

Supporting Information

Structure-Based Virtual Screening of Small-Molecule Antagonists of Platelet Integrin $\alpha\text{IIb}\beta\text{3}$ that Do Not Prime the Receptor to Bind Ligand

Ana Negri, Jihong Li, Sarasija Naini, Barry S. Coller, and Marta Filizola

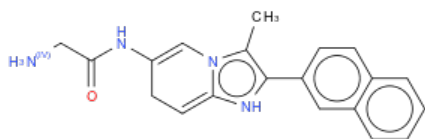
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Table S1

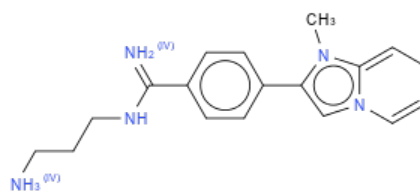
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1	<p>Chiral</p> <p>C13727245</p>	C13727245	2	<p>Chiral</p> <p>C13727253</p>	C13727253
3	<p>H</p> <p>Chiral</p> <p>C35483153</p> <p>H</p>	C35483153	4	<p>C20799873</p>	C20799873
5	<p>Chiral</p> <p>C13727248</p>	C13727248	6	<p>C00001763</p>	C00001763
7	<p>H H</p> <p>Chiral</p> <p>C32051969</p> <p>H</p>	C32051969	8	<p>Chiral</p> <p>C05394736</p>	C05394736

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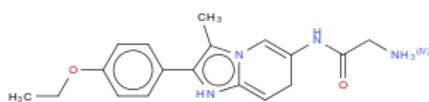
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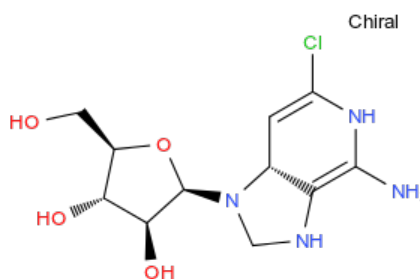
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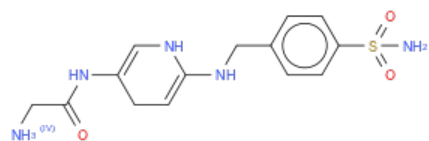
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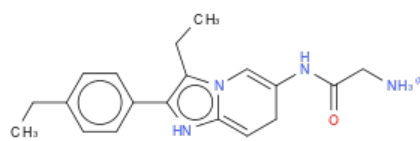
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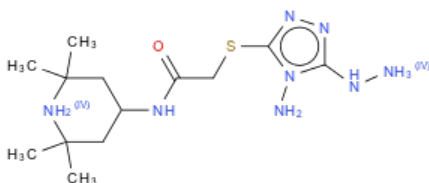
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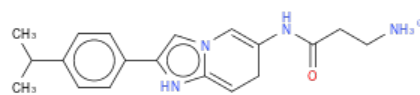
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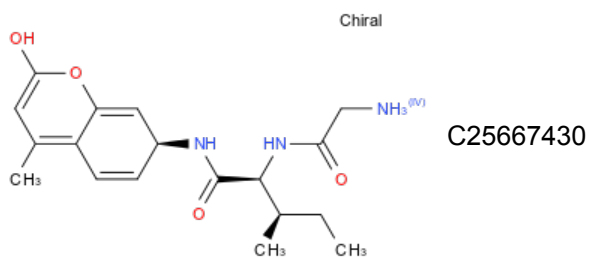
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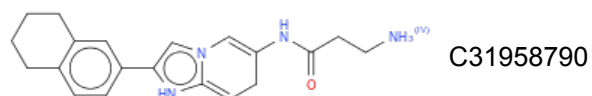


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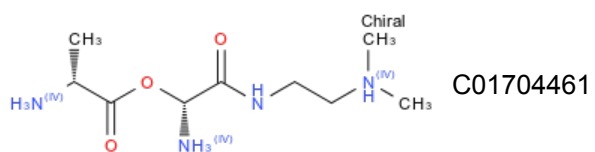
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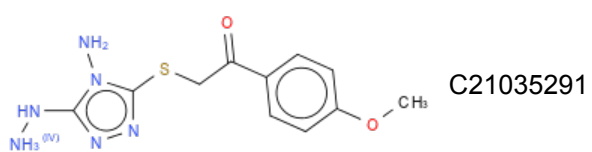
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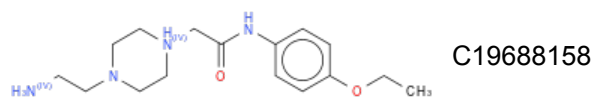
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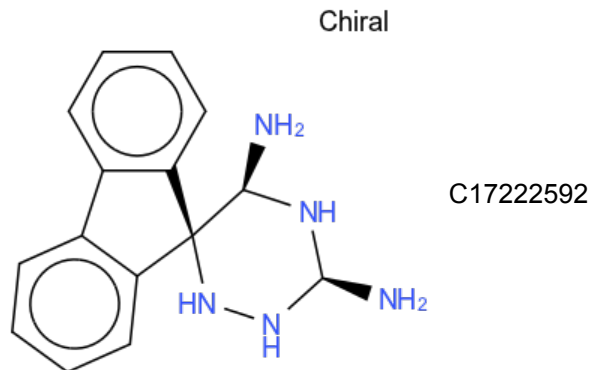
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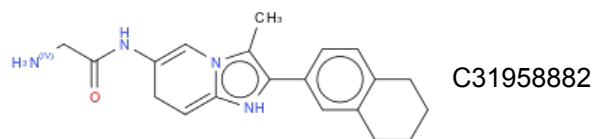
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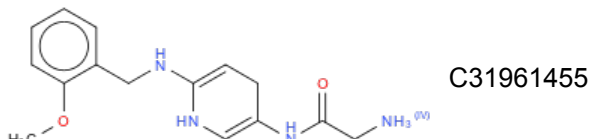
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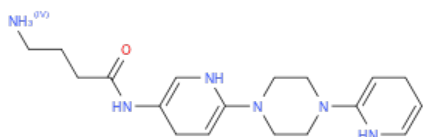
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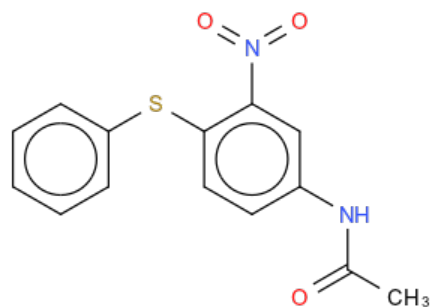


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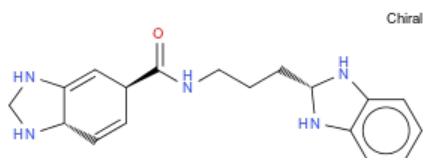
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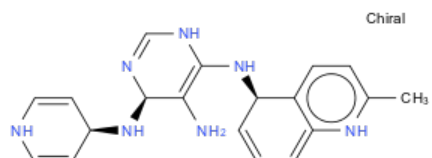
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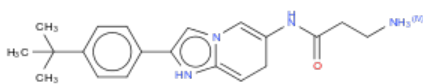
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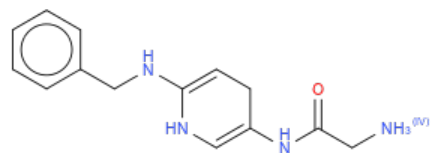
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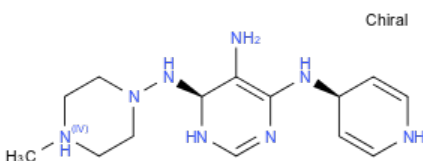
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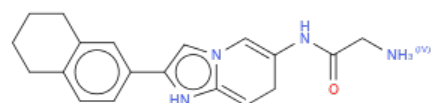
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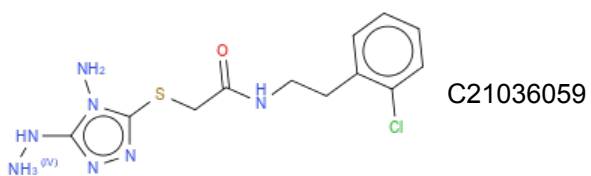
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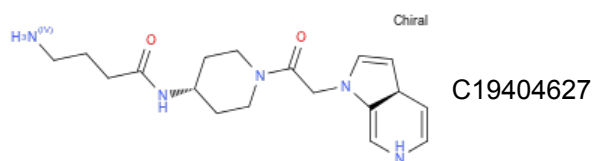


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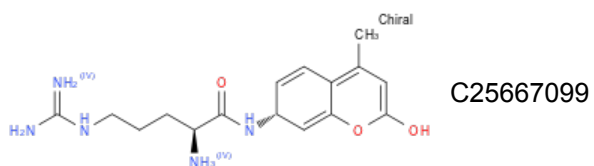
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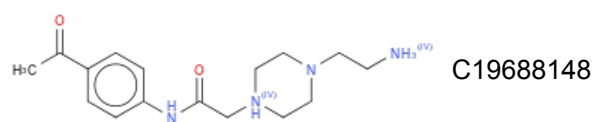
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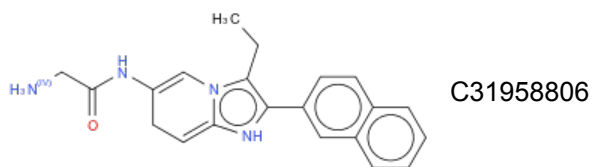
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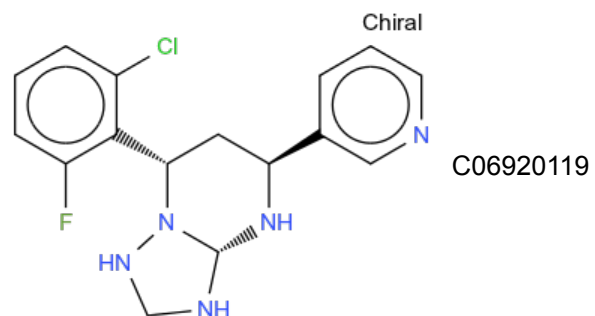
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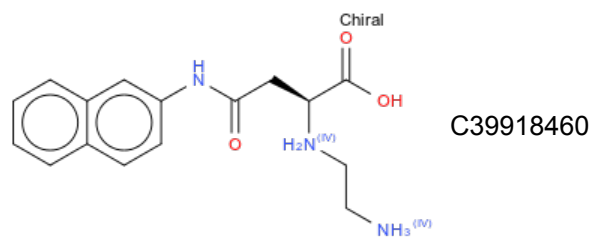
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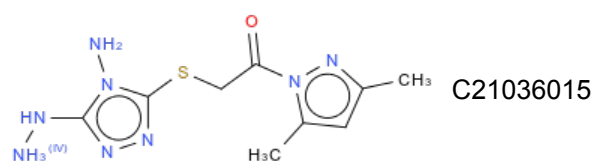
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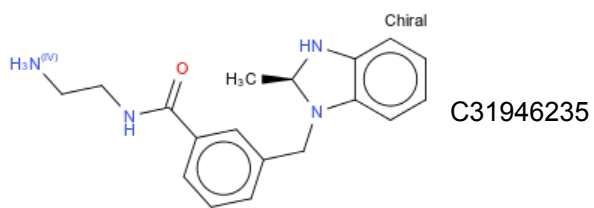
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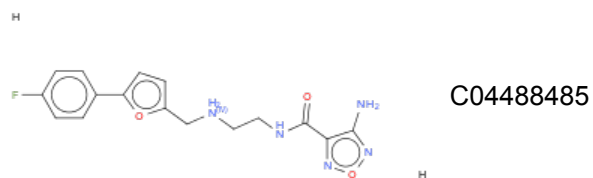
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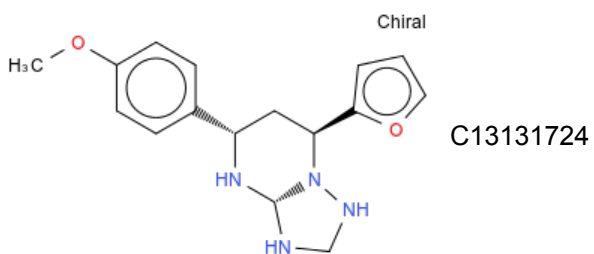
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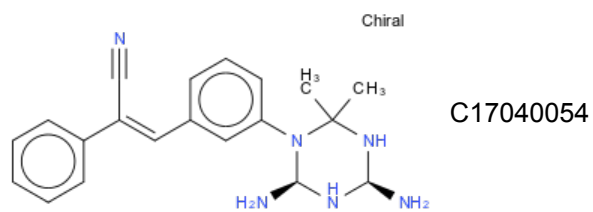
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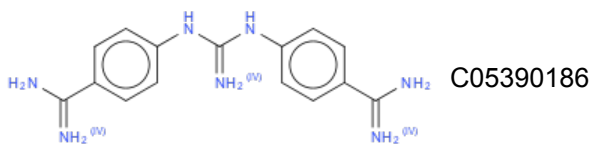
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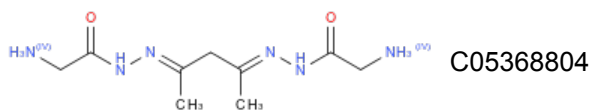
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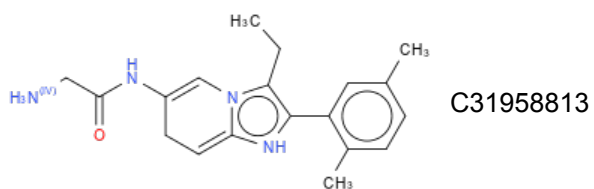
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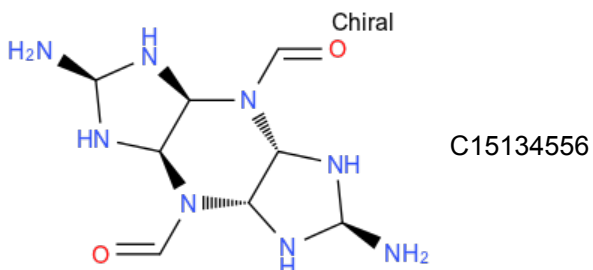
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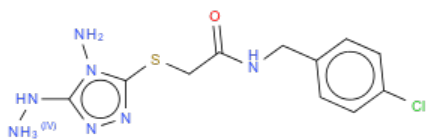
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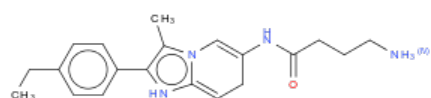


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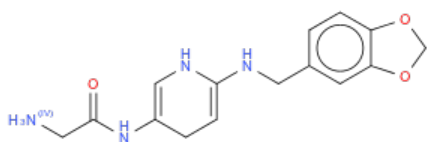
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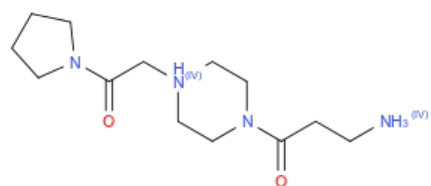
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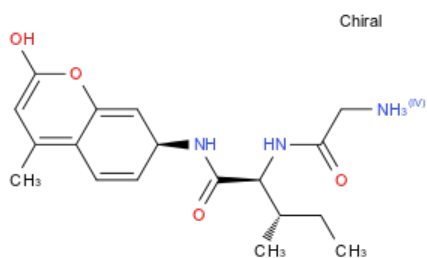
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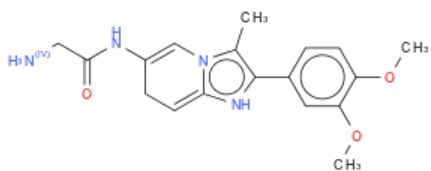
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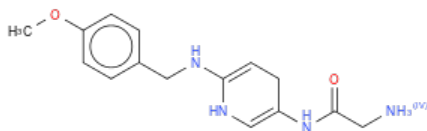
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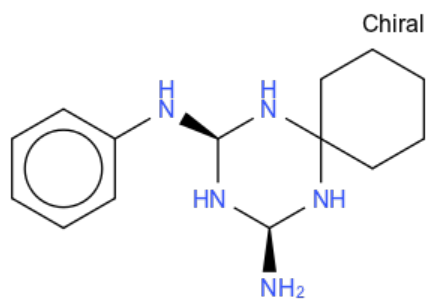
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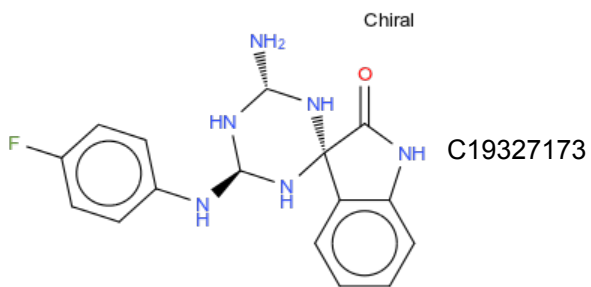
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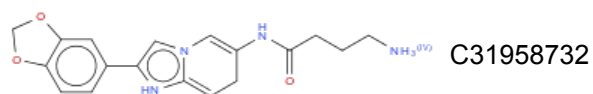


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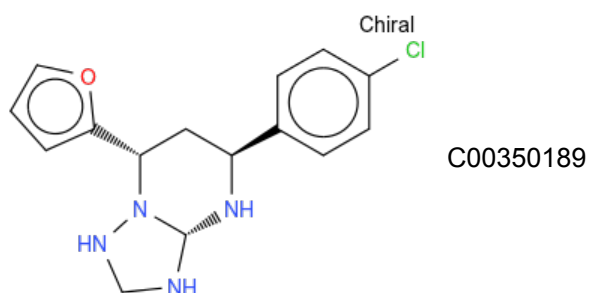
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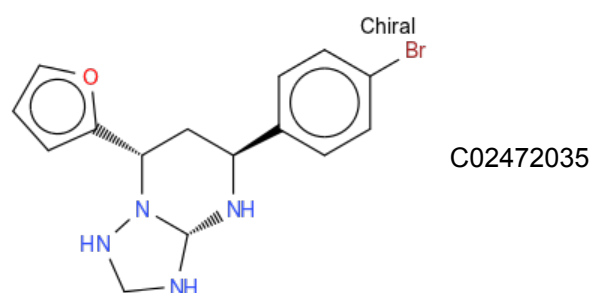
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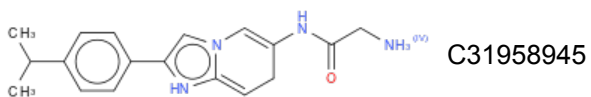
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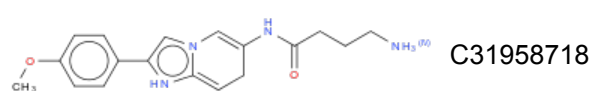
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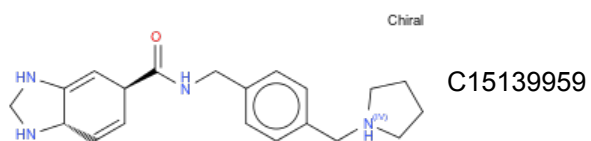
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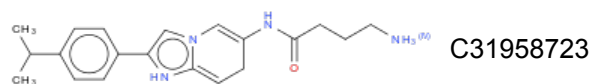
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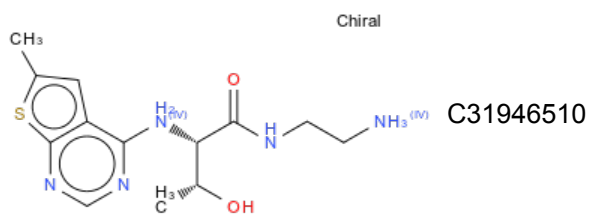
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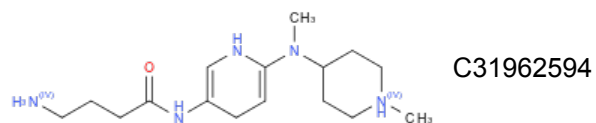
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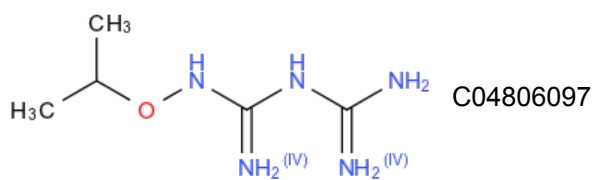
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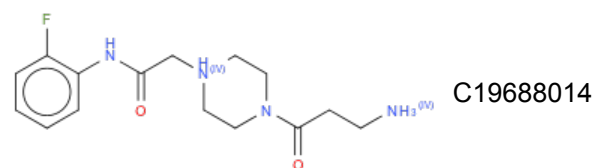
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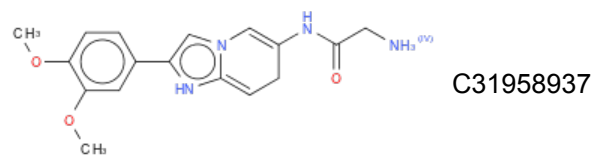
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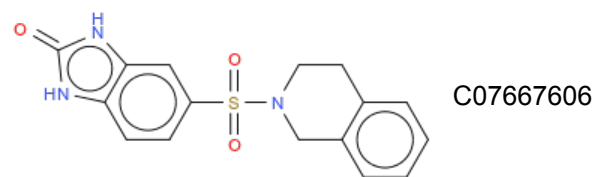
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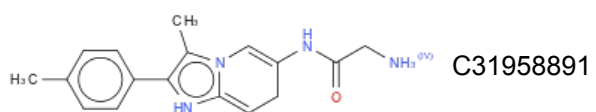
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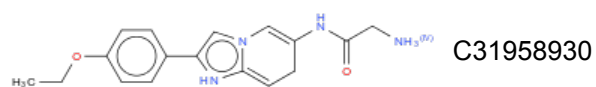
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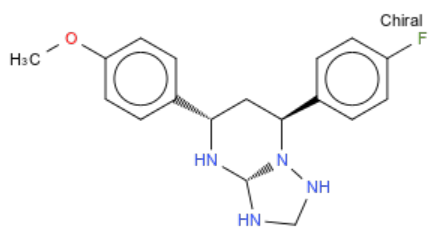
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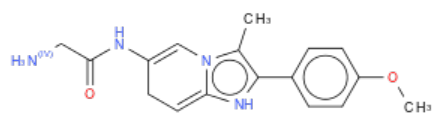


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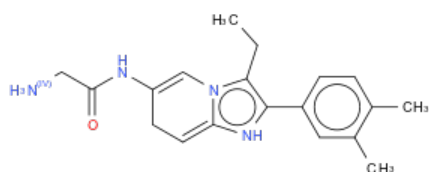
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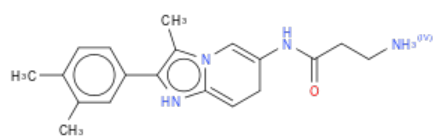
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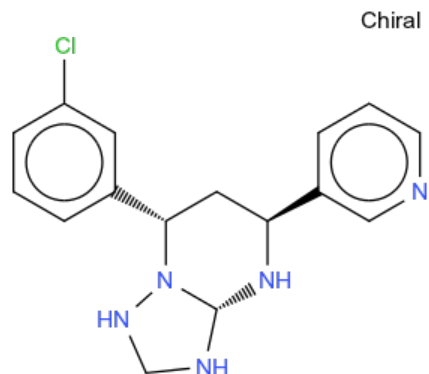
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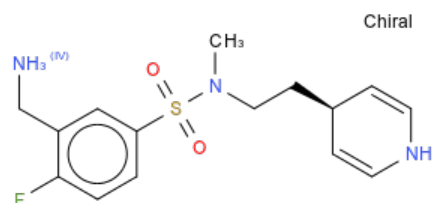
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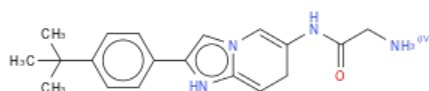
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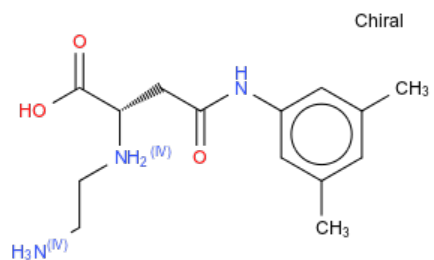
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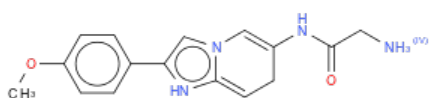
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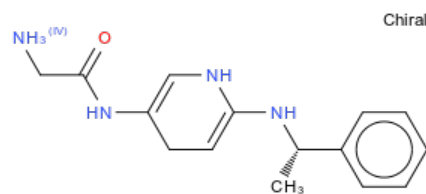
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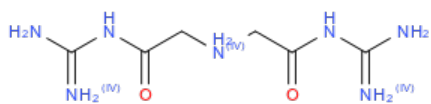
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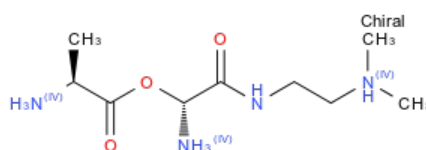
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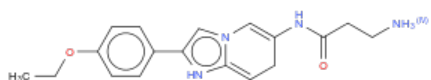
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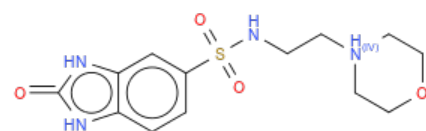
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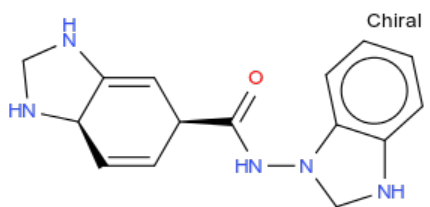
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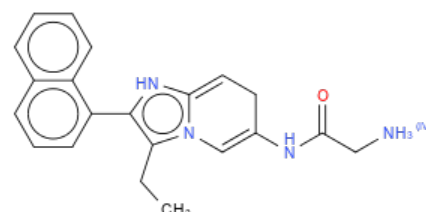
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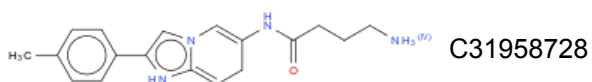
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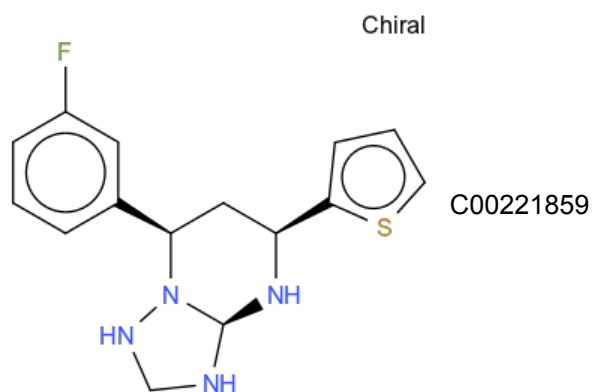


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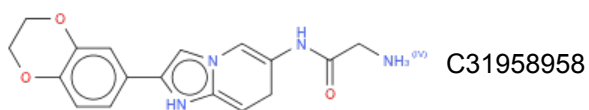
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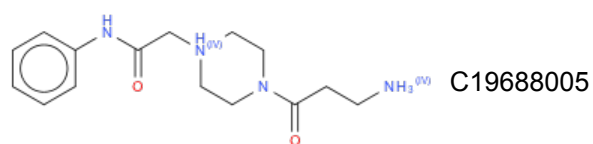
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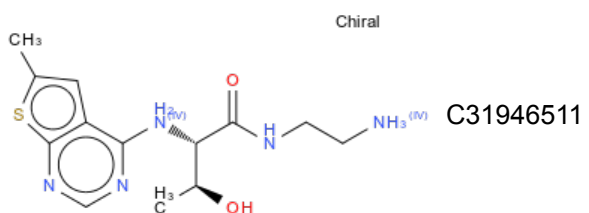
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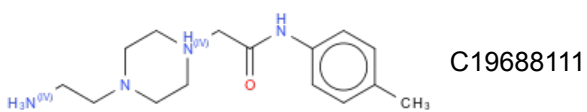
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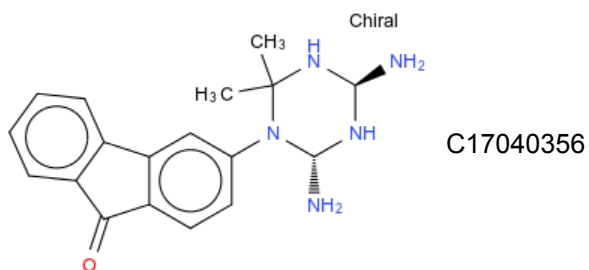
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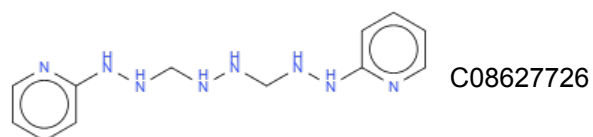
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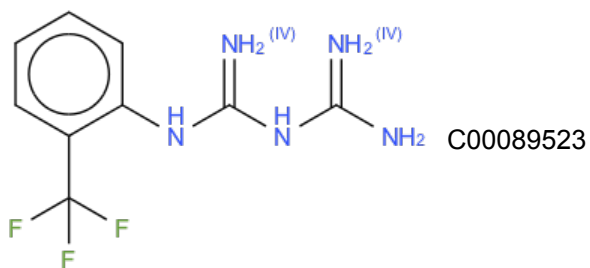
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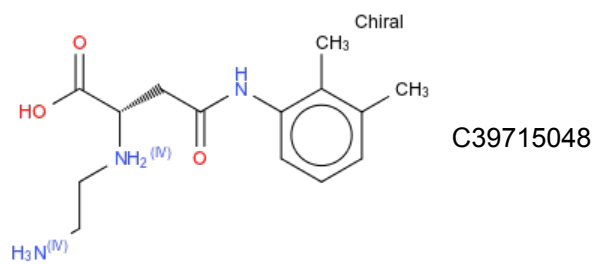
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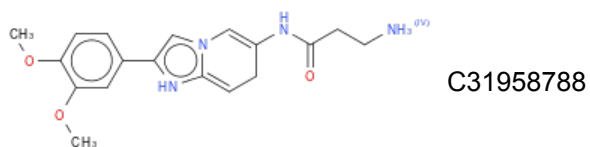
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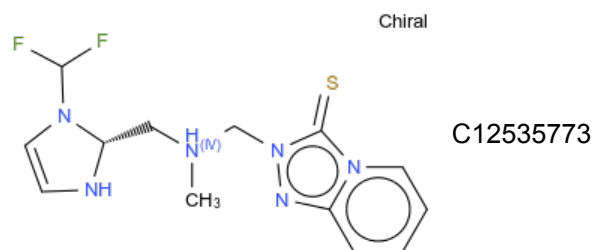
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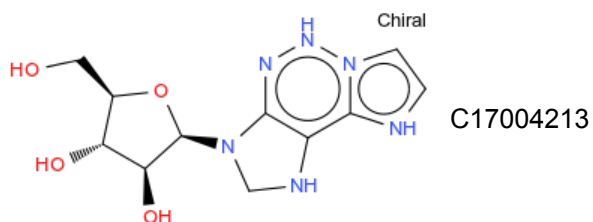
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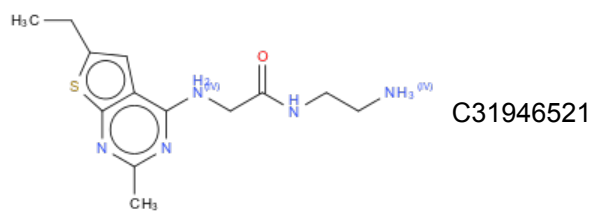
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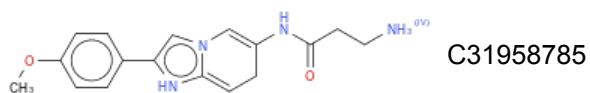
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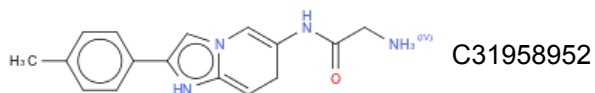
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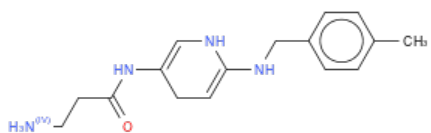
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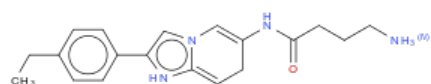


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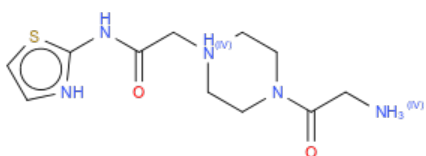
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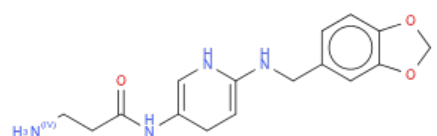
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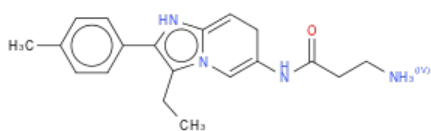
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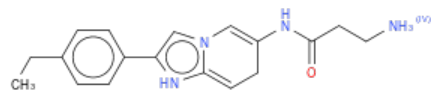
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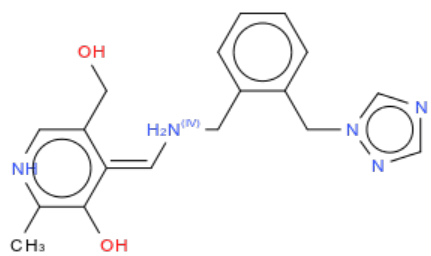
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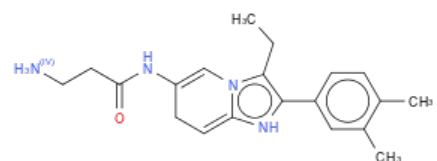
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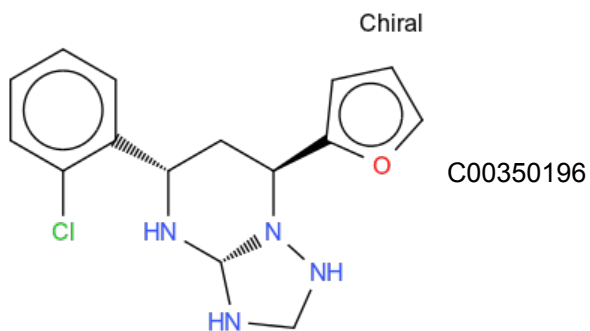
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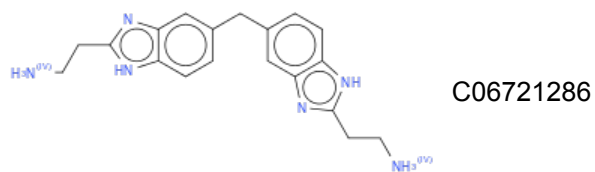


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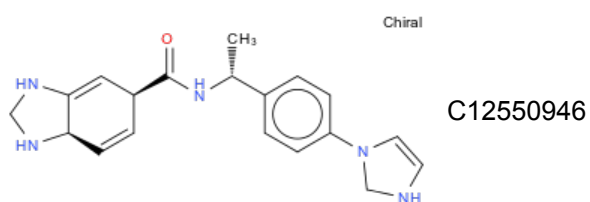
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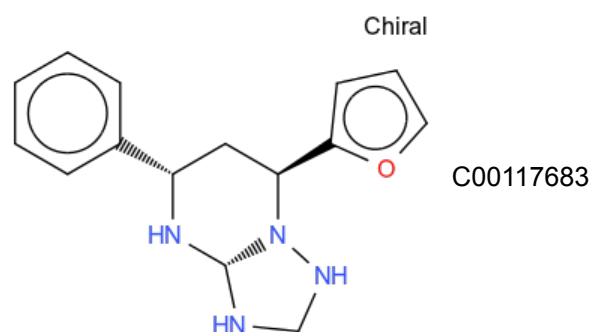
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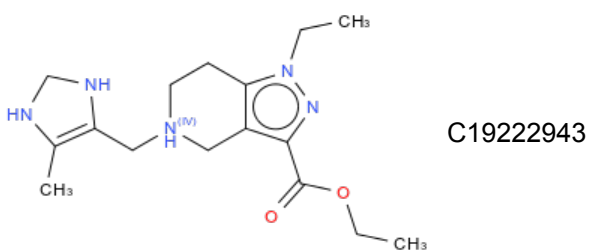
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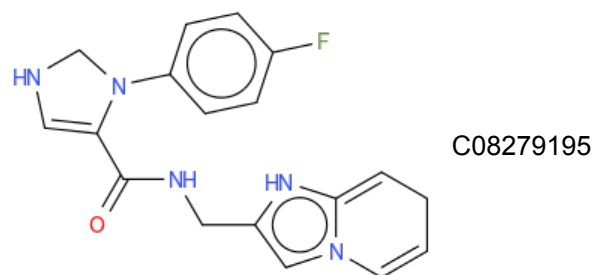
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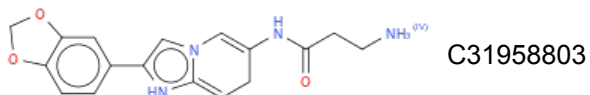
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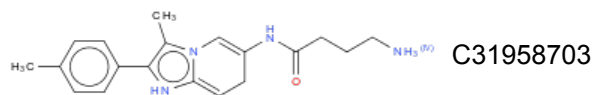
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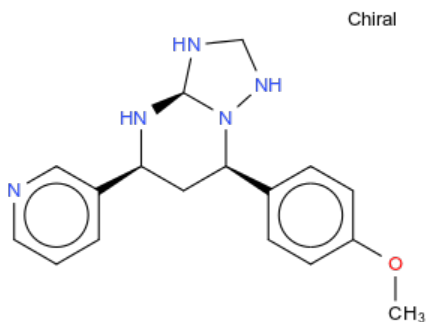
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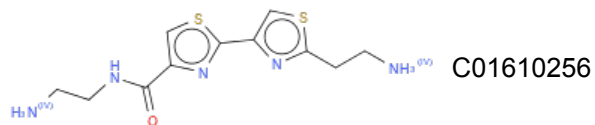
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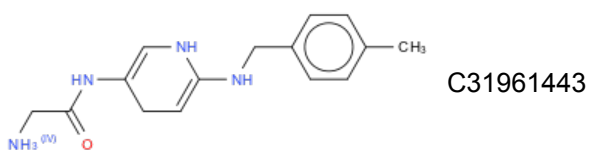
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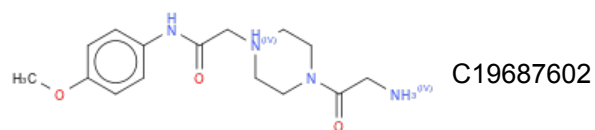
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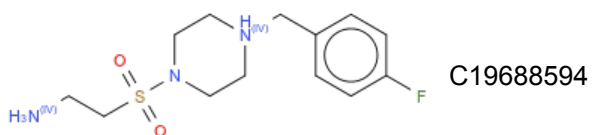
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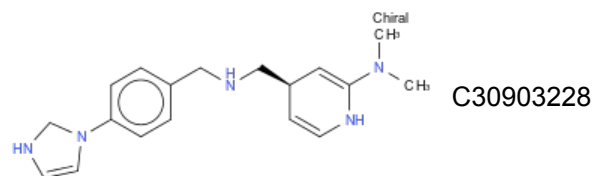
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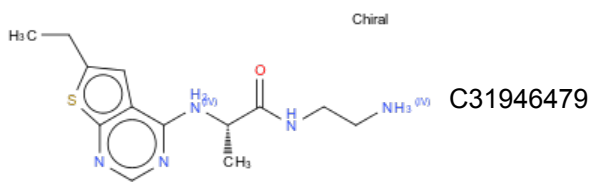
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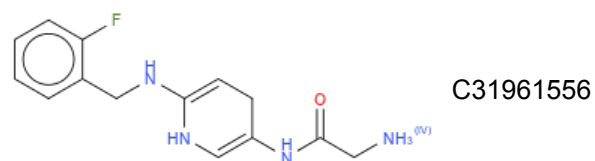
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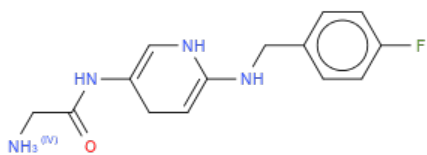
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128

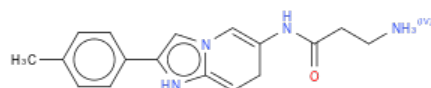


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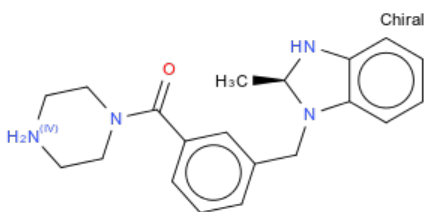
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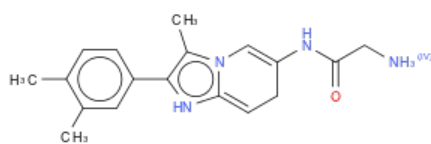
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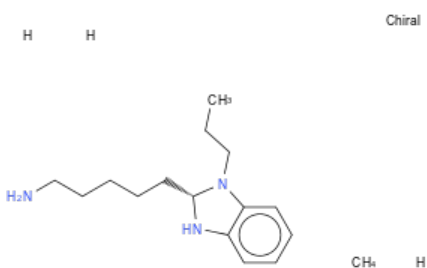
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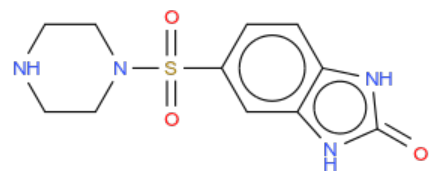
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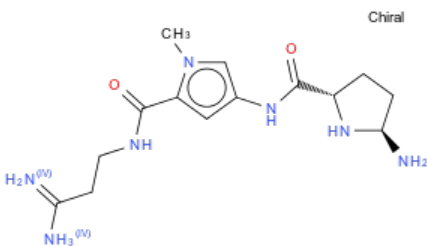
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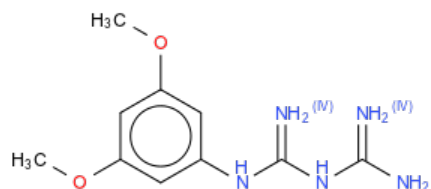
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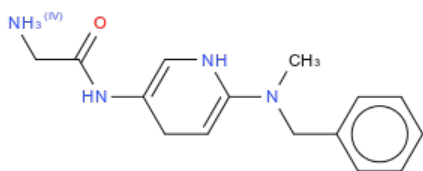
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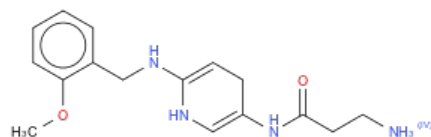
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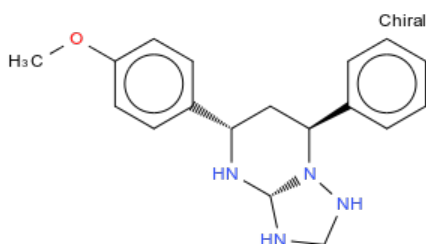
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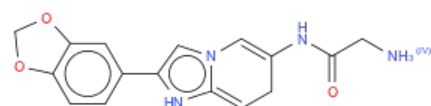
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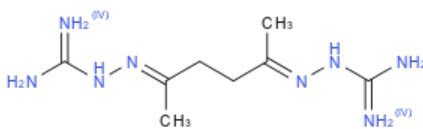
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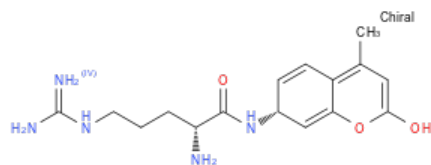
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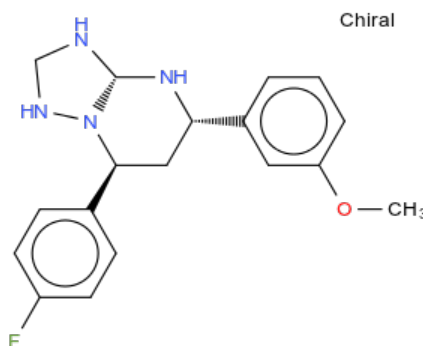
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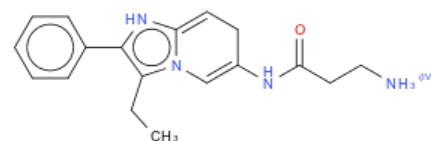
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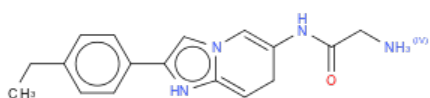
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144



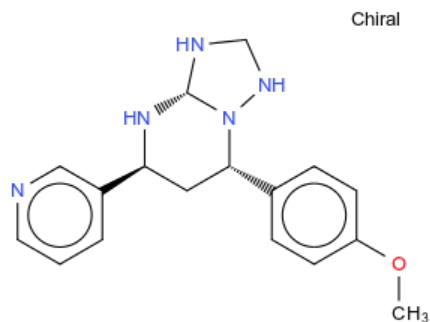
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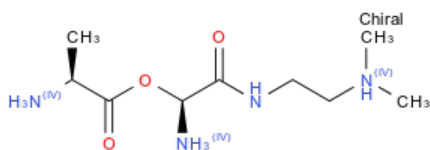
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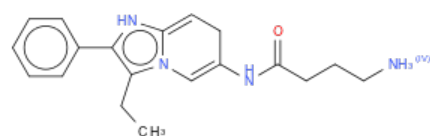
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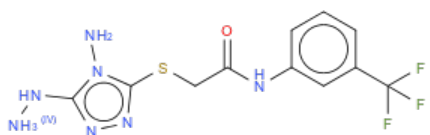
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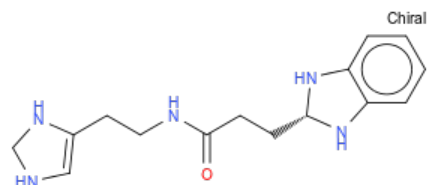
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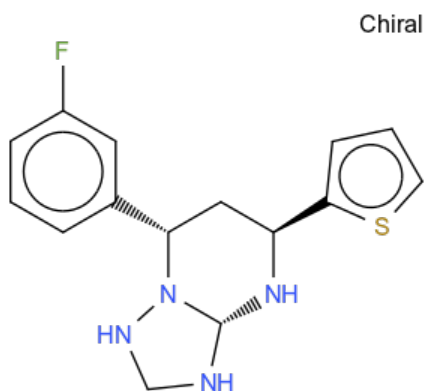
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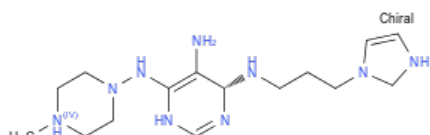
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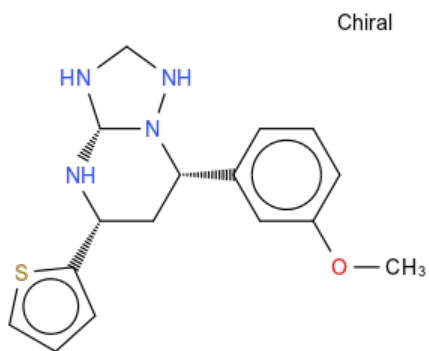
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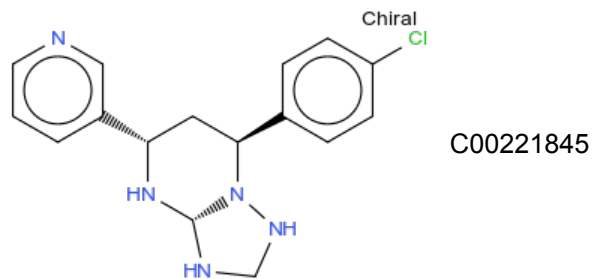


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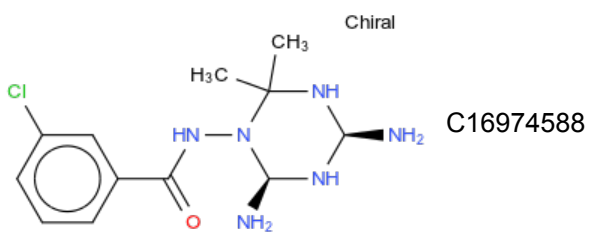
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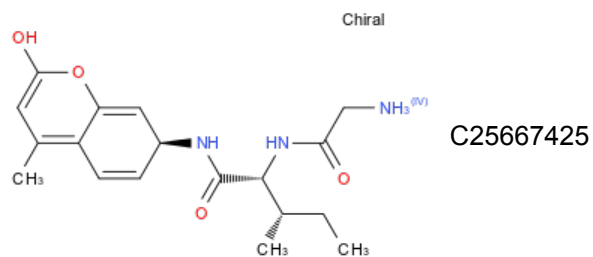
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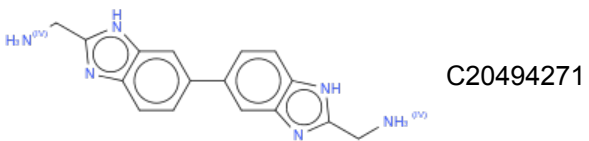
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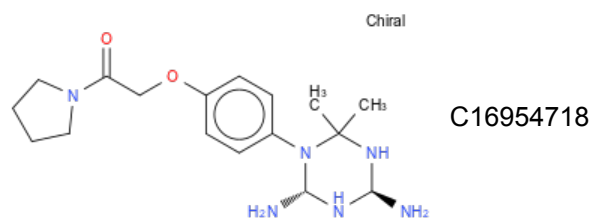
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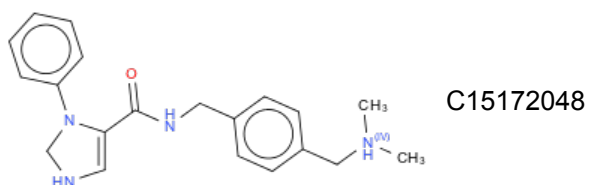
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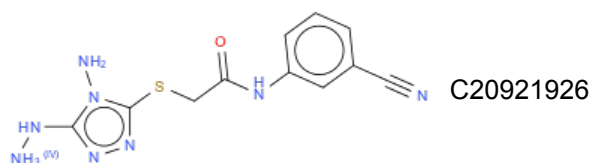
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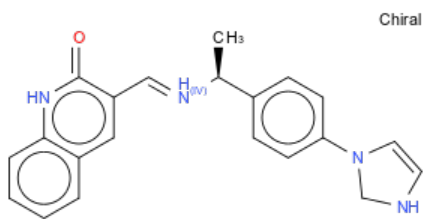
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160

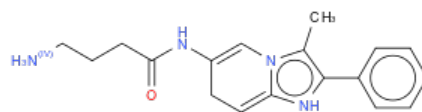


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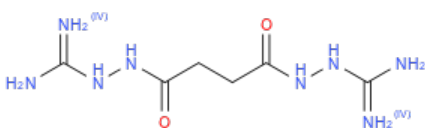
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162



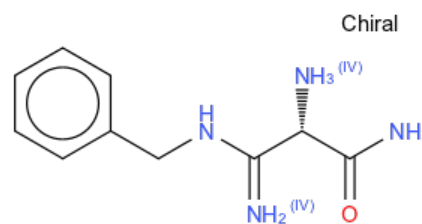
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163



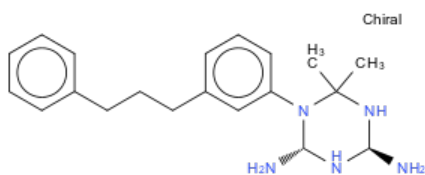
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164



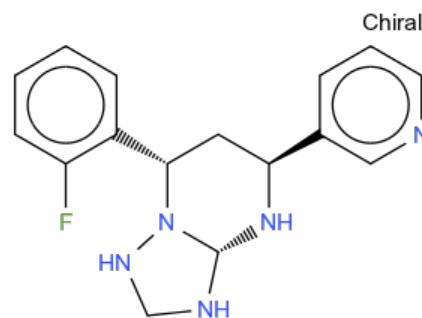
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165



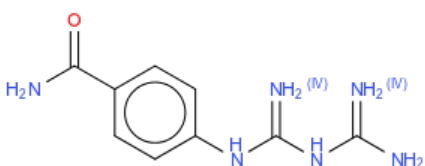
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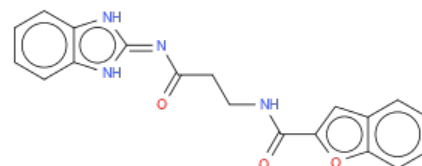
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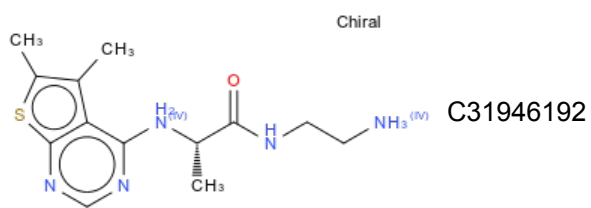
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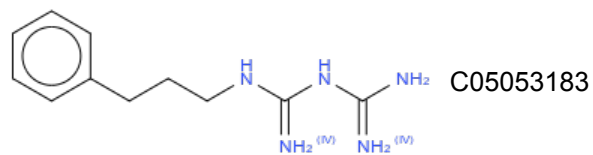


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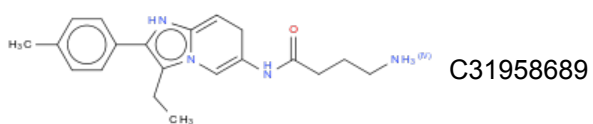
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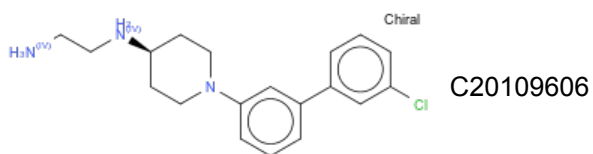
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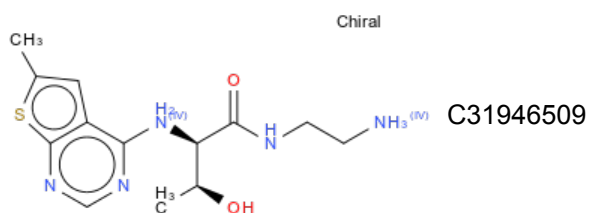
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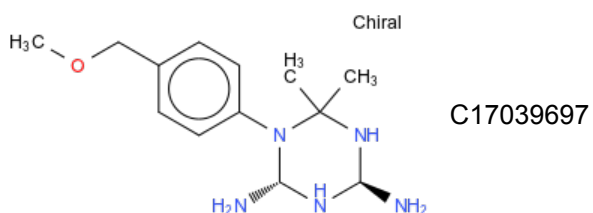
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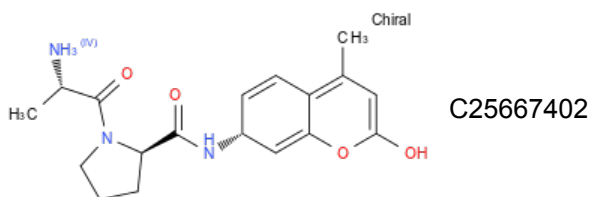
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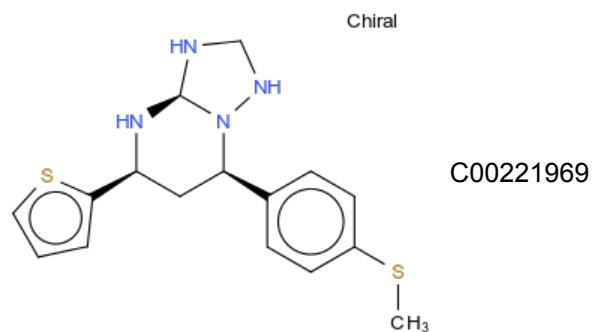
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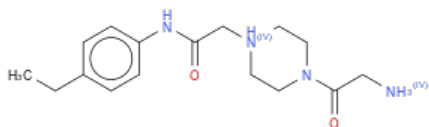
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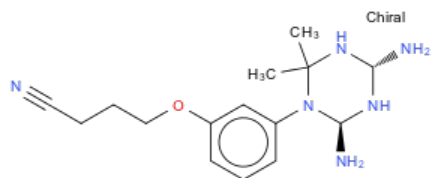


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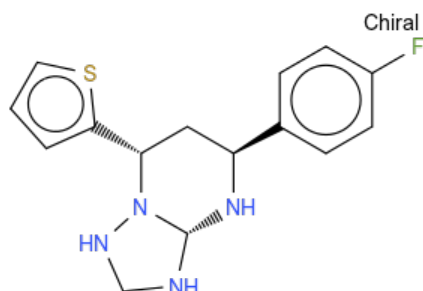
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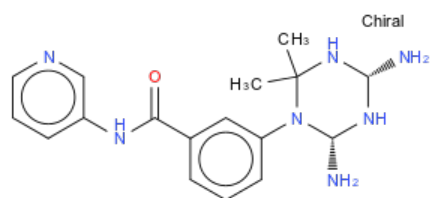
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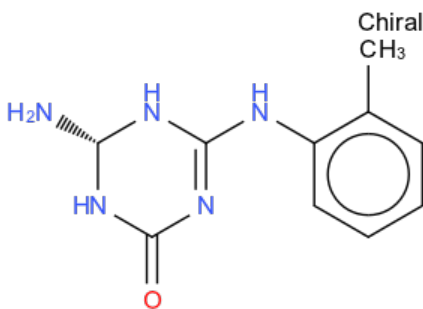
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188



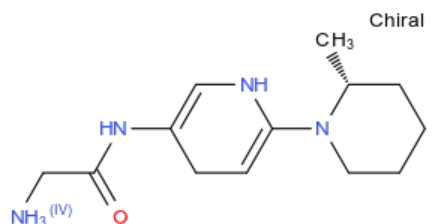
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189



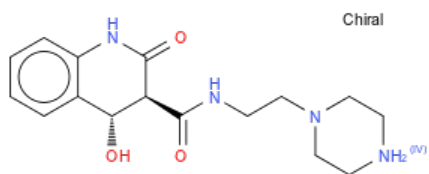
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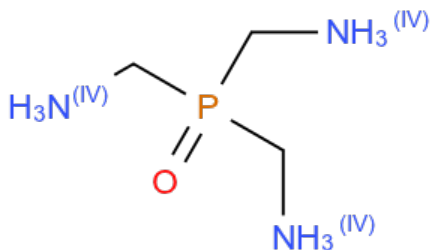
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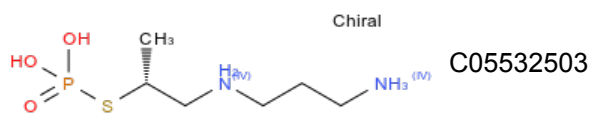
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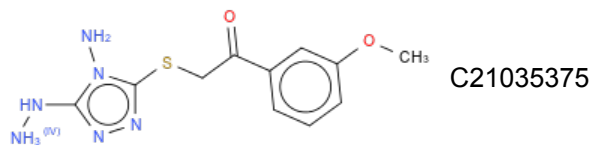


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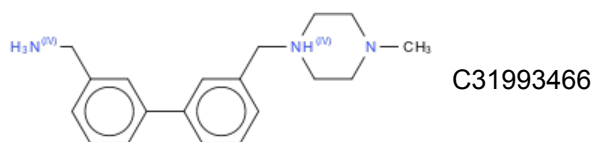
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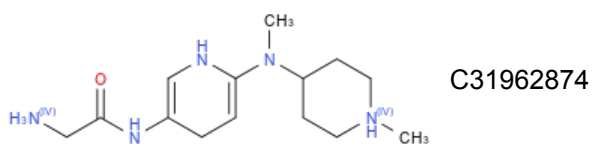
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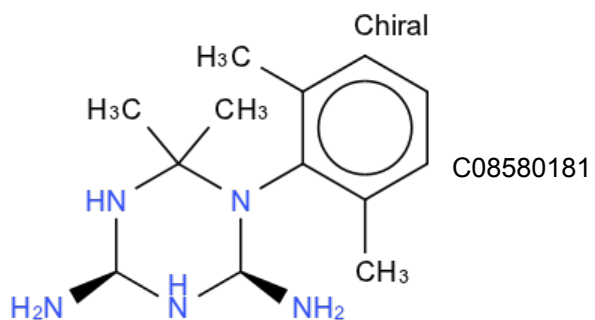
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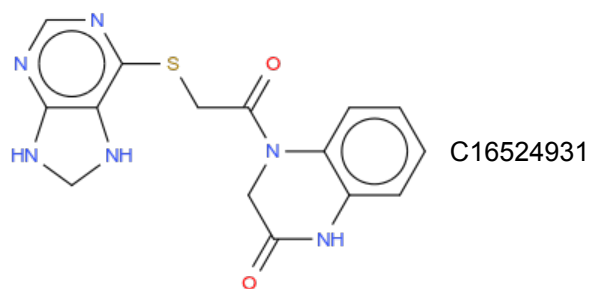
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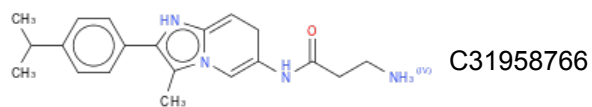
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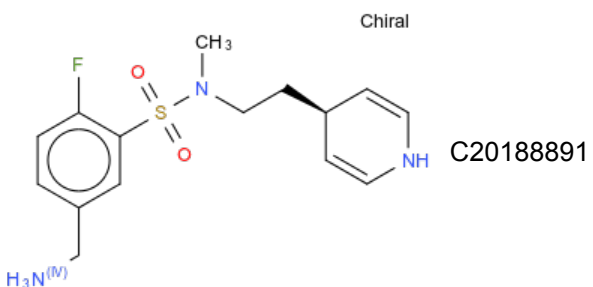
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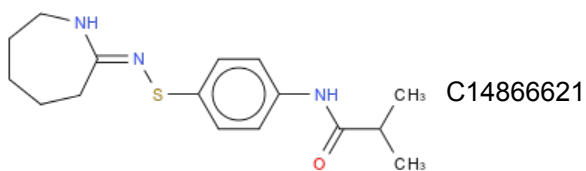
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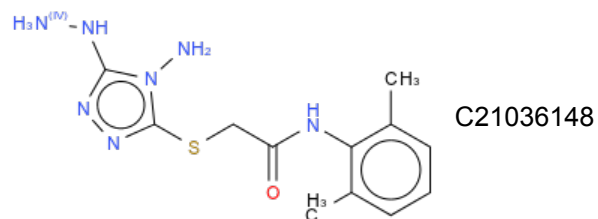
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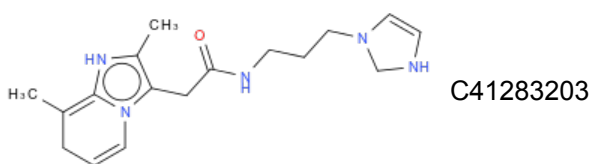
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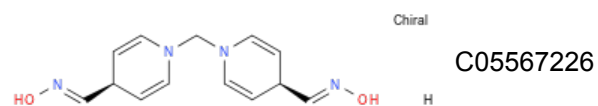
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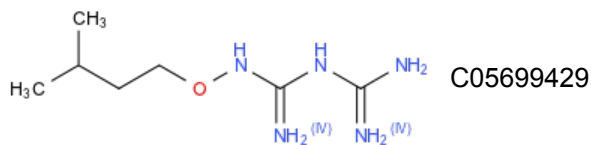
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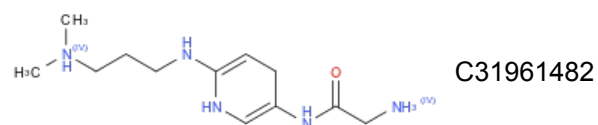
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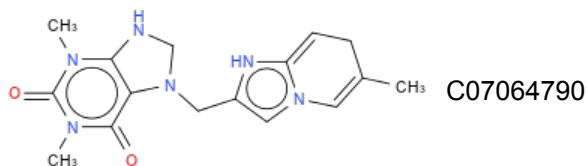
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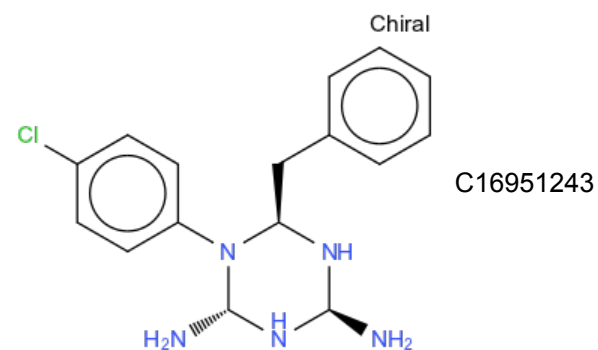
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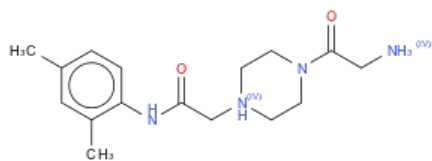
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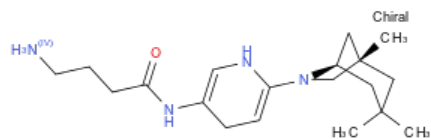


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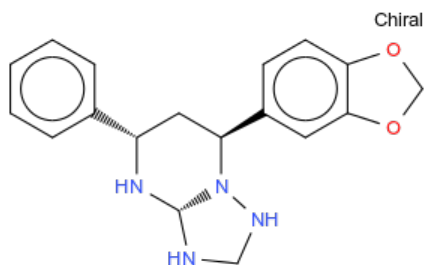
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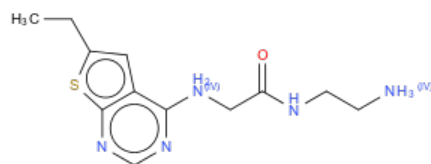
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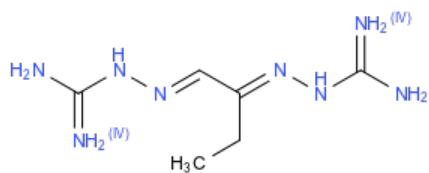
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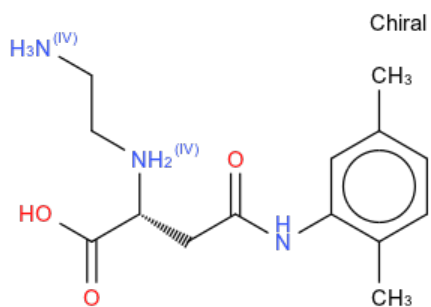
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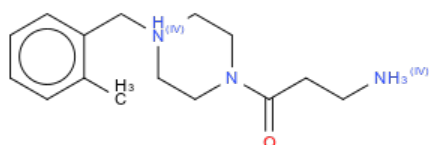
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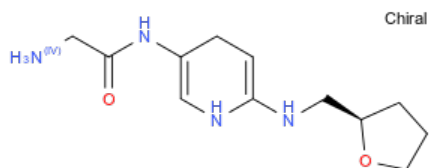
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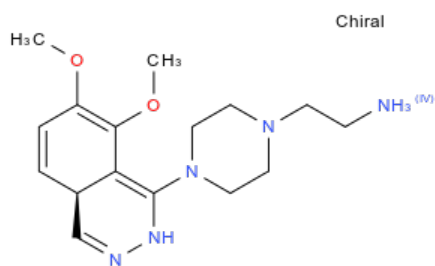
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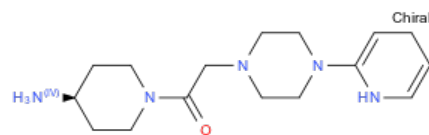
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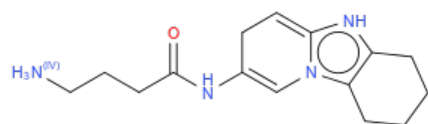
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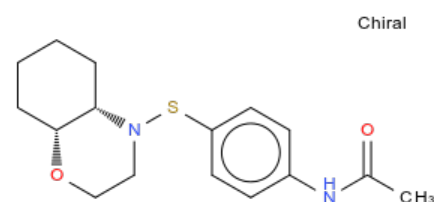
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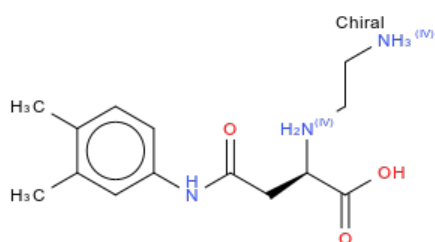
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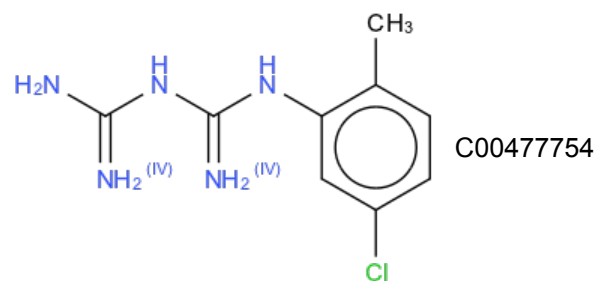
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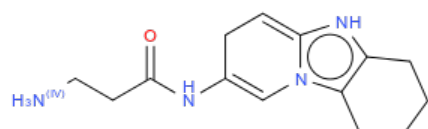
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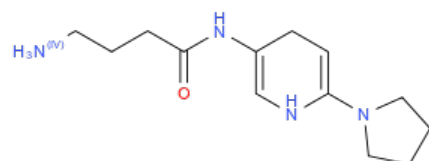
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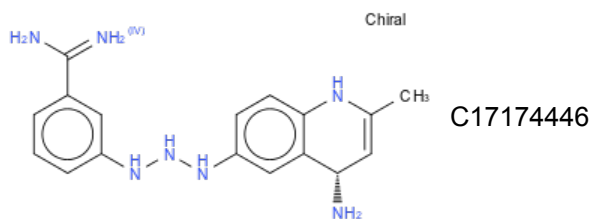
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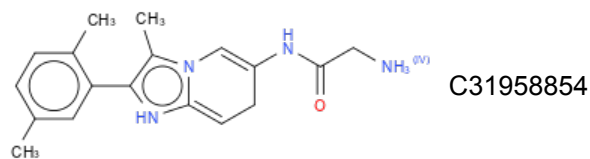


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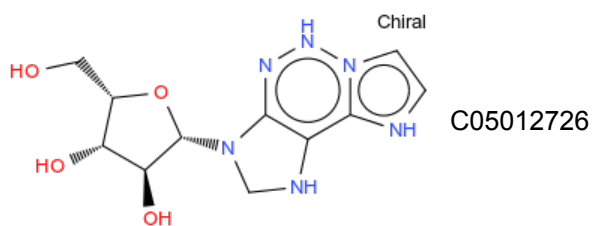
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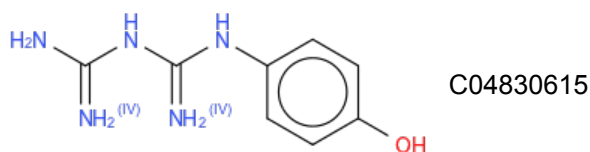
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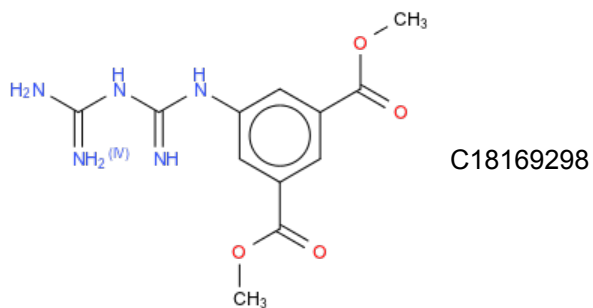
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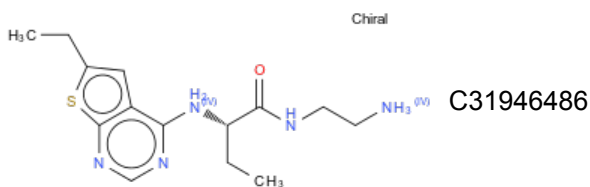
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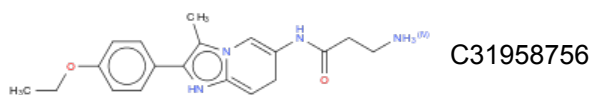
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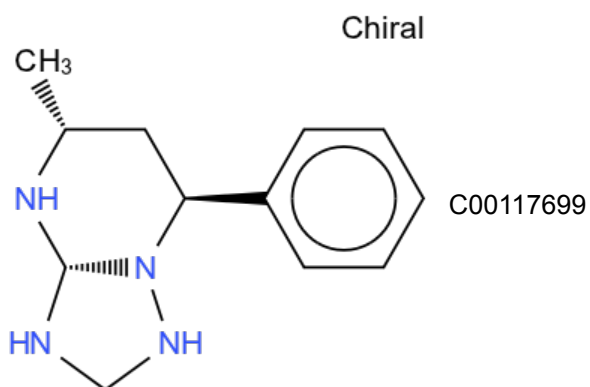
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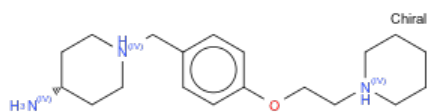
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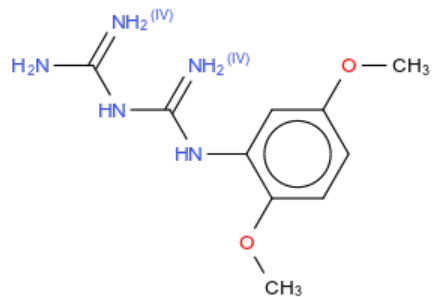


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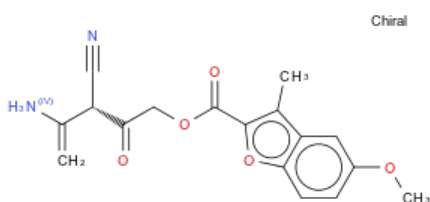
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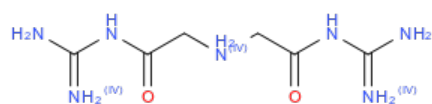
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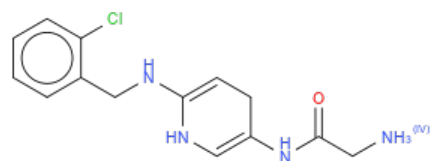
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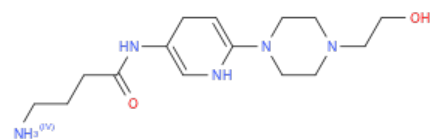
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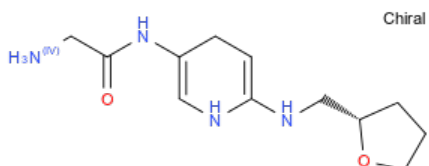
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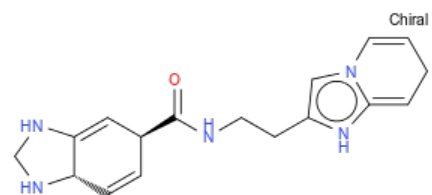
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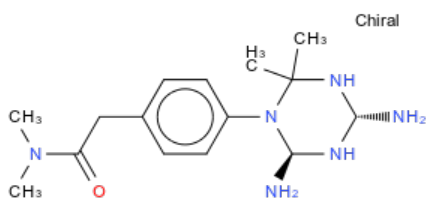
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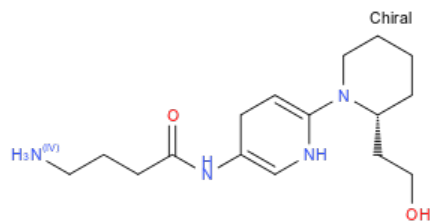
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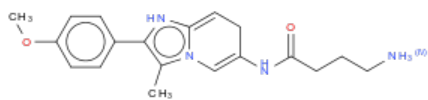
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242



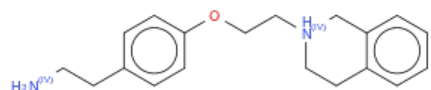
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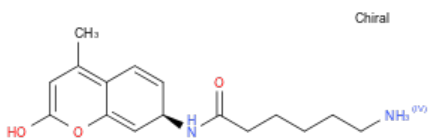
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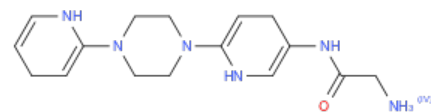
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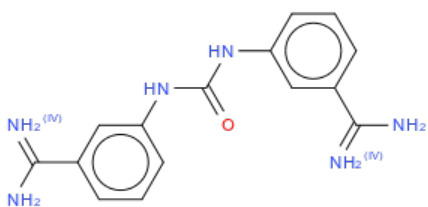
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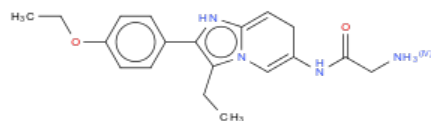
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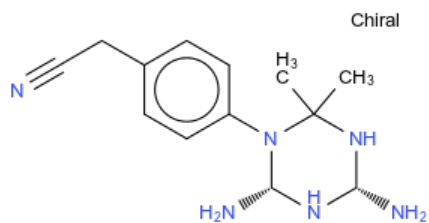
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248



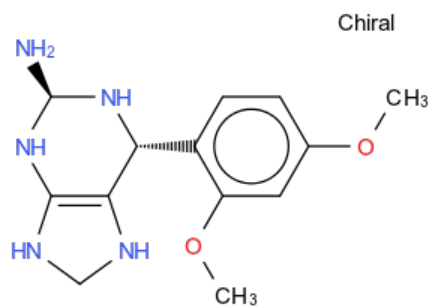
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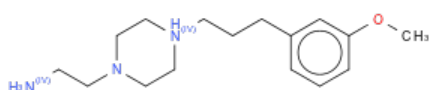
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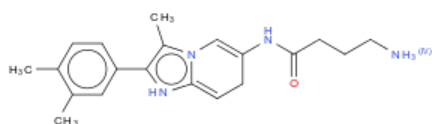
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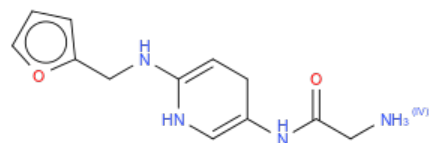
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252



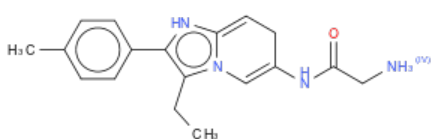
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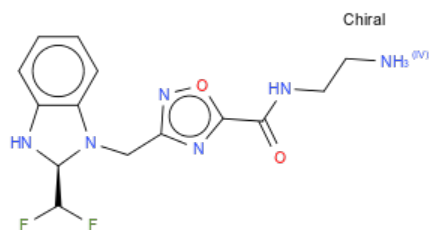
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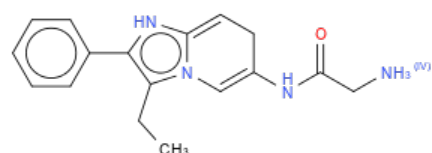
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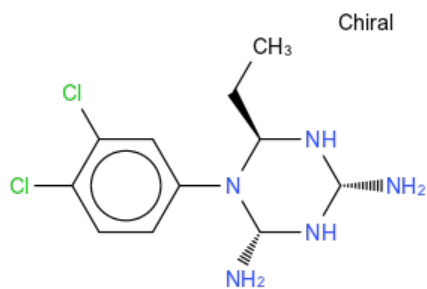
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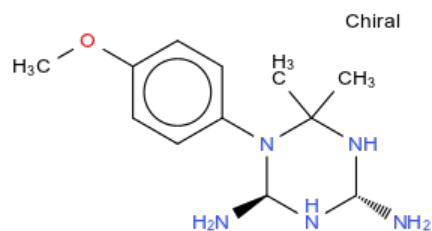
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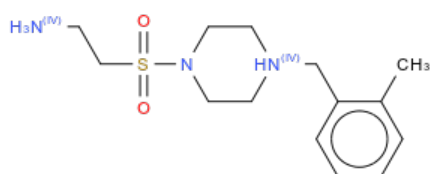
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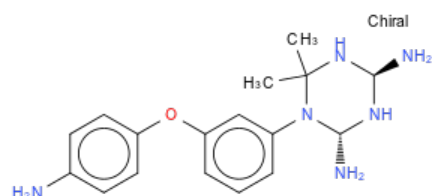
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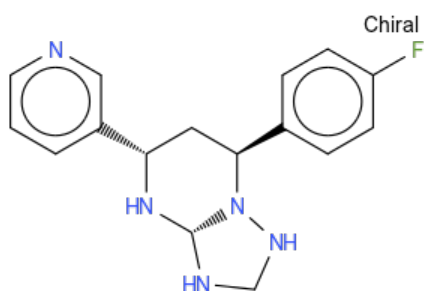
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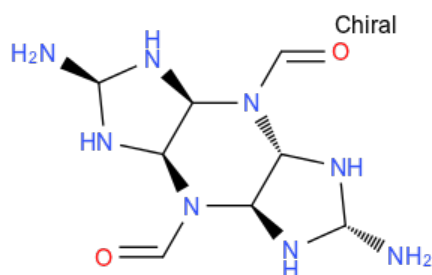
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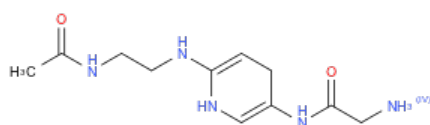
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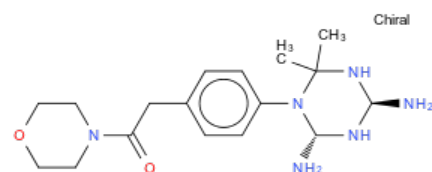
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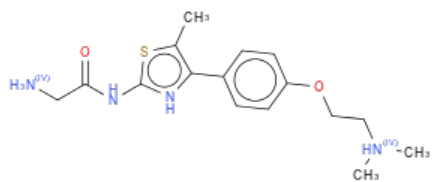
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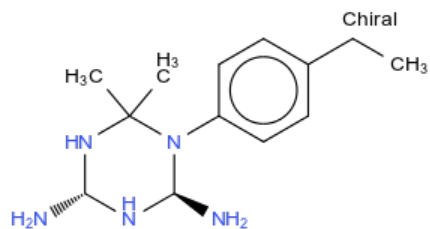
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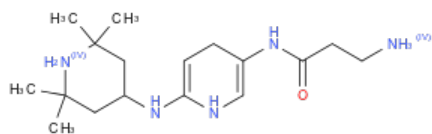
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266



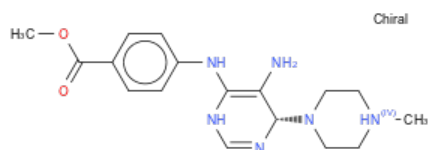
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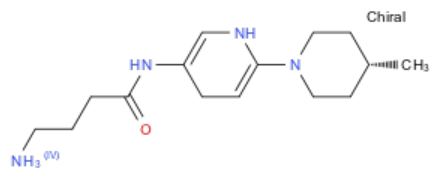
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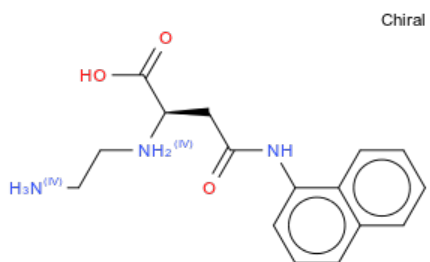
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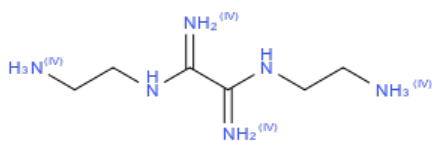
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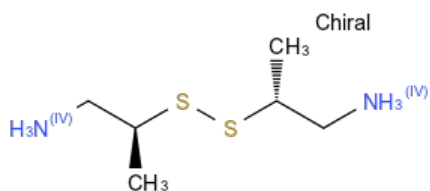
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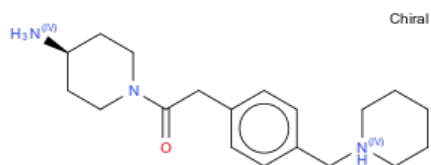
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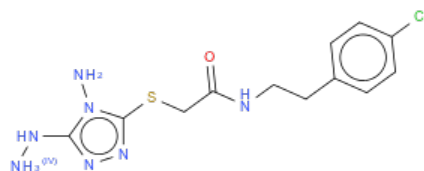
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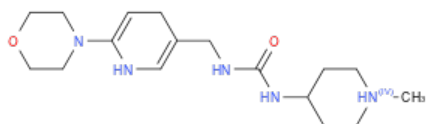
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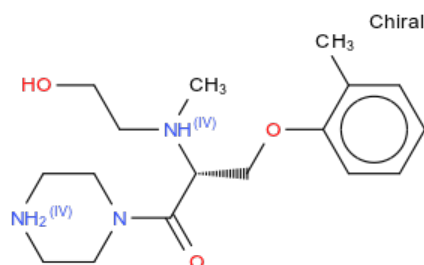
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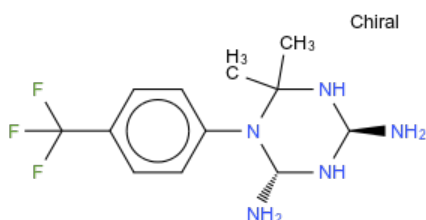
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276



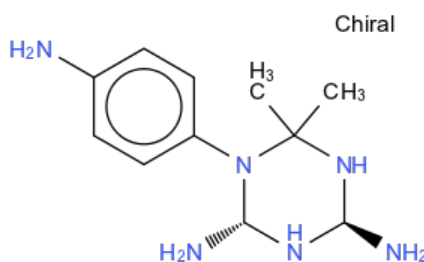
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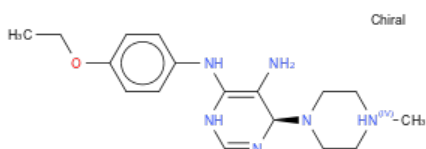
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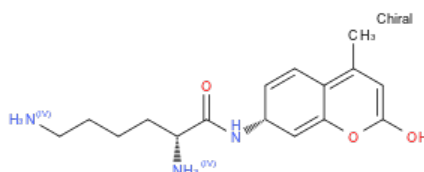
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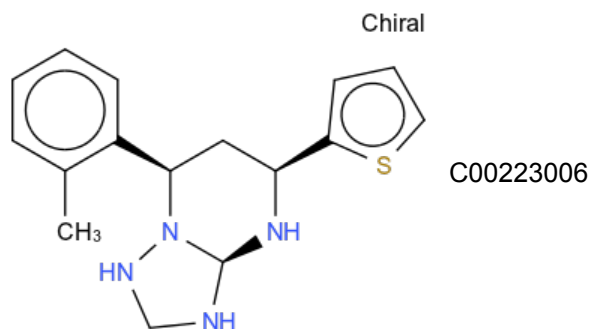
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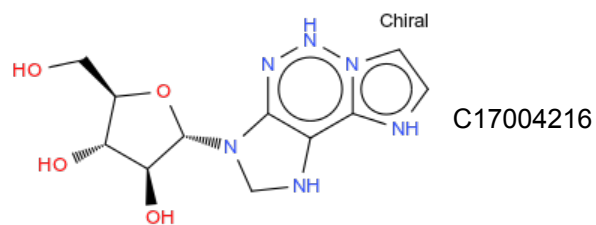


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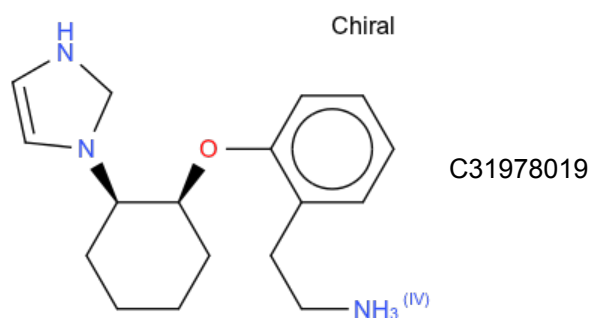
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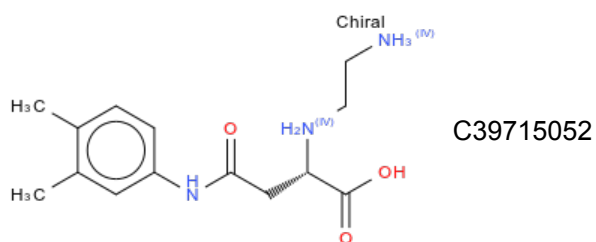
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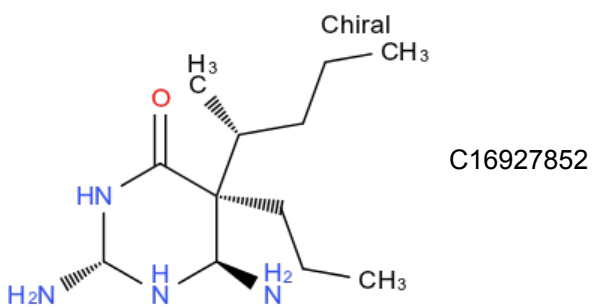
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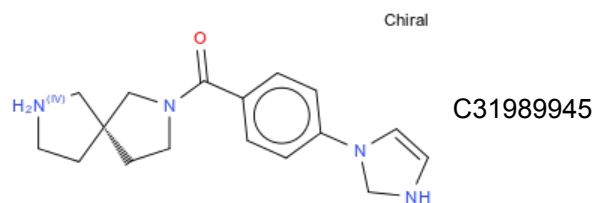
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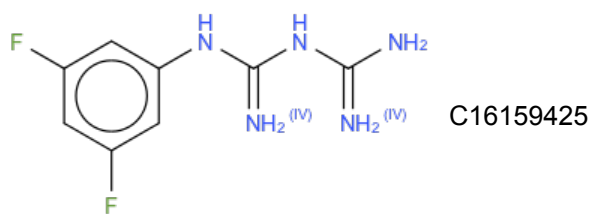
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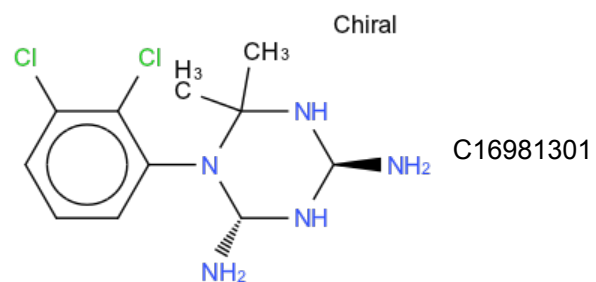
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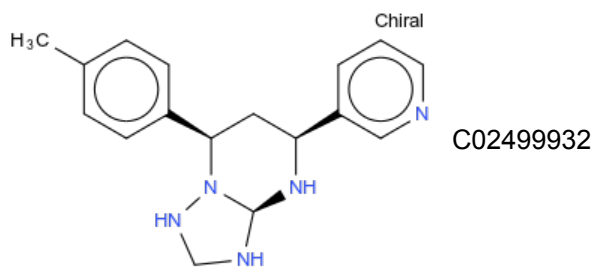
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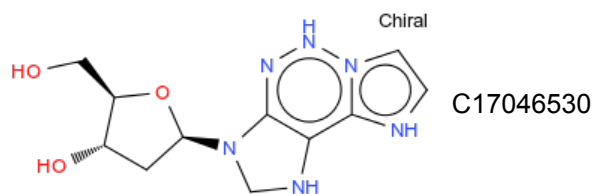
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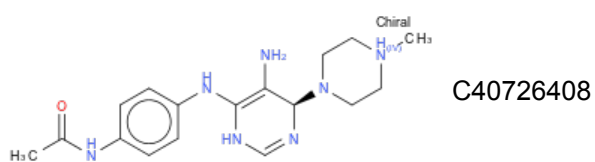
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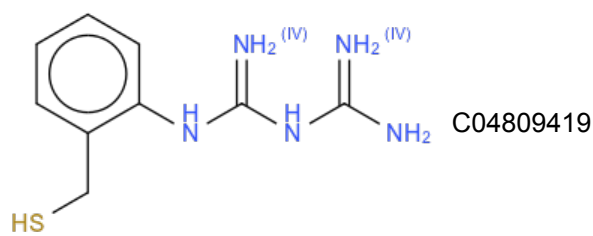
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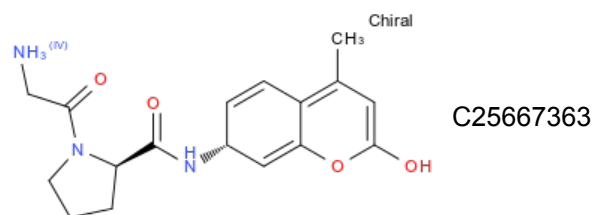
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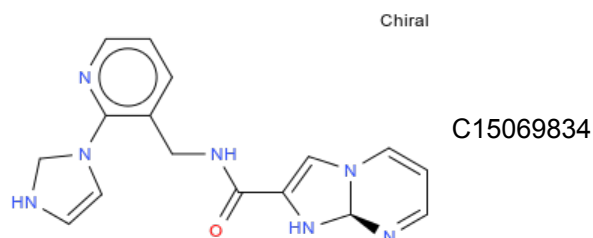
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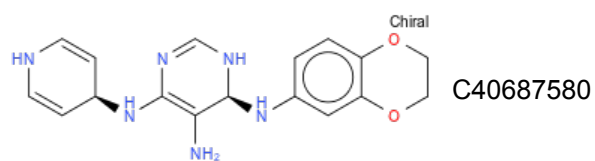
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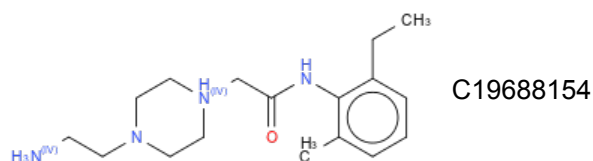
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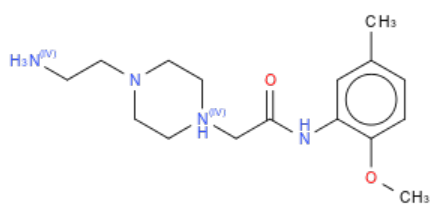
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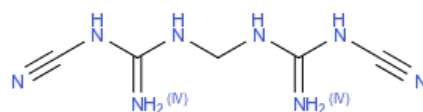


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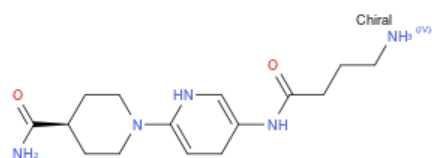
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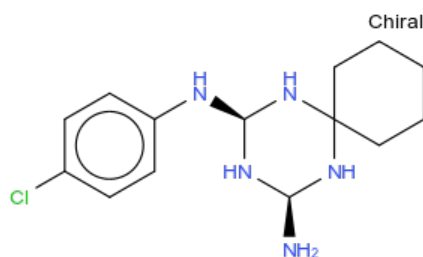
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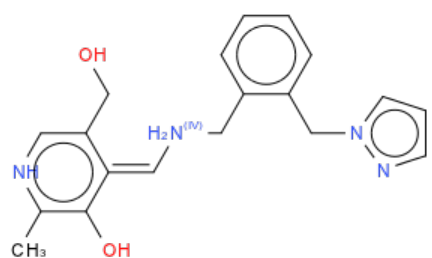
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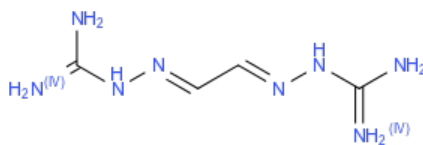
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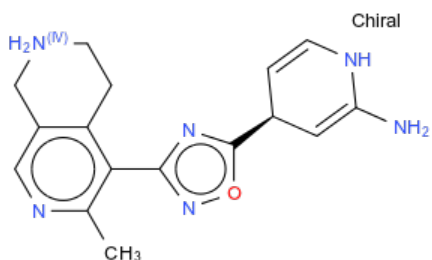
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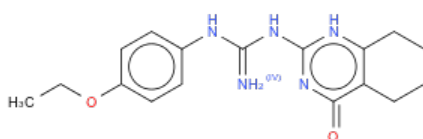
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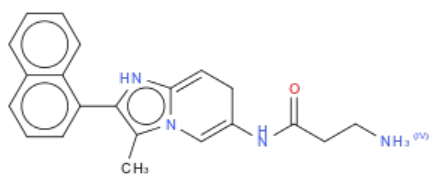
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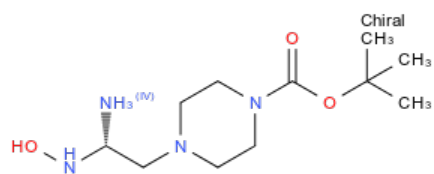
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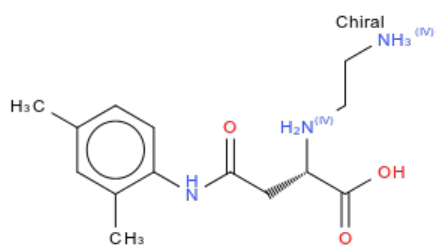
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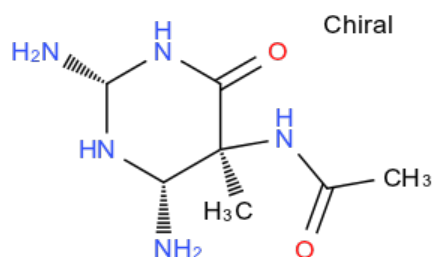
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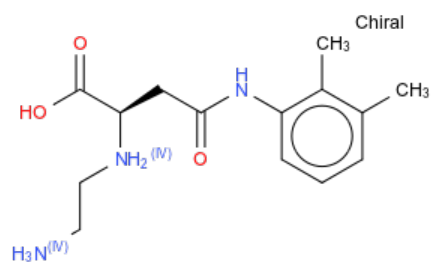
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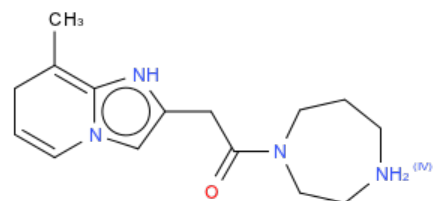
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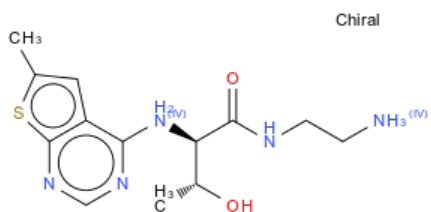
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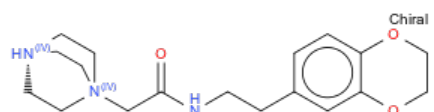
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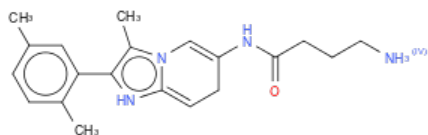
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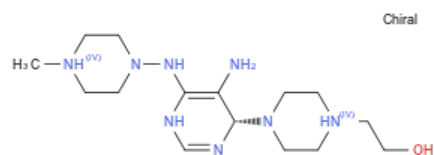
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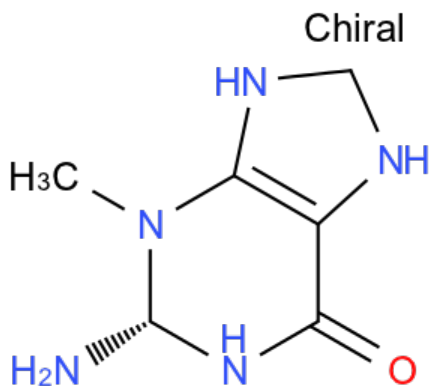
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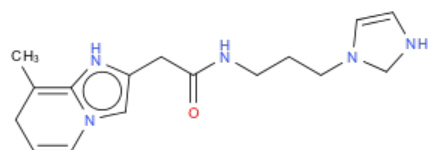
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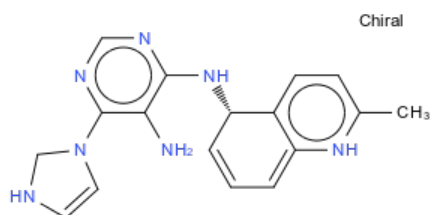
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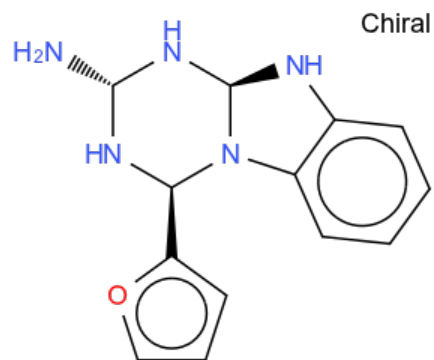
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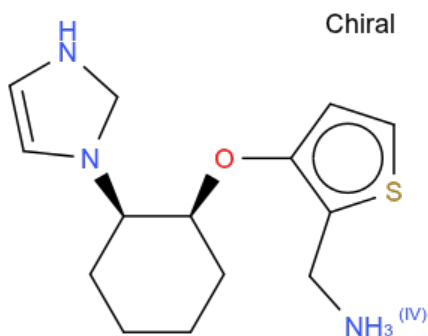
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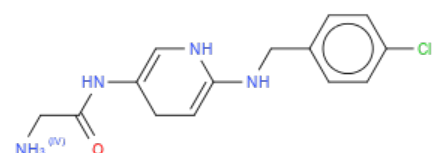
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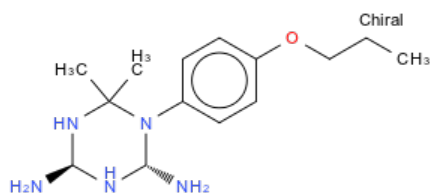
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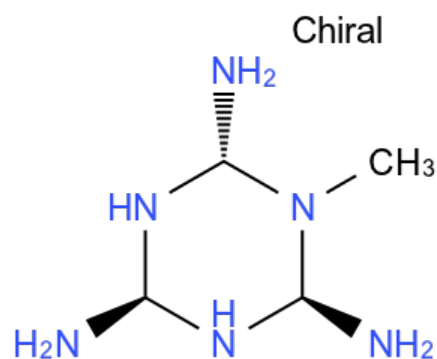
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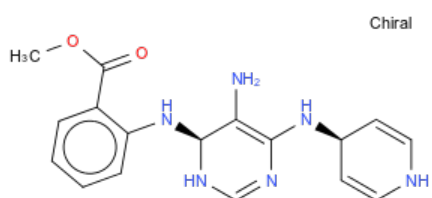
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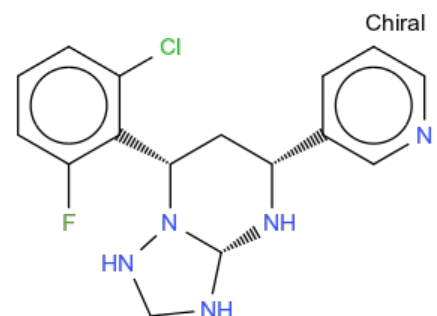
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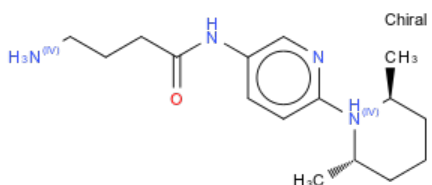
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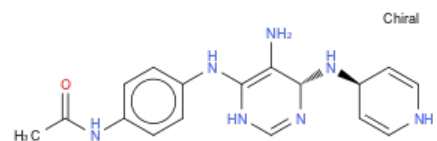
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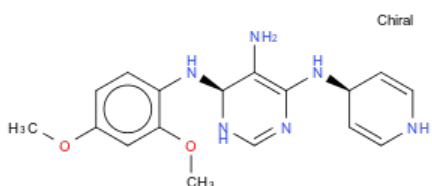
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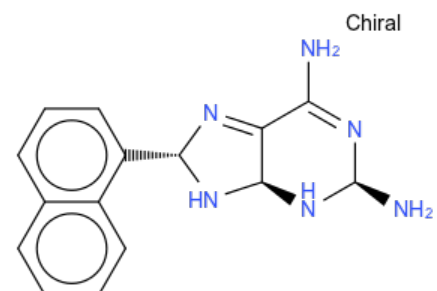
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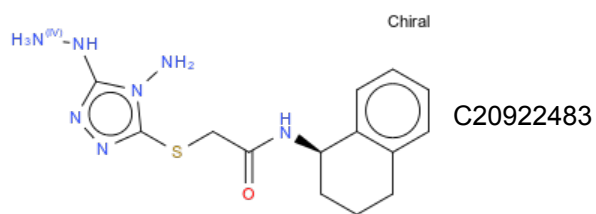
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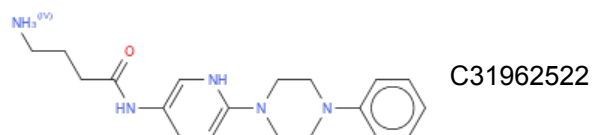


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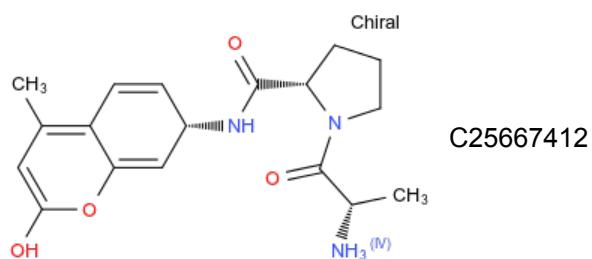
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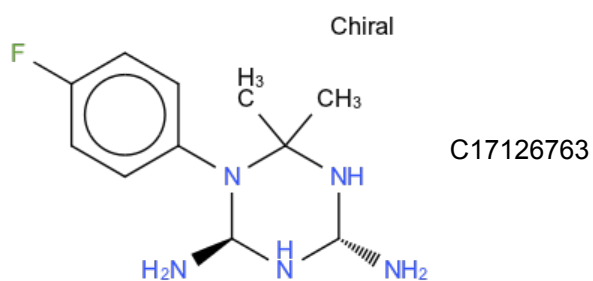
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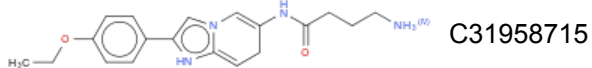
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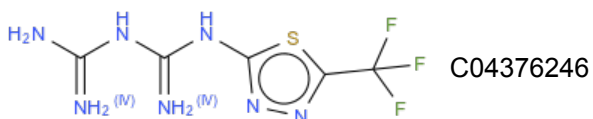
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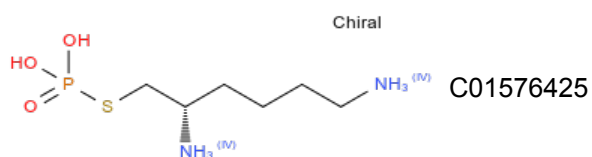
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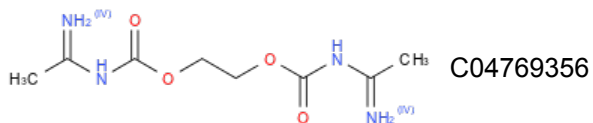
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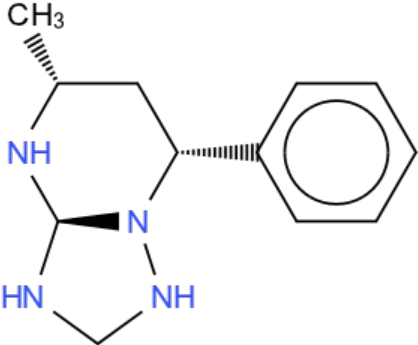
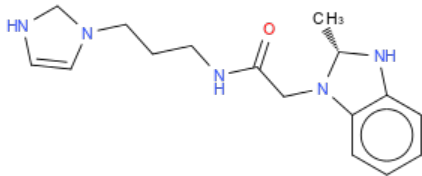
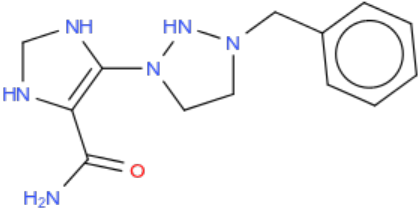
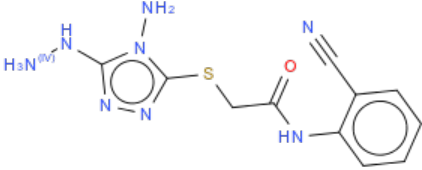
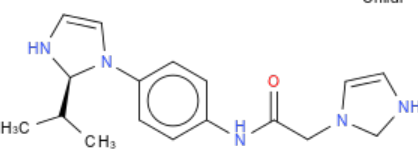
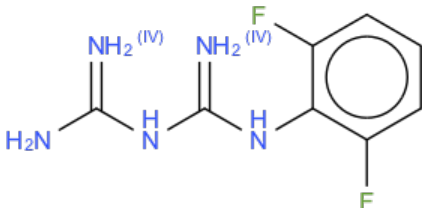
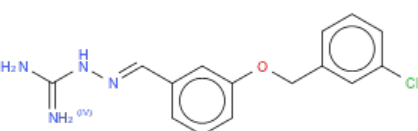
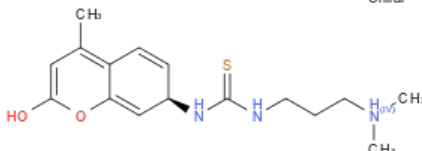


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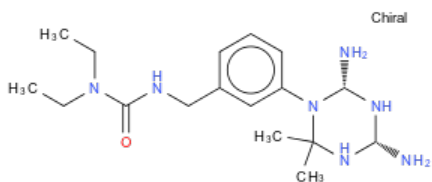


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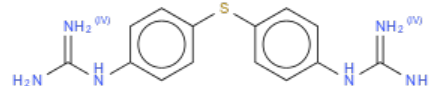
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339	 <p style="text-align: right;">C13283554</p>	340	 <p style="text-align: right;">C20922696</p>
341	<p style="text-align: center;">Chiral</p>  <p style="text-align: right;">C19454513</p>	342	 <p style="text-align: right;">C00089321</p>
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345



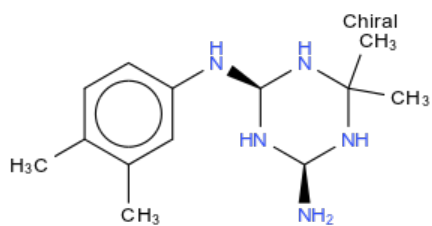
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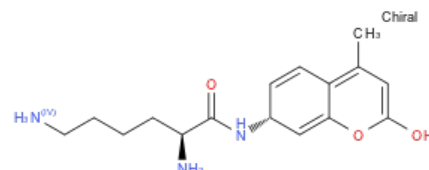
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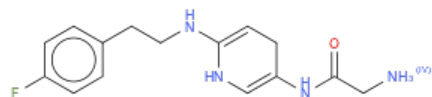
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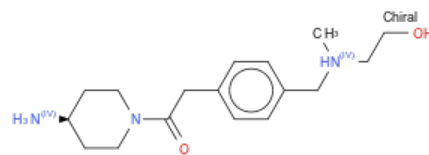
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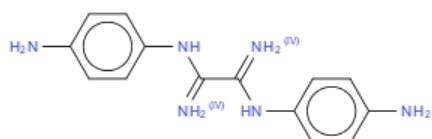
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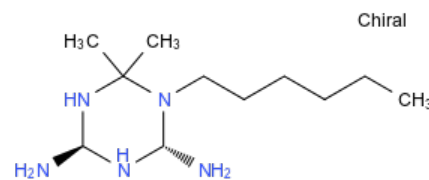
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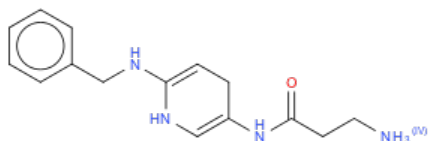
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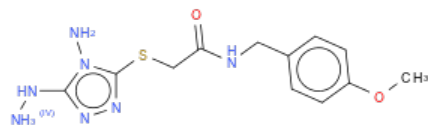
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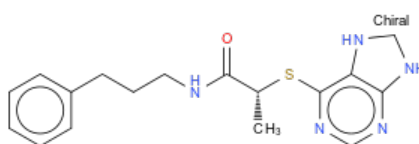
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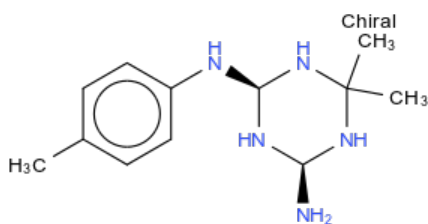
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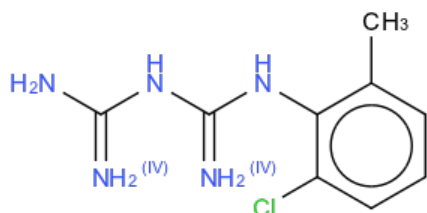
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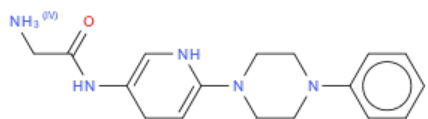
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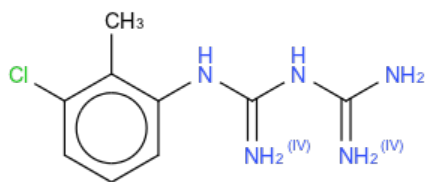
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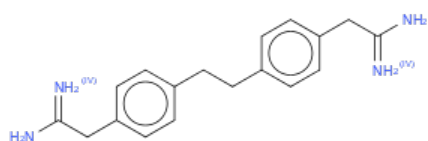
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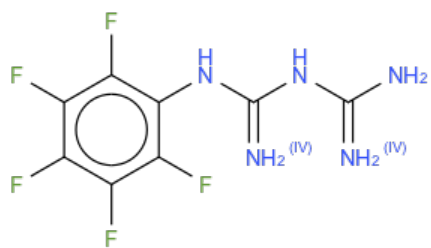
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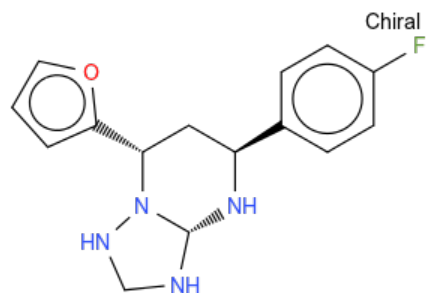
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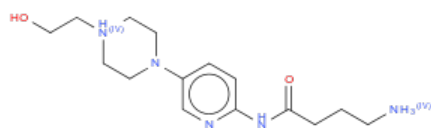
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362



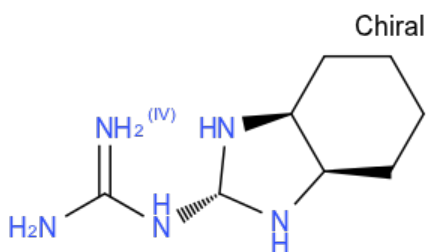
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363



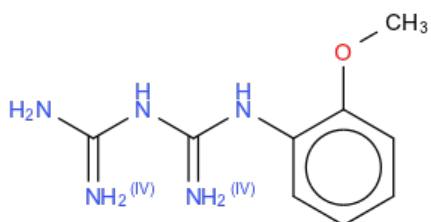
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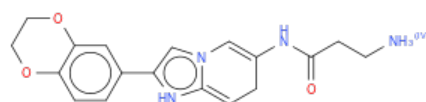
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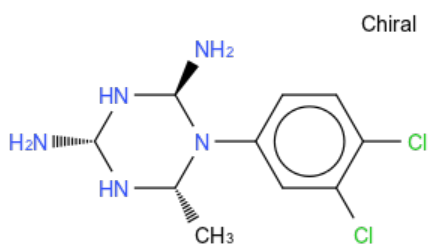
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366



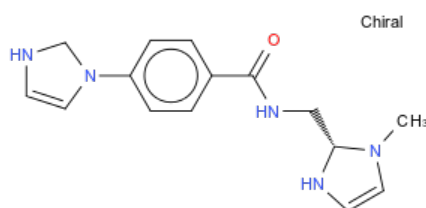
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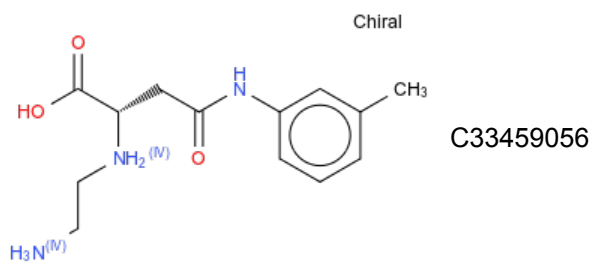
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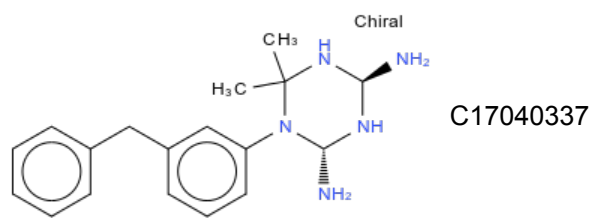


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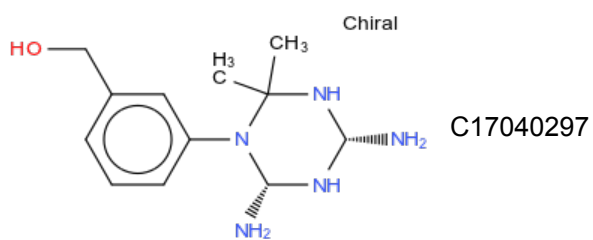
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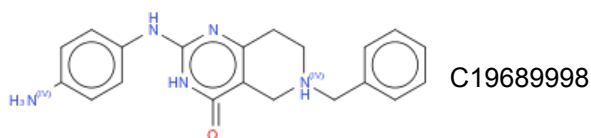
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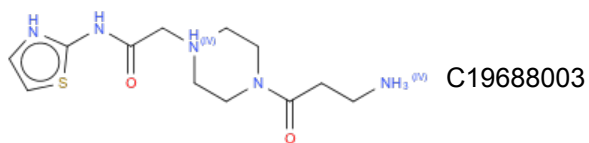
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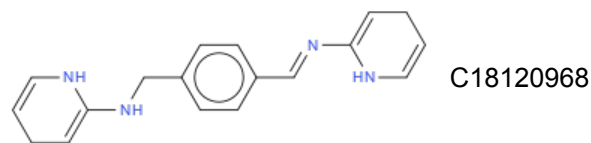
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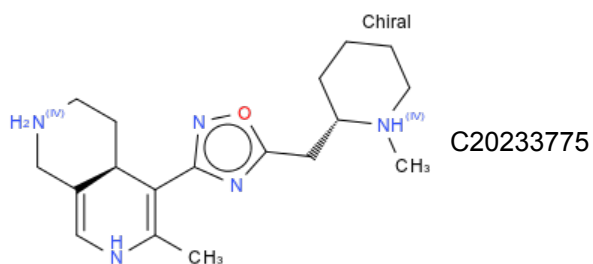
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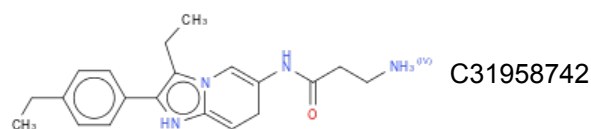
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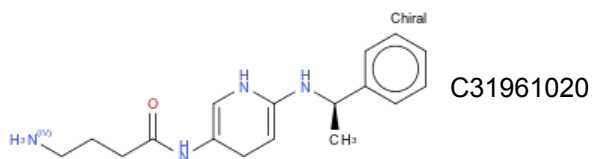
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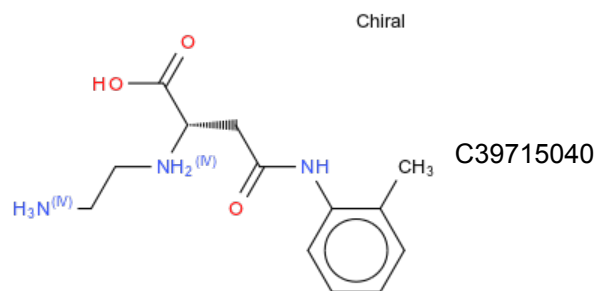


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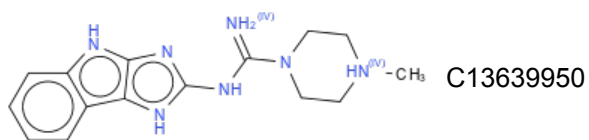
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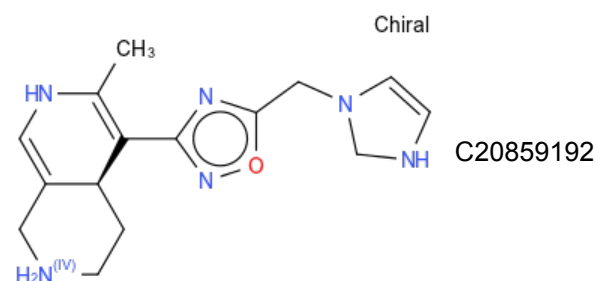
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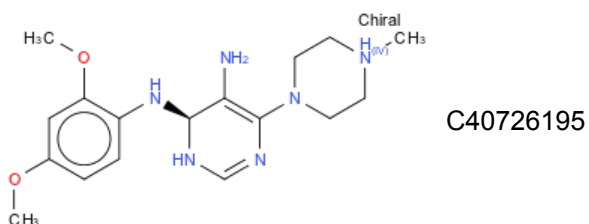
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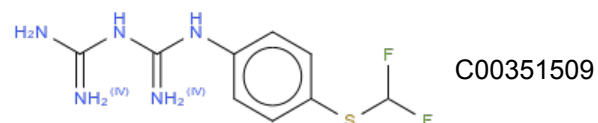
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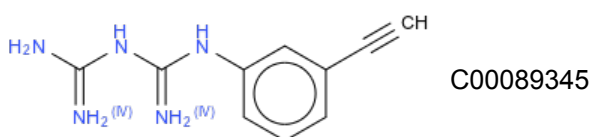
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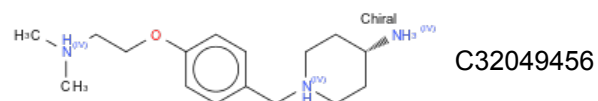
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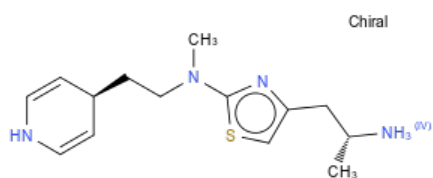
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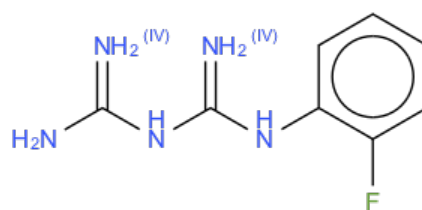
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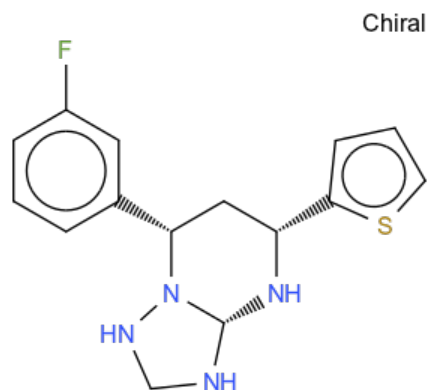
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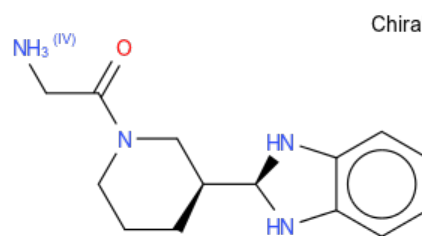
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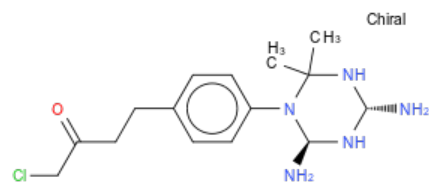
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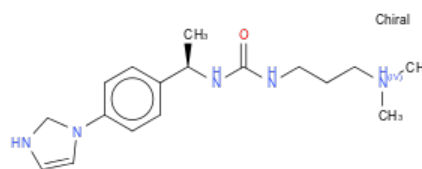
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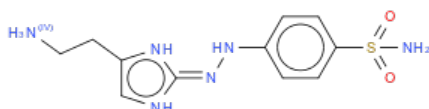
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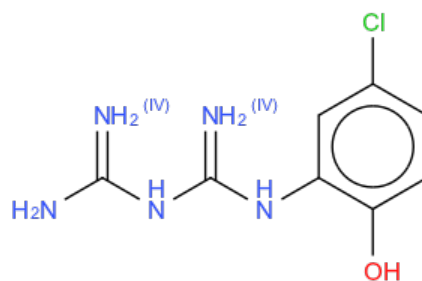
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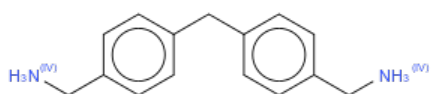
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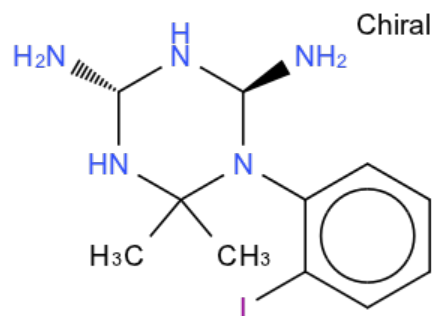
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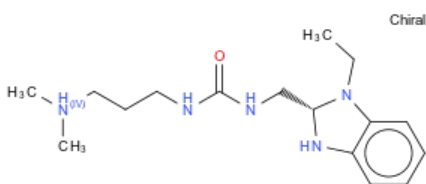
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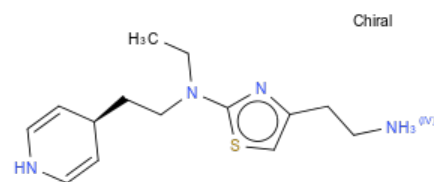
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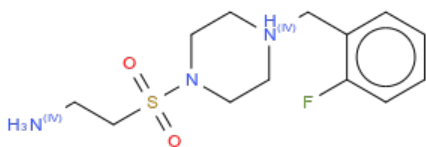
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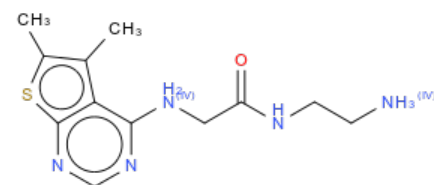
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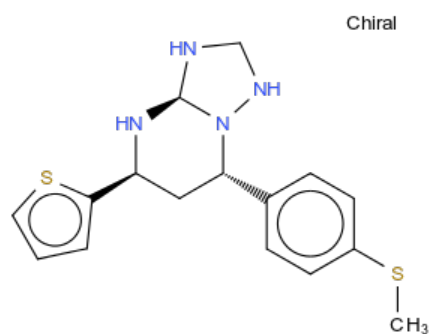
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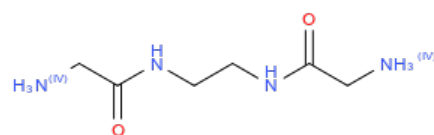
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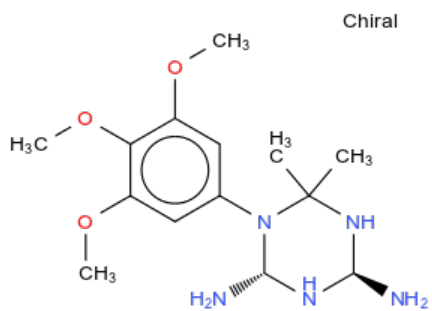
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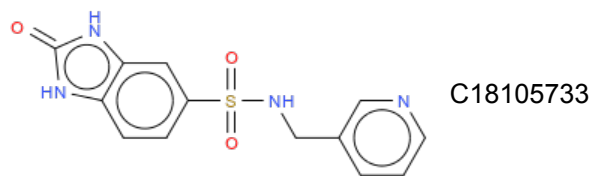


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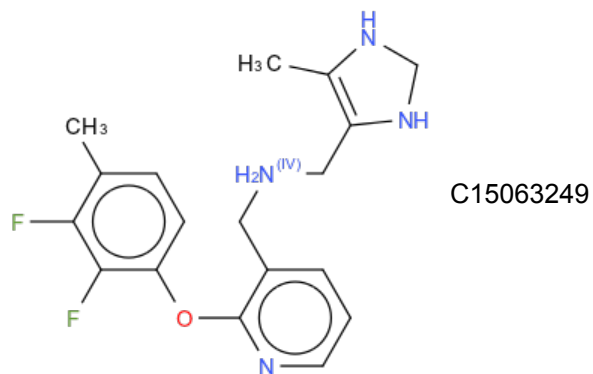
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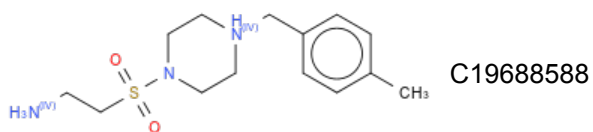
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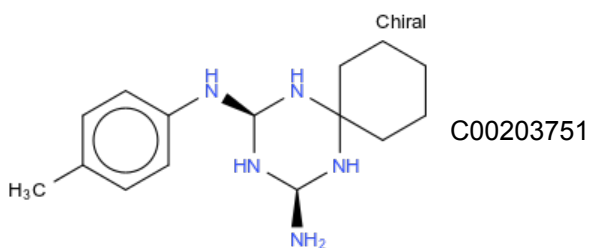
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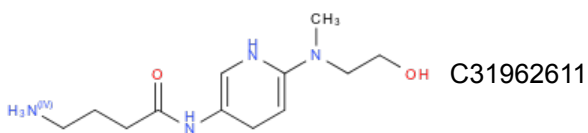
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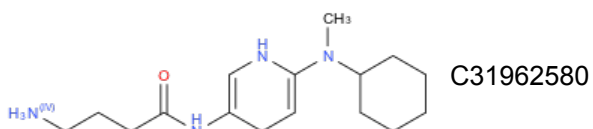
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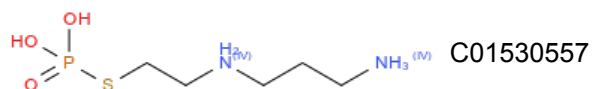
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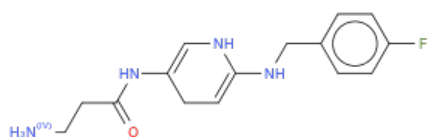
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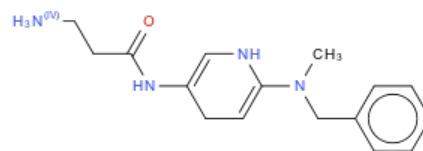


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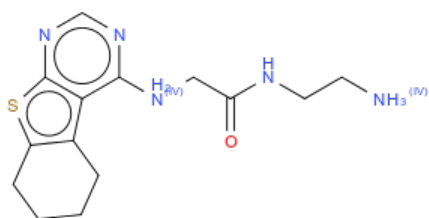
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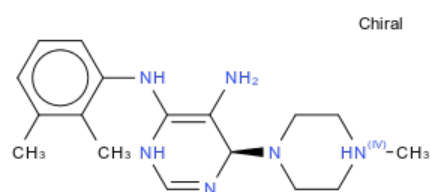
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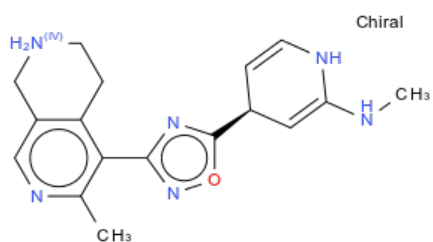
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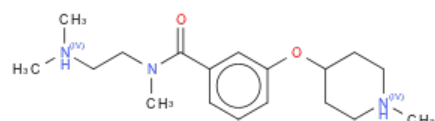
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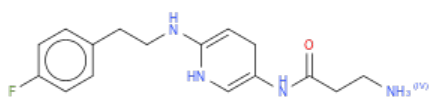
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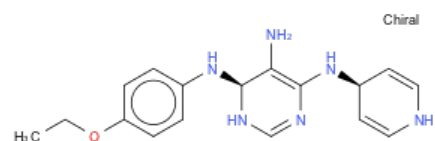
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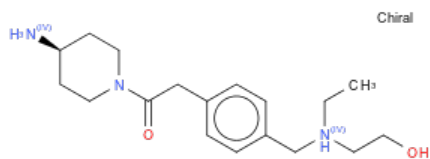
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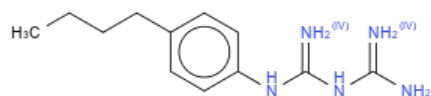
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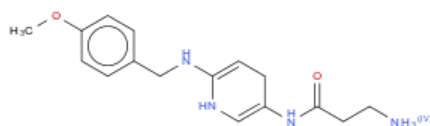
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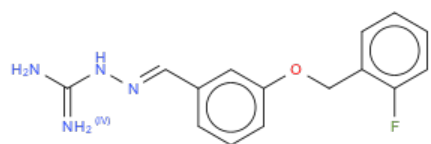
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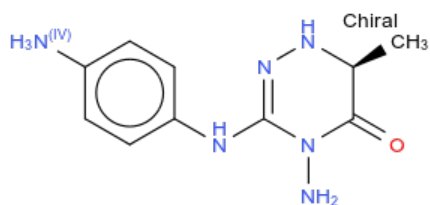
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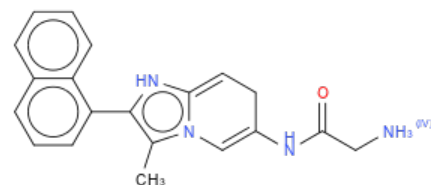
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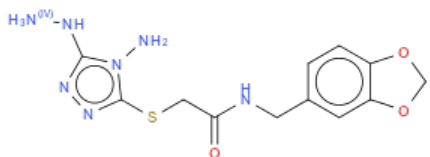
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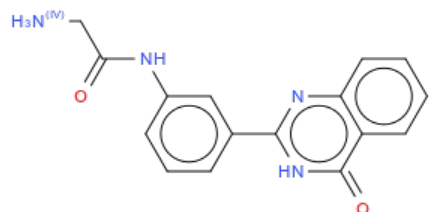
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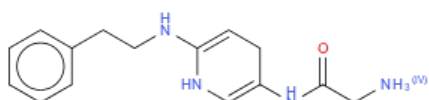
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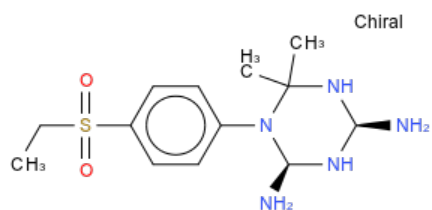
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425



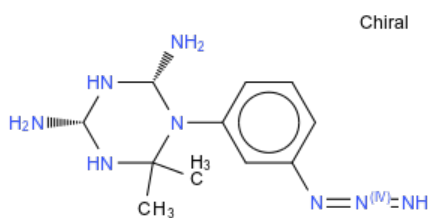
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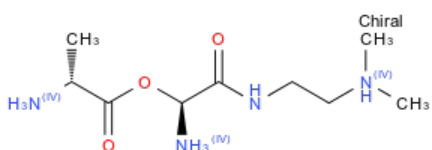
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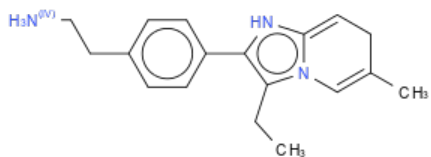
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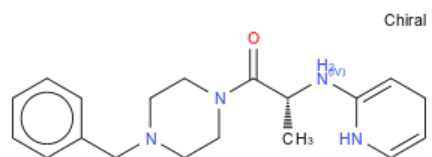
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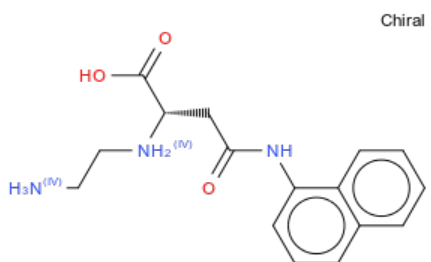
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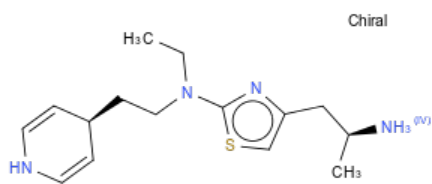
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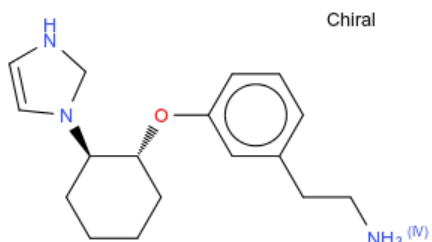
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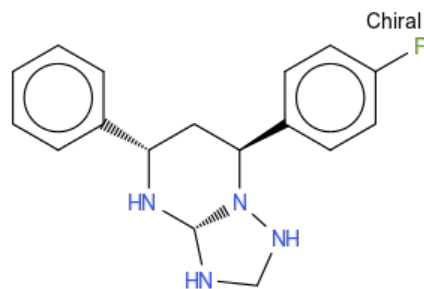
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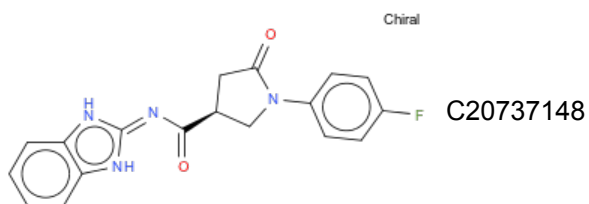
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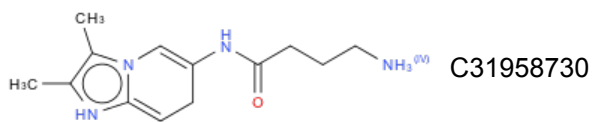
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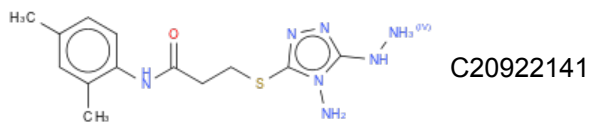
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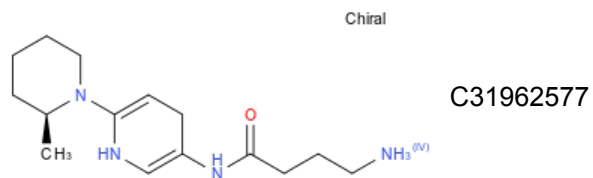
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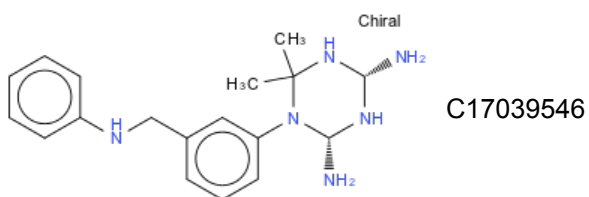
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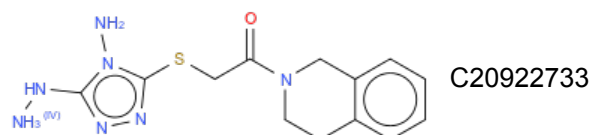
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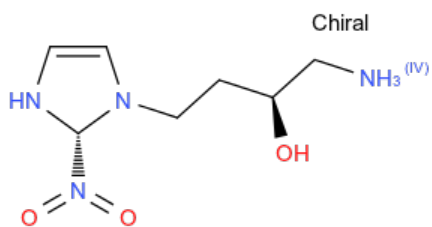
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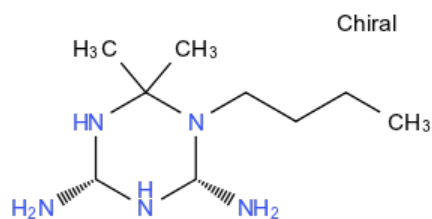
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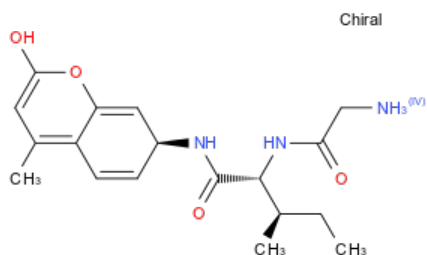
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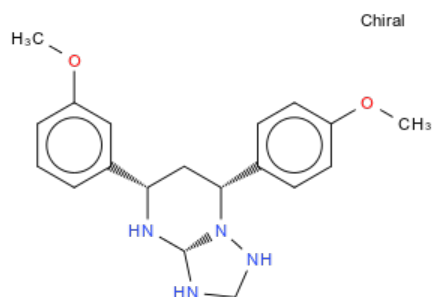
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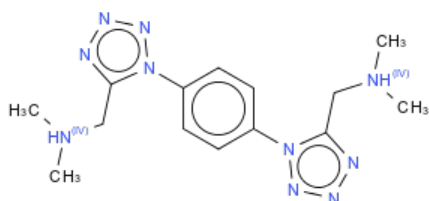
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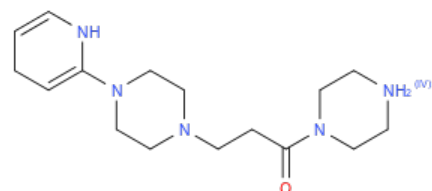
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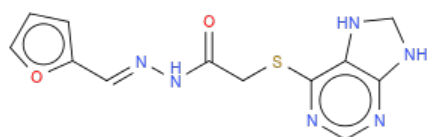
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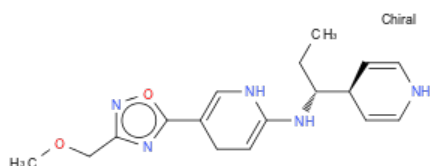
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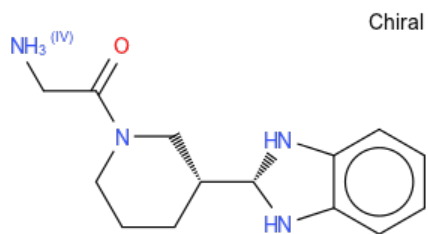
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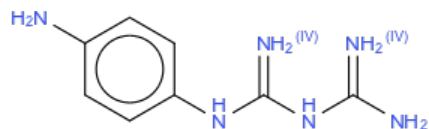
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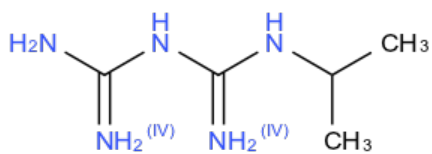
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450



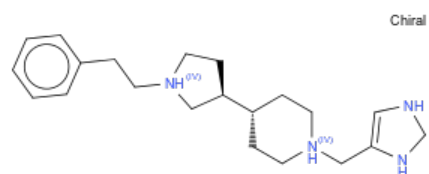
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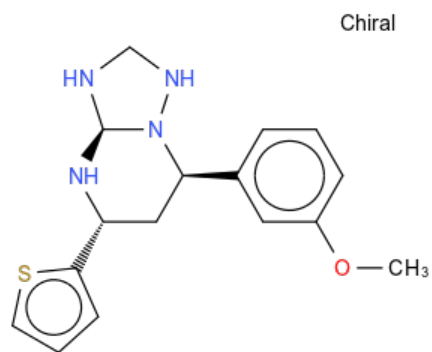
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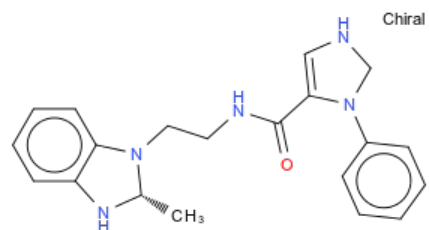
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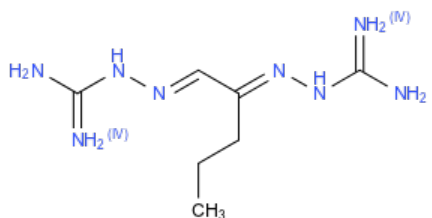
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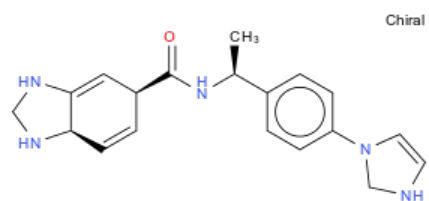
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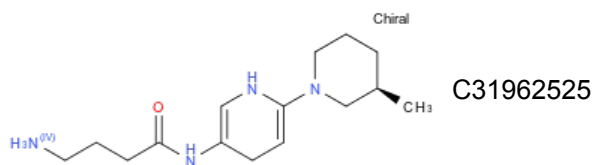
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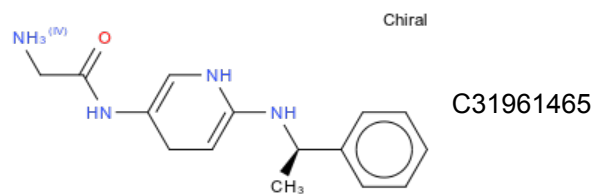


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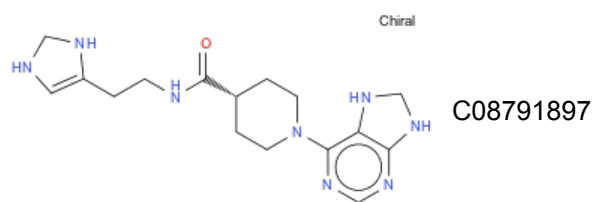
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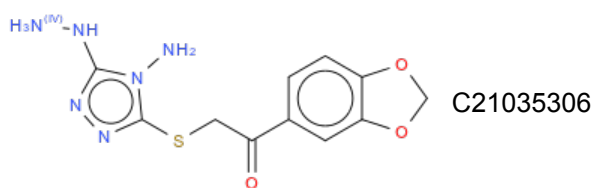
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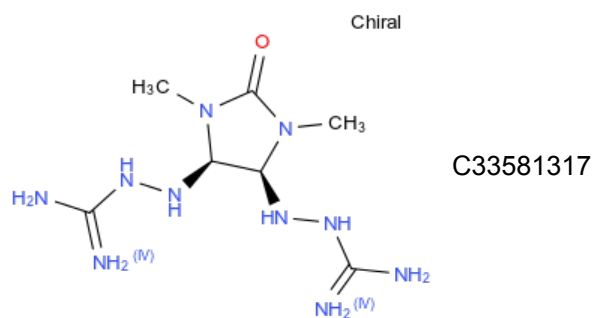
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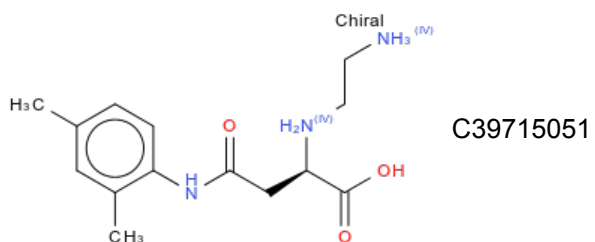
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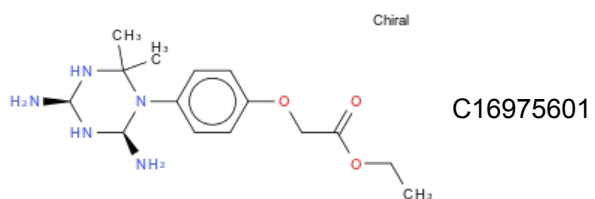
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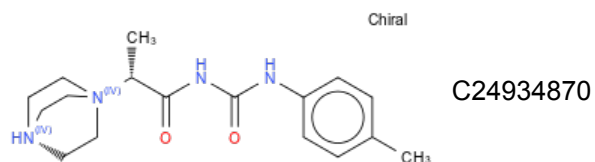
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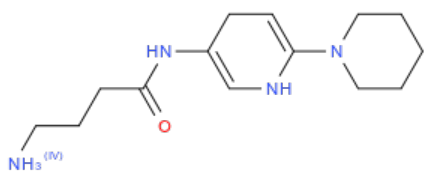
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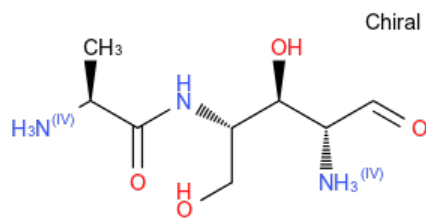


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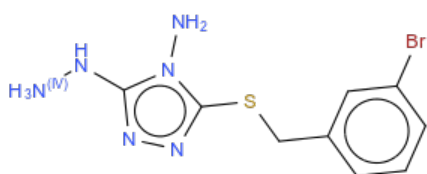
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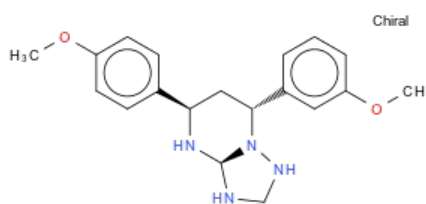
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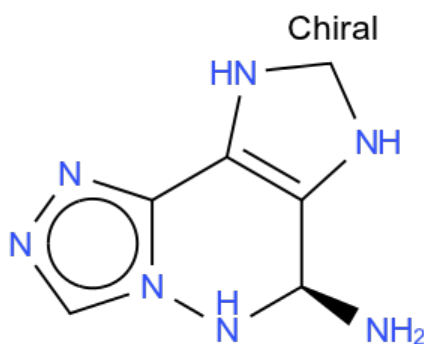
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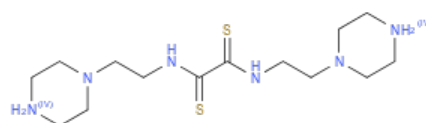
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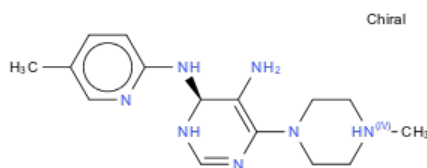
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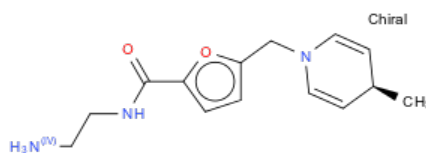
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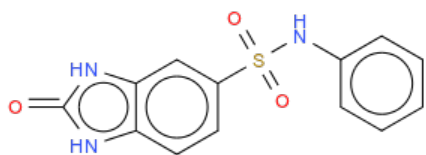
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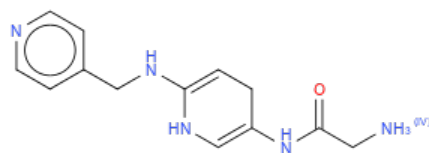
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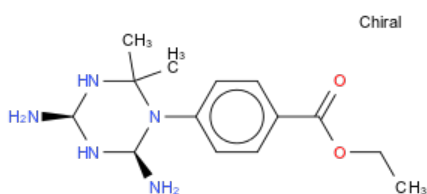
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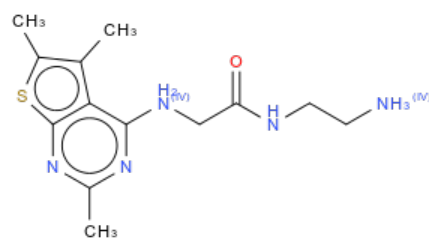
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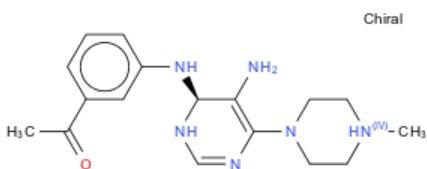
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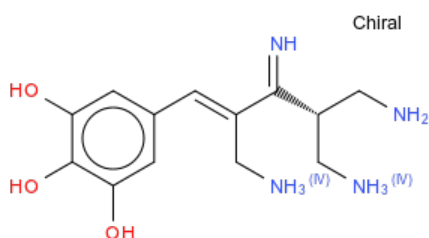
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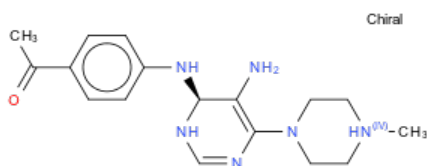
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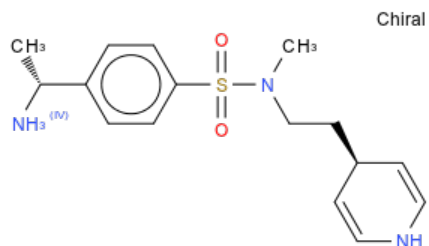
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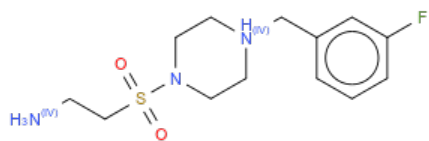
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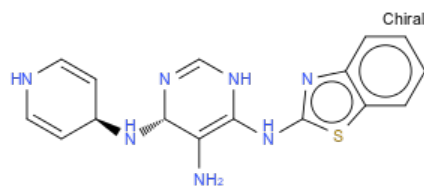
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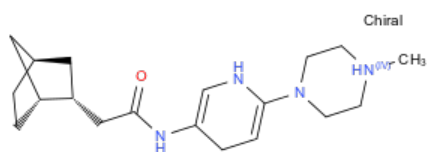
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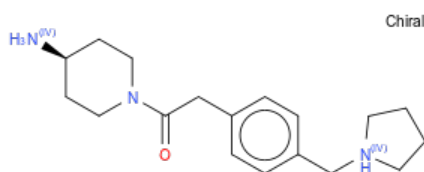
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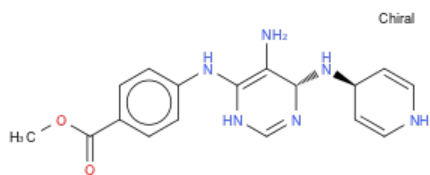
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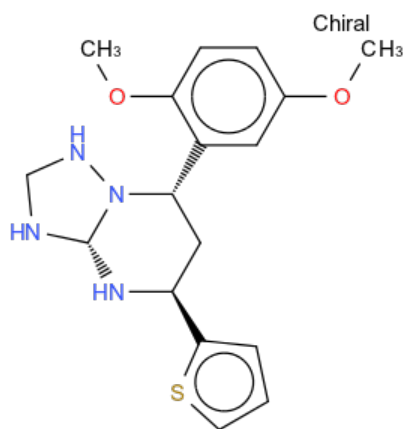
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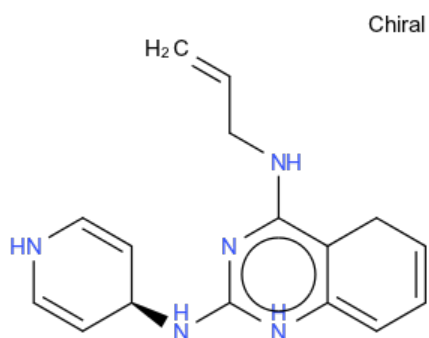
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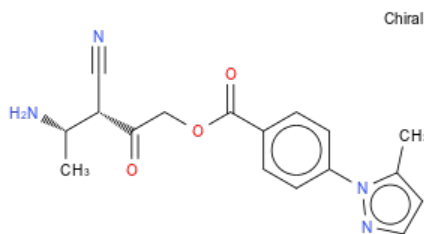
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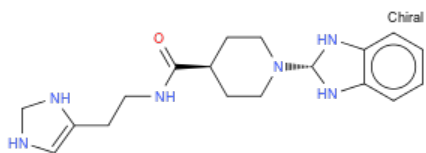
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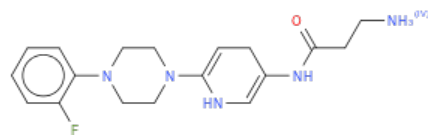
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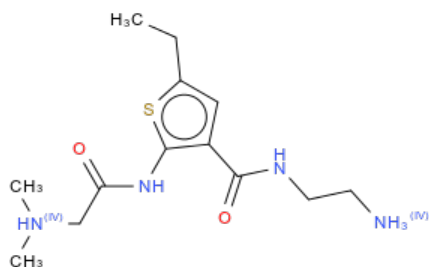
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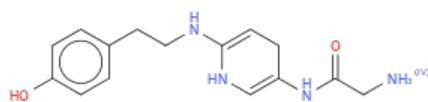
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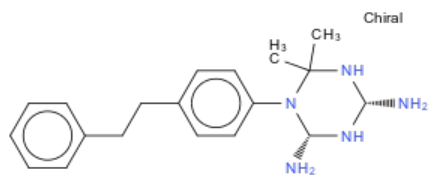
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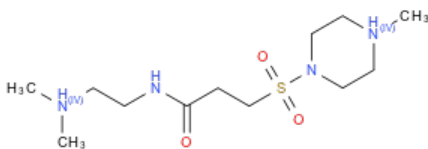
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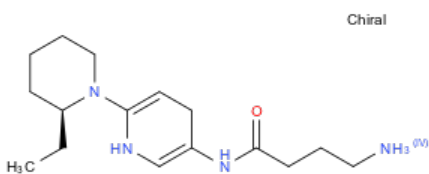
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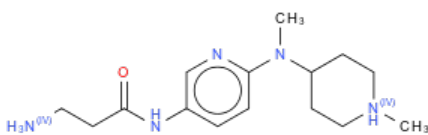
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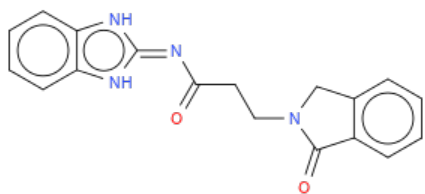
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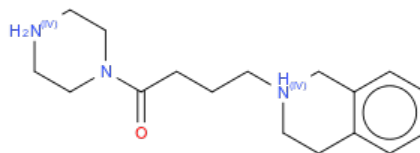
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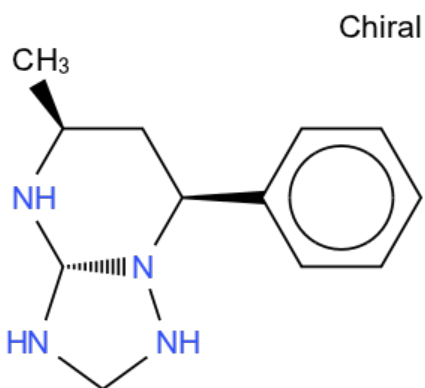
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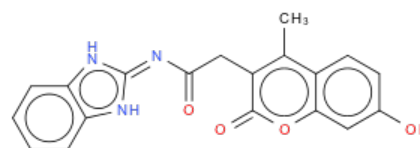
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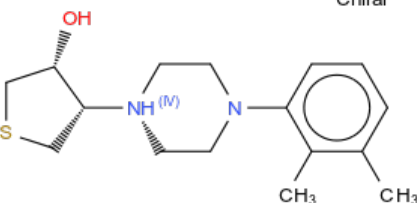
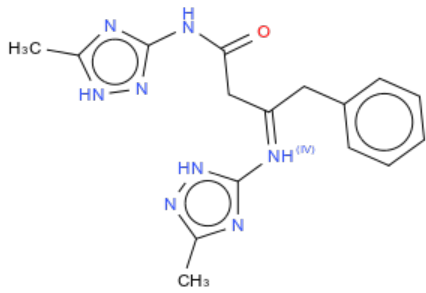
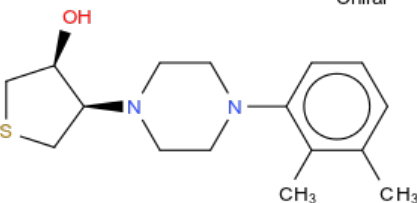
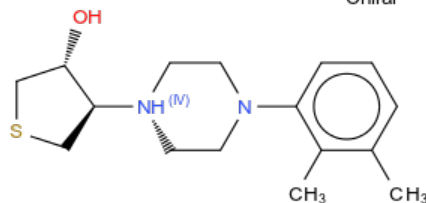
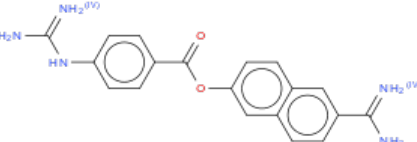
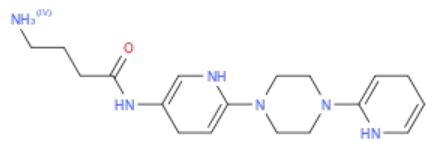
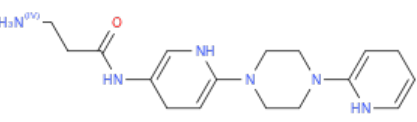
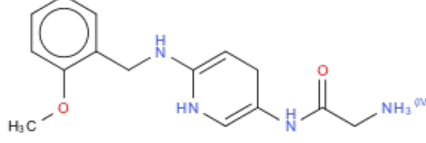
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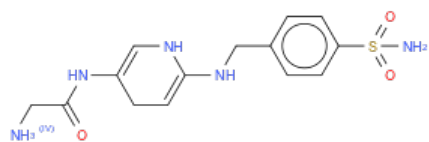


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Table S2

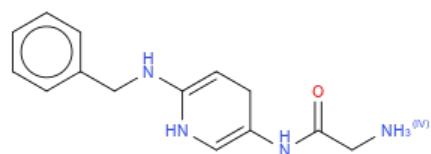
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3	<p>Chiral</p>  <p>C13727253</p>	C13727253	4	<p>Chiral</p>  <p>C13727248</p>	C13727248
5	 <p>C00001763</p>	C00001763	6	 <p>C31962462</p>	C31962462
7	 <p>C31962640</p>	C31962640	8	 <p>C31961455</p>	C31961455

9



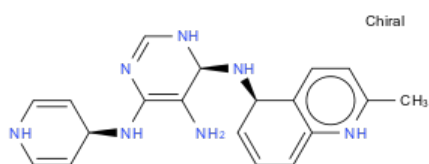
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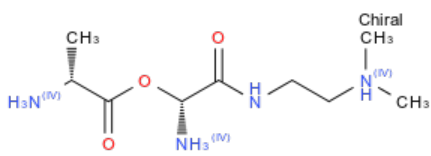
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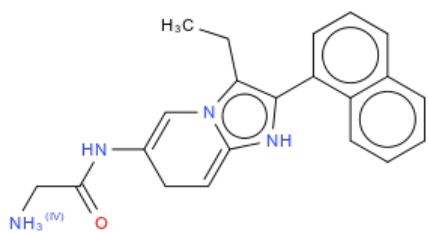
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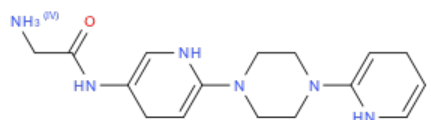
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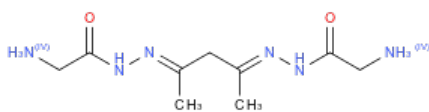
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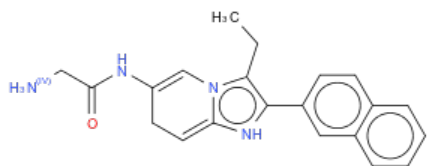
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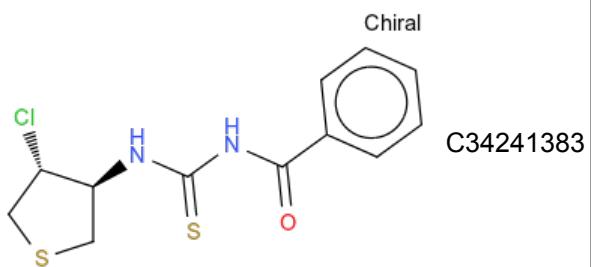
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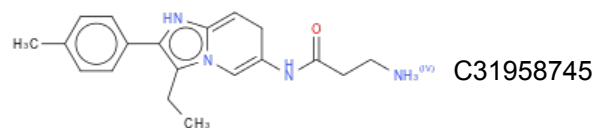


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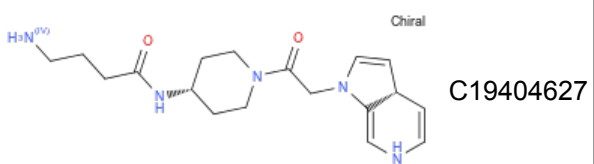
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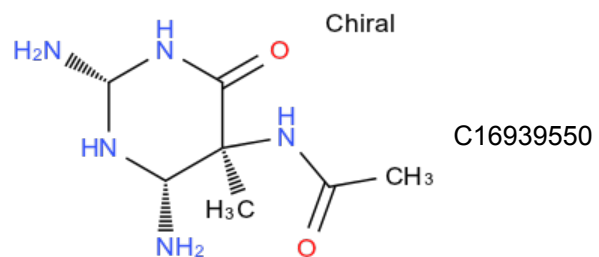
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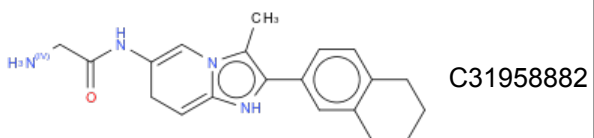
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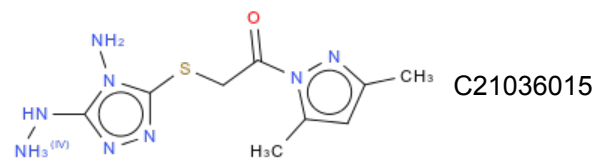
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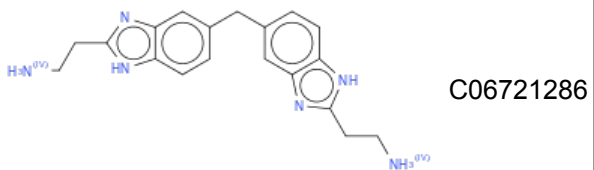
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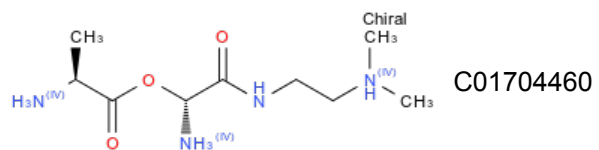
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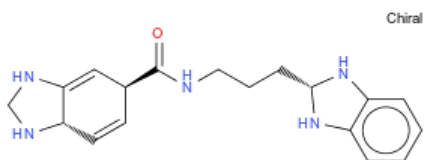
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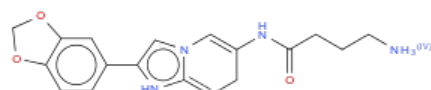


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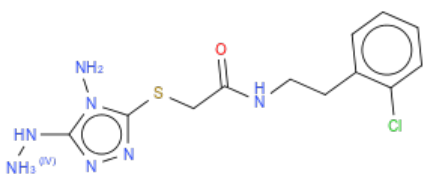
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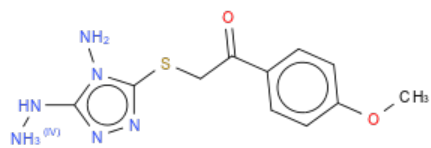
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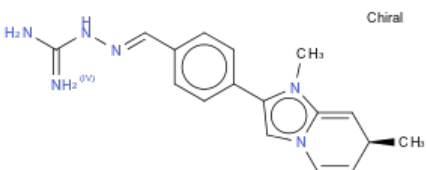
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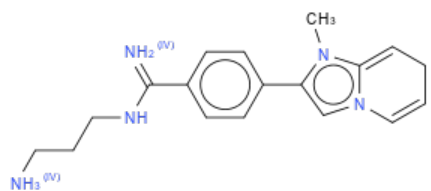
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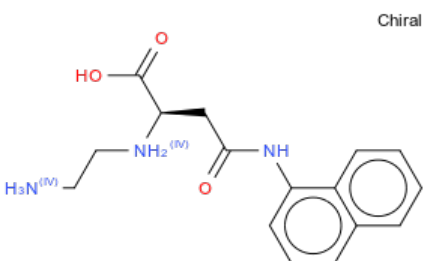
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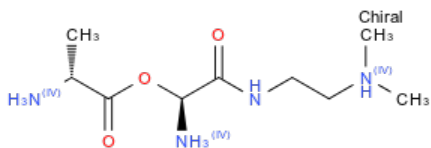
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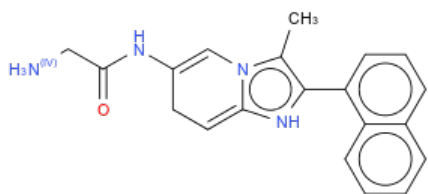
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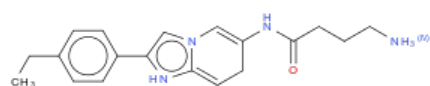
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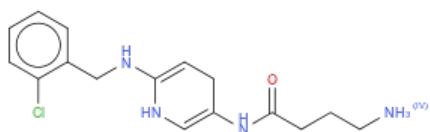
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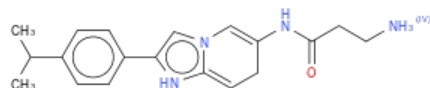
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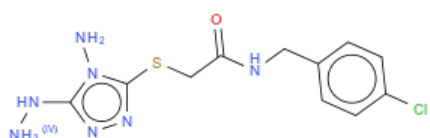
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36



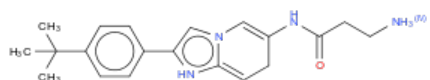
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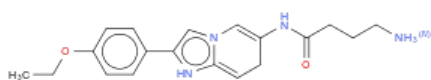
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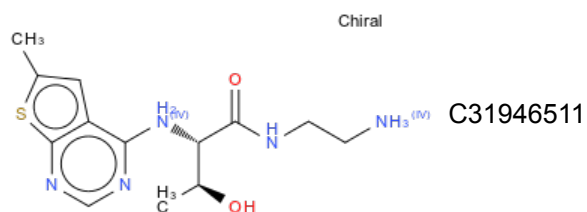
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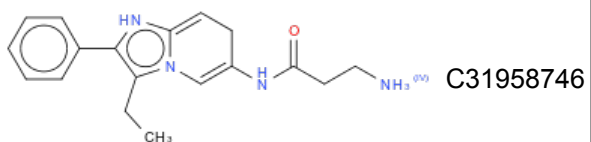
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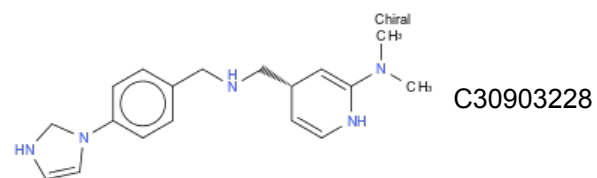


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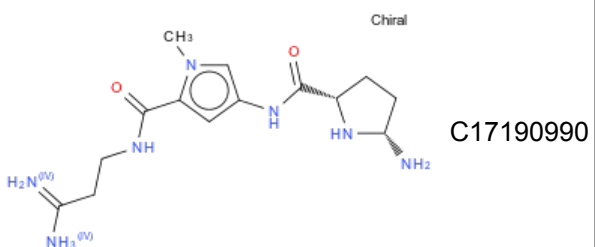
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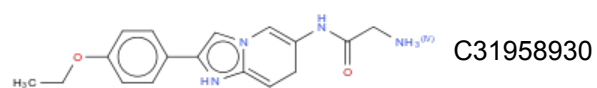
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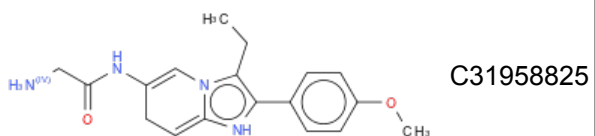
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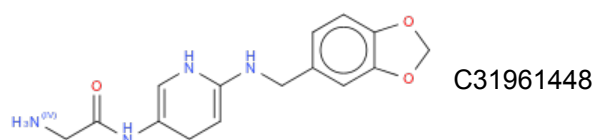
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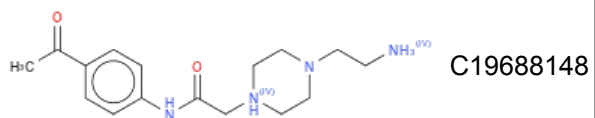
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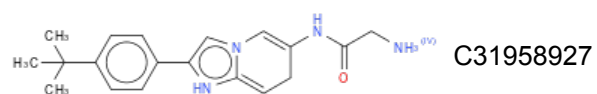
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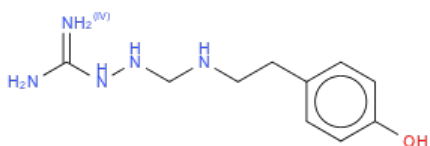
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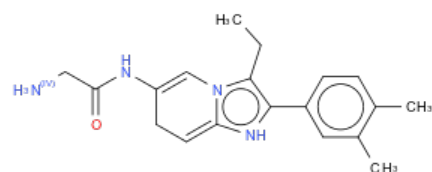


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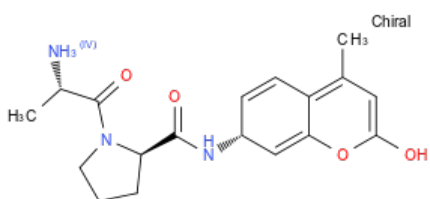
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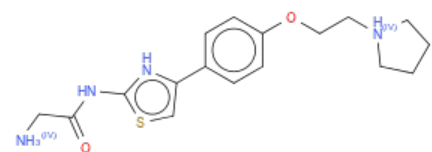
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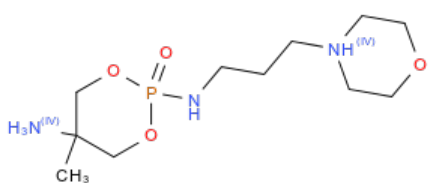
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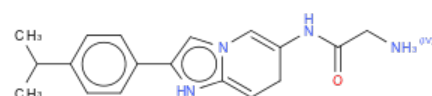
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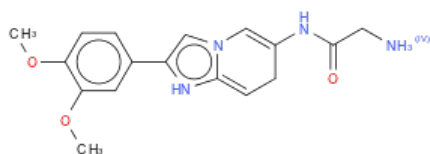
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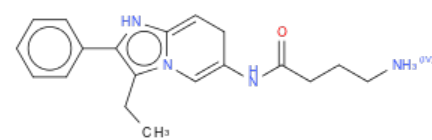
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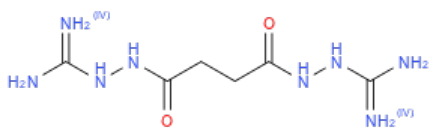
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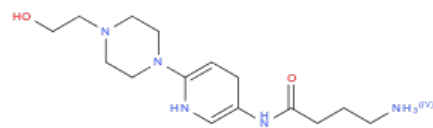
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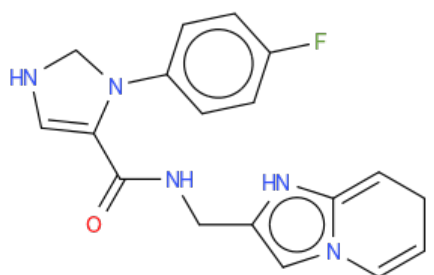
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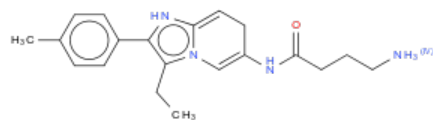
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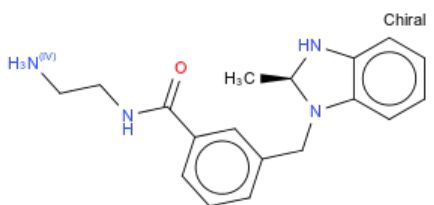
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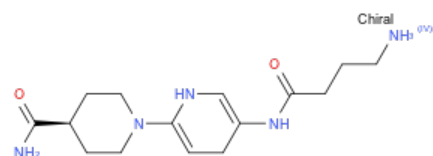
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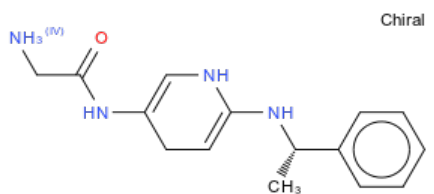
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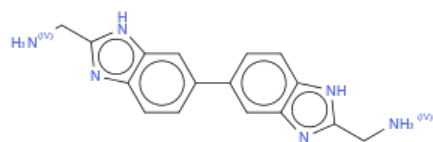
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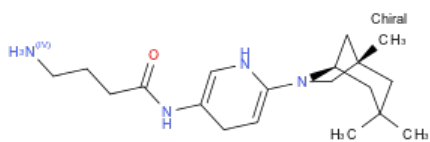
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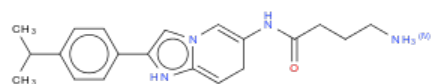
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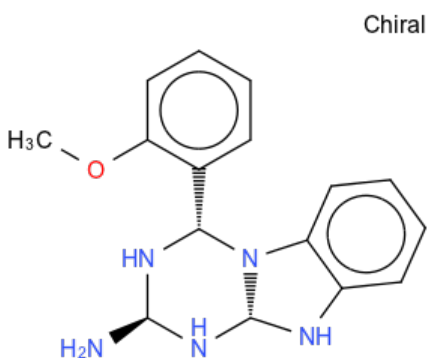
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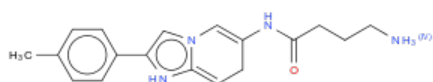
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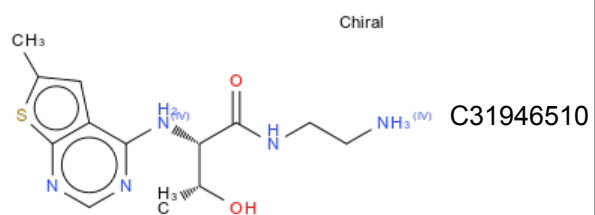
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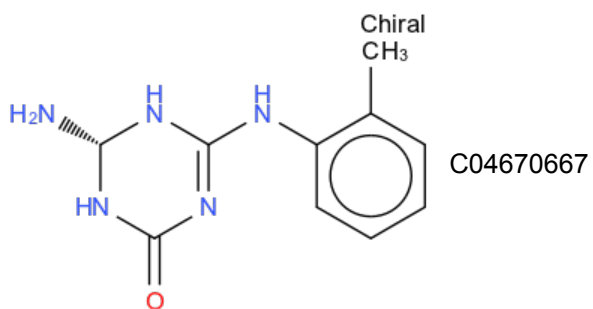
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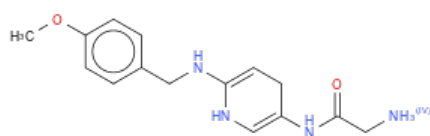
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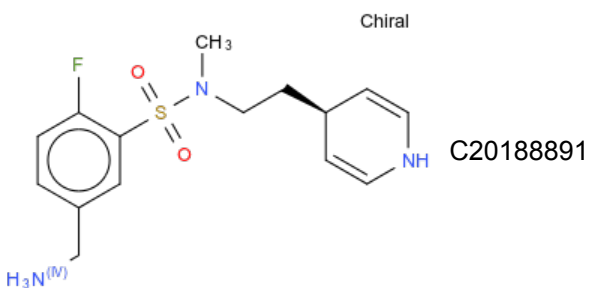
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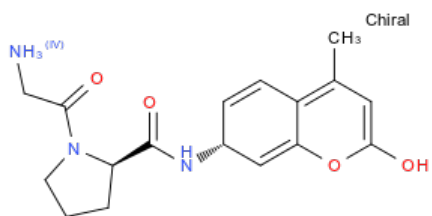
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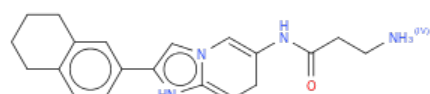
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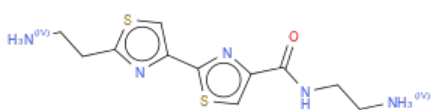
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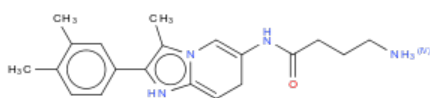
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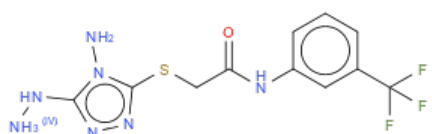
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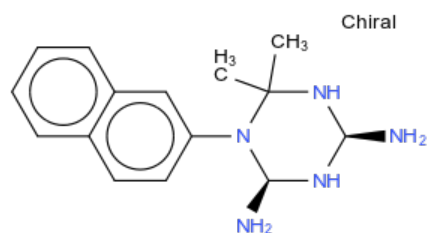
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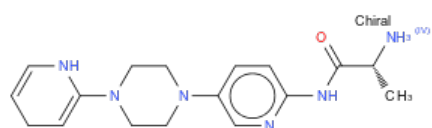
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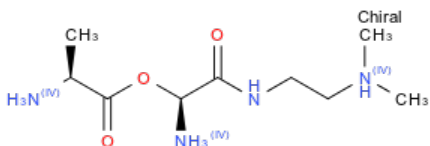
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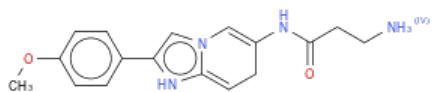
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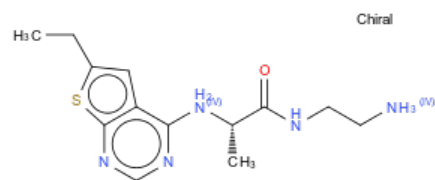
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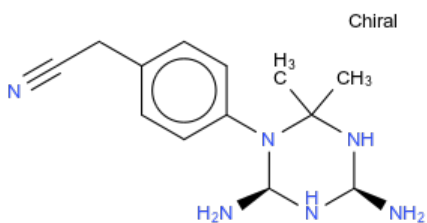
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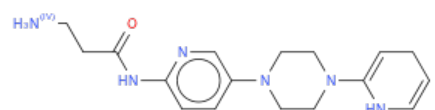
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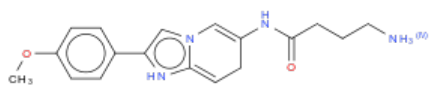
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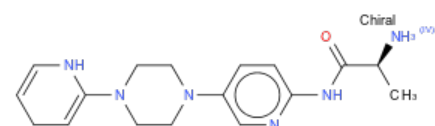
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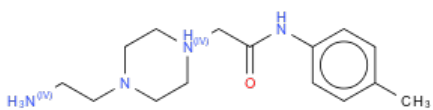
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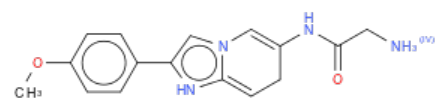
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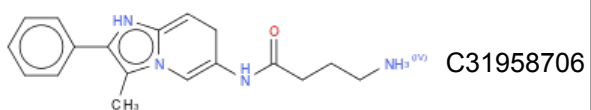
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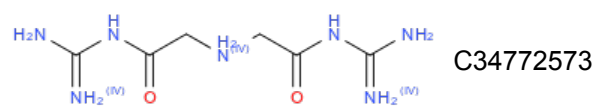


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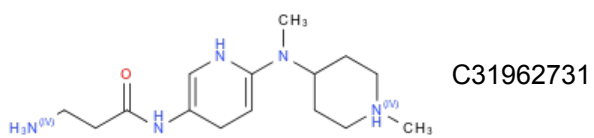
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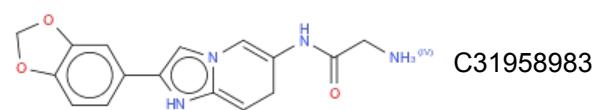
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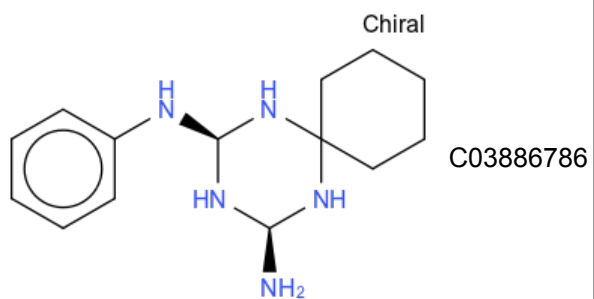
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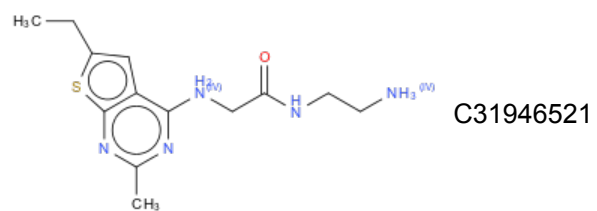
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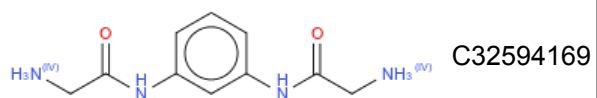
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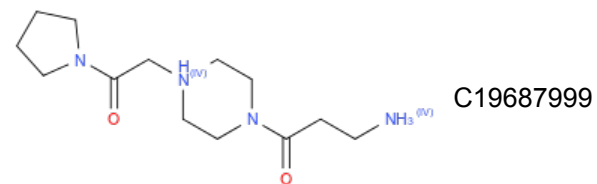
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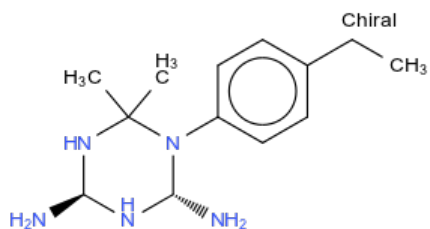
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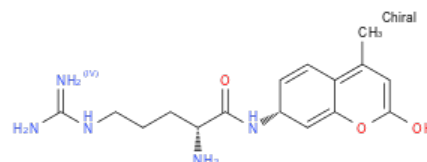


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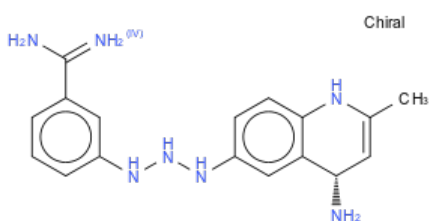
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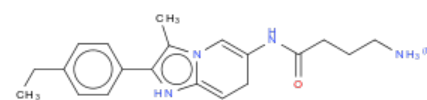
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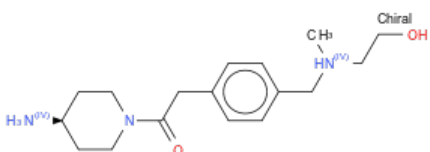
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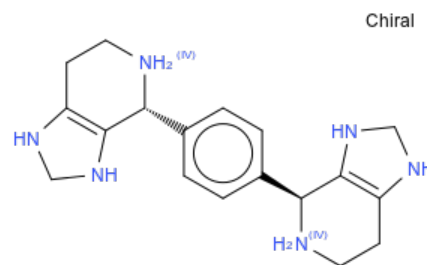
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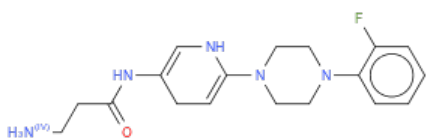
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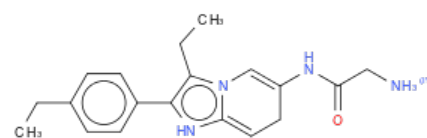
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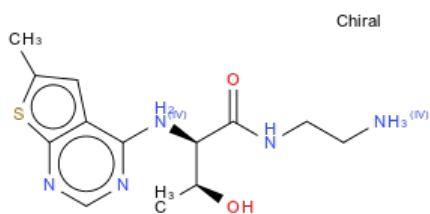
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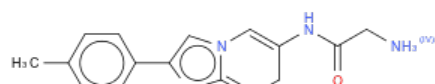
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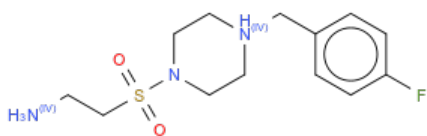
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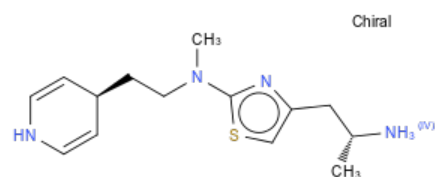
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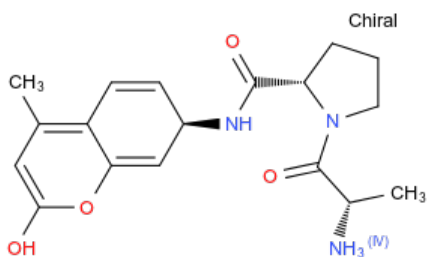
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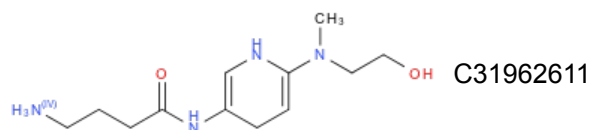
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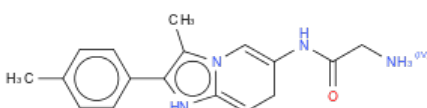
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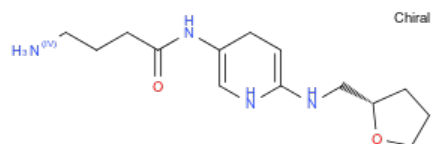
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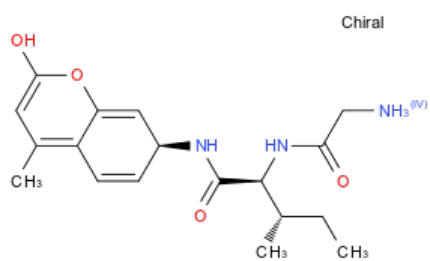
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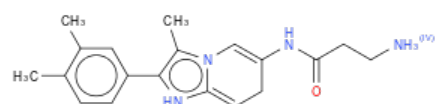
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113



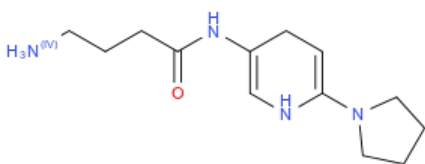
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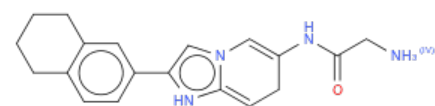
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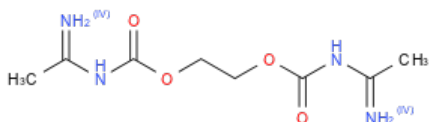
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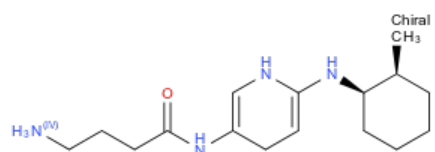
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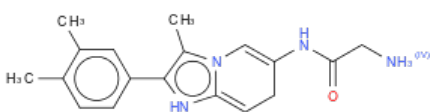
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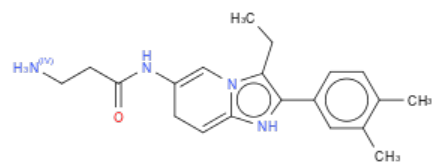
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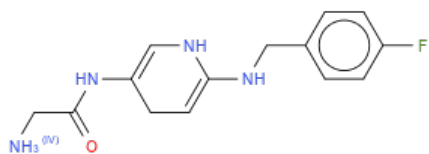
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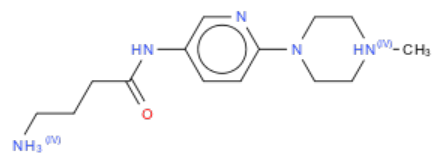
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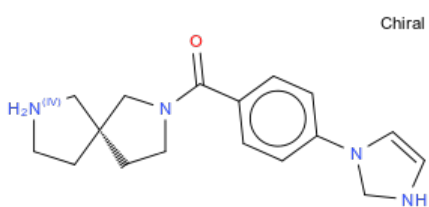
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122



C31962602

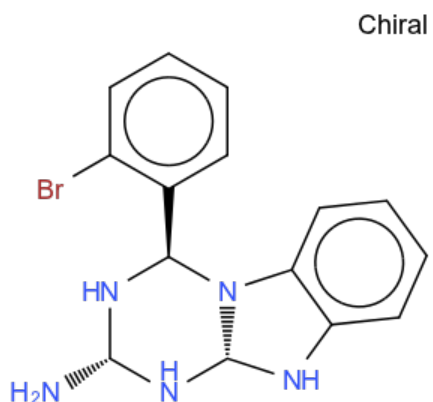
123



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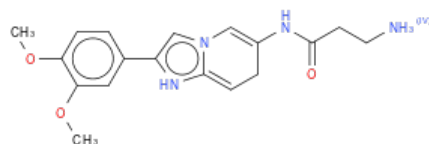
124



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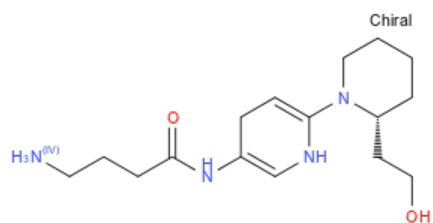
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125



C31958788

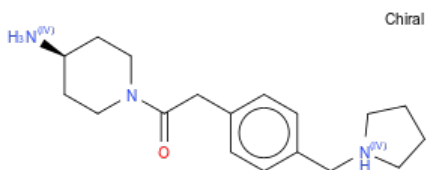
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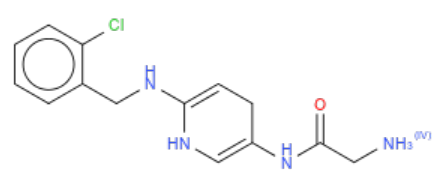
127



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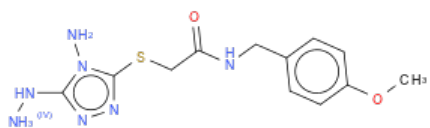
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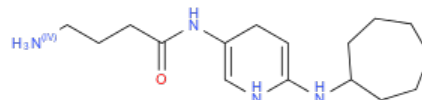
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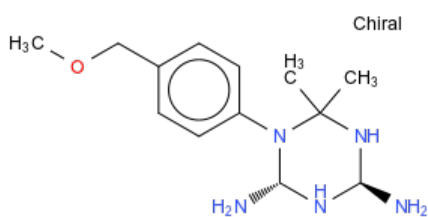
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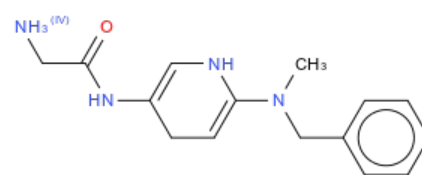
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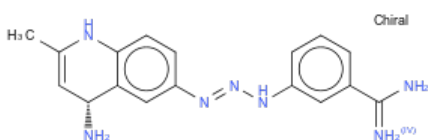
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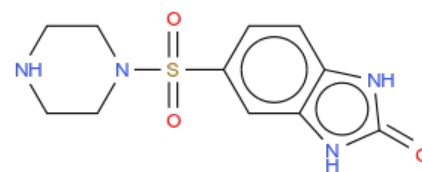
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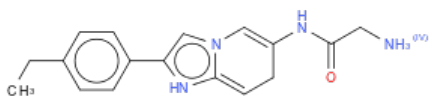
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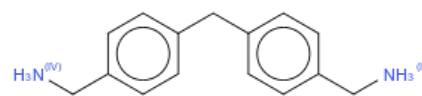
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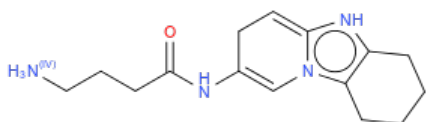
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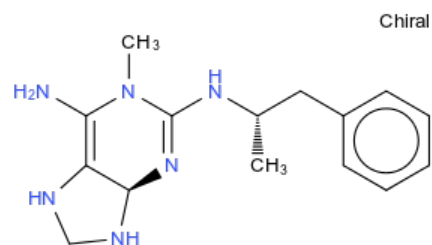
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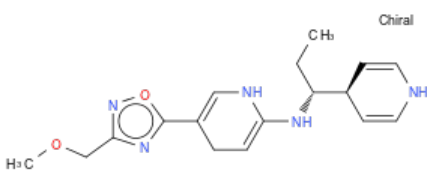
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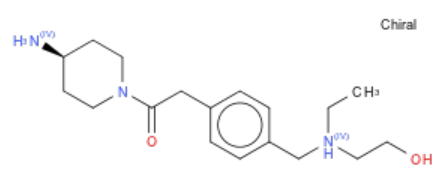
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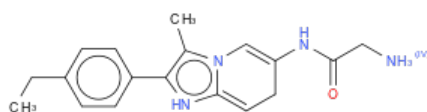
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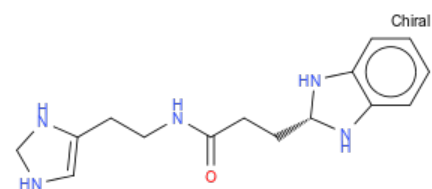
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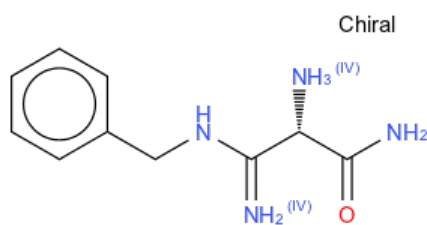
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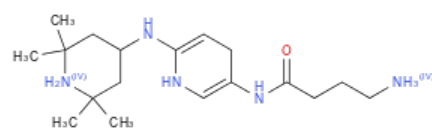
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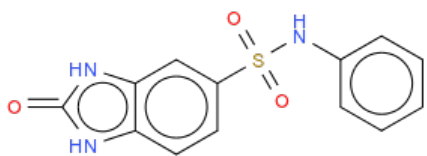
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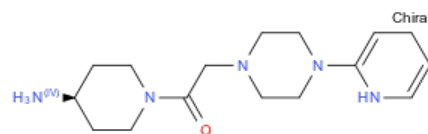
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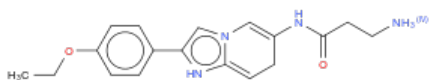
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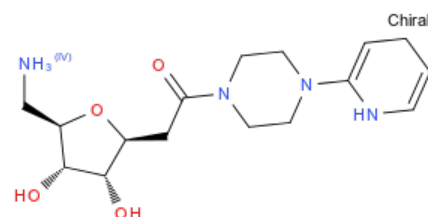
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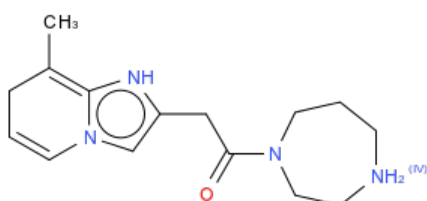
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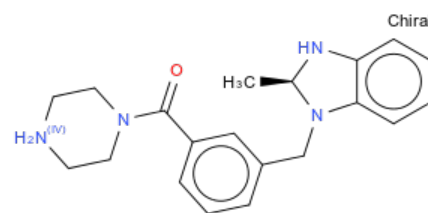
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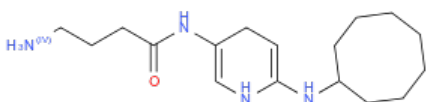
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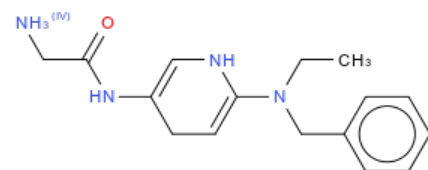
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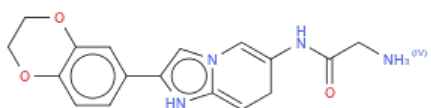
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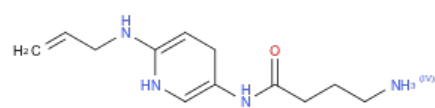
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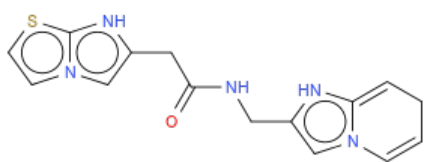
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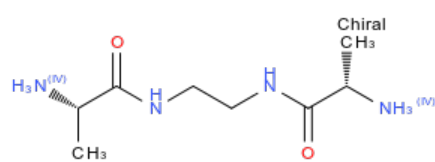
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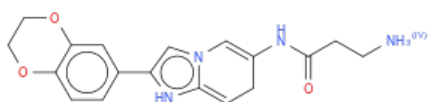
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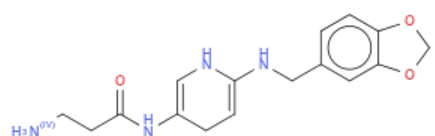
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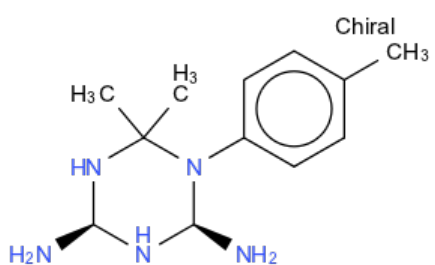
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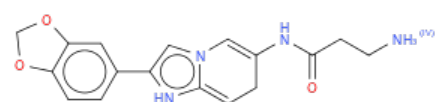
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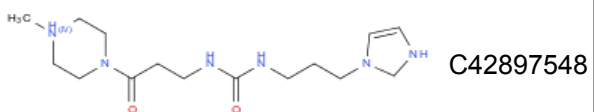
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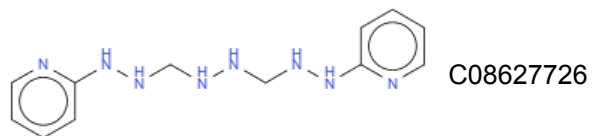


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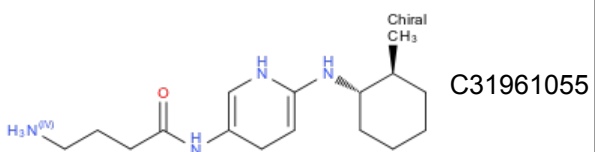
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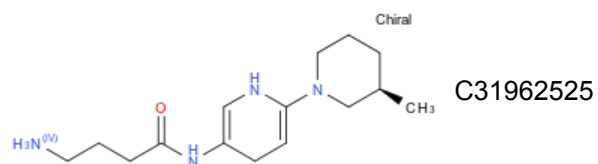
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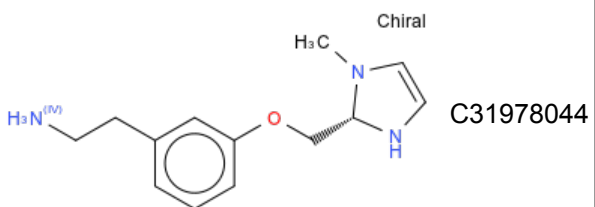
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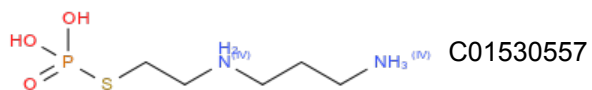
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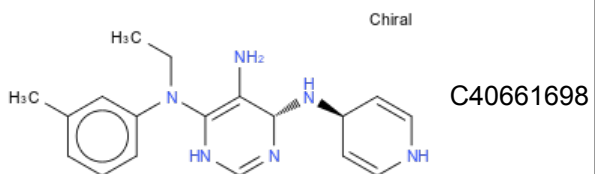
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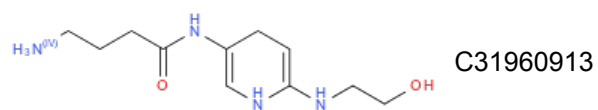
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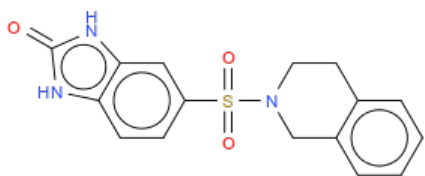
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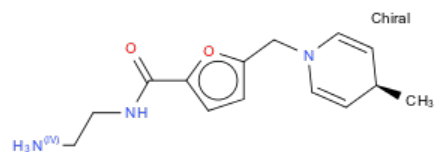


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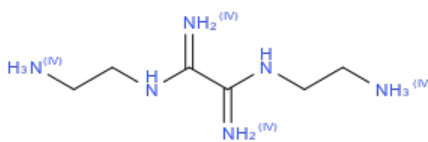
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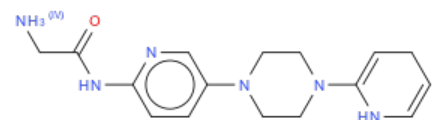
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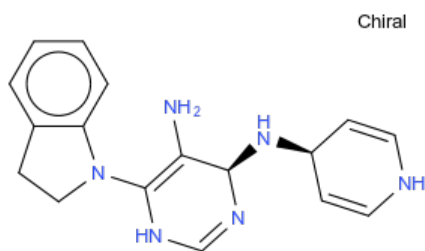
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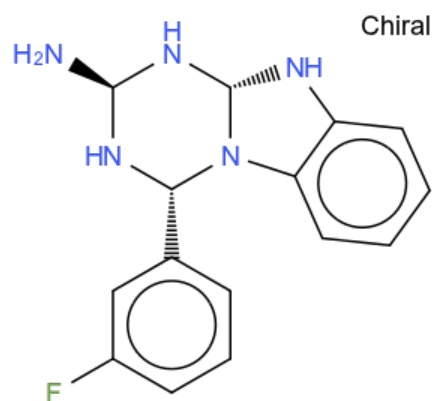
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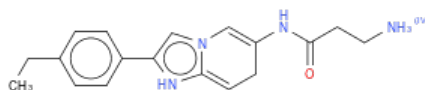
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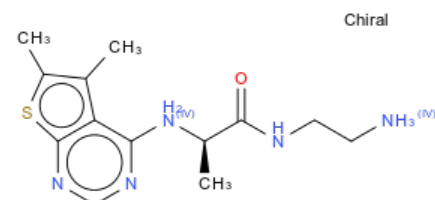
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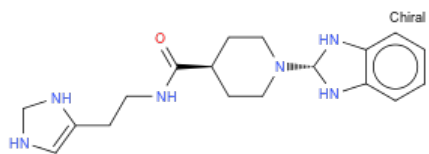
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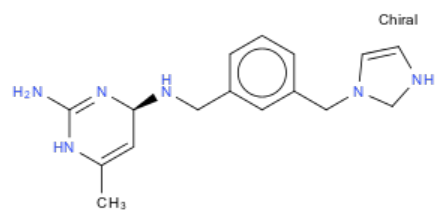
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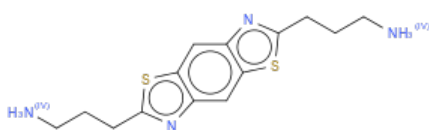
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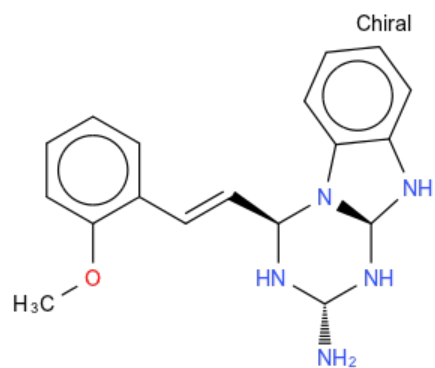
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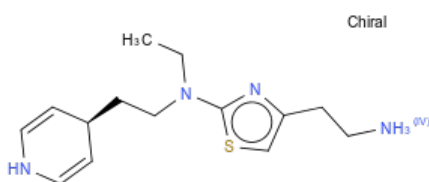
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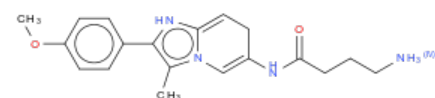
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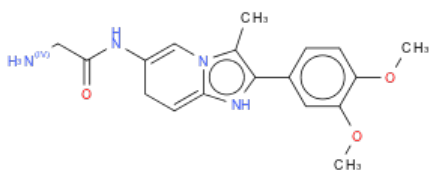
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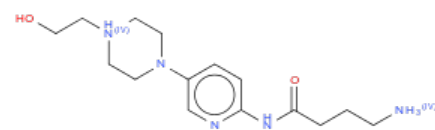
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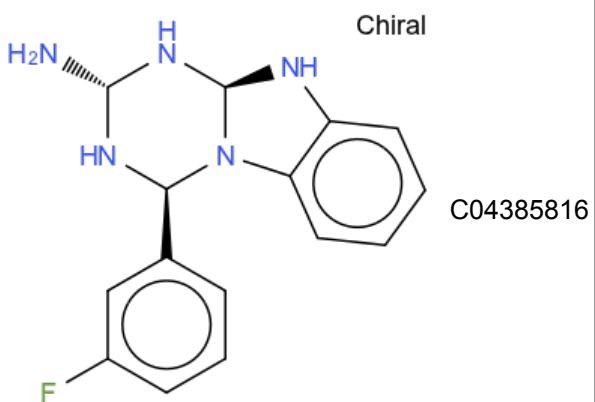
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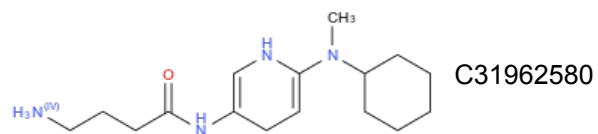
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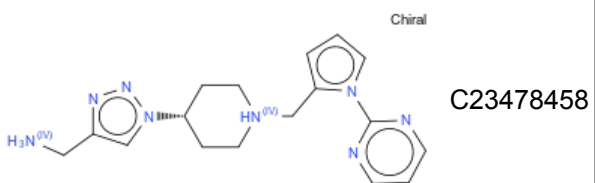
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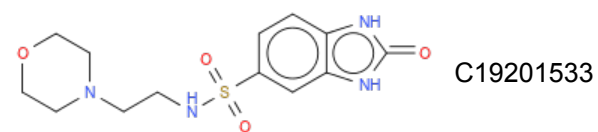
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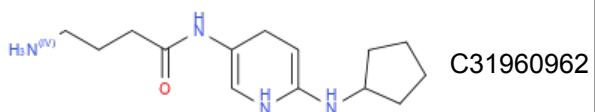
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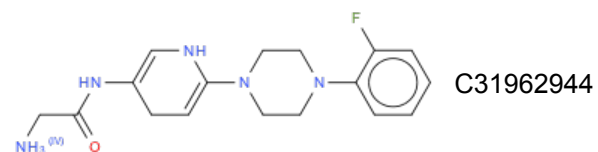
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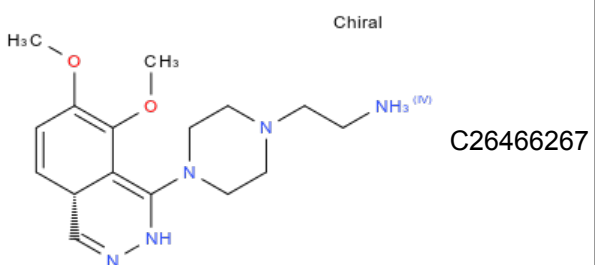
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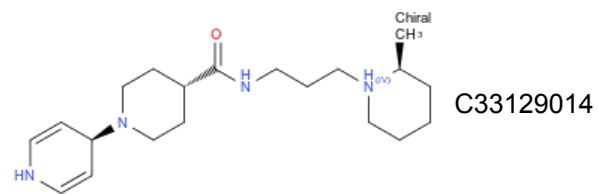
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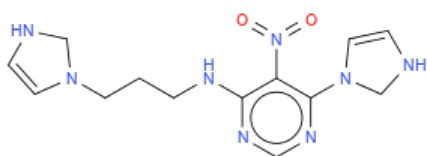
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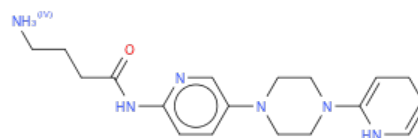


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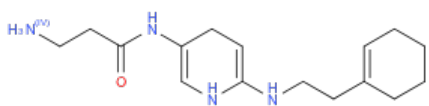
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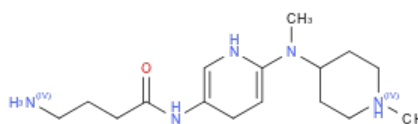
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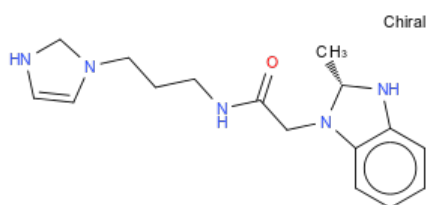
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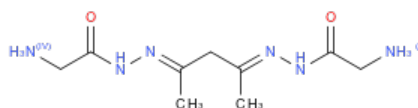
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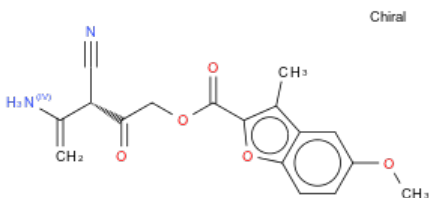
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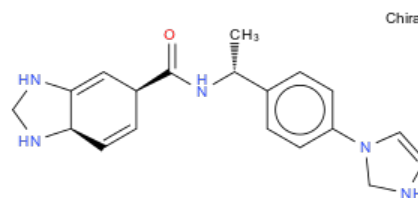
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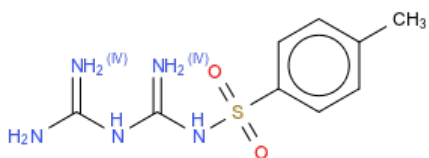
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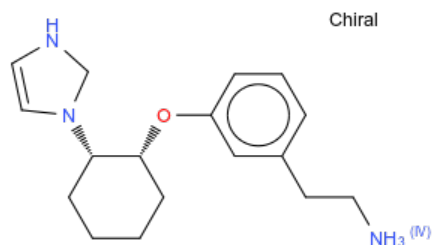
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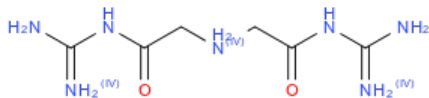
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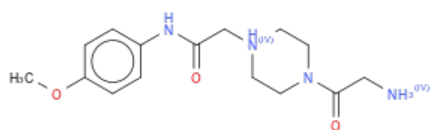
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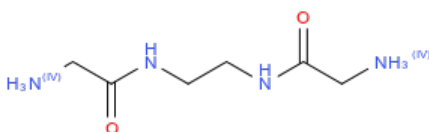
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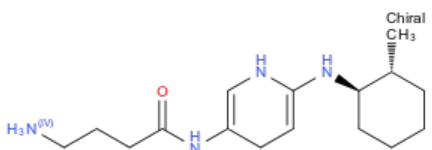
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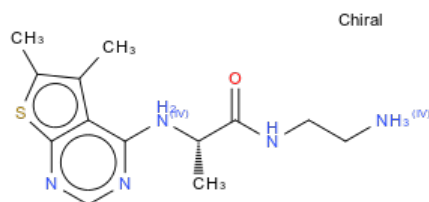
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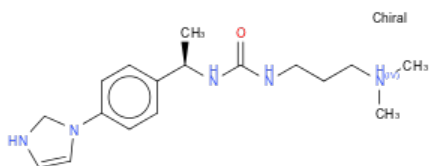
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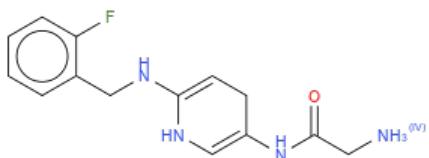
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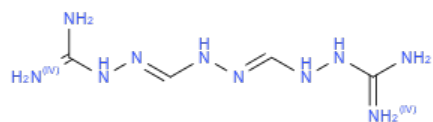
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209



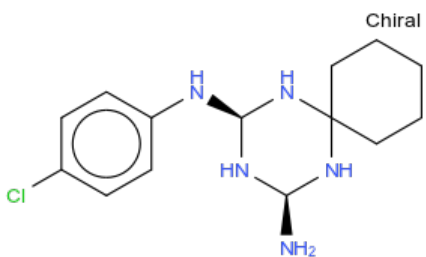
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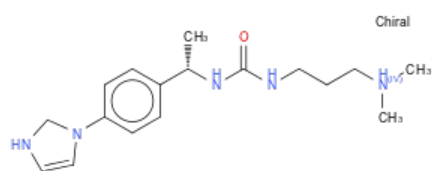
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211



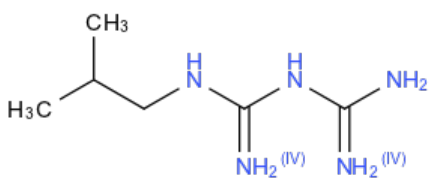
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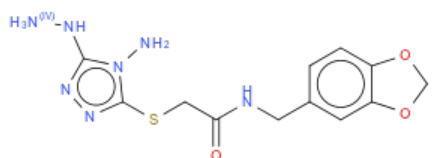
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213



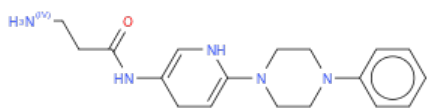
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214



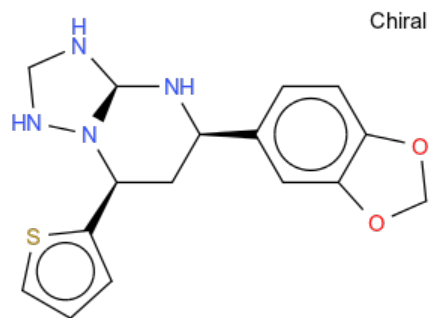
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215



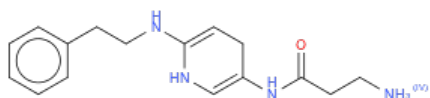
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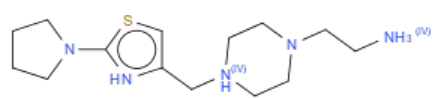
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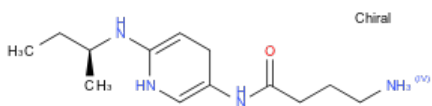
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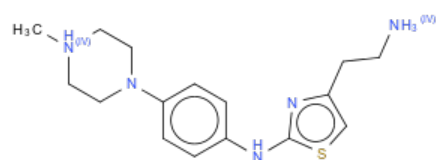
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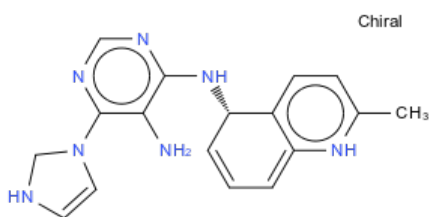
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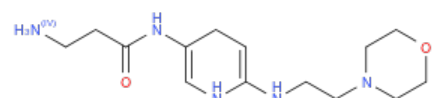
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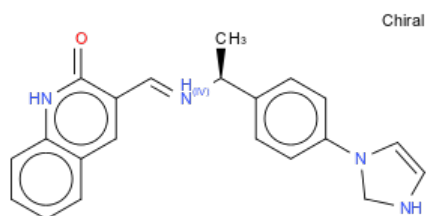
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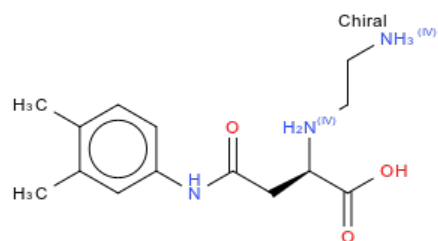
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223



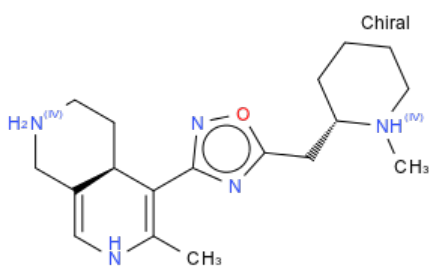
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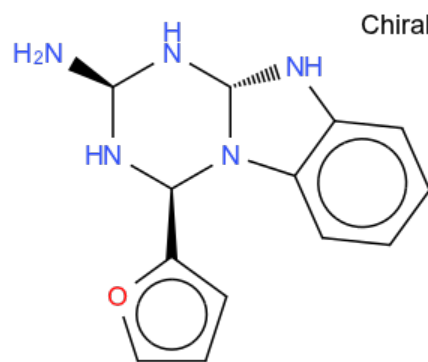
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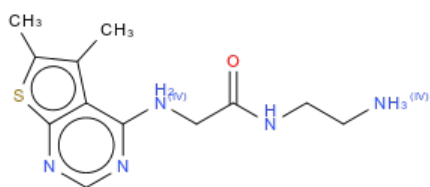
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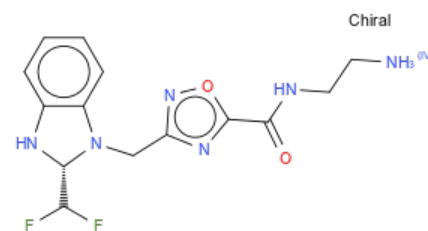
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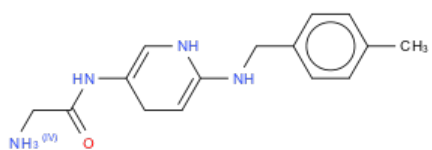
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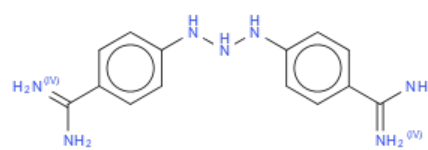
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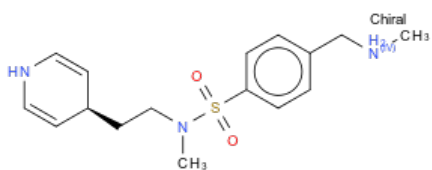
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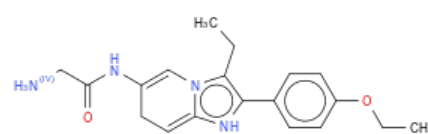
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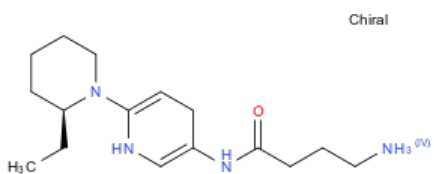
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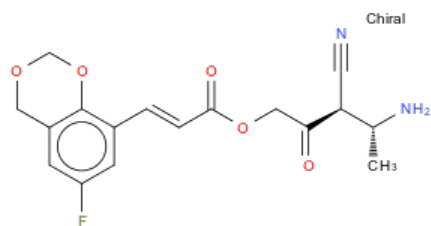
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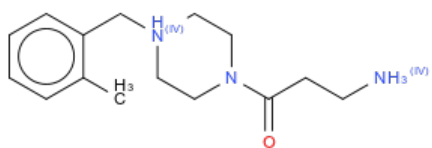
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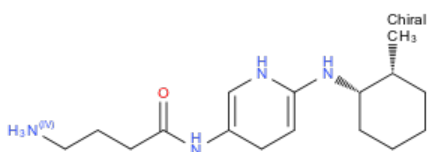
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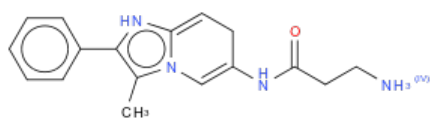
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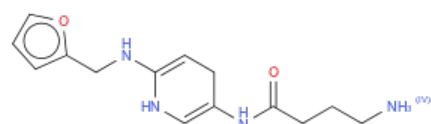
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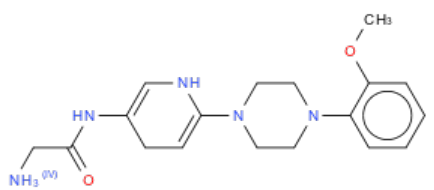
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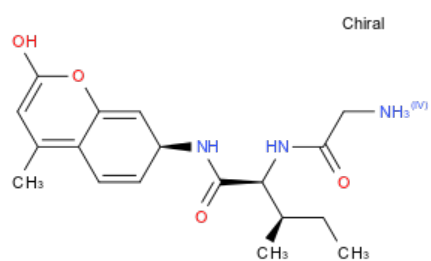
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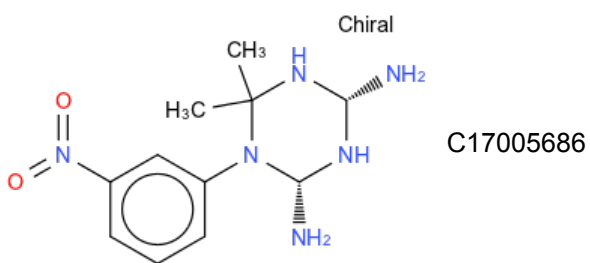
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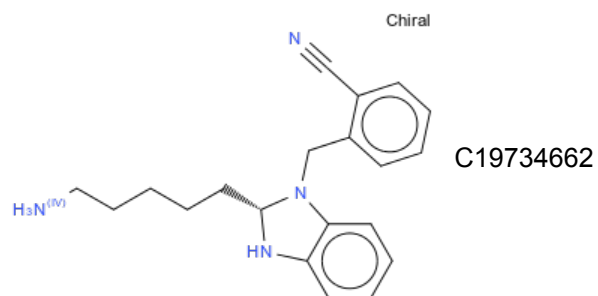


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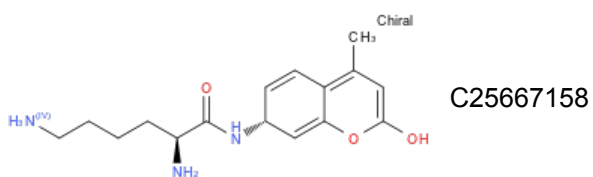
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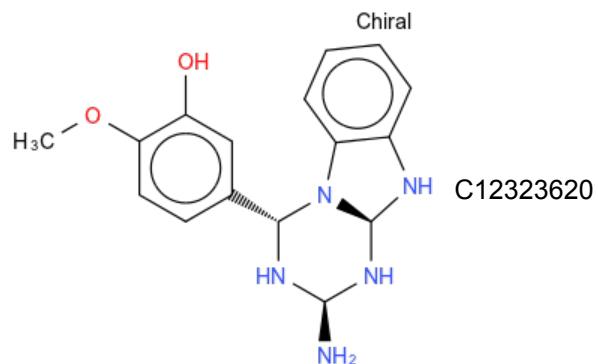
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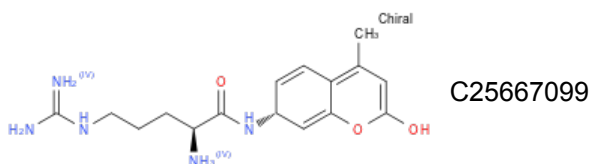
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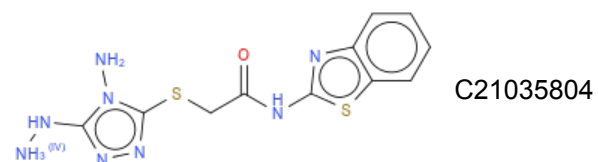
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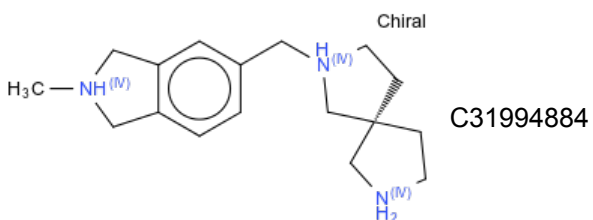
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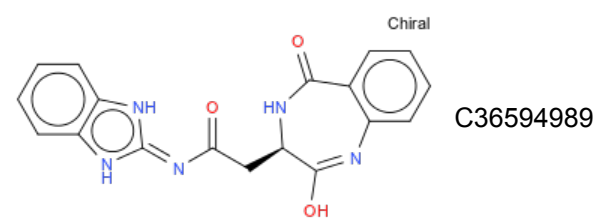
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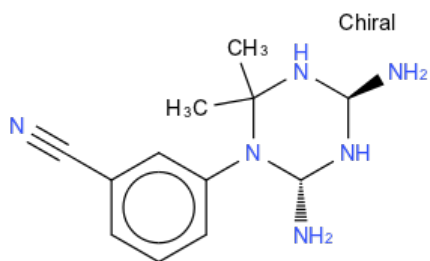
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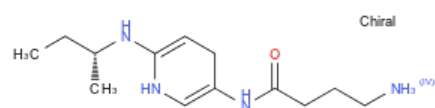


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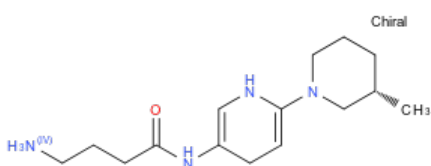
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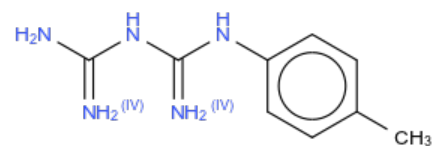
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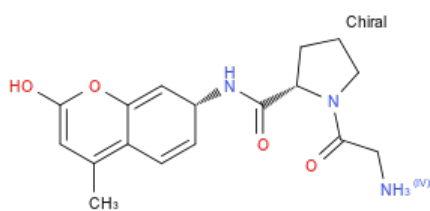
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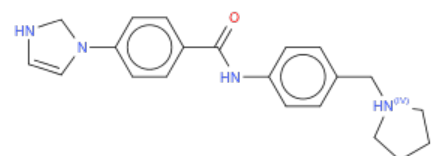
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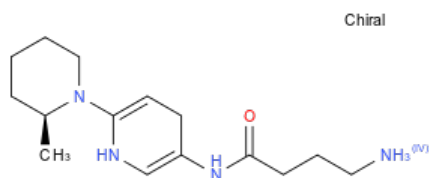
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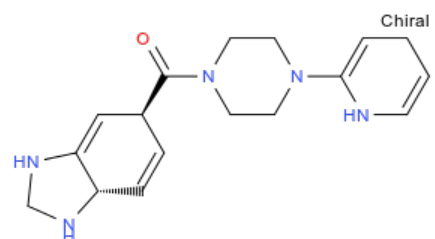
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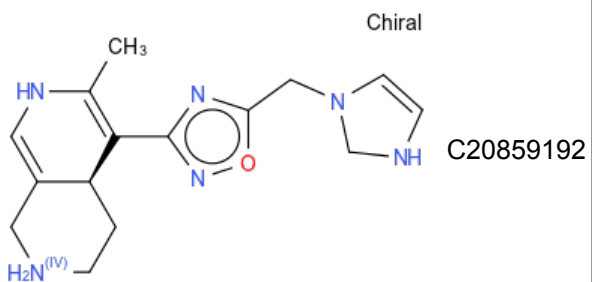
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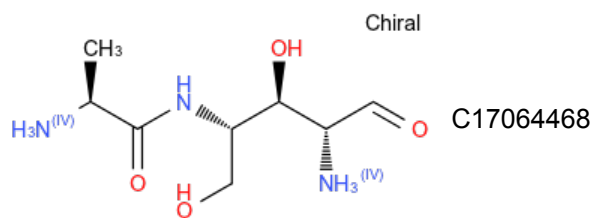


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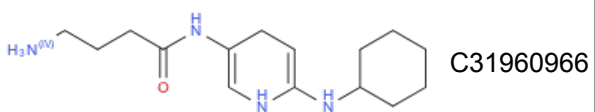
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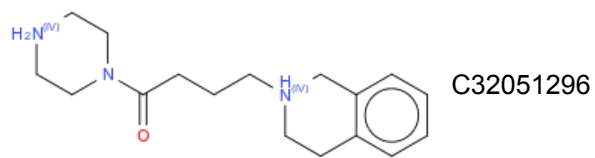
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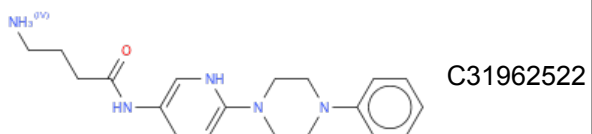
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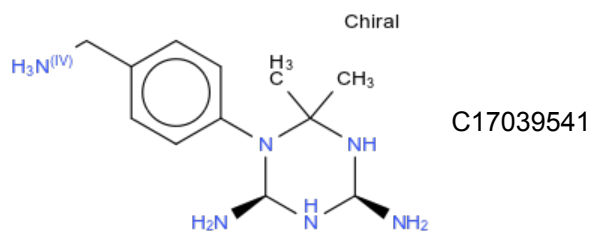
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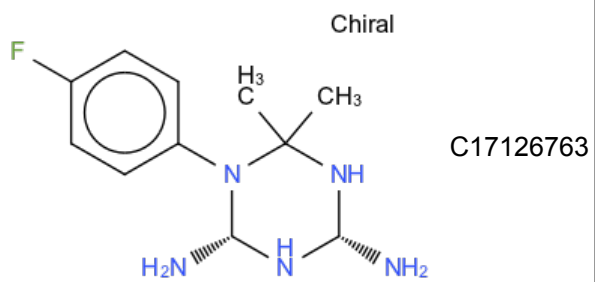
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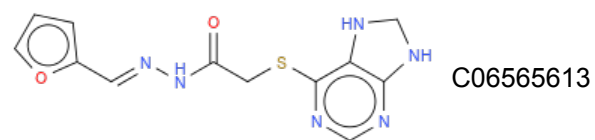
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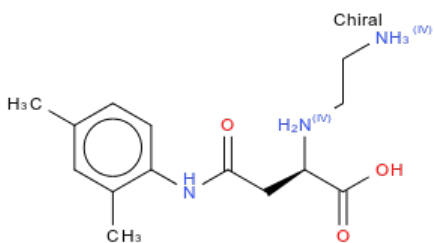
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264

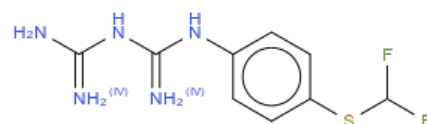


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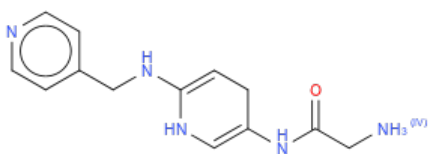
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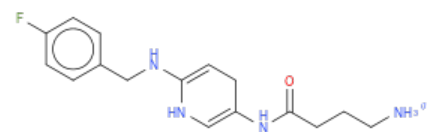
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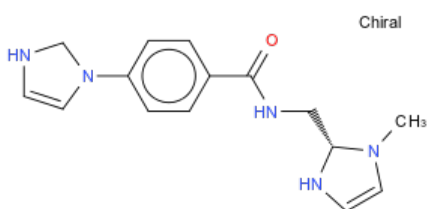
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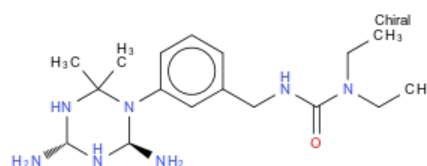
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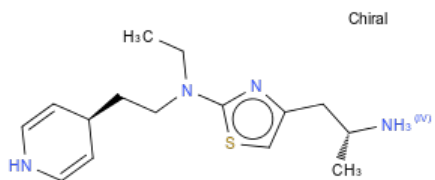
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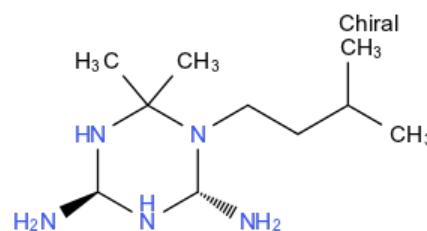
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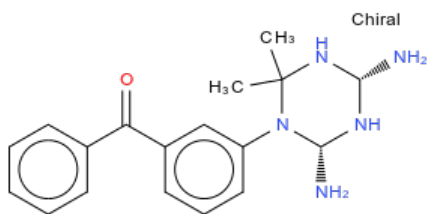
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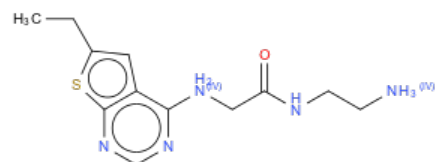
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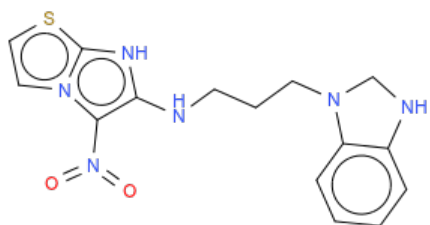
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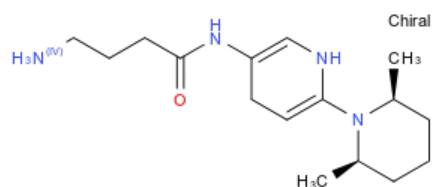
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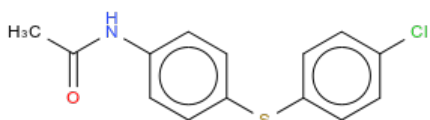
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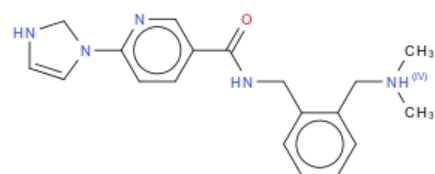
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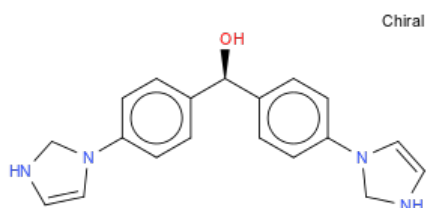
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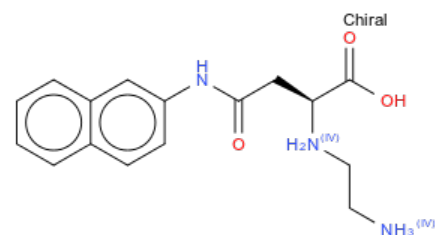
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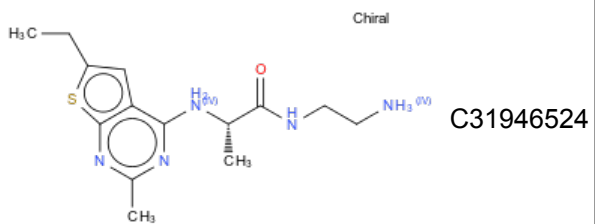
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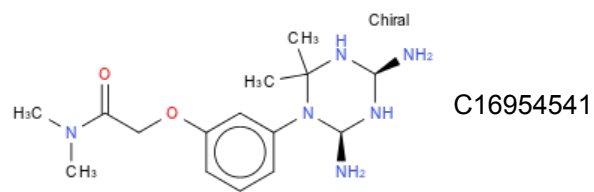


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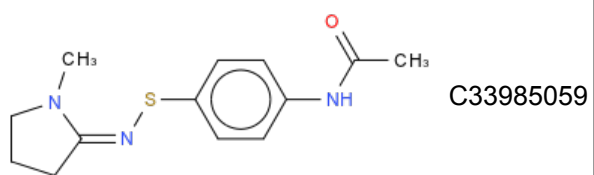
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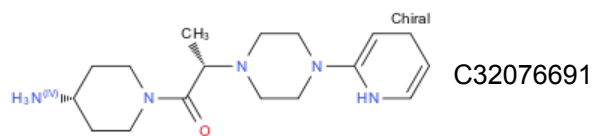
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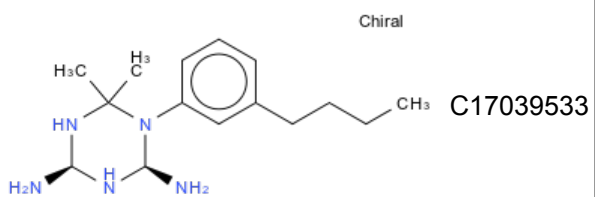
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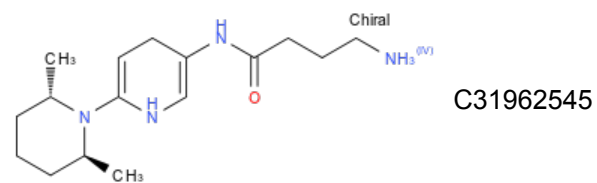
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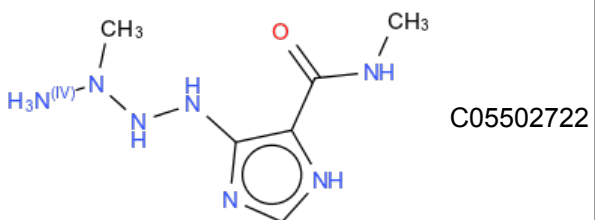
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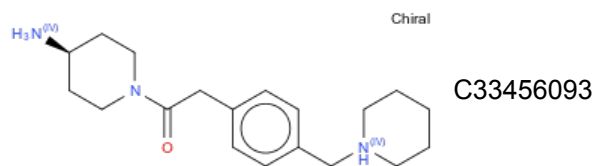
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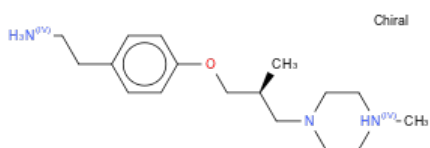
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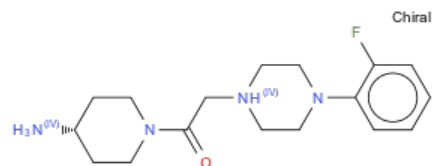


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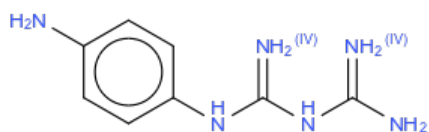
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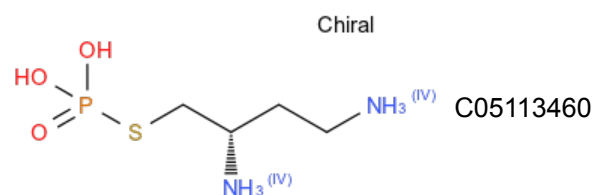
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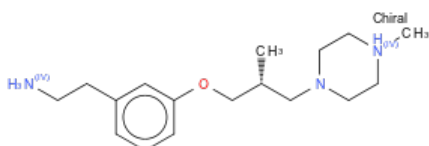
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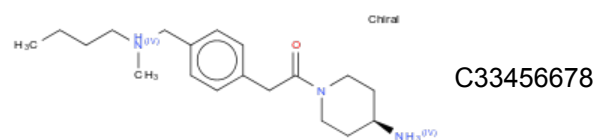
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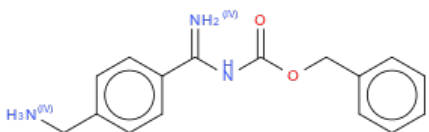
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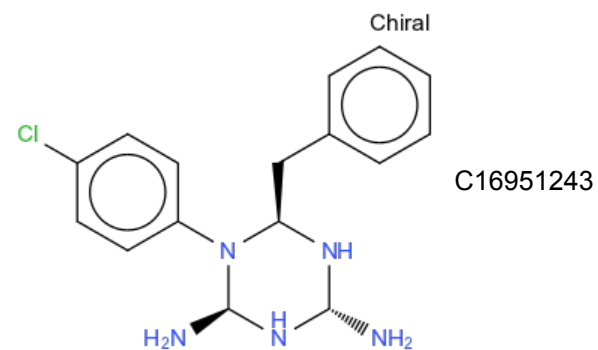
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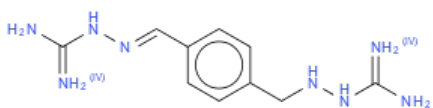
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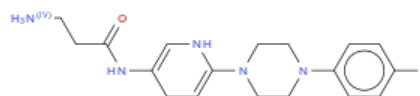
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297



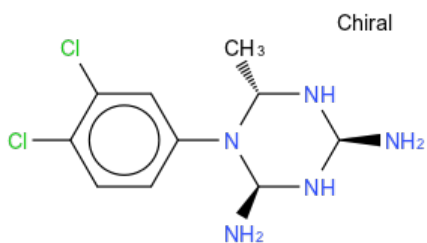
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298



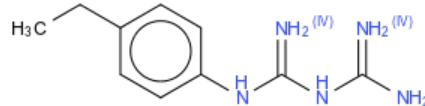
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299



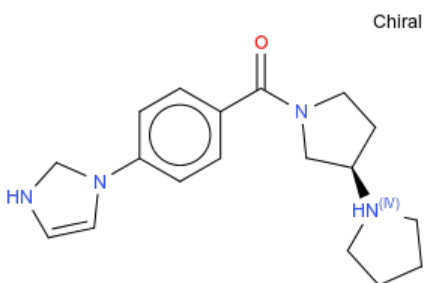
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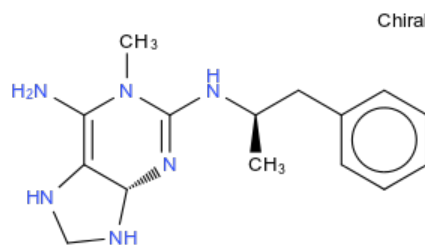
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301



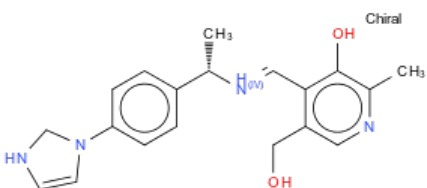
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302



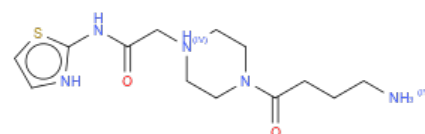
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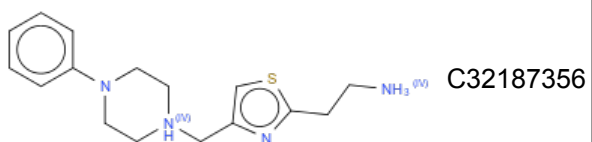
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304



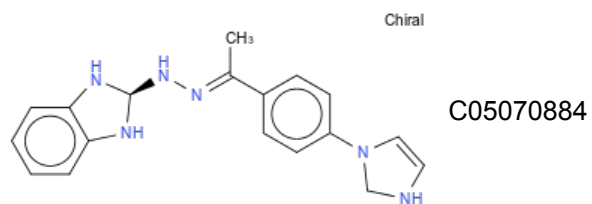
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305



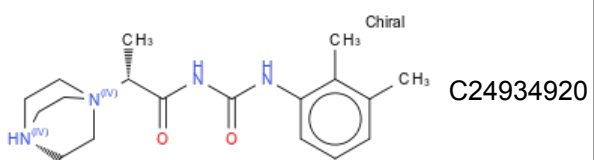
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306



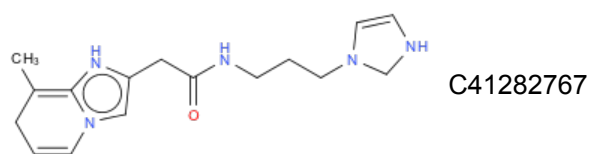
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307



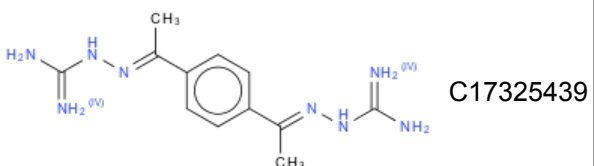
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308



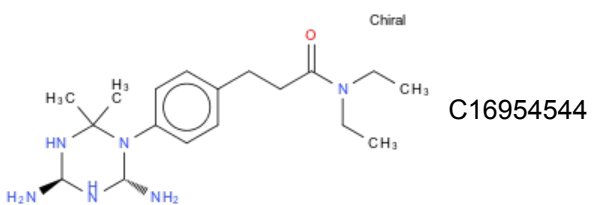
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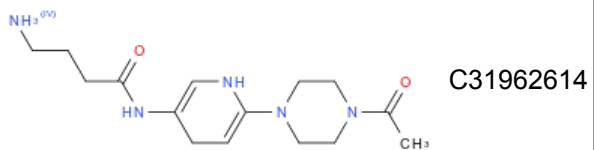
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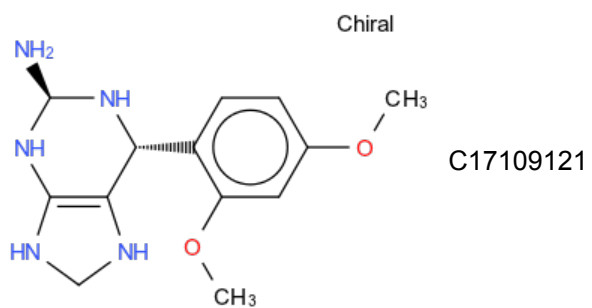
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311



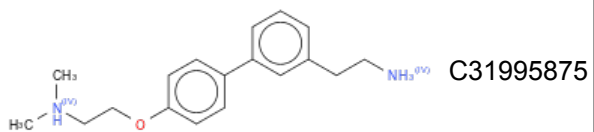
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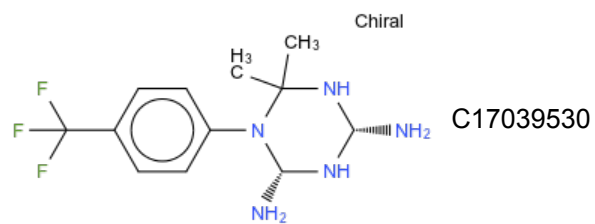


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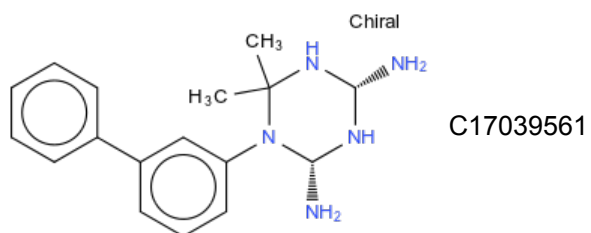
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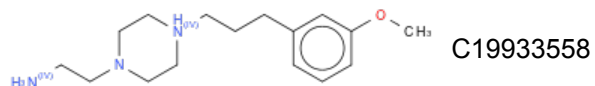
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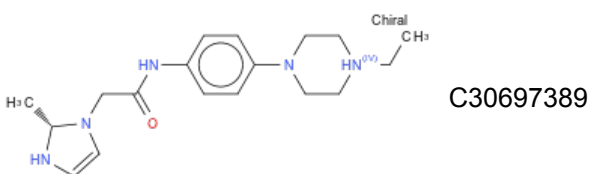
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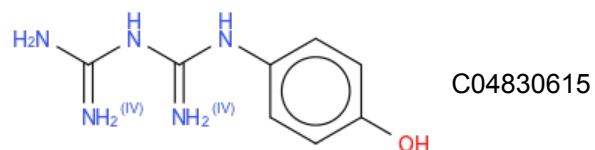
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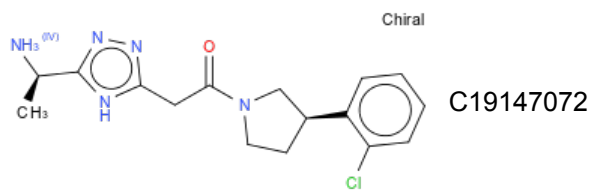
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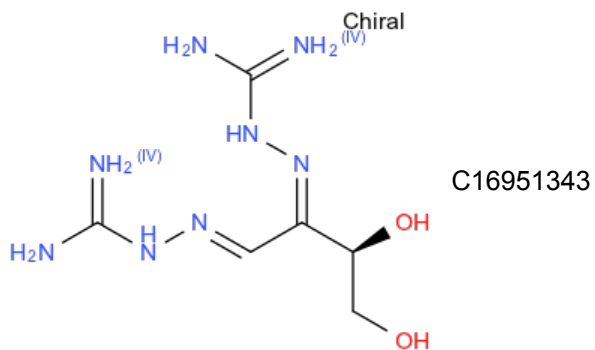
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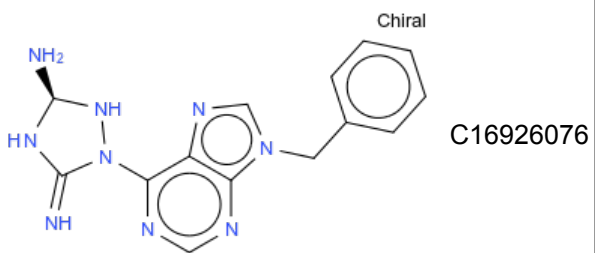
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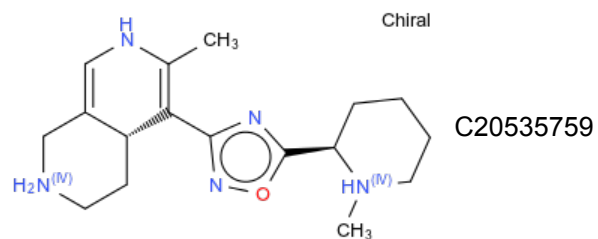
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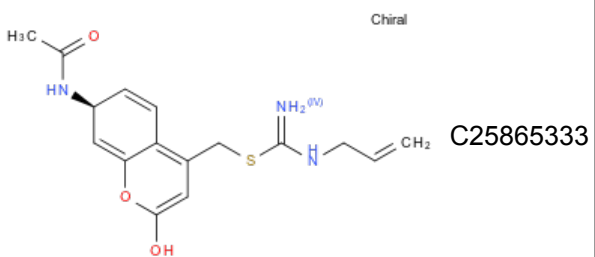
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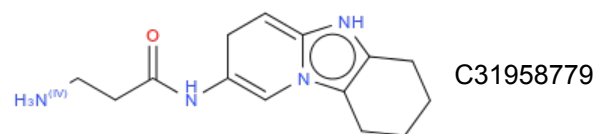
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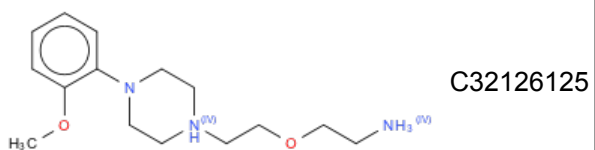
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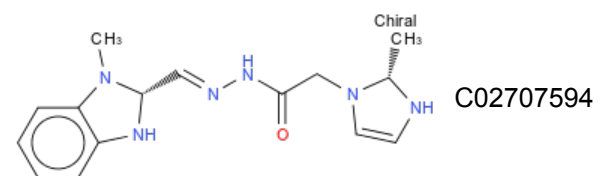
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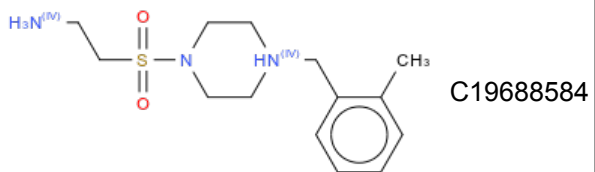
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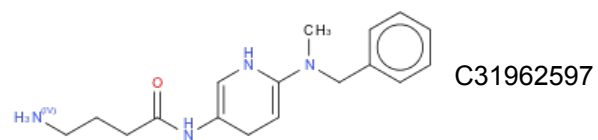
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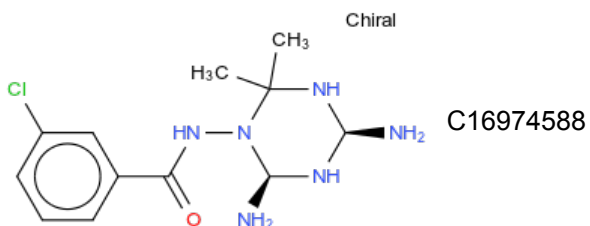
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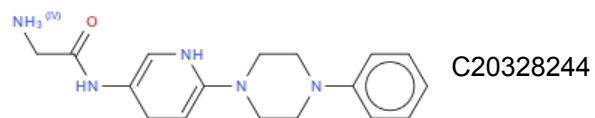
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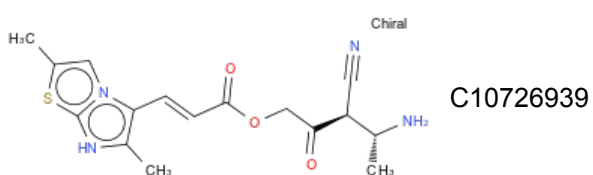
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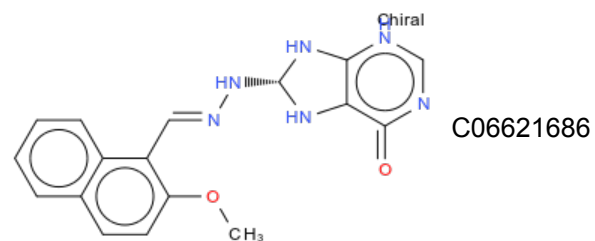
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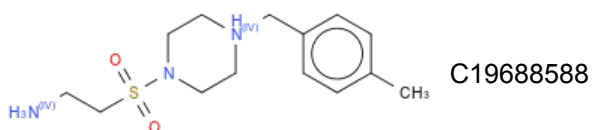
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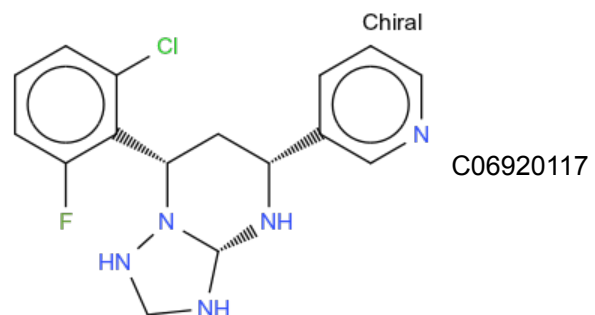
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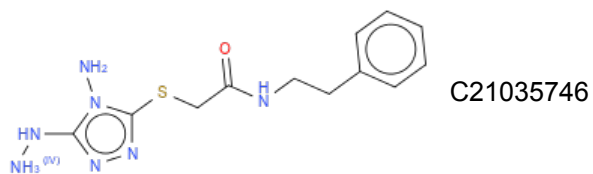
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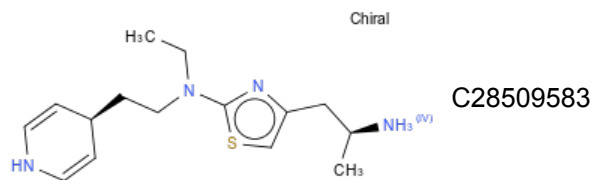
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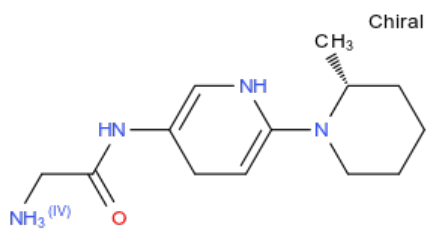
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336

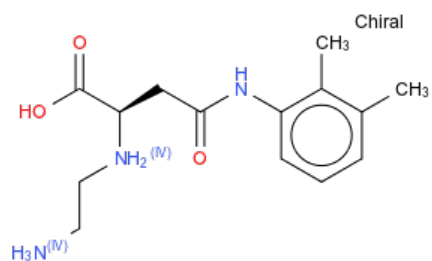


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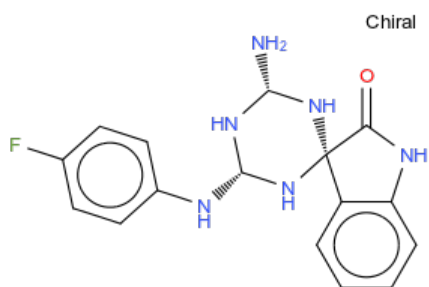
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338



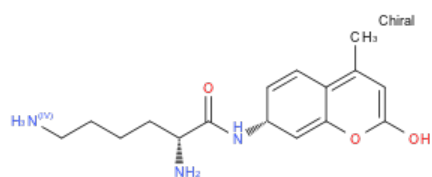
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339



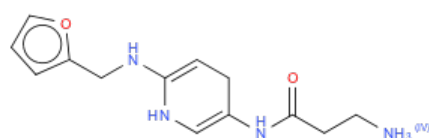
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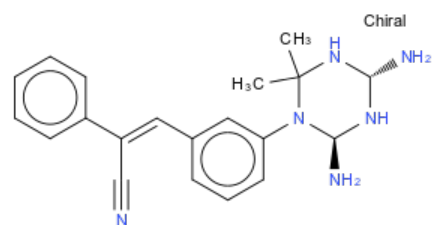
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341



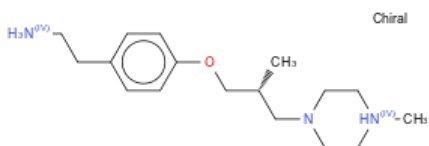
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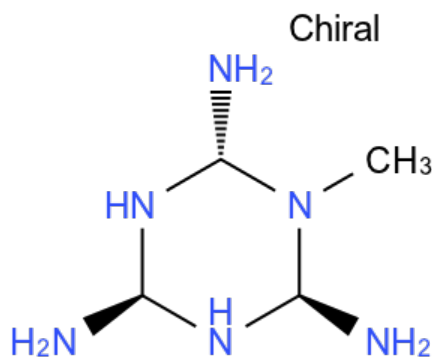
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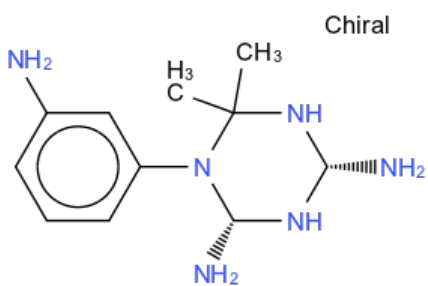
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344

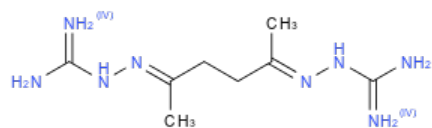


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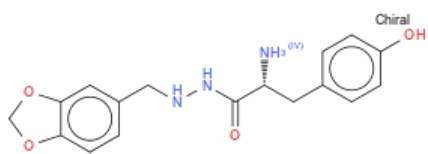
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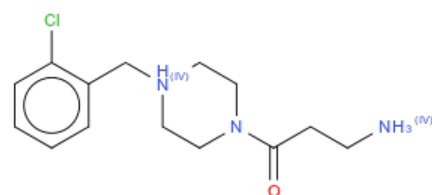
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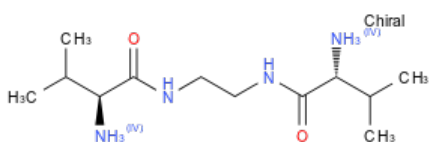
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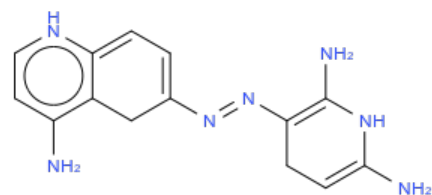
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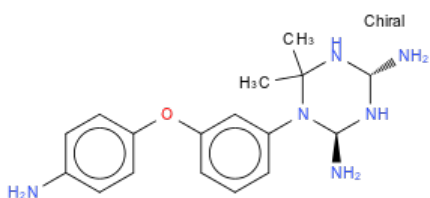
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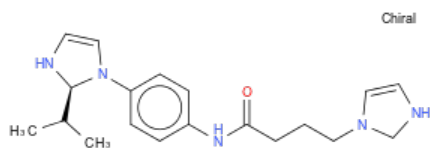
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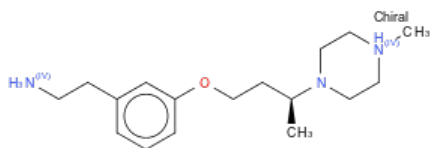
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352

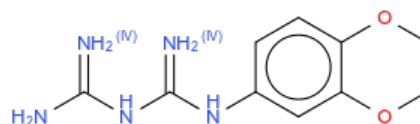


353



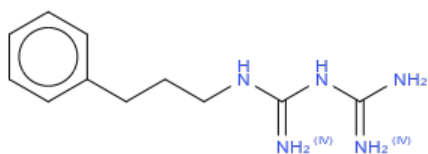
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354



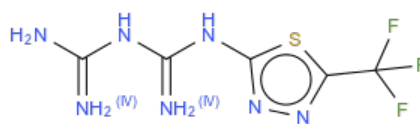
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355



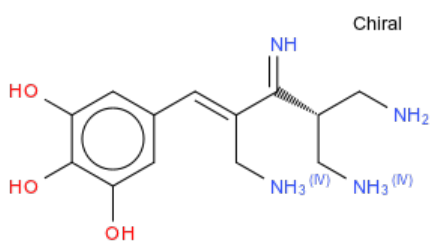
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356



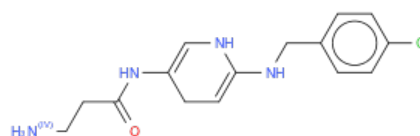
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357



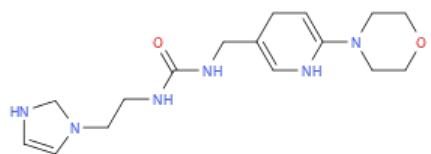
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358



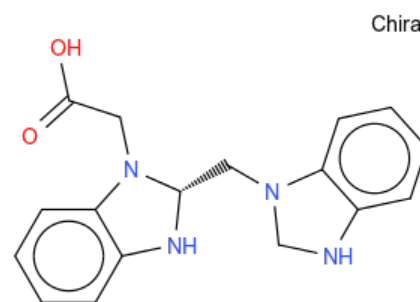
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359



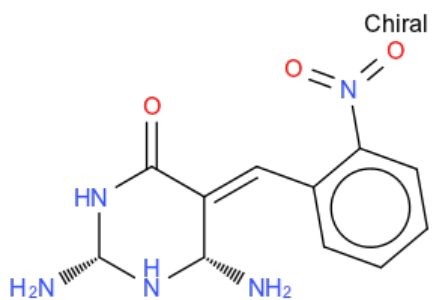
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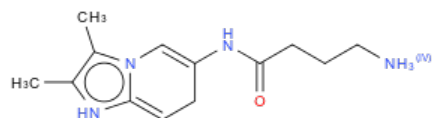
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361



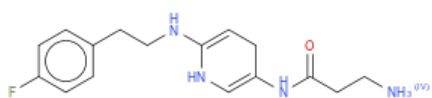
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362



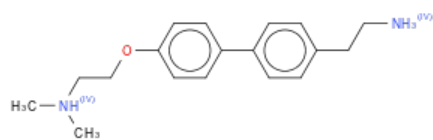
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363



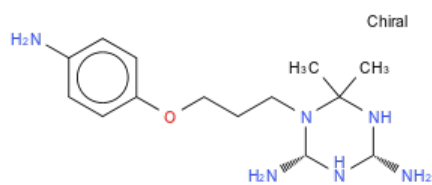
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364



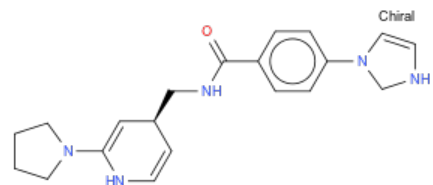
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365



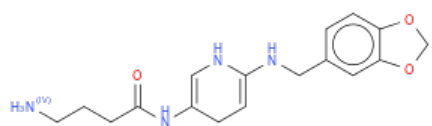
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366



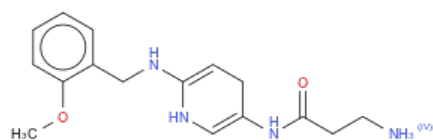
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367



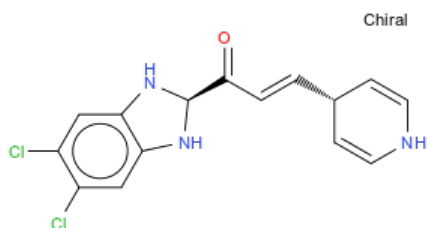
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368



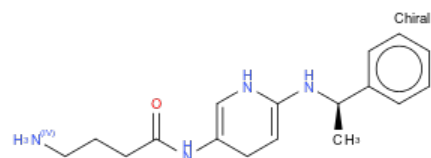
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369



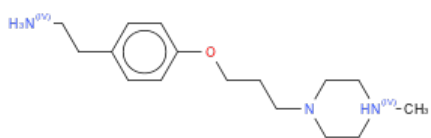
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370



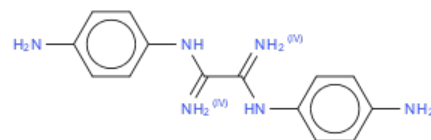
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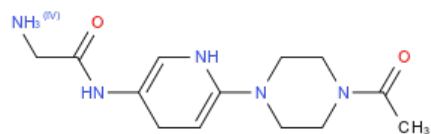
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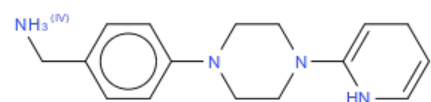
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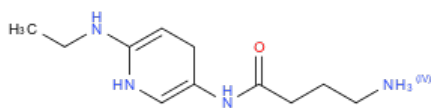
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374



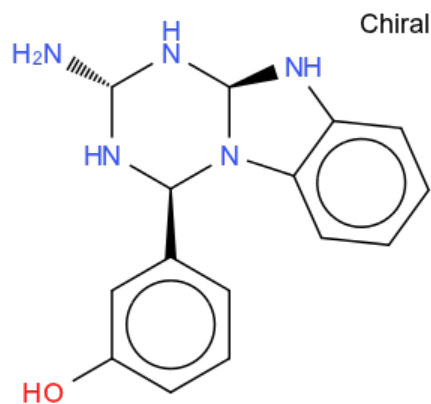
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375



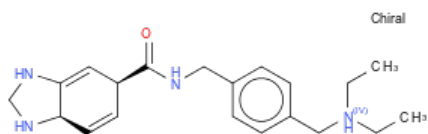
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376



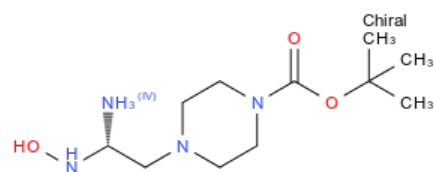
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377



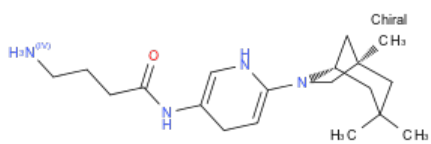
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378



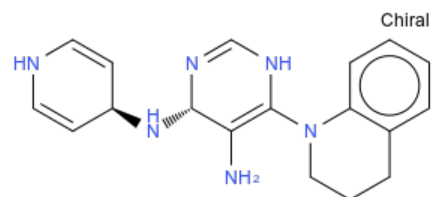
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379



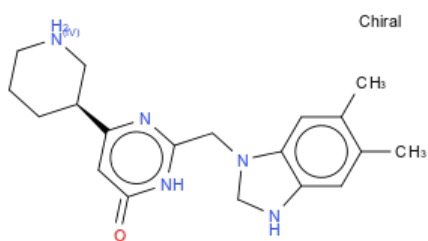
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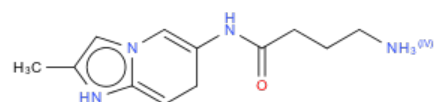
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381



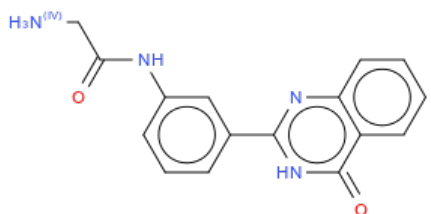
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382



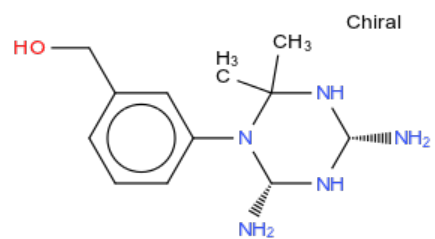
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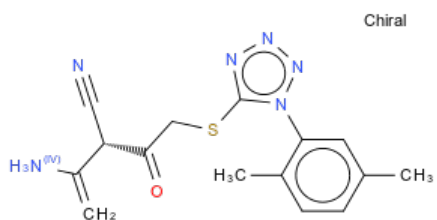
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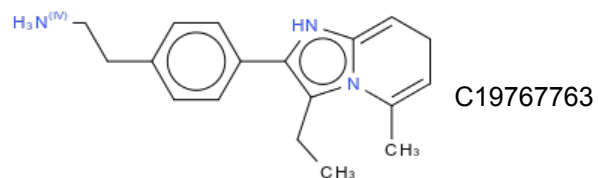


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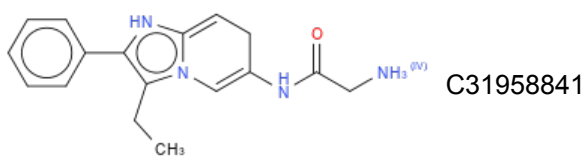
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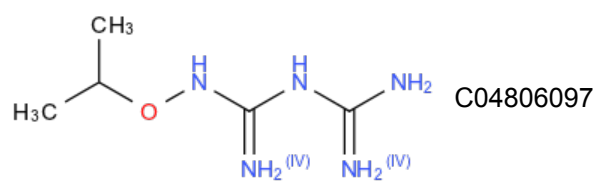
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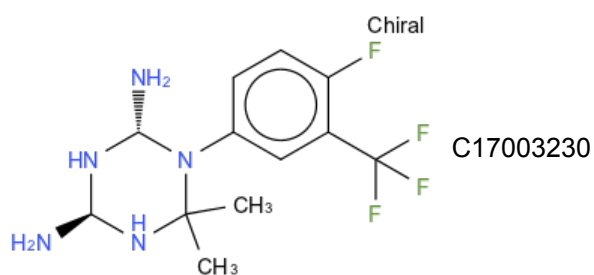
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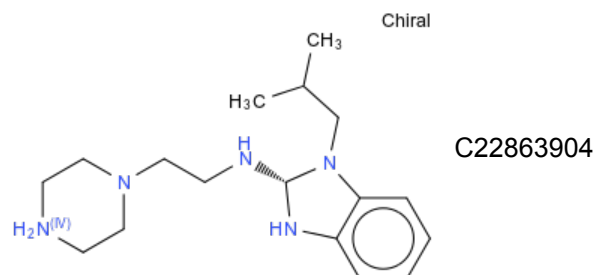
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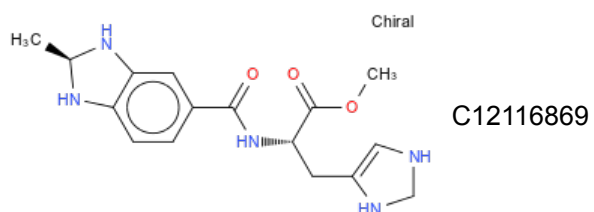
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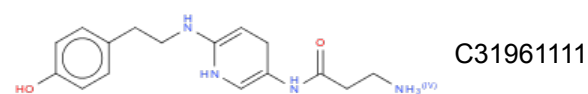
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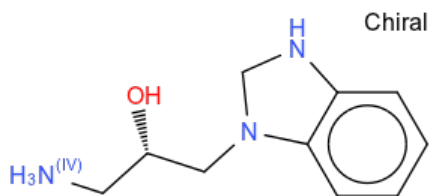
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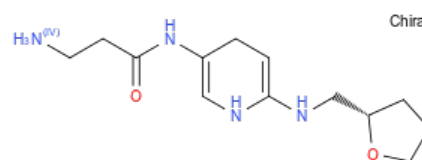


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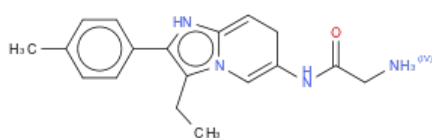
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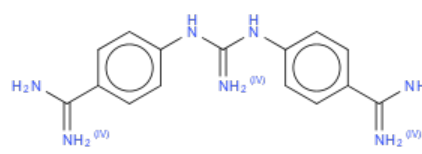
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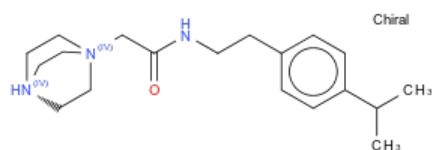
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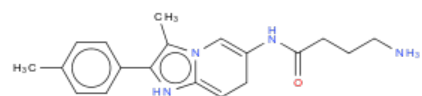
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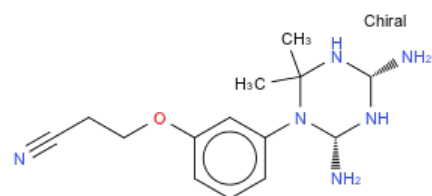
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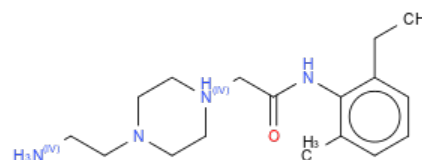
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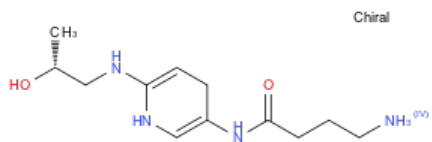
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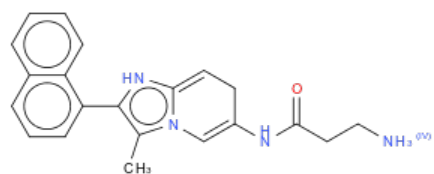
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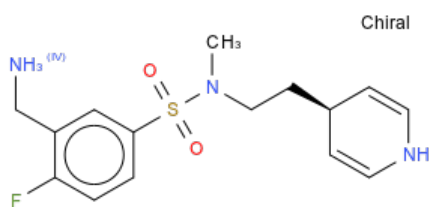
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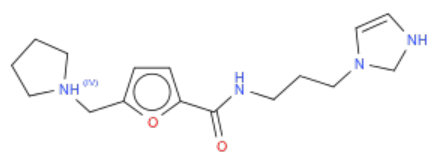
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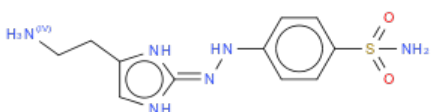
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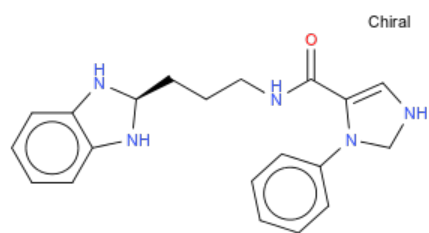
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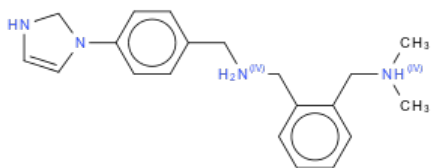
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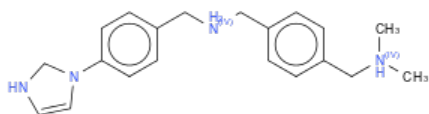
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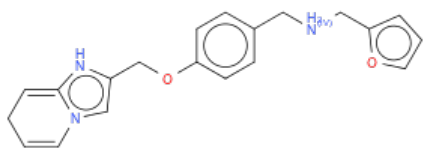
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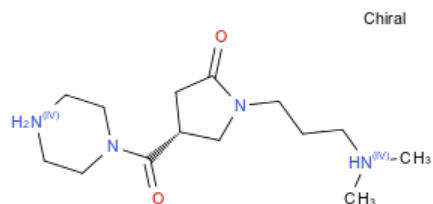
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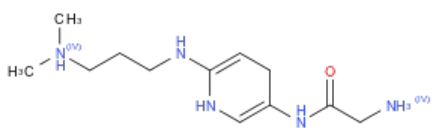
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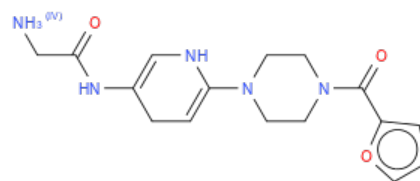
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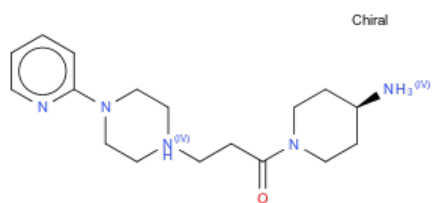
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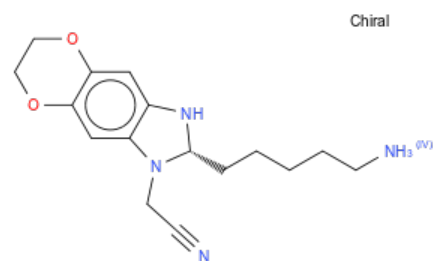
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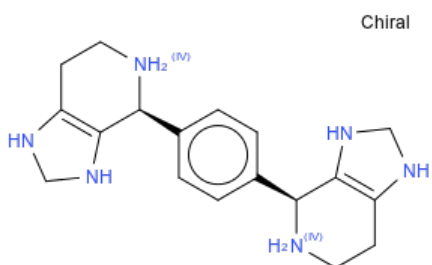
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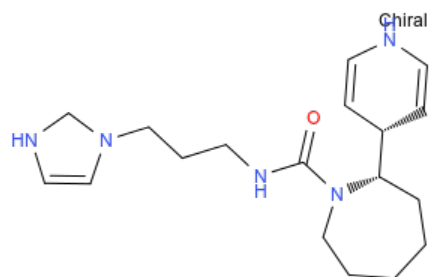
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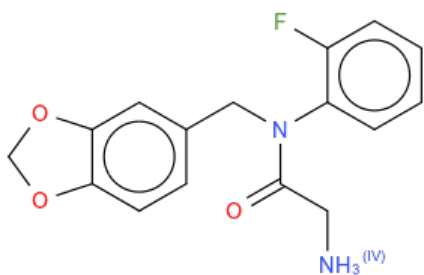
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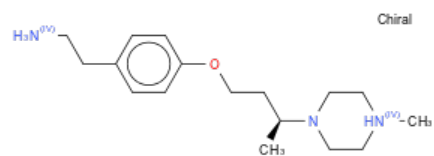
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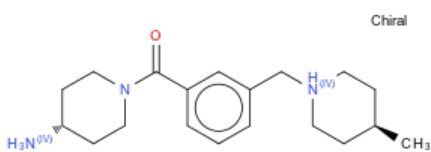
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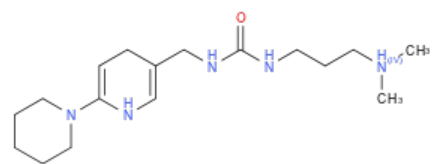
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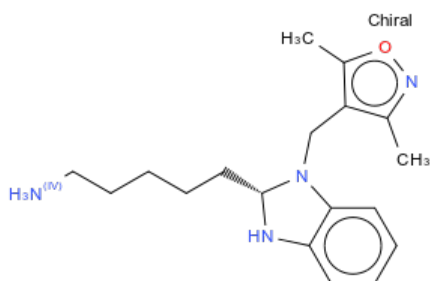
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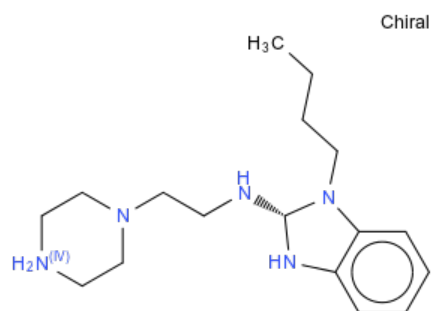
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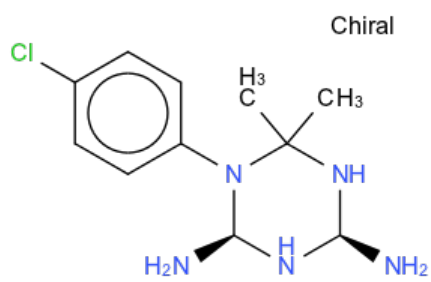
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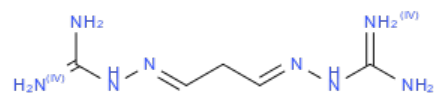
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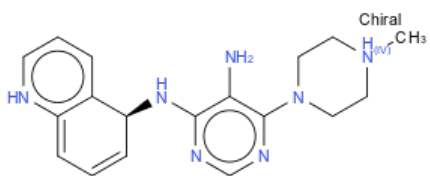
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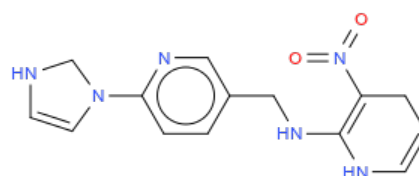
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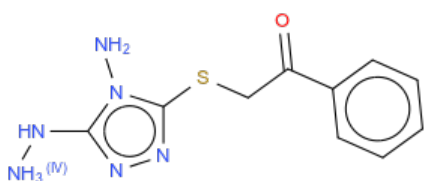
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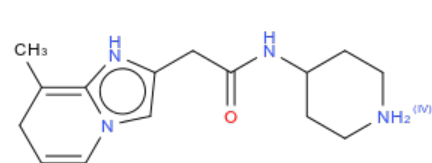
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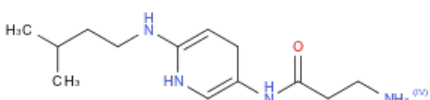
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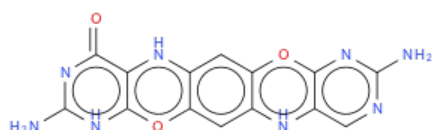
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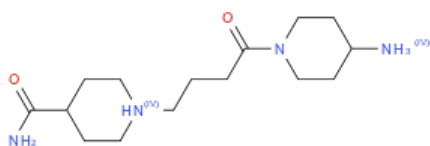
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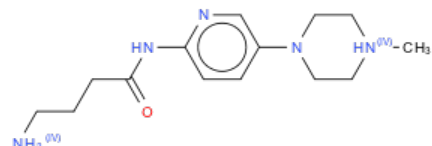
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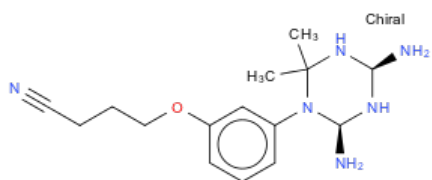
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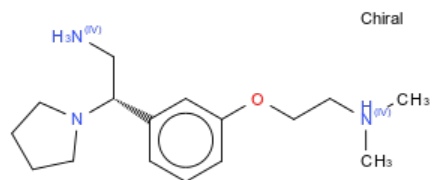
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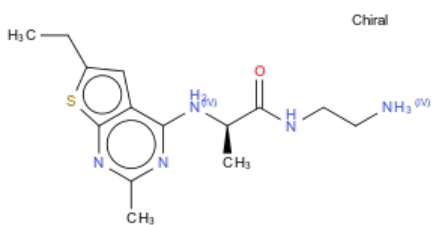
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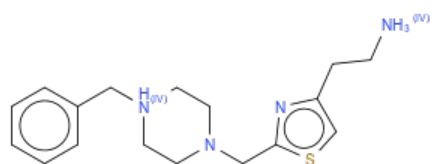
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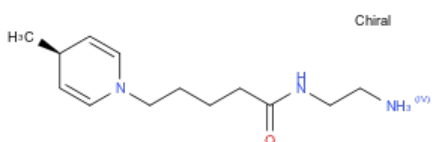
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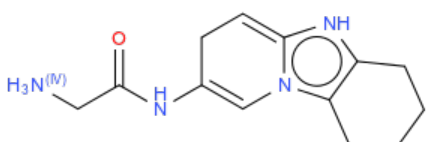
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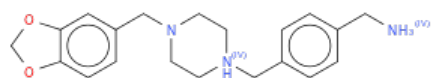
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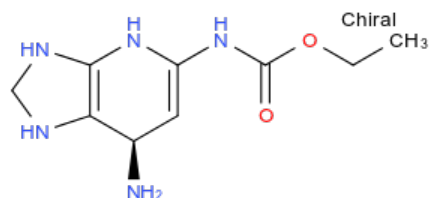
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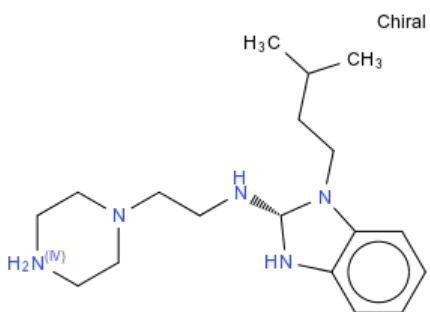
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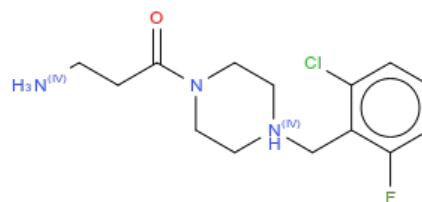
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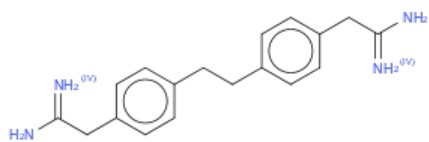
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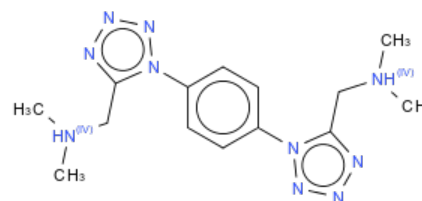
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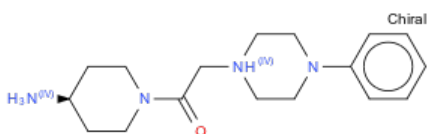
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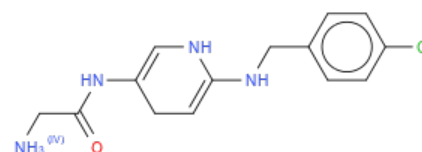
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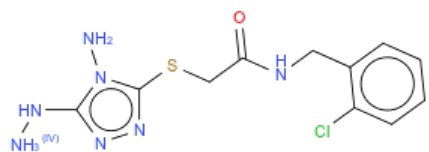
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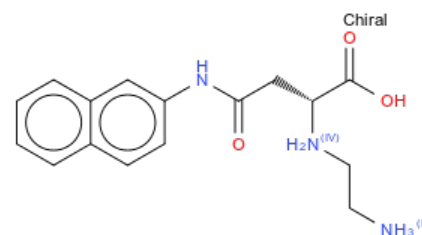
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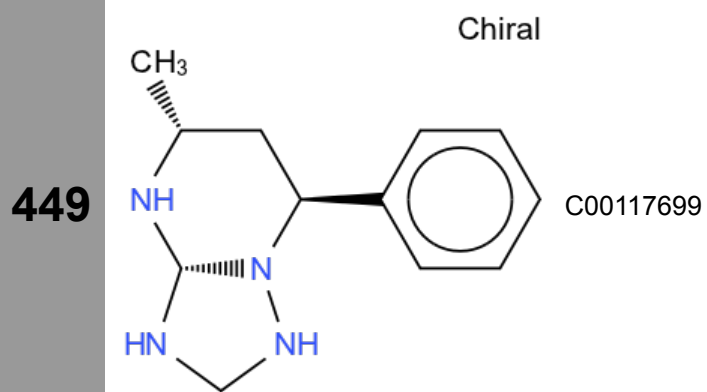
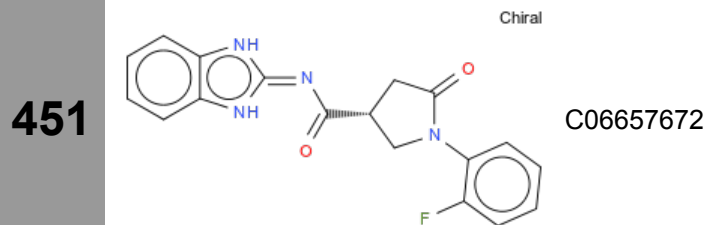
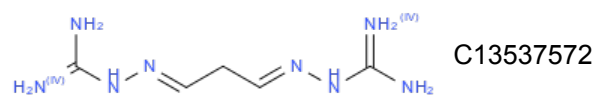
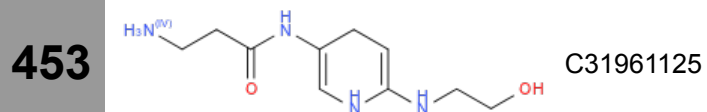
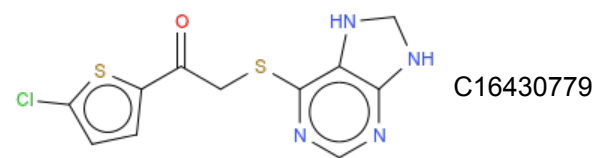
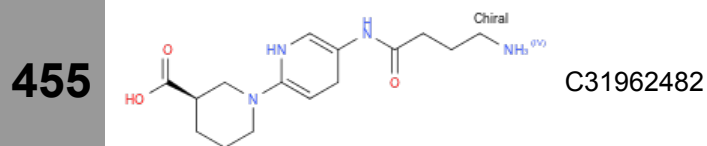
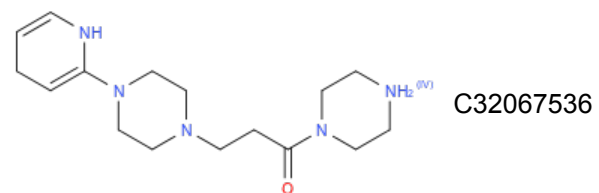
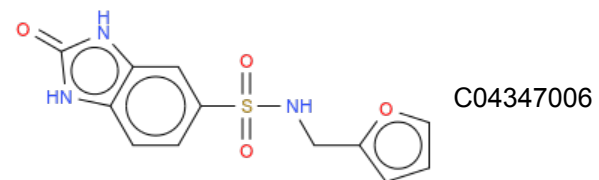


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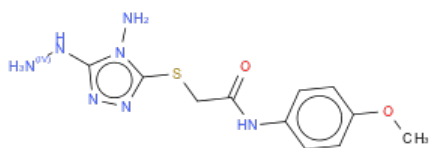
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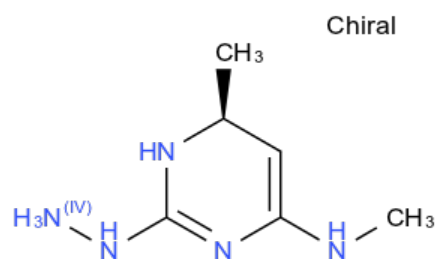
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457



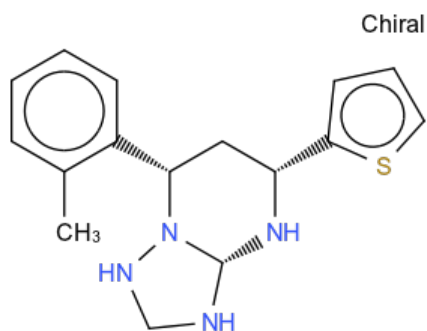
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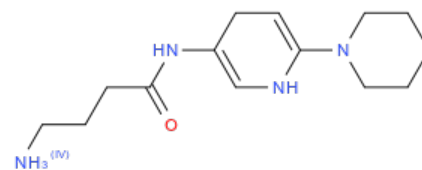
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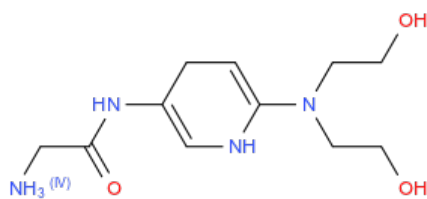
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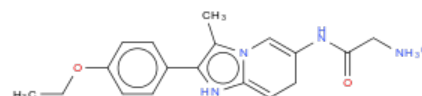
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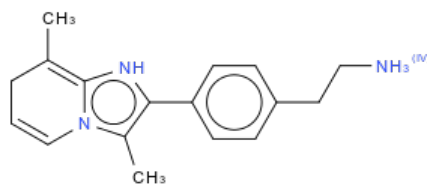
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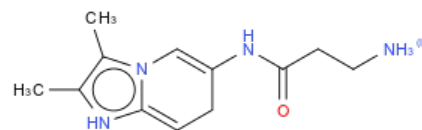
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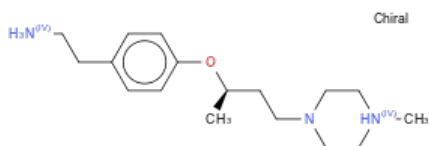
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464



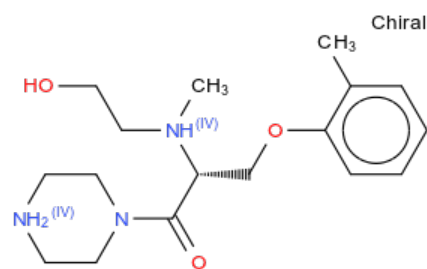
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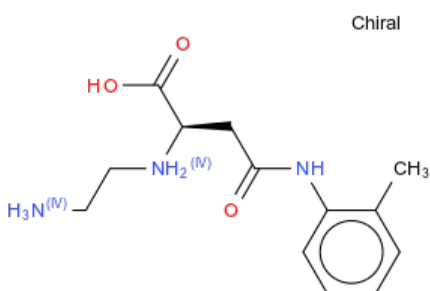
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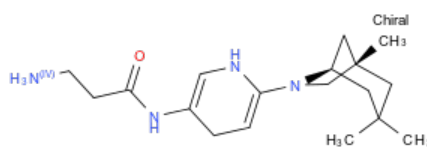
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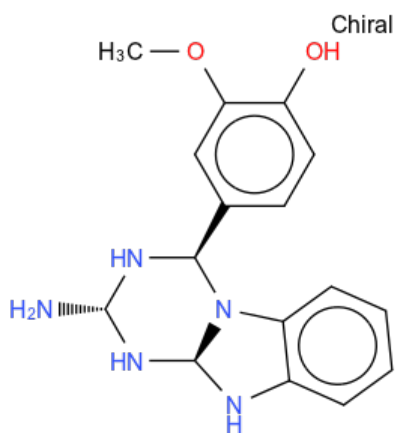
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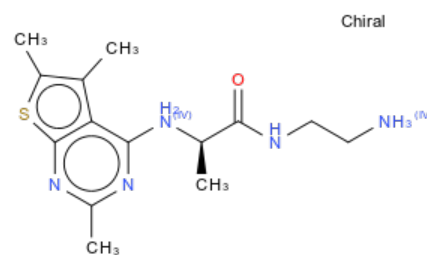
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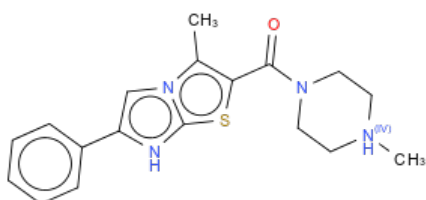
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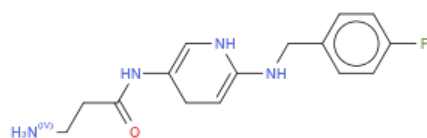
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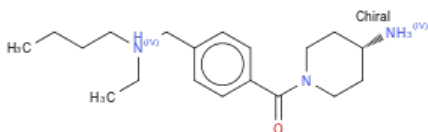
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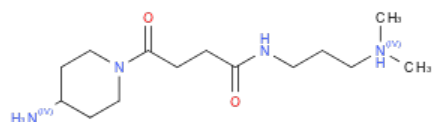
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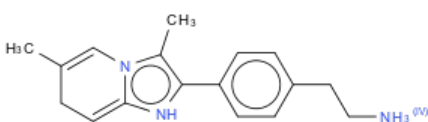
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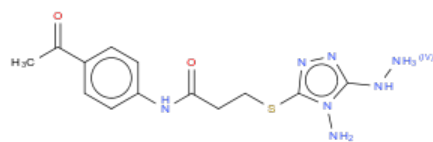
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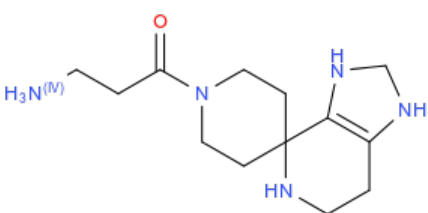
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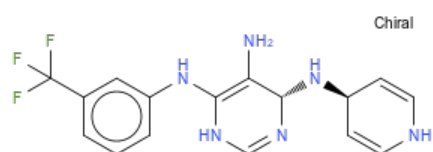
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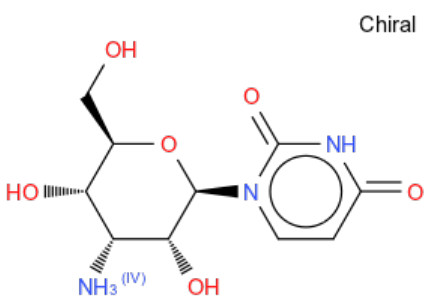
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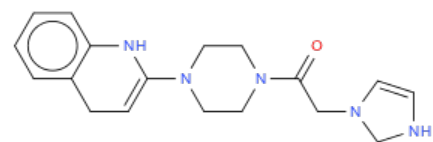
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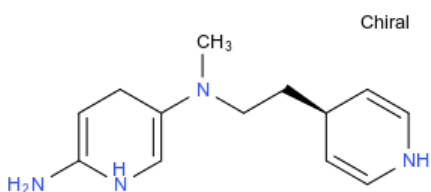
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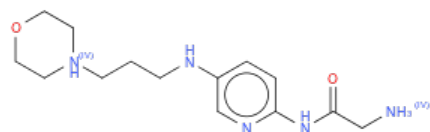
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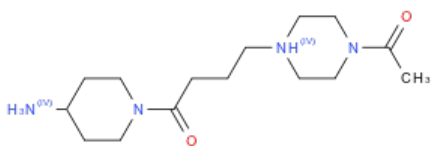
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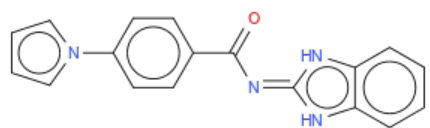
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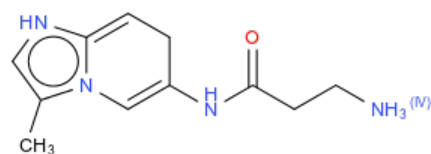
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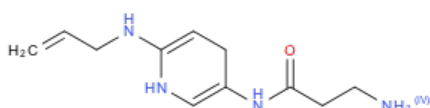
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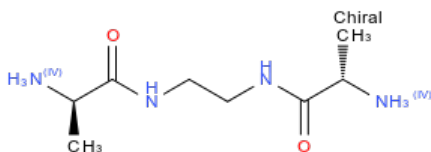
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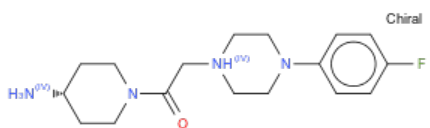
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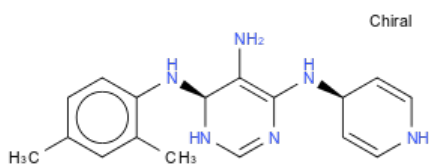
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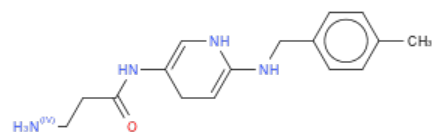
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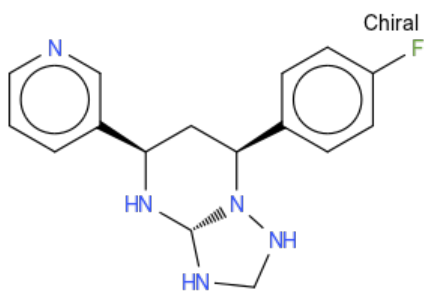
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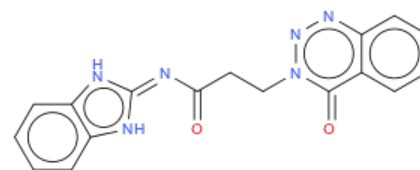
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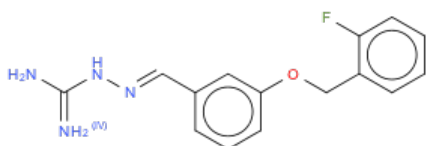
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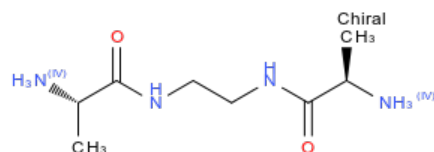
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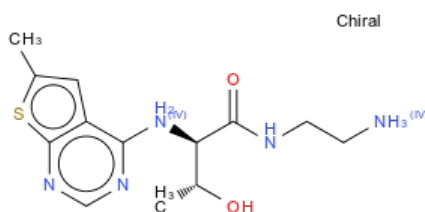
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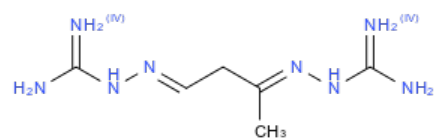
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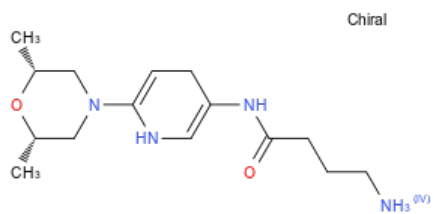
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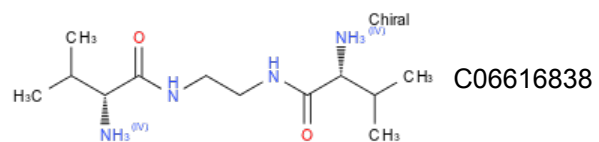
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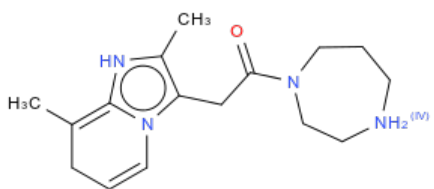
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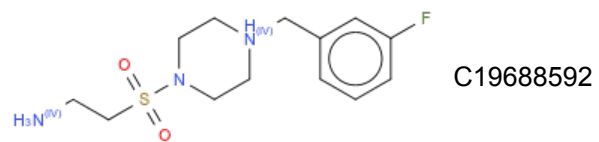
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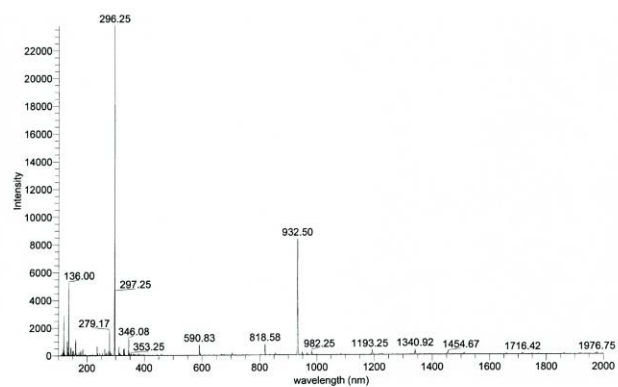
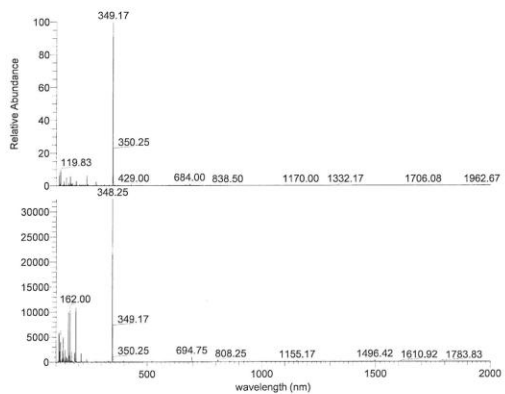
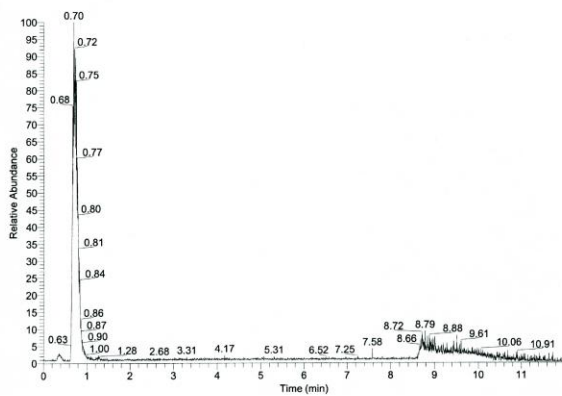
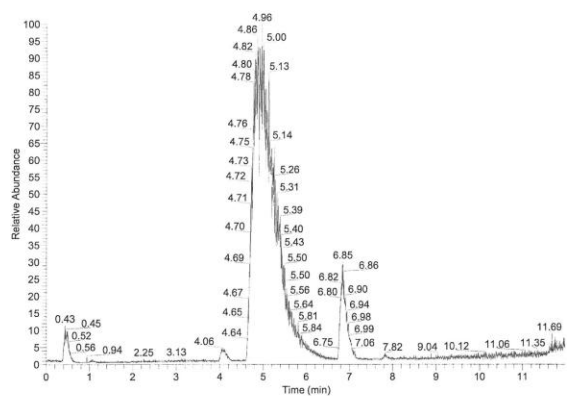


C41292566

500



C19688592



A

B

Figure S1. Liquid Chromatography/Mass Spectroscopy (LC/MS) analysis of the active compounds MSSM-1 and MSSM-2 (panel A and B, respectively).

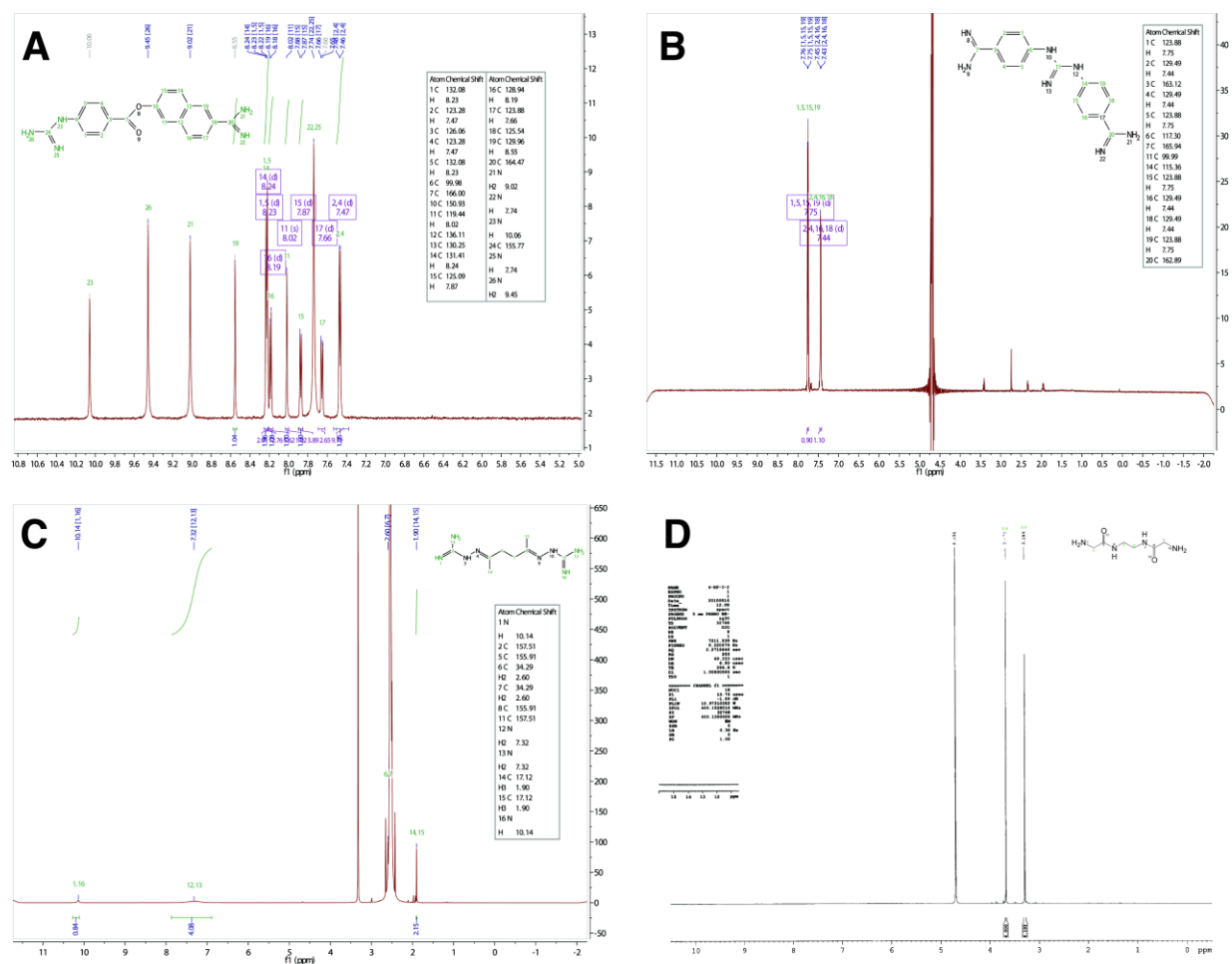


Figure S2. ¹H NMR analysis for each of the virtual screening hits, MSSM-1,2,3, and 5 (panel A, B, C and D, respectively).

```

read.table("database.ECFP4",sep=",") -> fingers
print(dim(fingers))
nst<-dim(fingers)[1]
cfinger<-as.matrix(fingers[,2:length(fingers[1,])])

read.table("subset-dataset.ECFP4",sep=",") -> selecfinger
print(dim(selecfinger))
nstselect<-dim(selecfinger)[1]
cselecfingerelec<-as.matrix(selecfinger[,2:length(selecfinger[1,])])

tanimotos<-matrix(NA,nrow=nstselect,ncol=nst)

for ( i in 1:nstselect){
  v1 <- cselecfingerelec[i,]
  print(i)
  norm1 <- v1 %*% v1
  for ( j in 1:nst){
    v2<- cfinger[j,]
    common <-v1 %*% v2
    norm2 <- v2 %*% v2
    tanimotos[i,j] <- common / (norm1+norm2 - common)
  }
}

mostsim<-NA*(1:6)
howsim<-NA*(1:6)

Nmostsim<-NA*(1:6)
Nhowsim<-NA*(1:6)

for ( i in 1:nstselect){
  mostsim[i]<-which.max(tanimotos[i,])
  howsim[i]<-max(tanimotos[i,])

  Nmostsim[i]<-order(tanimotos[i,],decreasing=TRUE)[2]
  Nhowsim[i]<-tanimotos[i,Nmostsim[i]]
}

cbind(1:6,mostsim,howsim, Nmostsim,Nhowsim)->results
colnames(results)<-c("Select","Best Mol.,""Best Tc","II Best. Mol.,""II
Best Tc")
results

```