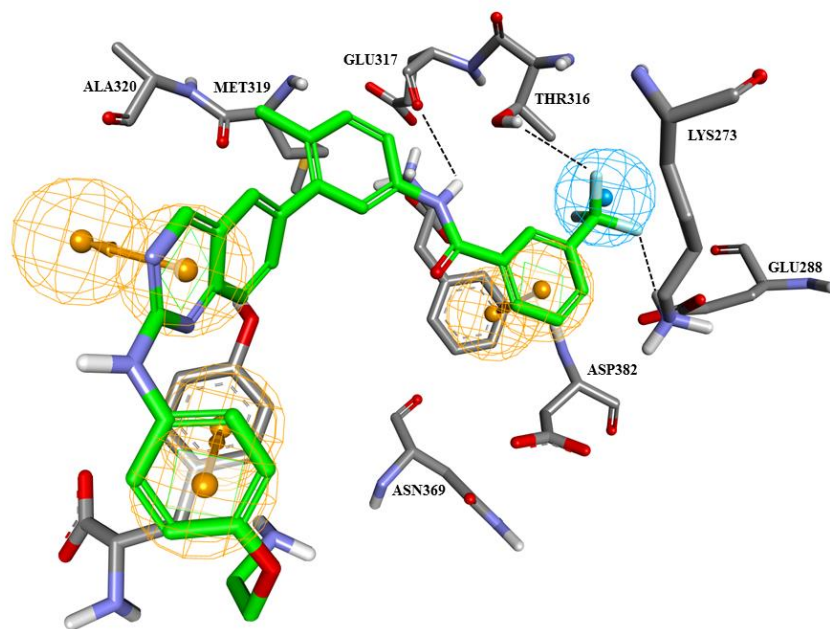


S1 Fig. Co-crystal (Gray; PDB ID: 2HK5) overlaid with its docked orientation (yellow).

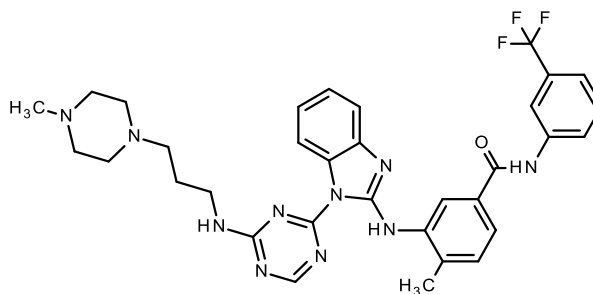


S2 Fig. Overlay of the pharmacophore model in the active site of the protein.

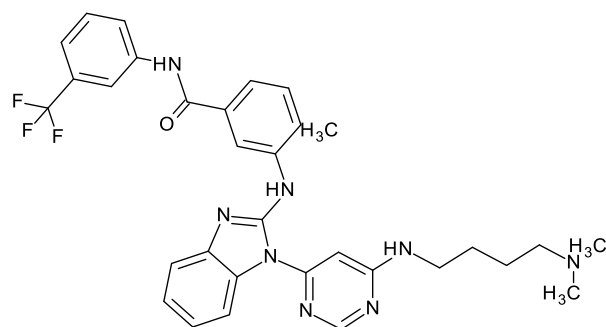
Supplementary Table 1. Chemical structures of test set compounds with their respective IC₅₀ values.

Compound No.	IC ₅₀ (nmol/L)	Structure
1	20	
2	27	
3	31	
4	43	
5	46	

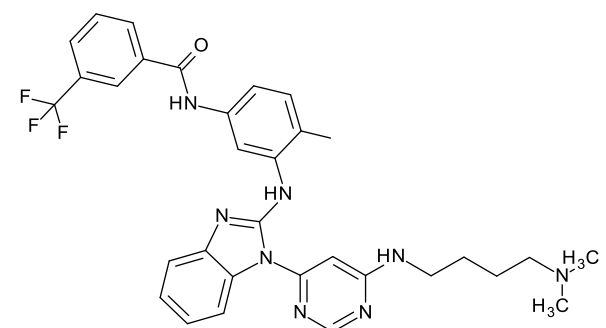
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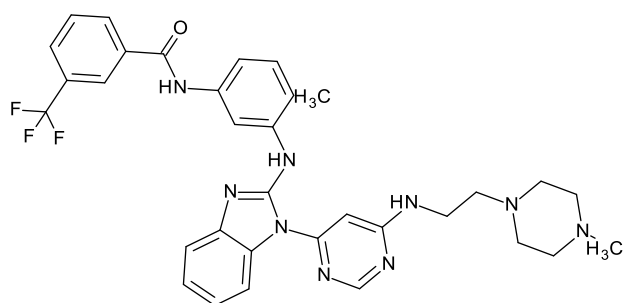
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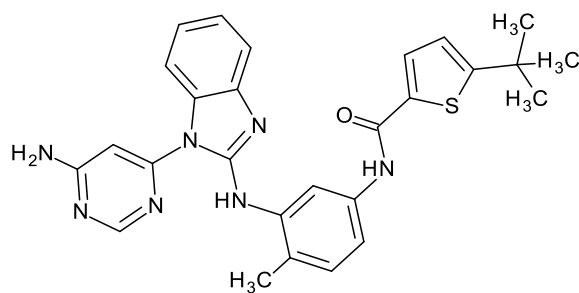
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9 69

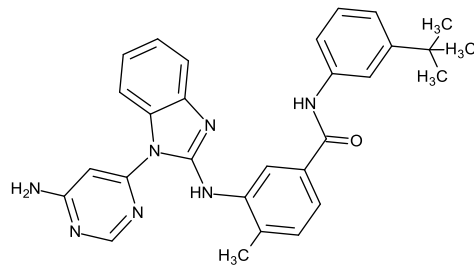


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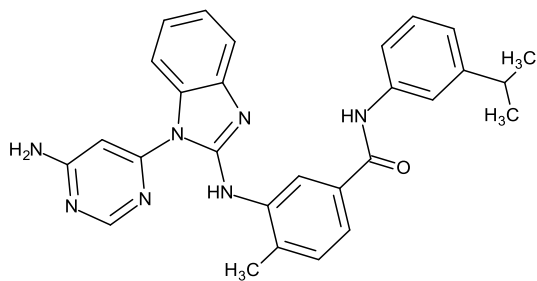
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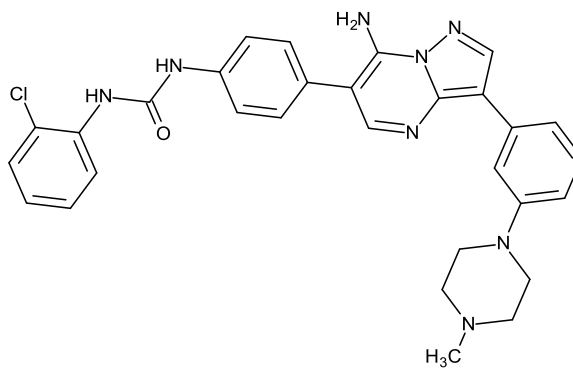
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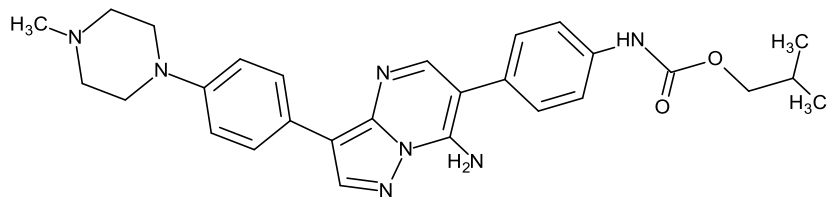
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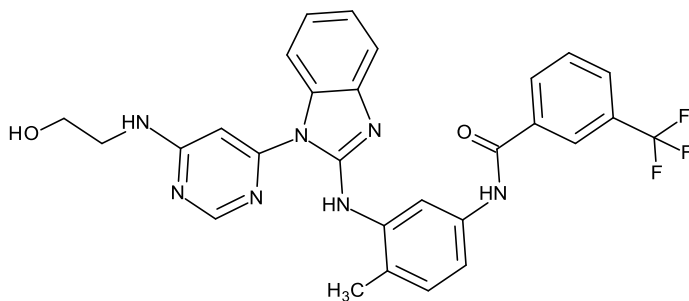
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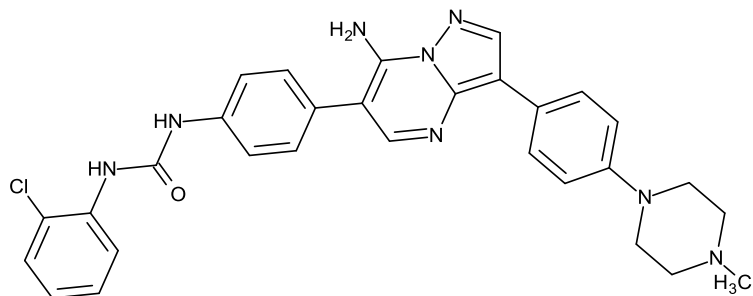
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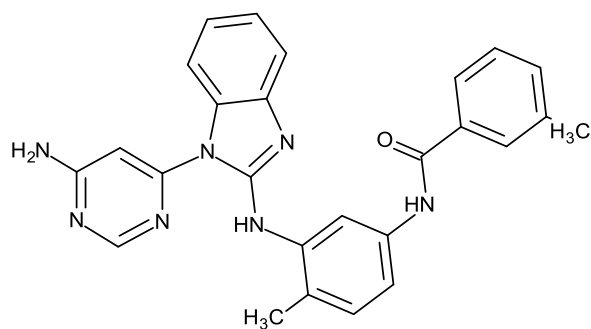
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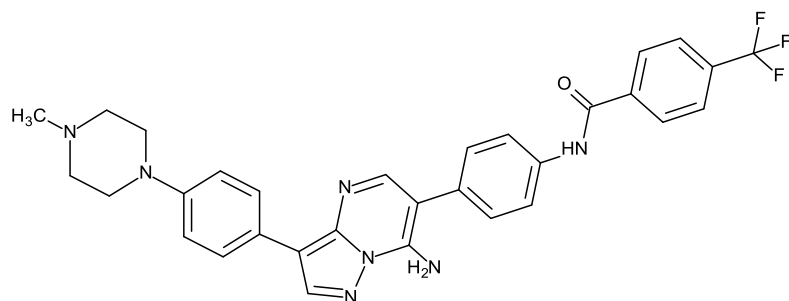
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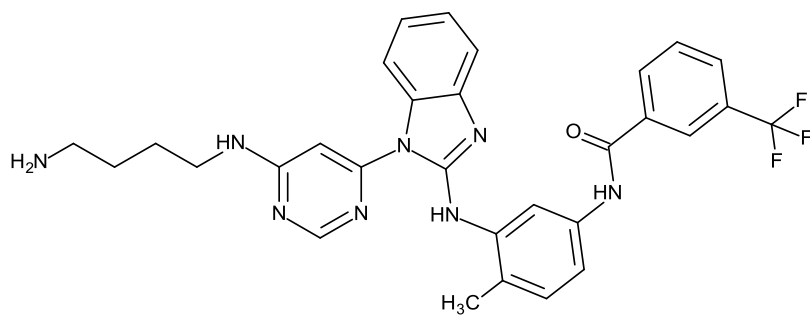
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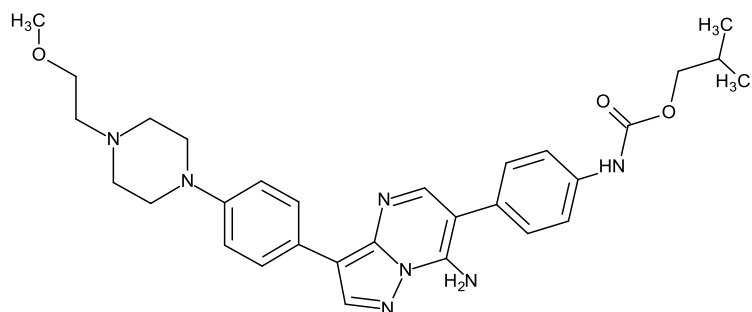
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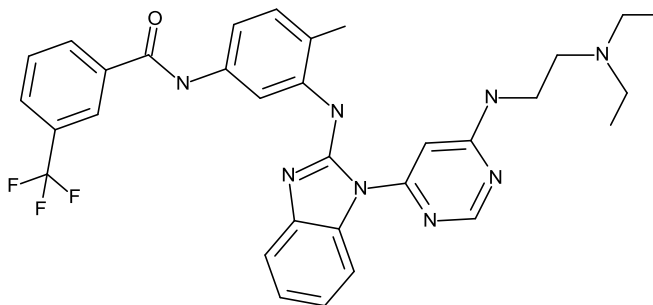
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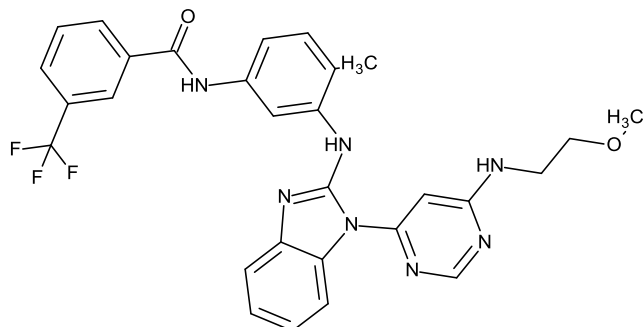
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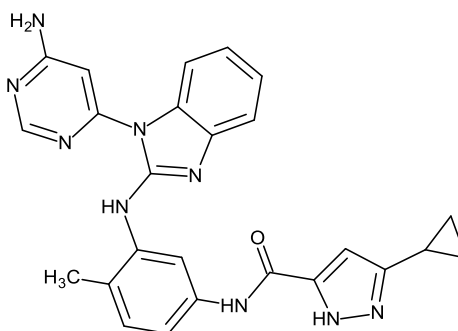
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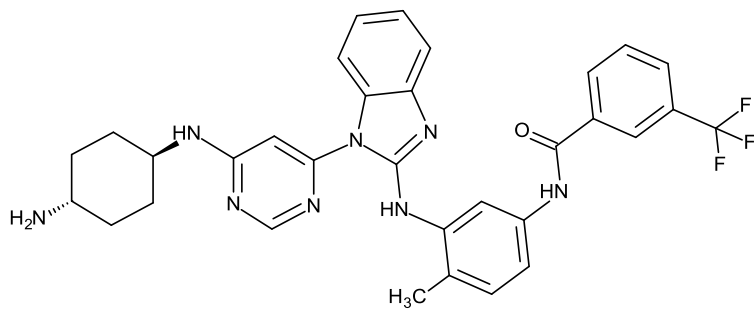
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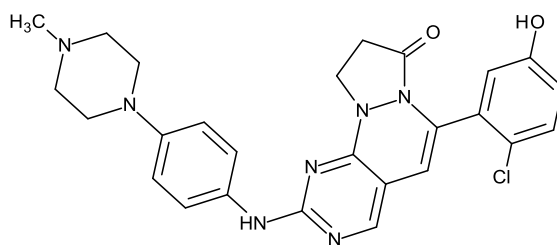
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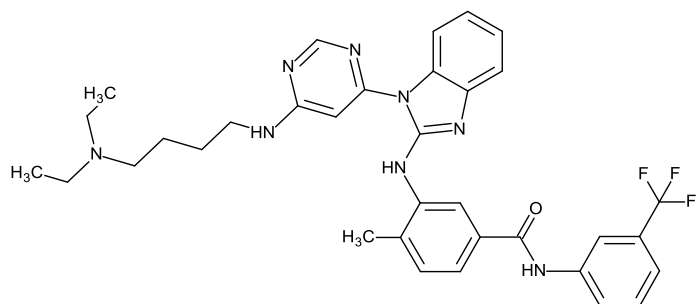
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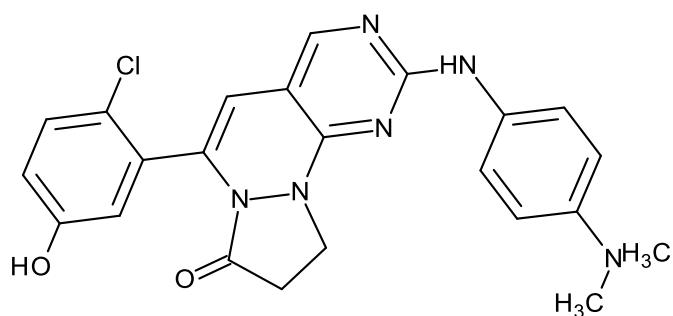
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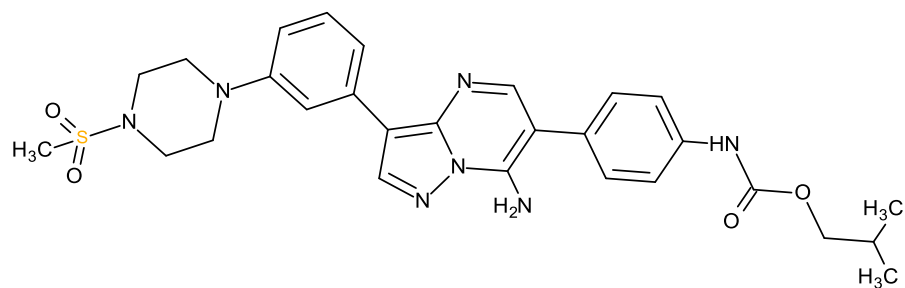
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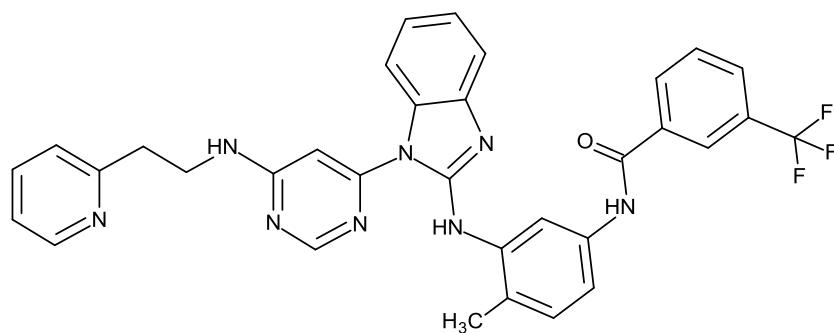
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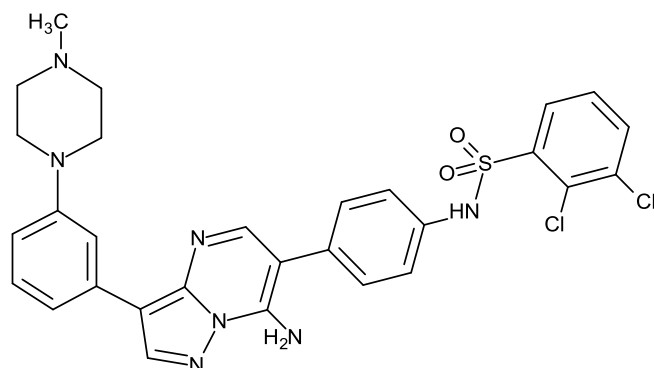
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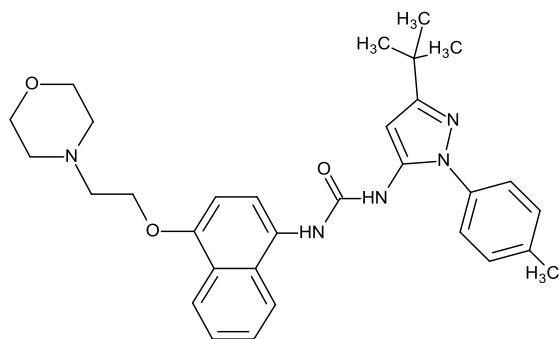
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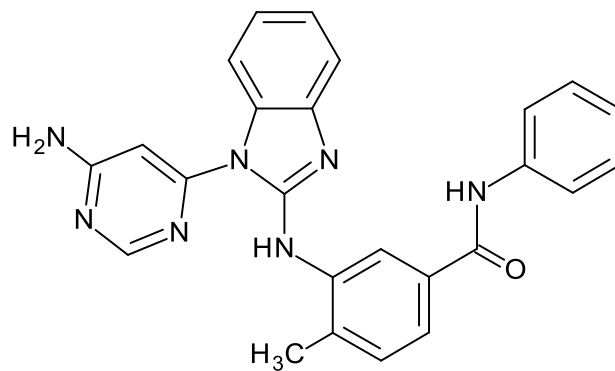
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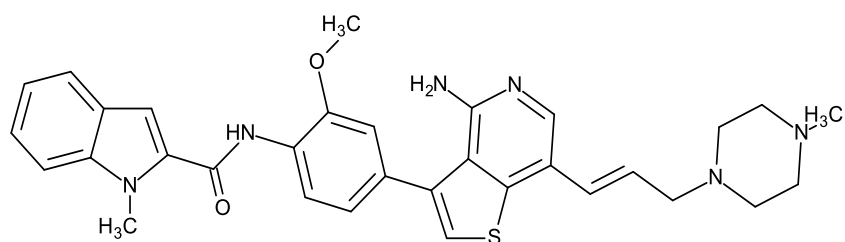
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33

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34

12900

