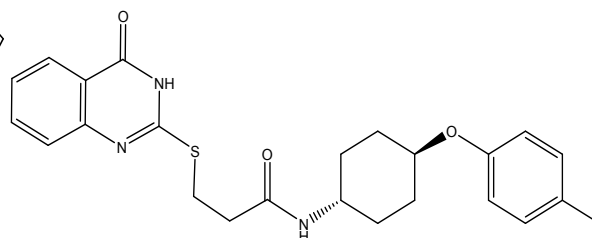
49 IC₅₀=0.1nM



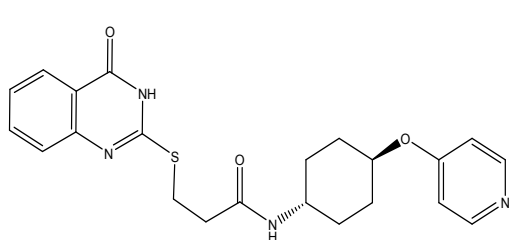
48 IC₅₀=0.1nM



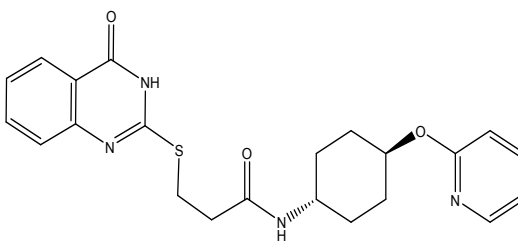
22 IC₅₀=0.1nM



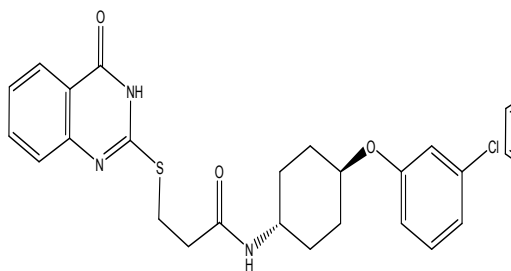
47 IC₅₀=0.2nM



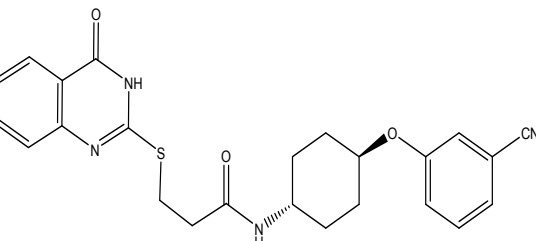
50 $IC_{50}=0.1nM$



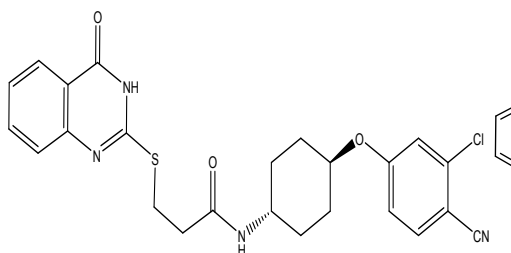
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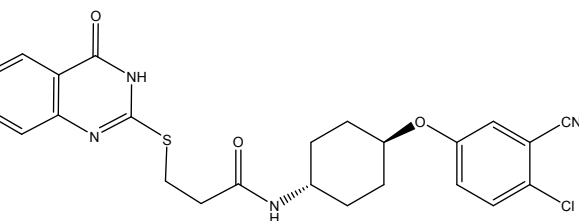
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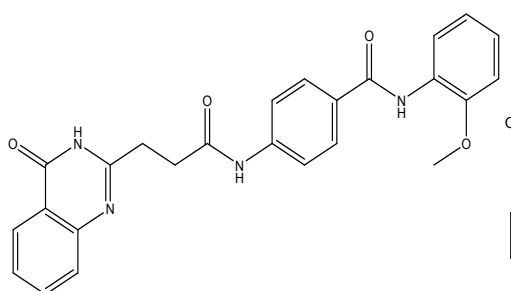
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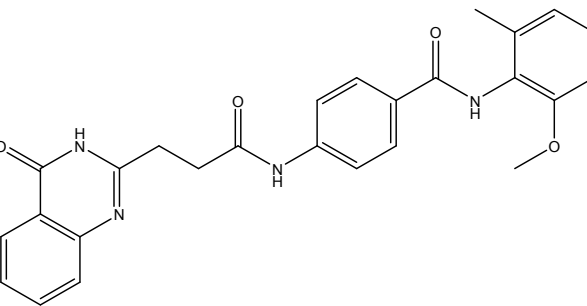
55 $IC_{50}=0.2nM$



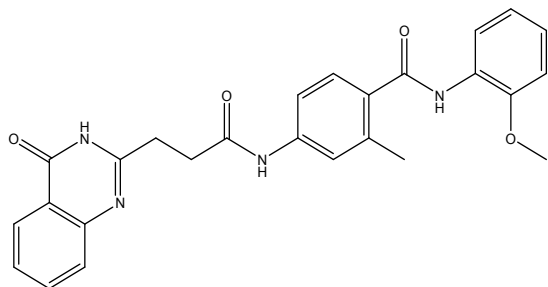
54 $IC_{50}=0.3nM$



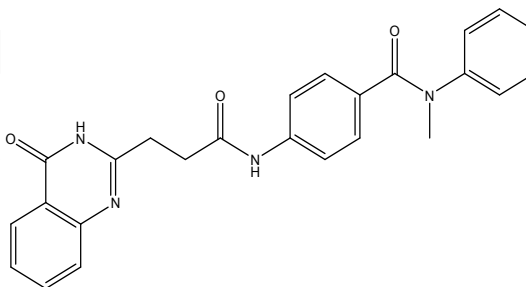
8 $IC_{50}=10nM$



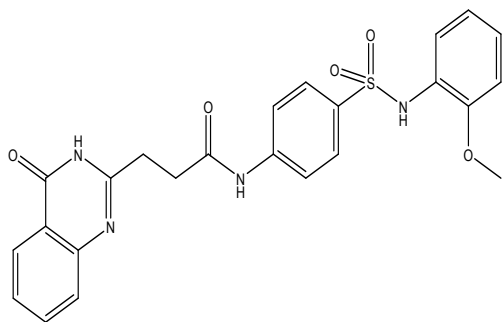
23 $IC_{50}=1.75\mu M$



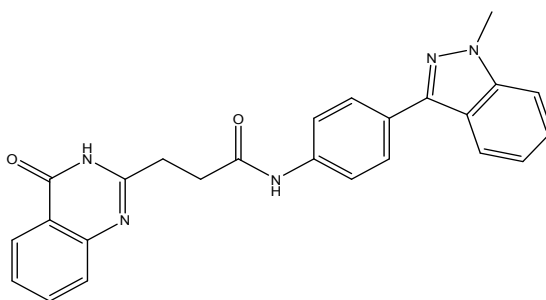
24 $IC_{50}=0.21\mu M$



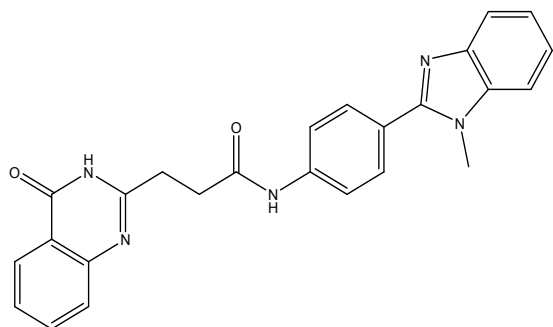
25 $IC_{50}=0.40\mu M$



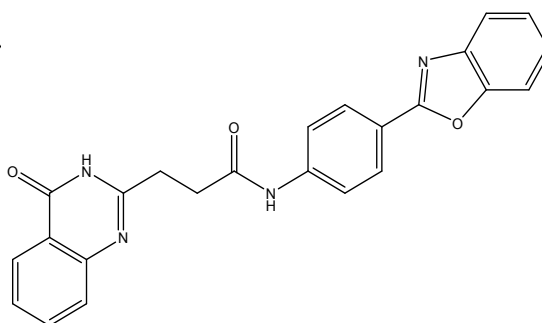
26 $IC_{50} > 46 \mu M$



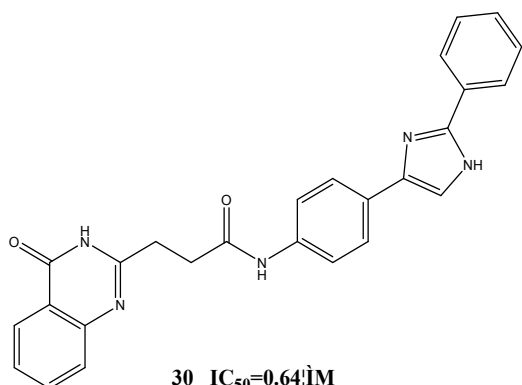
27 $IC_{50} = 0.40 \mu M$



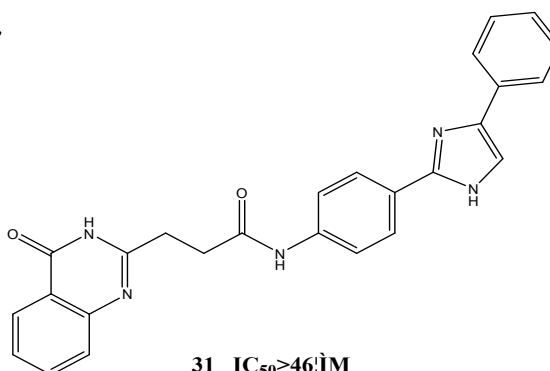
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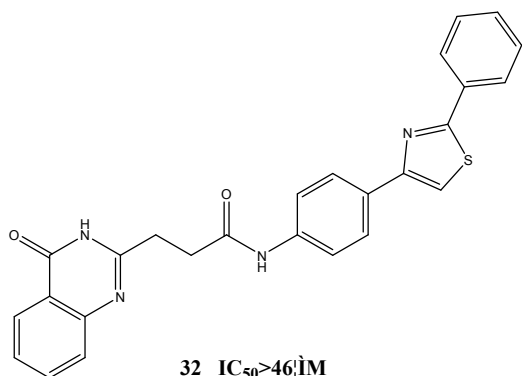
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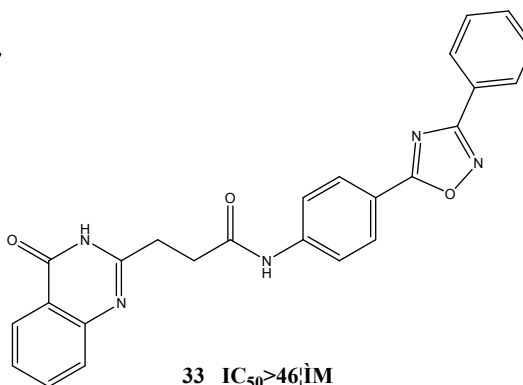
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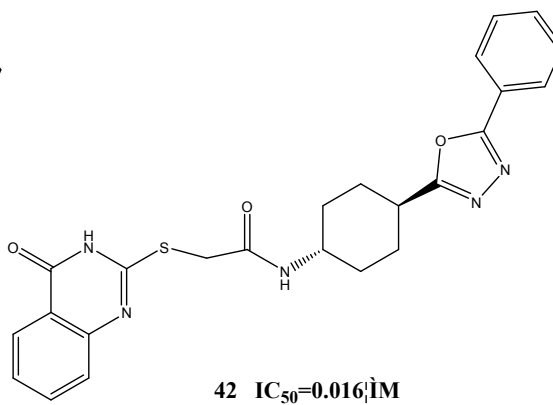
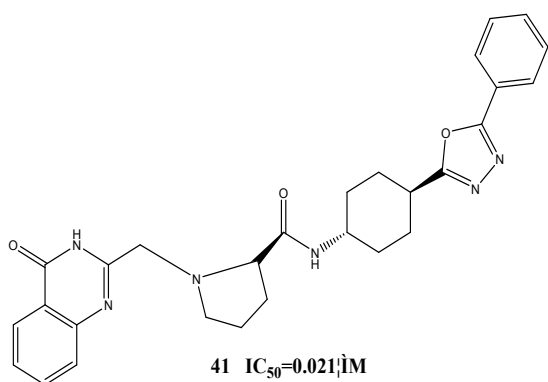
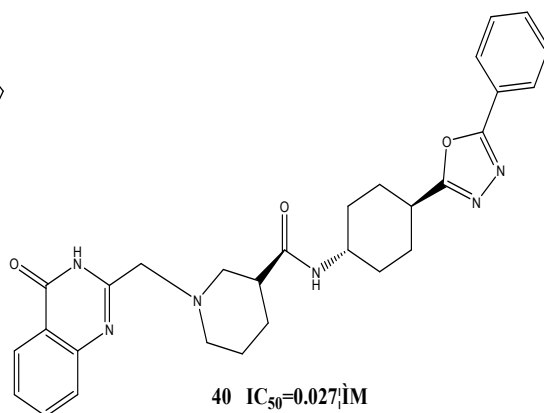
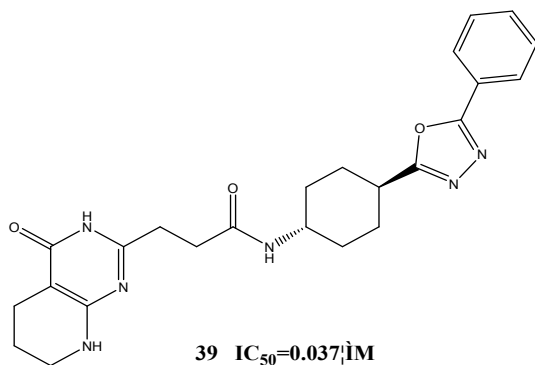
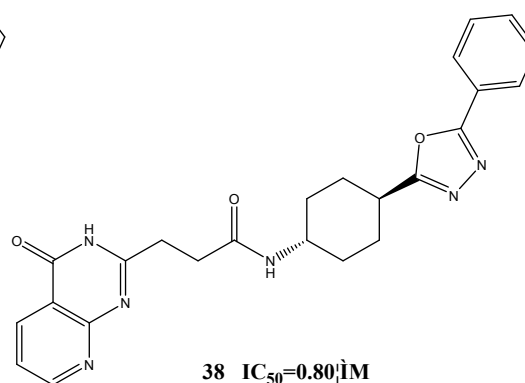
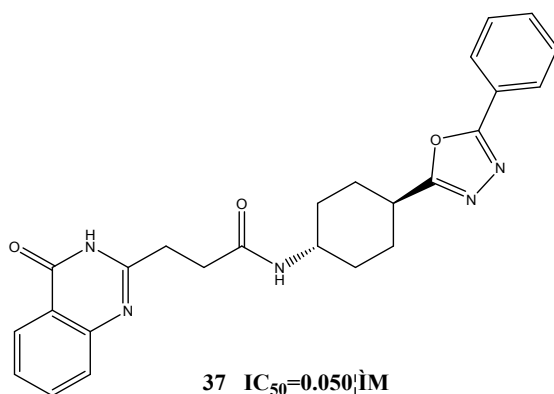
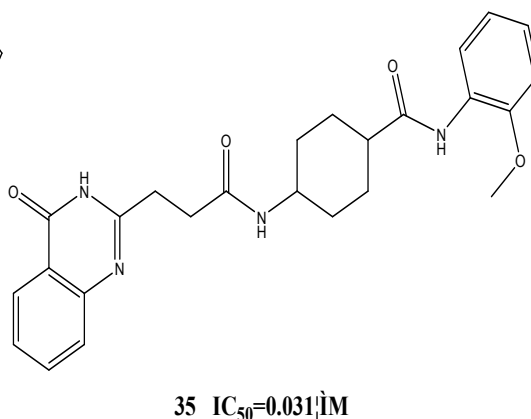
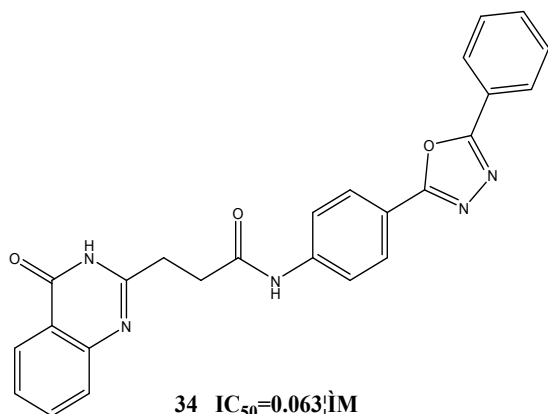
31 $IC_{50} > 46 \mu M$

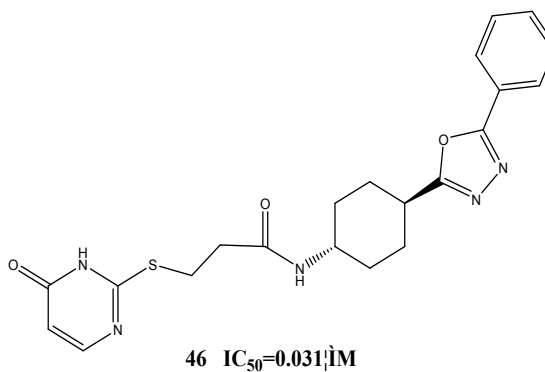
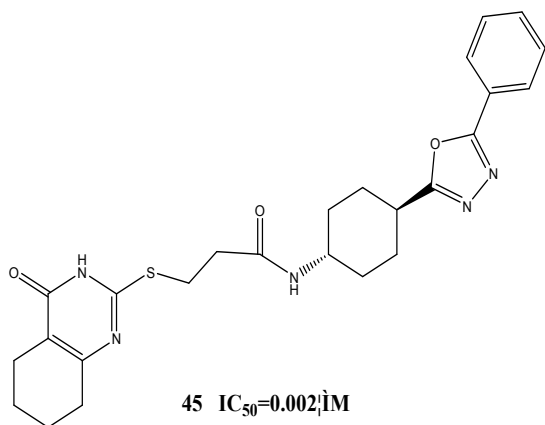
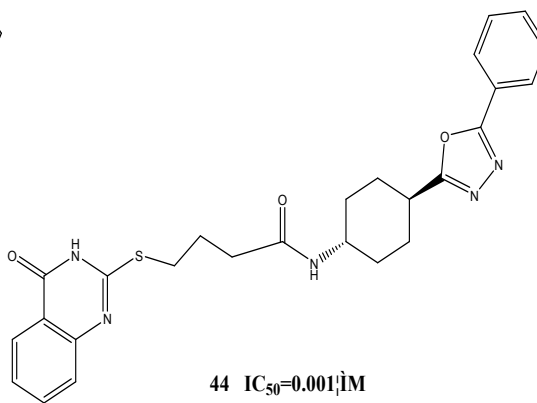
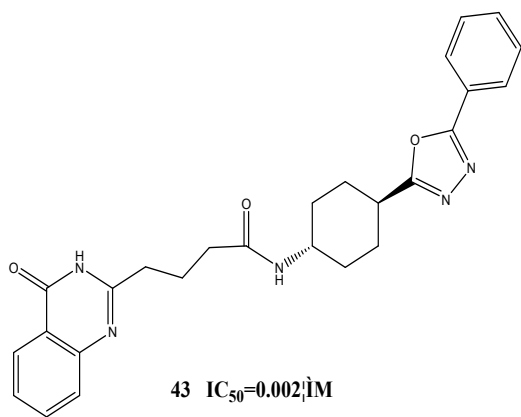


32 $IC_{50} > 46 \mu M$

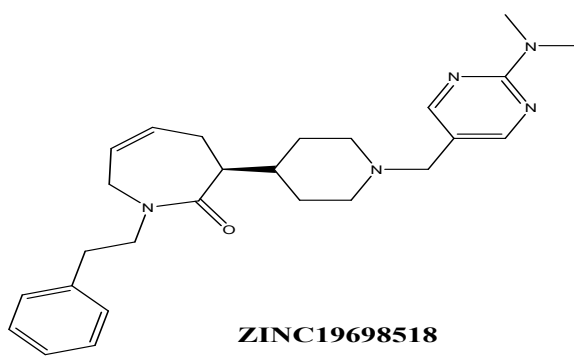
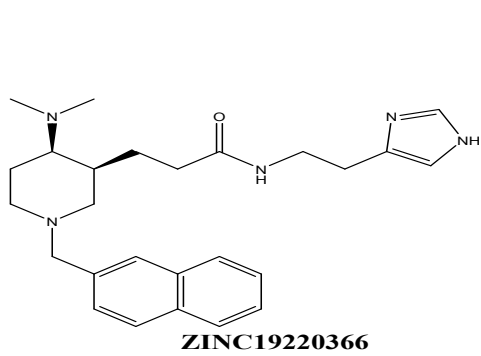


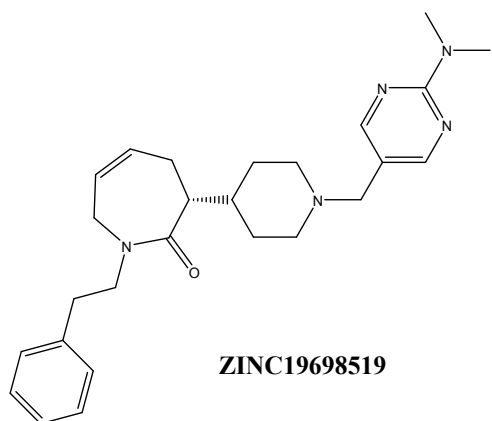
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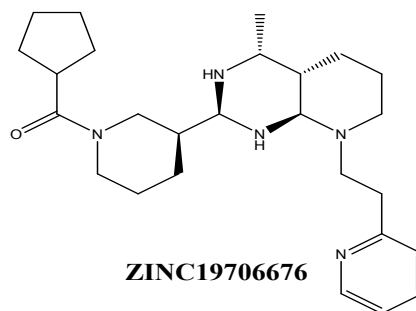


2. Inactive Molecules

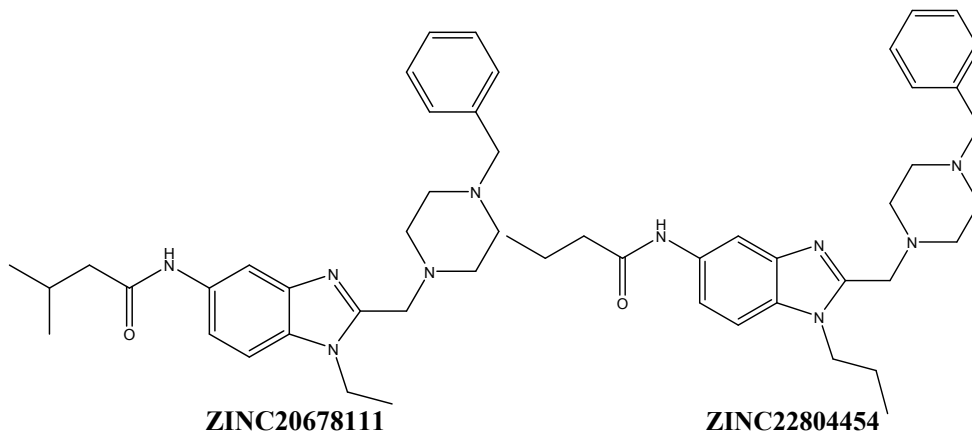




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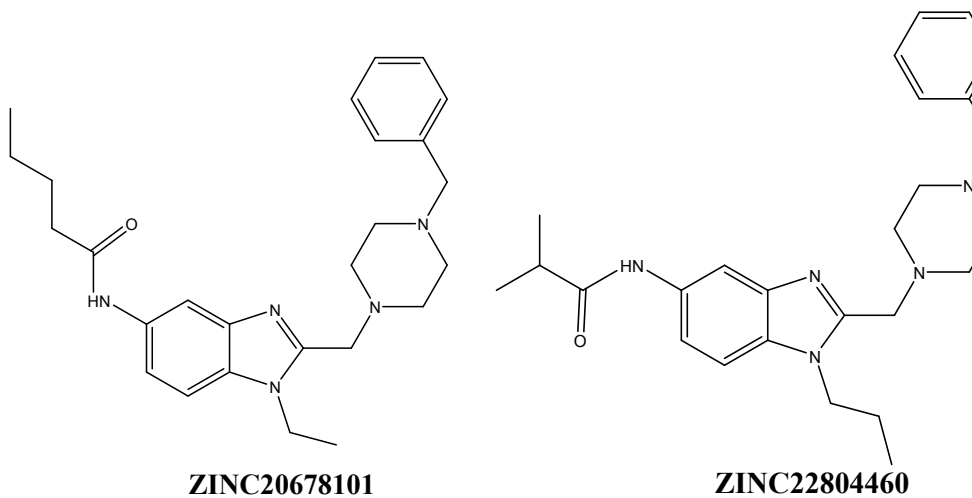


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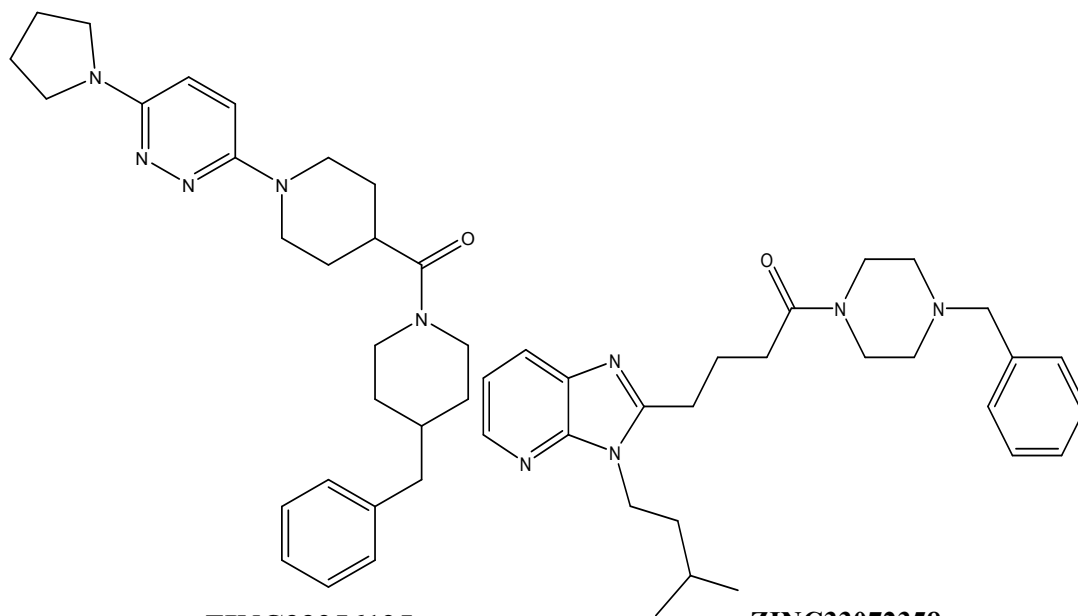
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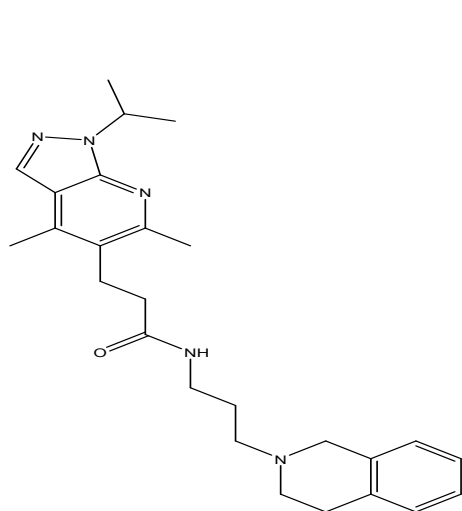
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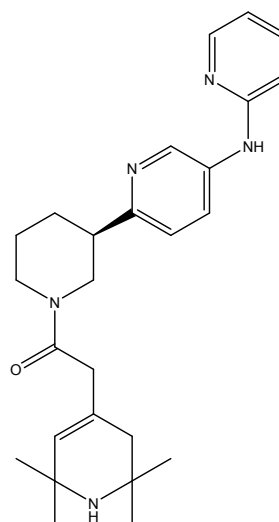


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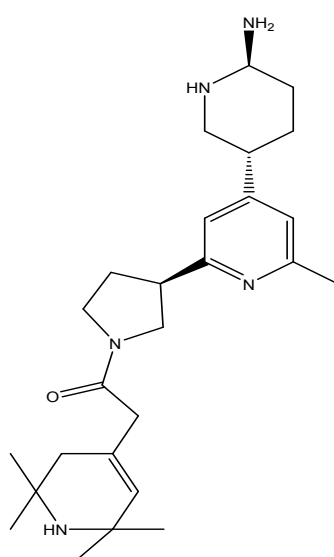
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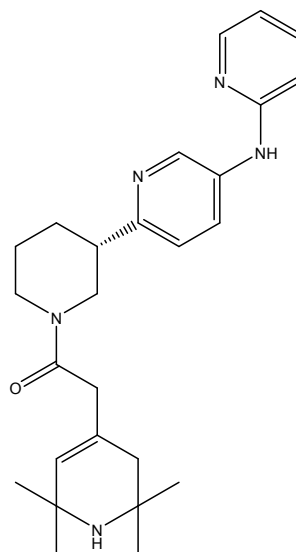
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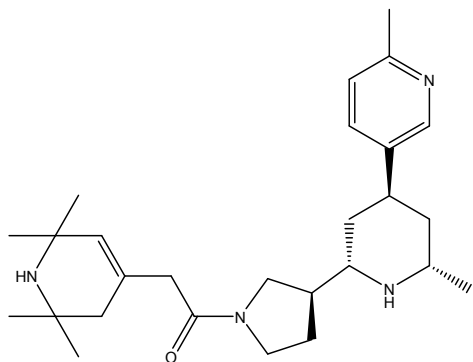
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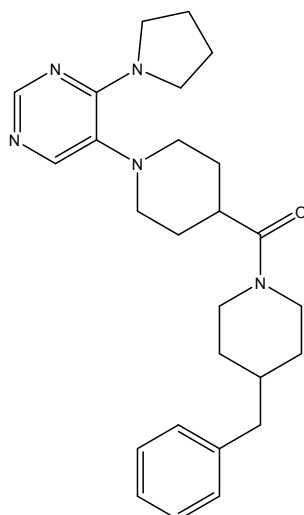
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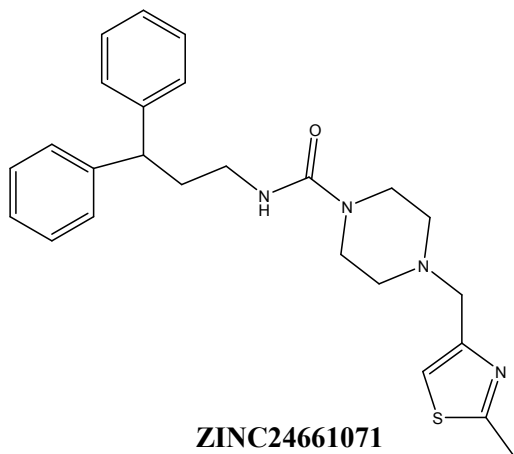
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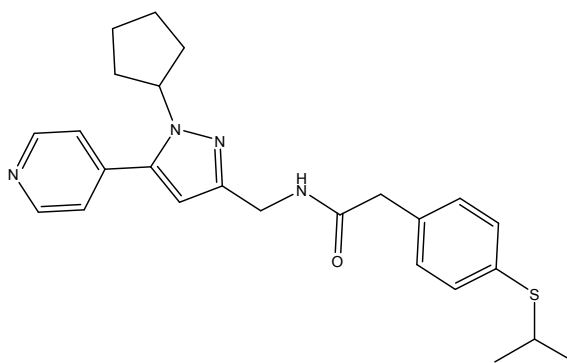
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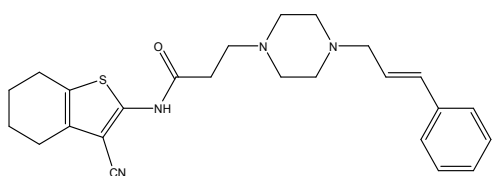
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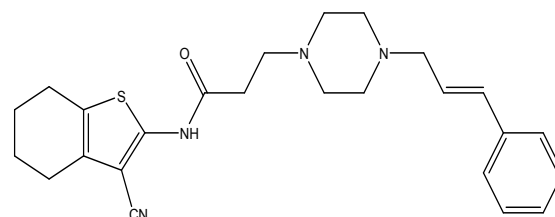
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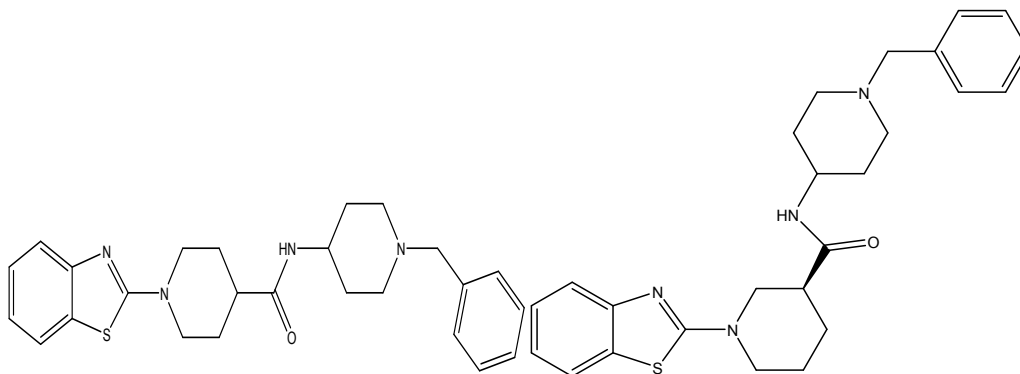
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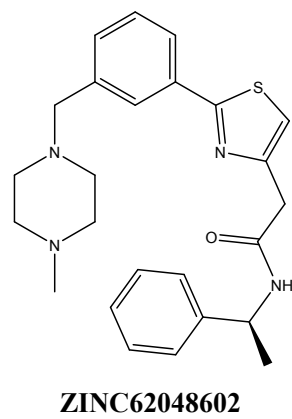
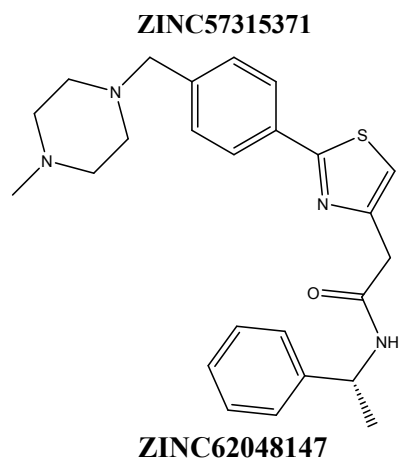
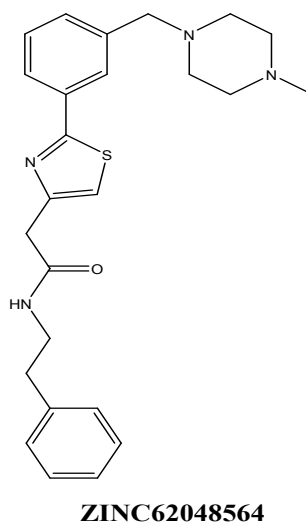
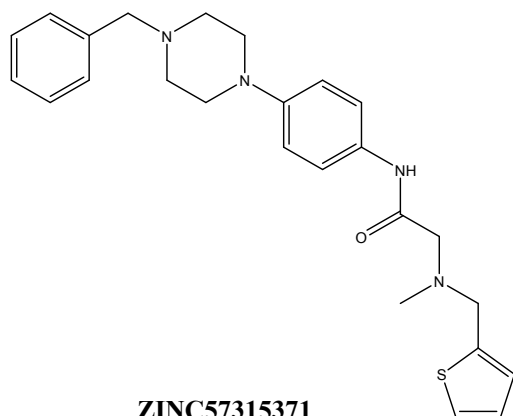
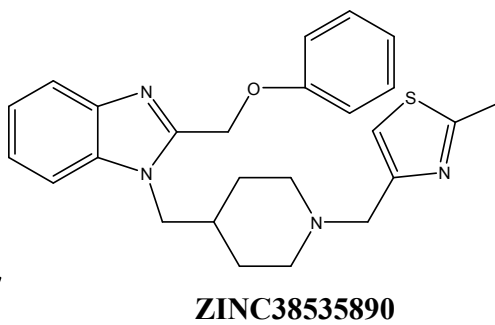
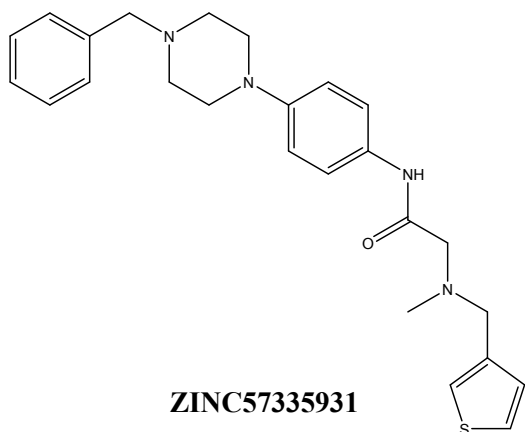


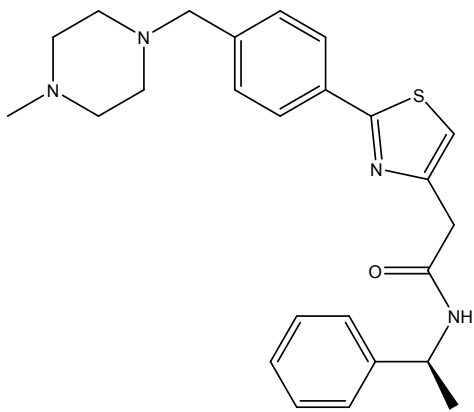
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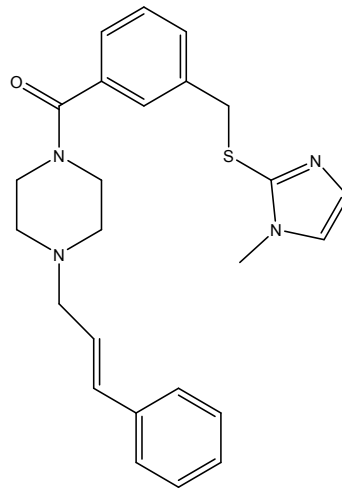
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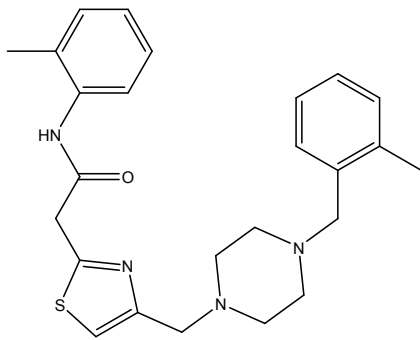




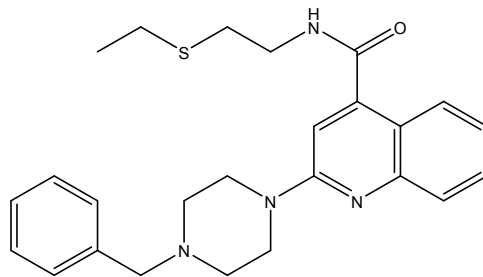
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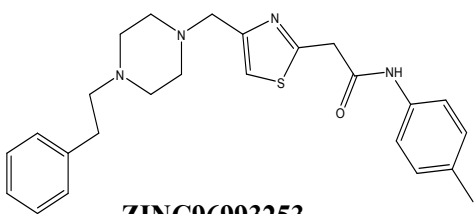
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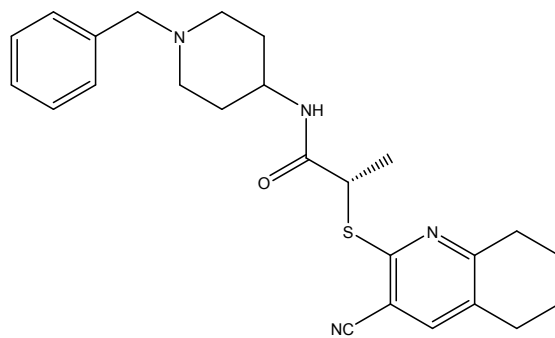
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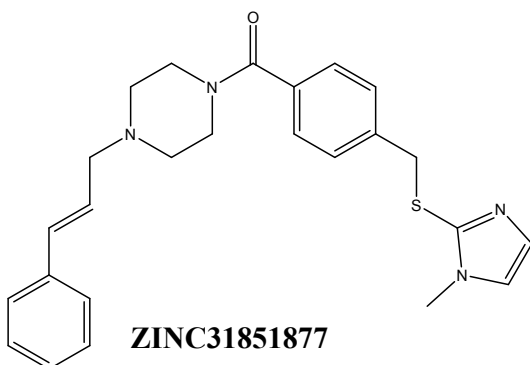
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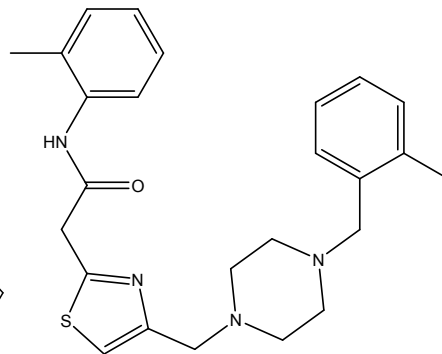
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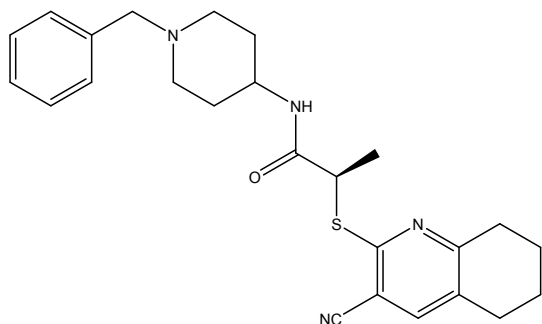
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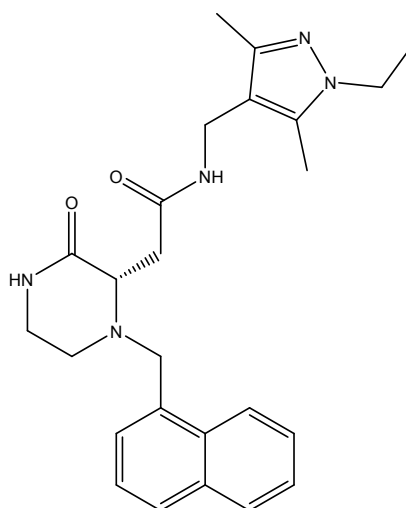
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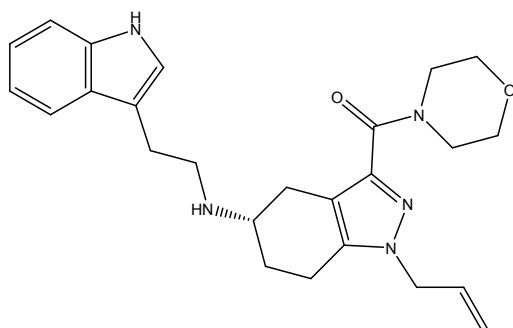
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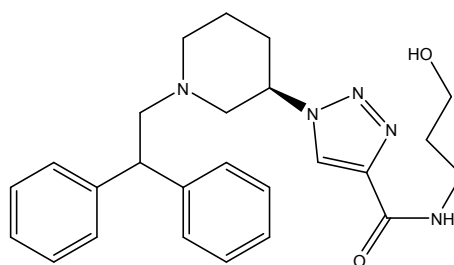
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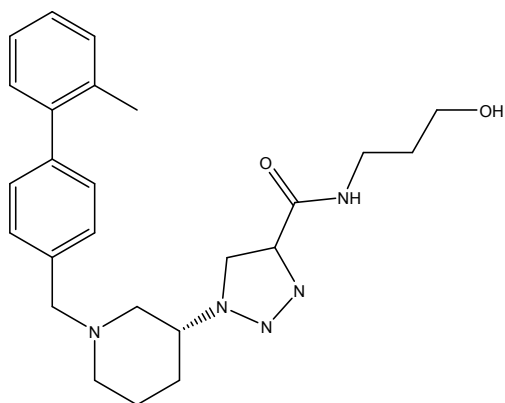
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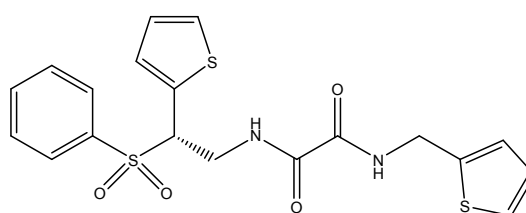
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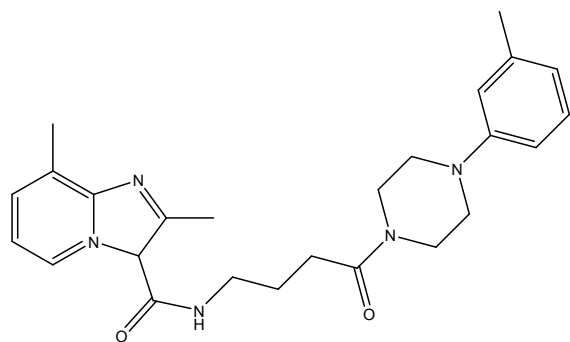
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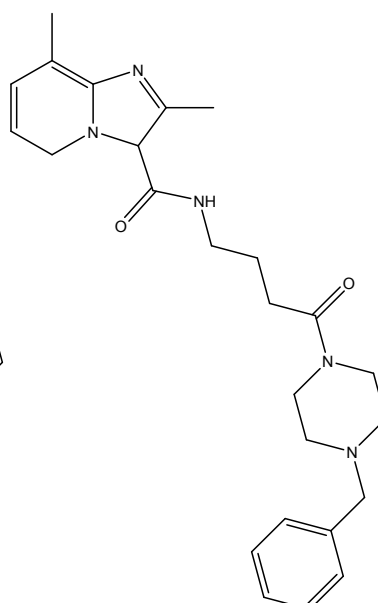
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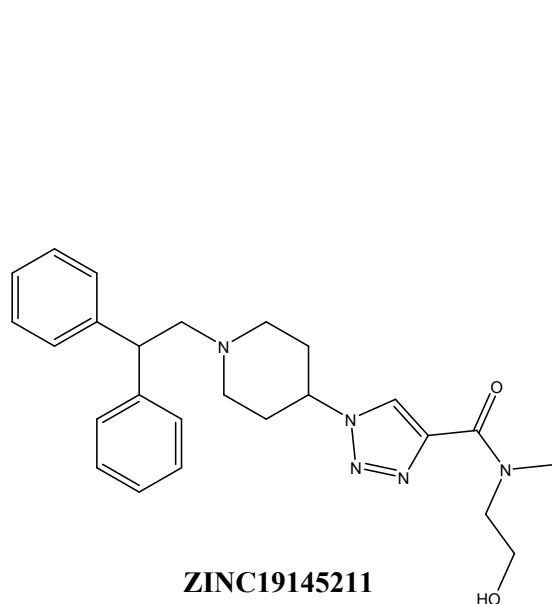
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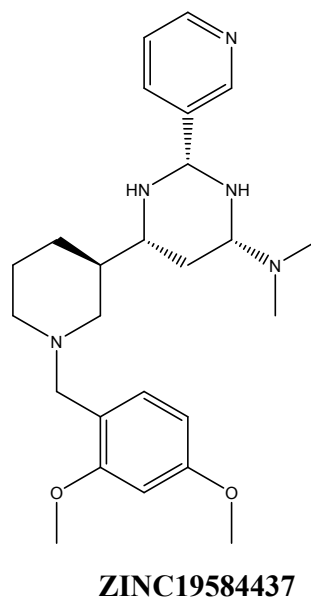
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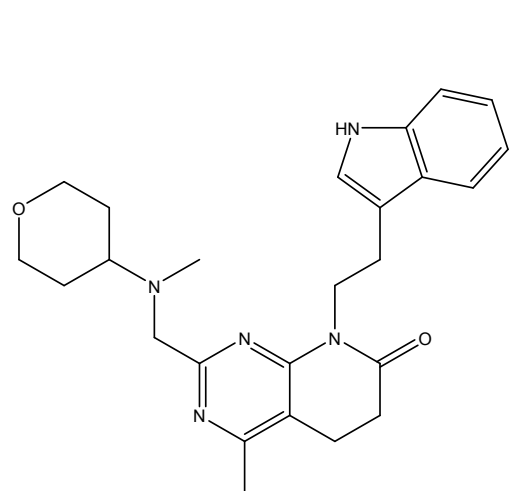
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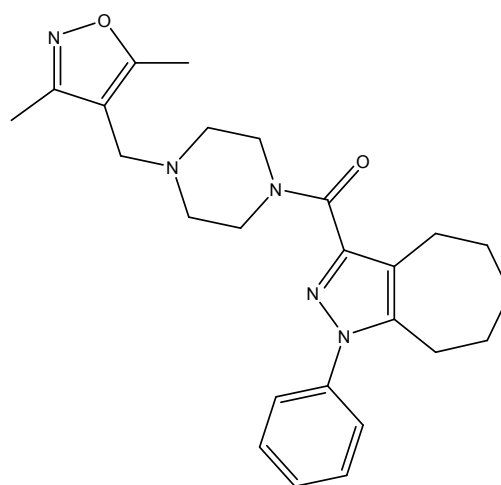
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