

[Supporting Information]

**Structure based virtual screening and molecular dynamic simulation studies to identify novel cytochrome  
bc1 inhibitors as antimalarial agents**

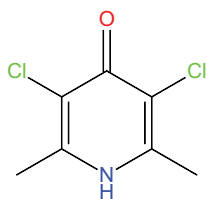
Rahul P. Gangwal,<sup>a</sup> Gaurao V. Dhole,<sup>a</sup> Mangesh V. Damre,<sup>a</sup> Kanchan Khandelwal,<sup>a</sup> Abhay .T. Sangamwar<sup>a,\*</sup>

<sup>a</sup>Department of Pharmacoinformatics, National Institute of Pharmaceutical Education and Research (NIPER),

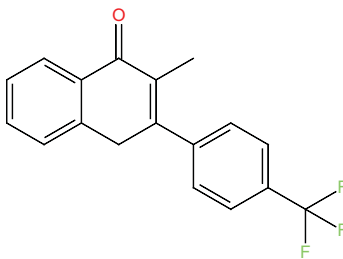
Sect-67, S.A.S. Nagar, Punjab-160 062, India

\* Corresponding author: Tel: 0172-2214682

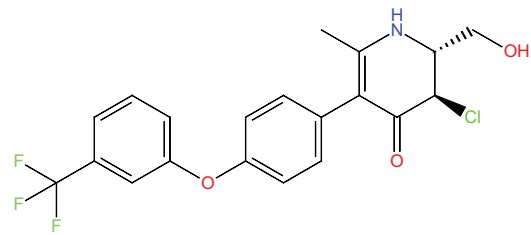
*E-mail: [abhays@niper.ac.in](mailto:abhays@niper.ac.in)*



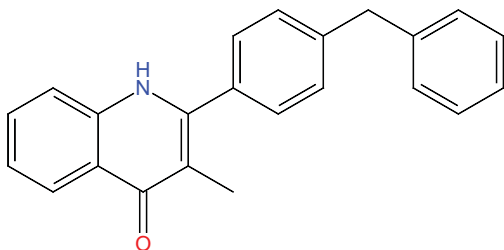
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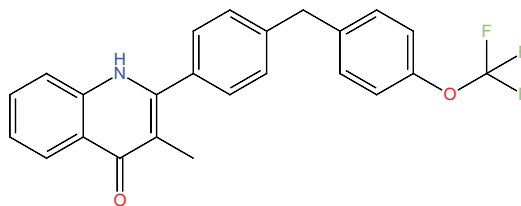
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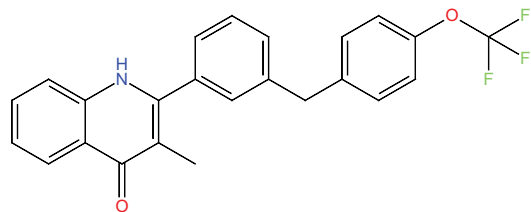
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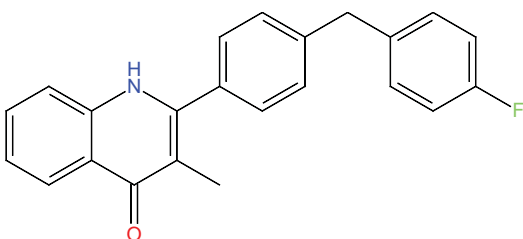
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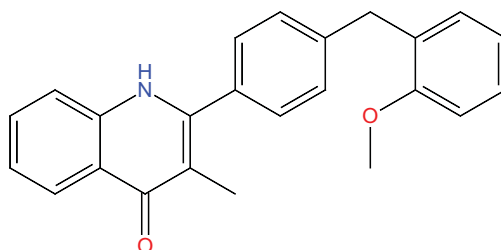
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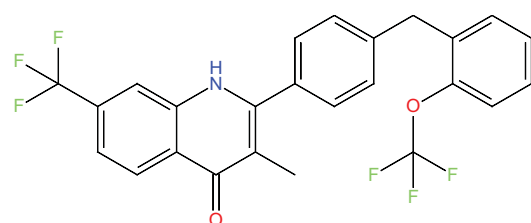
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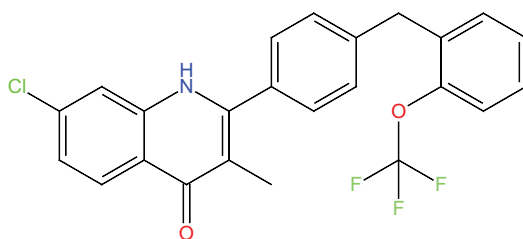
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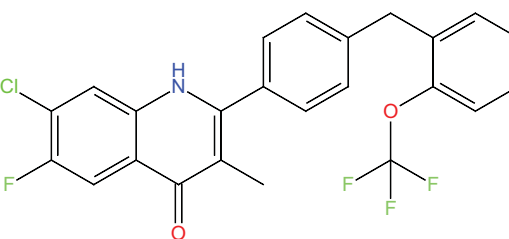
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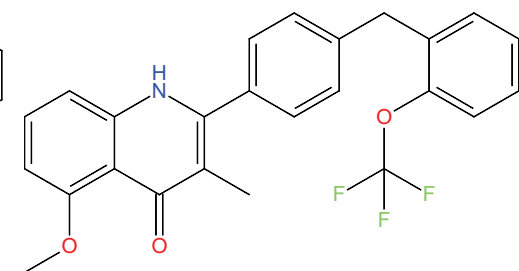
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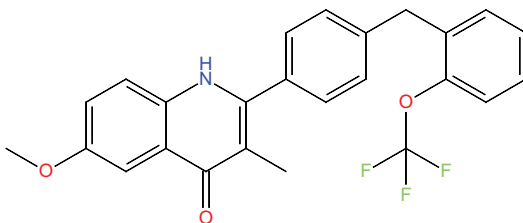
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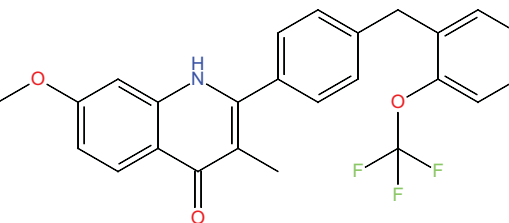
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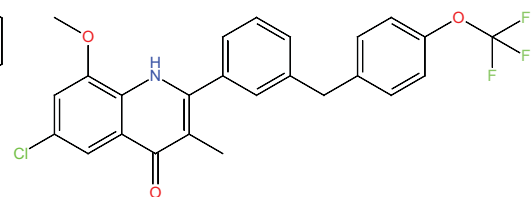
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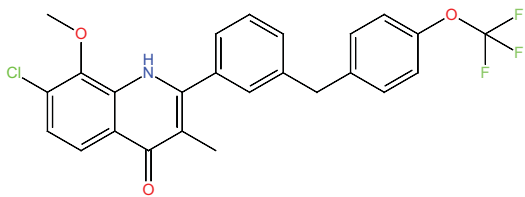
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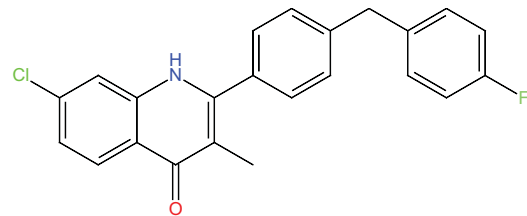
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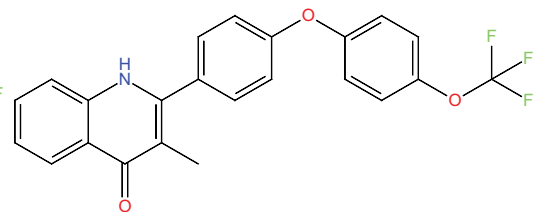
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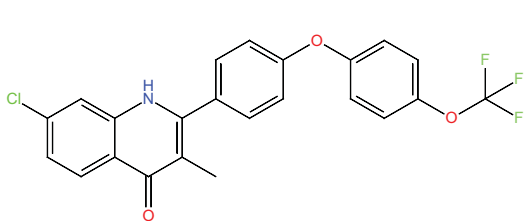
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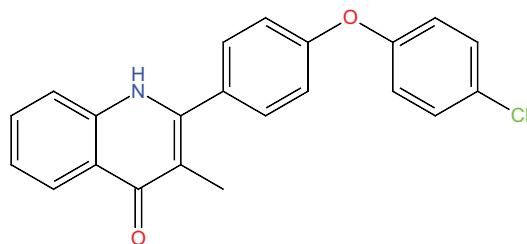
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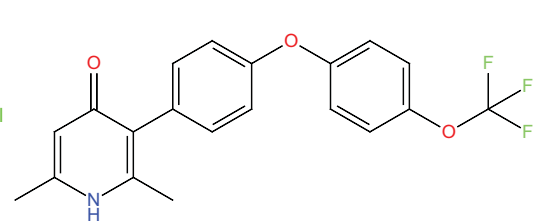
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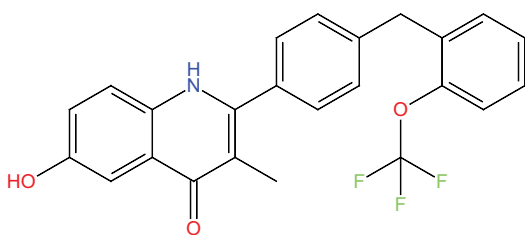
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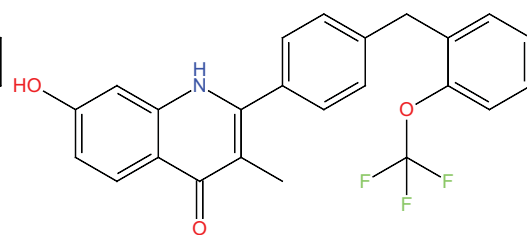
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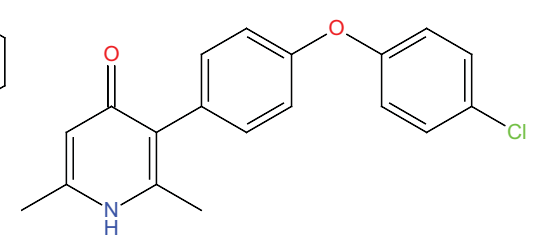
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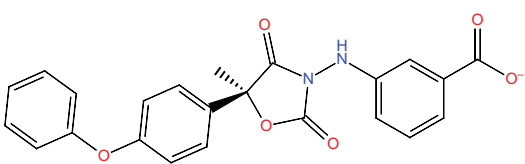
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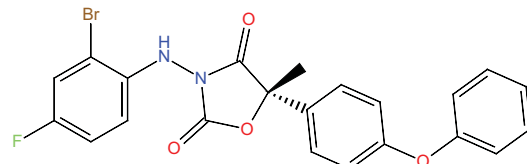
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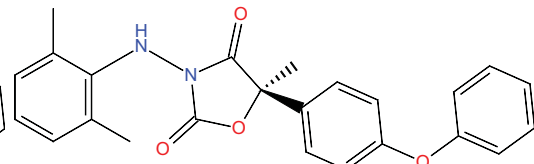
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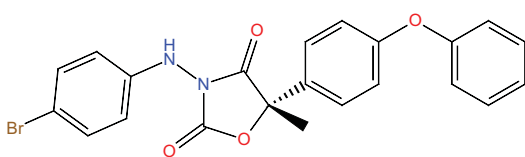
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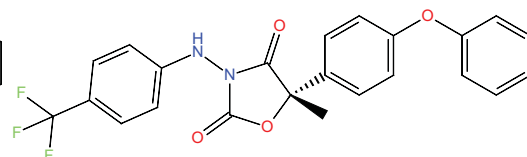
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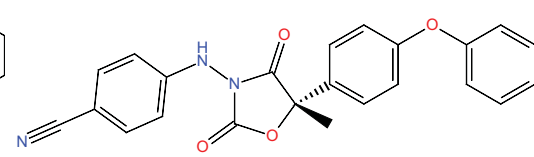
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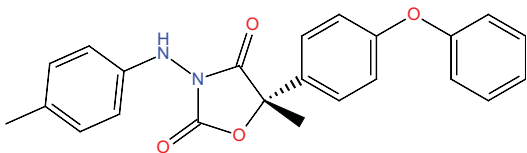
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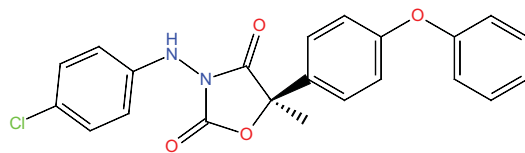
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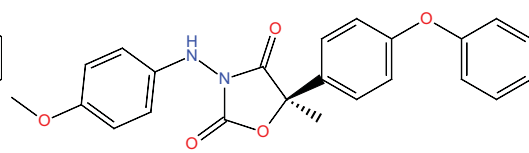
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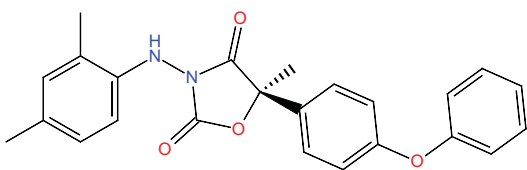
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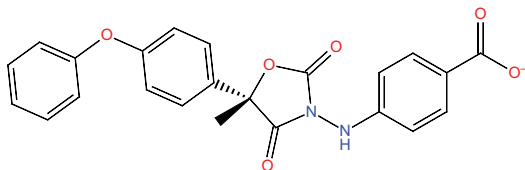
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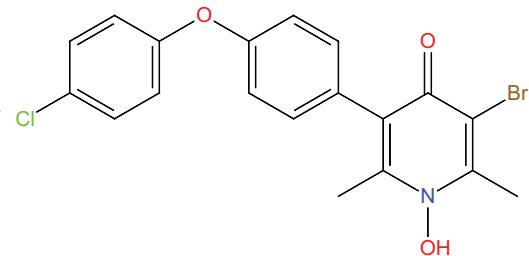
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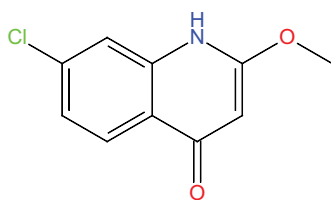
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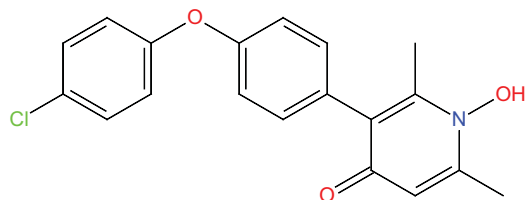
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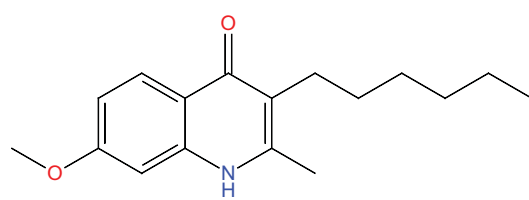
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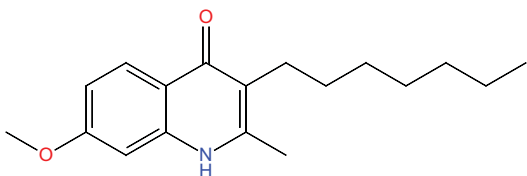
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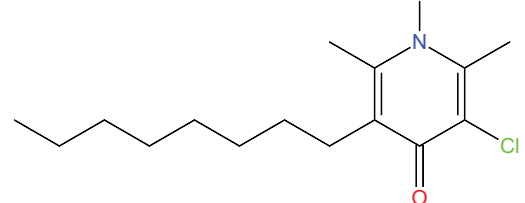
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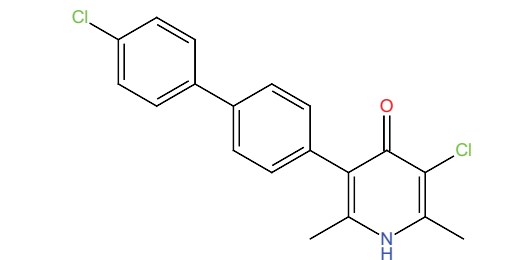
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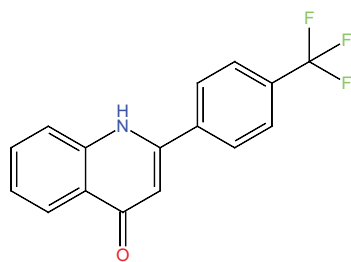
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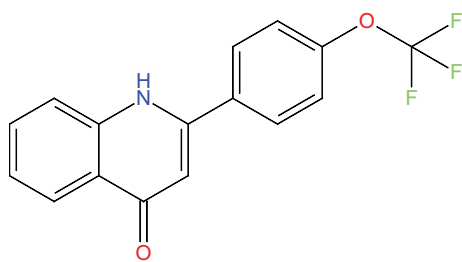
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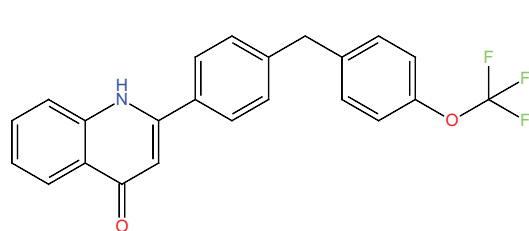
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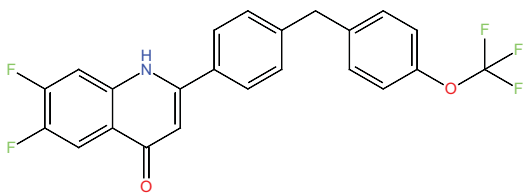
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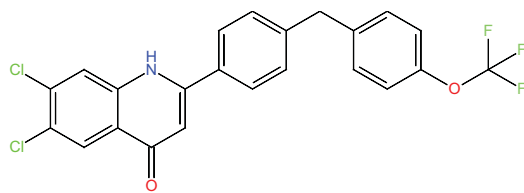
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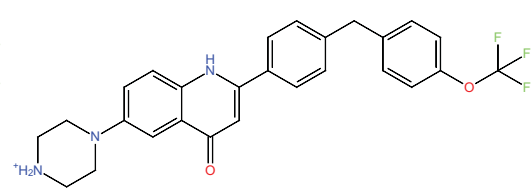
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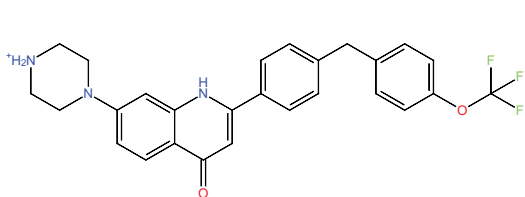
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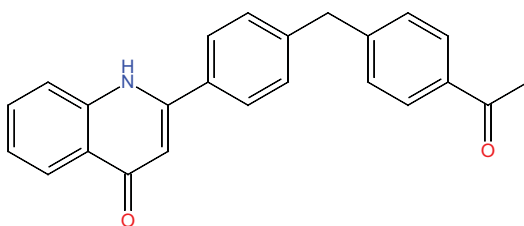
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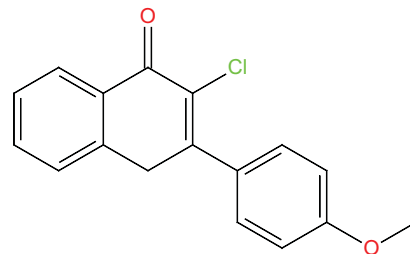
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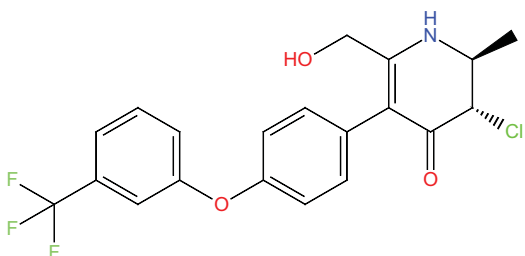
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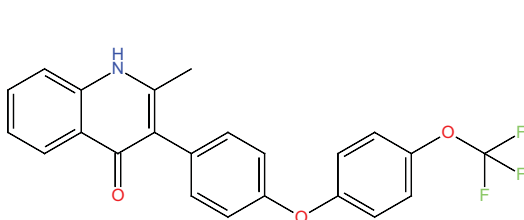
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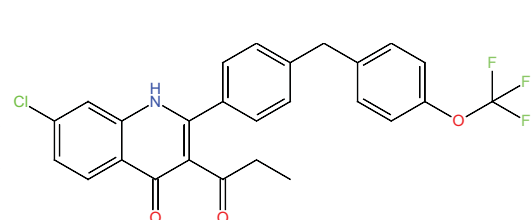
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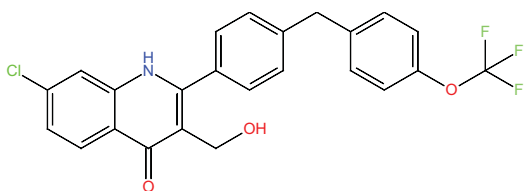
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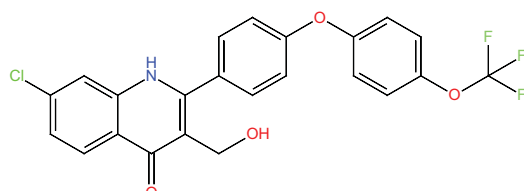
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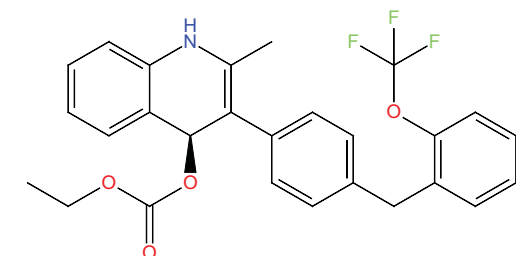
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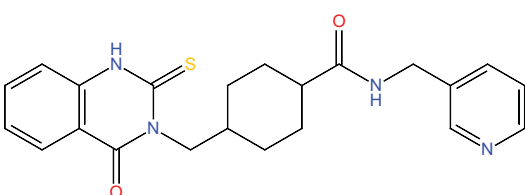
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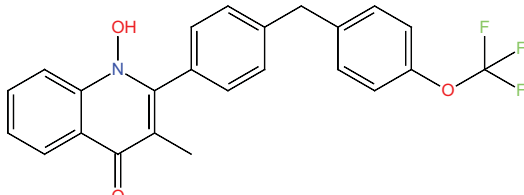
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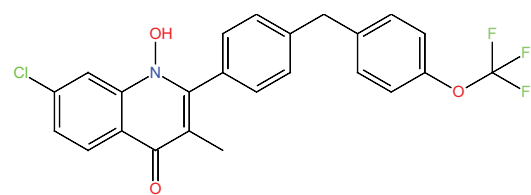
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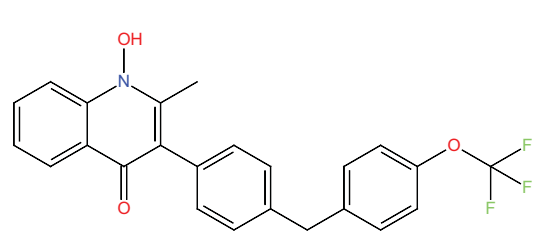
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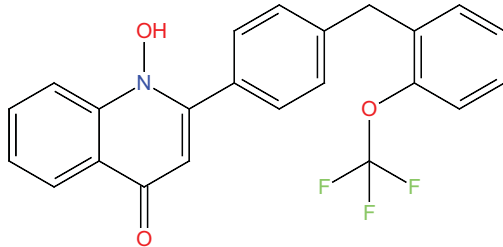
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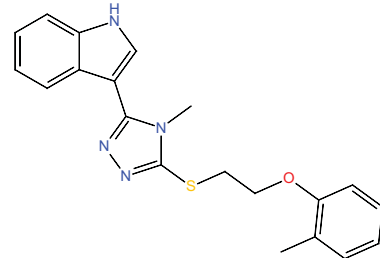
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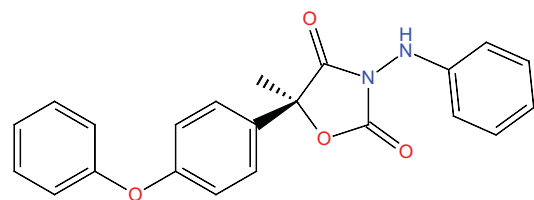
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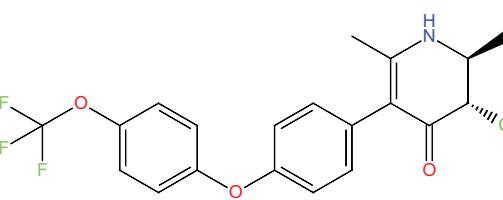
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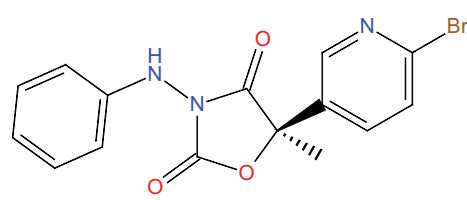
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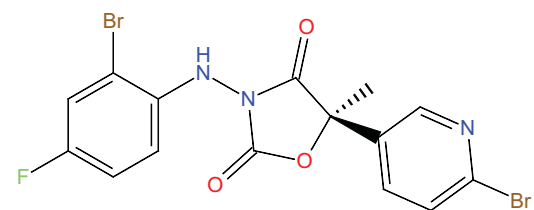
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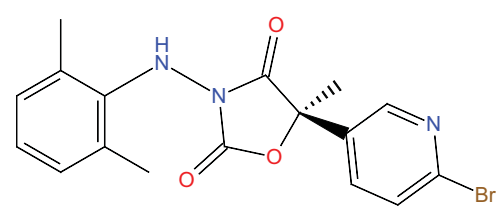
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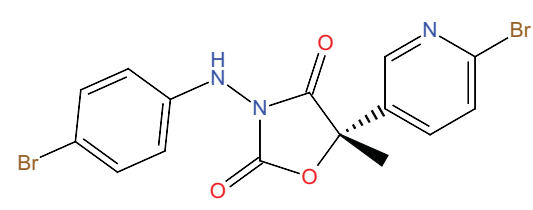
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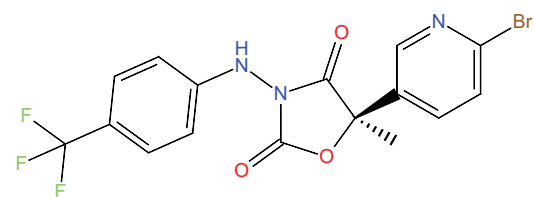
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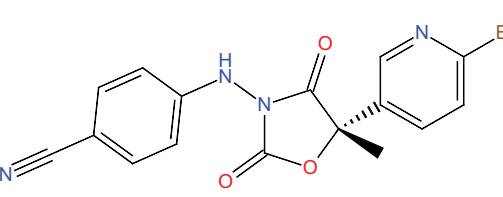
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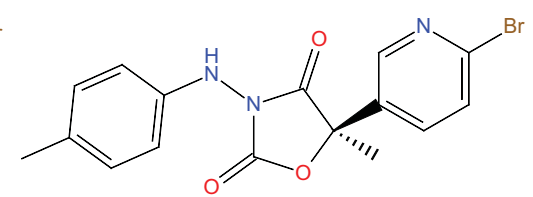
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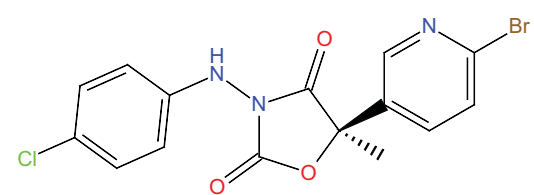
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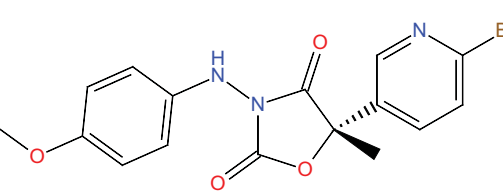
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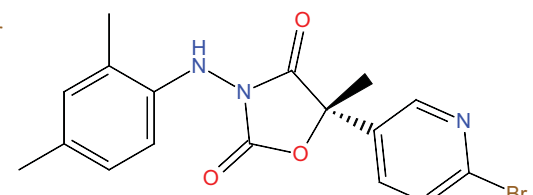
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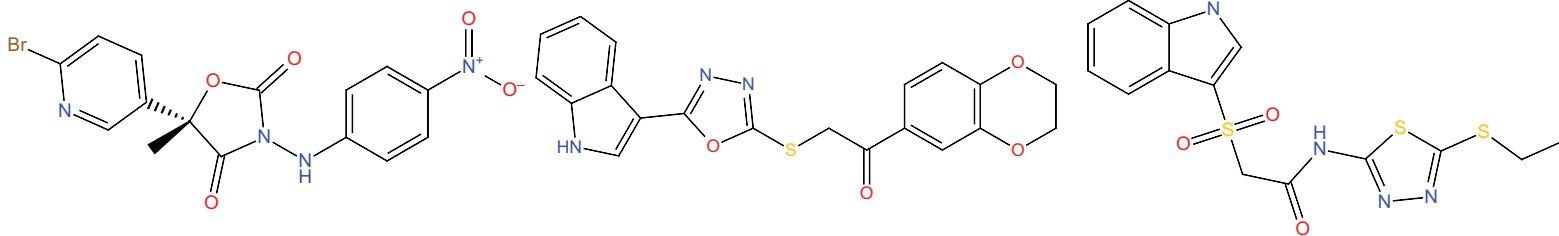
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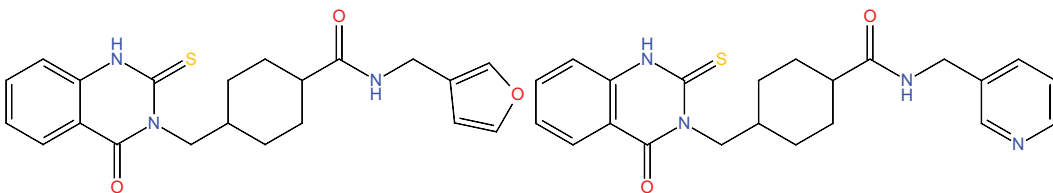
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title: 4k  
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Fig. S1 Chemical structure of test set compounds