

AB Test 1 – 3N-MCTS vs Literature Routes**AB Test Literature:**

mol_132: Tan, Haibo et al; Org. Biomol. Chem., 39, 9977-9983; 2015

mol_329: Jun 18, 2016; CA 2915356; A1

mol_341: Antimicrobial Agents and Chemotherapy, 2015 , vol. 59, # 2 p.
1110 - 1118

mol_538: Faming Zhuanli Shenqing; 49pp.; Patent 2016; CODEN:CNXXEV

mol_608: Fujiyasu, Jiro et al; From PCT Int. Appl., 2014142219, 18 Sep 2014

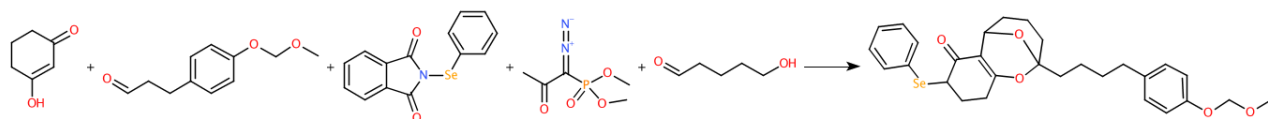
mol_706: Wu, Jing-Jing et al; Tetrahedron Letters, 58(10), 923-925; 2017

mol_716: Burnett, Duane A. et al; PCT Int. Appl., 2015066371, 07 May 2015

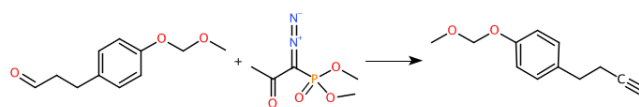
mol_752: Mueller, Anne et al, Chem. Eur. J, 21(39), 13723-13731; 2015

mol_841: Feb 11, 2016; WO 2016022460; A1

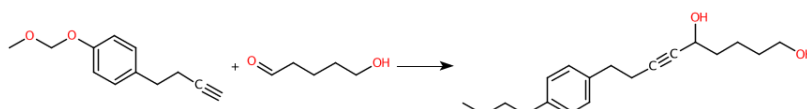
1 MCTS



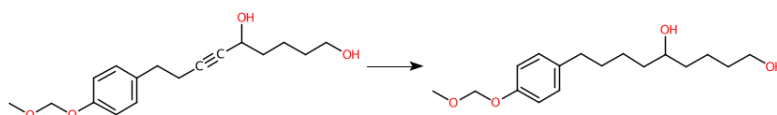
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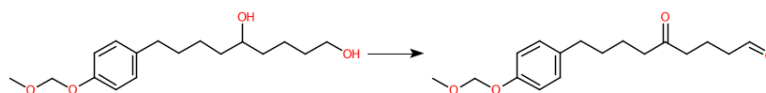
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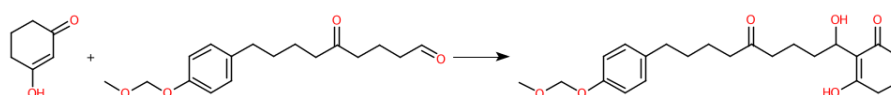
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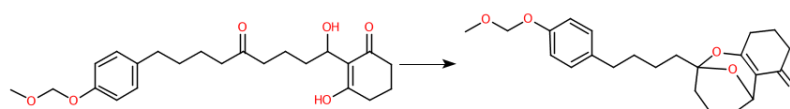
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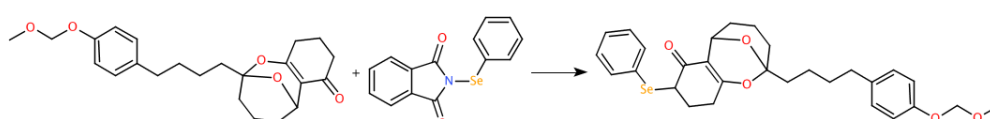
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step 3

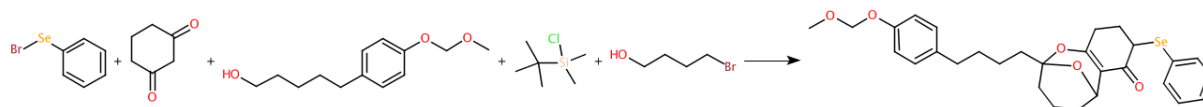


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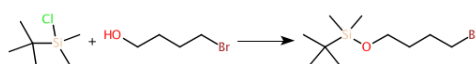


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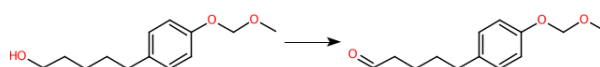
1 Literature



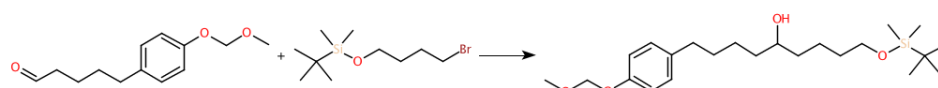
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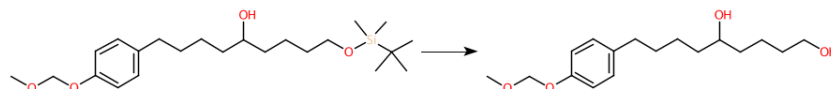
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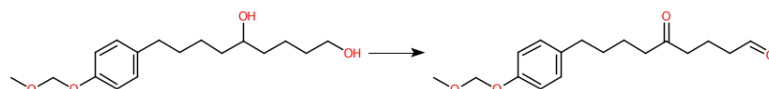
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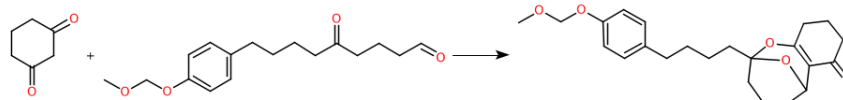
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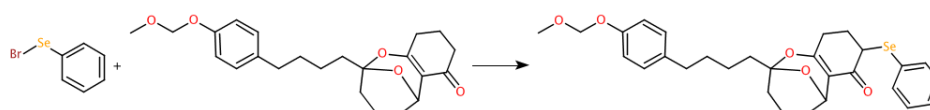
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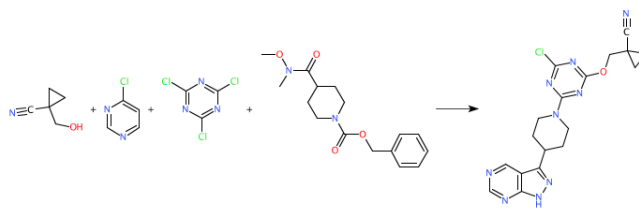


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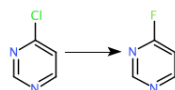


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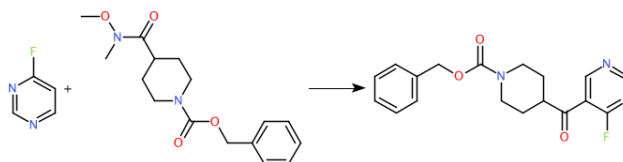
2 MCTS



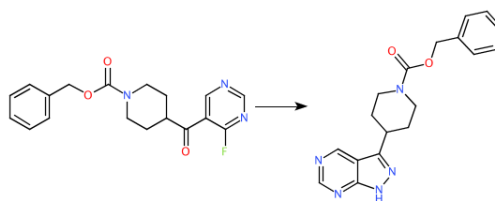
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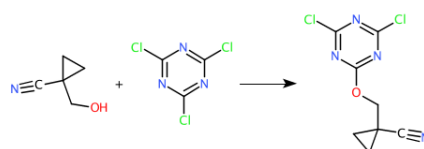
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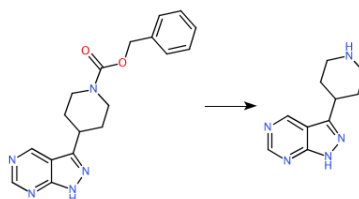
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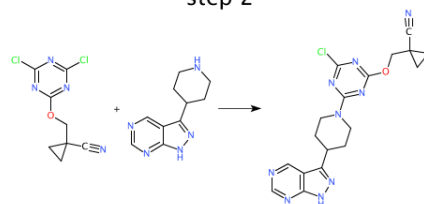
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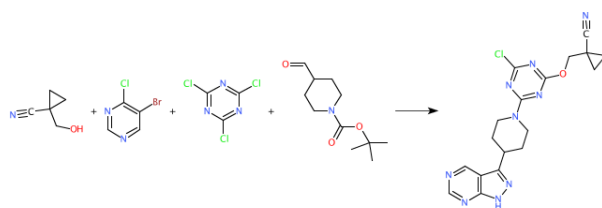


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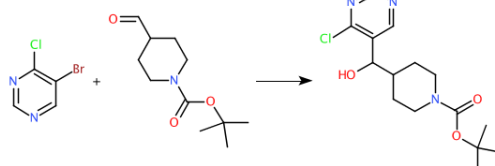


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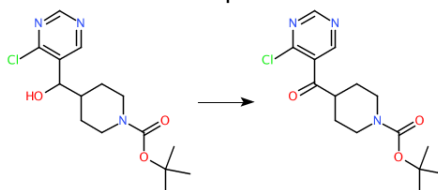
2 Literature



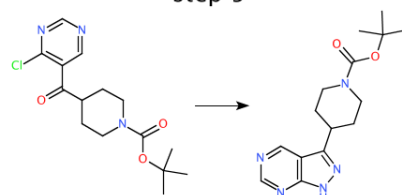
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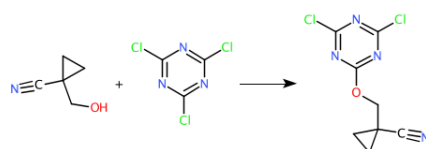
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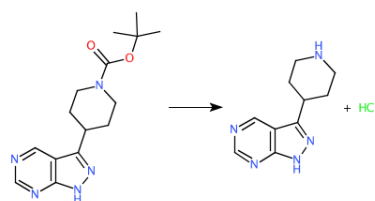
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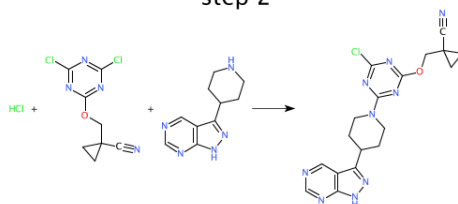
step 4



step 3



step 2



step 1

Chemical reaction scheme showing the conversion of 4-methoxycarbonylbenzotrile (4-methoxybenzocyanide) to 4-methoxybenzidine. The starting material is a benzene ring with a methoxycarbonyl group (-COOCH₃) at the para position and a cyano group (-C≡N) at the other para position. An arrow points to the product, which is a benzene ring with a methoxycarbonyl group (-COOCH₃) at the para position and a hydrazine group (-NH-NH₂) at the other para position.

The reaction scheme shows the synthesis of 2-(4-methoxybenzylidene)-1,3,4-oxadiazole. The starting materials are 4-methoxybenzohydrazide (a benzene ring with a methoxycarbonyl group at the para position and a hydrazide group at the other para position) and chloroacetaldehyde (ClCH₂CHO). The product is 2-(4-methoxybenzylidene)-1,3,4-oxadiazole, where the hydrazide group has cyclized to form a 1,3,4-oxadiazole ring, and the carbonyl oxygen has been replaced by the methoxy group.

Chemical reaction scheme showing the synthesis of compound 10. The reaction involves 1-(2-chloromethyl-1,3,4-oxadiazol-5-yl)benzoic acid methyl ester and 1-(2-aminoethyl)pyrrolidine. The product is 1-(2-(2-(2-methoxy-1-phenyl-1,3,4-oxadiazol-5-yl)ethylamino)ethyl)pyrrolidine.

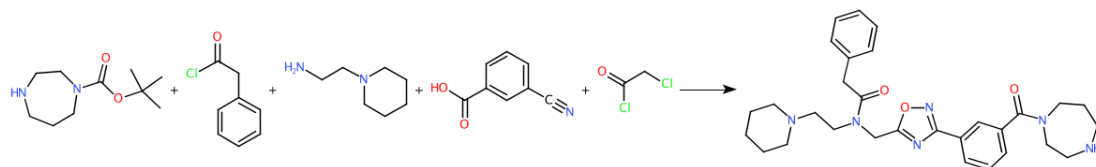
Chemical reaction scheme showing the synthesis of compound 10. The reaction involves the coupling of 2-chloro-1-phenylethan-1-one with 1-(4-methoxyphenyl)-5-((2-(4-morpholinyl)ethyl)hydrazono)-1H-imidazole-4-carboxylate. The product is 1-(4-methoxyphenyl)-5-((2-(4-morpholinyl)ethyl)hydrazono)-1H-imidazole-4-carboxylate-2-ylidene-1-phenylethan-1-one.

step 5

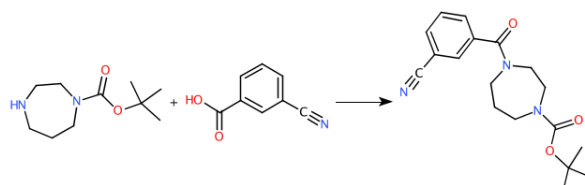
The reaction scheme shows the conversion of the methyl ester intermediate to the final carboxylic acid product. The starting material is the methyl ester of 1-(2-(4-(benzyl(2-(4-methoxybenzoyl)-1,2,4-oxadiazol-5-yl)ethyl)piperidin-1-yl)ethyl)benzoate. The reaction involves the removal of the methyl group from the ester, resulting in the formation of the carboxylic acid group. The product is 1-(2-(4-(benzyl(2-(4-carboxybenzoyl)-1,2,4-oxadiazol-5-yl)ethyl)piperidin-1-yl)ethyl)benzoic acid.

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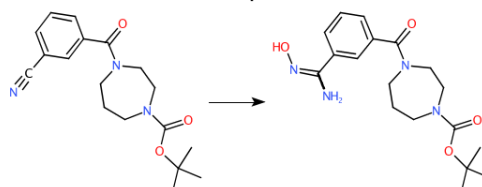
3 Literature



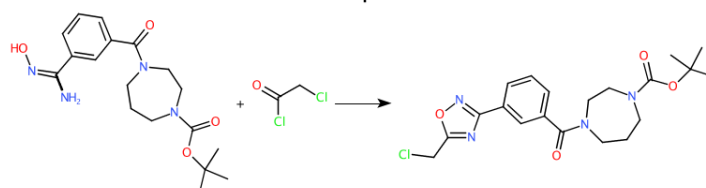
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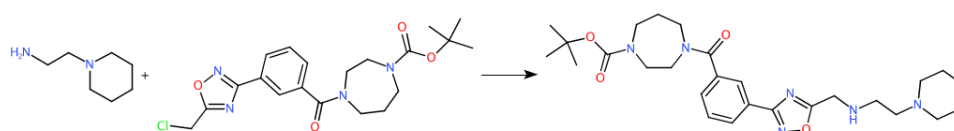
step 6



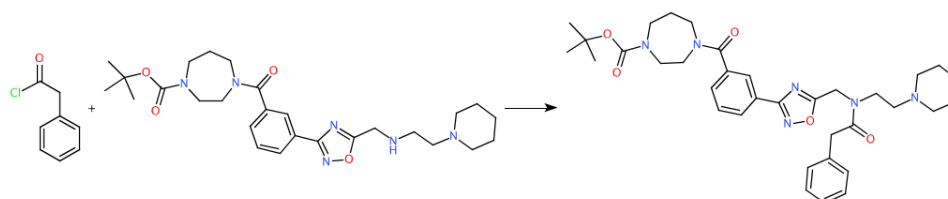
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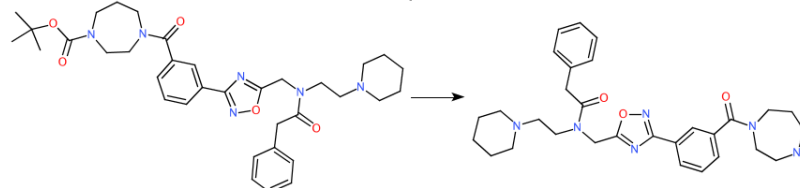
step 4



step 3

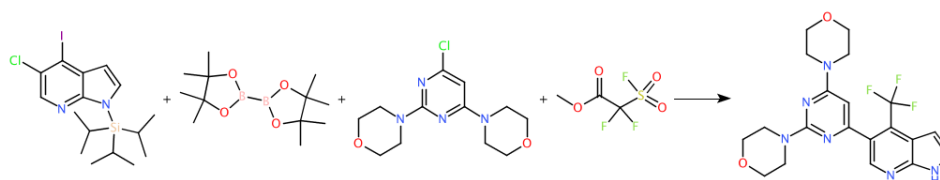


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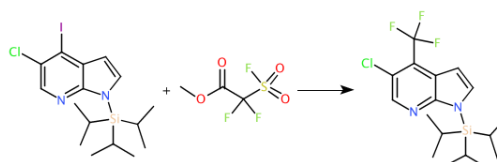


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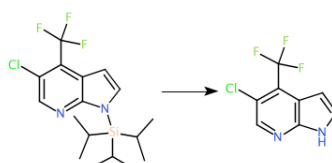
4 MCTS



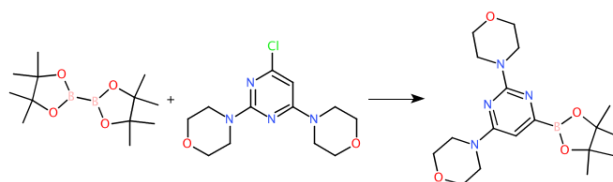
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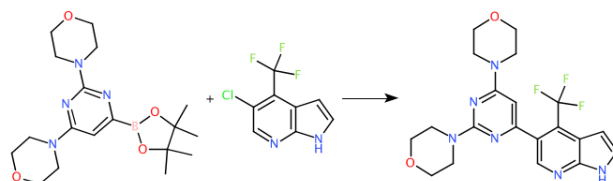
step 4



step 3

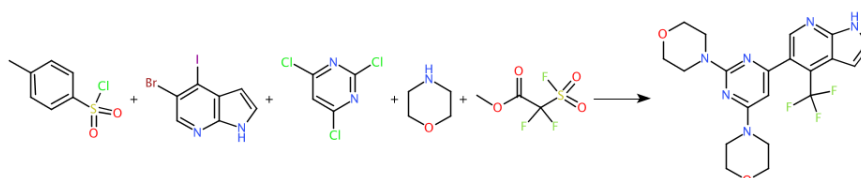


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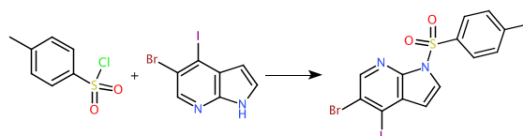


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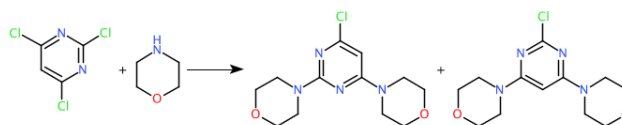
4 Literature



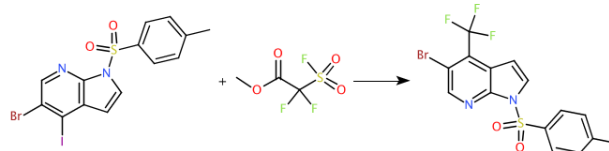
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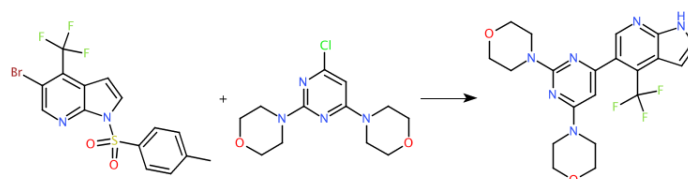
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step 3

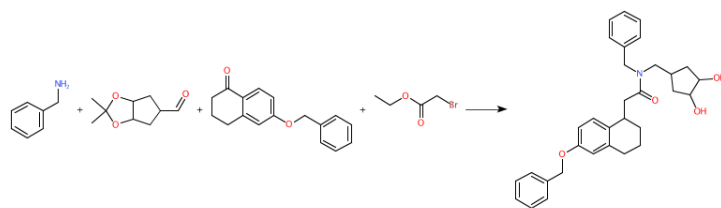


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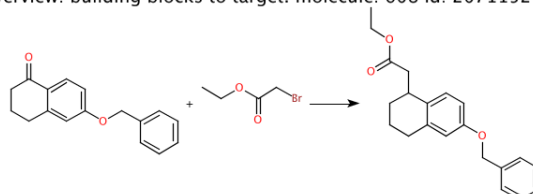


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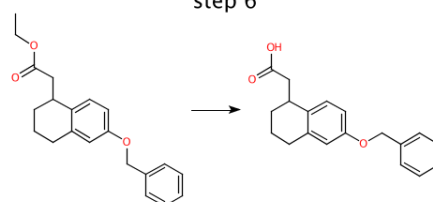
5 MCTS



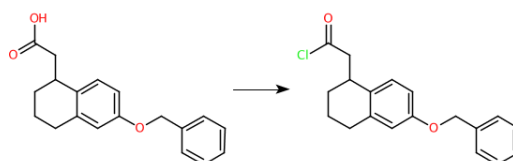
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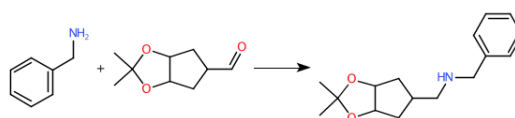
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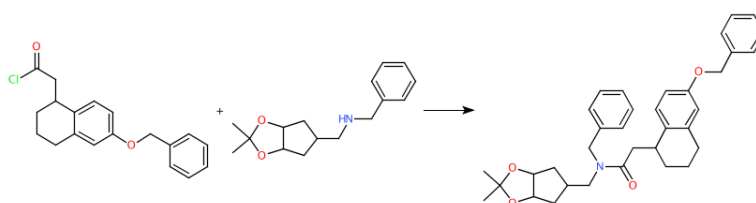
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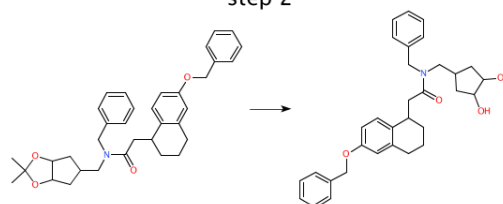
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step 3

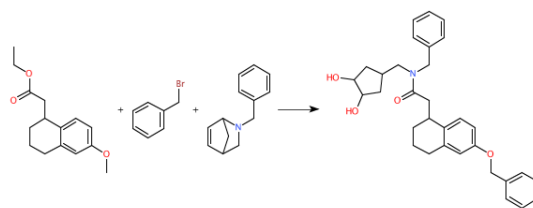


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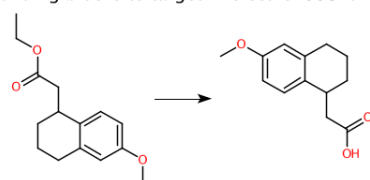


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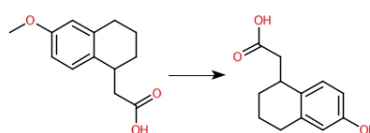
5 Literature



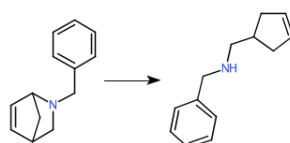
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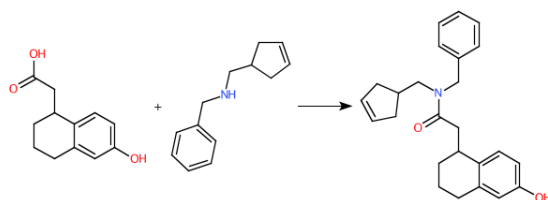
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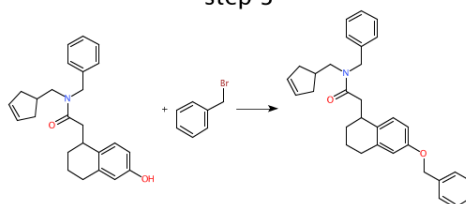
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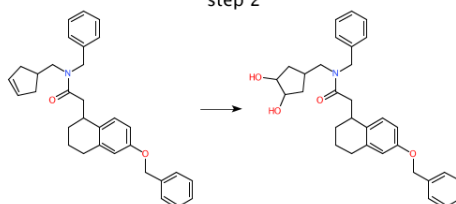
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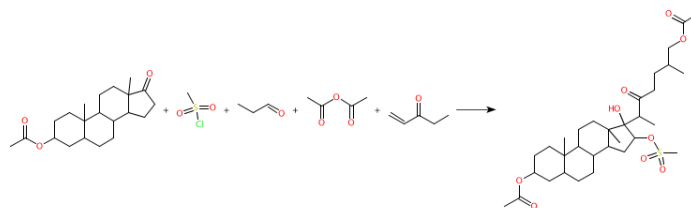


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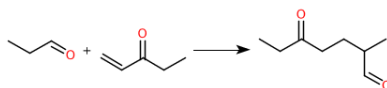


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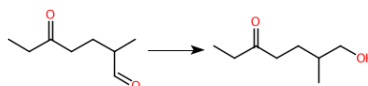
6 MCTS



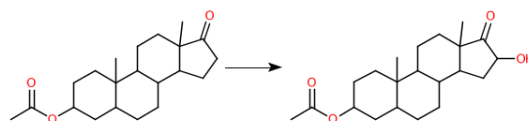
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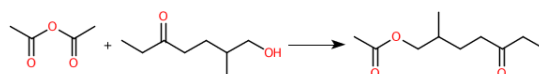
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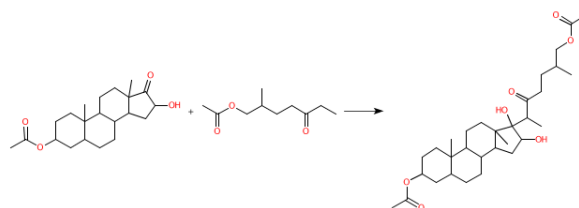
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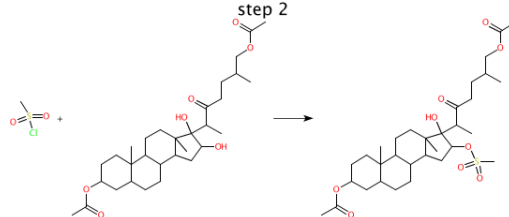
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step 3

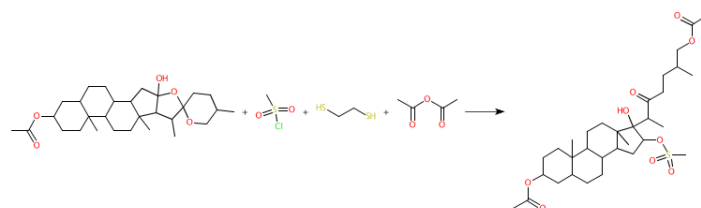


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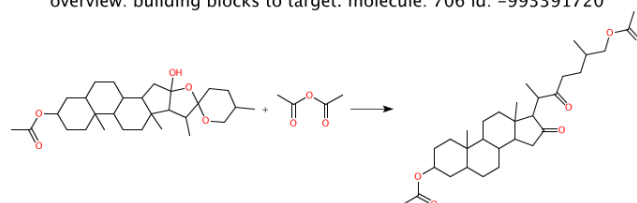


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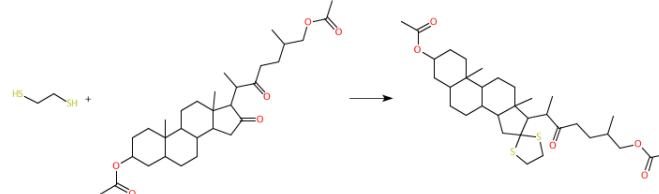
6 Literature



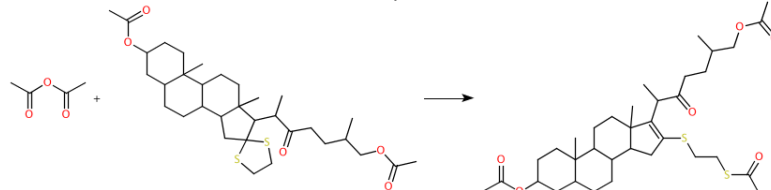
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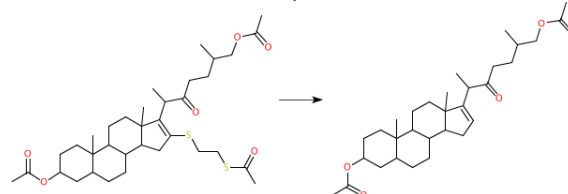
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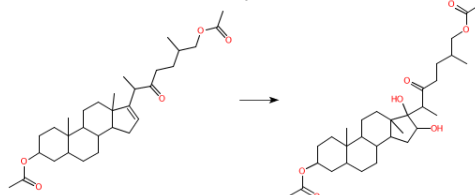
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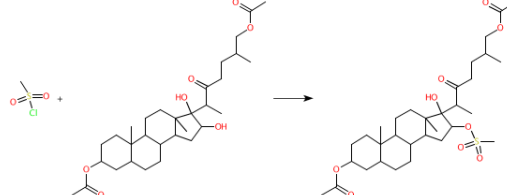
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step 3

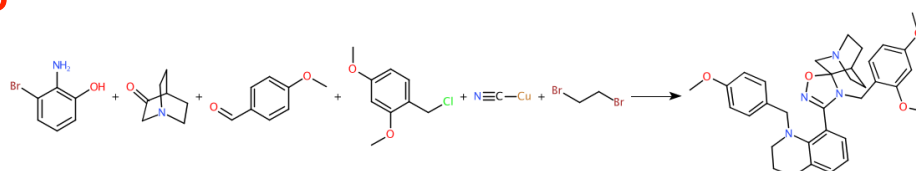


step 2

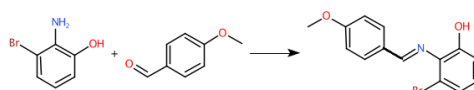


step 1

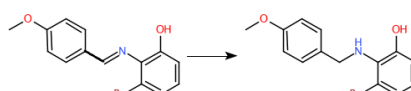
7 MCTS



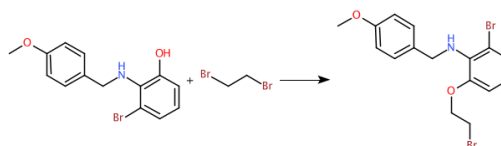
overview: building blocks to target. molecule: 716 id: 838806631



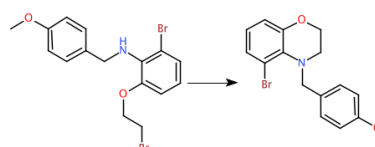
step 8



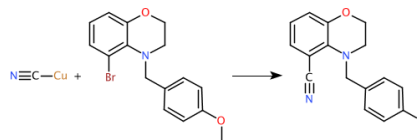
step 7



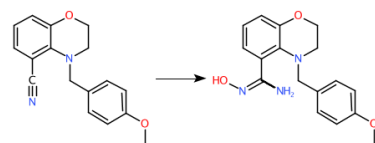
step 6



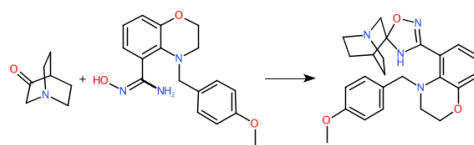
step 5



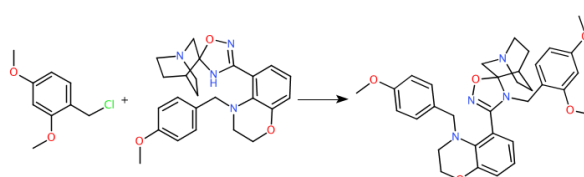
step 4



step 3

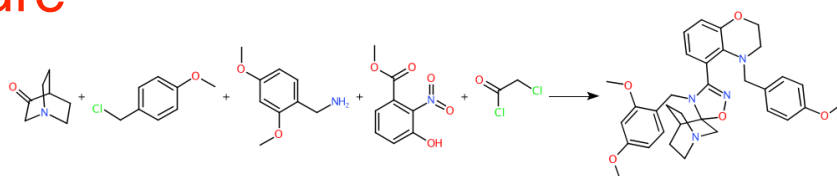


step 2

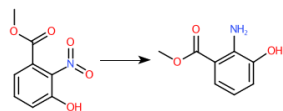


step 1

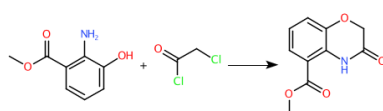
7 Literature



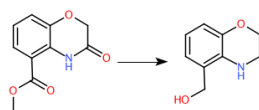
overview: building blocks to target. molecule: 716 id: -1861302227



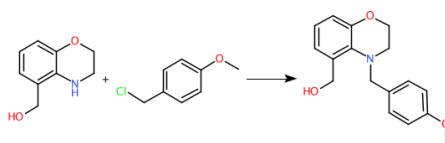
step 8



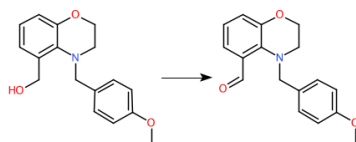
step 7



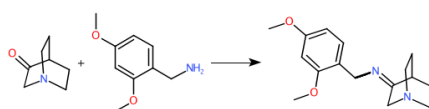
step 6



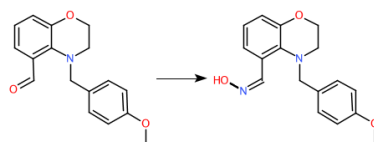
step 5



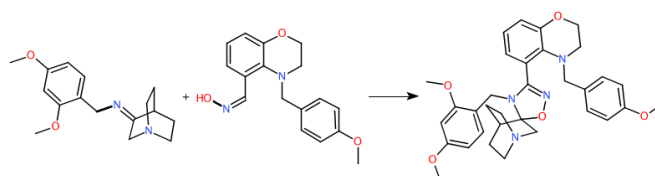
step 4



step 3

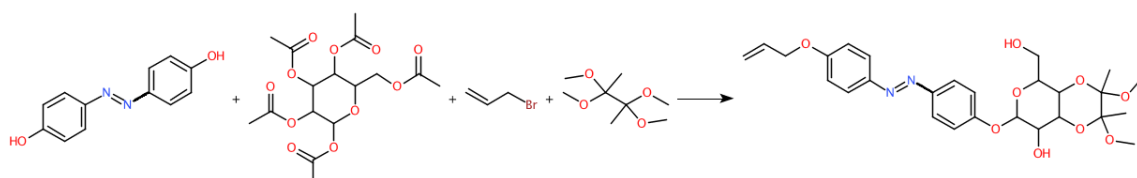


step 2

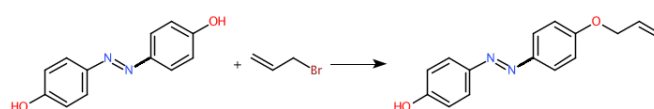


step 1

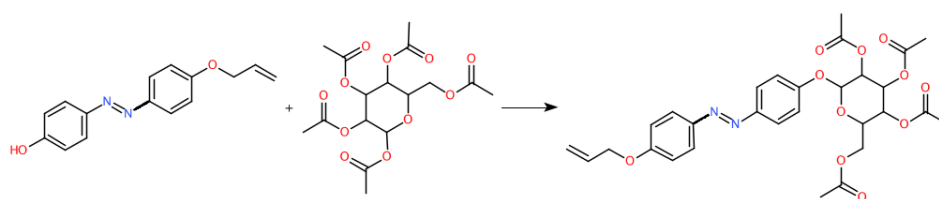
8 MCTS



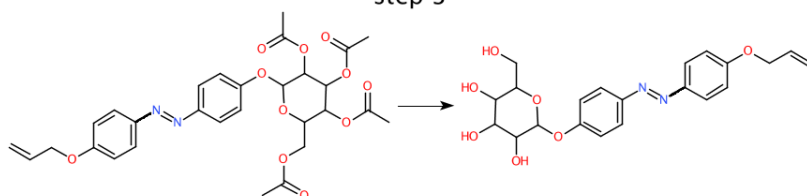
overview: building blocks to target. molecule: 752 id: -879018011



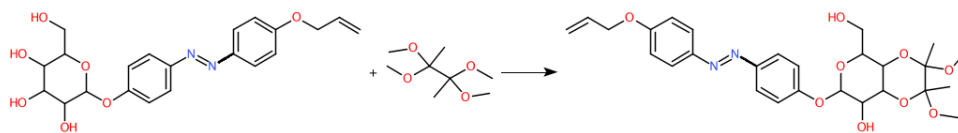
step 4



step 3

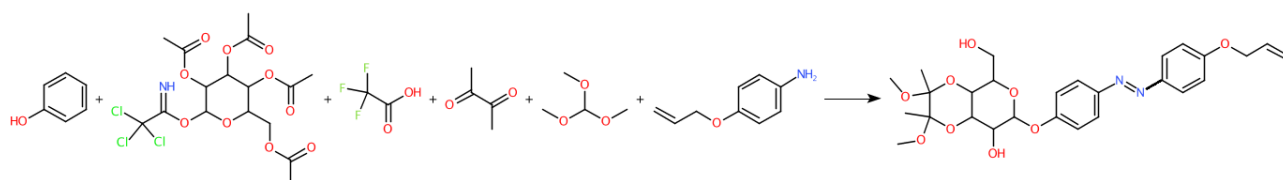


step 2

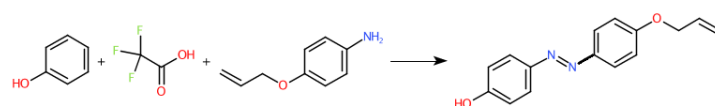


step 1

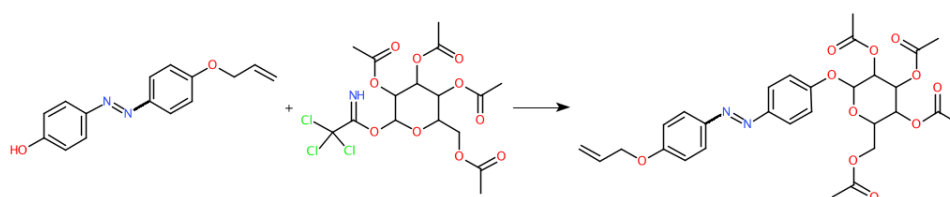
8 Literature



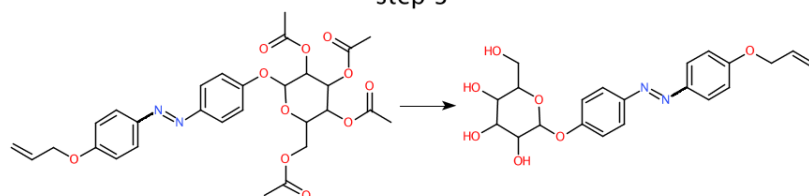
overview: building blocks to target. molecule: 752 id: -1778621489



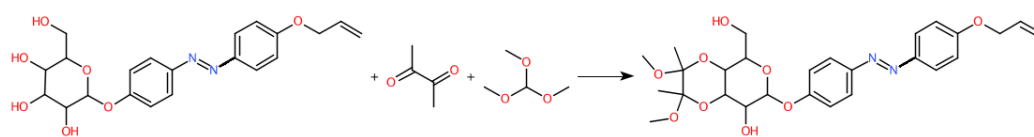
step 4



step 3

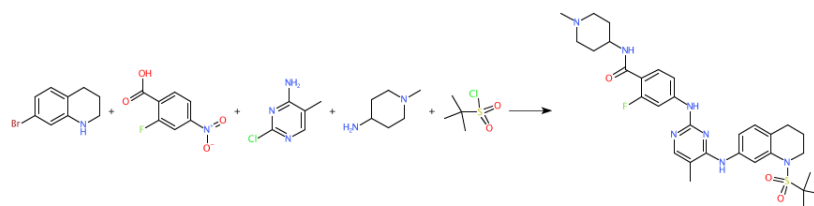


step 2

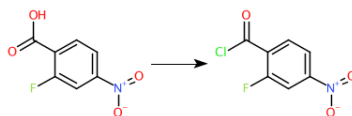


step 1

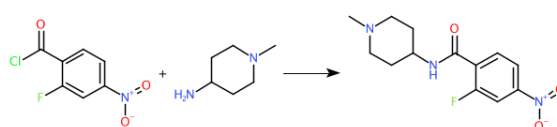
9 MCTS



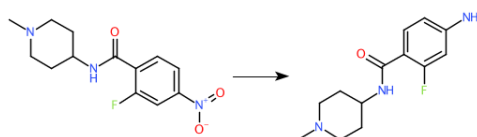
overview: building blocks to target. molecule: 841 id: 1619056472



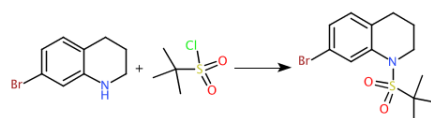
step 6



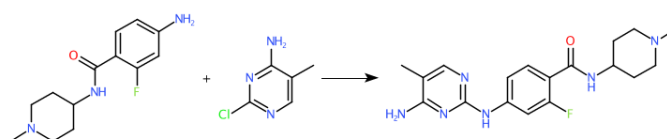
step 5



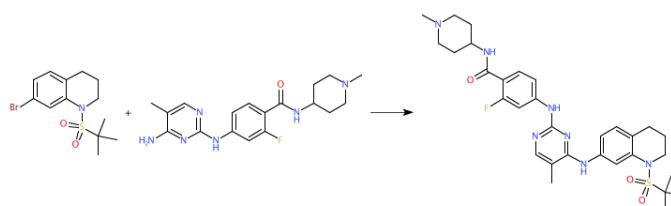
step 4



step 3

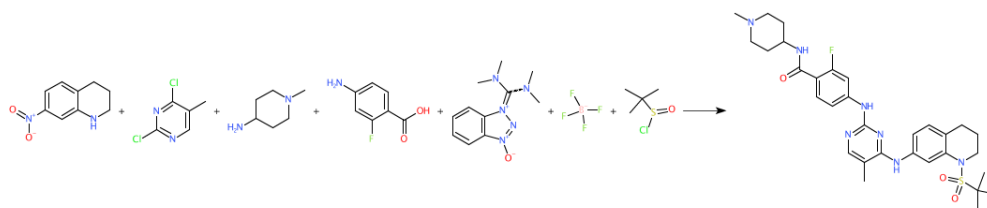


step 2

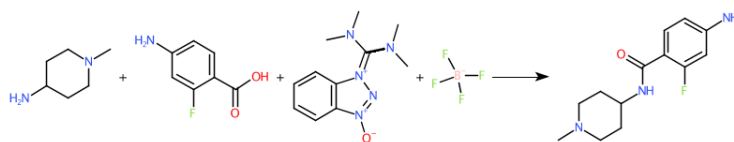


step 1

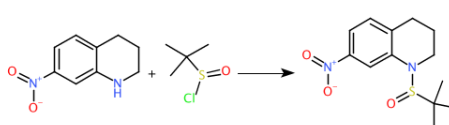
9 Literature



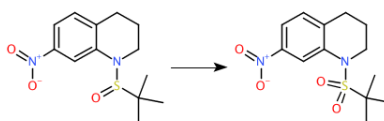
overview: building blocks to target. molecule: 841 id: -155621046



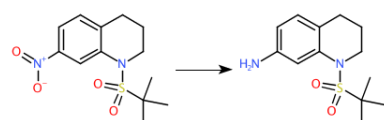
step 6



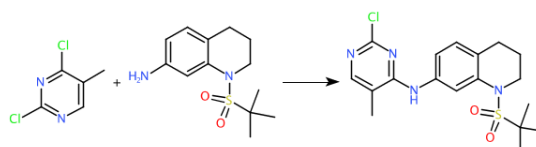
step 5



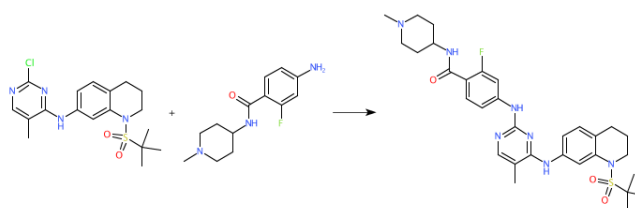
step 4



step 3



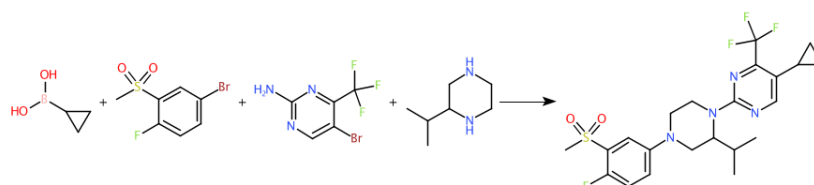
step 2



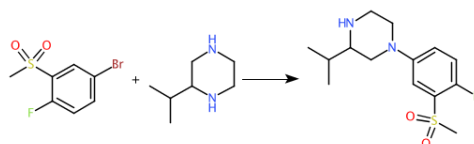
step 1

AB Test 2 – 3N-MCTS vs Heuristic BFS

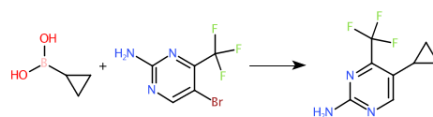
1 MCTS



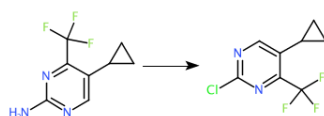
overview: building blocks to target. molecule: 15 id: -1642287589



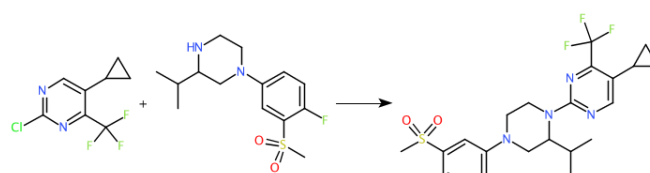
step 4



step 3

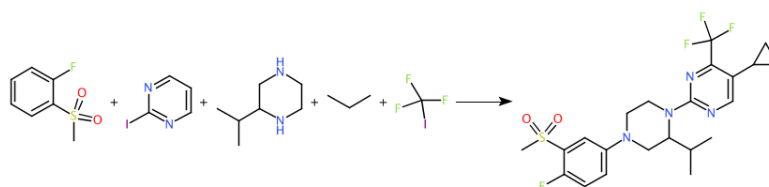


step 2

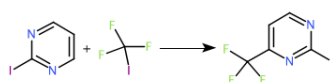


step 1

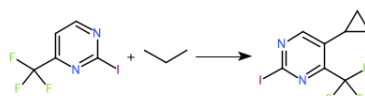
1 Heuristic BFS



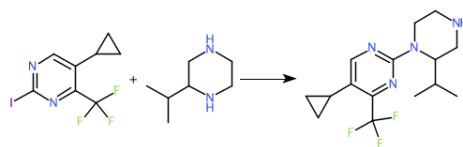
overview: building blocks to target. molecule: 15 id: -393970331



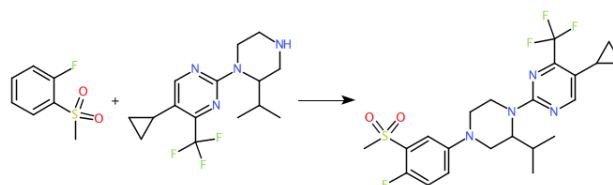
step 4



step 3

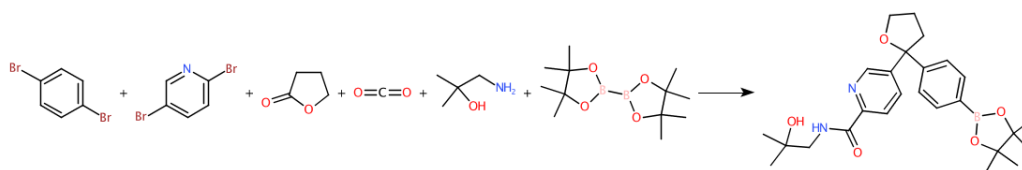


step 2

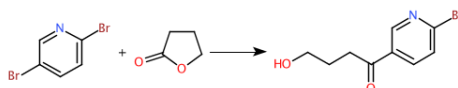


step 1

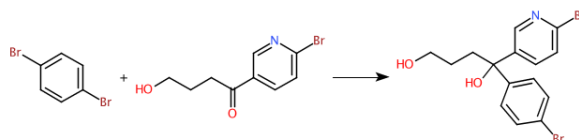
2 MCTS



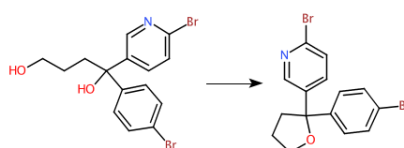
overview: building blocks to target. molecule: 291 id: -595446896



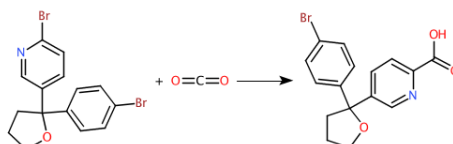
step 6



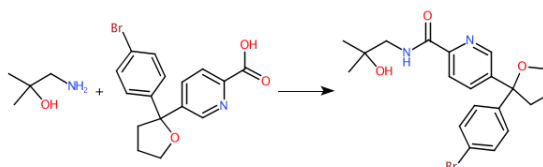
step 5



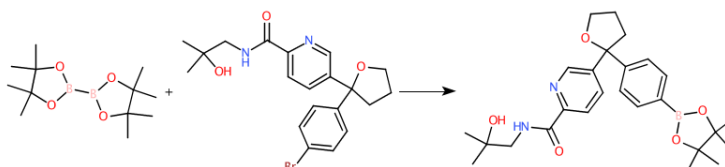
step 4



step 3

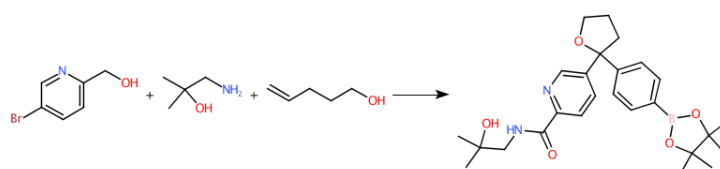


step 2

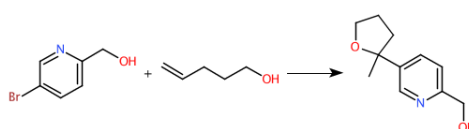


step 1

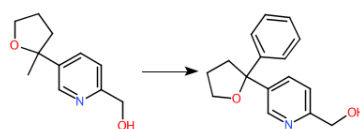
2 Heuristic BFS



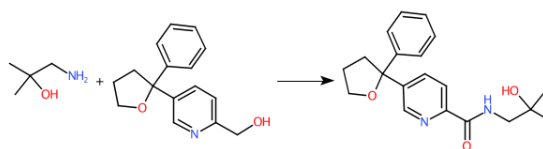
overview: building blocks to target. molecule: 291 id: 1651736554



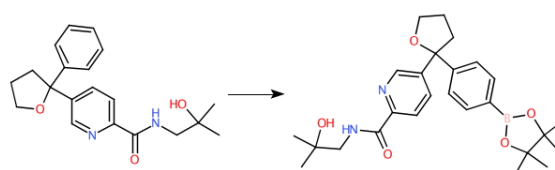
step 4



step 3

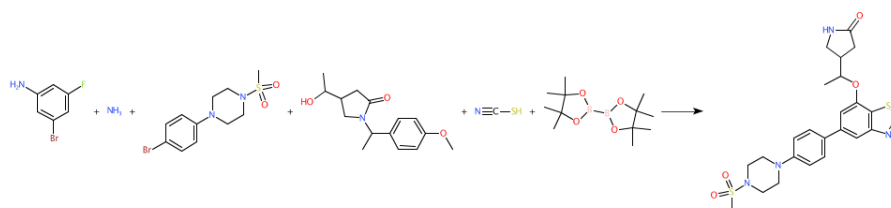


step 2

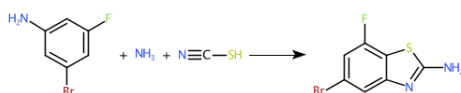


step 1

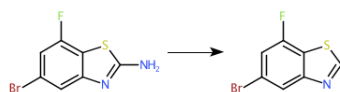
3 MCTS



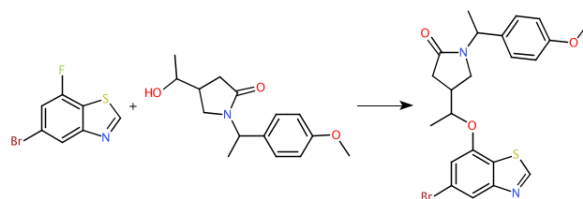
overview: building blocks to target. molecule: 591 id: -1458307292



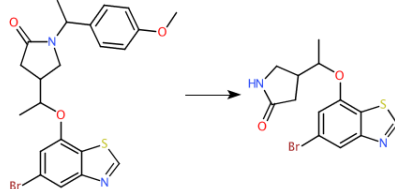
step 6



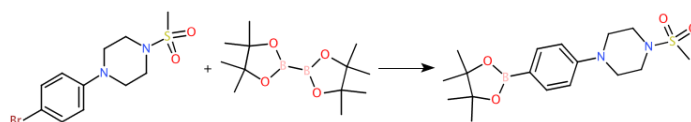
step 5



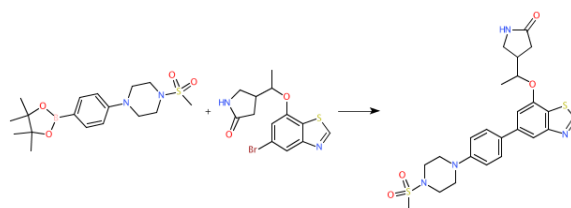
step 4



step 3

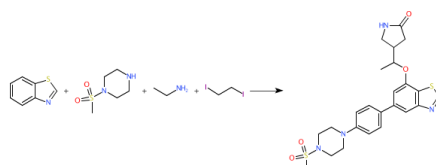


step 2

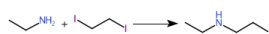


step 1

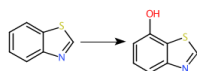
3 Heuristic BFS



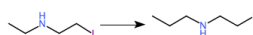
overview: building blocks to target. molecule: 591 id: 1329500428



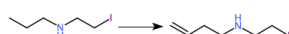
step 9



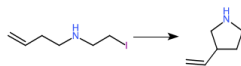
step 8



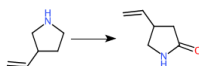
step 7



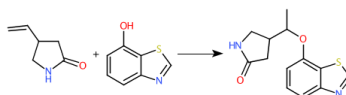
step 6



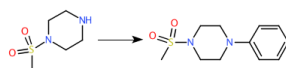
step 5



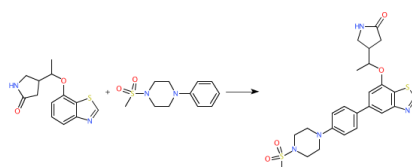
step 4



step 3

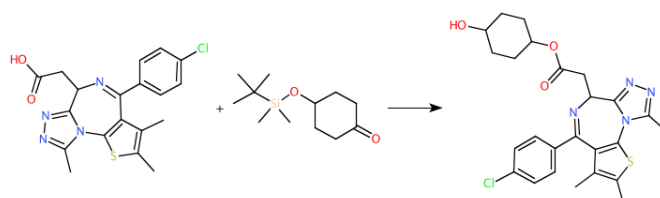


step 2

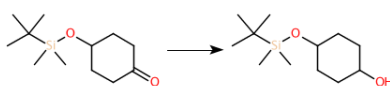


step 1

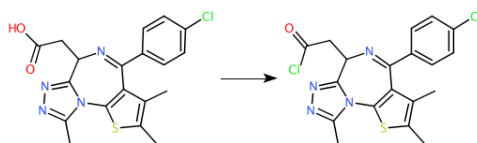
4 MCTS



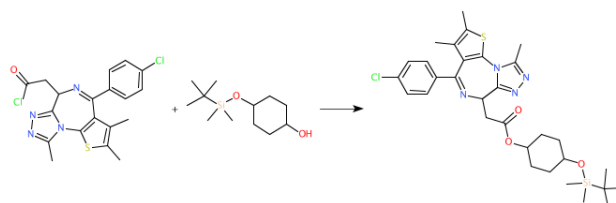
overview: building blocks to target. molecule: 616 id: 308054153



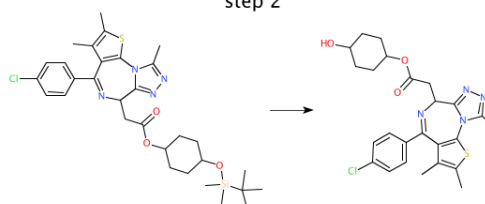
step 4



step 3

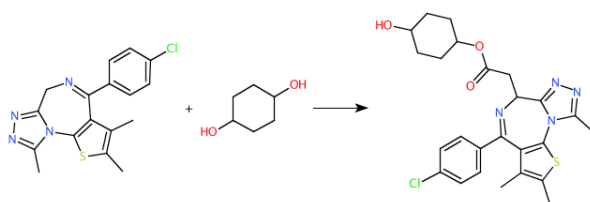


step 2

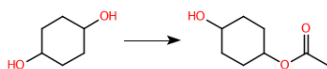


step 1

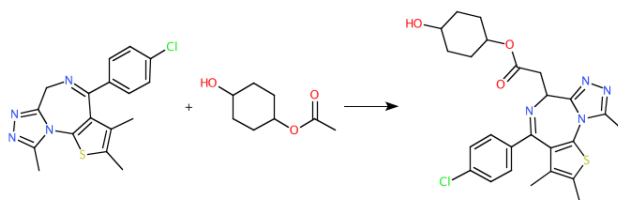
4 Heuristic BFS



overview: building blocks to target. molecule: 616 id: 1332906658

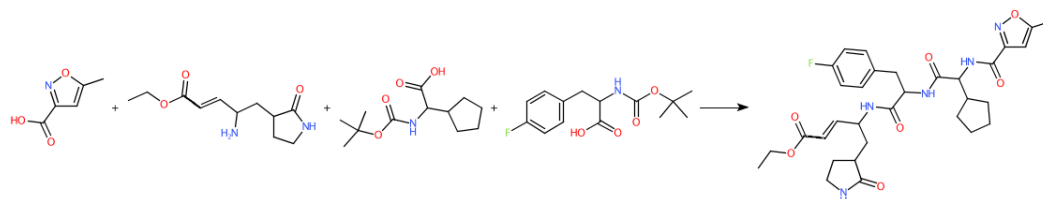


step 2

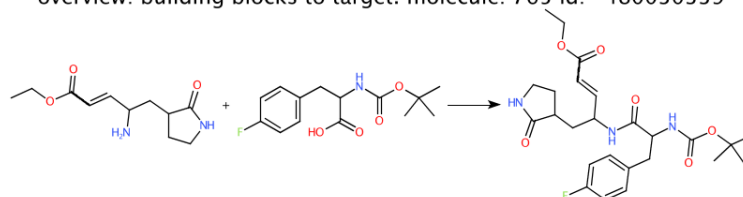


step 1

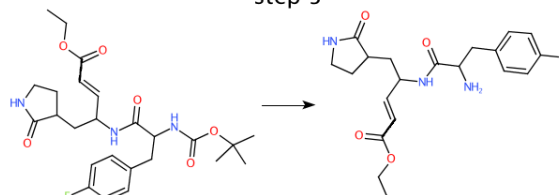
5 MCTS



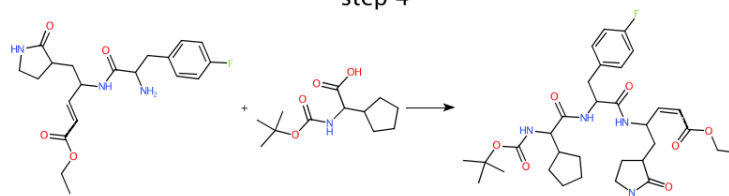
overview: building blocks to target. molecule: 765 id: -480030339



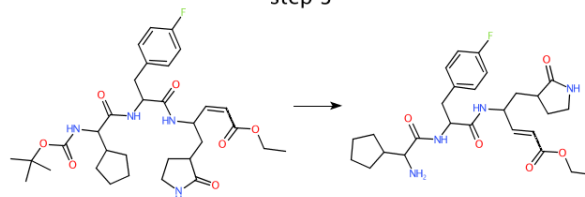
step 5



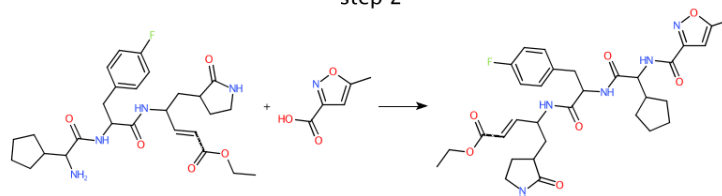
step 4



step 3

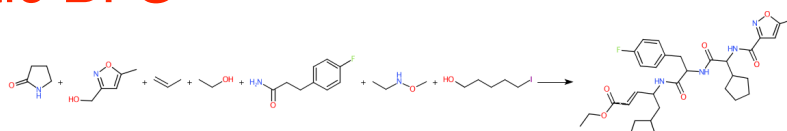


step 2



step 1

5 Heuristic BFS



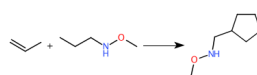
overview: building blocks to target. molecule: 765 id: -23963229



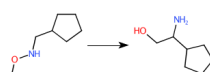
step 10



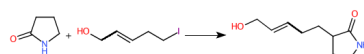
step 9



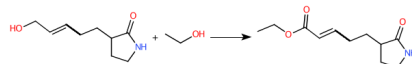
step 8



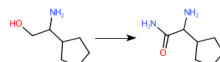
step 7



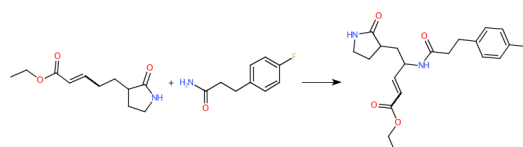
step 6



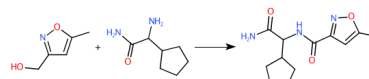
step 5



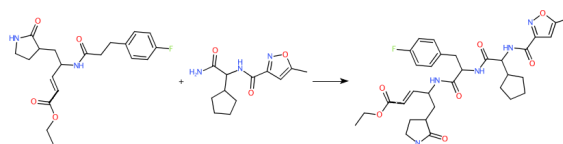
step 4



step 3

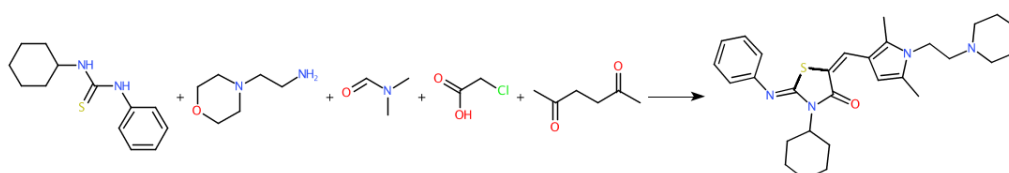


step 2

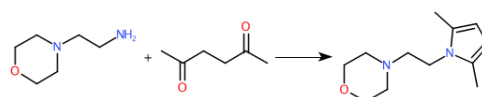


step 1

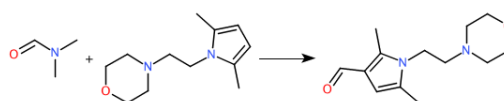
6 MCTS



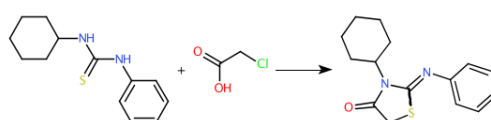
overview: building blocks to target. molecule: 833 id: -1806975545



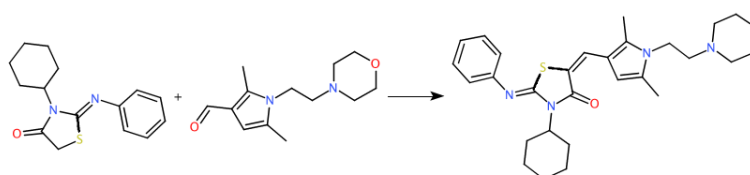
step 4



step 3

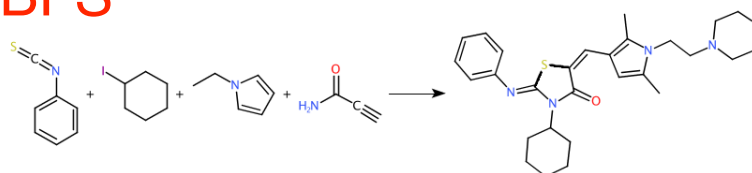


step 2

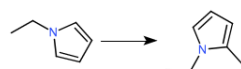


step 1

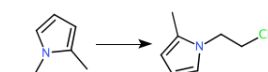
6 Heuristic BFS



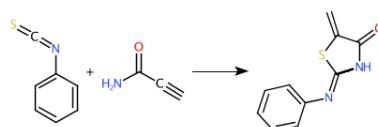
overview: building blocks to target. molecule: 833 id: -1715572566



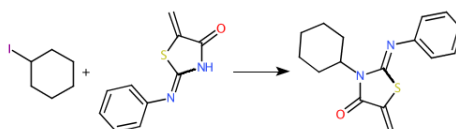
step 7



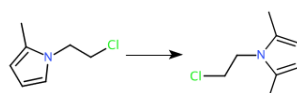
step 6



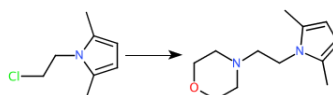
step 5



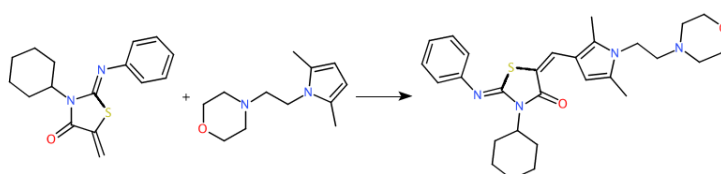
step 4



step 3

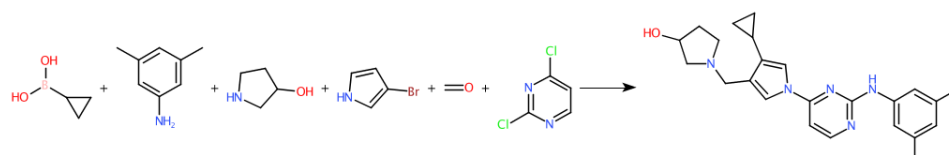


step 2

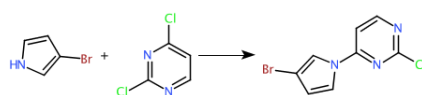


step 1

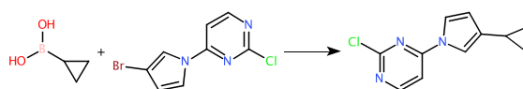
7 MCTS



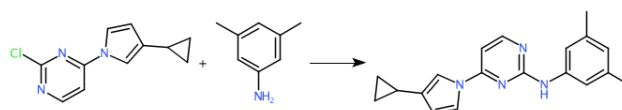
overview: building blocks to target. molecule: 845 id: -1912623546



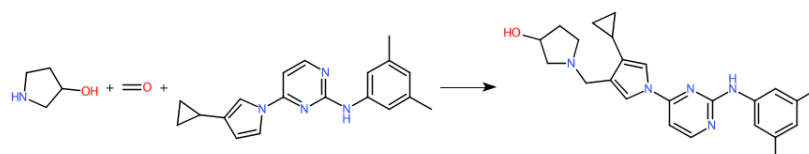
step 4



step 3

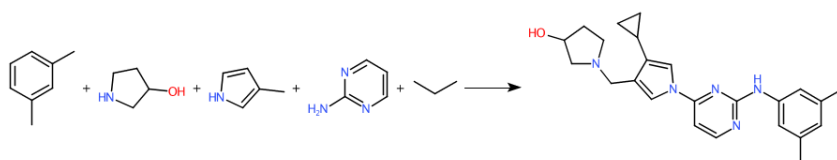


step 2

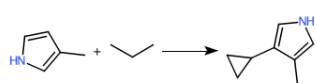


step 1

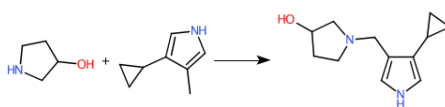
7 Heuristic BFS



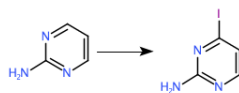
overview: building blocks to target. molecule: 845 id: -1608629638



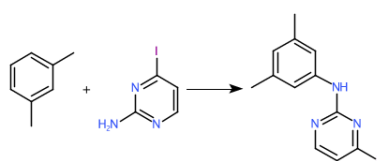
step 5



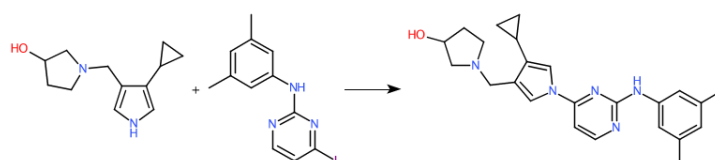
step 4



step 3

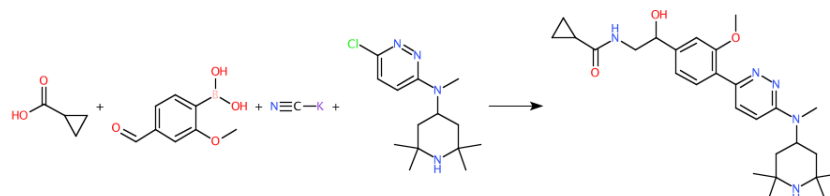


step 2

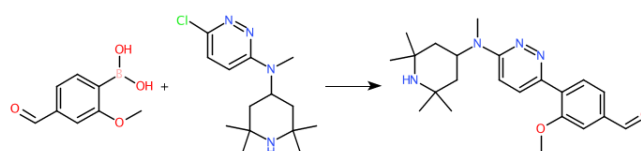


step 1

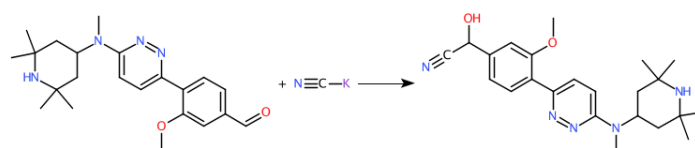
8 MCTS



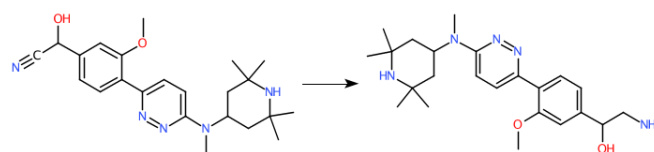
overview: building blocks to target. molecule: 850 id: -1045950342



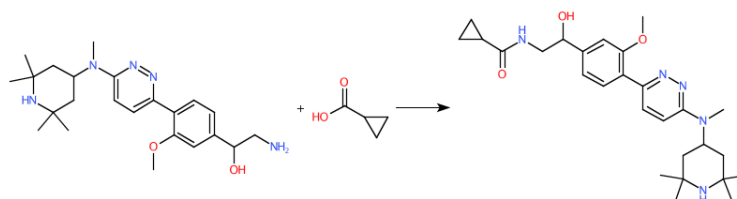
step 4



step 3

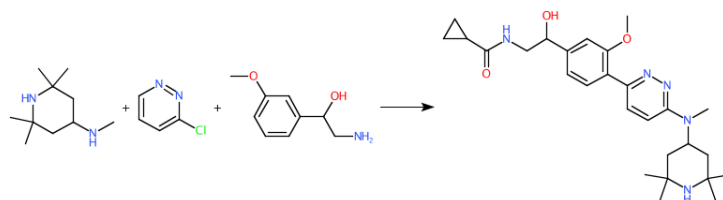


step 2

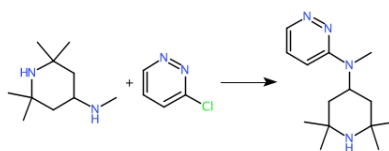


step 1

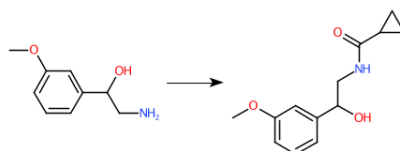
8 Heuristic BFS



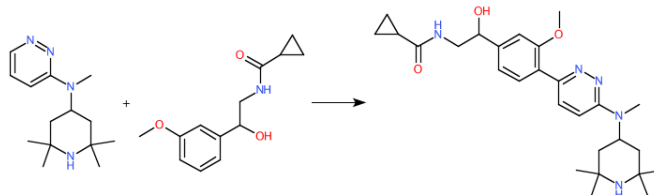
overview: building blocks to target. molecule: 850 id: -2075608617



step 3

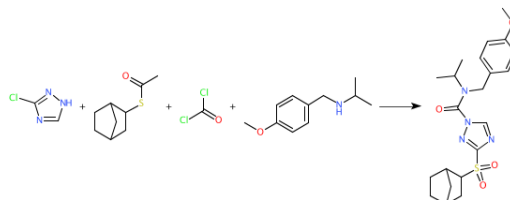


step 2

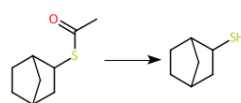


step 1

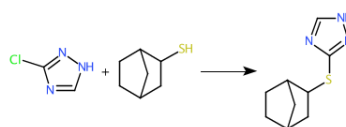
9 MCTS



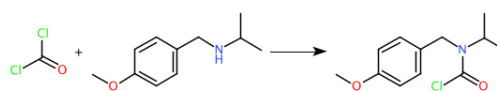
overview: building blocks to target. molecule: 944 id: -789174339



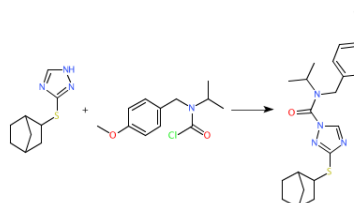
step 5



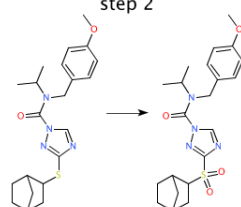
step 4



step 3

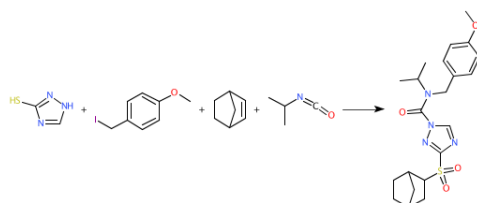


step 2

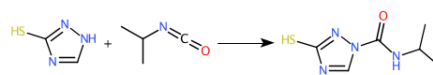


step 1

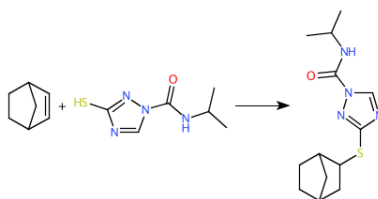
9 Heuristic BFS



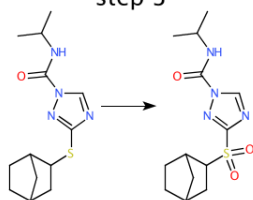
overview: building blocks to target. molecule: 944 id: 1295328237



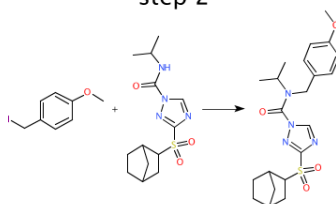
step 4



step 3

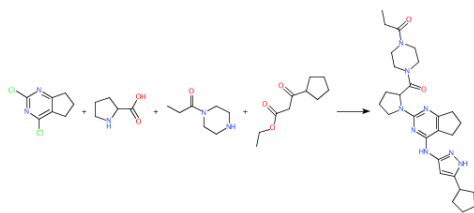


step 2

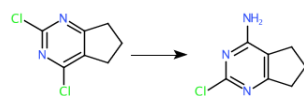


step 1

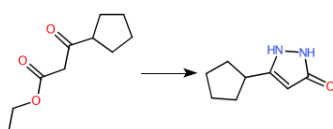
10 MCTS



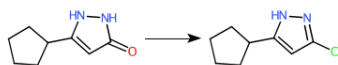
overview: building blocks to target. molecule: 945 id: -1366079493



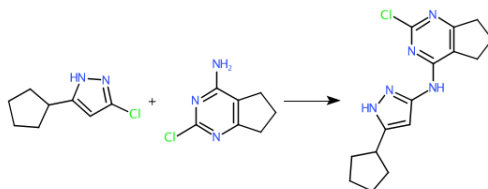
step 6



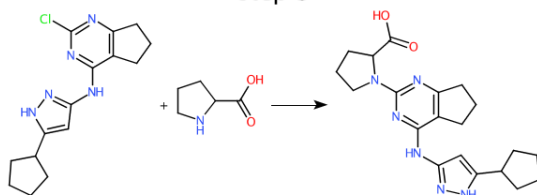
step 5



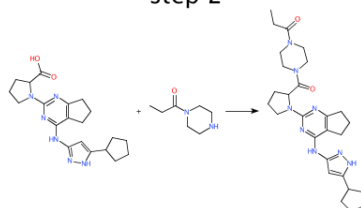
step 4



step 3

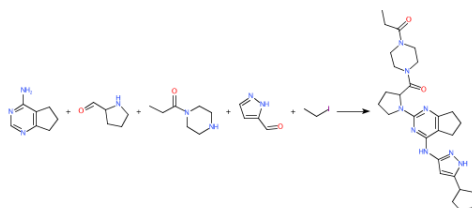


step 2

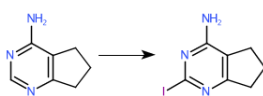


step 1

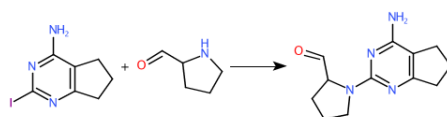
10 Heuristic BFS



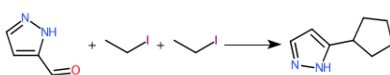
overview: building blocks to target. molecule: 945 id: -354976033



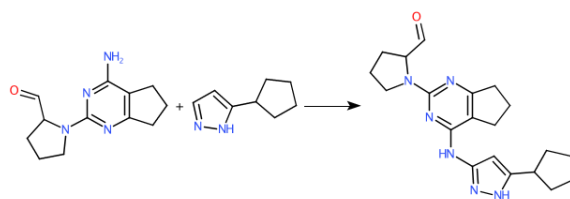
step 5



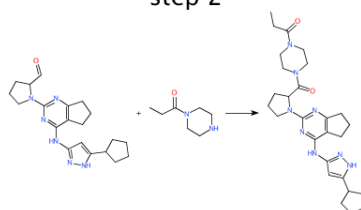
step 4



step 3



step 2



step 1