# Supporting Information: Predicting Retrosynthetic Pathways using Transformer-based Models and a Hyper-Graph Exploration Strategy

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## 1 Hypergraph exploration

Algorithm 1 provides an overview of the hyper-graph expansion strategy, where given a starting node ($N$), the graph is expanded by predicting the reactions and precursors ($R_i$) leading to the molecule $N$. The single-step retrosynthetic model uses a beam-search to explore the possible disconnections and we retain the top-15 predicted sets of precursors (thus, $i = \{1, 2, ..., 15\}$). The SMILES corresponding to these predictions are canonicalized and duplicate entries removed. Any SMILES that fails in the canonicalization step or contains the target molecule is also removed. The remaining sets of precursors are further filtered by using the forward model to assess reaction viability and selectivity. Regarding viability, we

retain only those precursors ($R_i$) whose top-1 forward model predictions match the molecule $N$. This guarantees that, in the presence of multiple functional groups, the recommended disconnection leads to the desired targets. While this is a necessary condition, it is not a sufficient one as competitive reactions (top-2 and following) may lead to a mixture of molecules different from the desired target. In order to enforce chemo-selectivity, we use the likelihood of the top-1 forward prediction model and select only top-1 predictions with a likelihood larger than the subsequent top-2 by at least 0.2. As the sum of likelihoods for the predictions of different sets of precursors ($R_i$) leading to a target $N$ is one, any prediction likelihood higher than 0.6 automatically satisfies the requirements above and passes our filter. This filtering protocol increases the occurrence of chemo-selective reactions along the retrosynthetic path, penalizing disconnections that are highly competitive.

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**Algorithm 1:** Hyper-graph expansion algorithm

**Data:** Existing Node $N$, Beam Size $B$, retrosynthesis model, forward model
**Result:** New Nodes connected to $N$
**begin**

    $R = \{R_i | i = 1..B\} \longleftarrow$ Predict possible retrosynthesis steps (top-$B$) // $R_i$ `are`
        `represented as SMILES`

    **for** $R_i \in R$ // `select precursor sets for expansion`
    **do**

        $R_i \longleftarrow$ Try to canonicalize $R_i$, discard if not canonicalizable
        Discard $R_i$, if $N$ is a precursor in $R_i$
        $L_{R_i \to N} \longleftarrow$ Compute likelihood of reaction $R_i \to N$
        **if** $L_{R_i \to N} > 0.6$ **then**
            Attach $R_i$ to $N$ with a hyper-arc
        **else**
            $F_{top-1}, F_{top-2} \longleftarrow$ Predict top-2 forward reactions from $R_i$
            **if** *Product of $F_{top-1}$ is $N$ and*
            $Likelihood(F_{top-1}) > 0.2 + Likelihood(F_{top-2})$ **then**
                Attach $R_i$ to $N$ with a hyper-arc
            **else**
                discard $R_i$

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Moreover, precursor sets are clustered together to identify similar disconnection strategies

and reduce tree complexity. Within the same cluster, the precursors related to the highest forward prediction likelihood are used as starting nodes for further tree expansion. Every precursor molecule, unless already present in the graph, will generate a new node, and every reaction will connect each of the reactants to the target molecule by means of a new hyper-arc.

Every hyper-arc in the tree is scored with a so-called optimization score, which is used to define the "best" retrosynthetic route. The total score of a retrosynthetic pathway is calculated by multiplying the scores of all the arcs contained in the path. The definition of the score for a single arc is:

$$S(\text{C} \Rightarrow \text{A} + \text{B}) = P(\text{A} + \text{B} \rightarrow \text{C}) \frac{s(\text{A}) * s(\text{B})}{s(\text{C})} \tag{1}$$

where $S(\text{C} \Rightarrow \text{A} + \text{B})$ denotes the score for a single retrosynthetic step: the higher the score the higher the preference towards that step. $P(\text{A} + \text{B} \rightarrow \text{C})$ is the likelihood of the forward chemical reaction computed by the forward prediction model. $s(\text{X})|\text{X} \in \{\text{A}, \text{B}, \text{C}\}$ is the simplicity score of molecule X:

$$s(\text{X}) = 1 - \frac{\text{SC}(\text{X}) - 1}{4} \tag{2}$$

where $SC(\text{X})$ is the SCScore[1] of molecule X. The SCScore of a molecule increases from 1 to 5 with an increasing complexity of the synthetic route. In this framework, the SCScore constitutes the driving force that pulls a retrosynthetic pathway towards simpler molecules.

Equation 1 closely resembles the definition of the Bayesian probability. In fact, assuming access to the set of all possible reactions, the likelihood of a retrosynthetic step would be defined as the conditional probability of observing the product when given the reactants, weighted by the ratio between the occurrence of the reagents and the occurrence of the product.

Even with a multi-million entry database, the evaluation of the individual components

would still be quite inaccurate. In fact, any molecule unreported in this database will contribute a value of zero to the evaluation of the Bayesian probability, with important drawbacks for the hyper-tree exploration. Therefore, the definition of the score for a single retrosynthetic step was only inspired by the Bayesian probability. We replaced the conditional probability with the likelihood of the forward prediction model and the probability of observing either reactants or products with a simplicity score. Similar to the Bayesian probability, the use of this heuristic favours those reaction that give more simple products (compared to reactants) under the same forward prediction likelihood.

The search for the optimal retrosynthetic route starts with the definition of a target molecule and uses a beam-search approach. The beam-search method is a greedy version of the best-first search: while best-first explores the entire graph and sorts all the possible paths according to some heuristic score, the beam search limits the exploration to a defined number of paths, thus limiting the computational cost without offering any guarantee of identifying the globally optimal path. The beam-search, as implemented in our software, relies on the following steps:

1. Expand the graph at every node contained in one of the possible pathways discovered up to this point and not yet expanded.

2. Create a new pathway for each of the arcs created by the last expansion.

3. Repeat steps 1 and 2 for a given number of times.

4. Assign a score to every pathway and discard the ones with the lowest score until the total number of "un-terminated" pathways correspond to the number of beams imposed by the user.

5. Restart from point 1 until all of the pathways meet one of the terminating conditions.

Each pathway of the beam-search may end because all the molecules needed to start the synthesis are found in a database of commercially available chemicals; or because the

number of synthetic steps (which corresponds to the number of "expansion phases") exceeds the number of maximum steps defined by the user; or finally because there is no possibility to further expand the needed nodes. The last condition may result from none of the set of precursors ($R_i$) surviving the filtering or from all the hyper-arcs generated by the expansion forming a cycle in the tree. From a chemical point of view, this means that one of the precursors of the product requires the product to synthesize itself.

Every time a pathway enters a cycle, the pathway itself is considered terminated. The tree exploration returns all the possible paths leading to a successful retrosynthesis, sorted by the optimization score.

## 2  Molecule representation

Similar to our previous works we use SMILES to represent molecules, taking more advantage of the auxiliary fragment information in which the grouped fragment indices are written after the label 'f:'. The different groups are separated by a ',' and the connected fragments within a group are separated by '.'. An example would be '|f:1.2,4.5|'. , where the fragments 1 and 2 as well as 4 and 5 belong together. There is nothing that enforces closeness of fragments in the SMILES string, hence different fragments belonging to the same compound could end up at opposite ends of the string. Typical examples are metallorganic compounds. Here, we relate the fragments within a group with a '∼' character instead of a '.'. Consequently, the fragmented molecules are kept together in the reaction string.

Atom-mapping as well as reactant-reagent roles, are a rich source of information generated by highly complicated tasks,[2] the assignment often being subjectively made by humans. Schwaller et al.[3] recently proposed to ignore reactant and reagent roles for the reaction prediction task. In contrast to previous works,[4–7] the single-step retrosynthetic model presented here predicts reactants and reagents. In an effort to simplify the prediction task, the most common precursors with a length of more than 50 tokens were replaced by molecule tokens.

Those molecules were turned back into the usual tokenization before calculating the likelihood with the forward model. Moreover, to ensure a basic tautomer standardization we inchified our molecules, as described in,[8] to improve the quality of the forward prediction model. In contrast to previous work,[9] we never use a reaction class token as input for the retrosynthesis model.

The data sets used to train the different models in this work are derived from the open source USPTO reaction database by Lowe[10,11] and the Pistachio database by NextMove Software.[12] We preprocessed both data sets to filter out incomplete reactions and keep 1M and 2M entries, respectively. As done previously in,[3,13] we added 800k textbook reactions to the training of specific forward and retrosynthetic models.

# 3  Models

## 3.1  Forward reaction prediction model

The forward prediction model was trained with the same hyperparameters as the original Molecular Transformer,[3] apart from the number of the attention layers, which was increased from 256 to 384. Thanks to the increase in capacity, a higher validation accuracy could be reached. For the final model we used a data set derived from Pistachio3.0[12] where all the molecules were inchified. As described in the work of Schwaller et al.[3] we augmented the training data with the addition of random SMILES and textbook reactions to the training set.

The forward prediction model can be used in two modes. First, when given a precursor set, the most likely products can be predicted. Second, when given a precursor set and a target product, the likelihood of this specific reaction can be estimated. In this work, we set the beam size of the forward model to 3.

As described previously, we use the forward chemical prediction model as a digital domain expert for evaluating the correctness of the predictions generated by the retrosynthetic model.

As recently published,[3] the accuracy of this model is higher than 90% when compared with a public data set. In order to calibrate the forward prediction model within the entire retrosynthetic framework, 50 random forward reaction predictions were analyzed by human experts. The assessment gave an accuracy of 78% which should be compared to an accuracy of 80% given by the trained model. Although the data set is too limited to claim any statistical relevance, this assessment offers strong evidence in favour of using the forward prediction model as a digital twin of human chemists.

## 3.2  Reaction classification model

To classify reactions, we used a data-driven reaction classification model[14] that was trained similarly to the Molecular Transformer forward and retrosynthetic model. It is characterized by four encoder layers and one decoder layer and trained using the same hyperparameters. The main difference is that the inputs were made up of the complete reaction string (precursors→products) and the outputs of the split reaction class identifier from NameRXN, consisting of three numbers corresponding to superclass, classes/categories and named reaction. More details on reaction classes can be found in.[15] The classification model used in this work matches the same class as the NameRXN tool[16] for 93.8% of the reactions.

## 3.3  Experiments on single-step retrosynthesis models

In Table 1 we show how different metrics develop during the training of the *stereo* retro model. After 100k time steps the round-trip accuracy and the coverage plateau and only a slight improvement of the invalid SMILES percentage can be observed, when training for longer.

Table 2 shows a comparison of models trained on different data sets and evaluated with the beam sizes 5, 10 and 20. The beam size defines how many precursor set suggestions output. The more data is used in the training set the less invalid SMILES the models tend to generate. As expected the coverage increases with larger beam sizes, while the round-trip

Table 1: Development of the round-trip accuracy, coverage and percentage of invalid SMILES during trainig of the retrosynthesis model, evaluated with a forward model trained on *stereo only*.

| Model | Beam | Total rxns | Round-trip accuracy | Coverage | Invalid SMILES |
|---|---|---|---|---|---|
| stereo only 10k | 10 | 100k | 56.9% | 87.4% | 4.03 % |
| stereo only 20k | 10 | 100k | 73.8% | 93.8% | 1.72 % |
| stereo only 50k | 10 | 100k | 78.7% | 95.0% | 0.81 % |
| stereo only 100k | 10 | 100k | 81.6% | 95.8% | 0.65 % |
| stereo only 150k | 10 | 100k | 81.3% | 95.8% | 0.62 % |
| stereo only 200k | 10 | 100k | 81.0% | 95.8% | 0.59 % |
| stereo only 250k | 10 | 100k | 81.5% | 95.9% | 0.58 % |

accuracy and the percentage of invalid SMILES worsen only slightly. *stereo only* means that the model was trained purely on the 1M reactions derived from the open USPTO dataset.[10,11] The *stereo* model was trained on the USPTO dataset and 800K textbook reactions from Nam & Kim.[13] For the *augmented* model we performed a SMILES data augmentation for the source molecules by using non canonical SMILES.[17] The target always consisted of canonical SMILES. In contrast to reaction prediction,[3] the augmentation seemed not to be beneficial in our retrosynthesis model training experiments.

Table 2: Evaluation of retrosynthesis models with different training data, evaluated on the same validation set with different beam sizes.

| Model | Beam | Total | Round-trip accuracy | Coverage | Invalid SMILES |
|---|---|---|---|---|---|
| stereo only | 5 | 50k | 82.4% | 93.5% | 0.57 % |
| stereo | 5 | 50k | 83.6% | 94.2% | 0.52 % |
| augmented | 5 | 50k | 81.8% | 94.0% | 0.43 % |
| stereo only | 10 | 100k | 81.5% | 95.9% | 0.59 % |
| stereo | 10 | 100k | 82.4% | 96.4% | 0.49 % |
| augmented | 10 | 100k | 80.7% | 96.2% | 0.42 % |
| stereo only | 20 | 200k | 79.8% | 97.1% | 0.65 % |
| stereo | 20 | 200k | 80.8% | 97.5% | 0.87 % |
| augmented | 20 | 200k | 78.9% | 97.5% | 0.49 % |

# 4 Synthesis routes

On the subsequent pages, the synthesis routes discussed in the main text are presented. The routes were predicted by the model (pistachio), which is openly available on the IBM RXN for Chemistry platform.[18] Figure 1 shows a screenshot of the results page for an example retrosynthesis route prediction.
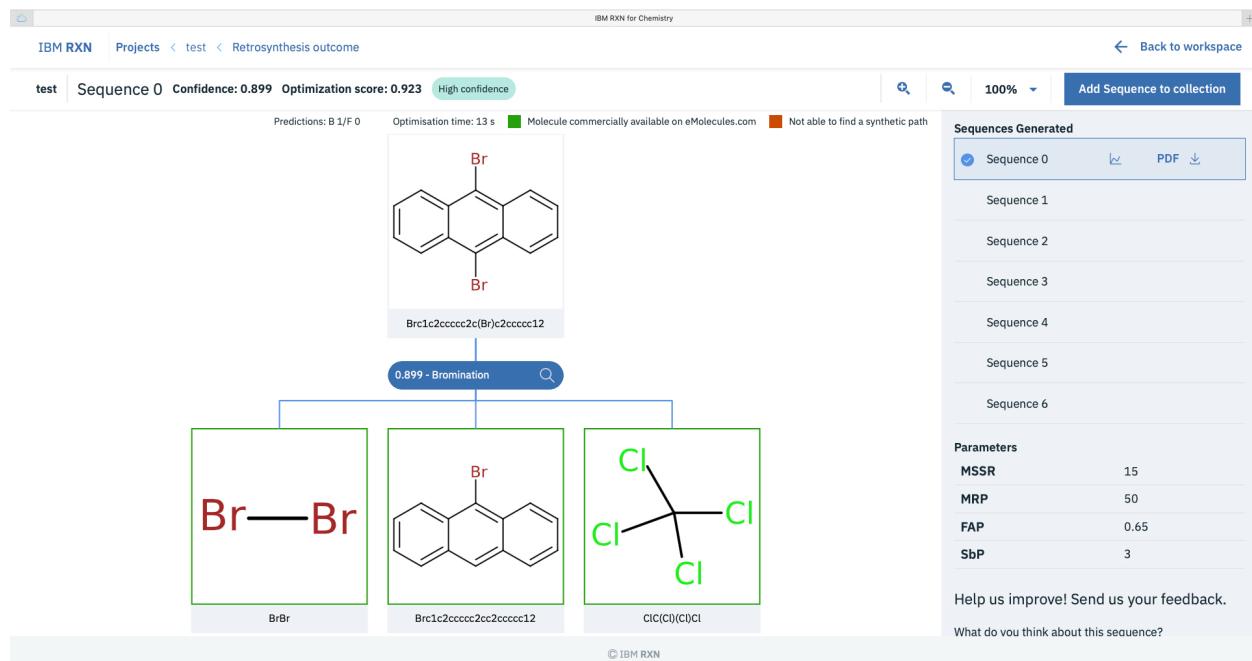


Figure 1: IBM RXN for Chemistry platform, retrosynthesis route prediction results view.

## 4.1 Index of generated retrosynthetic routes

The targets from Coley et al.[19] are extracted from: http://ibm.biz/Coley-Test, where corresponding retrosynthesis are also made available.

Both Segler Test-1 and Test-2 are instead from the supporting information:[20] http://ibm.biz/Segler-Test1-2 , with fully reported synthesis.

Here we list of the corresponding list of retrosynthetic routes generated by IBM RXN for Chemistry :

- S001-S006 : Molecule 1 (academic example)

- S007-S012 : Molecule 2 (academic example)

- S013-S014 : Molecule 3 (academic example)

- S015-S018 : Molecule 4 (academic example)

- S019-S027 : Molecule 5 (academic example)

- S028-S036 : Molecule 6 (academic example)

- S037-S046 : Molecule 7 (academic example)

- S047-S050 : Molecule 8 (academic example)

- S051-S059 : Molecule 9 (academic example)

- S060-S061 : Aspirin (Coley set)

- S062-S066 : Celecoxib (Coley set)

- S067-S073 : Diazepam (Coley set)

- S074-S077 : Lidocain (Coley set)

- S078-S079 : Quinapril (Coley set)

- S080-S084 : Safinamide (Coley set)

- S085-S086 : Secnidazole (Coley set)

- S087-S090 : (S)-warfarin (Coley set)

- S091-S092 : Molecule 1 - Test 1 (Segler set Test 1)

- S093-S095 : Molecule 2 - Test 1 (Segler set Test 1)

- S096-S098 : Molecule 3 - Test 1 (Segler set Test 1)

- S099-S112 : Molecule 4 - Test 1 (Segler set Test 1)

- S113-S128 : Molecule 5 - Test 1 (Segler set Test 1)

- S129-S134 : Molecule 6 - Test 1 (Segler set Test 1)

- S135-S142 : Molecule 7 - Test 1 (Segler set Test 1)

- S143-S148 : Molecule 8 - Test 1 (Segler set Test 1)

- S149-S151 : Molecule 9 - Test 1 (Segler set Test 1)

- S152-S153 : Molecule 1 - Test 2 (Segler set Test 2)

- S154-S156 : Molecule 2 - Test 2 (Segler set Test 2)

- S157-S160 : Molecule 3 - Test 2 (Segler set Test 2)

- S161-S162 : Molecule 4 - Test 2 (Segler set Test 2)

- S163-S169 : Molecule 5 - Test 2 (Segler set Test 2)

- S170-S171 : Molecule 6 - Test 2 (Segler set Test 2)

- S172-S184 : Molecule 7 - Test 2 (Segler set Test 2)

- S185-S187 : Molecule 8 - Test 2 (Segler set Test 2)

- S188-S190 : Molecule 9 - Test 2 (Segler set Test 2)

- S191-S193 : Molecule 10 - Test 2 (Segler set Test 2)

The last pages of the supporting information show three examples of failing retrosyntheses proposed by the stereo retrosynthesis model:

- S194-S195 : Example 1

- S196-S199 : Example 2

- S200-S201: Example 3

# References

(1) Coley, C. W.; Rogers, L.; Green, W. H.; Jensen, K. F. SCScore: Synthetic complexity learned from a reaction corpus. *Journal of chemical information and modeling* **2018**, *58*, 252–261.

(2) Schneider, N.; Stiefl, N.; Landrum, G. A. What's what: The (nearly) definitive guide to reaction role assignment. *Journal of chemical information and modeling* **2016**, *56*, 2336–2346.

(3) Schwaller, P.; Laino, T.; Gaudin, T.; Bolgar, P.; Hunter, C. A.; Bekas, C.; Lee, A. A. Molecular Transformer: A Model for Uncertainty-Calibrated Chemical Reaction Prediction. *ACS Central Science* **0**, *0*, null.

(4) Zheng, S.; Rao, J.; Zhang, Z.; Xu, J.; Yang, Y. Predicting Retrosynthetic Reaction using Self-Corrected Transformer Neural Networks. *arXiv preprint arXiv:1907.01356* **2019**,

(5) Karpov, P.; Godin, G.; Tetko, I. A Transformer Model for Retrosynthesis. **2019**,

(6) Lin, K.; Xu, Y.; Pei, J.; Lai, L. Automatic Retrosynthetic Pathway Planning Using Template-free Models. *arXiv preprint arXiv:1906.02308* **2019**,

(7) Lee, A. A.; Yang, Q.; Sresht, V.; Bolgar, P.; Hou, X.; Klug-McLeod, J. L.; Butler, C. R. Molecular Transformer unifies reaction prediction and retrosynthesis across pharma chemical space. *Chem. Commun.* **2019**, –.

(8) O'Boyle, N. M. Towards a Universal SMILES representation-A standard method to generate canonical SMILES based on the InChI. *Journal of cheminformatics* **2012**, *4*, 22.

(9) Liu, B.; Ramsundar, B.; Kawthekar, P.; Shi, J.; Gomes, J.; Luu Nguyen, Q.; Ho, S.;

Sloane, J.; Wender, P.; Pande, V. Retrosynthetic reaction prediction using neural sequence-to-sequence models. *ACS central science* **2017**, *3*, 1103–1113.

(10) Lowe, D. M. Extraction of Chemical Structures and Reactions from the Literature. Ph.D. thesis, University of Cambridge, 2012.

(11) Lowe, D. Chemical reactions from US patents (1976-Sep2016). **2017**,

(12) Nextmove Software Pistachio. `http://www.nextmovesoftware.com/pistachio.html`, (Accessed Jul 29, 2019).

(13) Nam, J.; Kim, J. Linking the neural machine translation and the prediction of organic chemistry reactions. *arXiv preprint arXiv:1612.09529* **2016**,

(14) Schwaller, P.; Vaucher, A.; Nair, V. H.; Laino, T. Data-Driven Chemical Reaction Classification with Attention-Based Neural Networks. **2019**,

(15) Schneider, N.; Lowe, D. M.; Sayle, R. A.; Tarselli, M. A.; Landrum, G. A. Big data from pharmaceutical patents: a computational analysis of medicinal chemists' bread and butter. *Journal of medicinal chemistry* **2016**, *59*, 4385–4402.

(16) Nextmove Software NameRXN. `http://www.nextmovesoftware.com/namerxn.html`, (Accessed Jul 29, 2019).

(17) Bjerrum, E. J. Smiles enumeration as data augmentation for neural network modeling of molecules. *arXiv preprint arXiv:1703.07076* **2017**,

(18) IBM RXN for Chemistry. `https://rxn.res.ibm.com`, (Accessed Oct 10, 2019).

(19) others,, et al. A robotic platform for flow synthesis of organic compounds informed by AI planning. *Science* **2019**, *365*, eaax1566.

(20) Segler, M. H. S.; Preuss, M.; Waller, M. P. Planning chemical syntheses with deep neural networks and symbolic AI. *Nature* **2018**, *555*, 604–610.
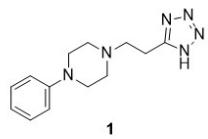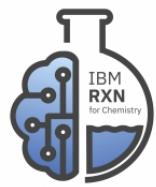
# Information about the retrosynthesis

Created On: 2019-09-27T10:22:21.359000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1C=CC(N2CCN(CCC3=NN=NN3)CC2)=CC=1
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1C=CC(N2CCN(CCC3=NN=NN3)CC2)=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.985

## *Step 1*

*Type: Tetrazole synthesis, Confidence: 0.991*
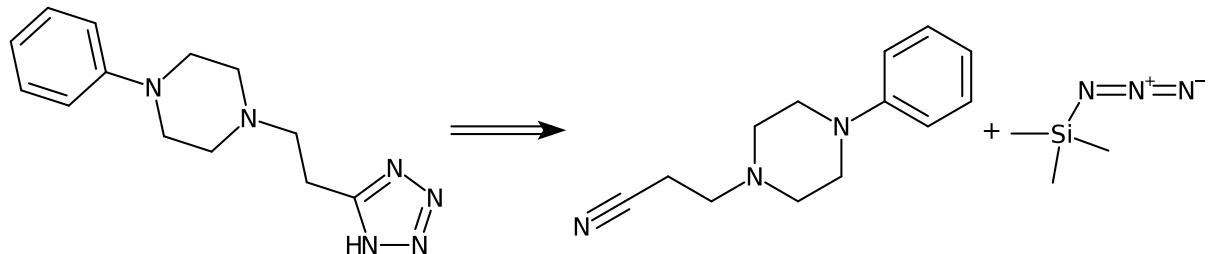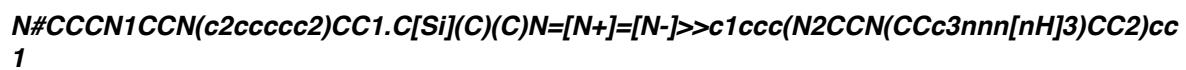
*N#CCCN1CCN(c2ccccc2)CC1.C[Si](C)(C)N=[N+]=[N-]>>c1ccc(N2CCN(CCc3nnn[nH]3)CC2)cc1*



## *Step 2*

*Type: Unrecognized, Confidence: 0.994*

*C=CC#N.Cc1ccccc1.c1ccc(N2CCNCC2)cc1>>N#CCCN1CCN(c2ccccc2)CC1*
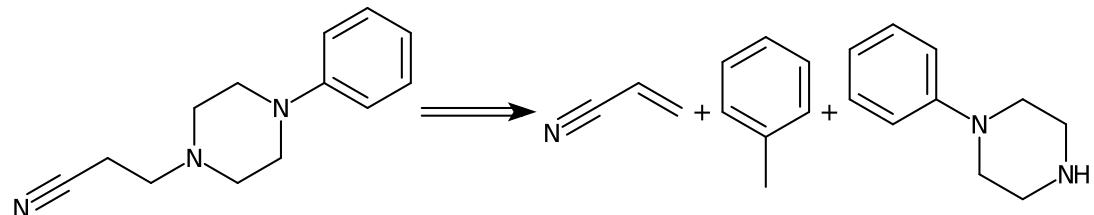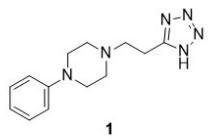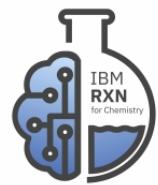
# Information about the retrosynthesis

Created On: 2019-09-27T10:22:21.359000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1C=CC(N2CCN(CCC3=NN=NN3)CC2)=CC=1
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1C=CC(N2CCN(CCC3=NN=NN3)CC2)=CC=1
Exclude substructures:

# Sequence 17, Confidence: 0.916

## Step 1

*Type: Tetrazole synthesis, Confidence: 0.991*

*N#CCCN1CCN(c2ccccc2)CC1.C[Si](C)(C)N=[N+]=[N-]>>c1ccc(N2CCN(CCc3nnn[nH]3)CC2)cc1*



## Step 2

*Type: Chloro N-alkylation, Confidence: 0.939*

*N#CCCCl.c1ccc(N2CCNCC2)cc1>>N#CCCN1CCN(c2ccccc2)CC1*
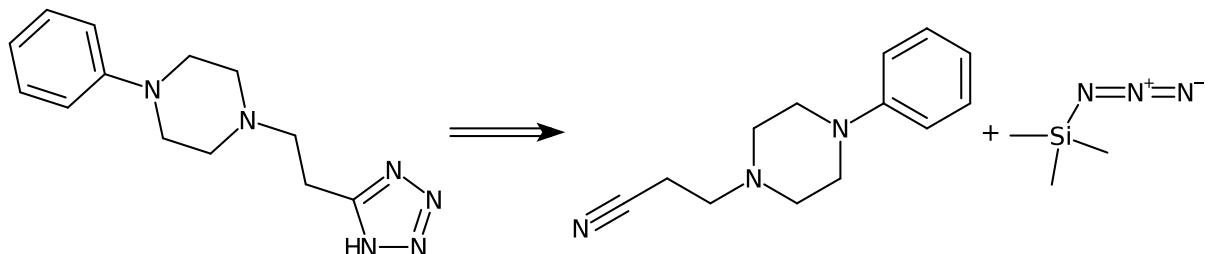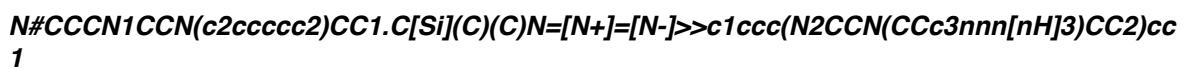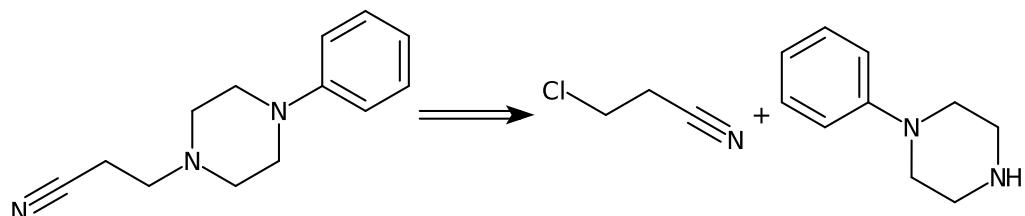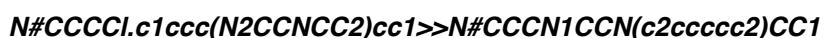


## Step 3

*Type: Hydroxy to chloro, Confidence: 0.984*
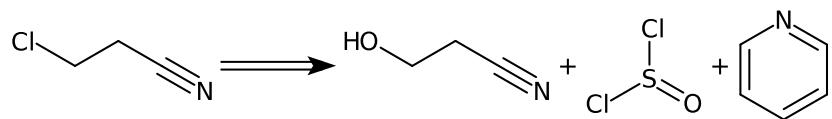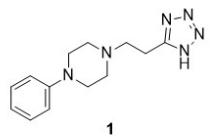
*N#CCCO.O=S(Cl)Cl.c1ccncc1>>N#CCCCl*

1

# Information about the retrosynthesis

Created On: 2019-09-27T10:22:21.359000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1C=CC(N2CCN(CCC3=NN=NN3)CC2)=CC=1
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1C=CC(N2CCN(CCC3=NN=NN3)CC2)=CC=1
Exclude substructures:

# Sequence 22, Confidence: 0.868

## *Step 1*

*Type: Tetrazole synthesis, Confidence: 0.991*

*N#CCCN1CCN(c2ccccc2)CC1.C[Si](C)(C)N=[N+]=[N-]>>c1ccc(N2CCN(CCc3nnn[nH]3)CC2)cc1*



## *Step 2*

*Type: Chloro N-alkylation, Confidence: 0.939*

*N#CCCCl.c1ccc(N2CCNCC2)cc1>>N#CCCN1CCN(c2ccccc2)CC1*
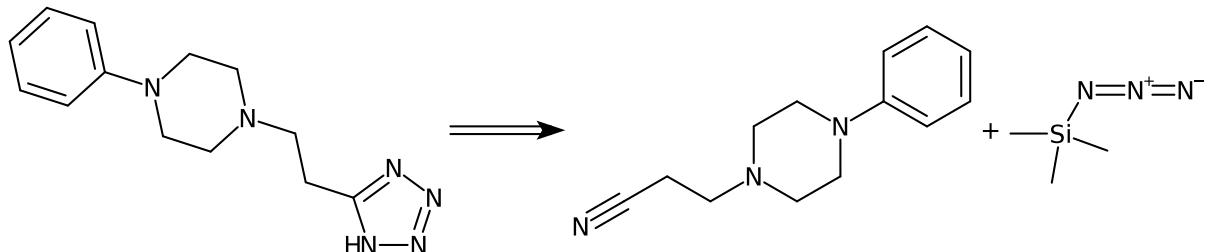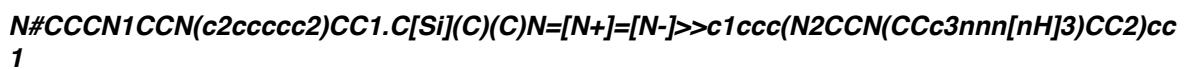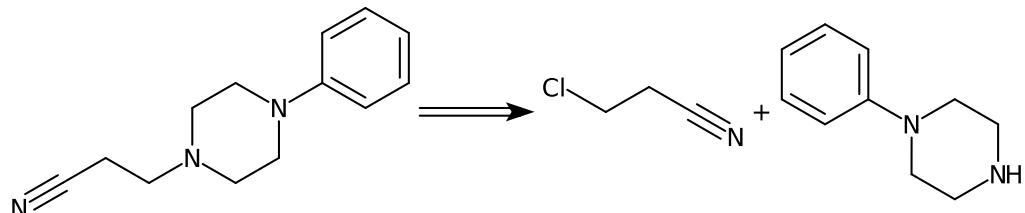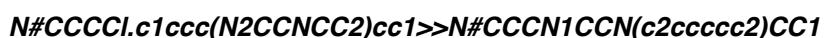


## *Step 3*

*Type: Carbamoyl to cyano, Confidence: 0.933*
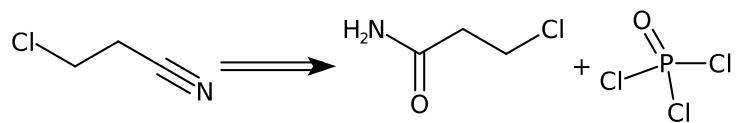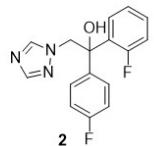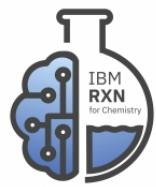
*NC(=O)CCCl.O=P(Cl)(Cl)Cl>>N#CCCCl*

# Information about the retrosynthesis

Created On: 2019-09-27T09:50:56.131000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: OC(C1C(F)=CC=CC=1)(C1C=CC(F)=CC=1)CN1N=CN=C1
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: OC(C1C(F)=CC=CC=1)(C1C=CC(F)=CC=1)CN1N=CN=C1
Exclude substructures:

# Sequence 0, Confidence: 0.88

## Step 1

*Type: Bromo Grignard reaction, Confidence: 0.965*

**O=C(Cn1cncn1)c1ccccc1F.C1CCOC1.Fc1ccc([Mg]Br)cc1>>OC(Cn1cncn1)(c1ccc(F)cc1)c1ccccc1F**
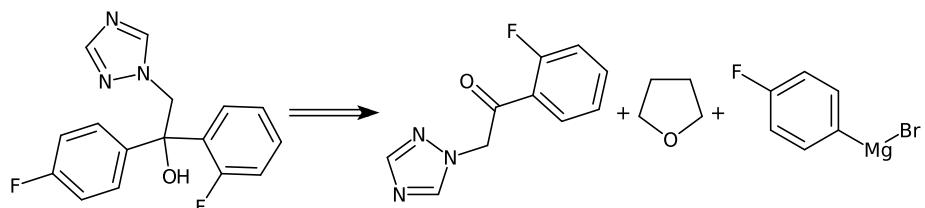


## Step 2

*Type: Bromo N-alkylation, Confidence: 0.912*
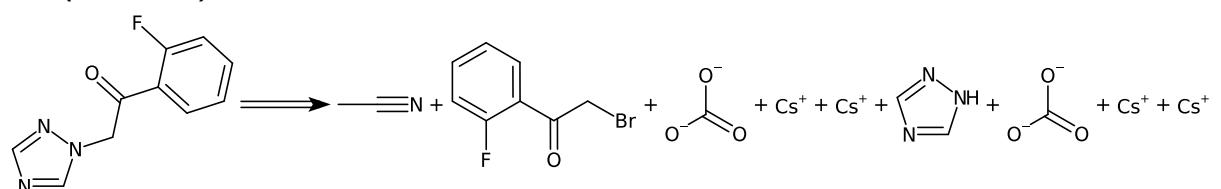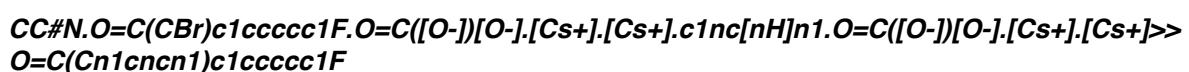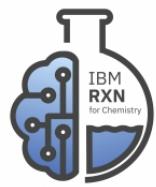
**CC#N.O=C(CBr)c1ccccc1F.O=C([O-])[O-].[Cs+].[Cs+].c1nc[nH]n1.O=C([O-])[O-].[Cs+].[Cs+]>>O=C(Cn1cncn1)c1ccccc1F**

# Information about the retrosynthesis

Created On: 2019-09-27T09:50:56.131000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: OC(C1C(F)=CC=CC=1)(C1C=CC(F)=CC=1)CN1N=CN=C1
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: OC(C1C(F)=CC=CC=1)(C1C=CC(F)=CC=1)CN1N=CN=C1
Exclude substructures:

## Sequence 5, Confidence: 0.845

### Step 1

*Type: Epoxide + amine coupling, Confidence: 0.95*

*Fc1ccc(C2(c3ccccc3F)CO2)cc1.c1nc[nH]n1>>OC(Cn1cncn1)(c1ccc(F)cc1)c1ccccc1F*
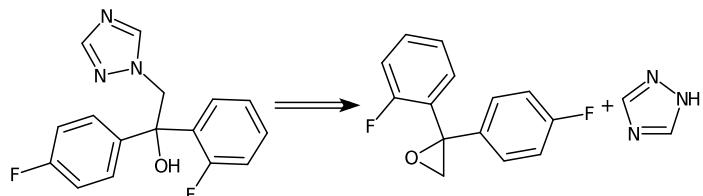


### Step 2

*Type: Johnson-Corey-Chaykovsky epoxidation, Confidence: 0.889*
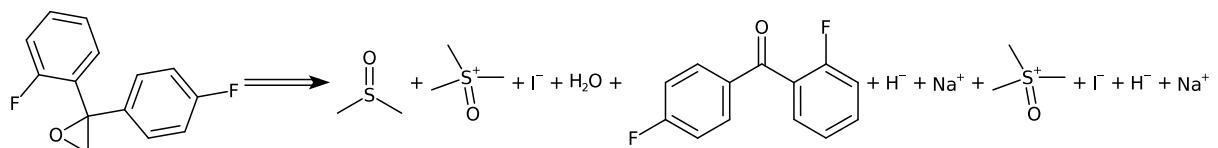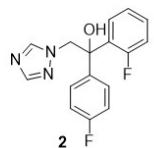
*CS(C)=O.C[S+](C)(C)=O.[I-].O.O=C(c1ccc(F)cc1)c1ccccc1F.[H-].[Na+].C[S+](C)(C)=O.[I-].[H-].[Na+]>>Fc1ccc(C2(c3ccccc3F)CO2)cc1*

# Information about the retrosynthesis

Created On: 2019-09-27T09:50:56.131000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: OC(C1C(F)=CC=CC=1)(C1C=CC(F)=CC=1)CN1N=CN=C1
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: OC(C1C(F)=CC=CC=1)(C1C=CC(F)=CC=1)CN1N=CN=C1
Exclude substructures:

# Sequence 23, Confidence: 0.759

## Step 1

*Type: Epoxide + amine coupling, Confidence: 0.95*

*Fc1ccc(C2(c3ccccc3F)CO2)cc1.c1nc[nH]n1>>OC(Cn1cncn1)(c1ccc(F)cc1)c1ccccc1F*
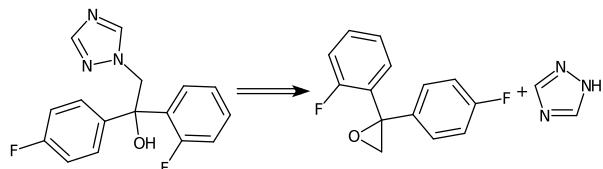


## Step 2

*Type: Prilezhaev epoxidation, Confidence: 0.815*
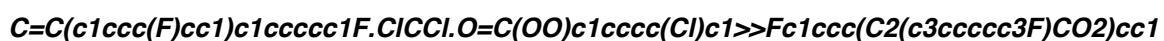
*C=C(c1ccc(F)cc1)c1ccccc1F.ClCCl.O=C(OO)c1cccc(Cl)c1>>Fc1ccc(C2(c3ccccc3F)CO2)cc1*



## Step 3

*Type: Wittig olefination, Confidence: 0.98*

*C1CCOC1.C[P+](c1ccccc1)(c1ccccc1)c1ccccc1.[Br-].O=C(c1ccc(F)cc1)c1ccccc1F.[Li]CCCC.*
*C[P+](c1ccccc1)(c1ccccc1)c1ccccc1.[Br-]>>C=C(c1ccc(F)cc1)c1ccccc1F*

**3**
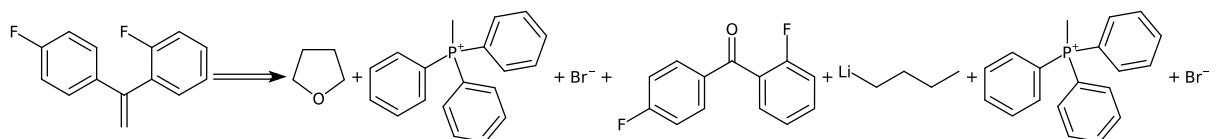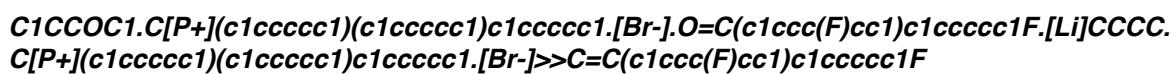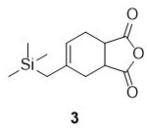
# Information about the retrosynthesis

Created On: 2019-09-27T15:37:32.099000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1C(C[Si](C)(C)C)=CCC2C(=O)OC(=O)C12
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1C(C[Si](C)(C)C)=CCC2C(=O)OC(=O)C12
Exclude substructures:

# Sequence 0, Confidence: 0.214

## Step 1

*Type: Diels-Alder cycloaddition, Confidence: 0.362*

*C=CC(=C)C[Si](C)(C)C.O=C1C=CC(=O)O1>>C[Si](C)(C)CC1=CCC2C(=O)OC(=O)C2C1*
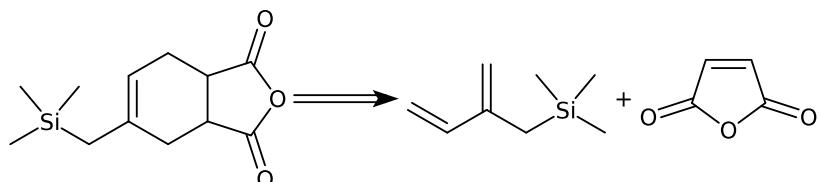
## Step 2

*Type: Wittig olefination, Confidence: 0.719*

*C=CC(=O)C[Si](C)(C)C.C1CCOC1.C[P+](c1ccccc1)(c1ccccc1)c1ccccc1.[Br-].[Li]CCCC>>C=CC(=C)C[Si](C)(C)C*
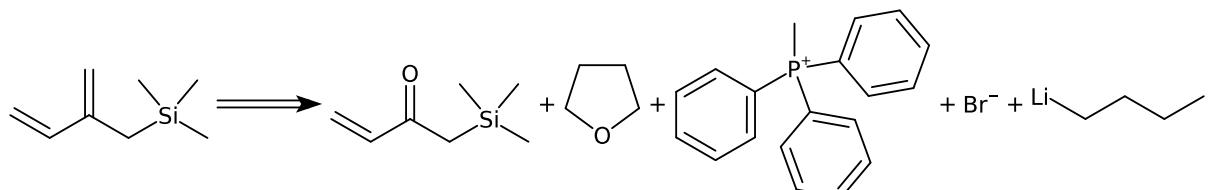
## Step 3

*Type: Weinreb ketone synthesis, Confidence: 0.857*

*CON(C)C(=O)C[Si](C)(C)C.C=C[Mg]Br.CCOCC>>C=CC(=O)C[Si](C)(C)C*

## Step 4

*Type: Weinreb amide synthesis, Confidence: 0.96*

*CNOC.Cl.C[Si](C)(C)CC(=O)O.CNOC.Cl>>CON(C)C(=O)C[Si](C)(C)C*
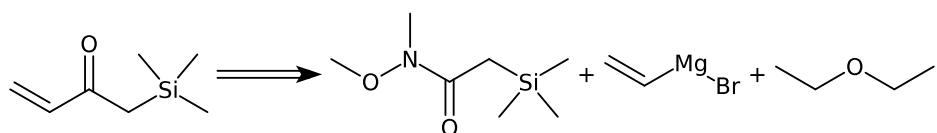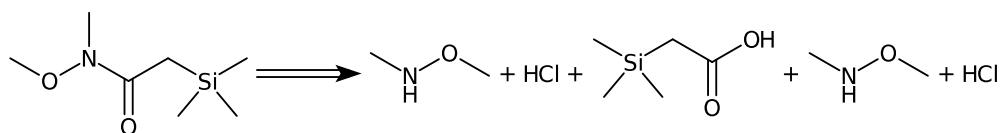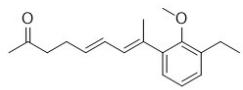
**4**

## Information about the retrosynthesis

Created On: 2019-09-27T09:41:56.899000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC(=O)CC/C=C/C=C(/C1=CC=CC(CC)=C1OC)\C
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: CC(=O)CC/C=C/C=C(/C1=CC=CC(CC)=C1OC)\C
Exclude substructures:

# Sequence 0, Confidence: 0.398

## Step 1

*Type: Ketone dioxolane deprotection, Confidence: 0.963*
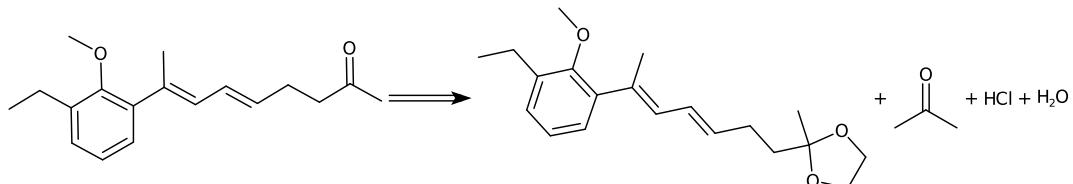
*CCc1cccc(/C(C)=C/C=C/CCC2(C)OCCO2)c1OC.CC(C)=O.Cl.O>>CCc1cccc(/C(C)=C/C=C/CCC(C)=O)c1OC*



## Step 2

*Type: Horner-Wadsworth-Emmons reaction, Confidence: 0.915*

*CC1(CCC=O)OCCO1.CCc1cccc(/C(C)=C/CP(=O)(OC)OC)c1OC.C1CCOC1.[H-].[Na+]>>CCc1cccc(/C(C)=C/C=C/CCC2(C)OCCO2)c1OC*



## Step 3

*Type: Aldehyde Collins oxidation, Confidence: 0.983*

*CC1(CCCO)OCCO1.ClCCl.O=[Cr](=O)([O-])Cl.c1cc[nH+]cc1.O=[Cr](=O)([O-])Cl.c1cc[nH+]cc1>>CC1(CCC=O)OCCO1*
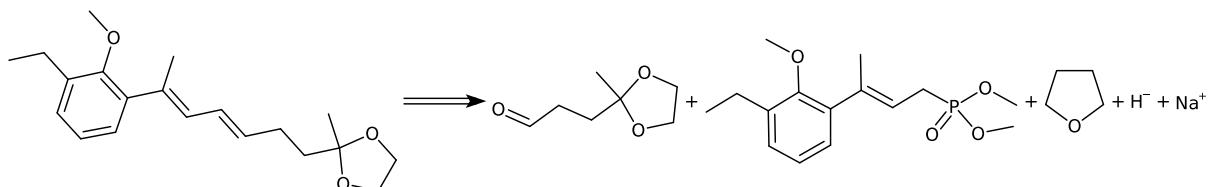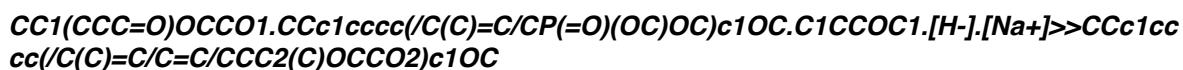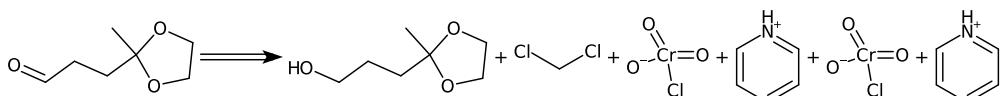


*Type: Michaelis-Arbuzov reaction, Confidence: 0.944*

*CCc1cccc(/C(C)=C/CCl)c1OC.C1CCOC1.COP(OC)OC>>CCc1cccc(/C(C)=C/CP(=O)(OC)OC)c1OC*
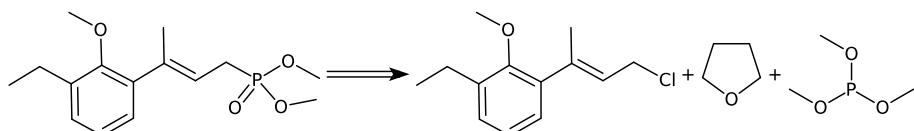


## Step 4

*Type: Hydroxy to chloro, Confidence: 0.971*

*CCc1cccc(/C(C)=C/CO)c1OC.ClCCl.O=S(Cl)Cl.c1ccncc1>>CCc1cccc(/C(C)=C/CCl)c1OC*
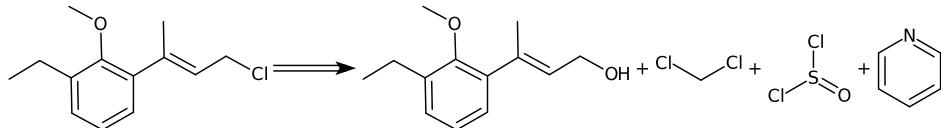


## Step 5

*Type: Aldehyde to alcohol reduction, Confidence: 0.94*

*CCc1cccc(/C(C)=C/C=O)c1OC.CO.[BH4-].[Na+]>>CCc1cccc(/C(C)=C/CO)c1OC*
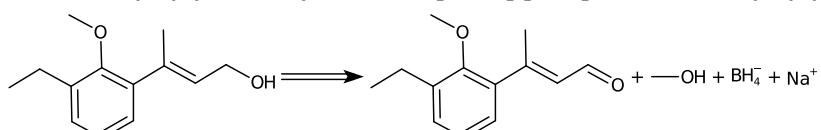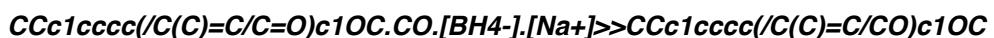


## Step 6

*Type: Cyano to formyl, Confidence: 0.92*
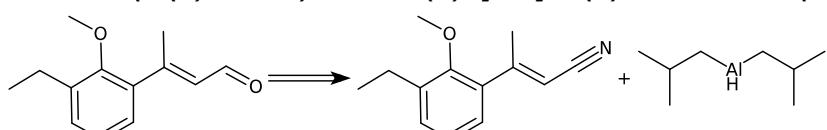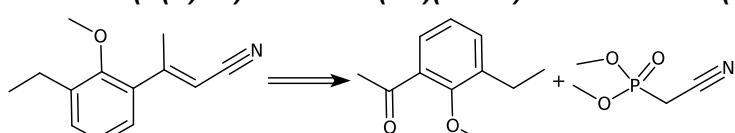
*CCc1cccc(/C(C)=C/C#N)c1OC.CC(C)C[AlH]CC(C)C>>CCc1cccc(/C(C)=C/C=O)c1OC*



## Step 7

*Type: Horner-Wadsworth-Emmons reaction, Confidence: 0.625*

*CCc1cccc(C(C)=O)c1OC.COP(=O)(CC#N)OC>>CCc1cccc(/C(C)=C/C#N)c1OC*



## Step 8

*Type: Alcohol to ketone oxidation, Confidence: 0.964*

*CCc1cccc(C(C)O)c1OC.ClCCl.O=[Mn]=O>>CCc1cccc(C(C)=O)c1OC*

## Step 9

*Type: Bromo Grignard reaction, Confidence: 0.99*

*CCc1cccc(C=O)c1OC.C[Mg+].[Br-]>>CCc1cccc(C(C)O)c1OC*
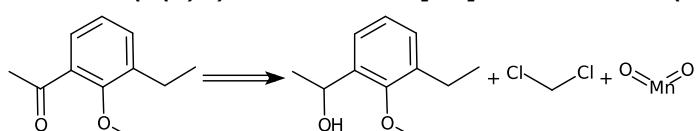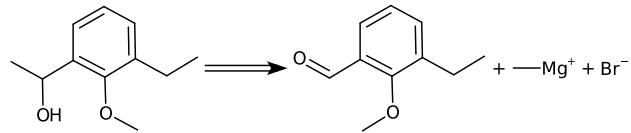


## Step 10

*Type: Hydroxy to methoxy, Confidence: 0.972*

*C1CCOC1.CCc1cccc(C=O)c1O.CI.[H-].[Na+].[H-].[Na+]>>CCc1cccc(C=O)c1OC*

**5**
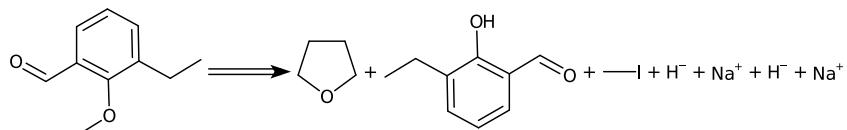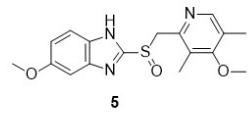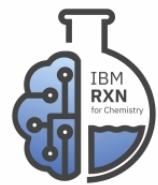
# Information about the retrosynthesis

Created On: 2019-10-01T14:57:31.373000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C(CS(=O)C1NC2=CC=C(OC)C=C2N=1)1=C(C)C(OC)=C(C)C=N1
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C(CS(=O)C1NC2=CC=C(OC)C=C2N=1)1=C(C)C(OC)=C(C)C=N1
Exclude substructures:

# Sequence 0, Confidence: 0.949

## *Step 1*

*Type: Sulfanyl to sulfinyl, Confidence: 0.949*

*CC(=O)O.COc1ccc2[nH]c(SCc3ncc(C)c(OC)c3C)nc2c1.OO>>COc1ccc2[nH]c(S(=O)Cc3ncc(C)c(OC)c3C)nc2c1*

**5**
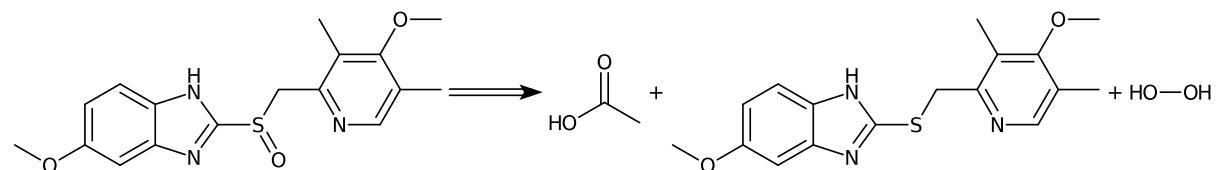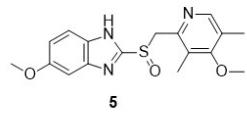
# Information about the retrosynthesis

Created On: 2019-10-01T15:01:50.922000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C(CS(=O)C1NC2=CC=C(OC)C=C2N=1)1=C(C)C(OC)=C(C)C=N1
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: C(CS(=O)C1NC2=CC=C(OC)C=C2N=1)1=C(C)C(OC)=C(C)C=N1
Exclude substructures:

# Sequence 0, Confidence: 0.579

Metadata:
Warnings: The retrosynthesis did not complete. Try increasing MSSR.

## Step 1

*Type: Sulfanyl to sulfinyl, Confidence: 0.943*

*COc1ccc2nc(SCc3ncc(C)c(OC)c3C)[nH]c2c1.ClCCl.O=C(OO)c1cccc(Cl)c1>>COc1ccc2[nH]c(S(=O)Cc3ncc(C)c(OC)c3C)nc2c1*
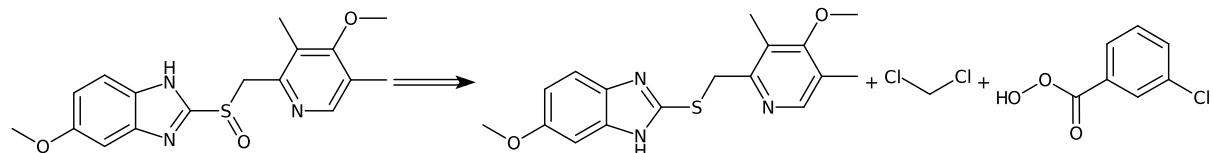
## Step 2

*Type: Thioether synthesis, Confidence: 0.947*

*COc1c(C)cnc(CBr)c1C.COc1ccc2nc(S)[nH]c2c1.CN(C)C=O.O=C([O-])[O-].[K+].[K+]>>COc1ccc2nc(SCc3ncc(C)c(OC)c3C)[nH]c2c1*
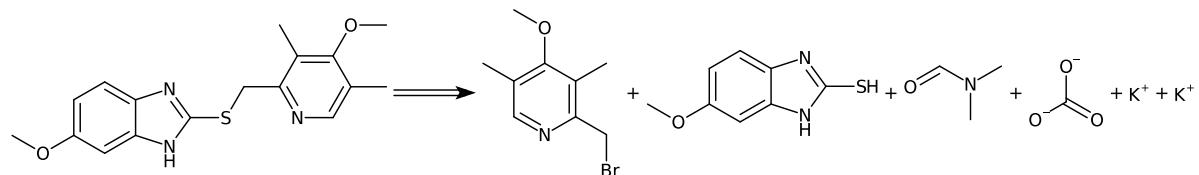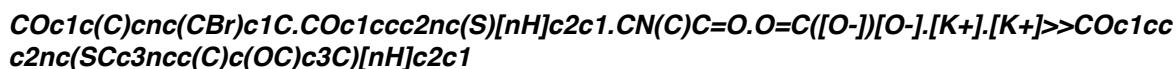
## Step 3

*Type: Appel bromination, Confidence: 0.981*
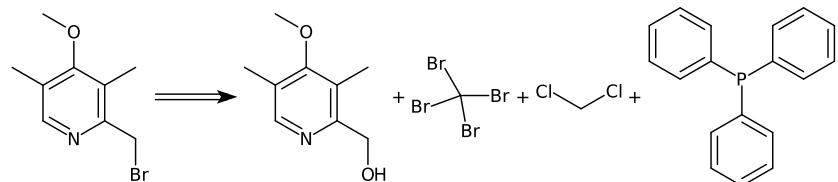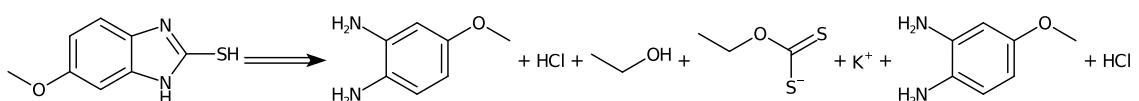
*COc1c(C)cnc(CO)c1C.BrC(Br)(Br)Br.ClCCl.c1ccc(P(c2ccccc2)c2ccccc2)cc1>>COc1c(C)cnc(CBr)c1C*

*Type: Unrecognized, Confidence: 0.968*

*COc1ccc(N)c(N)c1.Cl.CCO.CCOC(=S)[S-].[K+].COc1ccc(N)c(N)c1.Cl>>COc1ccc2nc(S)[nH]c2c1*

## Step 4

*Type: Ester to alcohol reduction, Confidence: 0.988*

*CCOC(=O)c1ncc(C)c(OC)c1C.C1CCOC1.[BH4-].[Li+]>>COc1c(C)cnc(CO)c1C*



*Type: Undefined, Confidence: 0.0*

*COc1ccc(N)c(N)c1.Cl>>COc1ccc(N)c(N)c1.Cl*



## Step 5

*Type: Fischer-Speier esterification, Confidence: 0.981*

*COc1c(C)cnc(C(=O)O)c1C.CCO.O=S(=O)(O)O>>CCOC(=O)c1ncc(C)c(OC)c1C*
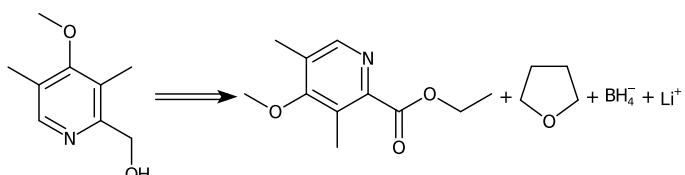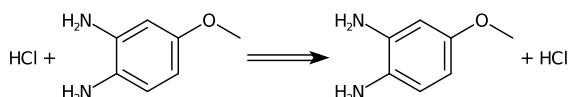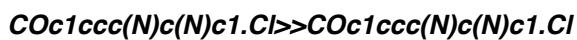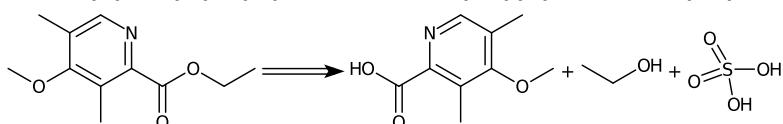


## Step 6

*Type: CO2H-Me deprotection, Confidence: 0.976*

*COC(=O)c1ncc(C)c(OC)c1C.CO.Cl.O.[Na+].[OH-]>>COc1c(C)cnc(C(=O)O)c1C*
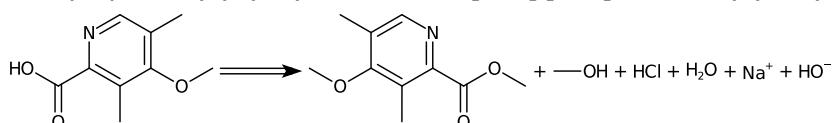


## Step 7

*Type: Pinner reaction, Confidence: 0.959*

*COc1c(C)cnc(C#N)c1C.CO.O=S(=O)(O)O>>COC(=O)c1ncc(C)c(OC)c1C*
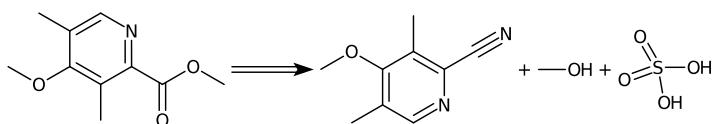
## Step 8

*Type: Unrecognized, Confidence: 0.966*

*COc1c(C)c[n+]([O-])cc1C.CN(C)C(=O)Cl.C[Si](C)(C)C#N.ClCCl>>COc1c(C)cnc(C#N)c1C*
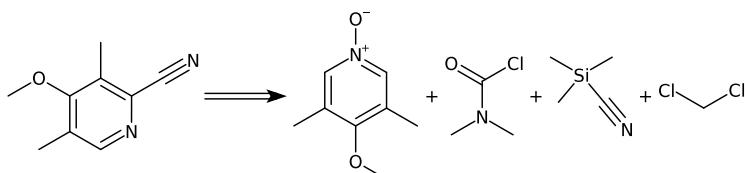


## Step 9

*Type: Unrecognized, Confidence: 0.94*

*Cc1c[n+]([O-])cc(C)c1[N+](=O)[O-].CO.C[O-].[Na+]>>COc1c(C)c[n+]([O-])cc1C*
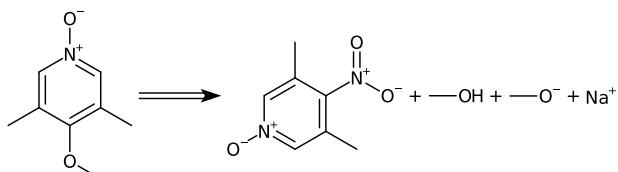


## Step 10

*Type: Nitration, Confidence: 0.955*

*Cc1cc(C)c[n+]([O-])c1.O=S(=O)(O)O.O=[N+]([O-])O.[Na+].[OH-]>>Cc1c[n+]([O-])cc(C)c1[N+](=O)[O-]*
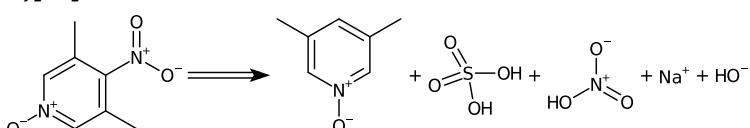


## Step 11

*Type: Nitrogen oxidation, Confidence: 0.901*

*Cc1cncc(C)c1.ClCCl.O=C(OO)c1cccc(Cl)c1>>Cc1cc(C)c[n+]([O-])c1*
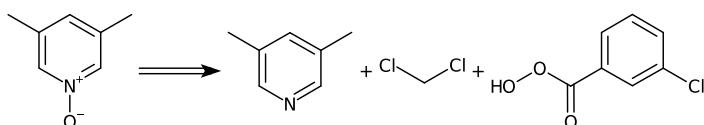


## Step 12

*Type: Aldehyde to alkane reduction, Confidence: 0.985*

*Cc1cncc(C=O)c1.NN.O.OCCOCCO.[K+].[OH-]>>Cc1cncc(C)c1*
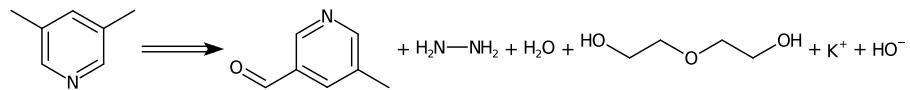


## Step 13

*Type: Alcohol to aldehyde oxidation, Confidence: 0.993*

*Cc1cncc(CO)c1.O=[Mn]=O>>Cc1cncc(C=O)c1*



## Step 14

*Type: Ester to alcohol reduction, Confidence: 0.991*
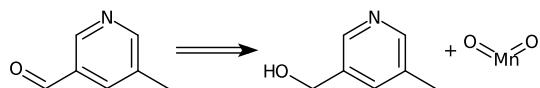
*COC(=O)c1cncc(C)c1.C1CCOC1.[BH4-].[Li+]>>Cc1cncc(CO)c1*



## Step 15

*Type: Fischer-Speier esterification, Confidence: 0.993*

*Cc1cncc(C(=O)O)c1.CO.O=C([O-])O.[Na+].O=S(=O)(O)O>>COC(=O)c1cncc(C)c1*

**5**
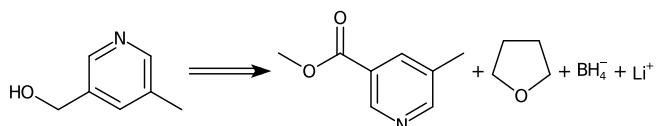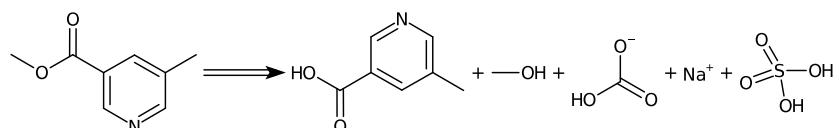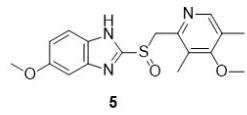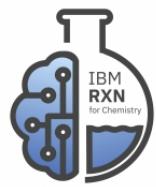
# Information about the retrosynthesis

Created On: 2019-10-01T20:33:01.477000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: N1=CC(C(=O)O)=CC(C)=C1
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: N1=CC(C(=O)O)=CC(C)=C1
Exclude substructures:

# Sequence 0, Confidence: 0.743

## Step 1

*Type: Bromo to carboxy, Confidence: 0.949*

*Cc1cncc(Br)c1.C1CCOC1.O=C=O.[Li]CCCC>>Cc1cncc(C(=O)O)c1*
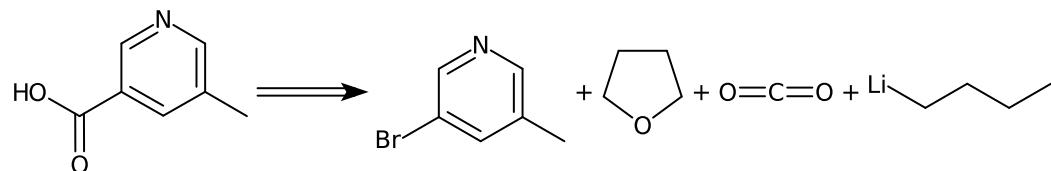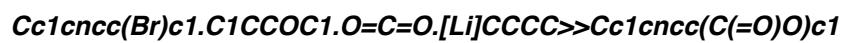


## Step 2

*Type: Wurtz-Fittig coupling, Confidence: 0.783*

*Brc1cncc(Br)c1.C1CCOC1.CCCCCC.Cl.[Li]CCCC>>Cc1cncc(Br)c1*
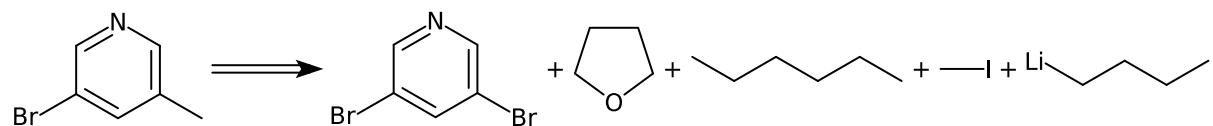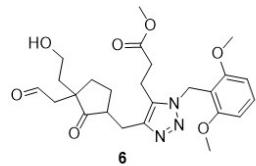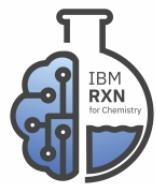
# Information about the retrosynthesis

Created On: 2019-09-27T07:41:29.805000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: COC(CCC1N(CC2C(OC)=CC=CC=2OC)N=NC=1CC1C(=O)C(CC=O)(CO)CC1)=O
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
COC(CCC1N(CC2C(OC)=CC=CC=2OC)N=NC=1CC1C(=O)C(CC=O)(CO)CC1)=O
Exclude substructures:

# Sequence 0, Confidence: 0.216

Metadata:
Warnings: 'UNFINISHED MESSAGE'

## *Step 1*

*Type: Ozonolysis, Confidence: 0.592*
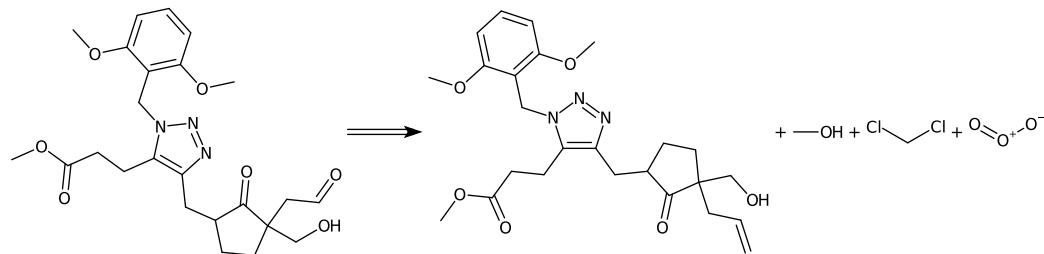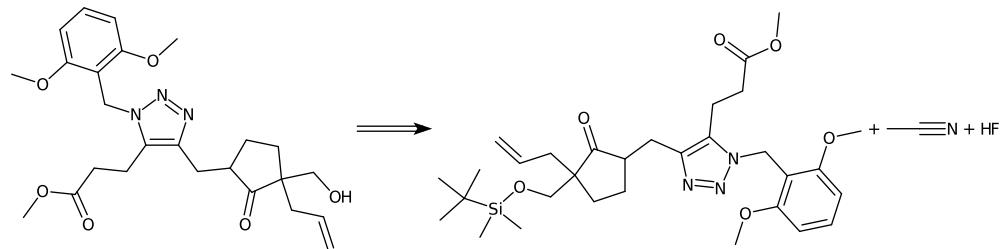
**C=CCC1(CO)CCC(Cc2nnn(Cc3c(OC)cccc3OC)c2CCC(=O)OC)C1=O.CO.ClCCl.O=[O+][O-]>>C
OC(=O)CCc1c(CC2CCC(CO)(CC=O)C2=O)nnn1Cc1c(OC)cccc1OC**



## *Step 2*

*Type: O-TBS deprotection, Confidence: 0.937*

**C=CCC1(CO[Si](C)(C)C(C)(C)C)CCC(Cc2nnn(Cc3c(OC)cccc3OC)c2CCC(=O)OC)C1=O.CC#N.
F>>C=CCC1(CO)CCC(Cc2nnn(Cc3c(OC)cccc3OC)c2CCC(=O)OC)C1=O**



## *Step 3*

*Type: Unrecognized, Confidence: 0.922*

**C=CCC1(CO[Si](C)(C)C(C)(C)C)CCCC1=O.COC(=O)CCc1c(Cl)nnn1Cc1c(OC)cccc1OC.C1CCO
C1.CC(C)[N-]C(C)C.[Li+]>>C=CCC1(CO[Si](C)(C)C(C)(C)C)CCC(Cc2nnn(Cc3c(OC)cccc3OC)c
2CCC(=O)OC)C1=O**

## Step 4

*Type: O-TBS protection, Confidence: 0.963*

*C=CCC1(CO)CCCC1=O.CC(C)(C)[Si](C)(C)Cl.CN(C)c1ccncc1.ClCCl>>C=CCC1(CO[Si](C)(C)C(C)(C)C)CCCC1=O*
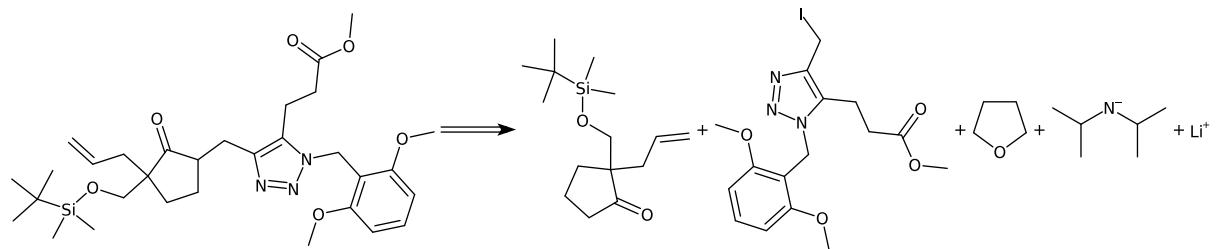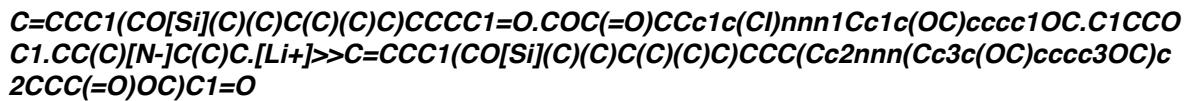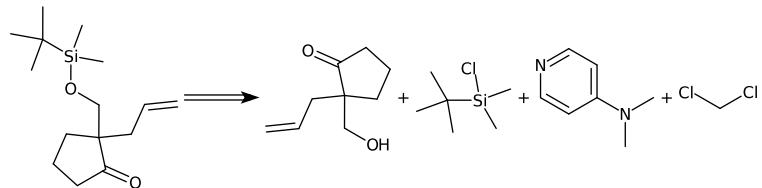


*Type: Chloro to iodo Finkelstein reaction, Confidence: 0.955*

*COC(=O)CCc1c(CCl)nnn1Cc1c(OC)cccc1OC.CC(C)=O.[I-].[Na+]>>COC(=O)CCc1c(CI)nnn1Cc1c(OC)cccc1OC*
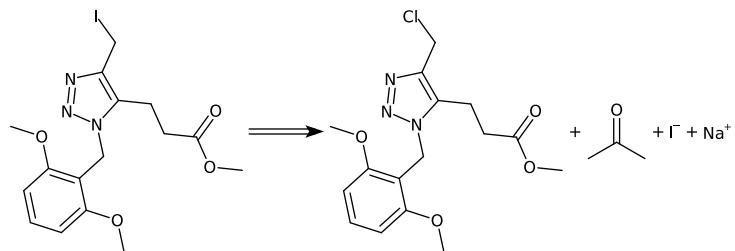


## Step 5

*Type: Ketone dioxolane deprotection, Confidence: 0.782*
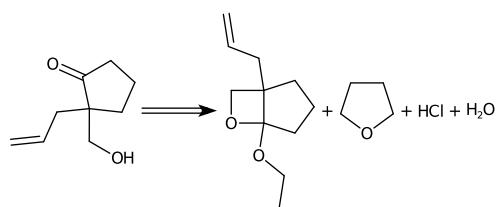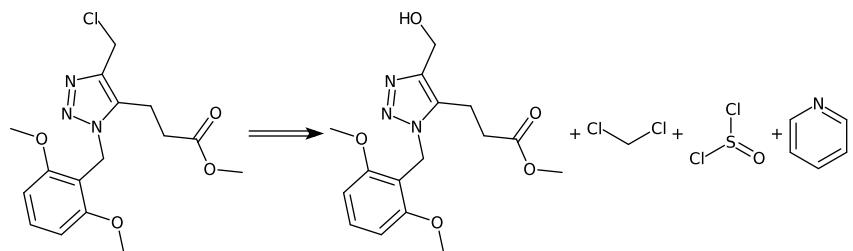
*C=CCC12CCCC1(OCC)OC2.C1CCOC1.Cl.O>>C=CCC1(CO)CCCC1=O*



*Type: Hydroxy to chloro, Confidence: 0.962*

*COC(=O)CCc1c(CO)nnn1Cc1c(OC)cccc1OC.ClCCl.O=S(Cl)Cl.c1ccncc1>>COC(=O)CCc1c(CCl)nnn1Cc1c(OC)cccc1OC*

## Step 6

*Type: Undefined, Confidence: 0.0*

*C=CCC12CCCC1(OCC)OC2>>C=CCC12CCCC1(OCC)OC2*



*Type: Alkene hydrogenation, Confidence: 0.788*

*COC(=O)/C=C/c1c(CO)nnn1Cc1c(OC)cccc1OC.[Pd]>>COC(=O)CCc1c(CO)nnn1Cc1c(OC)cccc1OC*
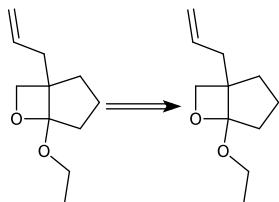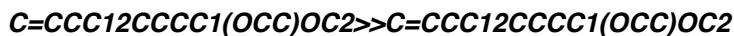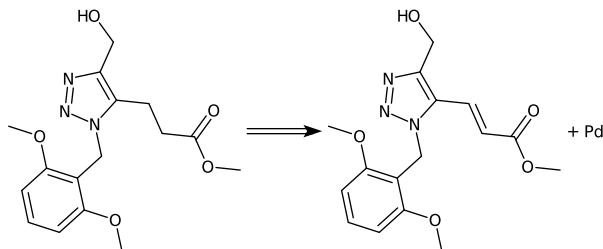


## Step 7

*Type: O-TBS deprotection, Confidence: 0.952*

*COC(=O)/C=C/c1c(CO[Si](C)(C)C(C)(C)C)nnn1Cc1c(OC)cccc1OC.C1CCOC1.CCCC[N+](CCCC)(CCCC)CCCC.[F-]>>COC(=O)/C=C/c1c(CO)nnn1Cc1c(OC)cccc1OC*
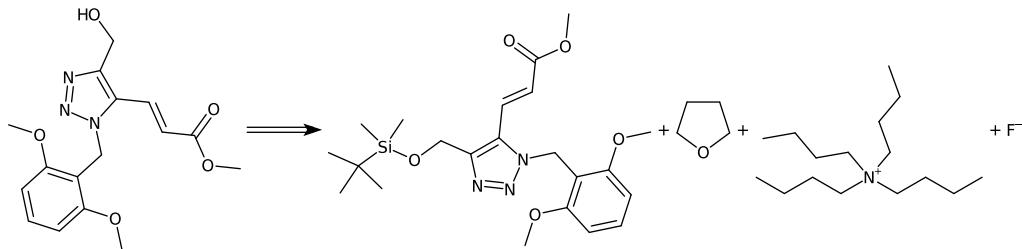


## Step 8

*Type: Horner-Wadsworth-Emmons reaction, Confidence: 0.878*

*COc1cccc(OC)c1Cn1nnc(CO[Si](C)(C)C(C)(C)C)c1C=O.COC(=O)CP(=O)(OC)OC.[NaH]>>COC(=O)/C=C/c1c(CO[Si](C)(C)C(C)(C)C)nnn1Cc1c(OC)cccc1OC*
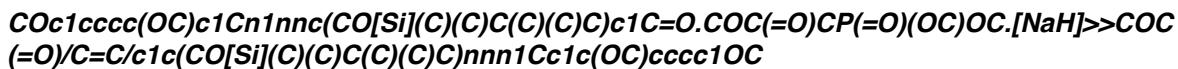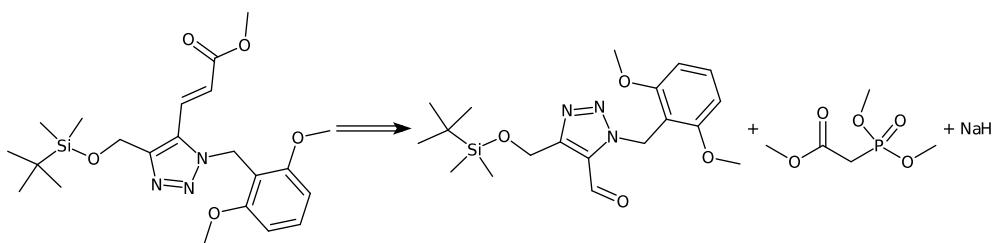
## Step 9

*Type: Alcohol to aldehyde oxidation, Confidence: 0.961*

*COc1cccc(OC)c1Cn1nnc(CO[Si](C)(C)C(C)(C)C)c1CO.ClCCl.O=[Mn]=O>>COc1cccc(OC)c1Cn1nnc(CO[Si](C)(C)C(C)(C)C)c1C=O*
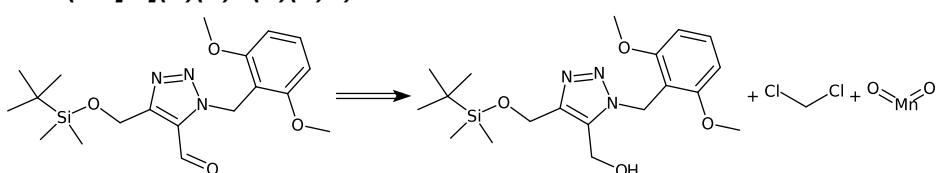


## Step 10

*Type: Ester to alcohol reduction, Confidence: 0.963*

*COC(=O)c1c(CO[Si](C)(C)C(C)(C)C)nnn1Cc1c(OC)cccc1OC.[BH4-].[Li+]>>COc1cccc(OC)c1Cn1nnc(CO[Si](C)(C)C(C)(C)C)c1CO*

**6**
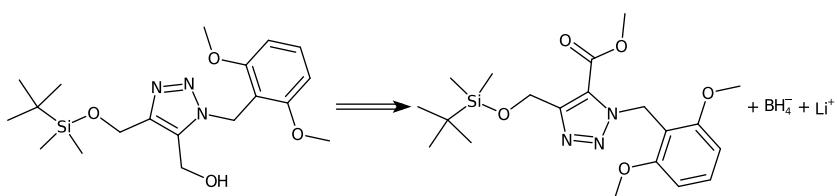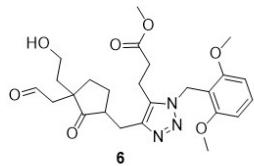
# Information about the retrosynthesis

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Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: COC(CCC1N(CC2C(OC)=CC=CC=2OC)N=NC=1CC1C(=O)C(CC=O)(CO)CC1)=O
MSSR: 15
FAP: 0.6
MRP: 20
SbP: 3
Available smiles:
Exclude smiles:
COC(CCC1N(CC2C(OC)=CC=CC=2OC)N=NC=1CC1C(=O)C(CC=O)(CO)CC1)=O
Exclude substructures:

# Sequence 0, Confidence: 0.204

## *Step 1*

*Type: Ozonolysis, Confidence: 0.592*
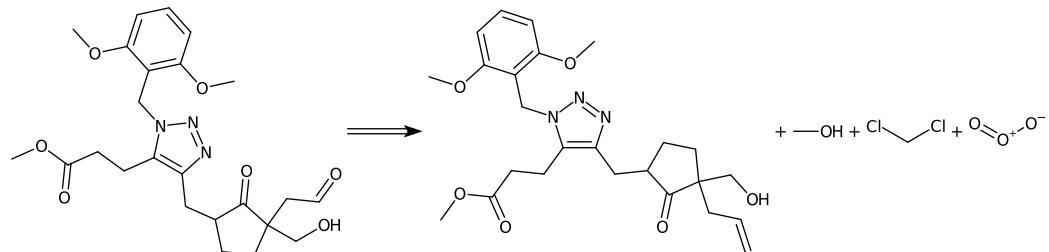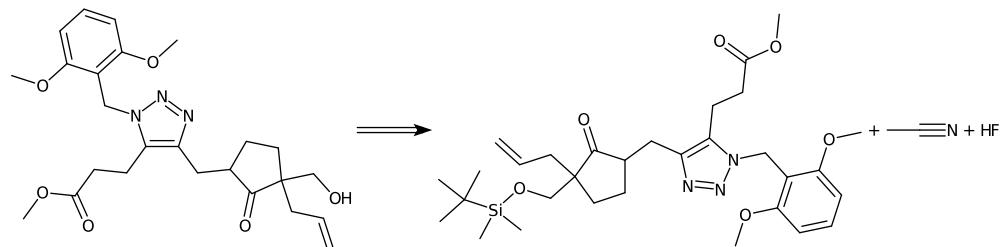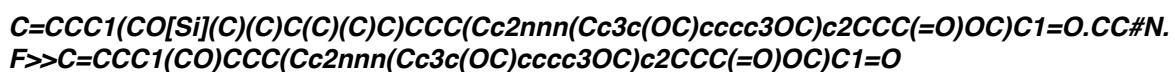
**C=CCC1(CO)CCC(Cc2nnn(Cc3c(OC)cccc3OC)c2CCC(=O)OC)C1=O.CO.ClCCl.O=[O+][O-]>>C OC(=O)CCc1c(CC2CCC(CO)(CC=O)C2=O)nnn1Cc1c(OC)cccc1OC**



## *Step 2*

*Type: O-TBS deprotection, Confidence: 0.937*

**C=CCC1(CO[Si](C)(C)C(C)(C)C)CCC(Cc2nnn(Cc3c(OC)cccc3OC)c2CCC(=O)OC)C1=O.CC#N. F>>C=CCC1(CO)CCC(Cc2nnn(Cc3c(OC)cccc3OC)c2CCC(=O)OC)C1=O**



## *Step 3*

*Type: Unrecognized, Confidence: 0.91*

**C=CCC1(CO[Si](C)(C)C(C)(C)C)CCCC1=O.COC(=O)CCc1c(CBr)nnn1Cc1c(OC)cccc1OC.C1C COC1.CC(C)[N-]C(C)C.[Li+]>>C=CCC1(CO[Si](C)(C)C(C)(C)C)CCC(Cc2nnn(Cc3c(OC)cccc3O C)c2CCC(=O)OC)C1=O**



## *Step 4*

*Type: O-TBS protection, Confidence: 0.963*

*C=CCC1(CO)CCCC1=O.CC(C)(C)[Si](C)(C)Cl.CN(C)c1ccncc1.ClCCl>>C=CCC1(CO[Si](C)(C)C(C)(C)C)CCCC1=O*
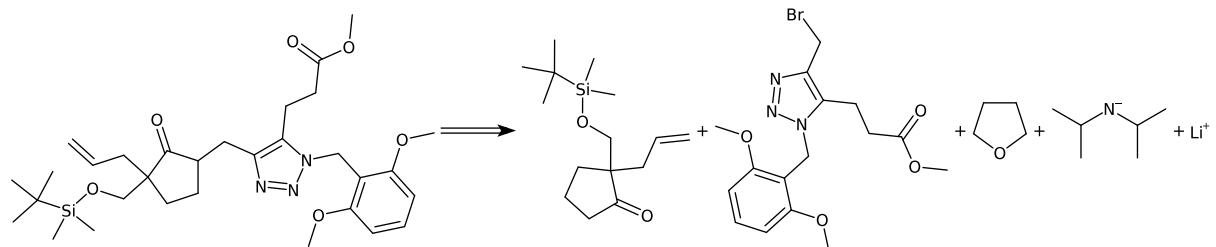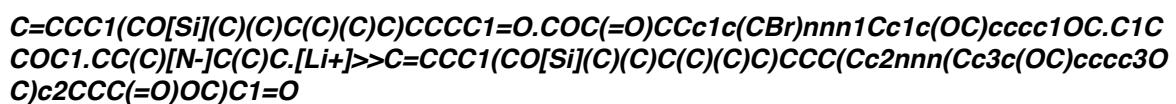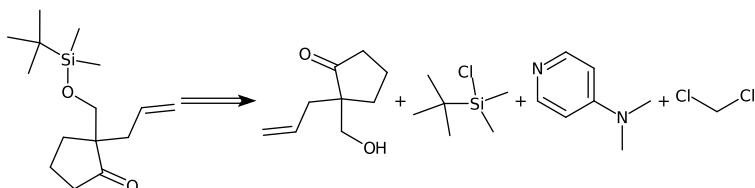


*Type: Wohl-Ziegler bromination, Confidence: 0.953*

*COC(=O)CCc1c(C)nnn1Cc1c(OC)cccc1OC.ClC(Cl)(Cl)Cl.O=C(OOC(=O)c1ccccc1)c1ccccc1.O=C1CCC(=O)N1Br>>COC(=O)CCc1c(CBr)nnn1Cc1c(OC)cccc1OC*



## Step 5

*Type: O-Ac deprotection, Confidence: 0.905*

*C=CCC1(COC(C)=O)CCCC1=O.CO.O=C([O-])[O-].[K+].[K+]>>C=CCC1(CO)CCCC1=O*
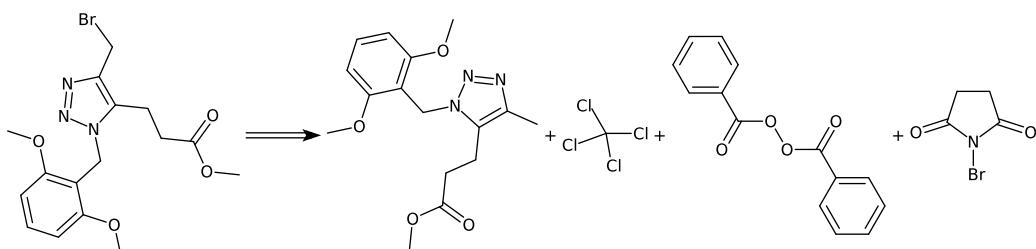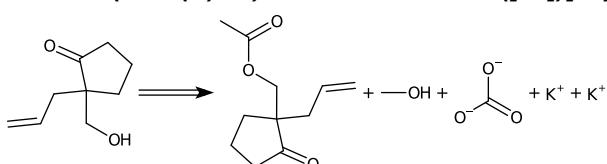


*Type: Azide-alkyne Huisgen cycloaddition, Confidence: 0.8*
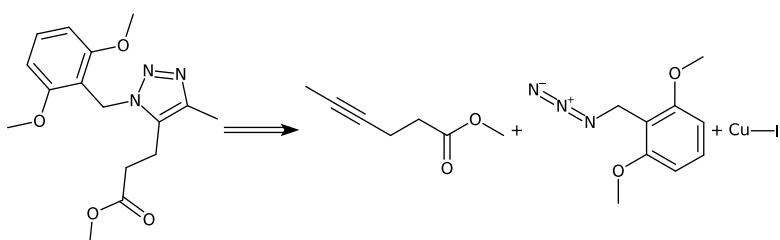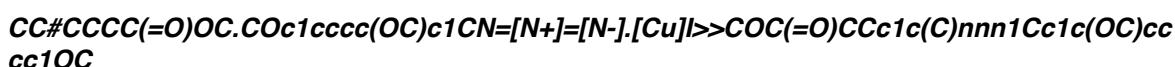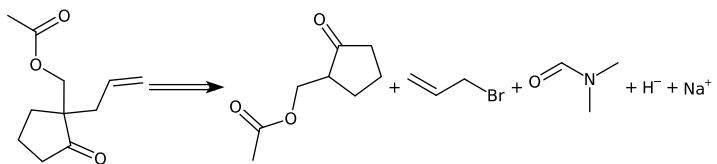
*CC#CCCC(=O)OC.COc1cccc(OC)c1CN=[N+]=[N-].[Cu]I>>COC(=O)CCc1c(C)nnn1Cc1c(OC)cccc1OC*



## Step 6

*Type: Unrecognized, Confidence: 0.639*

*CC(=O)OCC1CCCC1=O.C=CCBr.CN(C)C=O.[H-].[Na+]>>C=CCC1(COC(C)=O)CCCC1=O*



## Step 7

*Type: O-Ac protection, Confidence: 0.949*

*CC(=O)OC(C)=O.Cl.O=C1CCCC1CO.c1ccncc1>>CC(=O)OCC1CCCC1=O*
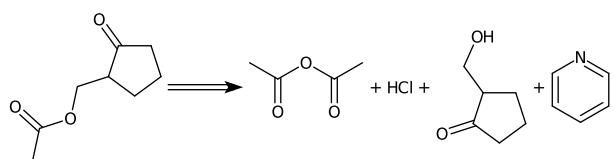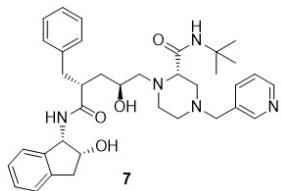
# Information about the retrosynthesis

Created On: 2019-09-27T07:36:16.955000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: O[C@H](CN1[C@H](C(NC(C)(C)C)=O)CN(CC2C=NC=CC=2)CC1)C[C@H](C(N[C@@H]1[C@H](O)CC2C1=CC=CC=2)=O)CC1C=CC=CC=1
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: O[C@H](CN1[C@H](C(NC(C)(C)C)=O)CN(CC2C=NC=CC=2)CC1)C[C@H](C(N[C@@H]1[C@H](O)CC2C1=CC=CC=2)=O)CC1C=CC=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.938

## *Step 1*

*Type: Aldehyde reductive amination, Confidence: 0.938*
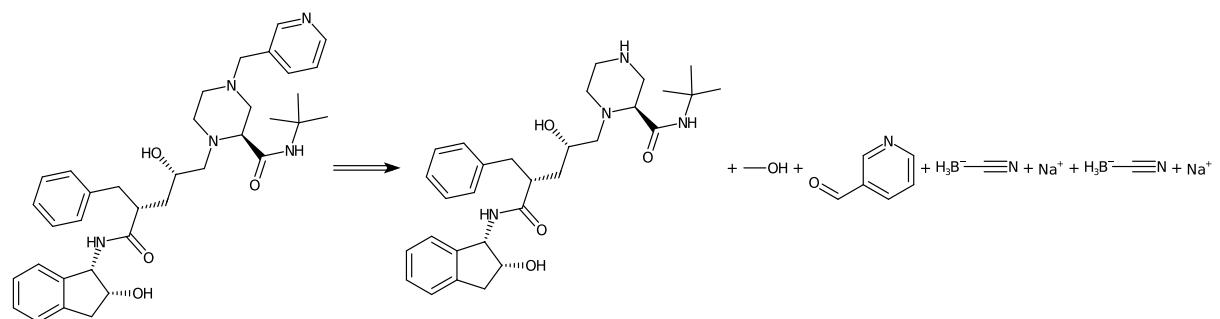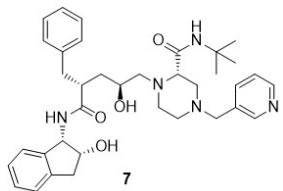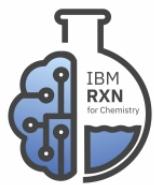
*CC(C)(C)NC(=O)[C@@H]1CNCCN1C[C@@H](O)C[C@@H](Cc1ccccc1)C(=O)N[C@H]1c2cccc c2C[C@H]1O.CO.O=Cc1cccnc1.[BH3-]C#N.[Na+].[BH3-]C#N.[Na+]>>CC(C)(C)NC(=O)[C@@H ]1CN(Cc2cccnc2)CCN1C[C@@H](O)C[C@@H](Cc1ccccc1)C(=O)N[C@H]1c2ccccc2C[C@H]1 O*

# Information about the retrosynthesis

Created On: 2019-09-27T07:36:16.955000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: O[C@H](CN1[C@H](C(NC(C)(C)C)=O)CN(CC2C=NC=CC=2)CC1)C[C@H](C(N[C@@H]1[C@H](O)CC2C1=CC=CC=2)=O)CC1C=CC=CC=1
MSSR: 10
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: O[C@H](CN1[C@H](C(NC(C)(C)C)=O)CN(CC2C=NC=CC=2)CC1)C[C@H](C(N[C@@H]1[C@H](O)CC2C1=CC=CC=2)=O)CC1C=CC=CC=1
Exclude substructures:

# Sequence 5, Confidence: 0.377

Metadata:
Warnings: 'UNFINISHED MESSAGE'

## Step 1

### Type: Epoxide + amine coupling, Confidence: 0.869
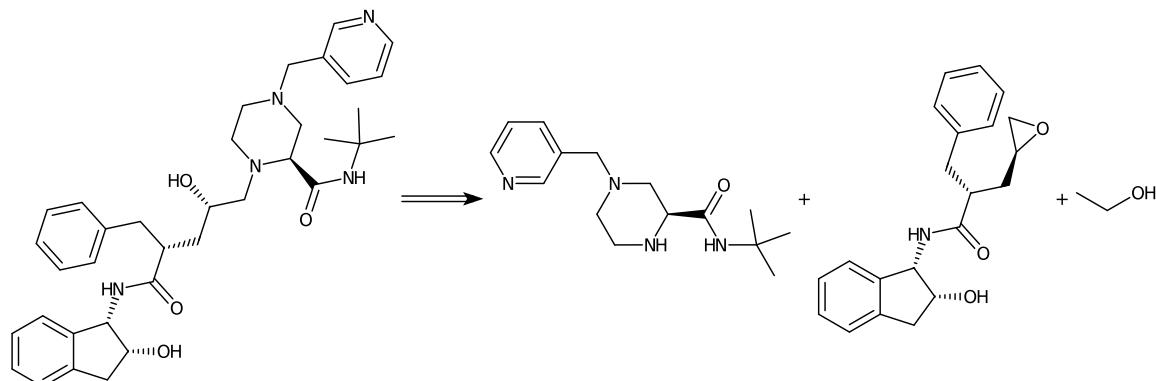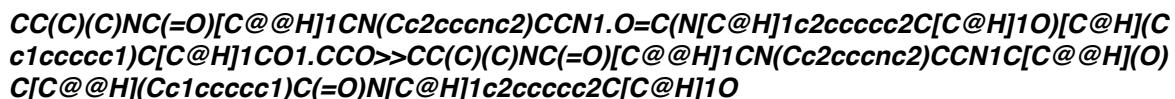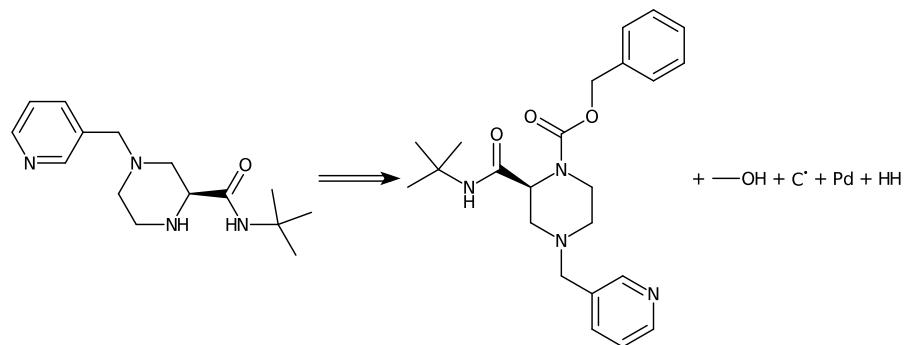
*CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1.O=C(N[C@H]1c2ccccc2C[C@H]1O)[C@H](Cc1ccccc1)C[C@H]1CO1.CCO>>CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C[C@@H](O)C[C@@H](Cc1ccccc1)C(=O)N[C@H]1c2ccccc2C[C@H]1O*



## Step 2

### Type: N-Cbz deprotection, Confidence: 0.935

*CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C(=O)OCc1ccccc1.CO.[C].[Pd].[HH]>>CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1*



### Type: Undefined, Confidence: 0.0

*O=C(N[C@H]1c2ccccc2C[C@H]1O)[C@H](Cc1ccccc1)C[C@H]1CO1>>O=C(N[C@H]1c2ccccc2C[C@H]1O)[C@H](Cc1ccccc1)C[C@H]1CO1*

## Step 3

*Type: Carboxylic acid + amine condensation, Confidence: 0.92*

*O=C(O)[C@@H]1CN(Cc2cccnc2)CCN1C(=O)OCc1ccccc1.CC(C)(C)N>>CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C(=O)OCc1ccccc1*
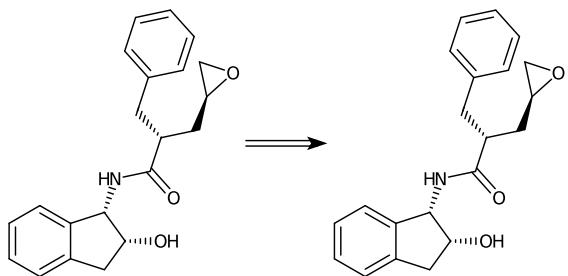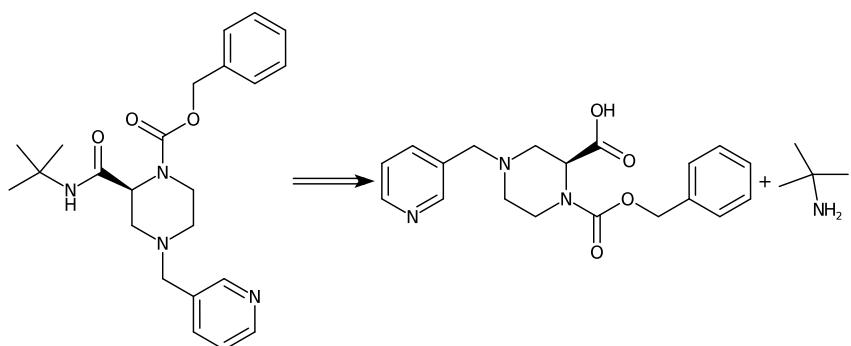


## Step 4

*Type: CO2H-Et deprotection, Confidence: 0.954*
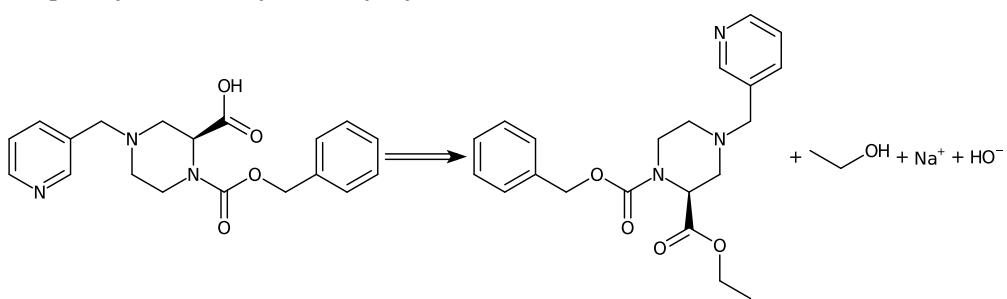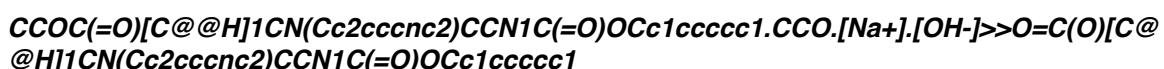
*CCOC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C(=O)OCc1ccccc1.CCO.[Na+].[OH-]>>O=C(O)[C@@H]1CN(Cc2cccnc2)CCN1C(=O)OCc1ccccc1*



## Step 5

*Type: Aldehyde reductive amination, Confidence: 0.923*

*CCOC(=O)[C@@H]1CNCCN1C(=O)OCc1ccccc1.CC(=O)O[BH-](OC(C)=O)OC(C)=O.[Na+].ClCCl.O=Cc1cccnc1>>CCOC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C(=O)OCc1ccccc1*

## Step 6

**Type: N-Boc deprotection, Confidence: 0.871**
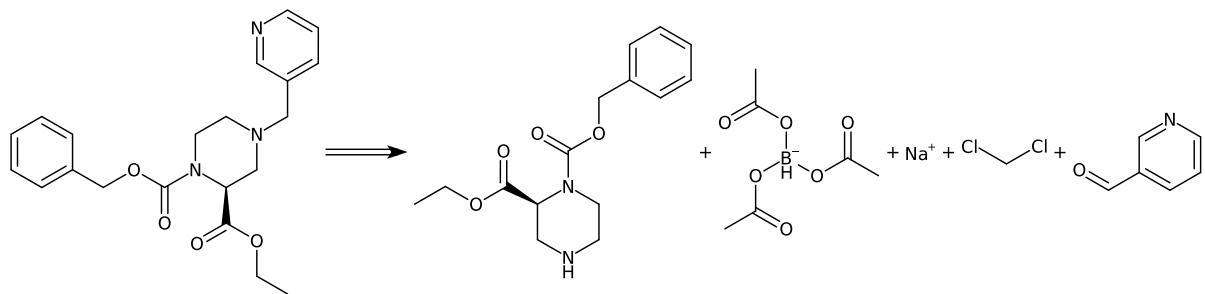
*CCOC(=O)[C@@H]1CN(C(=O)OC(C)(C)C)CCN1C(=O)OCc1ccccc1.O=C(O)C(F)(F)F>>CCOC(=O)[C@@H]1CNCCN1C(=O)OCc1ccccc1*



## Step 7

**Type: Amide Schotten-Baumann, Confidence: 0.94**

*CCOC(=O)[C@@H]1CN(C(=O)OC(C)(C)C)CCN1.CCN(C(C)C)C(C)C.ClCCl.O=C(Cl)OCc1ccccc1>>CCOC(=O)[C@@H]1CN(C(=O)OC(C)(C)C)CCN1C(=O)OCc1ccccc1*
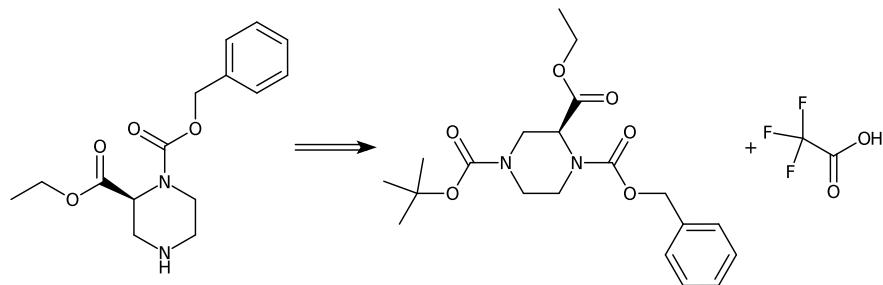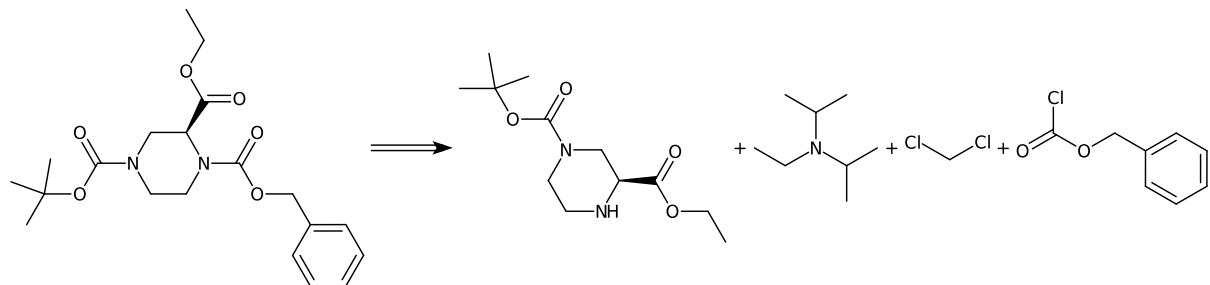


## Step 8

**Type: N-Boc protection, Confidence: 0.842**

*CCOC(=O)[C@@H]1CNCCN1.CC(C)(C)OC(=O)OC(=O)OC(C)(C)C.CCN(CC)CC.ClCCl>>CCOC(=O)[C@@H]1CN(C(=O)OC(C)(C)C)CCN1*
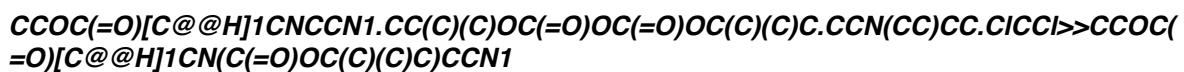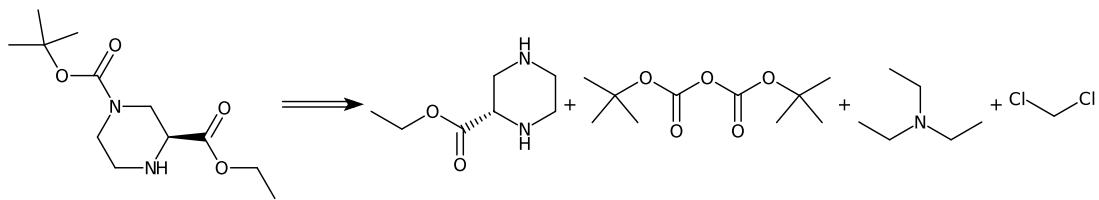
## Step 9

**Type: N-Bn deprotection, Confidence: 0.89**

*CCOC(=O)[C@@H]1CN(Cc2ccccc2)CCN1Cc1ccccc1.CCO.[HH].[Pd]>>CCOC(=O)[C@@H]1CNCCN1*
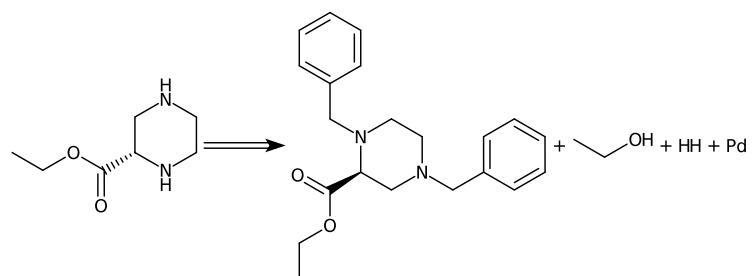


## Step 10

**Type: Fischer-Speier esterification, Confidence: 0.933**

*O=C(O)[C@@H]1CN(Cc2ccccc2)CCN1Cc1ccccc1.CCO.O=C([O-])O.[Na+].O=S(=O)(O)O>>CCOC(=O)[C@@H]1CN(Cc2ccccc2)CCN1Cc1ccccc1*
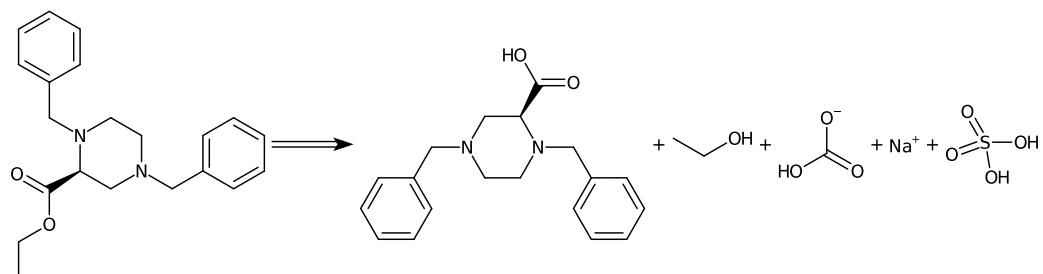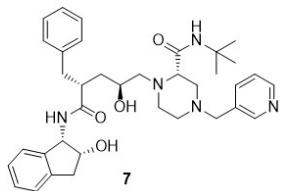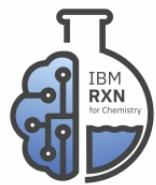
# Information about the retrosynthesis

Created On: 2019-10-01T08:58:35.823000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC(NC(C1N(CC(CC(C(NC2C(O)CC3C2=CC=CC=3)=O)CC2C=CC=CC=2)O)CCN(CC2C=NC=CC=2)C1)=O)(C)C
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: CC(NC(C1N(CC(CC(C(NC2C(O)CC3C2=CC=CC=3)=O)CC2C=CC=CC=2)O)CCN(CC2C=NC=CC=2)C1)=O)(C)C
Exclude substructures:

# Sequence 0, Confidence: 0.47

## Step 1

*Type: Epoxide + amine coupling, Confidence: 0.871*
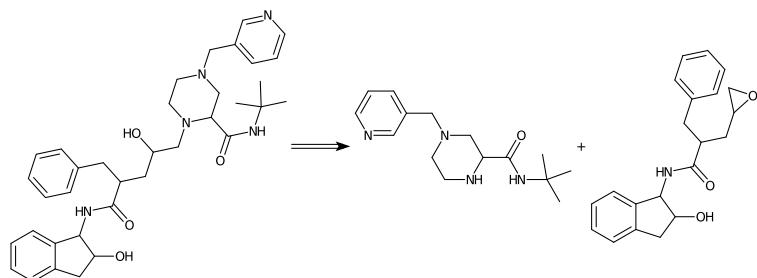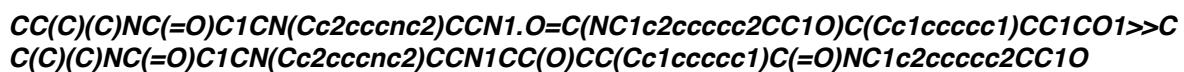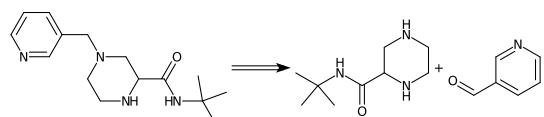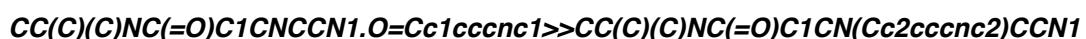
*CC(C)(C)NC(=O)C1CN(Cc2cccnc2)CCN1.O=C(NC1c2ccccc2CC1O)C(Cc1ccccc1)CC1CO1>>C C(C)(C)NC(=O)C1CN(Cc2cccnc2)CCN1CC(O)CC(Cc1ccccc1)C(=O)NC1c2ccccc2CC1O*



## Step 2

*Type: Aldehyde reductive amination, Confidence: 0.863*

*CC(C)(C)NC(=O)C1CNCCN1.O=Cc1cccnc1>>CC(C)(C)NC(=O)C1CN(Cc2cccnc2)CCN1*



*Type: Prilezhaev epoxidation, Confidence: 0.805*

*C=CCC(Cc1ccccc1)C(=O)NC1c2ccccc2CC1O.O=C(OO)c1cccc(Cl)c1>>O=C(NC1c2ccccc2CC 1O)C(Cc1ccccc1)CC1CO1*



## Step 3

*Type: Carboxylic acid + amine condensation, Confidence: 0.777*

*C=CCC(Cc1ccccc1)C(=O)O.CCN(C(C)C)C(C)C.CN(C)C(On1nnc2cccnc21)=[N+](C)C.F[P-](F)(F )(F)(F)F.ClCCl.NC1c2ccccc2CC1O.CN(C)C(On1nnc2cccnc21)=[N+](C)C.F[P-](F)(F)(F)(F)F>>C =CCC(Cc1ccccc1)C(=O)NC1c2ccccc2CC1O*

S 046
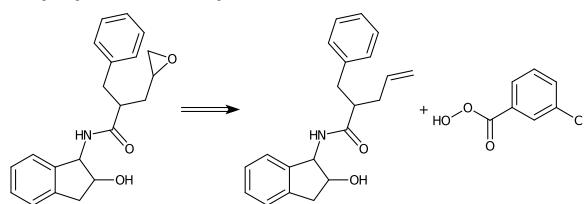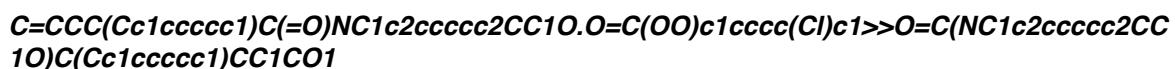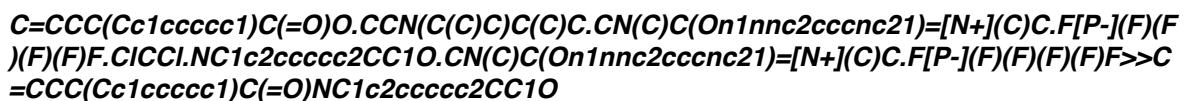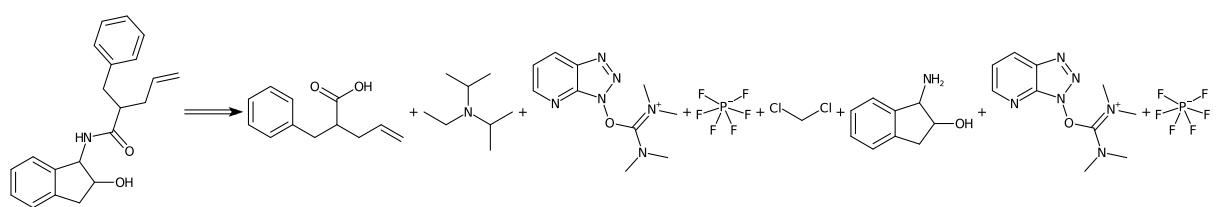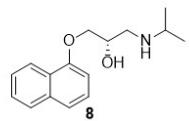
# Information about the retrosynthesis

Created On: 2019-10-01T08:32:01.771000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1=CC=CC2=CC=CC(OC[C@@H](O)CNC(C)C)=C12
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1=CC=CC2=CC=CC(OC[C@@H](O)CNC(C)C)=C12
Exclude substructures:

# Sequence 0, Confidence: 0.911

## *Step 1*

*Type: Epoxide + amine coupling, Confidence: 0.911*

*CC(C)N.c1ccc2c(OC[C@@H]3CO3)cccc2c1>>CC(C)NC[C@H](O)COc1cccc2ccccc12*
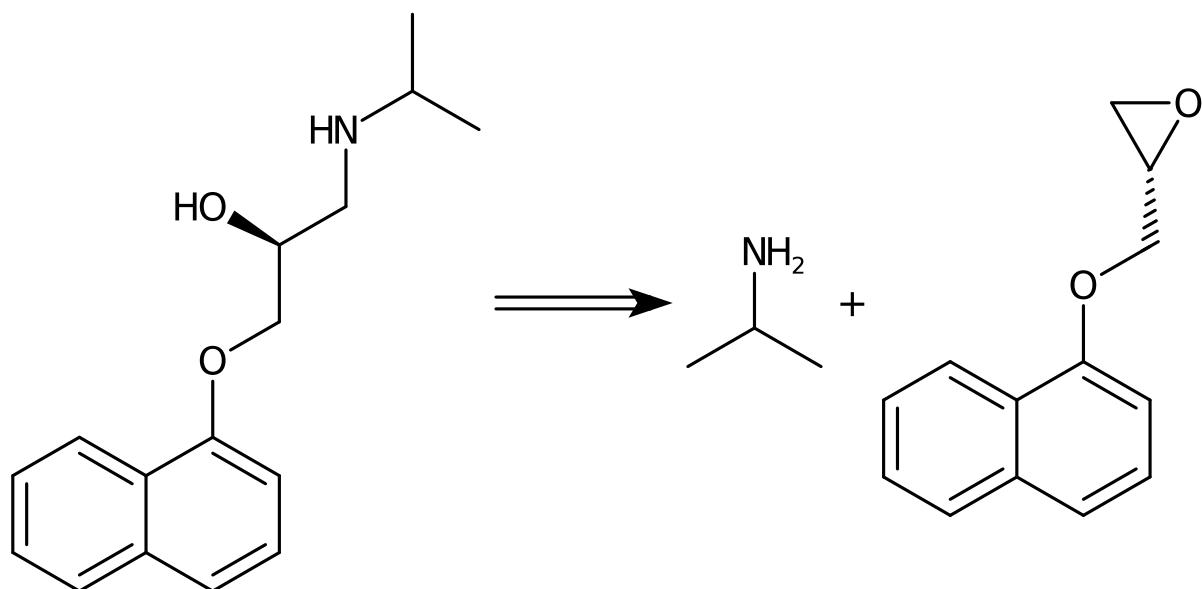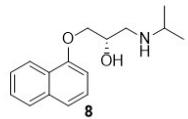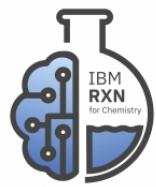
# Information about the retrosynthesis

Created On: 2019-10-01T10:21:04.636000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1=CC=CC2=CC=CC(OCC(CNC(C)C)O)=C12
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: C1=CC=CC2=CC=CC(OCC(CNC(C)C)O)=C12
Exclude substructures:

## Sequence 0, Confidence: 0.833

### Step 1

*Type: Epoxide + amine coupling, Confidence: 0.884*
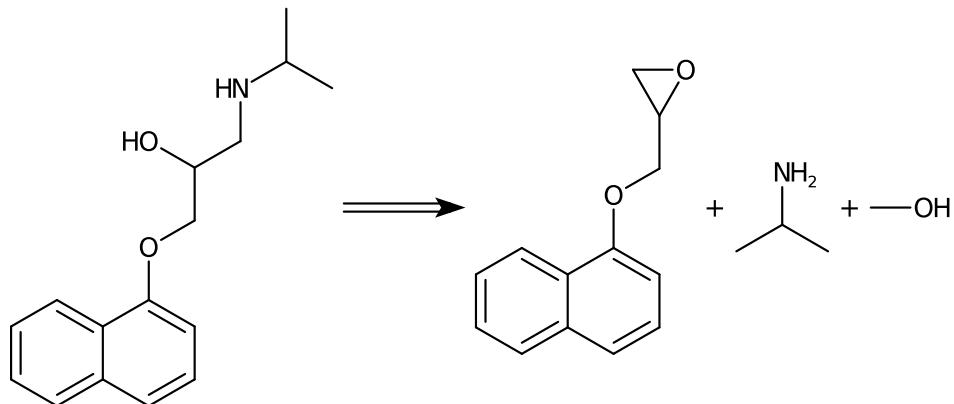
*c1ccc2c(OCC3CO3)cccc2c1.CC(C)N.CO>>CC(C)NCC(O)COc1cccc2ccccc12*



### Step 2

*Type: Williamson ether synthesis, Confidence: 0.943*

*CN(C)C=O.ClCC1CO1.Oc1cccc2ccccc12.[H-].[Na+].[H-].[Na+]>>c1ccc2c(OCC3CO3)cccc2c1*

9
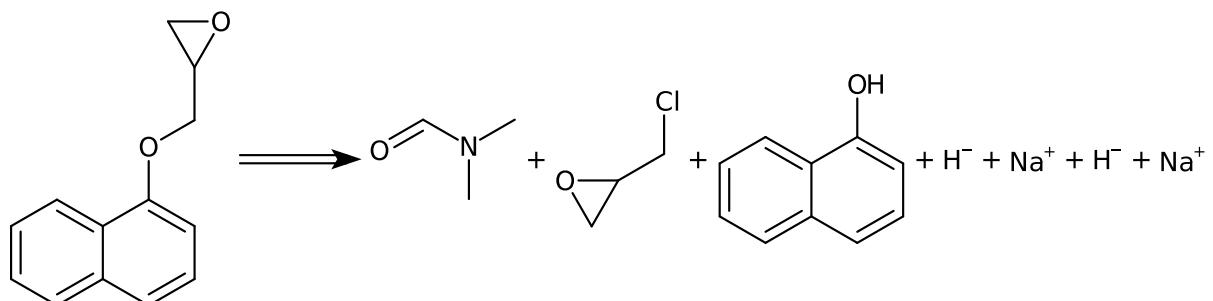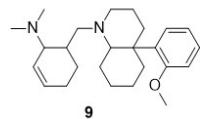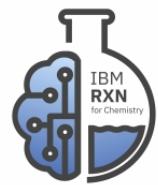
# Information about the retrosynthesis

Created On: 2019-10-02T09:38:18.325000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: COC1C(C23CCC(=O)CC2N(CC2C(N(C)C)C=CCC2)CCC3)=CC=CC=1
MSSR: 15
FAP: 0.6
MRP: 20
SbP: 3
Available smiles: C(=C/N(C)C)\C=C
Exclude smiles: COC1C(C23CCC(=O)CC2N(CC2C(N(C)C)C=CCC2)CCC3)=CC=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.0603

Metadata:
Warnings: The retrosynthesis did not complete. Try increasing MSSR.

## Step 1

*Type: Ketone dioxolane deprotection, Confidence: 0.759*
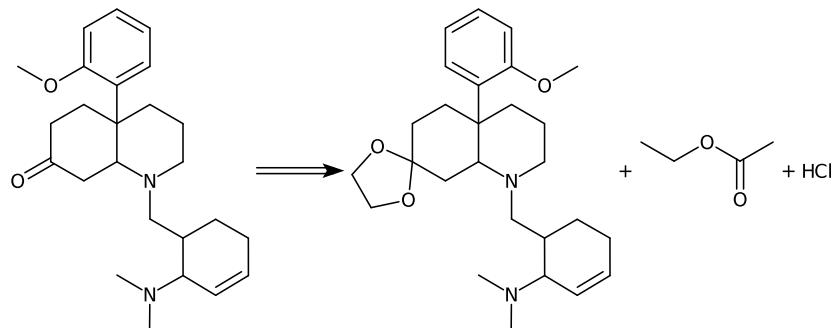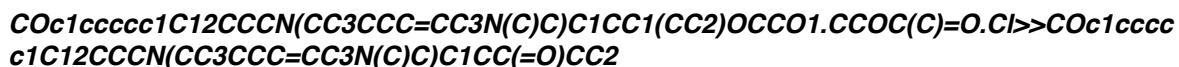
*COc1ccccc1C12CCCN(CC3CCC=CC3N(C)C)C1CC1(CC2)OCCO1.CCOC(C)=O.Cl>>COc1cccc c1C12CCCN(CC3CCC=CC3N(C)C)C1CC(=O)CC2*



## Step 2

*Type: Aldehyde reductive amination, Confidence: 0.763*

*CN(C)C1C=CCCC1C=O.COc1ccccc1C12CCCNC1CC1(CC2)OCCO1.[BH3-]C#N.[Na+]>>COc1c cccc1C12CCCN(CC3CCC=CC3N(C)C)C1CC1(CC2)OCCO1*



## Step 3

*Type: Aldehyde Collins oxidation, Confidence: 0.924*

*CN(C)C1C=CCCC1CO.ClCCl.O=[Cr](=O)([O-])Cl.c1cc[nH+]cc1>>CN(C)C1C=CCCC1C=O*
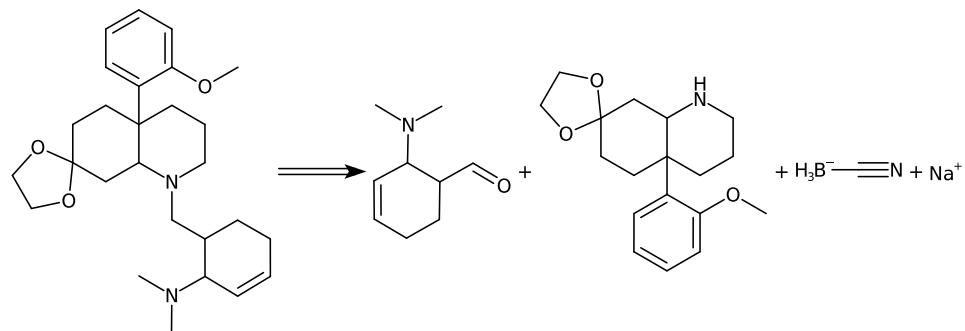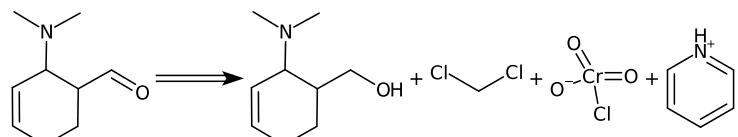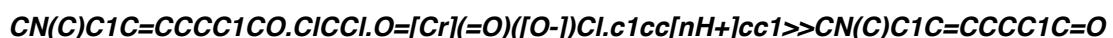
*Type: Amide to amine reduction, Confidence: 0.971*
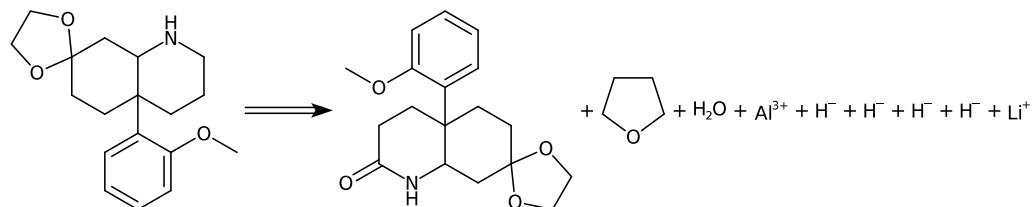
*COc1ccccc1C12CCC(=O)NC1CC1(CC2)OCCO1.C1CCOC1.O.[Al+3].[H-].[H-].[H-].[H-].[Li+]>>COc1ccccc1C12CCCNC1CC1(CC2)OCCO1*



## Step 4

*Type: Carboxylic acid to alcohol reduction, Confidence: 0.871*

*CN(C)C1C=CCCC1C(=O)O.C1CCOC1.[Al+3].[H-].[H-].[H-].[H-].[Li+]>>CN(C)C1C=CCCC1CO*



*Type: Undefined, Confidence: 0.0*

*COc1ccccc1C12CCC(=O)NC1CC1(CC2)OCCO1>>COc1ccccc1C12CCC(=O)NC1CC1(CC2)OCCO1*



## Step 5

*Type: CO2H-Me deprotection, Confidence: 0.879*

*COC(=O)C1CCC=CC1N(C)C.C1CCOC1.O.[Li+].[OH-]>>CN(C)C1C=CCCC1C(=O)O*
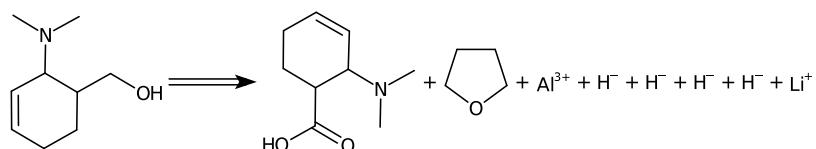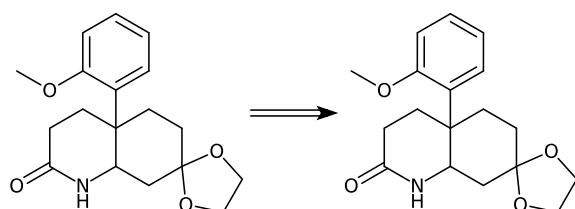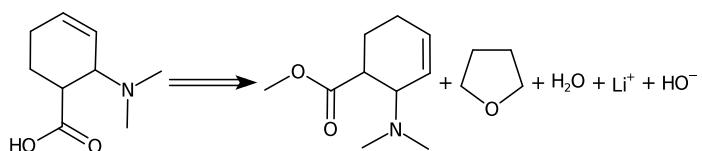


## Step 6

*Type: Bromo N-alkylation, Confidence: 0.64*
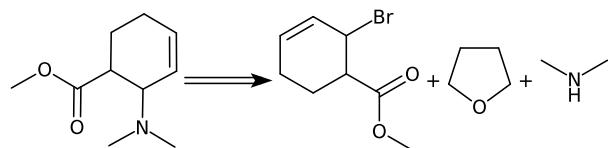
*COC(=O)C1CCC=CC1Br.C1CCOC1.CNC>>COC(=O)C1CCC=CC1N(C)C*



## Step 7

*Type: Methyl esterification, Confidence: 0.93*

*O=C(O)C1CCC=CC1Br.CO.O=S(Cl)Cl>>COC(=O)C1CCC=CC1Br*



## Step 8

*Type: CO2H-Et deprotection, Confidence: 0.902*

*CCOC(=O)C1CCC=CC1Br.C1CCOC1.O.[Li+].[OH-]>>O=C(O)C1CCC=CC1Br*
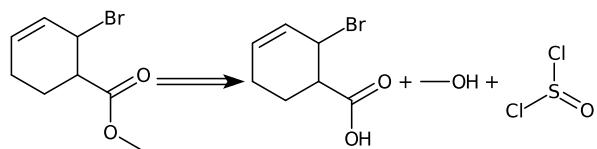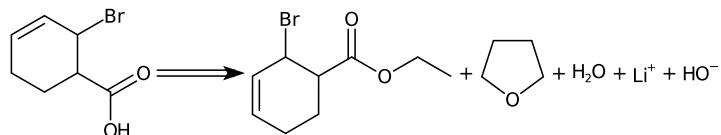


## Step 9

*Type: Hydroxy to bromo, Confidence: 0.795*

*CCOC(=O)C1CCC=CC1O.BrP(Br)Br>>CCOC(=O)C1CCC=CC1Br*
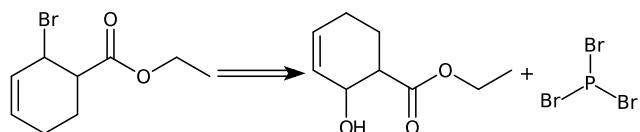


## Step 10

*Type: O-TBS deprotection, Confidence: 0.761*

*CCOC(=O)C1CCC=CC1O[Si](C)(C)C(C)(C)C.C1CCOC1.CCCC[N+](CCCC)(CCCC)CCCC.[F-]>>CCOC(=O)C1CCC=CC1O*
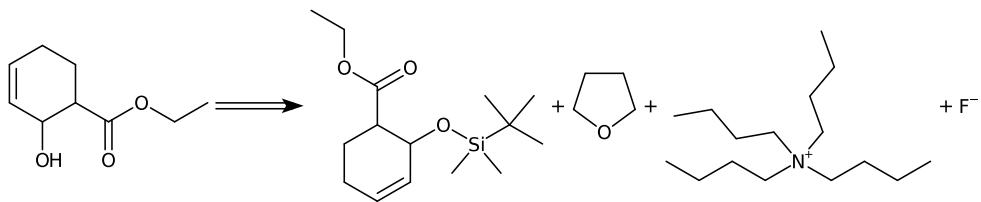
## Step 11

*Type: Olefin metathesis, Confidence: 0.784*

*C=CCCC(C(=O)OCC)C(C=C)O[Si](C)(C)C(C)(C)C.ClCCl>>CCOC(=O)C1CCC=CC1O[Si](C)(C)C(C)(C)C*
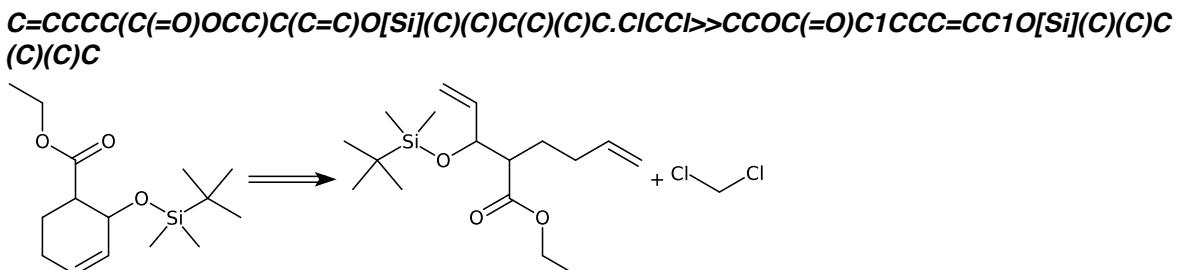


## Step 12

*Type: O-TBS protection, Confidence: 0.937*
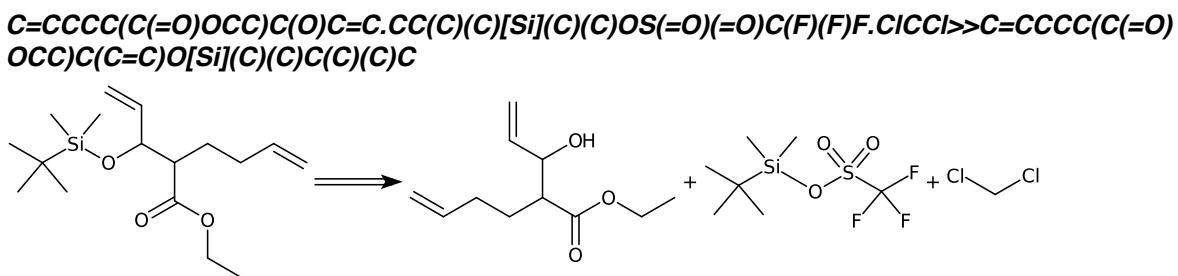
*C=CCCC(C(=O)OCC)C(O)C=C.CC(C)(C)[Si](C)(C)OS(=O)(=O)C(F)(F)F.ClCCl>>C=CCCC(C(=O)OCC)C(C=C)O[Si](C)(C)C(C)(C)C*



## Step 13

*Type: Unrecognized, Confidence: 0.649*

*C=CCCCC(=O)OCC.C1CCOC1.C=CC=O.CC(C)NC(C)C.[Li]CCCC>>C=CCCC(C(=O)OCC)C(O)C=C*
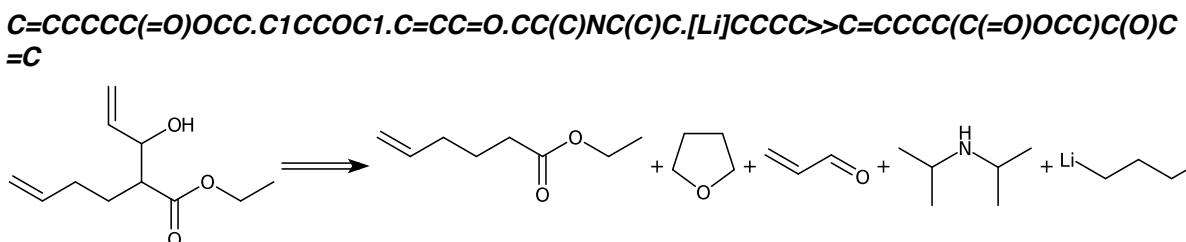


## Step 14

*Type: Fischer-Speier esterification, Confidence: 0.994*

*C=CCCC(=O)O.CCO.O=S(=O)(O)O>>C=CCCC(=O)OCC*
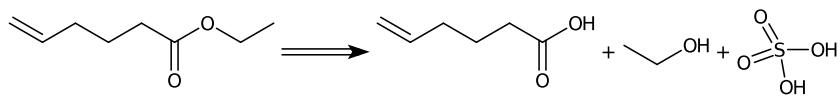
## Step 15

*Type: CO2H-Me deprotection, Confidence: 0.986*

*C=CCCCC(=O)OC.C1CCOC1.O.[Li]O>>C=CCCCC(=O)O*
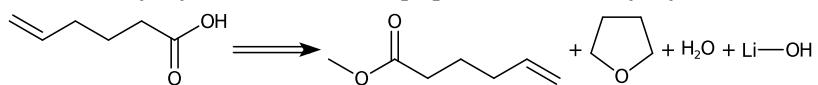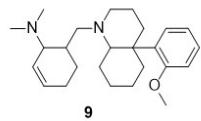
# Information about the retrosynthesis

Created On: 2019-09-27T15:37:13.273000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1CCNC2CCCCC12C1=C(OC)C=CC=C1
MSSR: 15
FAP: 0.6
MRP: 20
SbP: 3
Available smiles:
Exclude smiles: C1CCNC2CCCCC12C1=C(OC)C=CC=C1
Exclude substructures:

## Sequence 0, Confidence: 0.34

### Step 1

*Type: Secondary ketimine reduction, Confidence: 0.964*

*COc1ccccc1C12CCCCC1=NCCC2.CO.[BH4-].[Na+]>>COc1ccccc1C12CCCCC1NCCC2*
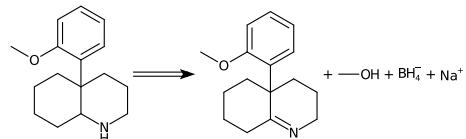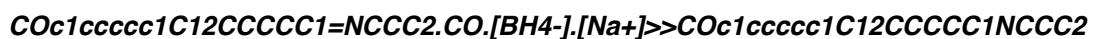


### Step 2

*Type: Alkylimino-de-oxo-bisubsitution, Confidence: 0.43*

*COc1ccccc1C1(CCCN)CCCCC1=O.Cc1ccccc1>>COc1ccccc1C12CCCCC1=NCCC2*
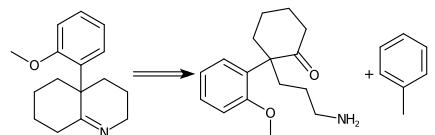


### Step 3

*Type: N-Phth deprotection, Confidence: 0.966*

*COc1ccccc1C1(CCCN2C(=O)c3ccccc3C2=O)CCCCC1=O.NN.O>>COc1ccccc1C1(CCCN)CCCCC1=O*
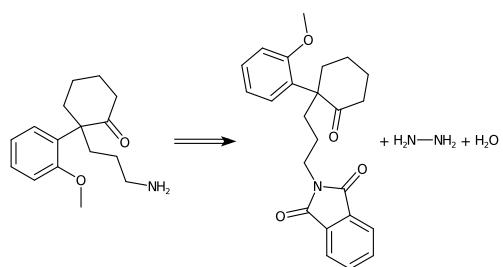


### Step 4

*Type: Chloro Gabriel alkylation, Confidence: 0.951*

*COc1ccccc1C1(CCCCl)CCCCC1=O.CN(C)C=O.O=C1NC(=O)c2ccccc21.[K]>>COc1ccccc1C1(CCCN2C(=O)c3ccccc3C2=O)CCCCC1=O*
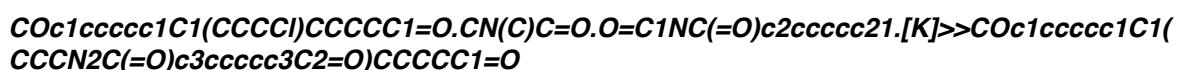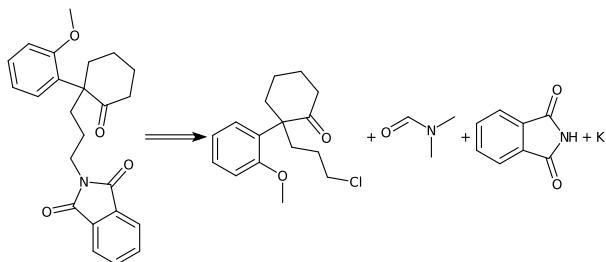
## Step 5

*Type: Unrecognized, Confidence: 0.949*

*COc1ccccc1C1CCCCC1=O.CN(C)C=O.ClCCCl.O.[H-].[Na+]>>COc1ccccc1C1(CCCCl)CCCCC1=O*
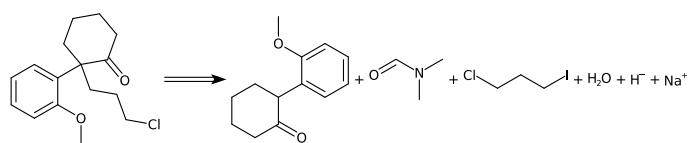


## Step 6

*Type: Unrecognized, Confidence: 0.939*

*CC(=O)[O-].CC(=O)[O-].[Pd+2].CC(C)(C)P(c1ccccc1-c1ccccc1)C(C)(C)C.CC(C)(C)[O-].[Na+].COc1ccccc1Br.Cc1ccccc1.O=C1CCCCC1.CC(=O)[O-].CC(=O)[O-].[Pd+2].CC(C)(C)[O-].[Na+]>>COc1ccccc1C1CCCCC1=O*
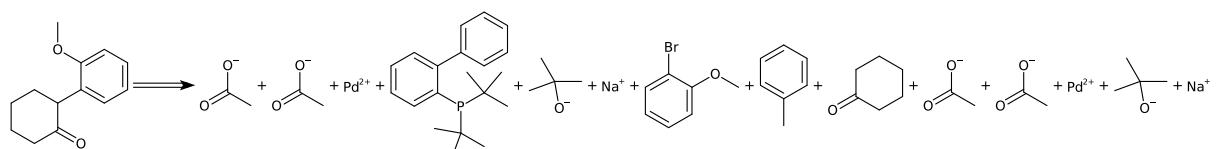
# Information about the retrosynthesis

Created On: 2019-09-27T09:06:14.426000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: O=C(OC1C(C(O)=O)=CC=CC=1)C
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: O=C(OC1C(C(O)=O)=CC=CC=1)C
Exclude substructures:

# Sequence 0, Confidence: 0.929

## *Step 1*

*Type: O-Ac protection, Confidence: 0.929*

*CC(=O)OC(C)=O.O.O=C(O)c1ccccc1O.c1ccncc1>>CC(=O)Oc1ccccc1C(=O)O*
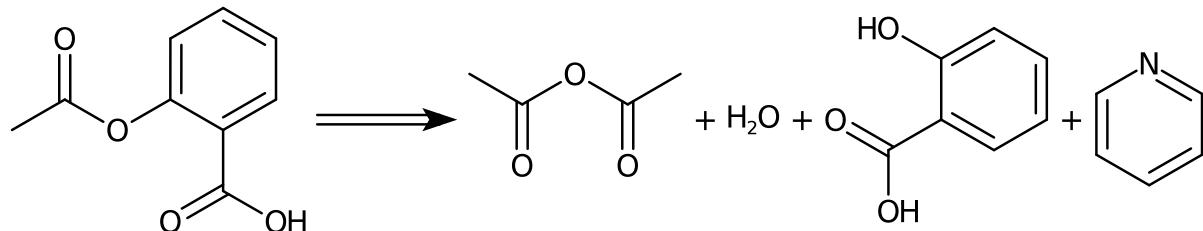
# Information about the retrosynthesis

Created On: 2019-09-27T09:08:04.135000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: O=S(N)(C1C=CC(N2C(C3C=CC(C)=CC=3)=CC(C(F)(F)F)=N2)=CC=1)=O
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: O=S(N)(C1C=CC(N2C(C3C=CC(C)=CC=3)=CC(C(F)(F)F)=N2)=CC=1)=O
Exclude substructures:

## Sequence 0, Confidence: 0.921

### Step 1

**Type: Fluoro N-arylation, Confidence: 0.921**

*Cc1ccc(-c2cc(C(F)(F)F)n[nH]2)cc1.NS(=O)(=O)c1ccc(F)cc1>>Cc1ccc(-c2cc(C(F)(F)F)nn2-c2cc(S(N)(=O)=O)cc2)cc1*
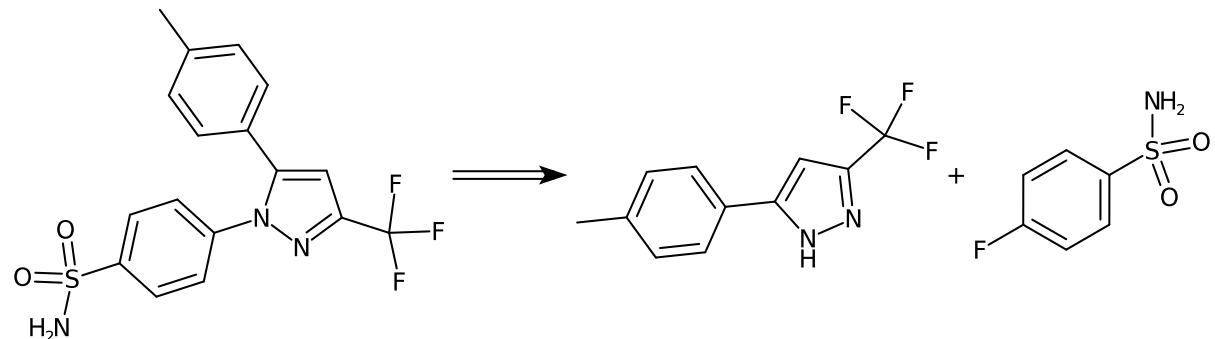
# Information about the retrosynthesis

Created On: 2019-10-01T11:46:30.813000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC1C=CC(C2N(C3C=CC(S(=O)(=O)N)=CC=3)N=C(C(F)(F)F)C=2)=CC=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: CC1C=CC(C2N(C3C=CC(S(=O)(=O)N)=CC=3)N=C(C(F)(F)F)C=2)=CC=1
Exclude substructures:

## Sequence 0, Confidence: 0.81

### Step 1

*Type: Knorr pyrazole synthesis, Confidence: 0.906*

*Cc1ccc(C(=O)CC(=O)C(F)(F)F)cc1.NNc1ccc(S(N)(=O)=O)cc1.O>>Cc1ccc(-c2cc(C(F)(F)F)nn2-c2ccc(S(N)(=O)=O)cc2)cc1*



### Step 2

*Type: Unrecognized, Confidence: 0.977*

*CC(=O)c1ccc(C)cc1.C1CCOC1.CCOC(=O)C(F)(F)F.Cl.[H-].[Na+]>>Cc1ccc(C(=O)CC(=O)C(F)F)cc1*
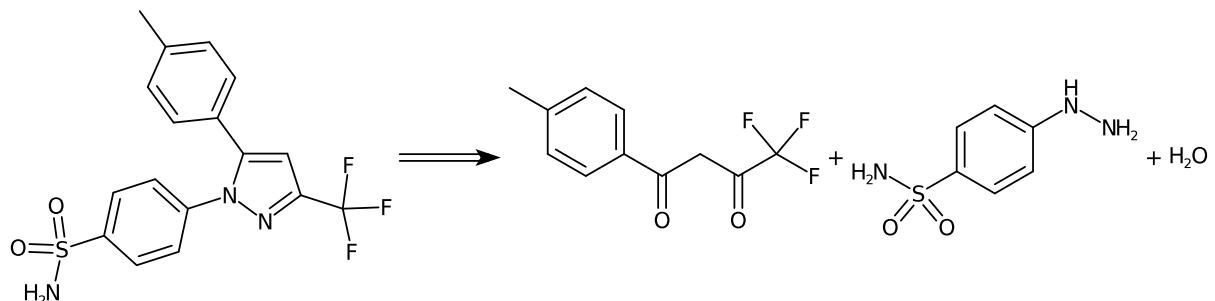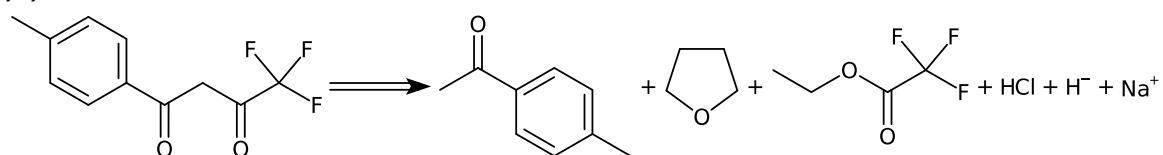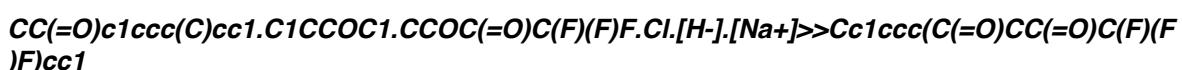


*Type: Fluoro to hydrazino, Confidence: 0.953*

*NS(=O)(=O)c1ccc(F)cc1.NN.O>>NNc1ccc(S(N)(=O)=O)cc1*
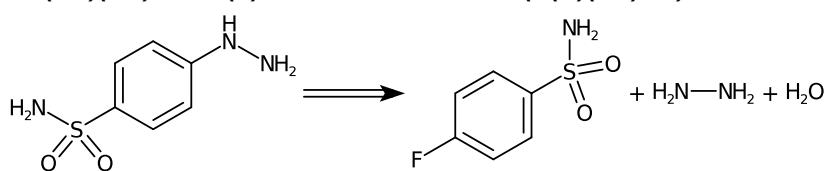


### Step 3

*Type: Bromo Grignard + nitrile ketone synthesis, Confidence: 0.997*

*Cc1ccc(C#N)cc1.C[Mg+].[Br-]>>CC(=O)c1ccc(C)cc1*
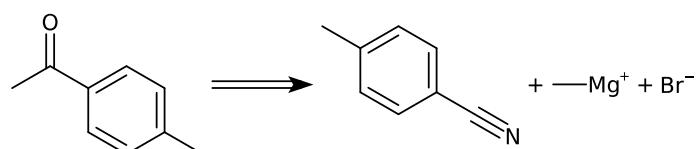
**Type: Chlorosulfonyl to sulfamoyl, Confidence: 0.985**

**C1CCOC1.O=S(=O)(Cl)c1ccc(F)cc1.[NH4+].[OH-].[NH4+].[OH-]>>NS(=O)(=O)c1ccc(F)cc1**
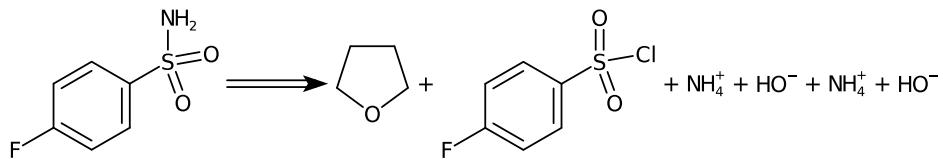


## Step 4

**Type: Rosenmund van Braun cyanation, Confidence: 0.978**

**Cc1ccc(Br)cc1.N#C[Cu]>>Cc1ccc(C#N)cc1**
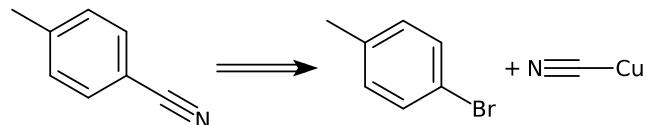
# Information about the retrosynthesis

Created On: 2019-09-27T09:07:08.967000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CN1C(=O)C/N=C(/C2C=CC=CC=2)\C2C=C(C=CC1=2)Cl
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: CN1C(=O)C/N=C(/C2C=CC=CC=2)\C2C=C(C=CC1=2)Cl
Exclude substructures:

# Sequence 0, Confidence: 0.977

## Step 1

*Type: Chloro Suzuki-type coupling, Confidence: 0.977*

*CN1C(=O)CN=C(Cl)c2cc(Cl)ccc21.OB(O)c1ccccc1>>CN1C(=O)CN=C(c2ccccc2)c2cc(Cl)ccc21*
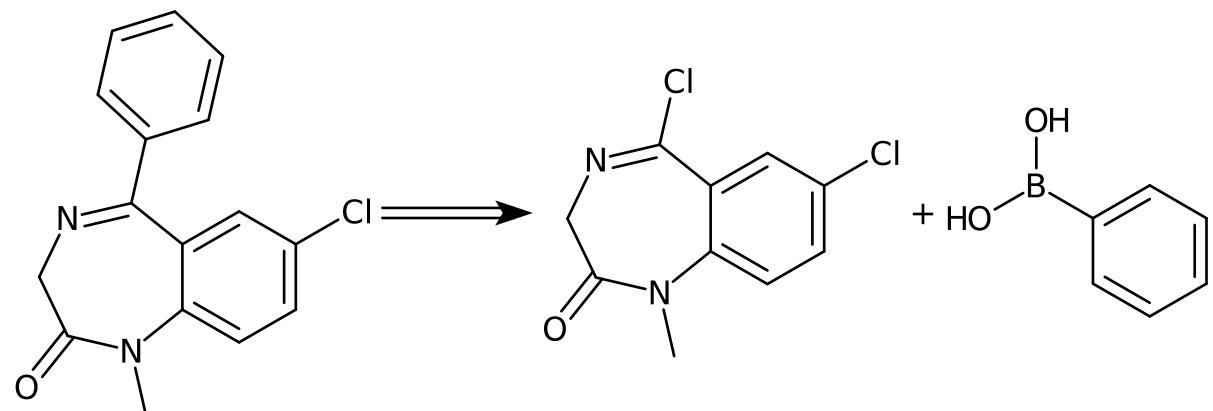
# Information about the retrosynthesis

Created On: 2019-09-27T09:07:08.967000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CN1C(=O)C/N=C(/C2C=CC=CC=2)\C2C=C(C=CC1=2)Cl
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: CN1C(=O)C/N=C(/C2C=CC=CC=2)\C2C=C(C=CC1=2)Cl
Exclude substructures:

# Sequence 1, Confidence: 0.762

## Step 1

*Type: Iodo N-methylation, Confidence: 0.967*
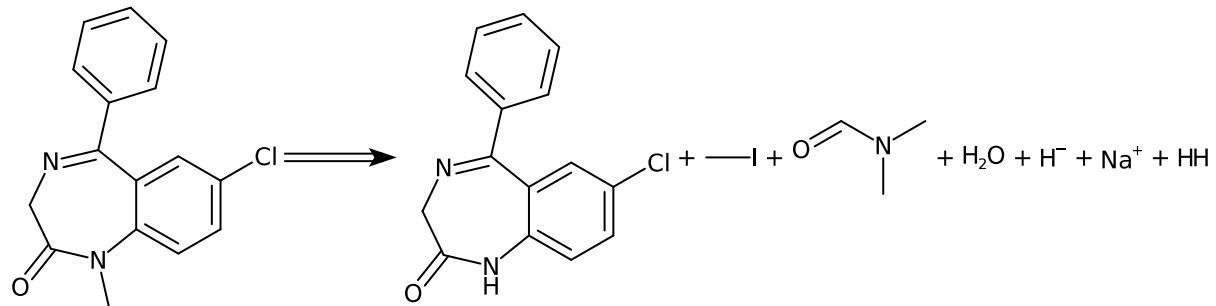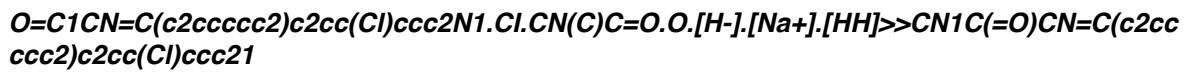
*O=C1CN=C(c2ccccc2)c2cc(Cl)ccc2N1.Cl.CN(C)C=O.O.[H-].[Na+].[HH]>>CN1C(=O)CN=C(c2ccccc2)c2cc(Cl)ccc21*



## Step 2

*Type: Unrecognized, Confidence: 0.788*

*O=C(CCl)Nc1ccc(Cl)cc1C(=O)c1ccccc1.[NH4+].[OH-].[NH4+].[OH-]>>O=C1CN=C(c2ccccc2)c2cc(Cl)ccc2N1*
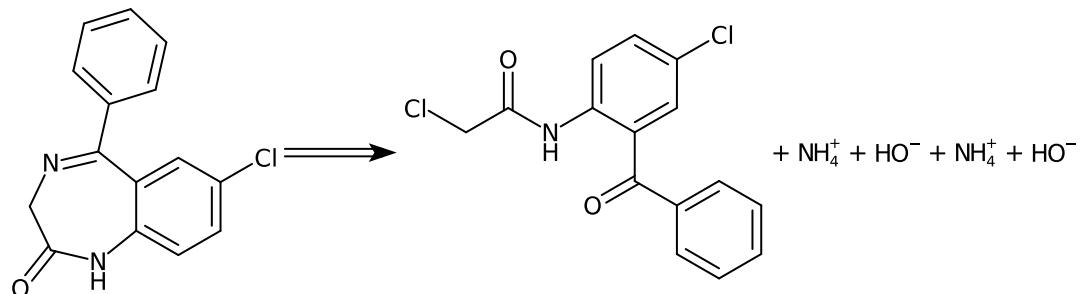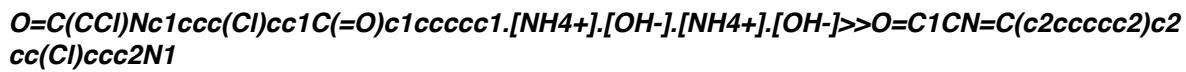
# Information about the retrosynthesis

Created On: 2019-10-01T12:22:08.704000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CN1C2C(=CC(=CC=2)Cl)/C(/C2C=CC=CC=2)=N\CC1=O
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: CN1C2C(=CC(=CC=2)Cl)/C(/C2C=CC=CC=2)=N\CC1=O
Exclude substructures:

# Sequence 0, Confidence: 0.679

## Step 1

*Type: Iodo N-methylation, Confidence: 0.967*
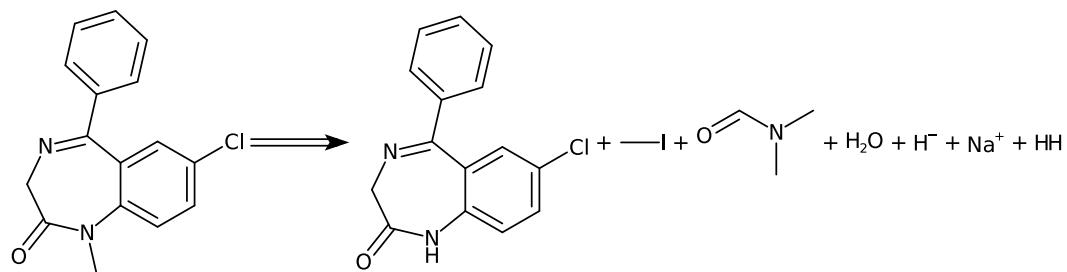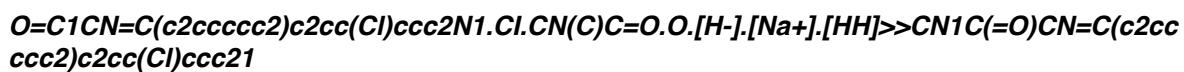
*O=C1CN=C(c2ccccc2)c2cc(Cl)ccc2N1.Cl.CN(C)C=O.O.[H-].[Na+].[HH]>>CN1C(=O)CN=C(c2ccccc2)c2cc(Cl)ccc21*



## Step 2

*Type: Unrecognized, Confidence: 0.788*

*O=C(CCl)Nc1ccc(Cl)cc1C(=O)c1ccccc1.[NH4+].[OH-]>>O=C1CN=C(c2ccccc2)c2cc(Cl)ccc2N1*



## Step 3

*Type: Amide Schotten-Baumann, Confidence: 0.966*

*Nc1ccc(Cl)cc1C(=O)c1ccccc1.ClCCl.O=C(Cl)CCl.O=C([O-])O.[Na+]>>O=C(CCl)Nc1ccc(Cl)cc1C(=O)c1ccccc1*
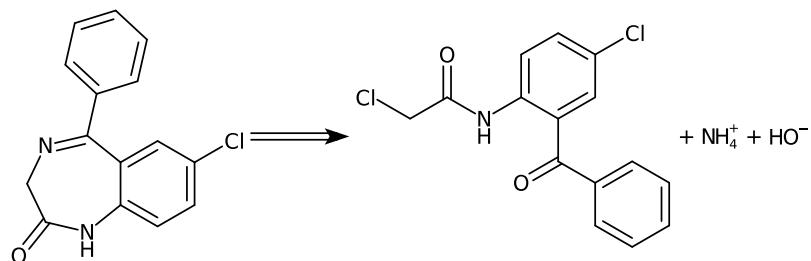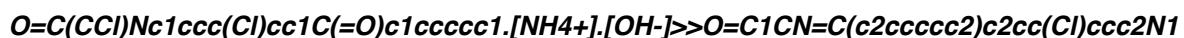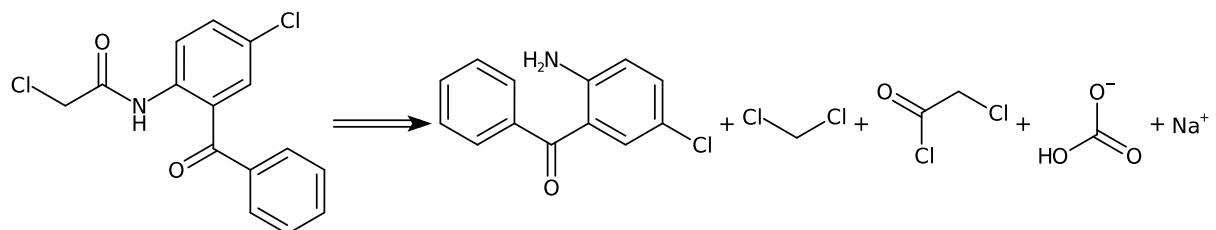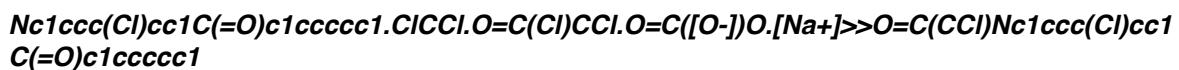


## Step 4

*Type: Bromo Grignard + nitrile ketone synthesis, Confidence: 0.964*

**N#Cc1cc(Cl)ccc1N.Br[Mg]c1ccccc1.C1CCOC1>>Nc1ccc(Cl)cc1C(=O)c1ccccc1**
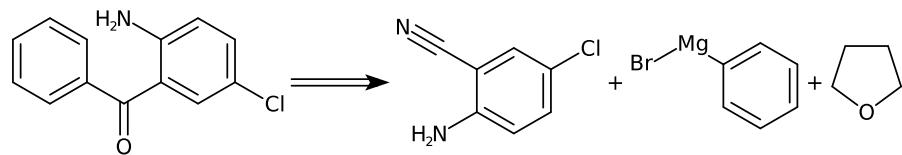


## Step 5

**Type: Chlorination, Confidence: 0.957**

**CC(=O)O.N#Cc1ccccc1N.O.O=C1CCC(=O)N1Cl>>N#Cc1cc(Cl)ccc1N**
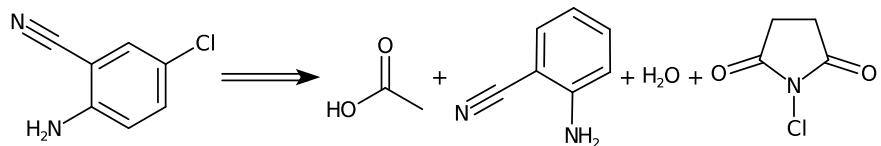
# Information about the retrosynthesis

Created On: 2019-09-27T09:06:41.671000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: O=C(CN(CC)CC)NC1C(C)=CC=CC=1C
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: O=C(CN(CC)CC)NC1C(C)=CC=CC=1C
Exclude substructures:

# Sequence 0, Confidence: 0.98

*Step 1*

*Type: Bromo N-alkylation, Confidence: 0.98*

*CCNCC.Cc1cccc(C)c1NC(=O)CBr>>CCN(CC)CC(=O)Nc1c(C)cccc1C*
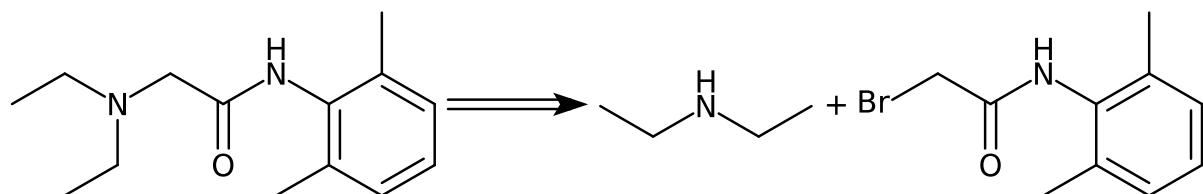
# Information about the retrosynthesis

Created On: 2019-10-01T12:37:41.867000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CCN(CC(NC1C(C)=CC=CC=1C)=O)CC
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: CCN(CC(NC1C(C)=CC=CC=1C)=O)CC
Exclude substructures:

## Sequence 0, Confidence: 0.959

### Step 1

*Type: Bromo N-alkylation, Confidence: 0.98*
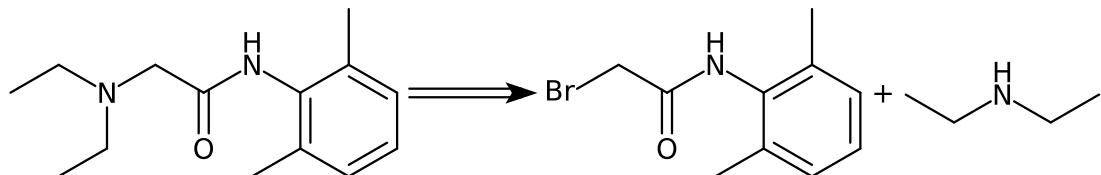
*Cc1cccc(C)c1NC(=O)CBr.CCNCC>>CCN(CC)CC(=O)Nc1c(C)cccc1C*



### Step 2

*Type: Amide Schotten-Baumann, Confidence: 0.978*

*Cc1cccc(C)c1N.ClCCl.O=C(Br)CBr.c1ccncc1>>Cc1cccc(C)c1NC(=O)CBr*
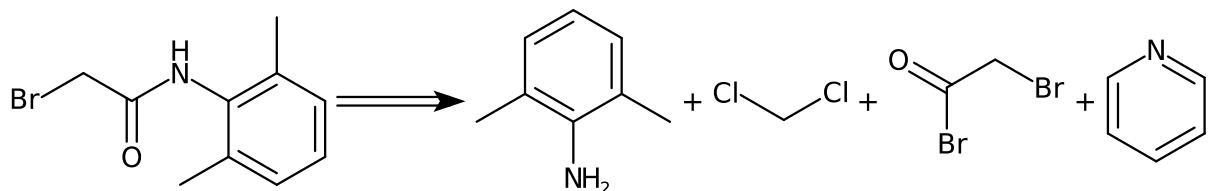
# Information about the retrosynthesis

Created On: 2019-09-27T09:07:50.027000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
O=C([C@H](CCC1C=CC=CC=1)N[C@@H](C)C(N1CC2C=CC=CC=2C[C@H]1C(O)=O)=O)OCC
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
O=C([C@H](CCC1C=CC=CC=1)N[C@@H](C)C(N1CC2C=CC=CC=2C[C@H]1C(O)=O)=O)OCC
Exclude substructures:

# Sequence 0, Confidence: 0.874

## Step 1

*Type: O-Bn deprotection, Confidence: 0.956*
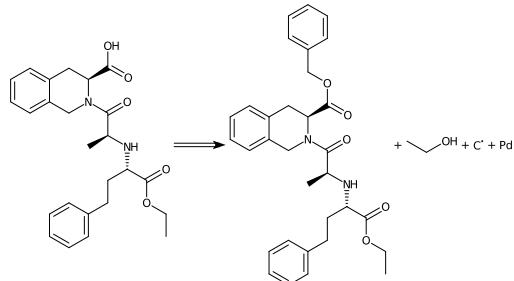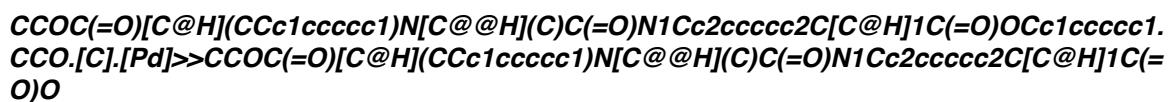
*CCOC(=O)[C@H](CCc1ccccc1)N[C@@H](C)C(=O)N1Cc2ccccc2C[C@H]1C(=O)OCc1ccccc1.*
*CCO.[C].[Pd]>>CCOC(=O)[C@H](CCc1ccccc1)N[C@@H](C)C(=O)N1Cc2ccccc2C[C@H]1C(=O)O*



## Step 2

*Type: Carboxylic acid + amine condensation, Confidence: 0.915*

*CCN(C(C)C)C(C)C.CCOC(=O)[C@H](CCc1ccccc1)N[C@@H](C)C(=O)O.CN(C)C(On1nnc2cccn*
*c21)=[N+](C)C.F[P-](F)(F)(F)(F)F.CN(C)C=O.O=C(OCc1ccccc1)[C@@H]1Cc2ccccc2CN1.CN(C*
*)C(On1nnc2cccnc21)=[N+](C)C.F[P-](F)(F)(F)(F)F>>CCOC(=O)[C@H](CCc1ccccc1)N[C@@H](*
*C)C(=O)N1Cc2ccccc2C[C@H]1C(=O)OCc1ccccc1*
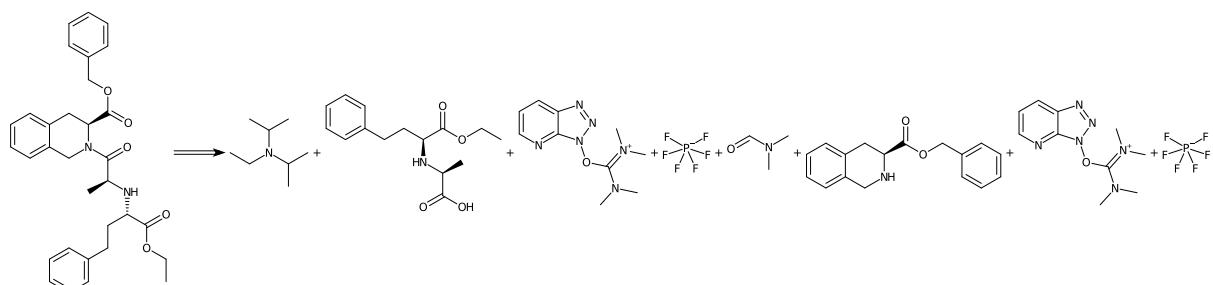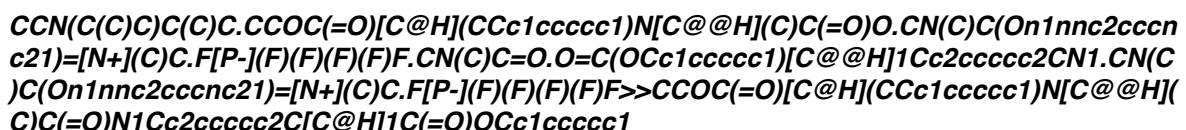
# Information about the retrosynthesis

Created On: 2019-09-27T09:07:36.533000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: O=C([C@H](C)NCC1C=CC(OCC2C=C(F)C=CC=2)=CC=1)N
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: O=C([C@H](C)NCC1C=CC(OCC2C=C(F)C=CC=2)=CC=1)N
Exclude substructures:

# Sequence 0, Confidence: 0.899

## Step 1

### Type: Aldehyde reductive amination, Confidence: 0.899

*CO.C[C@H](N)C(N)=O.O=Cc1ccc(OCc2cccc(F)c2)cc1.[BH3-]C#N.[Na+].[BH3-]C#N.[Na+]>>C[C@H](NCc1ccc(OCc2cccc(F)c2)cc1)C(N)=O*
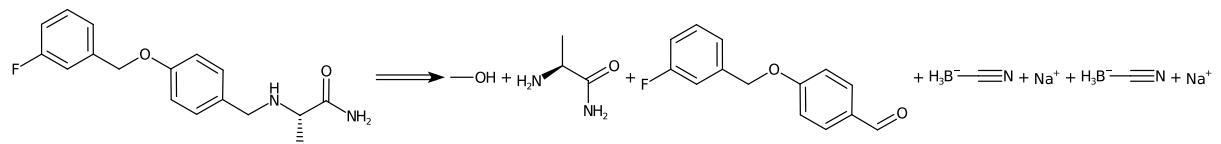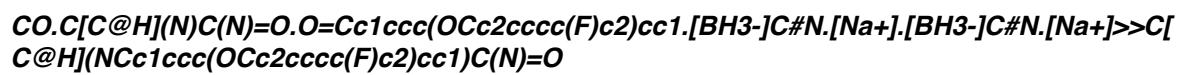
# Information about the retrosynthesis

Created On: 2019-10-01T12:47:48.394000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C[C@@H](C(=O)N)NCC1C=CC(OCC2C=C(F)C=CC=2)=CC=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: C[C@@H](C(=O)N)NCC1C=CC(OCC2C=C(F)C=CC=2)=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.666

## Step 1

*Type: Aldehyde reductive amination, Confidence: 0.899*
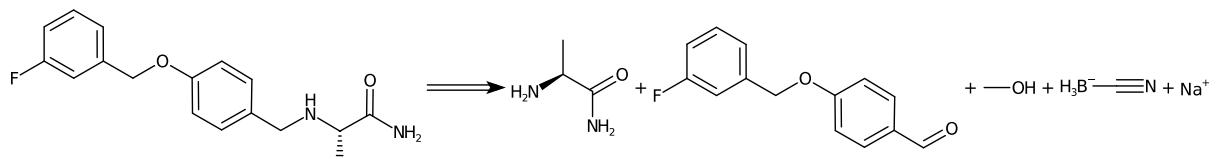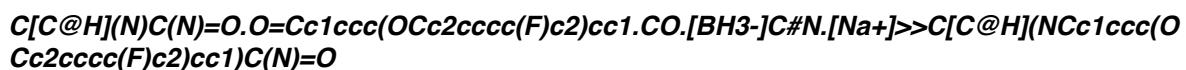
*C[C@H](N)C(N)=O.O=Cc1ccc(OCc2cccc(F)c2)cc1.CO.[BH3-]C#N.[Na+]>>C[C@H](NCc1ccc(OCc2cccc(F)c2)cc1)C(N)=O*

## Step 2

*Type: N-Cbz deprotection, Confidence: 0.919*

*C[C@H](NC(=O)OCc1ccccc1)C(N)=O.CO.[HH].[Pd]>>C[C@H](N)C(N)=O*

*Type: Williamson ether synthesis, Confidence: 0.97*

*CC(C)=O.Fc1cccc(CBr)c1.O=C([O-])[O-].[K+].[K+].O=Cc1ccc(O)cc1.O=C([O-])[O-].[K+].[K+]>>O=Cc1ccc(OCc2cccc(F)c2)cc1*
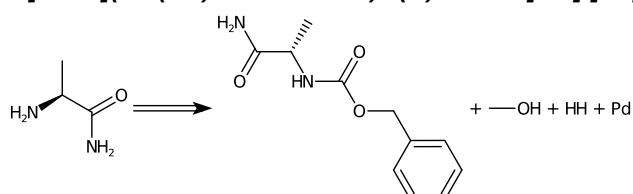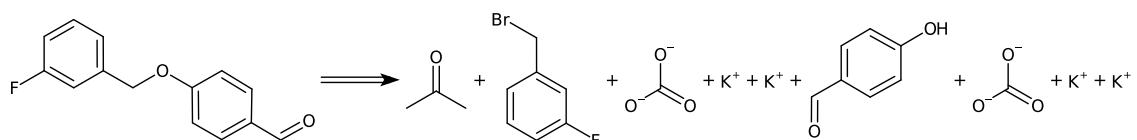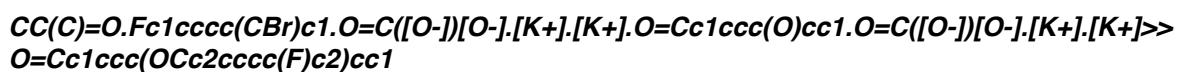
## Step 3

*Type: Carboxy ester to carbamoyl, Confidence: 0.94*

*COC(=O)[C@H](C)NC(=O)OCc1ccccc1.CO.N>>C[C@H](NC(=O)OCc1ccccc1)C(N)=O*

## Step 4

*Type: Fischer-Speier esterification, Confidence: 0.964*

*C[C@H](NC(=O)OCc1ccccc1)C(=O)O.CO.O=S(=O)(O)O>>COC(=O)[C@H](C)NC(=O)OCc1ccccc1*
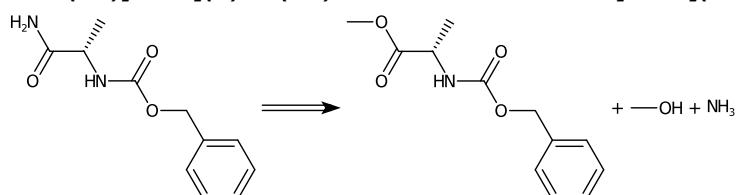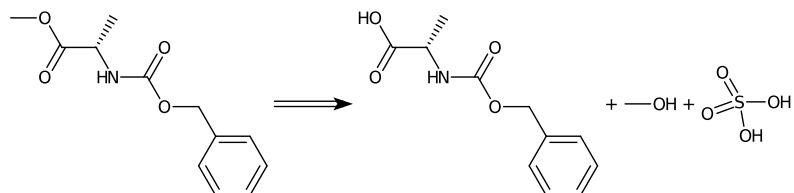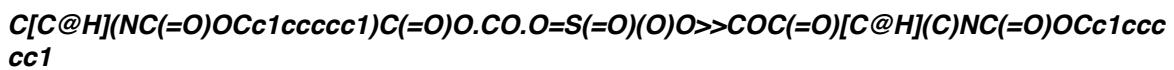


## Step 5

*Type: Amide Schotten-Baumann, Confidence: 0.917*

*C[C@H](N)C(=O)O.O.O=C(Cl)OCc1ccccc1.[Na+].[OH-].[Na+].[OH-]>>C[C@H](NC(=O)OCc1ccccc1)C(=O)O*
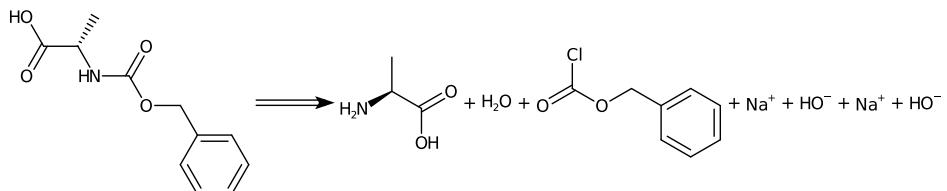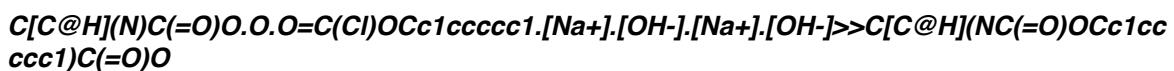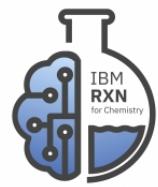
# Information about the retrosynthesis

Created On: 2019-09-27T09:06:28.528000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: [O-][N+](C1N(CC(C)O)C(C)=NC=1)=O
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: [O-][N+](C1N(CC(C)O)C(C)=NC=1)=O
Exclude substructures:

## Sequence 0, Confidence: 0.829

### *Step 1*

*Type: Unrecognized, Confidence: 0.888*

*Cc1ncc([N+](=O)[O-])o1.CC(O)CN.CCO>>Cc1ncc([N+](=O)[O-])n1CC(C)O*
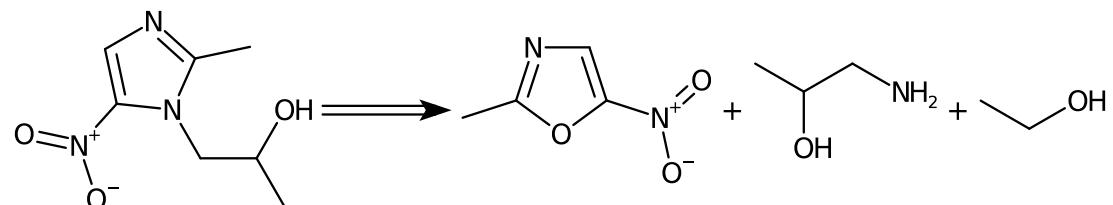


### *Step 2*

*Type: Nitration, Confidence: 0.934*

*Cc1ncco1.O=S(=O)(O)O.O=[N+]([O-])[O-].[K+].O=[N+]([O-])[O-].[K+]>>Cc1ncc([N+](=O)[O-])o1*

# Information about the retrosynthesis

Created On: 2019-09-30T16:22:07.824000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC(CC(C1C(=O)OC2C(=CC=CC=2)C=1O)C1C=CC=CC=1)=O
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: CC(CC(C1C(=O)OC2C(=CC=CC=2)C=1O)C1C=CC=CC=1)=O
Exclude substructures:

## Sequence 0, Confidence: 0.789

### *Step 1*

*Type: Unrecognized, Confidence: 0.789*

*CC(=O)/C=C/c1ccccc1.CCN(CC)CC.CO.O=c1cc(O)c2ccccc2o1>>CC(=O)CC(c1ccccc1)c1c(O)c2ccccc2oc1=O*

# Information about the retrosynthesis

Created On: 2019-09-30T16:22:07.824000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC(CC(C1C(=O)OC2C(=CC=CC=2)C=1O)C1C=CC=CC=1)=O
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: CC(CC(C1C(=O)OC2C(=CC=CC=2)C=1O)C1C=CC=CC=1)=O
Exclude substructures:

# Sequence 0, Confidence: 0.789

## *Step 1*

*Type: Unrecognized, Confidence: 0.789*

*CC(=O)/C=C/c1ccccc1.CCN(CC)CC.CO.O=c1cc(O)c2ccccc2o1>>CC(=O)CC(c1ccccc1)c1c(O)c2ccccc2oc1=O*

# Information about the retrosynthesis

Created On: 2019-09-26T17:08:00.636000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
C1C=CC([Se]C2C(=O)C3=C(OC4(CCCC3O4)CCCCC3C=CC(OCOC)=CC=3)CC2)=CC=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
C1C=CC([Se]C2C(=O)C3=C(OC4(CCCC3O4)CCCCC3C=CC(OCOC)=CC=3)CC2)=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.427

Metadata:
Warnings: 'ERROR MESSAGE'

## Step 1

### Type: Unrecognized, Confidence: 0.498

COCOc1ccc(CCCCC23CCCC(O2)C2=C(CCCC2=O)O3)cc1.C1CCOC1.CC(C)[N-]C(C)C.[Li+].[Cl-].[NH4+].c1ccc([Se][Se]c2ccccc2)cc1>>COCOc1ccc(CCCCC23CCCC(O2)C2=C(CCC([Se]c4ccccc4)C2=O)O3)cc1
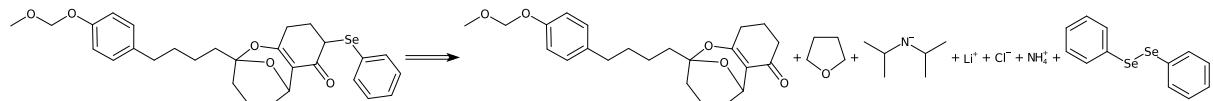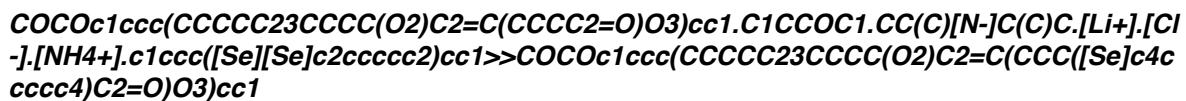


## Step 2

### Type: Alkyne to alkane hydrogenation, Confidence: 0.929

COCOc1ccc(C#CCCC23CCCC(O2)C2=C(CCCC2=O)O3)cc1.[HH].[Pd]>>COCOc1ccc(CCCCC23CCCC(O2)C2=C(CCCC2=O)O3)cc1
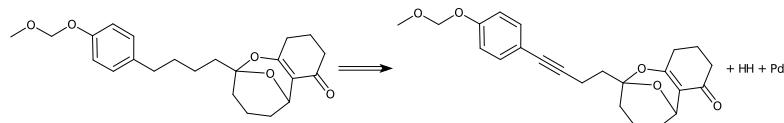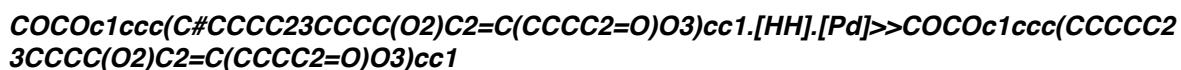


## Step 3

### Type: Iodo Sonogashira coupling, Confidence: 0.923
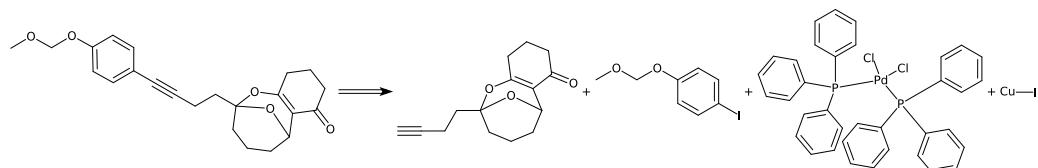
C#CCCC12CCCC(O1)C1=C(CCCC1=O)O2.COCOc1ccc(I)cc1.Cl[Pd](Cl)([P](c1ccccc1)(c1ccccc1)c1ccccc1)[P](c1ccccc1)(c1ccccc1)c1ccccc1.[Cu]I>>COCOc1ccc(C#CCCC23CCCC(O2)C2=C(CCCC2=O)O3)cc1



## Step 4

### Type: Undefined, Confidence: 0.0

C#CCCC12CCCC(O1)C1=C(CCCC1=O)O2>>C#CCCC12CCCC(O1)C1=C(CCCC1=O)O2
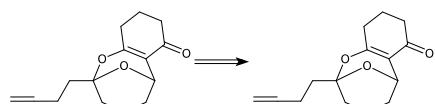
# Information about the retrosynthesis

Created On: 2019-09-26T17:08:12.317000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: N#CC1(CC1)COC1N=C(Cl)N=C(N2CCC(C3=NNC4=NC=NC=C34)CC2)N=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: N#CC1(CC1)COC1N=C(Cl)N=C(N2CCC(C3=NNC4=NC=NC=C34)CC2)N=1
Exclude substructures:

# Sequence 0, Confidence: 0.524

## Step 1

*Type: SNAr ether synthesis, Confidence: 0.926*

*Clc1nc(Cl)nc(N2CCC(c3n[nH]c4ncncc34)CC2)n1.N#CC1(CO)CC1>>N#CC1(COc2nc(Cl)nc(N3CCC(c4n[nH]c5ncncc45)CC3)n2)CC1*



## Step 2

*Type: Chloro N-arylation, Confidence: 0.862*

*c1ncc2c(C3CCNCC3)n[nH]c2n1.C1CCOC1.CCN(CC)CC.Clc1nc(Cl)nc(Cl)n1>>Clc1nc(Cl)nc(N2CCC(c3n[nH]c4ncncc34)CC2)n1*
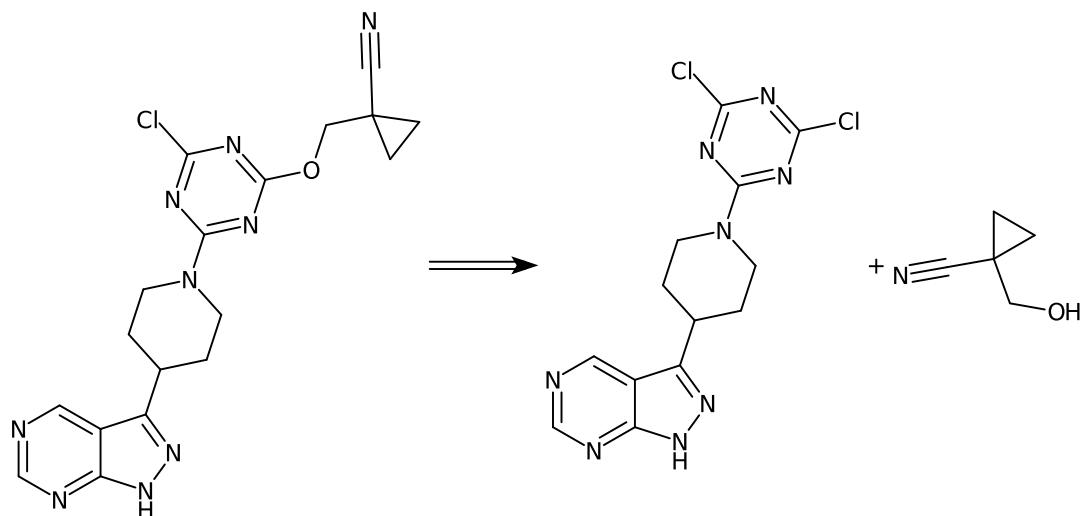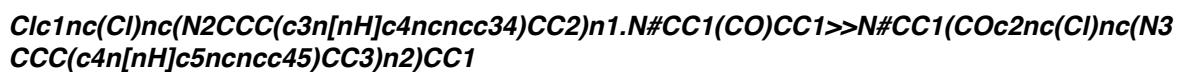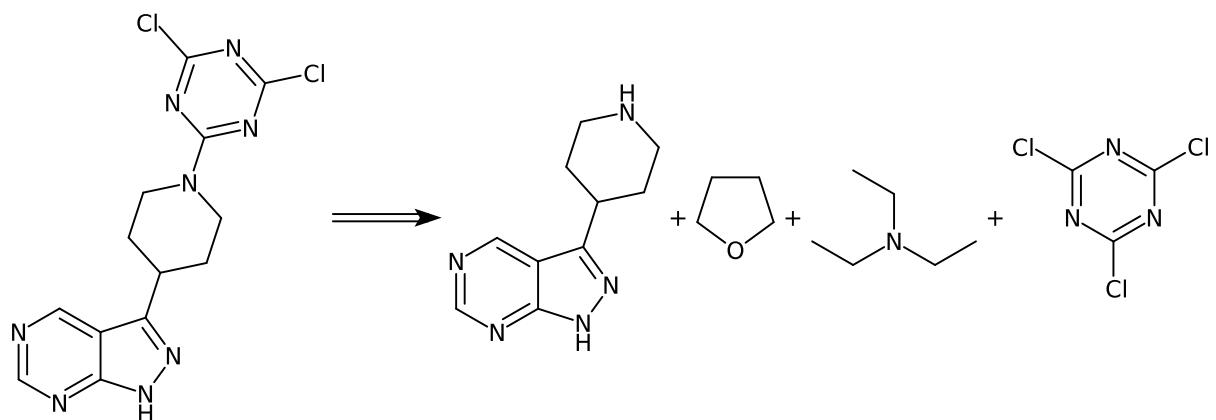


## Step 3

*Type: N-Boc deprotection, Confidence: 0.839*

*CC(C)(C)OC(=O)N1CCC(c2n[nH]c3ncncc23)CC1.Cl>>c1ncc2c(C3CCNCC3)n[nH]c2n1*
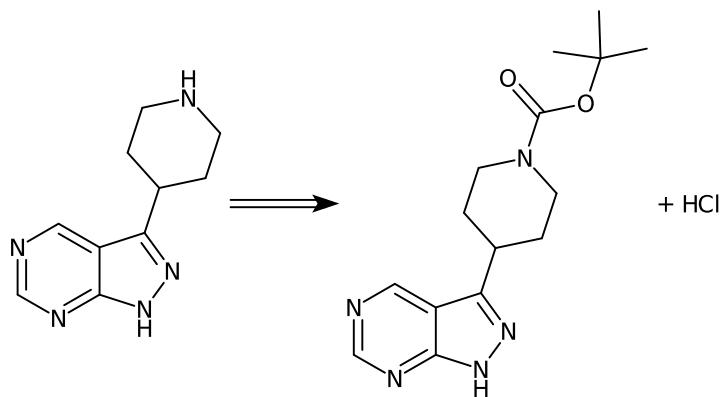
**Step 4**

*Type: Alkene hydrogenation, Confidence: 0.905*

*CC(C)(C)OC(=O)N1CC=C(c2n[nH]c3ncncc23)CC1.CCO.[Pd]>>CC(C)(C)OC(=O)N1CCC(c2n[nH]c3ncncc23)CC1*
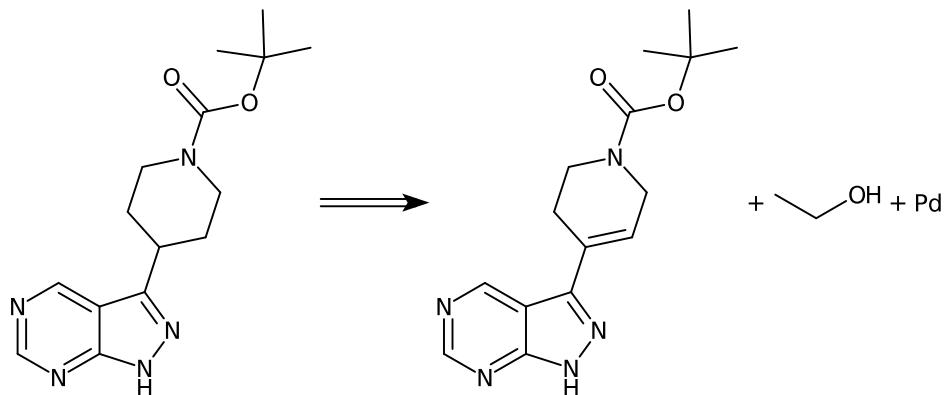


**Step 5**

*Type: Bromo Suzuki-type coupling, Confidence: 0.866*

*Brc1n[nH]c2ncncc12.CC(C)(C)OC(=O)N1CC=C(B2OC(C)(C)C(C)(C)O2)CC1>>CC(C)(C)OC(=O)N1CC=C(c2n[nH]c3ncncc23)CC1*
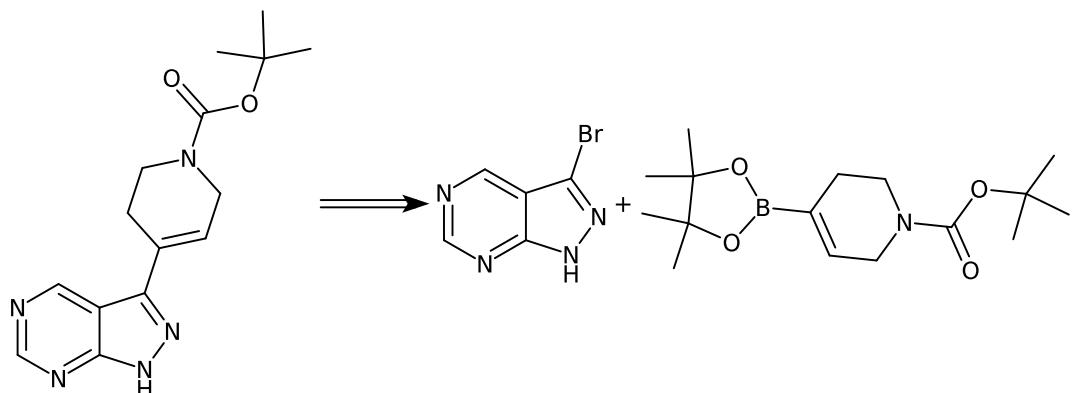
# Information about the retrosynthesis

Created On: 2019-09-26T17:08:24.616000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
C1NCCN(C(C2C=C(C3=NOC(CN(CCN4CCCCC4)C(CC4C=CC=CC=4)=O)=N3)C=CC=2)=O)CC1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
C1NCCN(C(C2C=C(C3=NOC(CN(CCN4CCCCC4)C(CC4C=CC=CC=4)=O)=N3)C=CC=2)=O)CC1
Exclude substructures:

## Sequence 0, Confidence: 0.723

### Step 1

*Type: N-Boc deprotection, Confidence: 0.929*
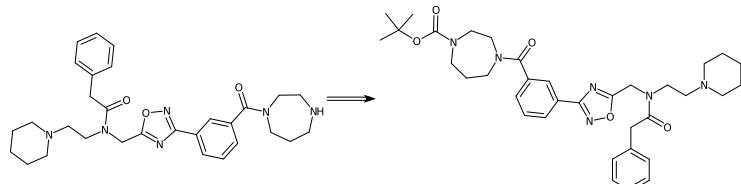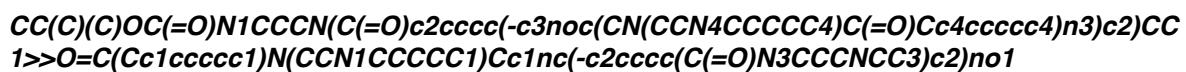
*CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CN(CCN4CCCCC4)C(=O)Cc4ccccc4)n3)c2)CC
1>>O=C(Cc1ccccc1)N(CCN1CCCCC1)Cc1nc(-c2cccc(C(=O)N3CCCNCC3)c2)no1*



### Step 2

*Type: Amide Schotten-Baumann, Confidence: 0.908*

*CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CNCCN4CCCCC4)n3)c2)CC1.O=C(Cl)Cc1cccc
c1.c1ccncc1>>CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CN(CCN4CCCCC4)C(=O)Cc4c
cccc4)n3)c2)CC1*



### Step 3

*Type: Chloro N-alkylation, Confidence: 0.902*

*CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CCl)n3)c2)CC1.CC#N.NCCN1CCCCC1.O=C([O
-])[O-].[K+].[K+]>>CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CNCCN4CCCCC4)n3)c2)CC
1*



### Step 4

*Type: Carboxylic acid + amine condensation, Confidence: 0.95*

*CC(C)(C)OC(=O)N1CCCNCC1.CCN(C(C)C)C(C)C.CN(C)C(On1nnc2cccnc21)=[N+](C)C.F[P-](F)
(F)(F)(F)F.ClCCl.O=C(O)c1cccc(-c2noc(CCl)n2)c1.CN(C)C(On1nnc2cccnc21)=[N+](C)C.F[P-](
F)(F)(F)(F)F>>CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CCl)n3)c2)CC1*

S 098
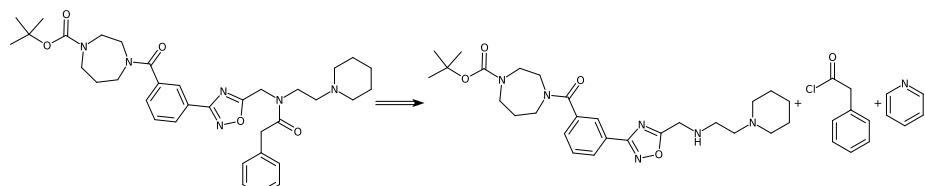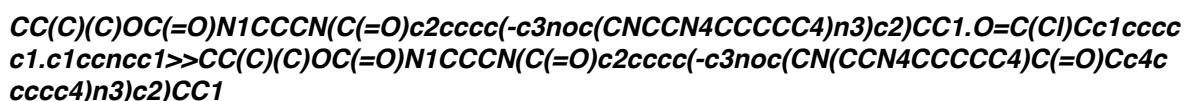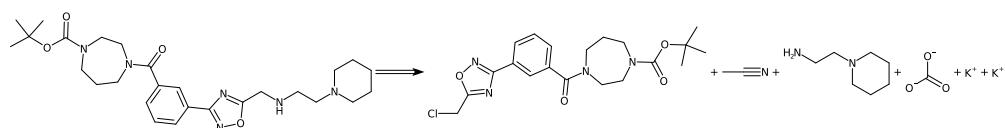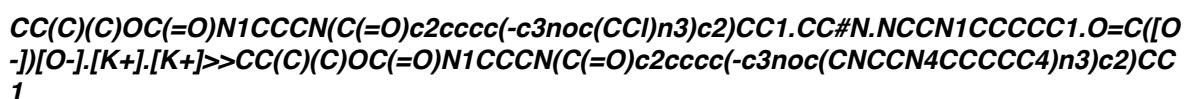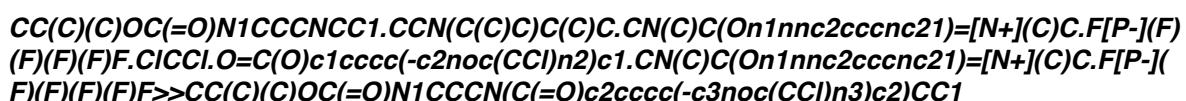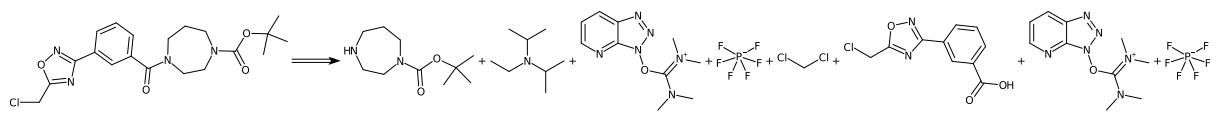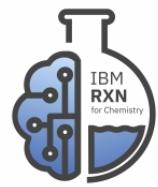
# Information about the retrosynthesis

Created On: 2019-10-01T13:05:14.059000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
O=C(N(CC1ON=C(C2C=C(C(N3CCNCCC3)=O)C=CC=2)N=1)CCN1CCCCC1)CC1C=CC=CC=1
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles:
O=C(N(CC1ON=C(C2C=C(C(N3CCNCCC3)=O)C=CC=2)N=1)CCN1CCCCC1)CC1C=CC=CC=1
Exclude substructures:

## Sequence 0, Confidence: 0.64

### Step 1

*Type: N-Boc deprotection, Confidence: 0.929*
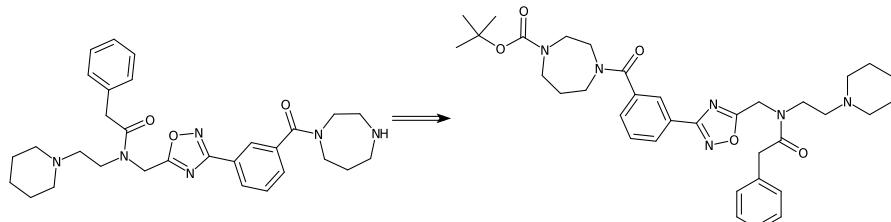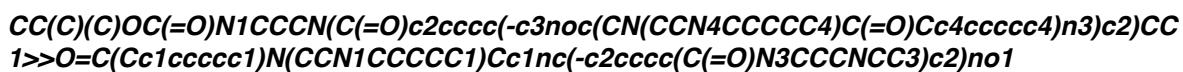
*CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CN(CCN4CCCCC4)C(=O)Cc4ccccc4)n3)c2)CC
1>>O=C(Cc1ccccc1)N(CCN1CCCCC1)Cc1nc(-c2cccc(C(=O)N3CCCNCC3)c2)no1*



### Step 2

*Type: Amide Schotten-Baumann, Confidence: 0.908*

*CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CNCCN4CCCCC4)n3)c2)CC1.O=C(Cl)Cc1cccc
c1.c1ccncc1>>CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CN(CCN4CCCCC4)C(=O)Cc4c
cccc4)n3)c2)CC1*



### Step 3

*Type: Chloro N-alkylation, Confidence: 0.902*

*CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CCl)n3)c2)CC1.CC#N.NCCN1CCCCC1.O=C([O
-])[O-].[K+].[K+]>>CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CNCCN4CCCCC4)n3)c2)CC
1*
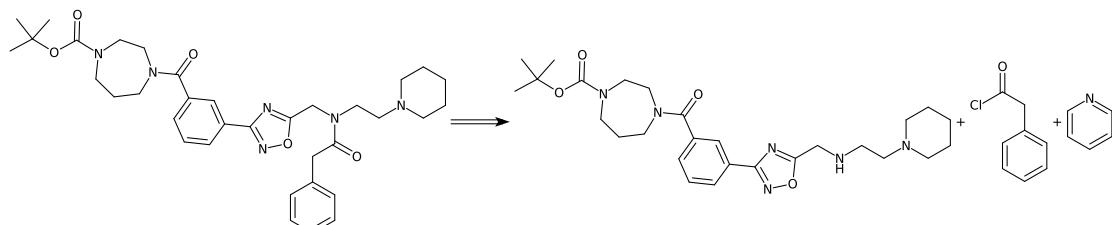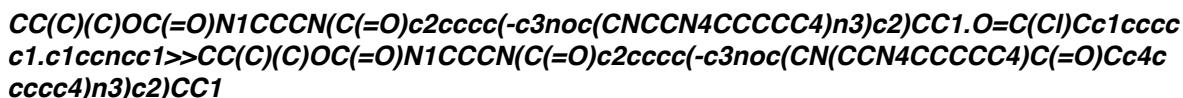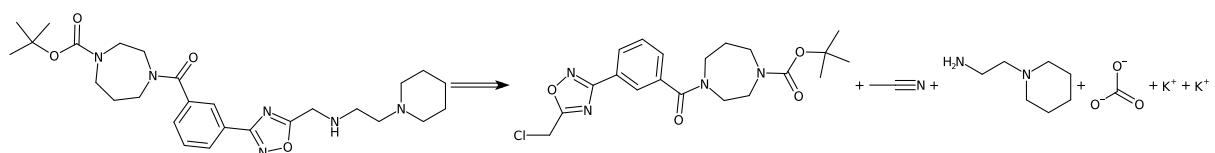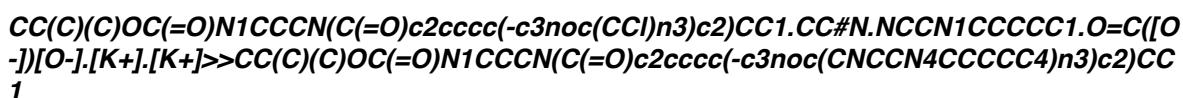


### Step 4

*Type: 1,2,4-Oxadiazole synthesis, Confidence: 0.938*

*CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(C(=N)NO)c2)CC1.C1CCOC1.CCN(CC)CC.O=C(Cl)CCl
>>CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(-c3noc(CCl)n3)c2)CC1*
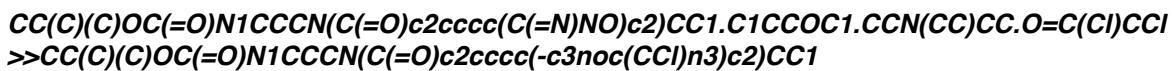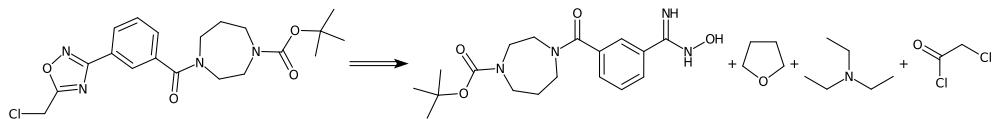
## Step 5

*Type: Cyano to Hydroxyamidino, Confidence: 0.979*
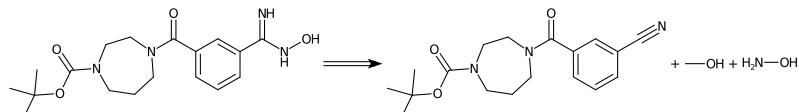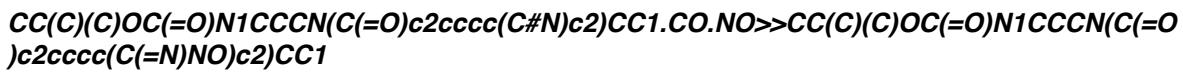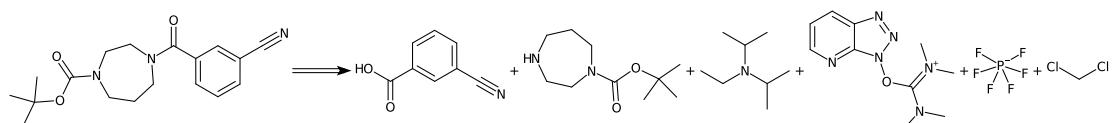
*CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(C#N)c2)CC1.CO.NO>>CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(C(=N)NO)c2)CC1*



## Step 6

*Type: Carboxylic acid + amine condensation, Confidence: 0.955*

*N#Cc1cccc(C(=O)O)c1.CC(C)(C)OC(=O)N1CCCNCC1.CCN(C(C)C)C(C)C.CN(C)C(On1nnc2cccnc21)=[N+](C)C.F[P-](F)(F)(F)(F)F.ClCCl>>CC(C)(C)OC(=O)N1CCCN(C(=O)c2cccc(C#N)c2)CC1*



## Step 7

*Type: Unrecognized, Confidence: 0.977*

*Cc1cccc(C#N)c1.O.O=[Mn](=O)(=O)[O-].[K+]>>N#Cc1cccc(C(=O)O)c1*



## Step 8

*Type: Rosenmund van Braun cyanation, Confidence: 0.984*
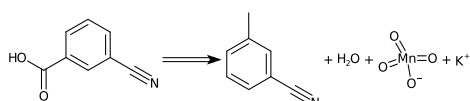
*Cc1cccc(Br)c1.N#C[Cu]>>Cc1cccc(C#N)c1*
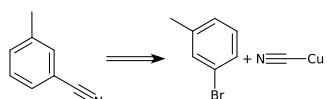


## Step 9

*Type: Amino to bromo, Confidence: 0.997*

**Br.Cc1cccc(N)c1.O=N[O-].[Na+].[Cu]Br.O=N[O-].[Na+]>>Cc1cccc(Br)c1**
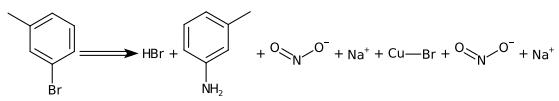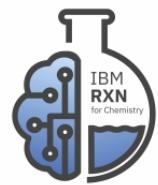
# Information about the retrosynthesis

Created On: 2019-09-26T17:09:14.562000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1N(C2N=C(N3CCOCC3)C=C(C3C(C(F)(F)F)=C4C(NC=C4)=NC=3)N=2)CCOC1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1N(C2N=C(N3CCOCC3)C=C(C3C(C(F)(F)F)=C4C(NC=C4)=NC=3)N=2)CCOC1
Exclude substructures:

# Sequence 0, Confidence: 0.9

## Step 1

**Type: Chloro Suzuki-type coupling, Confidence: 0.973**
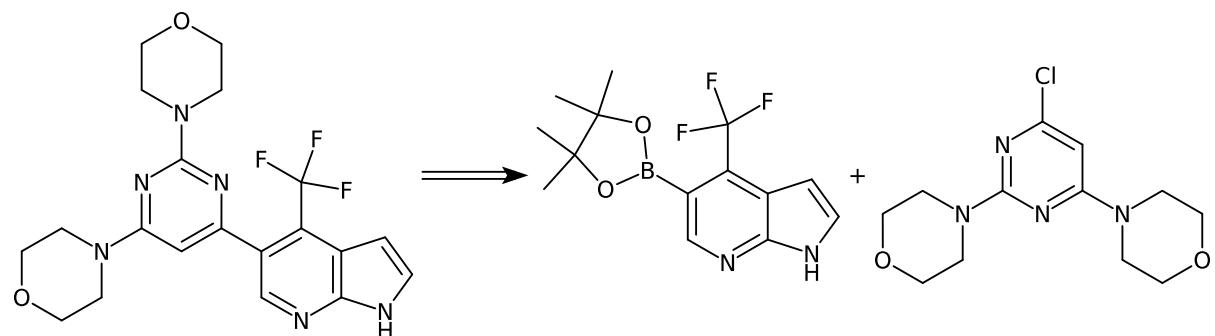
*CC1(C)OB(c2cnc3[nH]ccc3c2C(F)(F)F)OC1(C)C.Clc1cc(N2CCOCC2)nc(N2CCOCC2)n1>>FC(F)(F)c1c(-c2cc(N3CCOCC3)nc(N3CCOCC3)n2)cnc2[nH]ccc12*



## Step 2

**Type: Bromo Miyaura boration, Confidence: 0.926**

*CC1(C)OB(B2OC(C)(C)C(C)(C)O2)OC1(C)C.FC(F)(F)c1c(Br)cnc2[nH]ccc12>>CC1(C)OB(c2cnc3[nH]ccc3c2C(F)(F)F)OC1(C)C*
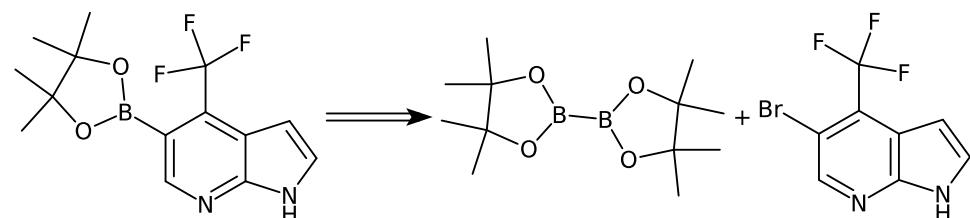
# Information about the retrosynthesis

Created On: 2019-10-01T13:20:26.992000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: FC(C1C2=C(NC=C2)N=CC=1C1N=C(N2CCOCC2)N=C(N2CCOCC2)C=1)(F)F
MSSR: 15
FAP: 0.7
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: FC(C1C2=C(NC=C2)N=CC=1C1N=C(N2CCOCC2)N=C(N2CCOCC2)C=1)(F)F
Exclude substructures:

# Sequence 0, Confidence: 0.467

Metadata:
Errors: No predictions above FAP. Reduce FAP, increase MRP or inspect siblings.

## Step 1

### Type: Mesyl N-arylation, Confidence: 0.986

CS(=O)(=O)c1nc(-c2cnc3[nH]ccc3c2C(F)(F)F)cc(N2CCOCC2)n1.C1COCCN1>>FC(F)(F)c1c(-c2cc(N3CCOCC3)nc(N3CCOCC3)n2)cnc2[nH]ccc12
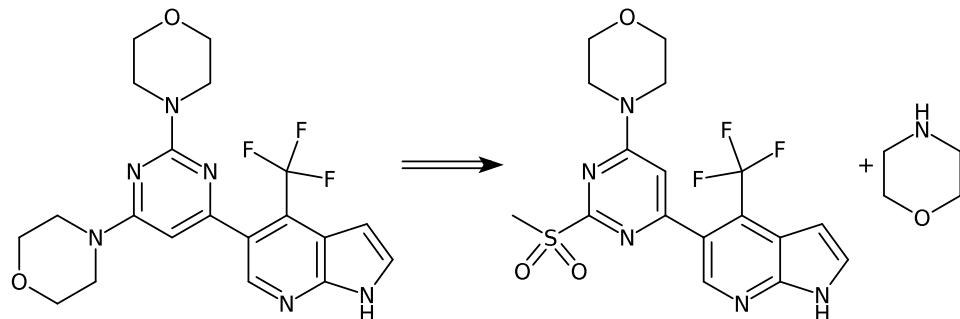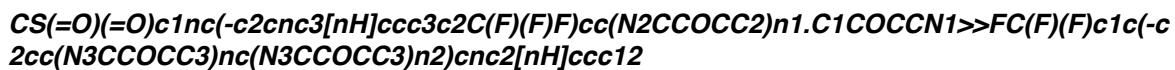


## Step 2

### Type: Sulfanyl to sulfonyl, Confidence: 0.901
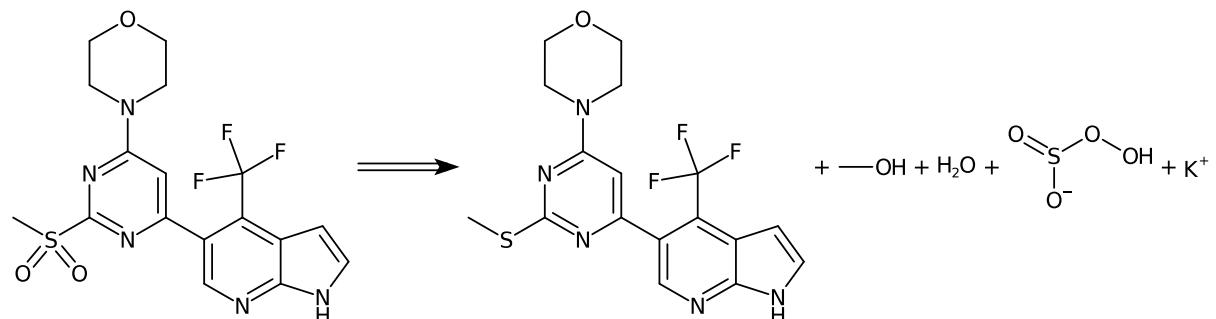
CSc1nc(-c2cnc3[nH]ccc3c2C(F)(F)F)cc(N2CCOCC2)n1.CO.O.O=S([O-])OO.[K+]>>CS(=O)(=O)c1nc(-c2cnc3[nH]ccc3c2C(F)(F)F)cc(N2CCOCC2)n1



## Step 3

### Type: Chloro Suzuki-type coupling, Confidence: 0.982

CSc1nc(Cl)cc(N2CCOCC2)n1.OB(O)c1cnc2[nH]ccc2c1C(F)(F)F>>CSc1nc(-c2cnc3[nH]ccc3c2C(F)(F)F)cc(N2CCOCC2)n1
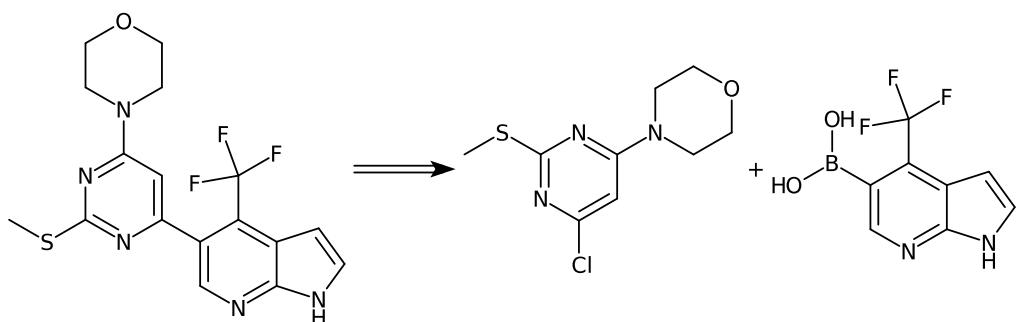
## Step 4

*Type: Chloro N-arylation, Confidence: 0.985*

*CSc1nc(Cl)cc(Cl)n1.C1COCCN1.O>>CSc1nc(Cl)cc(N2CCOCC2)n1*
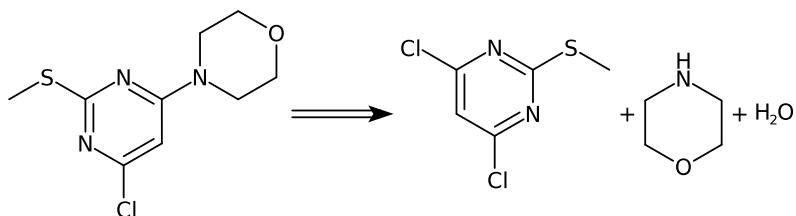


*Type: Bromo to borono, Confidence: 0.941*

*FC(F)(F)c1c(Br)cnc2[nH]ccc12.CC(C)OB(OC(C)C)OC(C)C.[Li]CCCC>>OB(O)c1cnc2[nH]ccc2c1C(F)(F)F*
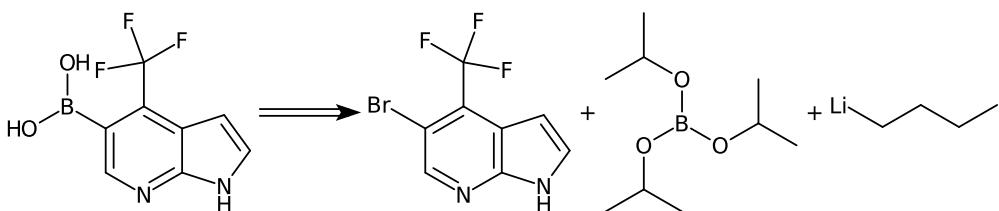


## Step 5

*Type: Hydroxy to chloro, Confidence: 0.983*

*CSc1nc(O)cc(O)n1.O=P(Cl)(Cl)Cl.[Na+].[OH-]>>CSc1nc(Cl)cc(Cl)n1*
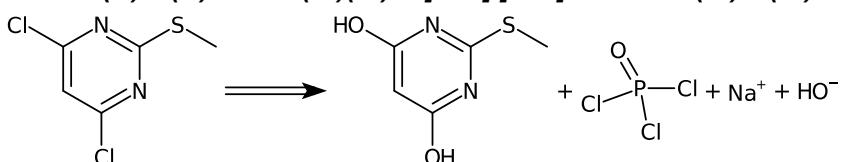


*Type: Unrecognized, Confidence: 0.973*

CC(C)[Si](C(C)C)(C(C)C)n1ccc2c(C(F)(F)F)c(Br)cnc21.CCCC[N+](CCCC)(CCCC)CCCC.[F-]>>F
C(F)(F)c1c(Br)cnc2[nH]ccc12



## Step 6

*Type: Unrecognized, Confidence: 0.848*

*CSC(=N)N.CCO.CCOC(=O)CC(=O)OCC>>CSc1nc(O)cc(O)n1*



*Type: Undefined, Confidence: 0.0*

CC(C)[Si](C(C)C)(C(C)C)n1ccc2c(C(F)(F)F)c(Br)cnc21>>CC(C)[Si](C(C)C)(C(C)C)n1ccc2c(C(F
)(F)F)c(Br)cnc21
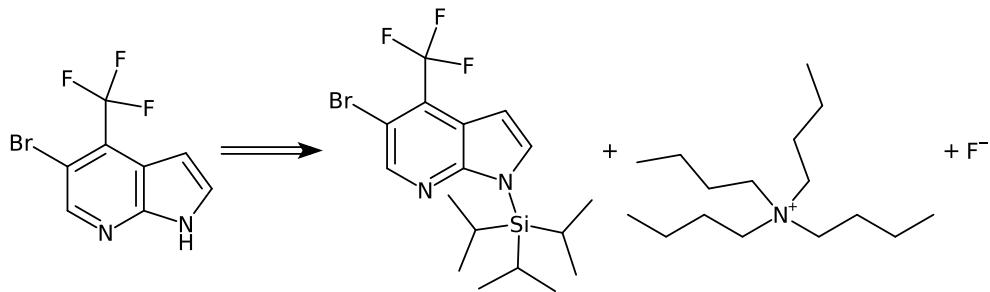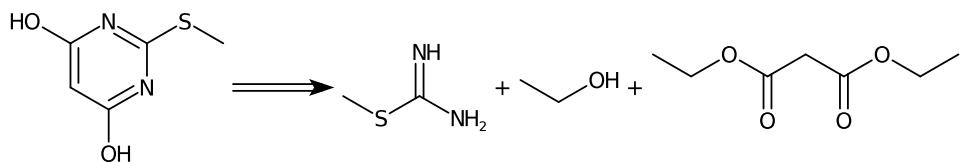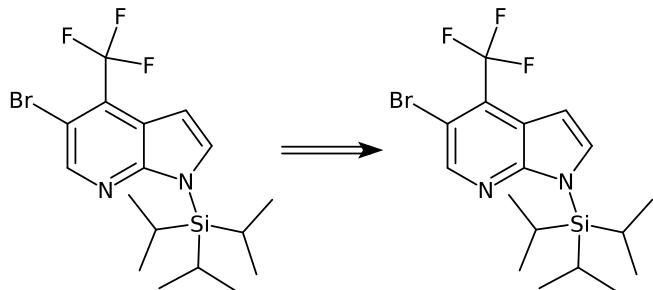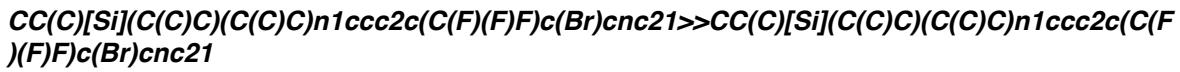


## Step 7

*Type: S-methylation, Confidence: 0.712*

*Cl.NC(N)=S.O=C([O-])[O-].[K+].[K+].O=C([O-])[O-].[K+].[K+]>>CSC(=N)N*
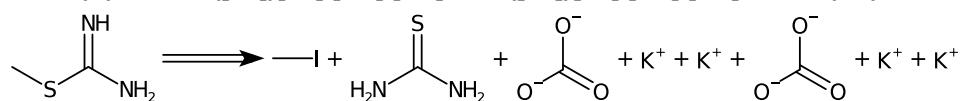
## Information about the retrosynthesis

Created On: 2019-10-01T19:46:55.746000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: FC(C1C2=C(NC=C2)N=CC=1C1N=C(N2CCOCC2)N=C(N2CCOCC2)C=1)(F)F
MSSR: 15
FAP: 0.6
MRP: 50
SbP: 3
Available smiles: C1=CC=CC=C1
Exclude smiles: FC(C1C2=C(NC=C2)N=CC=1C1N=C(N2CCOCC2)N=C(N2CCOCC2)C=1)(F)F
Exclude substructures:

# Sequence 0, Confidence: 0.181

## *Step 1*

**Type: Chloro N-arylation, Confidence: 0.973**
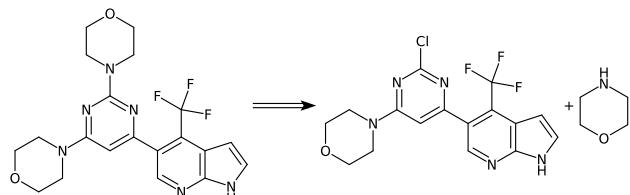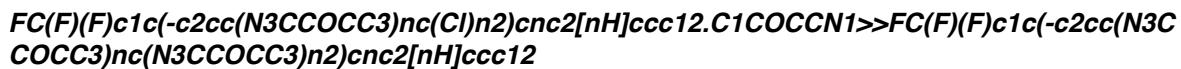
*FC(F)(F)c1c(-c2cc(N3CCOCC3)nc(Cl)n2)cnc2[nH]ccc12.C1COCCN1>>FC(F)(F)c1c(-c2cc(N3CCOCC3)nc(N3CCOCC3)n2)cnc2[nH]ccc12*



## *Step 2*

**Type: Chloro N-arylation, Confidence: 0.852**

*FC(F)(F)c1c(-c2cc(Cl)nc(Cl)n2)cnc2[nH]ccc12.C1COCCN1.O>>FC(F)(F)c1c(-c2cc(N3CCOCC3)nc(Cl)n2)cnc2[nH]ccc12*



## *Step 3*

**Type: Chloro Suzuki-type coupling, Confidence: 0.962**
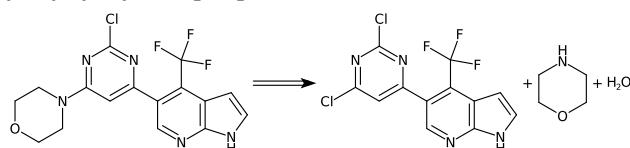
*CC1(C)OB(c2cnc3[nH]ccc3c2C(F)(F)F)OC1(C)C.Clc1cc(Cl)nc(Cl)n1>>FC(F)(F)c1c(-c2cc(Cl)nc(Cl)n2)cnc2[nH]ccc12*
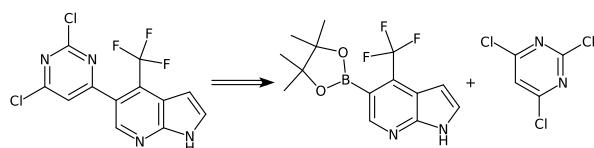


## *Step 4*

**Type: Iodo Miyaura boration, Confidence: 0.857**

*FC(F)(F)c1c(I)cnc2[nH]ccc12.C1COCCO1.CC(=O)[O-].[K+].CC1(C)OB(B2OC(C)(C)C(C)(C)O2)OC1(C)C.Cl[Pd]Cl.[Fe+2].c1ccc(P(c2ccccc2)[c-]2cccc2)cc1.c1ccc(P(c2ccccc2)[c-]2cccc2)cc1>>CC1(C)OB(c2cnc3[nH]ccc3c2C(F)(F)F)OC1(C)C*



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## Step 5

*Type: Unrecognized, Confidence: 0.96*

*CC(C)[Si](C(C)C)(C(C)C)n1ccc2c(C(F)(F)F)c(I)cnc21.C1CCOC1.CCCC[N+](CCCC)(CCCC)CCCC.[F-]>>FC(F)(F)c1c(I)cnc2[nH]ccc12*
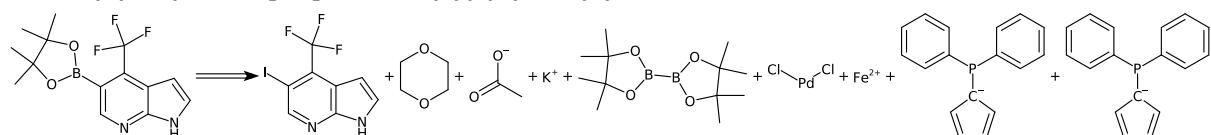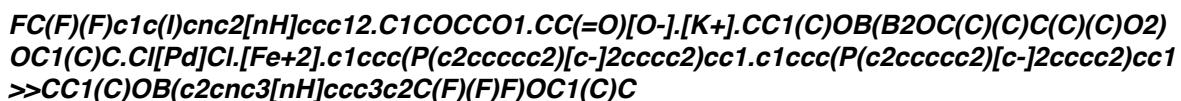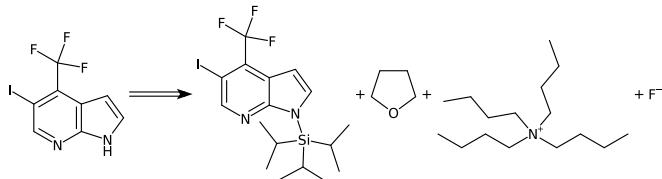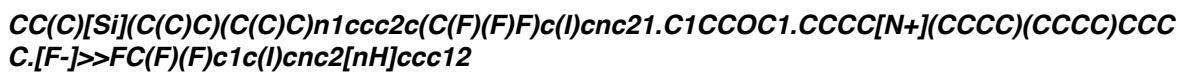


## Step 6

*Type: Iodination, Confidence: 0.673*

*CC(C)[Si](C(C)C)(C(C)C)n1ccc2c(C(F)(F)F)ccnc21.C1CCOC1.CC(C)[N-]C(C)C.[Li+].II.[Cl-].[NH4+]>>CC(C)[Si](C(C)C)(C(C)C)n1ccc2c(C(F)(F)F)c(I)cnc21*



## Step 7

*Type: Unrecognized, Confidence: 0.982*

*FC(F)(F)c1ccnc2[nH]ccc12.CC(C)[Si](Cl)(C(C)C)C(C)C.[NaH]>>CC(C)[Si](C(C)C)(C(C)C)n1ccc2c(C(F)(F)F)ccnc21*
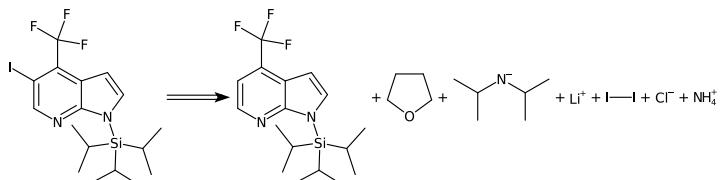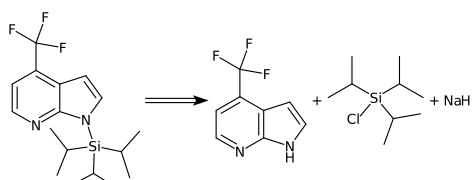


## Step 8

*Type: Indole synthesis, Confidence: 0.736*

*C[Si](C)(C)C#Cc1c(C(F)(F)F)ccnc1N.CN(C)C=O.[Cu]I>>FC(F)(F)c1ccnc2[nH]ccc12*
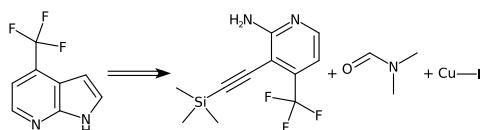


## Step 9

*Type: Bromo Sonogashira coupling, Confidence: 0.933*

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*Nc1nccc(C(F)(F)F)c1Br.C#C[Si](C)(C)C.CCN(CC)CC.Cl[Pd](Cl)([P](c1ccccc1)(c1ccccc1)c1ccc cc1)[P](c1ccccc1)(c1ccccc1)c1ccccc1.[Cu]I>>C[Si](C)(C)C#Cc1c(C(F)(F)F)ccnc1N*
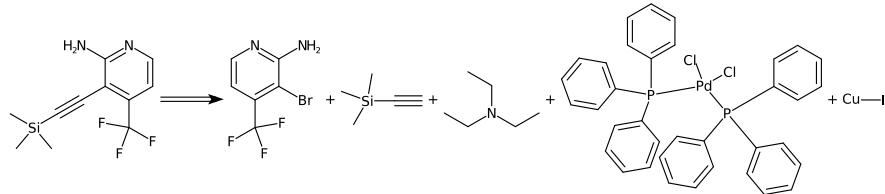


## Step 10

*Type: Chloro to amino, Confidence: 0.916*

*FC(F)(F)c1ccnc(Cl)c1Br.N>>Nc1nccc(C(F)(F)F)c1Br*
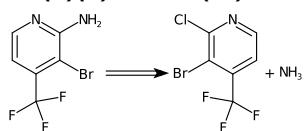


## Step 11

*Type: Unrecognized, Confidence: 0.766*

*[O-][n+]1ccc(C(F)(F)F)c(Br)c1.O=P(Cl)(Cl)Cl>>FC(F)(F)c1ccnc(Cl)c1Br*
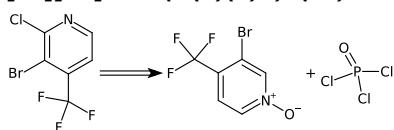


## Step 12

*Type: Nitrogen oxidation, Confidence: 0.992*

*FC(F)(F)c1ccncc1Br.ClCCl.O=C(OO)c1cccc(Cl)c1.[Na+].[OH-]>>[O-][n+]1ccc(C(F)(F)F)c(Br)c1*
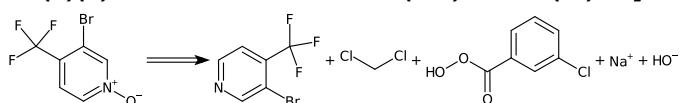


## Step 13

*Type: Unrecognized, Confidence: 0.872*

*Brc1cccnc1.C1CCOC1.CC(C)[N-]C(C)C.[Li+].FC(F)(F)I.CC(C)[N-]C(C)C.[Li+]>>FC(F)(F)c1ccnc c1Br*
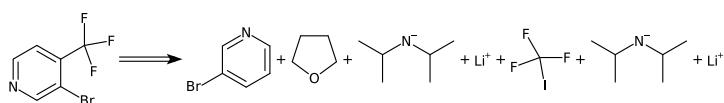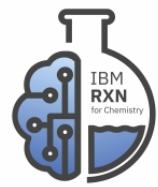
# Information about the retrosynthesis

Created On: 2019-09-26T17:09:25.559000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
C1C(COC2C=CC3=C(CCCC3CC(N(CC3C=CC=CC=3)CC3CC(O)C(O)C3)=O)C=2)=CC=CC=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
C1C(COC2C=CC3=C(CCCC3CC(N(CC3C=CC=CC=3)CC3CC(O)C(O)C3)=O)C=2)=CC=CC=1
Exclude substructures:

## Sequence 0, Confidence: 0.522

### *Step 1*

*Type: Upjohn dihydroxylation, Confidence: 0.771*
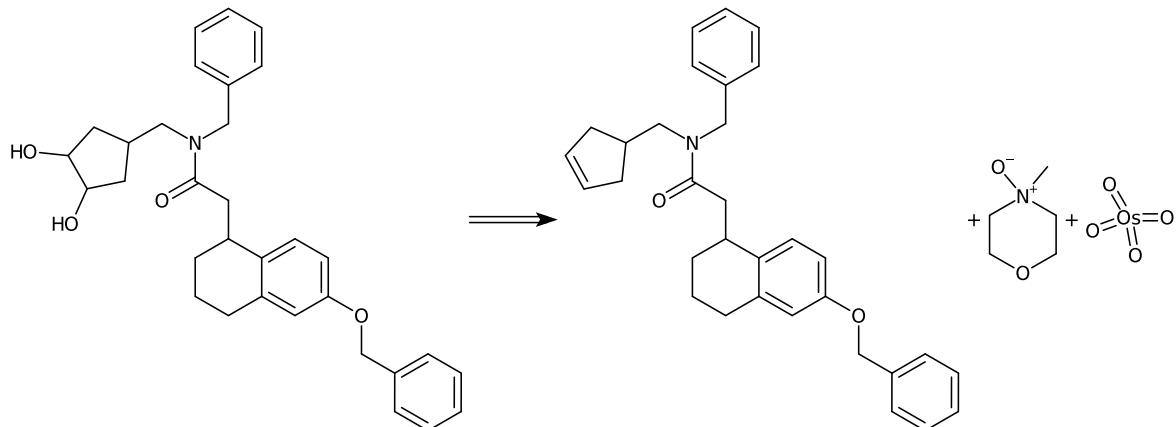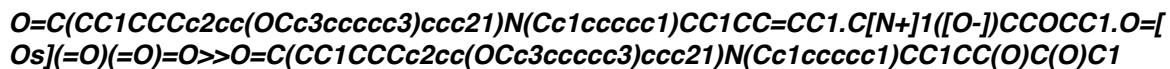
O=C(CC1CCCc2cc(OCc3ccccc3)ccc21)N(Cc1ccccc1)CC1CC=CC1.C[N+]1([O-])CCOCC1.O=[Os](=O)(=O)=O>>O=C(CC1CCCc2cc(OCc3ccccc3)ccc21)N(Cc1ccccc1)CC1CC(O)C(O)C1

### *Step 2*

*Type: Williamson ether synthesis, Confidence: 0.924*

O=C(CC1CCCc2cc(O)ccc21)N(Cc1ccccc1)CC1CC=CC1.BrCc1ccccc1.CN(C)C=O.[H-].[Na+]>>O=C(CC1CCCc2cc(OCc3ccccc3)ccc21)N(Cc1ccccc1)CC1CC=CC1

### *Step 3*

*Type: Carboxylic acid + amine condensation, Confidence: 0.884*

C1=CCC(CNCc2ccccc2)C1.O=C(O)CC1CCCc2cc(O)ccc21>>O=C(CC1CCCc2cc(O)ccc21)N(Cc1ccccc1)CC1CC=CC1
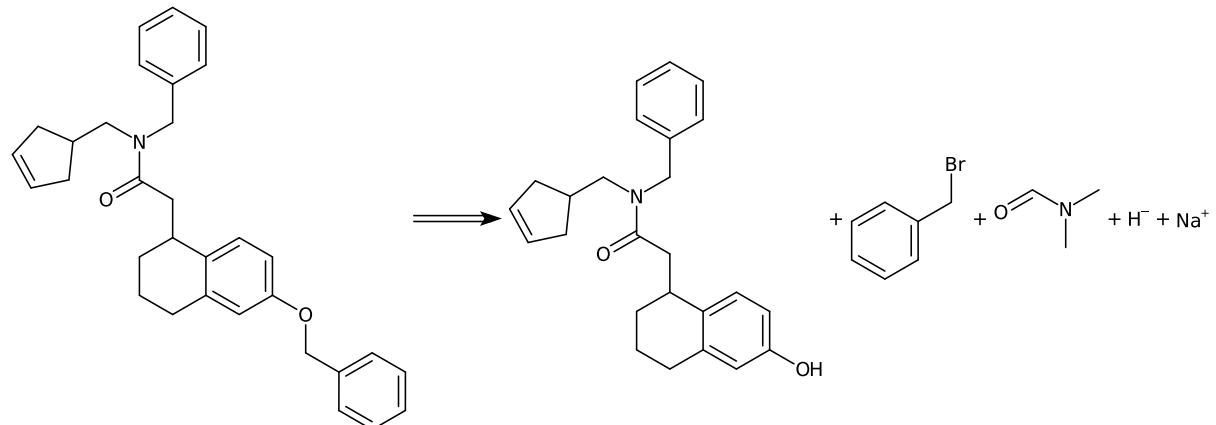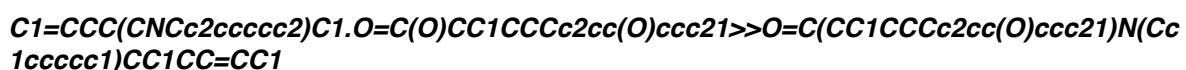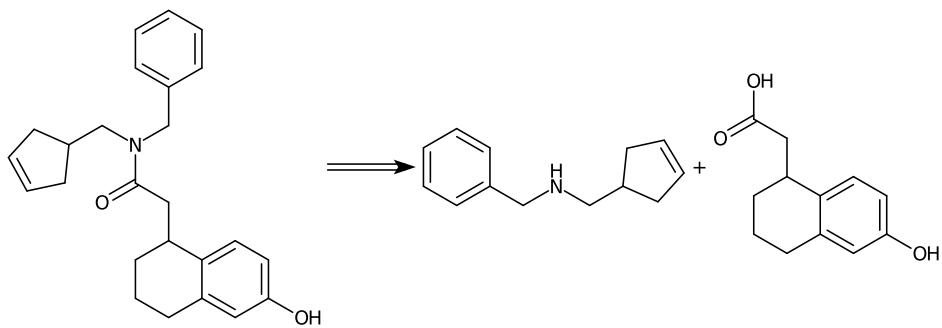
## Step 4

*Type: Aldehyde reductive amination, Confidence: 0.886*

*O=CC1CC=CC1.CC(=O)O[BH-](OC(C)=O)OC(C)=O.[Na+].ClCCl.NCc1ccccc1.O>>C1=CCC(CNCc2ccccc2)C1*
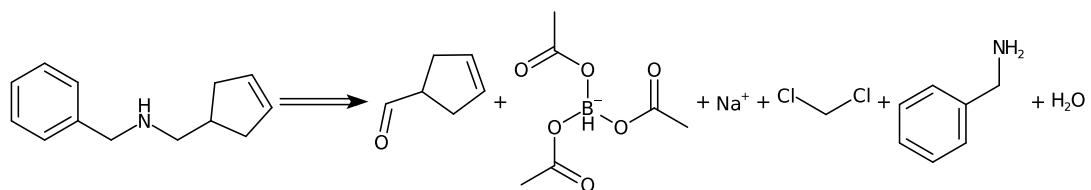


*Type: Methoxy to hydroxy, Confidence: 0.958*

*Br.COc1ccc2c(c1)CCCC2CC(=O)O.O>>O=C(O)CC1CCCc2cc(O)ccc21*
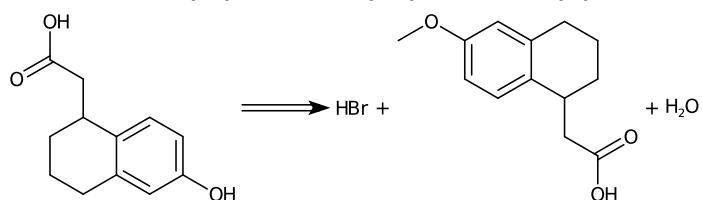


## Step 5

*Type: Aldehyde Collins oxidation, Confidence: 0.977*

*ClCCl.O=[Cr](=O)([O-])Cl.c1cc[nH+]cc1.OCC1CC=CC1.O=[Cr](=O)([O-])Cl.c1cc[nH+]cc1>>O=CC1CC=CC1*
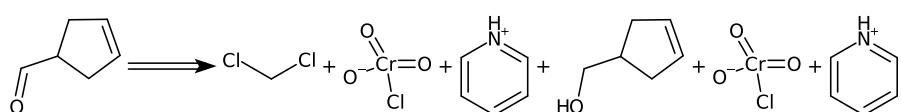
# Information about the retrosynthesis

Created On: 2019-10-01T13:35:23.042000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
O=C(N(CC1CC(O)C(O)C1)CC1C=CC=CC=1)CC1C2C(=CC(=CC=2)OCC2C=CC=CC=2)CCC1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles:
O=C(N(CC1CC(O)C(O)C1)CC1C=CC=CC=1)CC1C2C(=CC(=CC=2)OCC2C=CC=CC=2)CCC1
Exclude substructures:

# Sequence 0, Confidence: 0.267

Metadata:
Warnings: The retrosynthesis did not complete. Try increasing MSSR.

## Step 1

**Type: Upjohn dihydroxylation, Confidence: 0.771**
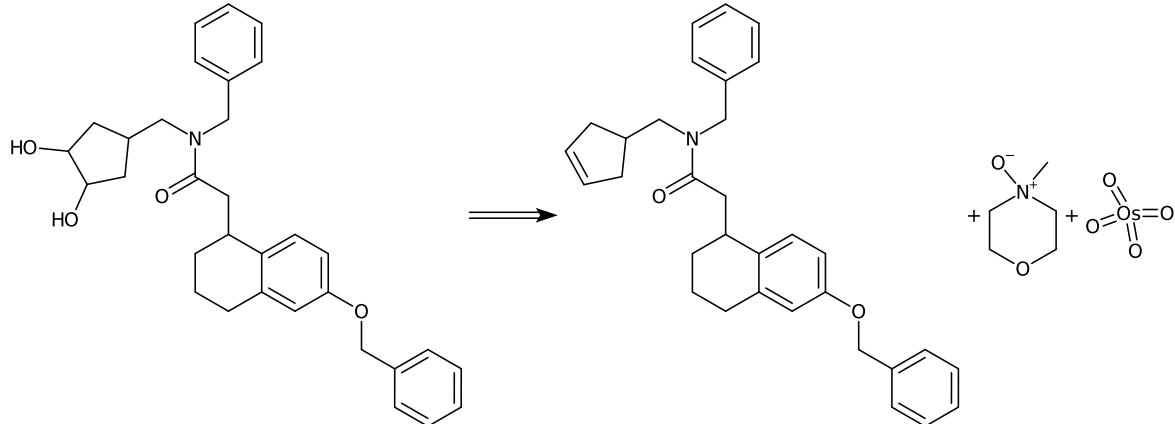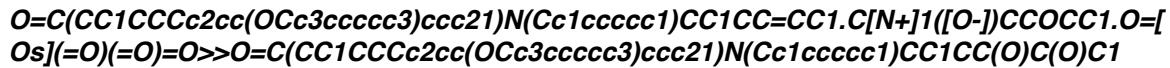
*O=C(CC1CCCc2cc(OCc3ccccc3)ccc21)N(Cc1ccccc1)CC1CC=CC1.C[N+]1([O-])CCOCC1.O=[Os](=O)(=O)=O>>O=C(CC1CCCc2cc(OCc3ccccc3)ccc21)N(Cc1ccccc1)CC1CC(O)C(O)C1*



## Step 2

**Type: Williamson ether synthesis, Confidence: 0.924**

*O=C(CC1CCCc2cc(O)ccc21)N(Cc1ccccc1)CC1CC=CC1.BrCc1ccccc1.CN(C)C=O.[H-].[Na+]>>O=C(CC1CCCc2cc(OCc3ccccc3)ccc21)N(Cc1ccccc1)CC1CC=CC1*



## Step 3

**Type: Carboxylic acid + amine condensation, Confidence: 0.884**

*C1=CCC(CNCc2ccccc2)C1.O=C(O)CC1CCCc2cc(O)ccc21>>O=C(CC1CCCc2cc(O)ccc21)N(Cc1ccccc1)CC1CC=CC1*



## Step 4

*Type: Aldehyde reductive amination, Confidence: 0.886*

*O=CC1CC=CC1.CC(=O)O[BH-](OC(C)=O)OC(C)=O.[Na+].ClCCl.NCc1ccccc1.O>>C1=CCC(CNCc2ccccc2)C1*



*Type: Methoxy to hydroxy, Confidence: 0.958*

*COc1ccc2c(c1)CCCC2CC(=O)O.Br.O>>O=C(O)CC1CCCc2cc(O)ccc21*



## Step 5

*Type: Aldehyde Collins oxidation, Confidence: 0.977*

*OCC1CC=CC1.ClCCl.O=[Cr](=O)([O-])Cl.c1cc[nH+]cc1>>O=CC1CC=CC1*



*Type: CO2H-Me deprotection, Confidence: 0.985*

*COC(=O)CC1CCCc2cc(OC)ccc21.CO.Cl.[Na+].[OH-]>>COc1ccc2c(c1)CCCC2CC(=O)O*
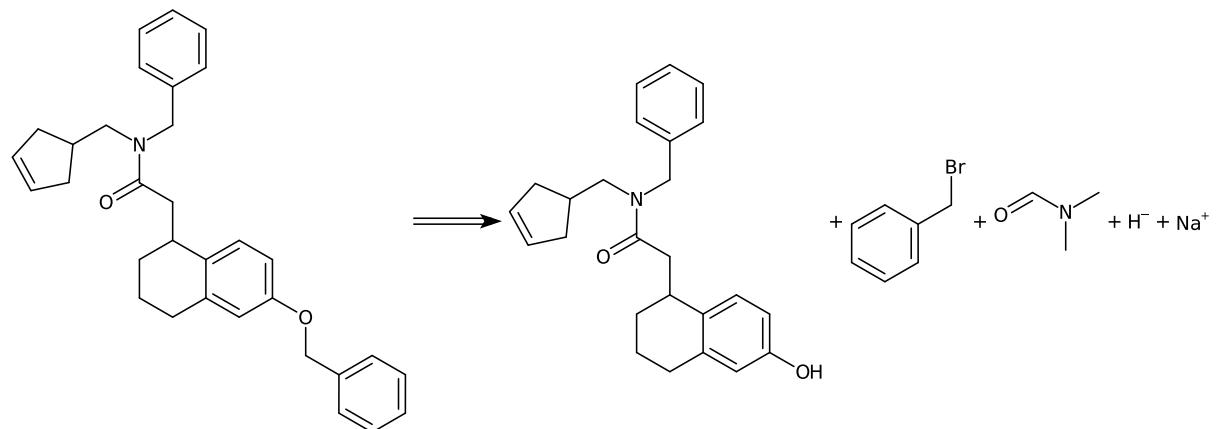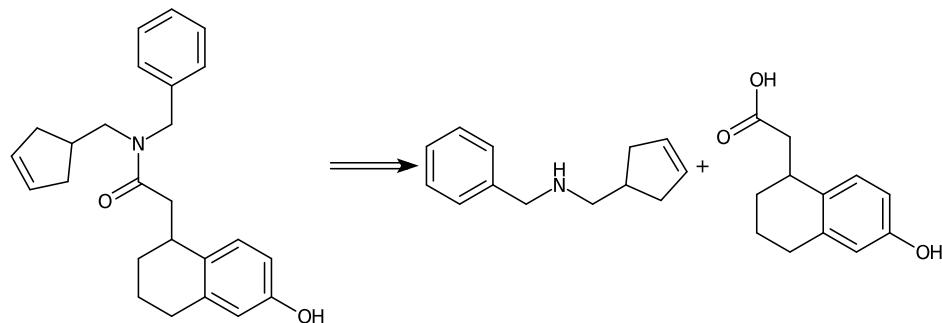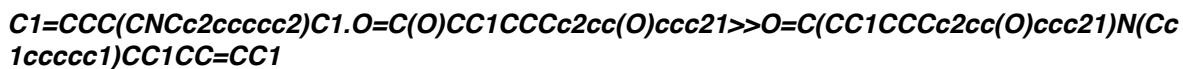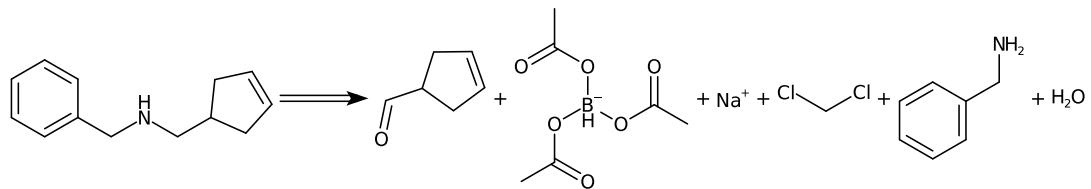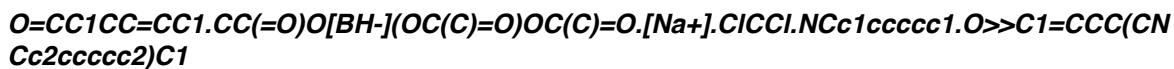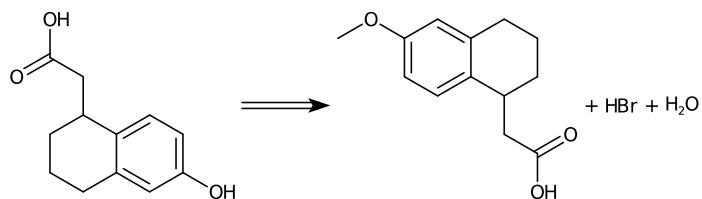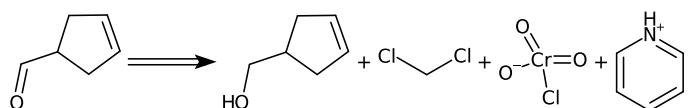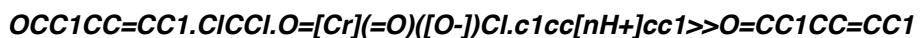
## Step 6

**Type: Ester to alcohol reduction, Confidence: 0.982**

**CCOC(=O)C1CC=CC1.[Al+3].[H-].[H-].[H-].[H-].[Li+]>>OCC1CC=CC1**



**Type: Alkene hydrogenation, Confidence: 0.979**

**COC(=O)C=C1CCCc2cc(OC)ccc21.CO.[HH].[Pd]>>COC(=O)CC1CCCc2cc(OC)ccc21**
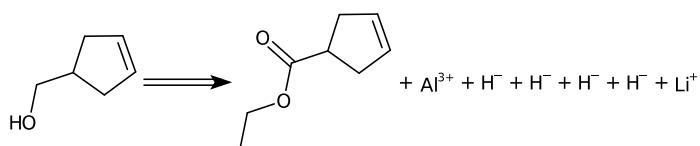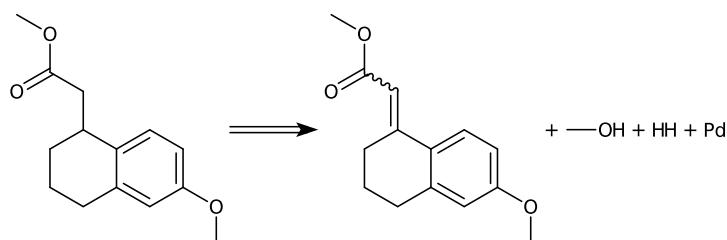


## Step 7

**Type: Ethyl esterification, Confidence: 0.936**

**O=C([O-])C1CC=CC1.CCO.Cc1ccc(S(=O)(=O)O)cc1>>CCOC(=O)C1CC=CC1**



**Type: Horner-Wadsworth-Emmons reaction, Confidence: 0.792**

**COc1ccc2c(c1)CCCC2=O.C1CCOC1.COC(=O)CP(=O)(OC)OC.[Li]CCCC>>COC(=O)C=C1CCC c2cc(OC)ccc21**
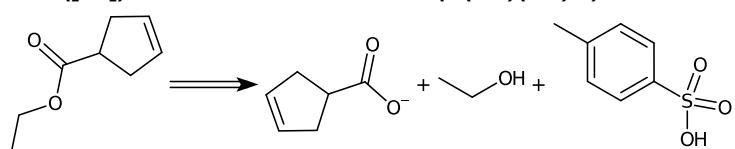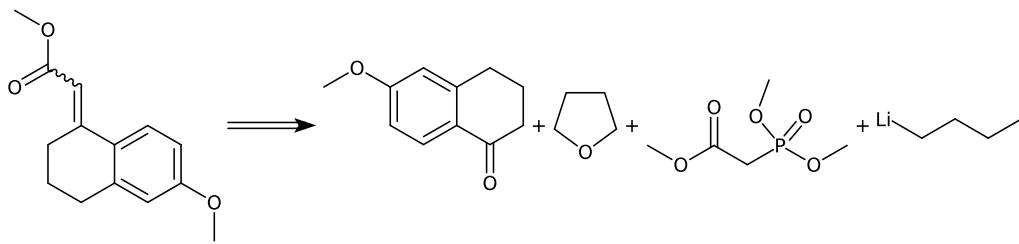
## Step 8

*Type: Undefined, Confidence: 0.0*

*O=C([O-])C1CC=CC1>>O=C([O-])C1CC=CC1*



*Type: Unrecognized, Confidence: 0.953*

*COc1cccc(CCCC(=O)O)c1.O=S(Cl)Cl.[Al+3].[Cl-].[Cl-].[Cl-]>>COc1ccc2c(c1)CCCC2=O*
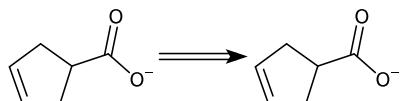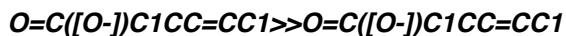


## Step 9

*Type: CO2H-Me deprotection, Confidence: 0.981*
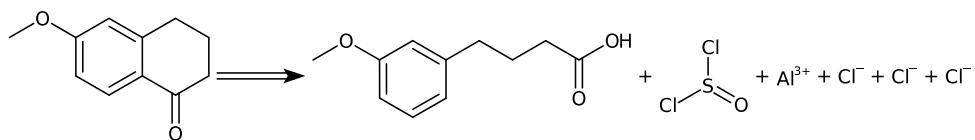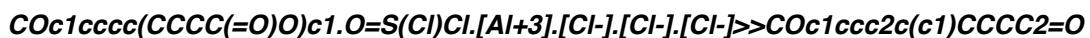
*COC(=O)CCCc1cccc(OC)c1.CO.[Na+].[OH-]>>COc1cccc(CCCC(=O)O)c1*
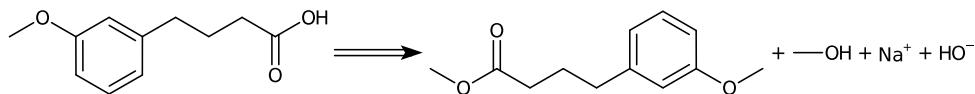


## Step 10

*Type: Alkene hydrogenation, Confidence: 0.973*

*COC(=O)/C=C/Cc1cccc(OC)c1.CO.[HH].[Pd]>>COC(=O)CCCc1cccc(OC)c1*



## Step 11

*Type: Horner-Wadsworth-Emmons reaction, Confidence: 0.843*

*COc1cccc(CC=O)c1.COC(=O)CP(=O)(OC)OC.[NaH]>>COC(=O)/C=C/Cc1cccc(OC)c1*
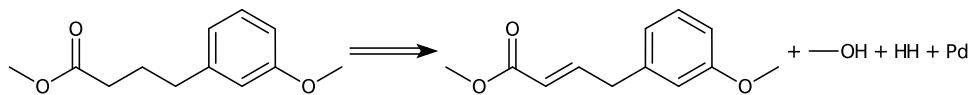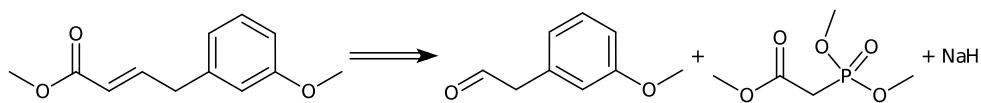
## Step 12

*Type: Cyano to formyl, Confidence: 0.98*

*COc1cccc(CC#N)c1.CC(C)C[AlH]CC(C)C.ClCCl>>COc1cccc(CC=O)c1*
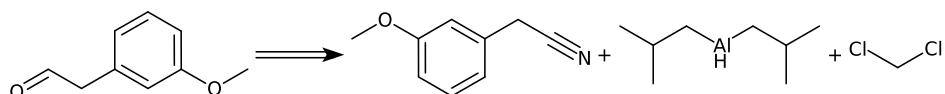


## Step 13

*Type: Bromo Kolbe nitrile synthesis, Confidence: 0.988*

*COc1cccc(CBr)c1.[C-]#N.[Na+]>>COc1cccc(CC#N)c1*
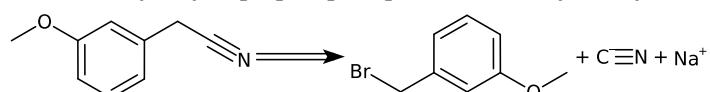


## Step 14

*Type: Hydroxy to bromo, Confidence: 0.992*

*COc1cccc(CO)c1.BrP(Br)Br>>COc1cccc(CBr)c1*
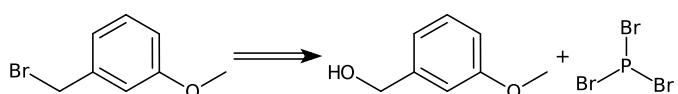


## Step 15

*Type: Carboxylic acid to alcohol reduction, Confidence: 0.99*

*COc1cccc(C(=O)O)c1.B.C1CCOC1>>COc1cccc(CO)c1*
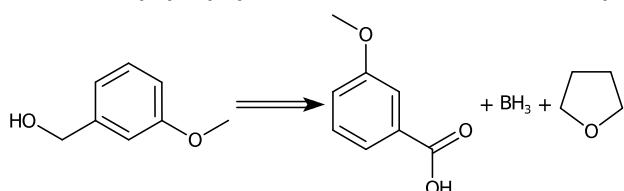
# Information about the retrosynthesis

Created On: 2019-10-01T19:53:53.373000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
O=C(N(CC1CC(O)C(O)C1)CC1C=CC=CC=1)CC1C2C(=CC(=CC=2)OCC2C=CC=CC=2)CCC1
MSSR: 15
FAP: 0.6
MRP: 50
SbP: 3
Available smiles: C1=CC=CC=C1
Exclude smiles:
O=C(N(CC1CC(O)C(O)C1)CC1C=CC=CC=1)CC1C2C(=CC(=CC=2)OCC2C=CC=CC=2)CCC1
Exclude substructures:

# Sequence 0, Confidence: 0.267

Metadata:
Warnings: The retrosynthesis did not complete. Try increasing MSSR.

## Step 1

*Type: Unrecognized, Confidence: 0.919*

*CC1(C)OC2CC(CN(Cc3ccccc3)C(=O)CC3CCCc4cc(OCc5ccccc5)ccc43)CC2O1.CO.Cl>>O=C(CC1CCCc2cc(OCc3ccccc3)ccc21)N(Cc1ccccc1)CC1CC(O)C(O)C1*



## Step 2

*Type: Amide Schotten-Baumann, Confidence: 0.83*

*CC1(C)OC2CC(CNCc3ccccc3)CC2O1.O=C(Cl)CC1CCCc2cc(OCc3ccccc3)ccc21>>CC1(C)OC2CC(CN(Cc3ccccc3)C(=O)CC3CCCc4cc(OCc5ccccc5)ccc43)CC2O1*
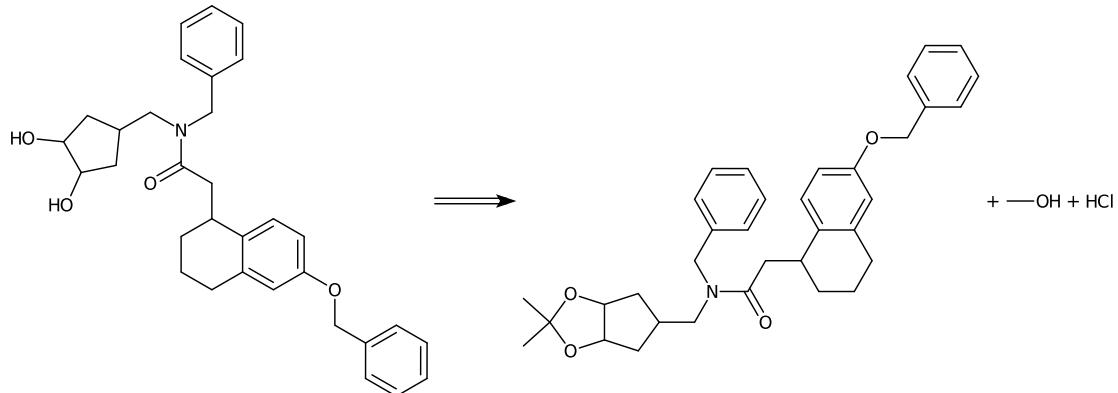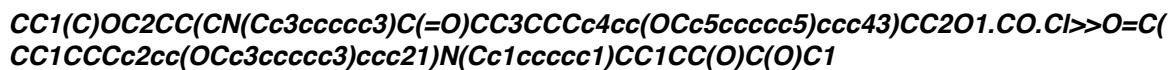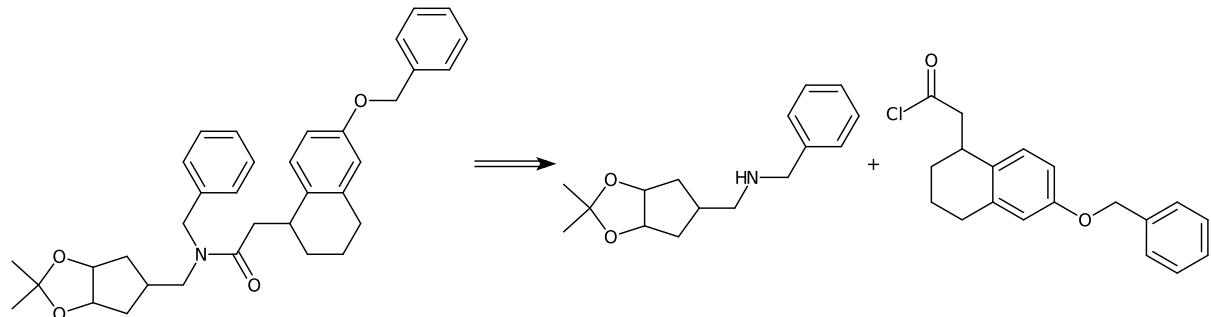


## Step 3

*Type: Tosyloxy N-alkylation, Confidence: 0.877*

*Cc1ccc(S(=O)(=O)OCC2CC3OC(C)(C)OC3C2)cc1.NCc1ccccc1>>CC1(C)OC2CC(CNCc3ccccc3)CC2O1*
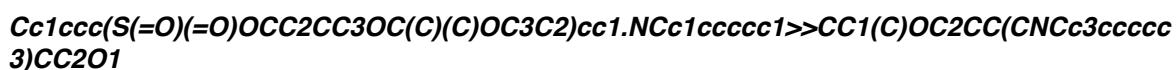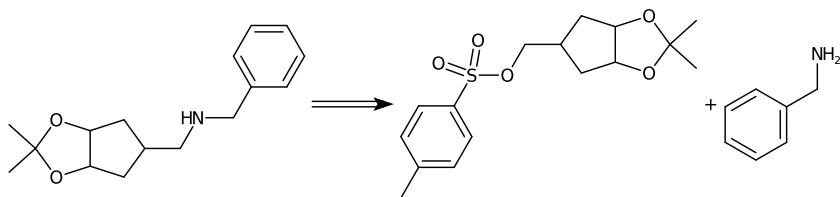
**Type: Carboxylic acid to acid chloride, Confidence: 0.896**

*O=C(O)CC1CCCc2cc(OCc3ccccc3)ccc21.ClCCl.O=S(Cl)Cl>>O=C(Cl)CC1CCCc2cc(OCc3ccccc3)ccc21*
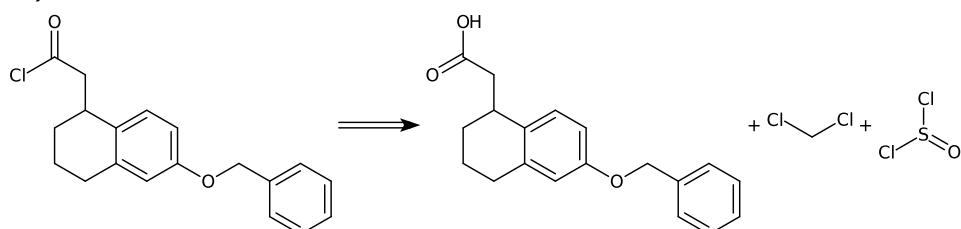


## Step 4

**Type: Sulfonic ester Schotten-Baumann, Confidence: 0.969**

*CC1(C)OC2CC(CO)CC2O1.Cc1ccc(S(=O)(=O)Cl)cc1>>Cc1ccc(S(=O)(=O)OCC2CC3OC(C)(C)OC3C2)cc1*
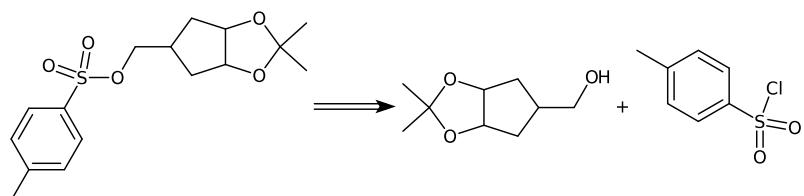


**Type: CO2H-Et deprotection, Confidence: 0.984**

*CCOC(=O)CC1CCCc2cc(OCc3ccccc3)ccc21.CO.O.[Na+].[OH-]>>O=C(O)CC1CCCc2cc(OCc3ccccc3)ccc21*
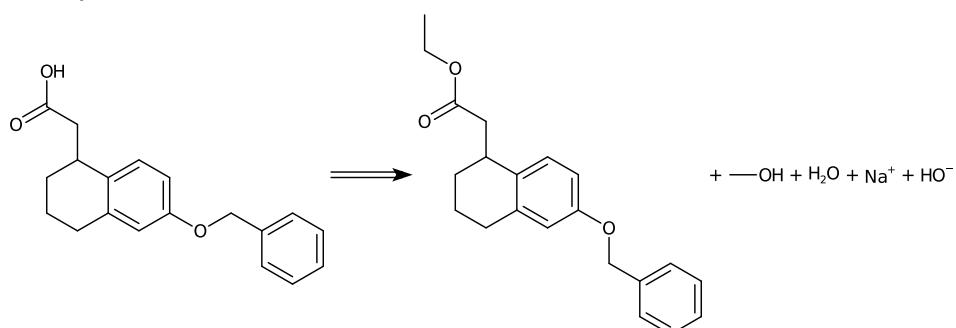


## Step 5

*Type: Ester to alcohol reduction, Confidence: 0.931*
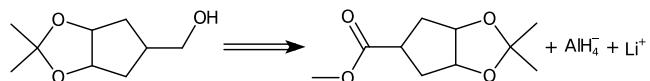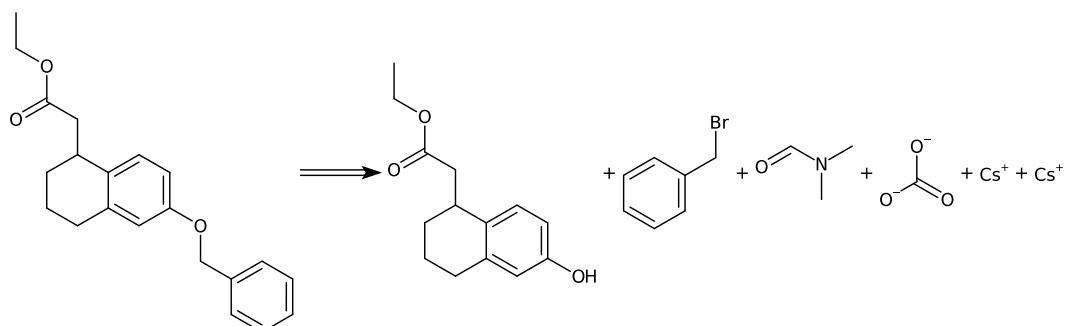
*COC(=O)C1CC2OC(C)(C)OC2C1.[AlH4-].[Li+]>>CC1(C)OC2CC(CO)CC2O1*



*Type: Williamson ether synthesis, Confidence: 0.948*

*CCOC(=O)CC1CCCc2cc(O)ccc21.BrCc1ccccc1.CN(C)C=O.O=C([O-])[O-].[Cs+].[Cs+]>>CCOC(=O)CC1CCCc2cc(OCc3ccccc3)ccc21*



## Step 6

*Type: Methyl esterification, Confidence: 0.97*

*CC1(C)OC2CC(C(=O)O)CC2O1.CI.CN(C)C=O.O=C([O-])[O-].[K+].[K+]>>COC(=O)C1CC2OC(C)(C)OC2C1*



*Type: Fischer-Speier esterification, Confidence: 0.987*

*O=C(O)CC1CCCc2cc(O)ccc21.CCO.O=S(=O)(O)O>>CCOC(=O)CC1CCCc2cc(O)ccc21*



## Step 7

*Type: CO2H-Et deprotection, Confidence: 0.915*

*CCOC(=O)C1CC2OC(C)(C)OC2C1.CO.[Na+].[OH-]>>CC1(C)OC2CC(C(=O)O)CC2O1*
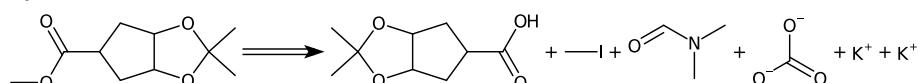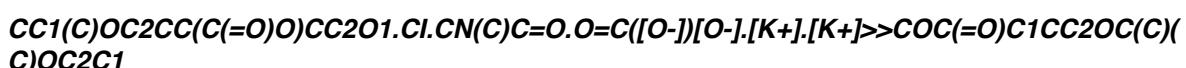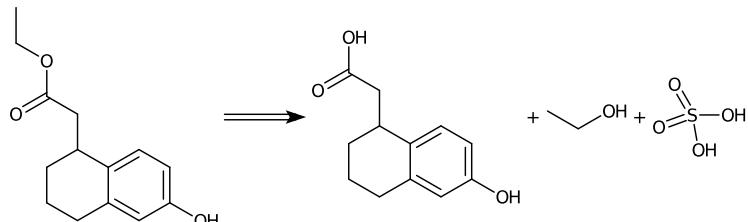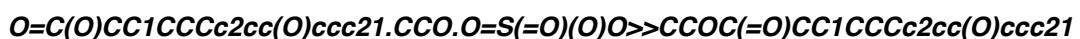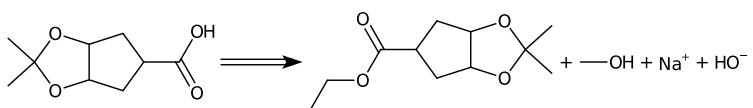
*Type: Methoxy to hydroxy, Confidence: 0.958*

**COc1ccc2c(c1)CCCC2CC(=O)O.Br.O>>O=C(O)CC1CCCc2cc(O)ccc21**
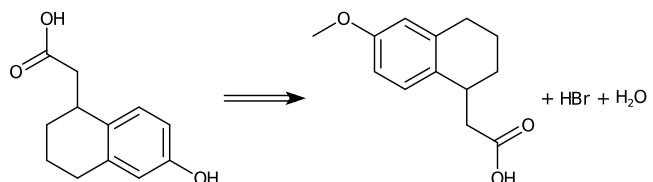


## Step 8

*Type: Unrecognized, Confidence: 0.893*

**CCOC(=O)C1CC(O)C(O)C1.COC(C)(C)OC.Cc1ccc(S(=O)(=O)O)cc1.Cc1ccccc1>>CCOC(=O)C1CC2OC(C)(C)OC2C1**
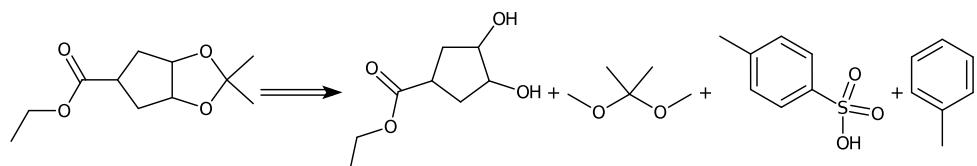


*Type: Alkene hydrogenation, Confidence: 0.948*

**COc1ccc2c(c1)CCC=C2CC(=O)O.[HH].[Pd]>>COc1ccc2c(c1)CCCC2CC(=O)O**
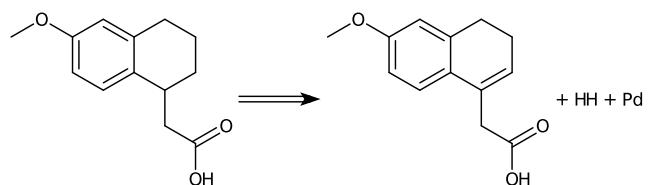


## Step 9

*Type: Milas hydroxylation, Confidence: 0.963*

**CCOC(=O)C1CC=CC1.O=[Os](=O)(=O)=O>>CCOC(=O)C1CC(O)C(O)C1**
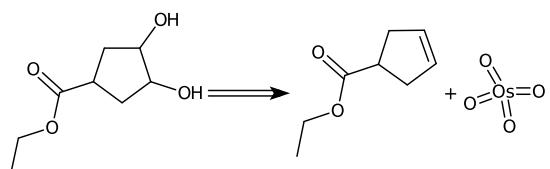
*Type: CO2H-Me deprotection, Confidence: 0.974*
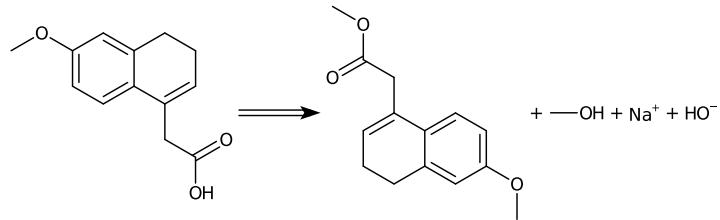
*COC(=O)CC1=CCCc2cc(OC)ccc21.CO.[Na+].[OH-]>>COc1ccc2c(c1)CCC=C2CC(=O)O*



## Step 10

*Type: Fischer-Speier esterification, Confidence: 0.991*

*O=C(O)C1CC=CC1.CCO.O=S(=O)(O)O>>CCOC(=O)C1CC=CC1*



*Type: Undefined, Confidence: 0.0*

*COC(=O)CC1=CCCc2cc(OC)ccc21>>COC(=O)CC1=CCCc2cc(OC)ccc21*



## Step 11

*Type: CO2H-Me deprotection, Confidence: 0.966*

*COC(=O)C1CC=CC1.C1CCOC1.O.[Li+].[OH-]>>O=C(O)C1CC=CC1*
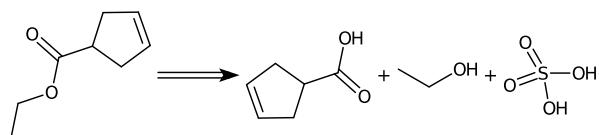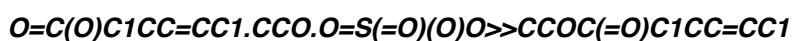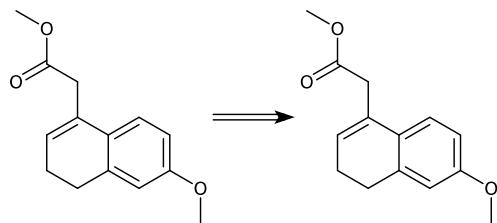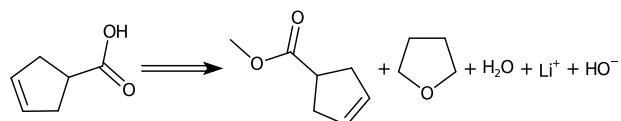


## Step 12

*Type: Olefin metathesis, Confidence: 0.931*

*C=CCC(CC=C)C(=O)OC.ClCCl>>COC(=O)C1CC=CC1*

## Step 13

*Type: Unrecognized, Confidence: 0.915*

*C=CCCC(=O)OC.C1CCOC1.C=CCBr.CC(C)NC(C)C.[Li]CCCC>>C=CCC(CC=C)C(=O)OC*
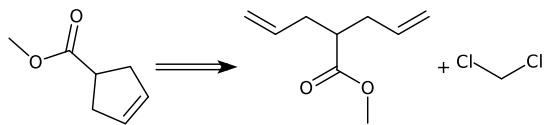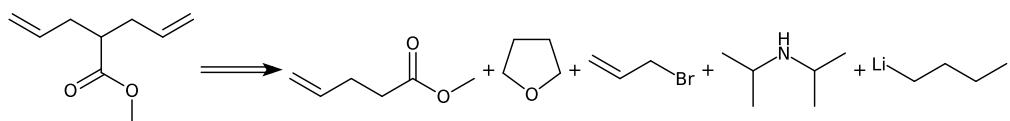


## Step 14

*Type: Methyl esterification, Confidence: 0.995*

*C=CCCC(=O)O.CO.C[Si](C)(C)C=[N+]=[N-].ClCCl>>C=CCCC(=O)OC*
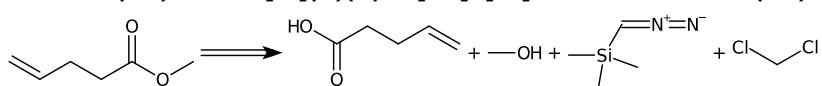


## Step 15

*Type: CO2H-Et deprotection, Confidence: 0.98*

*C=CCCC(=O)OCC.C1CCOC1.O.[Li]O>>C=CCC(=O)O*
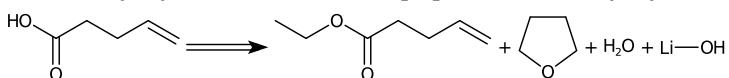
## Information about the retrosynthesis

Created On: 2019-09-26T17:09:37.740000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1C2(C(CCC3C2CCC2(C3CC(C2(O)C(C(CCC(COC(C)=O)C)=O)C)OS(=O)(=O)C)C)CC(OC(C)=O)C1)C
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1C2(C(CCC3C2CCC2(C3CC(C2(O)C(C(CCC(COC(C)=O)C)=O)C)OS(=O)(=O)C)C)CC(OC(C)=O)C1)C
Exclude substructures:

# Sequence 0, Confidence: 0.734

Metadata:
Warnings: 'ERROR MESSAGE'
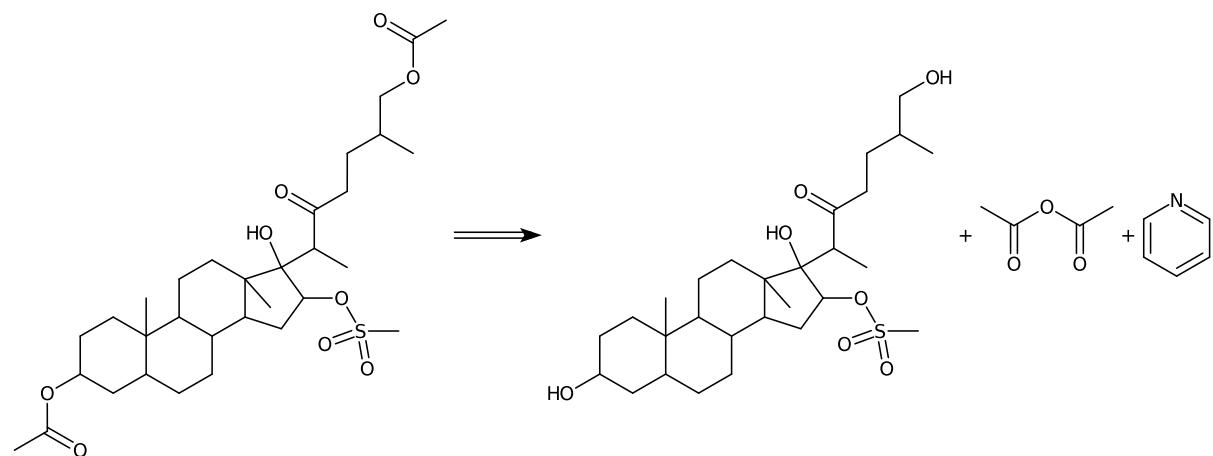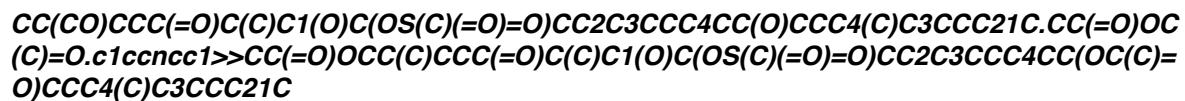
## *Step 1*

*Type: Unrecognized, Confidence: 0.734*

*CC(CO)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C.CC(=O)OC
(C)=O.c1ccncc1>>CC(=O)OCC(C)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(OC(C)=
O)CCC4(C)C3CCC21C*



## *Step 2*

*Type: Undefined, Confidence: 0.0*

*CC(CO)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C>>CC(CO)
CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C*
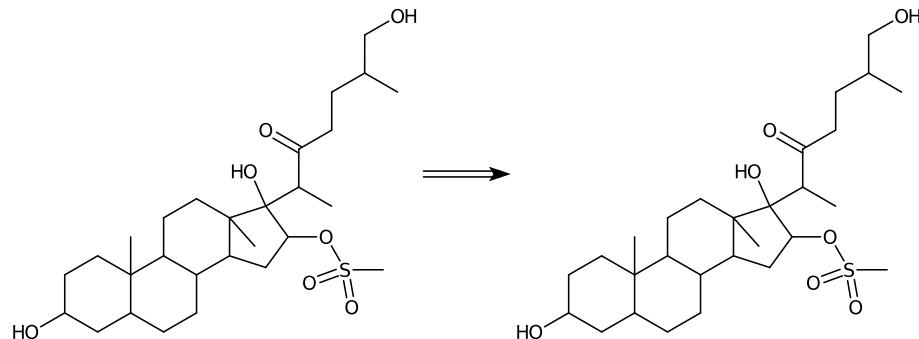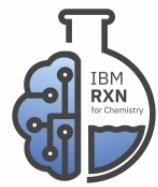
# Information about the retrosynthesis

Created On: 2019-10-01T13:32:30.614000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC(OCC(CCC(C(C1(C2(C(C3C(CC2)C2(C(CC(CC2)OC(=O)C)CC3)C)CC1OS(=O)(=O)C)C)O)C)=O)C)=O
MSSR: 15
FAP: 0.6
MRP: 50
SbP: 3
Available smiles:
Exclude smiles: CC(OCC(CCC(C(C1(C2(C(C3C(CC2)C2(C(CC(CC2)OC(=O)C)CC3)C)CC1OS(=O)(=O)C)C)O)C)=O)C)=O
Exclude substructures:

# Sequence 0, Confidence: 0.734

Metadata:
Errors: No predictions above FAP. Reduce FAP, increase MRP or inspect siblings.

## *Step 1*

*Type: Unrecognized, Confidence: 0.734*

*CC(CO)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C.CC(=O)OC(C)=O.c1ccncc1>>CC(=O)OCC(C)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(OC(C)=O)CCC4(C)C3CCC21C*



## *Step 2*

*Type: Undefined, Confidence: 0.0*

*CC(CO)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C>>CC(CO)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C*
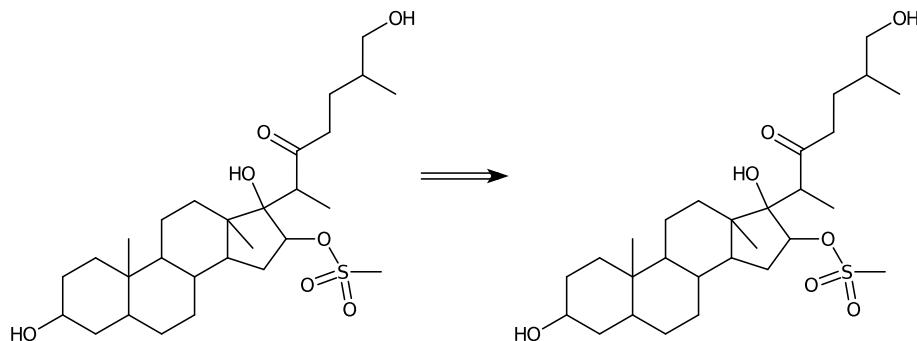
# Information about the retrosynthesis

Created On: 2019-10-01T19:56:40.172000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC(OCC(CCC(C(C1(C2(C(C3C(CC2)C2(C(CC(CC2)OC(=O)C)CC3)C)CC1OS(=O)(=O)C)C)O)C)=O)C)=O
MSSR: 15
FAP: 0.6
MRP: 50
SbP: 3
Available smiles: C(=O)1C2(C(C3C(CC2)C2(C(CC(CC2)OC(=O)C)CC3)C)CC1)C
Exclude smiles: CC(OCC(CCC(C(C1(C2(C(C3C(CC2)C2(C(CC(CC2)OC(=O)C)CC3)C)CC1OS(=O)(=O)C)C)O)C)=O)C)=O
Exclude substructures:

# Sequence 0, Confidence: 0.734

Metadata:
Errors: No predictions above FAP. Reduce FAP, increase MRP or inspect siblings.

## Step 1

**Type: Unrecognized, Confidence: 0.734**

*CC(CO)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C.CC(=O)OC(C)=O.c1ccncc1>>CC(=O)OCC(C)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(OC(C)=O)CCC4(C)C3CCC21C*



## Step 2

**Type: Undefined, Confidence: 0.0**

*CC(CO)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C>>CC(CO)CCC(=O)C(C)C1(O)C(OS(C)(=O)=O)CC2C3CCC4CC(O)CCC4(C)C3CCC21C*
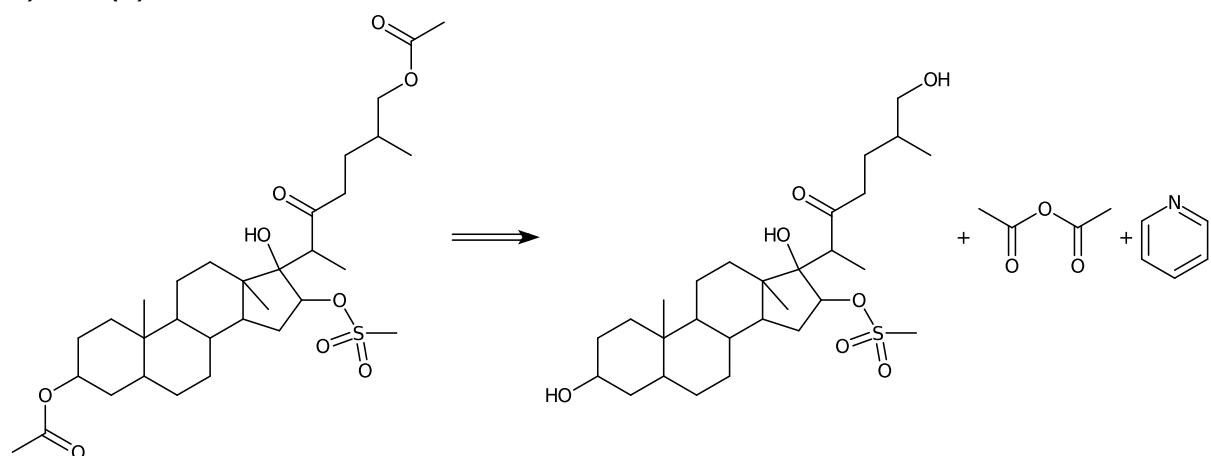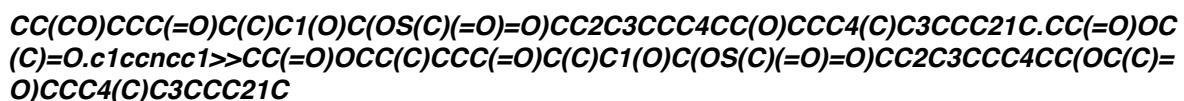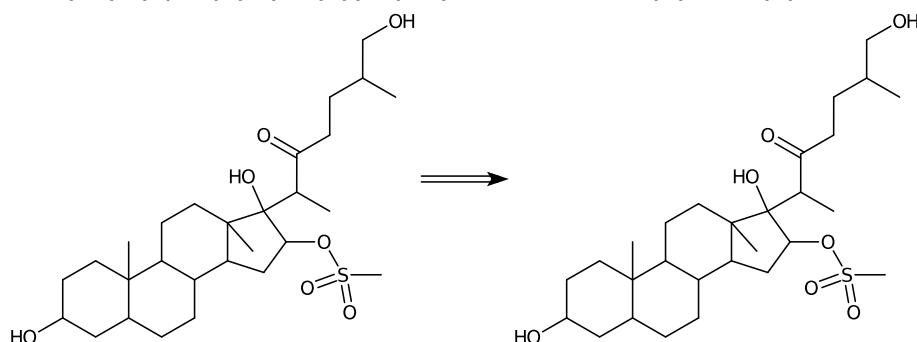
# Information about the retrosynthesis

Created On: 2019-09-26T17:09:48.283000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: COC1C=CC(CN2C3C(=CC=CC=3C3N(CC4C(OC)=CC(OC)=CC=4)C(C4C5CCN(CC5)C4)ON=3)OCC2)=CC=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: COC1C=CC(CN2C3C(=CC=CC=3C3N(CC4C(OC)=CC(OC)=CC=4)C(C4C5CCN(CC5)C4)ON=3)OCC2)=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.13

Metadata:
Warnings: 'ERROR MESSAGE'

## Step 1

### Type: Mitsunobu aryl ether synthesis, Confidence: 0.427

COc1ccc(CN(CCO)c2c(O)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1>>COc1
ccc(CN2CCOc3cccc(C4=NOC(C5CN6CCC5CC6)N4Cc4ccc(OC)cc4OC)c32)cc1



## Step 2

### Type: O-TBS deprotection, Confidence: 0.86

COc1ccc(CN(CCO[Si](C)(C)C(C)(C)C)c2c(O)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)c
c2OC)cc1.C1CCOC1.CCCC[N+](CCCC)(CCCC)CCCC.[F-]>>COc1ccc(CN(CCO)c2c(O)cccc2C
2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1



## Step 3

### Type: O-Bn deprotection, Confidence: 0.65

COc1ccc(CN(CCO[Si](C)(C)C(C)(C)C)c2c(OCc3ccccc3)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc
2ccc(OC)cc2OC)cc1.C1CCOC1.[Pd]>>COc1ccc(CN(CCO[Si](C)(C)C(C)(C)C)c2c(O)cccc2C2=
NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1

## Step 4

*Type: Bromo N-alkylation, Confidence: 0.807*

*COc1ccc(CNc2c(OCc3ccccc3)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1.CC(C)(C)[Si](C)(C)OCCBr.CN(C)C=O.[H-].[Na+]>>COc1ccc(CN(CCO[Si](C)(C)C(C)(C)C)c2c(OCc3ccccc3)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1*



## Step 5

*Type: Aldehyde reductive amination, Confidence: 0.724*

*COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3N)=NOC2C2CN3CCC2CC3)c(OC)c1.CC(=O)O[BH-](OC(C)=O)OC(C)=O.[Na+].COc1ccc(C=O)cc1.ClCCl>>COc1ccc(CNc2c(OCc3ccccc3)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1*



## Step 6

*Type: Nitro to amino, Confidence: 0.934*

S 137

COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3[N+](=O)[O-])=NOC2C2CN3CCC2CC3)c(OC)c1.CCO.Cl[Sn]Cl.O.O>>COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3N)=NOC2C2CN3CCC2CC3)c(OC)c1



### Step 7

*Type: Undefined, Confidence: 0.0*

COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3[N+](=O)[O-])=NOC2C2CN3CCC2CC3)c(OC)c1>>COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3[N+](=O)[O-])=NOC2C2CN3CCC2CC3)c(OC)c1

# Information about the retrosynthesis

Created On: 2019-10-01T13:59:59.566000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: COC1C=CC(CN2C3C(=CC=CC=3C3N(CC4C(OC)=CC(OC)=CC=4)C(C4C5CCN(CC5)C4)ON=3)OCC2)=CC=1
MSSR: 15
FAP: 0.6
MRP: 50
SbP: 3
Available smiles:
Exclude smiles: COC1C=CC(CN2C3C(=CC=CC=3C3N(CC4C(OC)=CC(OC)=CC=4)C(C4C5CCN(CC5)C4)ON=3)OCC2)=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.13

Metadata:
Errors: No predictions above FAP. Reduce FAP, increase MRP or inspect siblings.

## *Step 1*

*Type: Mitsunobu aryl ether synthesis, Confidence: 0.427*

*COc1ccc(CN(CCO)c2c(O)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1>>COc1ccc(CN2CCOc3cccc(C4=NOC(C5CN6CCC5CC6)N4Cc4ccc(OC)cc4OC)c32)cc1*



## *Step 2*

*Type: O-TBS deprotection, Confidence: 0.86*

*COc1ccc(CN(CCO[Si](C)(C)C(C)(C)C)c2c(O)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1.C1CCOC1.CCCC[N+](CCCC)(CCCC)CCCC.[F-]>>COc1ccc(CN(CCO)c2c(O)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1*



## *Step 3*

*Type: O-Bn deprotection, Confidence: 0.65*

*COc1ccc(CN(CCO[Si](C)(C)C(C)(C)C)c2c(OCc3ccccc3)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1.C1CCOC1.[Pd]>>COc1ccc(CN(CCO[Si](C)(C)C(C)(C)C)c2c(O)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1*

## Step 4

*Type: Bromo N-alkylation, Confidence: 0.807*

*COc1ccc(CNc2c(OCc3ccccc3)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1.CC(C)(C)[Si](C)(C)OCCBr.CN(C)C=O.[H-].[Na+]>>COc1ccc(CN(CCO[Si](C)(C)C(C)(C)C)c2c(OCc3ccccc3)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1*



## Step 5

*Type: Aldehyde reductive amination, Confidence: 0.724*

*COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3N)=NOC2C2CN3CCC2CC3)c(OC)c1.CC(=O)O[BH-](OC(C)=O)OC(C)=O.[Na+].COc1ccc(C=O)cc1.ClCCl>>COc1ccc(CNc2c(OCc3ccccc3)cccc2C2=NOC(C3CN4CCC3CC4)N2Cc2ccc(OC)cc2OC)cc1*



## Step 6

*Type: Nitro to amino, Confidence: 0.934*

COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3[N+](=O)[O-])=NOC2C2CN3CCC2CC3)c(OC)c1.CCO.Cl[Sn]Cl.O.O>>COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3N)=NOC2C2CN3CCC2CC3)c(OC)c1



## Step 7

*Type: Undefined, Confidence: 0.0*

COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3[N+](=O)[O-])=NOC2C2CN3CCC2CC3)c(OC)c1>>COc1ccc(CN2C(c3cccc(OCc4ccccc4)c3[N+](=O)[O-])=NOC2C2CN3CCC2CC3)c(OC)c1

# Information about the retrosynthesis

Created On: 2019-09-26T17:09:59.309000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
C1C=C(/N=N/C2C=CC(OC3OC(CO)C4C(OC(C)(OC)C(O4)(C)OC)C3O)=CC=2)C=CC=1OCC=C
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
C1C=C(/N=N/C2C=CC(OC3OC(CO)C4C(OC(C)(OC)C(O4)(C)OC)C3O)=CC=2)C=CC=1OCC=C
Exclude substructures:

# Sequence 0, Confidence: 0.428

Metadata:
Warnings: 'ERROR MESSAGE'

## Step 1

*Type: O-Ac deprotection, Confidence: 0.922*
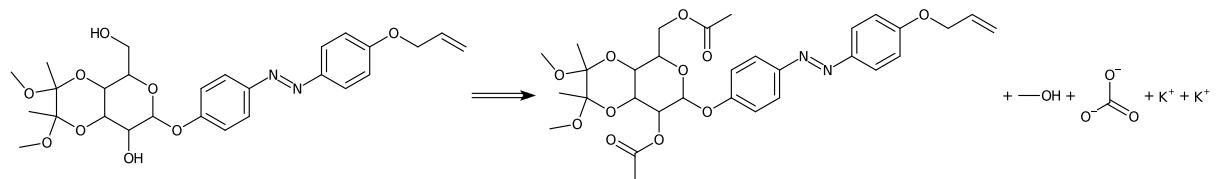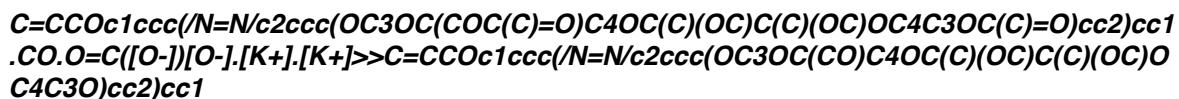
*C=CCOc1ccc(/N=N/c2ccc(OC3OC(COC(C)=O)C4OC(C)(OC)C(C)(OC)OC4C3OC(C)=O)cc2)cc1
.CO.O=C([O-])[O-].[K+].[K+]>>C=CCOc1ccc(/N=N/c2ccc(OC3OC(CO)C4OC(C)(OC)C(C)(OC)O
C4C3O)cc2)cc1*



## Step 2

*Type: Williamson ether synthesis, Confidence: 0.716*

*C=CCOc1ccc(/N=N/c2ccc(O)cc2)cc1.COC1(C)OC2C(COC(C)=O)OC(Br)C(OC(C)=O)C2OC1(C)
OC.CN(C)C=O.[H-].[Na+]>>C=CCOc1ccc(/N=N/c2ccc(OC3OC(COC(C)=O)C4OC(C)(OC)C(C)(O
C)OC4C3OC(C)=O)cc2)cc1*



## Step 3

*Type: Methoxy to hydroxy, Confidence: 0.895*

*C=CCOc1ccc(/N=N/c2ccc(OC)cc2)cc1.BrB(Br)Br.ClCCl>>C=CCOc1ccc(/N=N/c2ccc(O)cc2)cc
1*



*Type: Unrecognized, Confidence: 0.787*

*COC1(C)OC2C(CO)OC(Br)C(O)C2OC1(C)OC.CC(=O)OC(C)=O.c1ccncc1>>COC1(C)OC2C(CO
C(C)=O)OC(Br)C(OC(C)=O)C2OC1(C)OC*
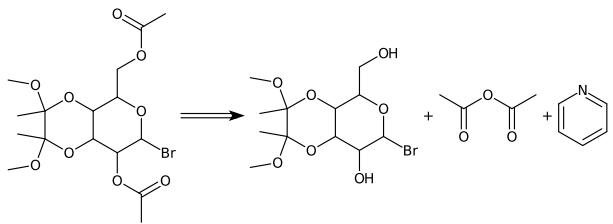
## Step 4

*Type: Williamson ether synthesis, Confidence: 0.92*

*COc1ccc(/N=N/c2ccc(O)cc2)cc1.C=CCBr.[NaH]>>C=CCOc1ccc(/N=N/c2ccc(OC)cc2)cc1*
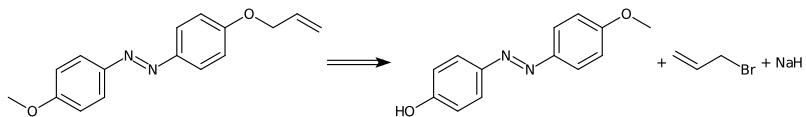


*Type: Undefined, Confidence: 0.0*

*COC1(C)OC2C(CO)OC(Br)C(O)C2OC1(C)OC>>COC1(C)OC2C(CO)OC(Br)C(O)C2OC1(C)OC*
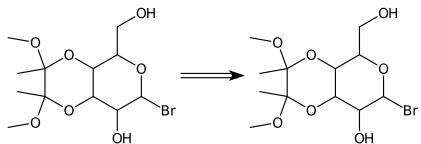
# Information about the retrosynthesis

Created On: 2019-10-01T14:05:49.729000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
C=CCOC1C=CC(/N=N/C2C=CC(OC3C(O)C4C(OC(C(O4)(OC)C)(OC)C)C(CO)O3)=CC=2)=CC=1
MSSR: 15
FAP: 0.6
MRP: 50
SbP: 3
Available smiles:
Exclude smiles:
C=CCOC1C=CC(/N=N/C2C=CC(OC3C(O)C4C(OC(C(O4)(OC)C)(OC)C)C(CO)O3)=CC=2)=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.428

Metadata:
Errors: No predictions above FAP. Reduce FAP, increase MRP or inspect siblings.

## Step 1

*Type: O-Ac deprotection, Confidence: 0.922*
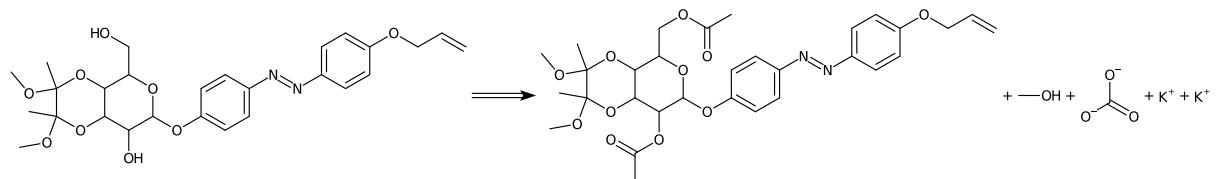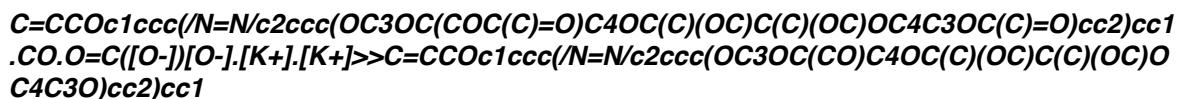
*C=CCOc1ccc(/N=N/c2ccc(OC3OC(COC(C)=O)C4OC(C)(OC)C(C)(OC)OC4C3OC(C)=O)cc2)cc1
.CO.O=C([O-])[O-].[K+].[K+]>>C=CCOc1ccc(/N=N/c2ccc(OC3OC(CO)C4OC(C)(OC)C(C)(OC)O
C4C3O)cc2)cc1*



## Step 2

*Type: Williamson ether synthesis, Confidence: 0.716*

*C=CCOc1ccc(/N=N/c2ccc(O)cc2)cc1.COC1(C)OC2C(COC(C)=O)OC(Br)C(OC(C)=O)C2OC1(C)
OC.CN(C)C=O.[H-].[Na+]>>C=CCOc1ccc(/N=N/c2ccc(OC3OC(COC(C)=O)C4OC(C)(OC)C(C)(O
C)OC4C3OC(C)=O)cc2)cc1*



## Step 3

*Type: Methoxy to hydroxy, Confidence: 0.895*

*C=CCOc1ccc(/N=N/c2ccc(OC)cc2)cc1.BrB(Br)Br.ClCCl>>C=CCOc1ccc(/N=N/c2ccc(O)cc2)cc
1*



*Type: Unrecognized, Confidence: 0.787*

*COC1(C)OC2C(CO)OC(Br)C(O)C2OC1(C)OC.CC(=O)OC(C)=O.c1ccncc1>>COC1(C)OC2C(CO
C(C)=O)OC(Br)C(OC(C)=O)C2OC1(C)OC*
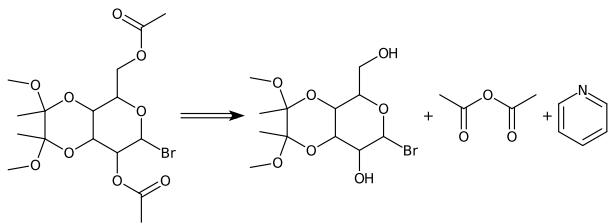
## Step 4

*Type: Williamson ether synthesis, Confidence: 0.92*

*COc1ccc(/N=N/c2ccc(O)cc2)cc1.C=CCBr.[NaH]>>C=CCOc1ccc(/N=N/c2ccc(OC)cc2)cc1*
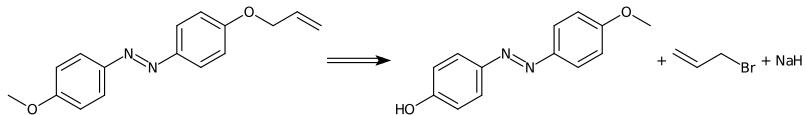


*Type: Undefined, Confidence: 0.0*

*COC1(C)OC2C(CO)OC(Br)C(O)C2OC1(C)OC>>COC1(C)OC2C(CO)OC(Br)C(O)C2OC1(C)OC*
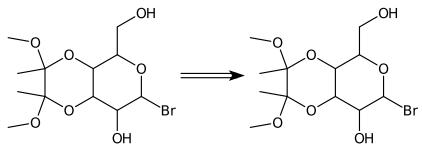
# Information about the retrosynthesis

Created On: 2019-09-26T17:10:10.302000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1N(C)CCC(NC(=O)C2C(F)=CC(NC3N=CC(C)=C(NC4C=C5N(S(C(C)(C)C)(=O)=O)CCC
C5=CC=4)N=3)=CC=2)C1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1N(C)CCC(NC(=O)C2C(F)=CC(NC3N=CC(C)=C(NC4C=C5N(S(C(C)(C)C)(=O)=
O)CCCC5=CC=4)N=3)=CC=2)C1
Exclude substructures:

## Sequence 0, Confidence: 0.835

### Step 1

*Type: Chloro N-arylation, Confidence: 0.968*

*CN1CCC(NC(=O)c2ccc(N)cc2F)CC1.Cc1cnc(Cl)nc1Nc1ccc2c(c1)N(S(=O)(=O)C(C)(C)C)CCC2.*
*CC(C)O>>Cc1cnc(Nc2ccc(C(=O)NC3CCN(C)CC3)c(F)c2)nc1Nc1ccc2c(c1)N(S(=O)(=O)C(C)(C)*
*C)CCC2*
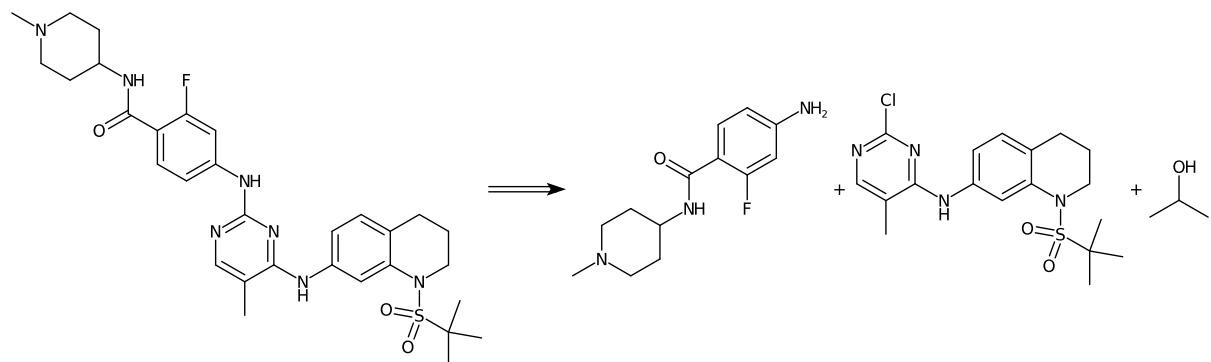


### Step 2

*Type: Carboxylic acid + amine condensation, Confidence: 0.957*

*CN1CCC(N)CC1.Nc1ccc(C(=O)O)c(F)c1>>CN1CCC(NC(=O)c2ccc(N)cc2F)CC1*
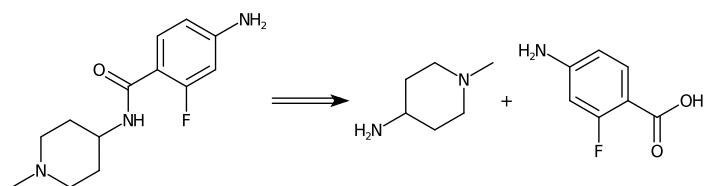


*Type: Chloro N-arylation, Confidence: 0.942*

*CC(C)(C)S(=O)(=O)N1CCCc2ccc(N)cc21.CN(C)C=O.Cc1cnc(Cl)nc1Cl>>Cc1cnc(Cl)nc1Nc1ccc*
*2c(c1)N(S(=O)(=O)C(C)(C)C)CCC2*



### Step 3

*Type: Nitro to amino, Confidence: 0.988*

*CC(C)(C)S(=O)(=O)N1CCCc2ccc([N+](=O)[O-])cc21.CCOC(C)=O.[Pd]>>CC(C)(C)S(=O)(=O)N1CCCc2ccc(N)cc21*
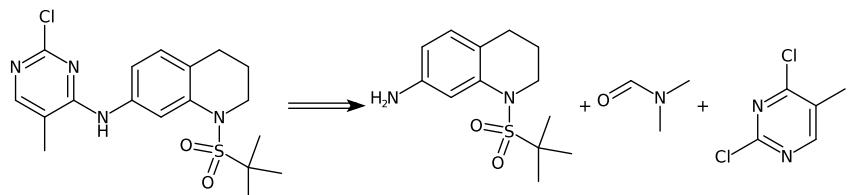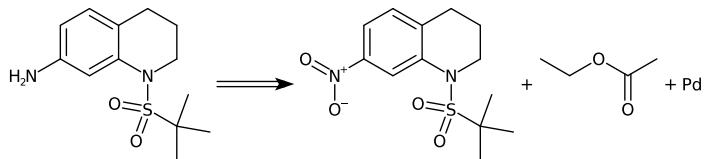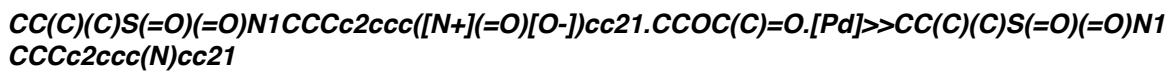


## Step 4

*Type: Sulfonamide Schotten-Baumann, Confidence: 0.968*

*CC(C)(C)S(=O)(=O)Cl.ClCCl.O=[N+]([O-])c1ccc2c(c1)NCCC2>>CC(C)(C)S(=O)(=O)N1CCCc2ccc([N+](=O)[O-])cc21*
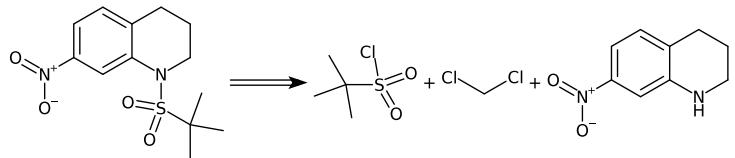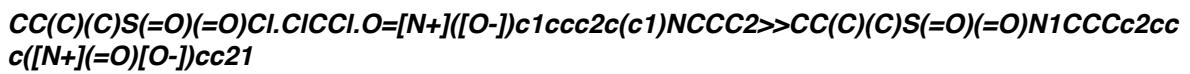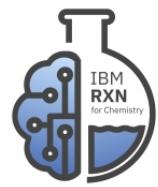
# Information about the retrosynthesis

Created On: 2019-09-26T19:42:38.407000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: C1C(N2CCN(C3N=C(C(F)(F)F)C(C4CC4)=CN=3)C(C(C)C)C2)=CC=C(F)C=1S(=O)(=O)C
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
C1C(N2CCN(C3N=C(C(F)(F)F)C(C4CC4)=CN=3)C(C(C)C)C2)=CC=C(F)C=1S(=O)(=O)C
Exclude substructures:

## Sequence 0, Confidence: 0.875

### Step 1

*Type: Chloro N-arylation, Confidence: 0.949*

*CC(C)C1CN(c2ccc(F)c(S(C)(=O)=O)c2)CCN1.FC(F)(F)c1nc(Cl)ncc1C1CC1.O=C([O-])[O-].[K+].[K+]>>CC(C)C1CN(c2ccc(F)c(S(C)(=O)=O)c2)CCN1c1ncc(C2CC2)c(C(F)(F)F)n1*
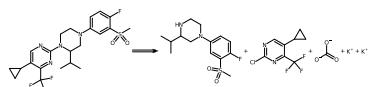


### Step 2

*Type: Bromo Buchwald-Hartwig amination, Confidence: 0.938*
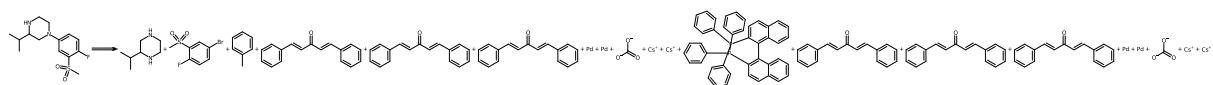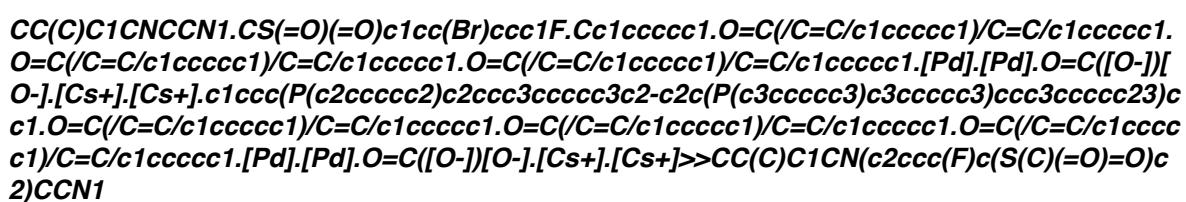
*CC(C)C1CNCCN1.CS(=O)(=O)c1cc(Br)ccc1F.Cc1ccccc1.O=C(/C=C/c1ccccc1)/C=C/c1ccccc1.O=C(/C=C/c1ccccc1)/C=C/c1ccccc1.O=C(/C=C/c1ccccc1)/C=C/c1ccccc1.[Pd].[Pd].O=C([O-])[O-].[Cs+].[Cs+].c1ccc(P(c2ccccc2)c2ccc3ccccc3c2-c2c(P(c3ccccc3)c3ccccc3)ccc3ccccc23)cc1.O=C(/C=C/c1ccccc1)/C=C/c1ccccc1.O=C(/C=C/c1ccccc1)/C=C/c1ccccc1.O=C(/C=C/c1ccccc1)/C=C/c1ccccc1.[Pd].[Pd].O=C([O-])[O-].[Cs+].[Cs+]>>CC(C)C1CN(c2ccc(F)c(S(C)(=O)=O)c2)CCN1*



*Type: Bromo Suzuki-type coupling, Confidence: 0.983*

*C1CCC(P(C2CCCCC2)C2CCCCC2)CC1.Cc1ccccc1.FC(F)(F)c1nc(Cl)ncc1Br.O.O=P([O-])([O-])[O-].[K+].[K+].[K+].OB(O)C1CC1.O=P([O-])([O-])[O-].[K+].[K+].[K+]>>FC(F)(F)c1nc(Cl)ncc1C1CC1*
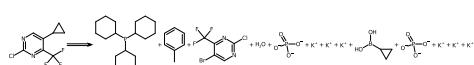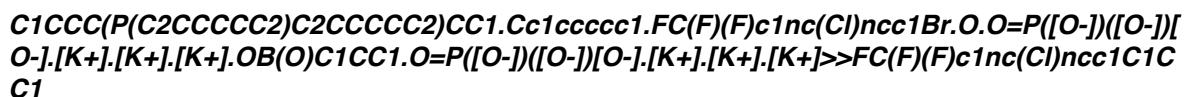
# Information about the retrosynthesis

Created On: 2019-09-26T19:42:54.341000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
CC(C)(O)CNC(=O)C1N=CC(C2(OCCC2)C2C=CC(B3OC(C)(C)C(C)(C)O3)=CC=2)=CC=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
CC(C)(O)CNC(=O)C1N=CC(C2(OCCC2)C2C=CC(B3OC(C)(C)C(C)(C)O3)=CC=2)=CC=1
Exclude substructures:

## Sequence 0, Confidence: 0.673

### Step 1

*Type: Bromo Miyaura boration, Confidence: 0.966*
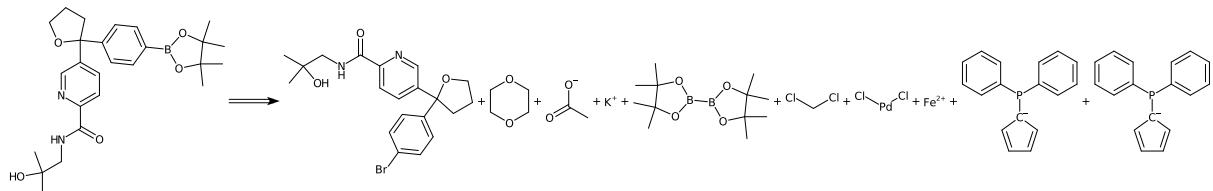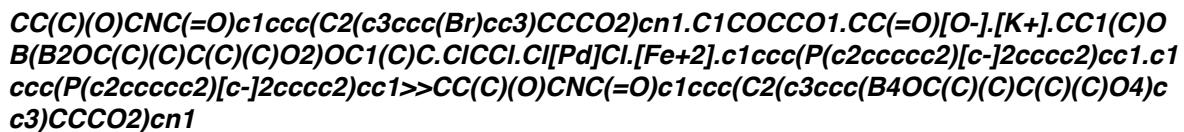
*CC(C)(O)CNC(=O)c1ccc(C2(c3ccc(Br)cc3)CCCO2)cn1.C1COCCO1.CC(=O)[O-].[K+].CC1(C)O B(B2OC(C)(C)C(C)(C)O2)OC1(C)C.ClCCl.Cl[Pd]Cl.[Fe+2].c1ccc(P(c2ccccc2)[c-]2cccc2)cc1.c1 ccc(P(c2ccccc2)[c-]2cccc2)cc1>>CC(C)(O)CNC(=O)c1ccc(C2(c3ccc(B4OC(C)(C)C(C)(C)O4)c c3)CCCO2)cn1*



### Step 2

*Type: Carboxylic acid + amine condensation, Confidence: 0.984*

*O=C(O)c1ccc(C2(c3ccc(Br)cc3)CCCO2)cn1.CC(C)(O)CN>>CC(C)(O)CNC(=O)c1ccc(C2(c3ccc( Br)cc3)CCCO2)cn1*



### Step 3

*Type: CO2H-Me deprotection, Confidence: 0.98*

*COC(=O)c1ccc(C2(c3ccc(Br)cc3)CCCO2)cn1.[Li]O>>O=C(O)c1ccc(C2(c3ccc(Br)cc3)CCCO2) cn1*



### Step 4

*Type: Unrecognized, Confidence: 0.952*

*COC(=O)c1ccc(C(O)(CCCO)c2ccc(Br)cc2)cn1.CS(=O)(=O)O.ClCCl>>COC(=O)c1ccc(C2(c3ccc (Br)cc3)CCCO2)cn1*
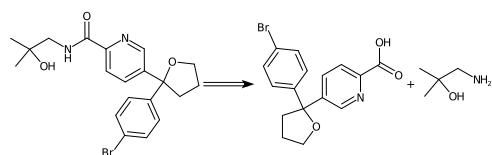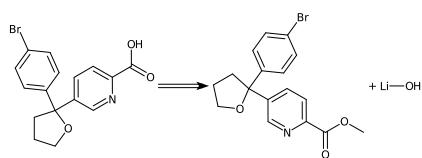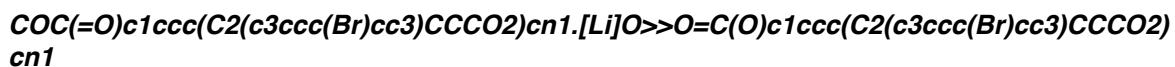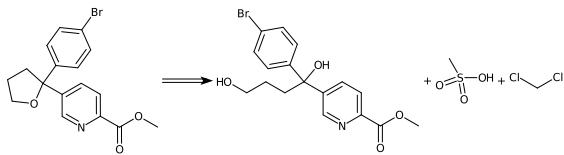
## Step 5

*Type: Alkene hydration, Confidence: 0.979*

*C=CCC(O)(c1ccc(Br)cc1)c1ccc(C(=O)OC)nc1.B.C1CCOC1.C1CCOC1.OO.[Na+].[OH-]>>COC(=O)c1ccc(C(O)(CCCO)c2ccc(Br)cc2)cn1*
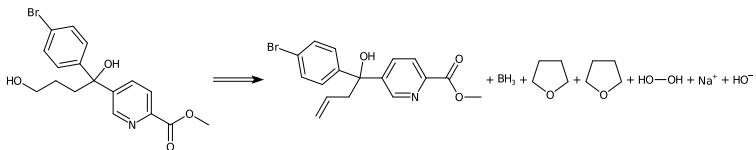


## Step 6

*Type: Bromo ketone Barbier reaction, Confidence: 0.95*
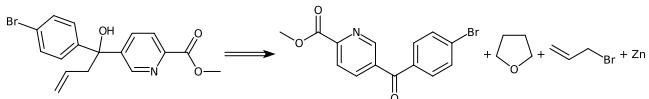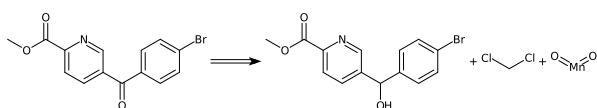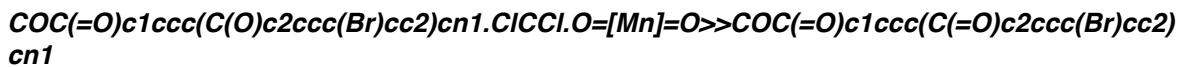
*COC(=O)c1ccc(C(=O)c2ccc(Br)cc2)cn1.C1CCOC1.C=CCBr.[Zn]>>C=CCC(O)(c1ccc(Br)cc1)c1ccc(C(=O)OC)nc1*



## Step 7

*Type: Alcohol to ketone oxidation, Confidence: 0.983*

*COC(=O)c1ccc(C(O)c2ccc(Br)cc2)cn1.ClCCl.O=[Mn]=O>>COC(=O)c1ccc(C(=O)c2ccc(Br)cc2)cn1*



## Step 8

*Type: Unrecognized, Confidence: 0.829*

*C1CCOC1.COC(=O)c1ccc(Br)cn1.O=Cc1ccc(Br)cc1.[Li]CCCC>>COC(=O)c1ccc(C(O)c2ccc(Br)cc2)cn1*
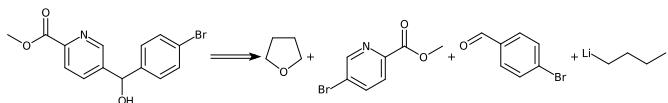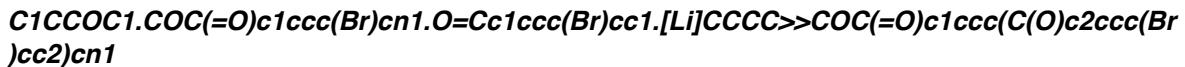
# Information about the retrosynthesis

Created On: 2019-09-26T19:43:08.998000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
C1(C2=C(N=CS2)C=C(C2C=CC(N3CCN(S(C)(=O)=O)CC3)=CC=2)C=1)OC(C)C1CNC(=O)C1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
C1(C2=C(N=CS2)C=C(C2C=CC(N3CCN(S(C)(=O)=O)CC3)=CC=2)C=1)OC(C)C1CNC(=O)C1
Exclude substructures:

## Sequence 0, Confidence: 0.696

### Step 1

**Type: Bromo Suzuki-type coupling, Confidence: 0.963**

*CC(Oc1cc(Br)cc2ncsc12)C1CNC(=O)C1.CC1(C)OB(c2ccc(N3CCN(S(C)(=O)=O)CC3)cc2)OC1(C)C>>CC(Oc1cc(-c2ccc(N3CCN(S(C)(=O)=O)CC3)cc2)cc2ncsc12)C1CNC(=O)C1*
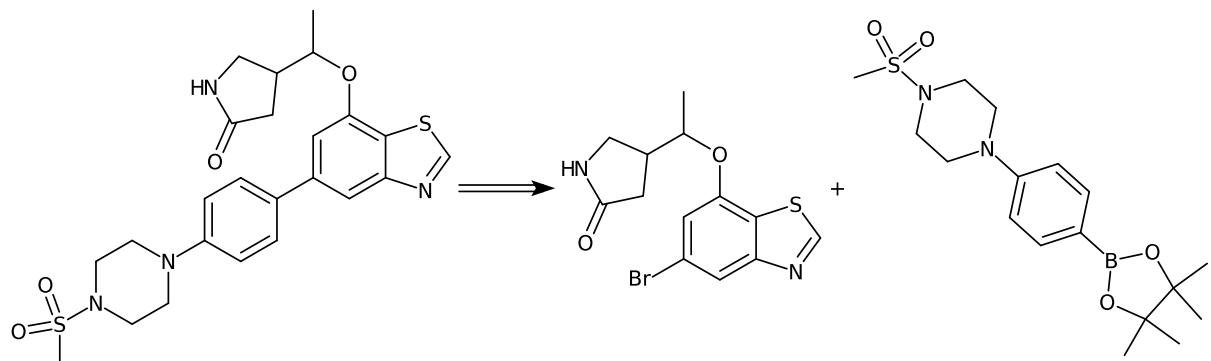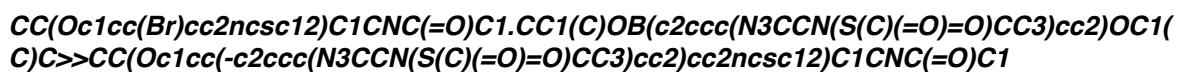


### Step 2

**Type: SNAr ether synthesis, Confidence: 0.961**
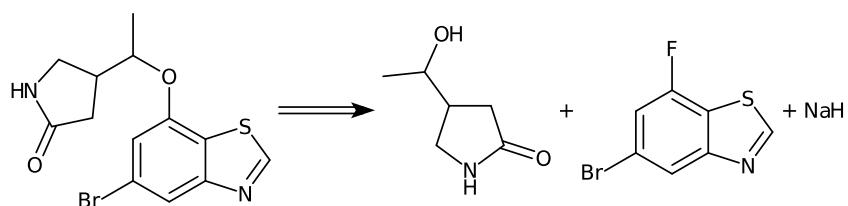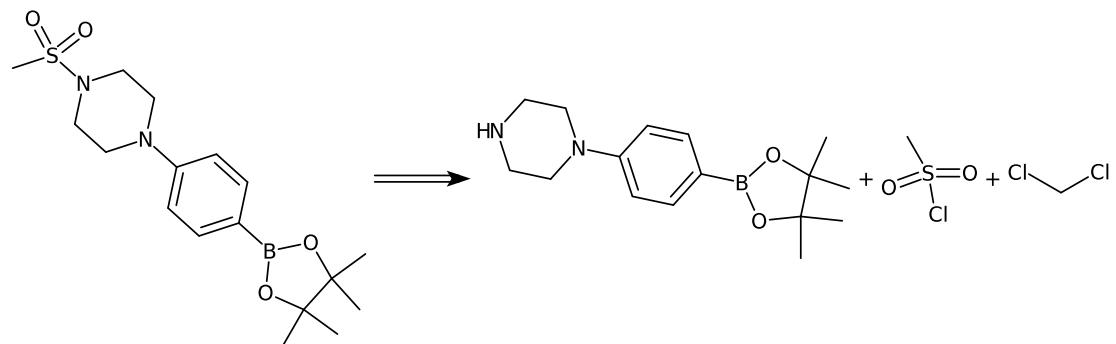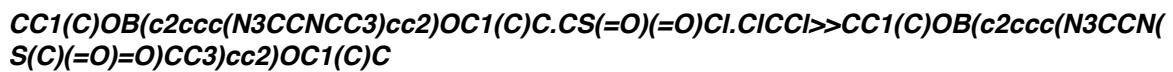
*CC(O)C1CNC(=O)C1.Fc1cc(Br)cc2ncsc12.[NaH]>>CC(Oc1cc(Br)cc2ncsc12)C1CNC(=O)C1*



**Type: Sulfonamide Schotten-Baumann, Confidence: 0.989**

*CC1(C)OB(c2ccc(N3CCNCC3)cc2)OC1(C)C.CS(=O)(=O)Cl.ClCCl>>CC1(C)OB(c2ccc(N3CCN(S(C)(=O)=O)CC3)cc2)OC1(C)C*



### Step 3

*Type: Ketone to alcohol reduction, Confidence: 0.974*

*CC(=O)C1CNC(=O)C1.CCO.O.[BH4-].[Na+]>>CC(O)C1CNC(=O)C1*



*Type: Unrecognized, Confidence: 0.989*

*Nc1cc(Br)cc(F)c1S.CCOC(OCC)OCC>>Fc1cc(Br)cc2ncsc12*



## Step 4

*Type: Unrecognized, Confidence: 0.986*

*CON(C)C(=O)C1CNC(=O)C1.[Li]C>>CC(=O)C1CNC(=O)C1*
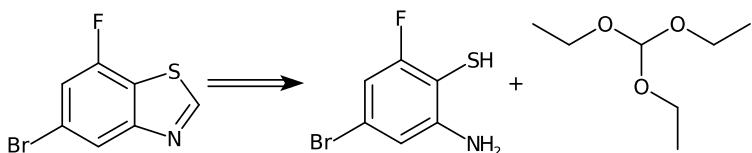


*Type: Nitro to amino, Confidence: 0.975*
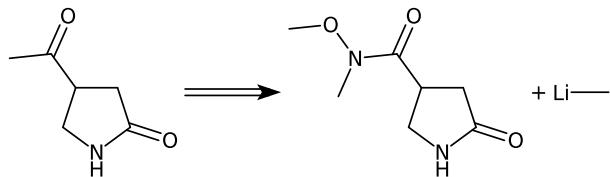
*O=[N+]([O-])c1cc(Br)cc(F)c1S.CO.[Cl-].[NH4+].[Fe]>>Nc1cc(Br)cc(F)c1S*
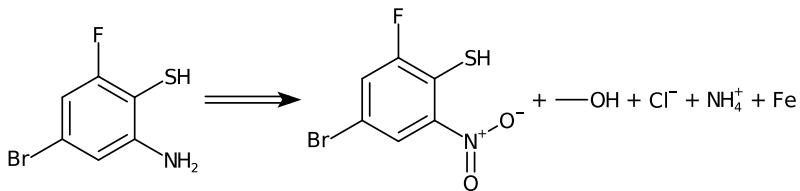


## Step 5

*Type: Weinreb amide synthesis, Confidence: 0.963*

*CNOC.Cl.O=C1CC(C(=O)O)CN1.CNOC.Cl>>CON(C)C(=O)C1CNC(=O)C1*
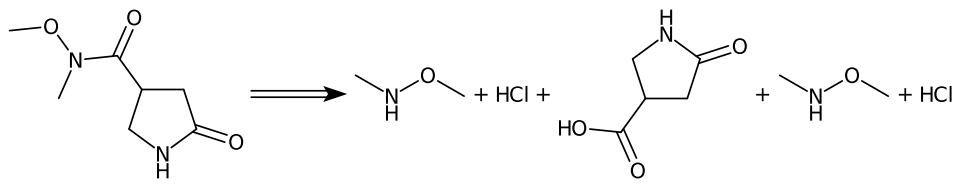
**Type: Fluoro to sulfanyl, Confidence: 0.852**

*CN(C)C=O.O.O=[N+]([O-])c1cc(Br)cc(F)c1F.S.[Na].S.[Na]>>O=[N+]([O-])c1cc(Br)cc(F)c1S*
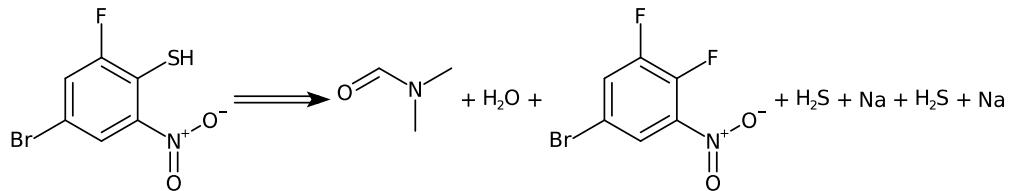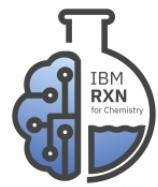
# Information about the retrosynthesis

Created On: 2019-09-30T15:04:42.289000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
CC1=C(C)C2/C(=N\C(C3N(C=2S1)C(C)=NN=3)CC(OC1CCC(O)CC1)=O)/C1C=CC(Cl)=CC=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
CC1=C(C)C2/C(=N\C(C3N(C=2S1)C(C)=NN=3)CC(OC1CCC(O)CC1)=O)/C1C=CC(Cl)=CC=1
Exclude substructures:

## Sequence 0, Confidence: 0.684

### *Step 1*

**Type: Esterification, Confidence: 0.739**

*Cc1sc2c(c1C)C(c1ccc(Cl)cc1)=NC(CC(=O)O)c1nnc(C)n1-2.CN(C)C=O.O=C(n1ccnc1)n1ccnc1.OC1CCC(O)CC1>>Cc1sc2c(c1C)C(c1ccc(Cl)cc1)=NC(CC(=O)OC1CCC(O)CC1)c1nnc(C)n1-2*
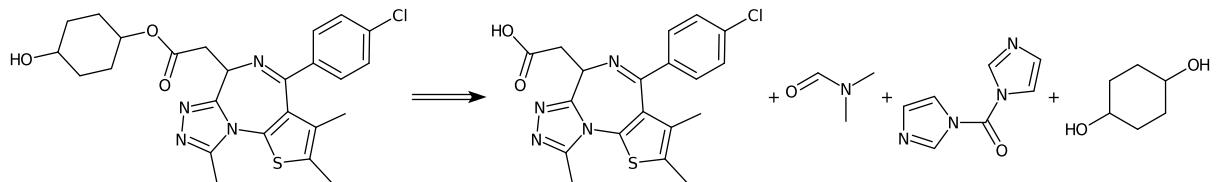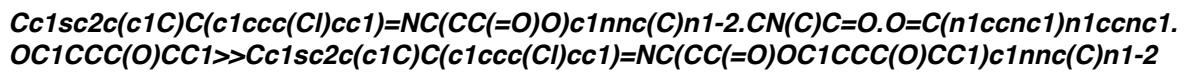


### *Step 2*

**Type: CO2H-tBu deprotection, Confidence: 0.926**

*Cc1sc2c(c1C)C(c1ccc(Cl)cc1)=NC(CC(=O)OC(C)(C)C)c1nnc(C)n1-2.O=C(O)C(F)(F)F>>Cc1sc2c(c1C)C(c1ccc(Cl)cc1)=NC(CC(=O)O)c1nnc(C)n1-2*
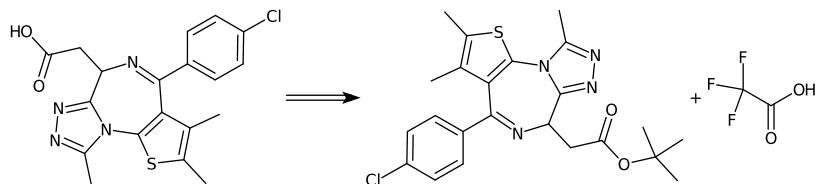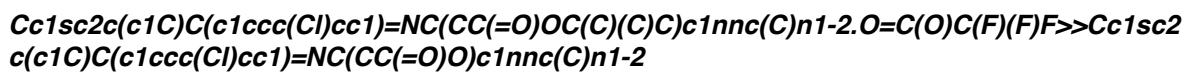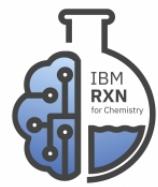
# Information about the retrosynthesis

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Product: CCOC(=O)/C=C/C(NC(=O)C(NC(=O)C(NC(C1=NOC(C)=C1)=O)C1CCCC1)CC1C=CC(F)=CC=1)CC1C(=O)NCC1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: CCOC(=O)/C=C/C(NC(=O)C(NC(=O)C(NC(C1=NOC(C)=C1)=O)C1CCCC1)CC1C=CC(F)=CC=1)CC1C(=O)NCC1
Exclude substructures:

# Sequence 0, Confidence: 0.77

Metadata:
Warnings: 'ERROR MESSAGE'

## Step 1

*Type: Carboxylic acid + amine condensation, Confidence: 0.829*
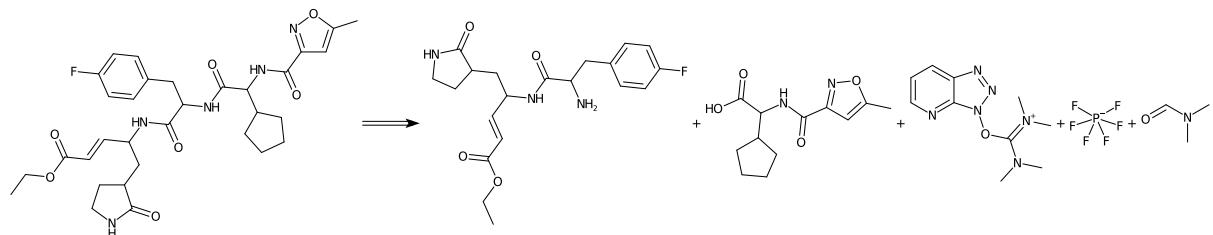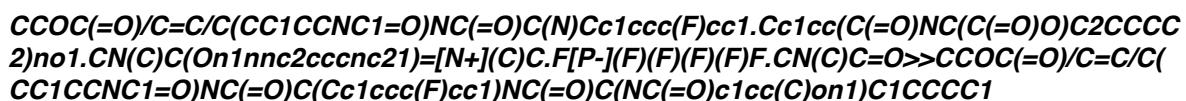
*CCOC(=O)/C=C/C(CC1CCNC1=O)NC(=O)C(N)Cc1ccc(F)cc1.Cc1cc(C(=O)NC(C(=O)O)C2CCCC2)no1.CN(C)C(On1nnc2cccnc21)=[N+](C)C.F[P-](F)(F)(F)(F)F.CN(C)C=O>>CCOC(=O)/C=C/C(CC1CCNC1=O)NC(=O)C(Cc1ccc(F)cc1)NC(=O)C(NC(=O)c1cc(C)on1)C1CCCC1*



## Step 2

*Type: Undefined, Confidence: 0.0*

*CCOC(=O)/C=C/C(CC1CCNC1=O)NC(=O)C(N)Cc1ccc(F)cc1>>CCOC(=O)/C=C/C(CC1CCNC1=O)NC(=O)C(N)Cc1ccc(F)cc1*



*Type: Amide Schotten-Baumann, Confidence: 0.929*

*Cc1cc(C(=O)Cl)no1.NC(C(=O)O)C1CCCC1>>Cc1cc(C(=O)NC(C(=O)O)C2CCCC2)no1*
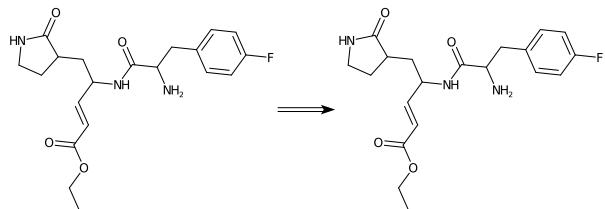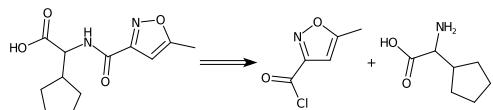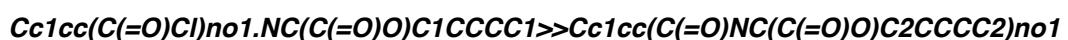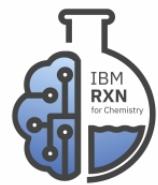
# Information about the retrosynthesis

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Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CCOC(/C=C/C(NC(C(NC(C(C1CCCC1)NC(C1=NOC(C)=C1)=O)=O)CC1C=CC(F)=CC=1
)=O)CC1C(=O)NCC1)=O
MSSR: 15
FAP: 0.6
MRP: 50
SbP: 3
Available smiles:
Exclude smiles: CCOC(/C=C/C(NC(C(NC(C(C1CCCC1)NC(C1=NOC(C)=C1)=O)=O)CC1C=CC(F)
=CC=1)=O)CC1C(=O)NCC1)=O
Exclude substructures:

# Sequence 0.0805, Confidence: 0.121

## Step 1

*Type: Carboxylic acid + amine condensation, Confidence: 0.829*

*CCOC(=O)/C=C/C(CC1CCNC1=O)NC(=O)C(N)Cc1ccc(F)cc1.Cc1cc(C(=O)NC(C(=O)O)C2CCCC 2)no1.CN(C)C(On1nnc2cccnc21)=[N+](C)C.F[P-](F)(F)(F)(F)F.CN(C)C=O>>CCOC(=O)/C=C/C( CC1CCNC1=O)NC(=O)C(Cc1ccc(F)cc1)NC(=O)C(NC(=O)c1cc(C)on1)C1CCCC1*
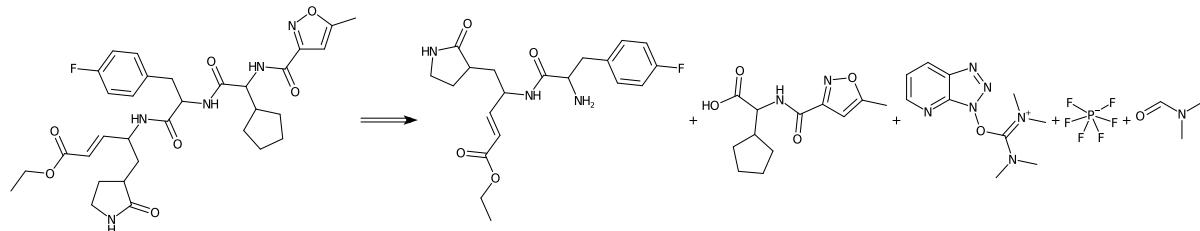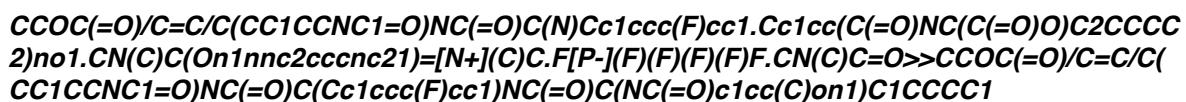


## Step 2

*Type: N-Boc deprotection, Confidence: 0.607*
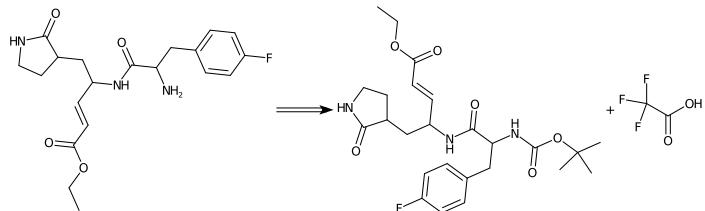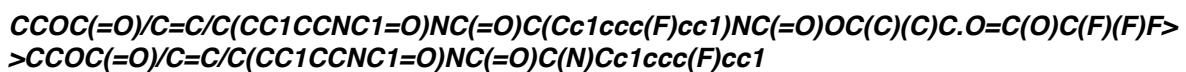
*CCOC(=O)/C=C/C(CC1CCNC1=O)NC(=O)C(Cc1ccc(F)cc1)NC(=O)OC(C)(C)C.O=C(O)C(F)(F)F> >CCOC(=O)/C=C/C(CC1CCNC1=O)NC(=O)C(N)Cc1ccc(F)cc1*



*Type: Amide Schotten-Baumann, Confidence: 0.929*

*Cc1cc(C(=O)Cl)no1.NC(C(=O)O)C1CCCC1>>Cc1cc(C(=O)NC(C(=O)O)C2CCCC2)no1*



## Step 3

*Type: Carboxylic acid + amine condensation, Confidence: 0.836*

*CCOC(=O)/C=C/C(N)CC1CCNC1=O.CC(C)(C)OC(=O)NC(Cc1ccc(F)cc1)C(=O)O.CCN(C(C)C)C( C)C.CN(C)C(On1nnc2cccnc21)=[N+](C)C.F[P-](F)(F)(F)(F)F.ClCCl>>CCOC(=O)/C=C/C(CC1CC NC1=O)NC(=O)C(Cc1ccc(F)cc1)NC(=O)OC(C)(C)C*
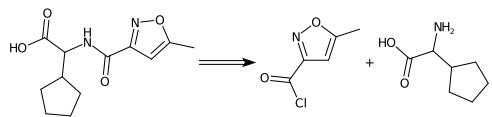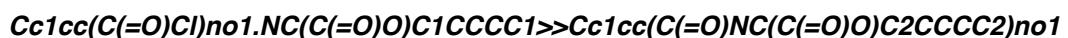
S 166
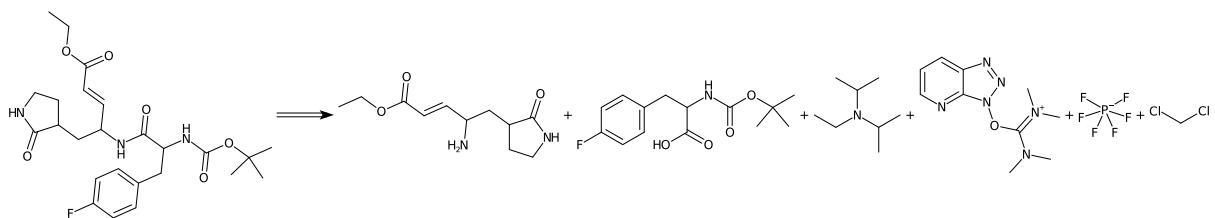
## Step 4

**Type: Ketone reductive amination, Confidence: 0.855**

*CCOC(=O)/C=C/C(=O)CC1CCNC1=O.CC(=O)[O-].[NH4+].CO.[BH3-]C#N.[Na+]>>CCOC(=O)/C=C/C(N)CC1CCNC1=O*
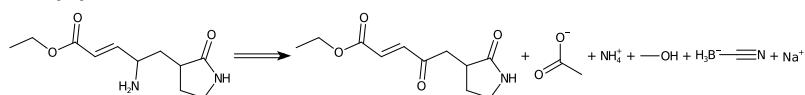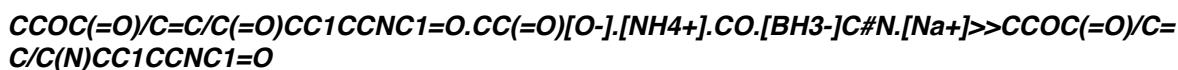


## Step 5

**Type: Alcohol to ketone oxidation, Confidence: 0.962**
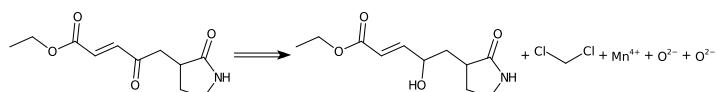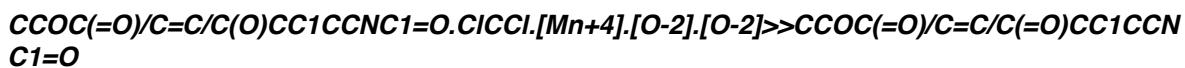
*CCOC(=O)/C=C/C(O)CC1CCNC1=O.ClCCl.[Mn+4].[O-2].[O-2]>>CCOC(=O)/C=C/C(=O)CC1CCNC1=O*



## Step 6

**Type: O-TBS deprotection, Confidence: 0.843**

*CCOC(=O)/C=C/C(CC1CCNC1=O)O[Si](C)(C)C(C)(C)C.C1CCOC1.CCCC[N+](CCCC)(CCCC)CCCC.[F-]>>CCOC(=O)/C=C/C(O)CC1CCNC1=O*



## Step 7

**Type: Horner-Wadsworth-Emmons reaction, Confidence: 0.668**

*CC(C)(C)[Si](C)(C)OC(C=O)CC1CCNC1=O.C1CCOC1.CCOC(=O)CP(=O)(OCC)OCC.[H-].[Na+]>>CCOC(=O)/C=C/C(CC1CCNC1=O)O[Si](C)(C)C(C)(C)C*
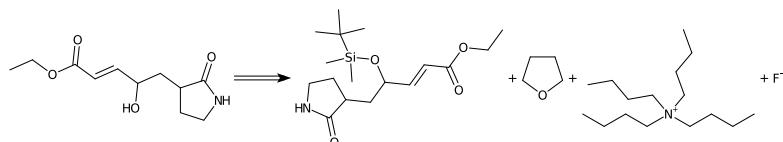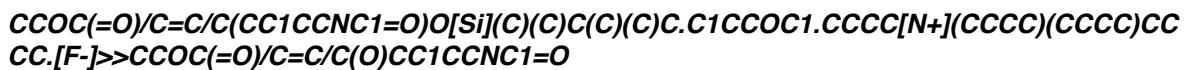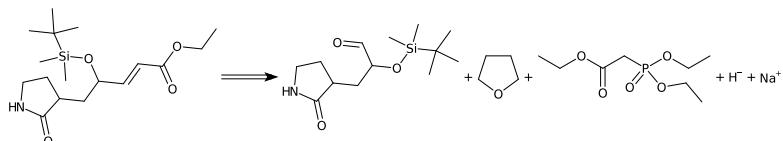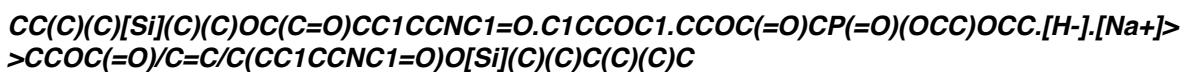
## Step 8

*Type: Aldehyde Dess-Martin oxidation, Confidence: 0.961*

*CC(C)(C)[Si](C)(C)OC(CO)CC1CCNC1=O.CC(=O)OI1(OC(C)=O)(OC(C)=O)OC(=O)c2ccccc21.ClCCl>>CC(C)(C)[Si](C)(C)OC(C=O)CC1CCNC1=O*



## Step 9

*Type: O-Bn deprotection, Confidence: 0.961*

*CC(C)(C)[Si](C)(C)OC(COCc1ccccc1)CC1CCNC1=O.CO.[HH].[Pd]>>CC(C)(C)[Si](C)(C)OC(CO)CC1CCNC1=O*
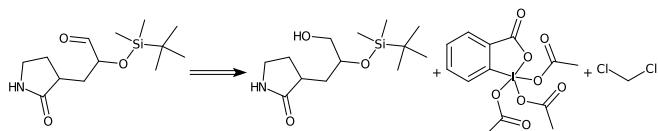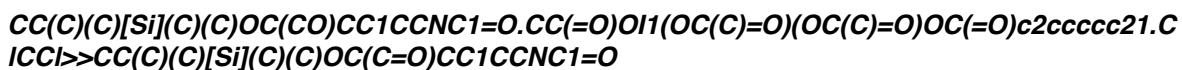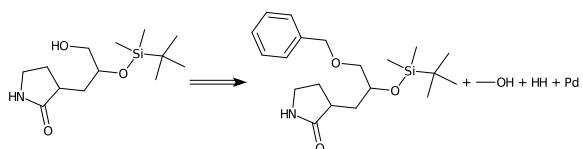


## Step 10

*Type: O-TBS protection, Confidence: 0.948*

*O=C1NCCC1CC(O)COCc1ccccc1.CC(C)(C)[Si](C)(C)Cl.c1c[nH]cn1>>CC(C)(C)[Si](C)(C)OC(COCc1ccccc1)CC1CCNC1=O*
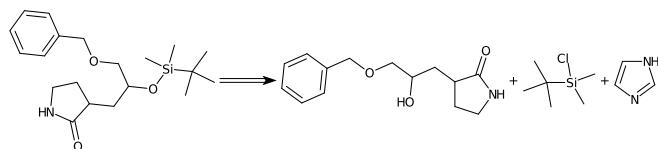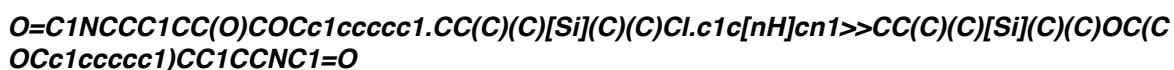


## Step 11

*Type: Ketone to alcohol reduction, Confidence: 0.971*

*O=C(COCc1ccccc1)CC1CCNC1=O.CO.[BH4-].[Na+]>>O=C1NCCC1CC(O)COCc1ccccc1*
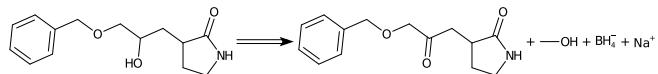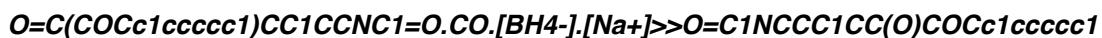


## Step 12

*Type: N-Boc deprotection, Confidence: 0.858*

*CC(C)(C)OC(=O)N1CCC(CC(=O)COCc2ccccc2)C1=O.ClCCl.O=C(O)C(F)(F)F>>O=C(COCc1ccccc1)CC1CCNC1=O*
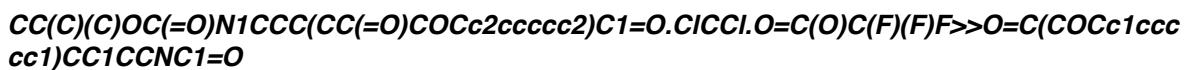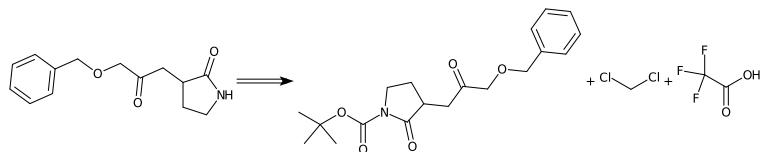
### Step 13

*Type: Unrecognized, Confidence: 0.918*

*C1CCOC1.CC(C)(C)OC(=O)N1CCCC1=O.C[Si](C)(C)[N-][Si](C)(C)C.[Li+].O=C(CBr)COCc1ccc
cc1.C[Si](C)(C)[N-][Si](C)(C)C.[Li+]>>CC(C)(C)OC(=O)N1CCC(CC(=O)COCc2ccccc2)C1=O*
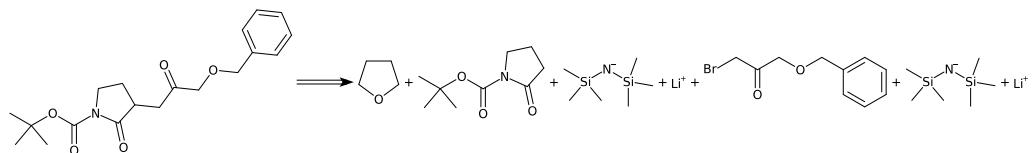
# Information about the retrosynthesis

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Product:
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MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
C1C=CC=CC=1/N=C1\S/C(=C/C2=C(C)N(CCN3CCOCC3)C(C)=C2)/C(=O)N\1C1CCCCC1
Exclude substructures:

# Sequence 0, Confidence: 0.0

Metadata:
Errors: 'ERROR MESSAGE'

## *Step 1*

*Type: Unrecognized, Confidence: 0.0*

*Cc1cc(/C=C2/S/C(=N\c3ccccc3)N(C3CCCCC3)C2=O)c(C)n1CCN1CCOCC1>>Cc1cc(/C=C2/S/C(=N\c3ccccc3)N(C3CCCCC3)C2=O)c(C)n1CCN1CCOCC1*
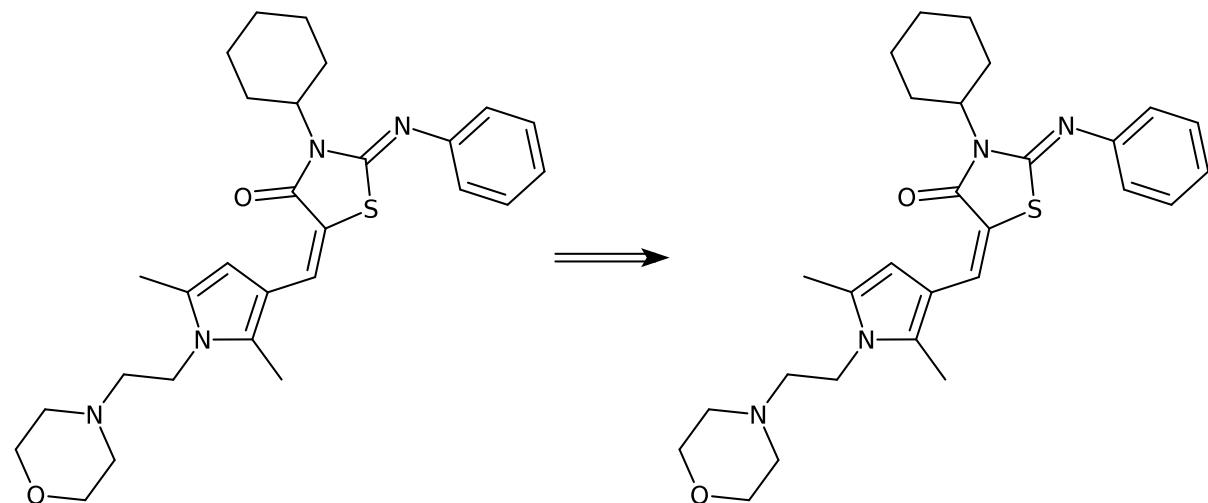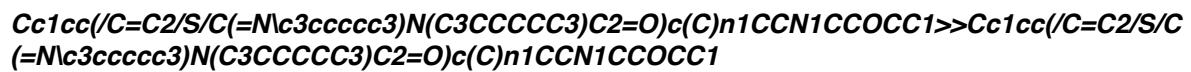
# Information about the retrosynthesis

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Product: C1C(C)=CC(C)=CC=1NC1N=CC=C(N2C=C(CN3CC(O)CC3)C(C3CC3)=C2)N=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: C1C(C)=CC(C)=CC=1NC1N=CC=C(N2C=C(CN3CC(O)CC3)C(C3CC3)=C2)N=1
Exclude substructures:

# Sequence 0, Confidence: 0.887

## Step 1

*Type: Aldehyde reductive amination, Confidence: 0.983*

**Cc1cc(C)cc(Nc2nccc(-n3cc(C=O)c(C4CC4)c3)n2)c1.C1CCOC1.OC1CCNC1.[BH3-]C#N.[Na+]>
>Cc1cc(C)cc(Nc2nccc(-n3cc(CN4CCC(O)C4)c(C4CC4)c3)n2)c1**



## Step 2

*Type: Chloro N-arylation, Confidence: 0.977*

**Cc1cc(C)cc(Nc2nccc(Cl)n2)c1.O=Cc1c[nH]cc1C1CC1.CN(C)C=O.O=C([O-])[O-].[Cs+].[Cs+]>>
Cc1cc(C)cc(Nc2nccc(-n3cc(C=O)c(C4CC4)c3)n2)c1**
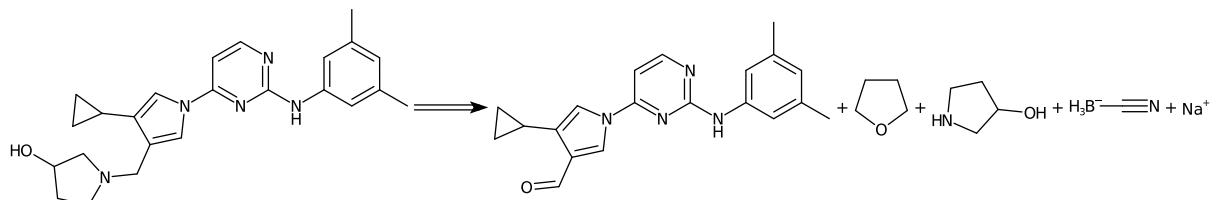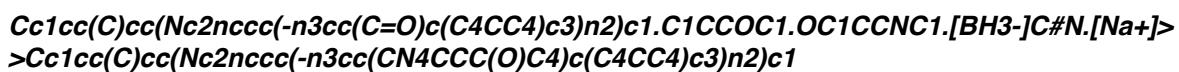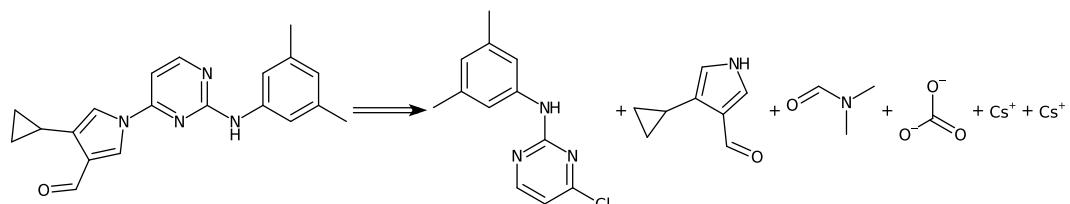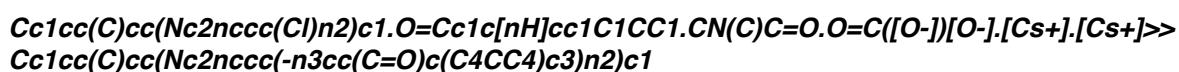


## Step 3

*Type: Pyridone to chloropyridine, Confidence: 0.967*
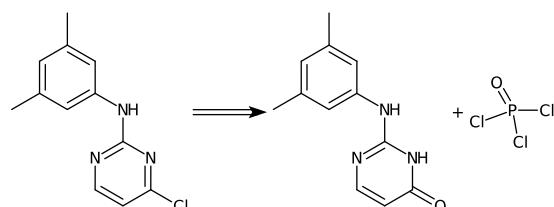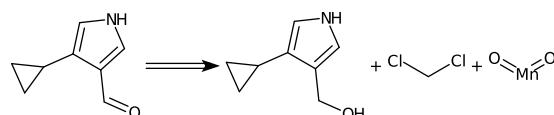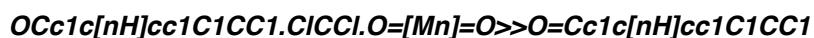
**Cc1cc(C)cc(Nc2nccc(=O)[nH]2)c1.O=P(Cl)(Cl)Cl>>Cc1cc(C)cc(Nc2nccc(Cl)n2)c1**



*Type: Alcohol to aldehyde oxidation, Confidence: 0.987*

**OCc1c[nH]cc1C1CC1.ClCCl.O=[Mn]=O>>O=Cc1c[nH]cc1C1CC1**

# Step 4

*Type: Unrecognized, Confidence: 0.985*

*CCO.CSc1nccc(=O)[nH]1.Cc1cc(C)cc(N)c1>>Cc1cc(C)cc(Nc2nccc(=O)[nH]2)c1*



*Type: Ester to alcohol reduction, Confidence: 0.983*

*C1CCOC1.CCOC(=O)c1c[nH]cc1C1CC1.[Al+3].[H-].[H-].[H-].[H-].[Li+].[Al+3].[H-].[H-].[H-].[H-].[Li+]>>OCc1c[nH]cc1C1CC1*
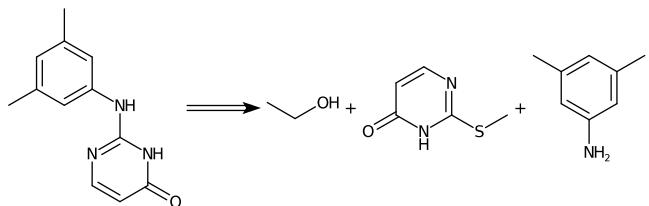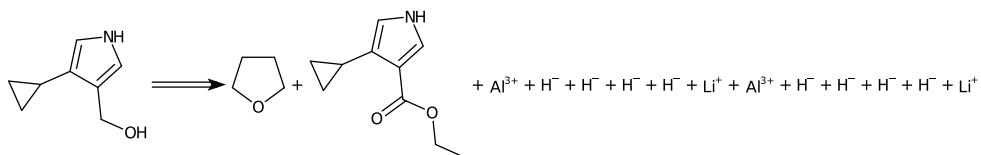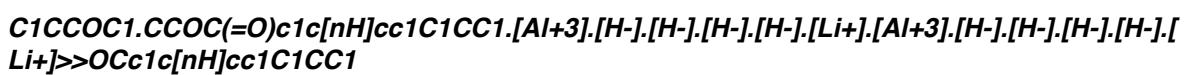
## Information about the retrosynthesis

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Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC1C=C(NC2N=C(N3C=C(C4CC4)C(CN4CC(O)CC4)=C3)C=CN=2)C=C(C)C=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles: C1=CC=CC=C1
Exclude smiles: CC1C=C(NC2N=C(N3C=C(C4CC4)C(CN4CC(O)CC4)=C3)C=CN=2)C=C(C)C=1
Exclude substructures:

# Sequence 0, Confidence: 0.758

Metadata:
Errors: No predictions above FAP. Reduce FAP, increase MRP or inspect siblings.

## Step 1

*Type: Aldehyde reductive amination, Confidence: 0.983*

**Cc1cc(C)cc(Nc2nccc(-n3cc(C=O)c(C4CC4)c3)n2)c1.C1CCOC1.OC1CCNC1.[BH3-]C#N.[Na+]>
>Cc1cc(C)cc(Nc2nccc(-n3cc(CN4CCC(O)C4)c(C4CC4)c3)n2)c1**



## Step 2

*Type: Alcohol to aldehyde oxidation, Confidence: 0.991*
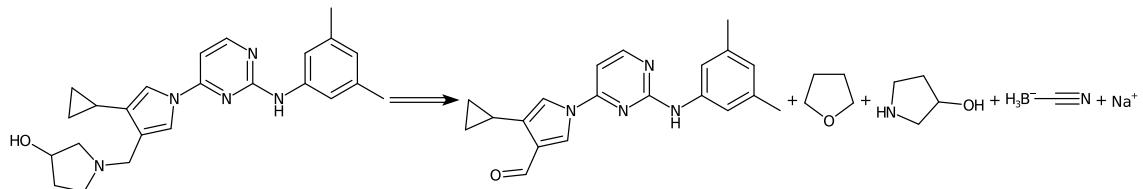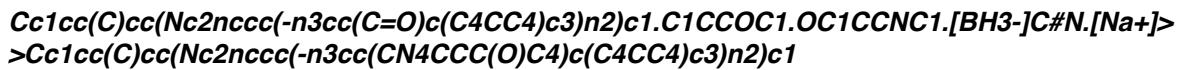
**Cc1cc(C)cc(Nc2nccc(-n3cc(CO)c(C4CC4)c3)n2)c1.ClCCl.O=[Mn]=O>>Cc1cc(C)cc(Nc2nccc(-n3cc(C=O)c(C4CC4)c3)n2)c1**



## Step 3

*Type: Ester to alcohol reduction, Confidence: 0.991*

**CCOC(=O)c1cn(-c2ccnc(Nc3cc(C)cc(C)c3)n2)cc1C1CC1.C1CCOC1.[Al+3].[H-].[H-].[H-].[H-].[Li+]>>Cc1cc(C)cc(Nc2nccc(-n3cc(CO)c(C4CC4)c3)n2)c1**



## Step 4

*Type: Chloro N-arylation, Confidence: 0.947*
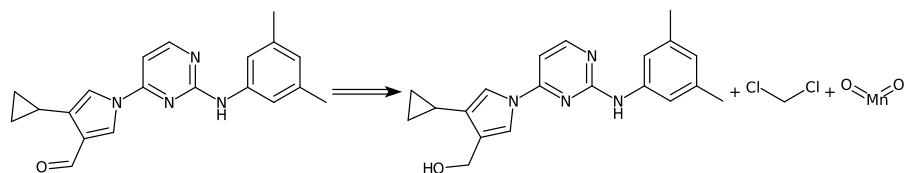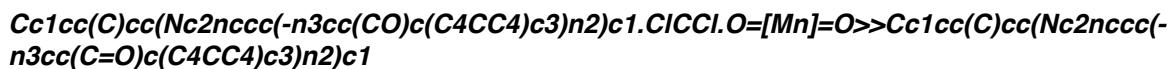
**CCOC(=O)c1cn(-c2ccnc(Cl)n2)cc1C1CC1.Cc1cc(C)cc(N)c1.Cl>>CCOC(=O)c1cn(-c2ccnc(Nc3cc(C)cc(C)c3)n2)cc1C1CC1**
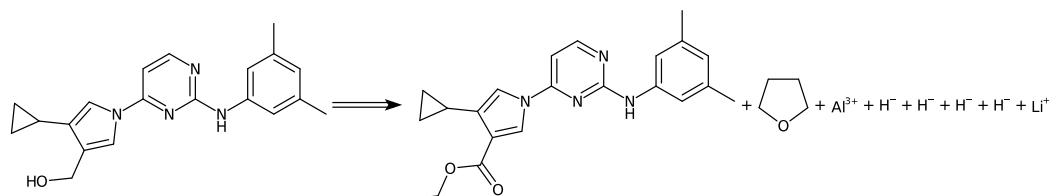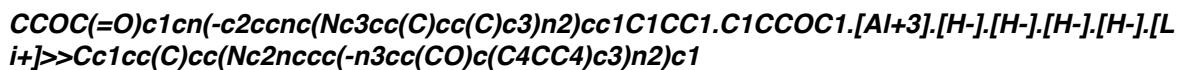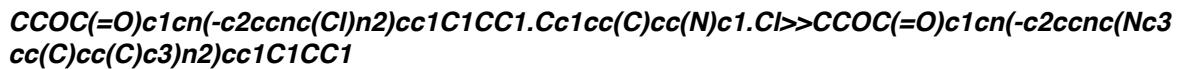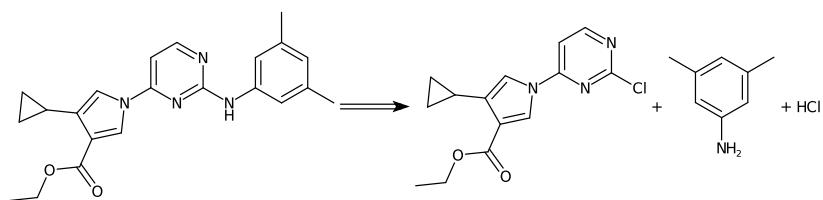
## Step 5

*Type: Chloro N-arylation, Confidence: 0.961*

*CCOC(=O)c1c[nH]cc1C1CC1.CS(C)=O.Clc1ccnc(Cl)n1.O=C([O-])[O-].[K+].[K+]>>CCOC(=O)c1cn(-c2ccnc(Cl)n2)cc1C1CC1*
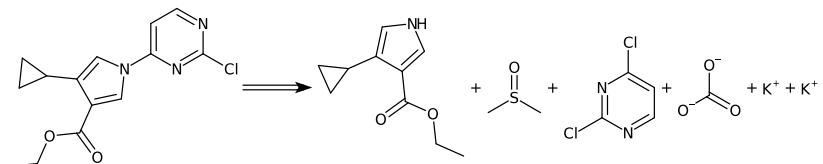


*Type: Nitro to amino, Confidence: 0.965*

*Cc1cc(C)cc([N+](=O)[O-])c1.[HH].[Ni]>>Cc1cc(C)cc(N)c1*
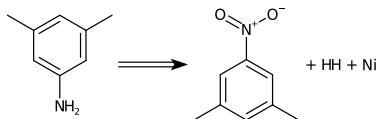


## Step 6

*Type: Iodo Suzuki coupling, Confidence: 0.98*

*CCOC(=O)c1c[nH]cc1I.C1CCC(P(C2CCCCC2)C2CCCCC2)CC1.CC(=O)[O-].CC(=O)[O-].[Pd+2].Cc1ccccc1.O.O=P([O-])([O-])[O-].[K+].[K+].[K+].OB(O)C1CC1>>CCOC(=O)c1c[nH]cc1C1CC1*
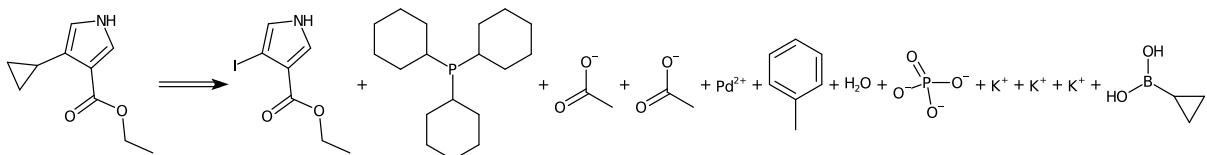


*Type: Undefined, Confidence: 0.0*
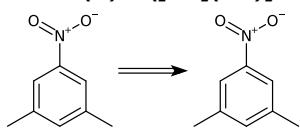
*Cc1cc(C)cc([N+](=O)[O-])c1>>Cc1cc(C)cc([N+](=O)[O-])c1*



## Step 7

*Type: Amino to iodo, Confidence: 0.975*
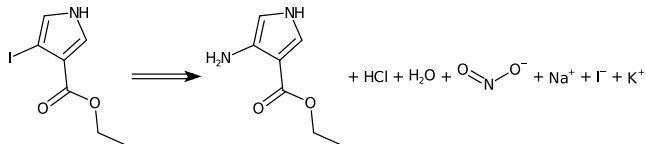
*CCOC(=O)c1c[nH]cc1N.Cl.O.O=N[O-].[Na+].[I-].[K+]>>CCOC(=O)c1c[nH]cc1I*



## Step 8

*Type: Nitro to amino, Confidence: 0.983*

*CCOC(=O)c1c[nH]cc1[N+](=O)[O-].CCO.[C].[Pd]>>CCOC(=O)c1c[nH]cc1N*



## Step 9

*Type: Fischer-Speier esterification, Confidence: 0.987*

*O=C(O)c1c[nH]cc1[N+](=O)[O-].CCO.O=S(=O)(O)O>>CCOC(=O)c1c[nH]cc1[N+](=O)[O-]*
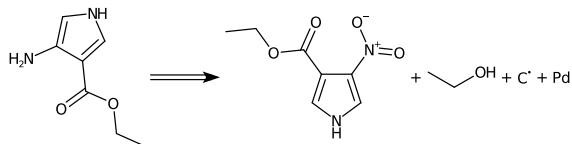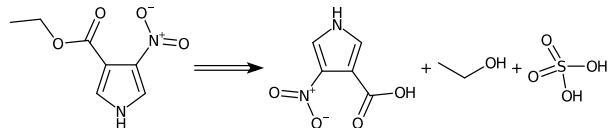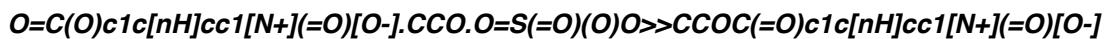


## Step 10

*Type: CO2H-Me deprotection, Confidence: 0.963*
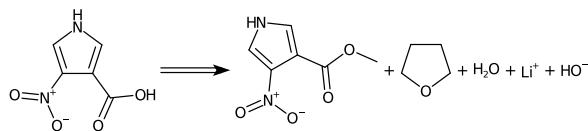
*COC(=O)c1c[nH]cc1[N+](=O)[O-].C1CCOC1.O.[Li+].[OH-]>>O=C(O)c1c[nH]cc1[N+](=O)[O-]*



## Step 11

*Type: Undefined, Confidence: 0.0*

*COC(=O)c1c[nH]cc1[N+](=O)[O-]>>COC(=O)c1c[nH]cc1[N+](=O)[O-]*
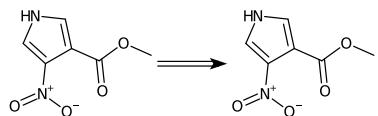
# Information about the retrosynthesis

Created On: 2019-10-01T14:26:41.757000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: CC1C=C(NC2N=C(N3C=C(C4CC4)C(CN4CC(O)CC4)=C3)C=CN=2)C=C(C)C=1
MSSR: 15
FAP: 0.6
MRP: 50
SbP: 3
Available smiles: C1=CC=CC=C1
Exclude smiles: CC1C=C(NC2N=C(N3C=C(C4CC4)C(CN4CC(O)CC4)=C3)C=CN=2)C=C(C)C=1
Exclude substructures:

# Sequence 0, Confidence: 0.406

Metadata:
Warnings: The retrosynthesis did not complete. Try increasing MSSR.

## Step 1

*Type: Aldehyde reductive amination, Confidence: 0.983*

**Cc1cc(C)cc(Nc2nccc(-n3cc(C=O)c(C4CC4)c3)n2)c1.C1CCOC1.OC1CCNC1.[BH3-]C#N.[Na+]>>Cc1cc(C)cc(Nc2nccc(-n3cc(CN4CCC(O)C4)c(C4CC4)c3)n2)c1**

## Step 2

*Type: Alcohol to aldehyde oxidation, Confidence: 0.991*
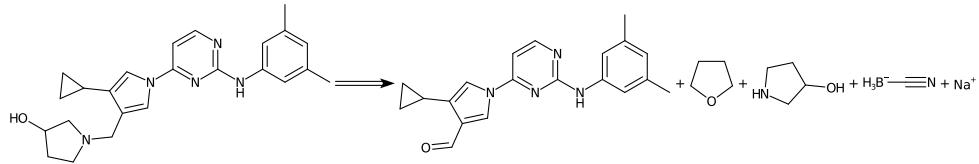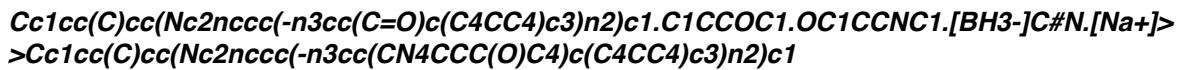
**Cc1cc(C)cc(Nc2nccc(-n3cc(CO)c(C4CC4)c3)n2)c1.ClCCl.O=[Mn]=O>>Cc1cc(C)cc(Nc2nccc(-n3cc(C=O)c(C4CC4)c3)n2)c1**

## Step 3

*Type: Mesyl N-arylation, Confidence: 0.986*

**CS(=O)(=O)c1nccc(-n2cc(CO)c(C3CC3)c2)n1.Cc1cc(C)cc(N)c1>>Cc1cc(C)cc(Nc2nccc(-n3cc(CO)c(C4CC4)c3)n2)c1**
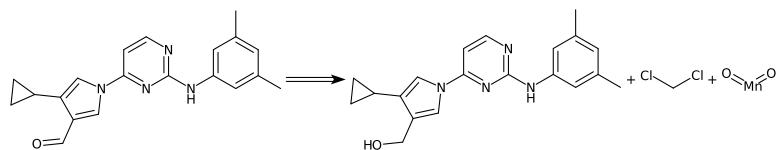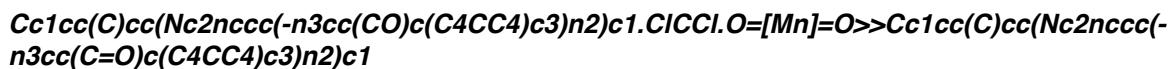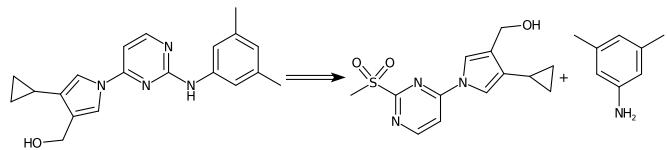
## Step 4

*Type: Sulfanyl to sulfonyl, Confidence: 0.908*

**CSc1nccc(-n2cc(CO)c(C3CC3)c2)n1.CO.O.O=S([O-])OO.[K+]>>CS(=O)(=O)c1nccc(-n2cc(CO)c(C3CC3)c2)n1**
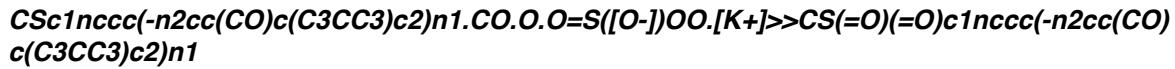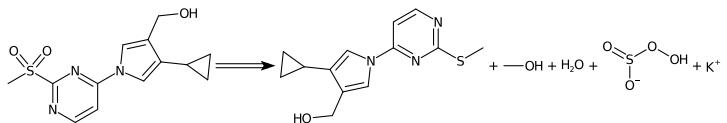
**Type: Nitro to amino, Confidence: 0.965**

**Cc1cc(C)cc([N+](=O)[O-])c1.[HH].[Ni]>>Cc1cc(C)cc(N)c1**
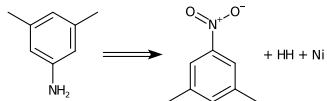


## Step 5

**Type: Ester to alcohol reduction, Confidence: 0.985**

**COC(=O)c1cn(-c2ccnc(SC)n2)cc1C1CC1.C1CCOC1.[Al+3].[H-].[H-].[H-].[H-].[Li+]>>CSc1nccc(-n2cc(CO)c(C3CC3)c2)n1**
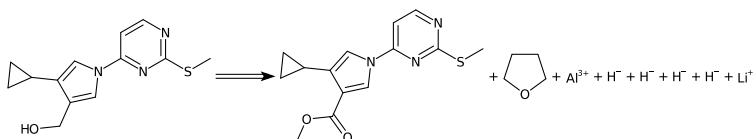


**Type: Undefined, Confidence: 0.0**

**Cc1cc(C)cc([N+](=O)[O-])c1>>Cc1cc(C)cc([N+](=O)[O-])c1**
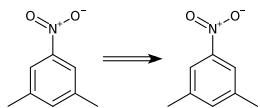


## Step 6

**Type: Chloro N-arylation, Confidence: 0.957**

**COC(=O)c1c[nH]cc1C1CC1.CSc1nccc(Cl)n1.CC#N.O=C([O-])[O-].[Cs+].[Cs+]>>COC(=O)c1cn(-c2ccnc(SC)n2)cc1C1CC1**
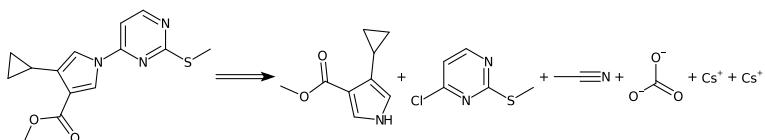


## Step 7

**Type: Fischer-Speier esterification, Confidence: 0.991**

**O=C(O)c1c[nH]cc1C1CC1.CO.O=S(=O)(O)O>>COC(=O)c1c[nH]cc1C1CC1**
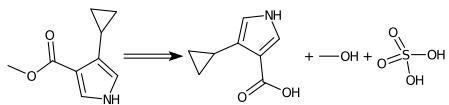
**Type: Hydroxy to chloro, Confidence: 0.989**

*CSc1nccc(=O)[nH]1.O=P(Cl)(Cl)Cl.[Na+].[OH-]>>CSc1nccc(Cl)n1*
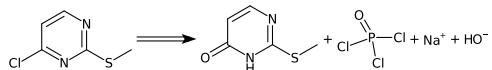


## Step 8

**Type: CO2H-Et deprotection, Confidence: 0.981**

*CCOC(=O)c1c[nH]cc1C1CC1.C1CCOC1.O.[Li]O>>O=C(O)c1c[nH]cc1C1CC1*
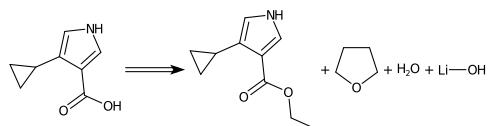


**Type: S-methylation, Confidence: 0.977**

*O=c1cc[nH]c(=S)[nH]1.CI.CO.O.[Na+].[OH-]>>CSc1nccc(=O)[nH]1*
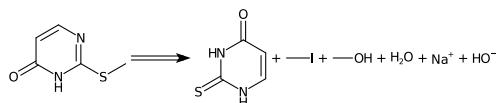


## Step 9

**Type: N-Boc deprotection, Confidence: 0.911**

*CCOC(=O)c1cn(C(=O)OC(C)(C)C)cc1C1CC1.ClCCl.O=C(O)C(F)(F)F>>CCOC(=O)c1c[nH]cc1C1CC1*
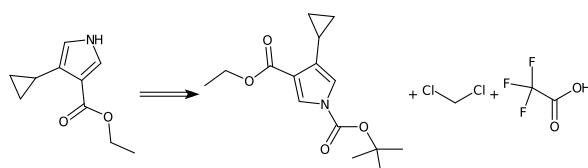


**Type: Unrecognized, Confidence: 0.794**

*CCOC(=O)/C=C/N(C)C.CO.C[O-].[Na+].NC(N)=S>>O=c1cc[nH]c(=S)[nH]1*
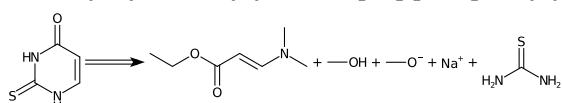
## Step 10

*Type: Iodo Suzuki coupling, Confidence: 0.846*

*CCOC(=O)c1cn(C(=O)OC(C)(C)C)cc1I.C1CCC(P(C2CCCCC2)C2CCCCC2)CC1.CC(=O)[O-].CC(=O)[O-].[Pd+2].Cc1ccccc1.O.O=P([O-])([O-])[O-].[K+].[K+].[K+].OB(O)C1CC1>>CCOC(=O)c1cn(C(=O)OC(C)(C)C)cc1C1CC1*



*Type: Undefined, Confidence: 0.0*

*CCOC(=O)/C=C/N(C)C>>CCOC(=O)/C=C/N(C)C*
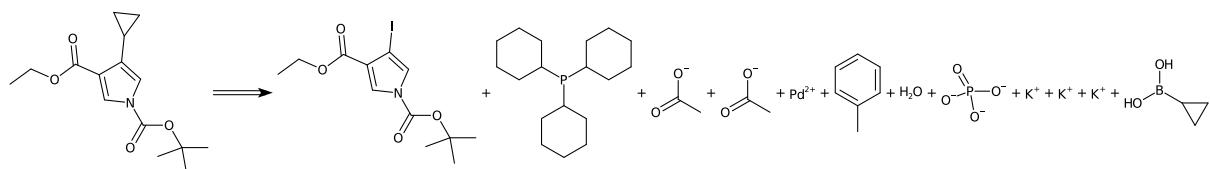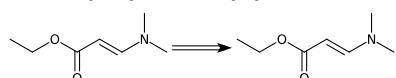


## Step 11

*Type: N-Boc protection, Confidence: 0.978*

*CCOC(=O)c1c[nH]cc1I.C1CCOC1.CC(C)(C)OC(=O)OC(=O)OC(C)(C)C.[H-].[Na+]>>CCOC(=O)c1cn(C(=O)OC(C)(C)C)cc1I*
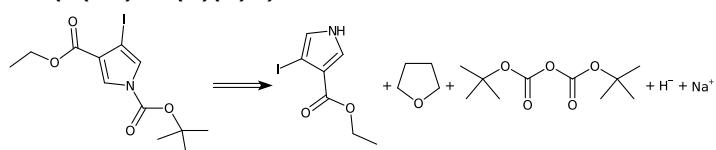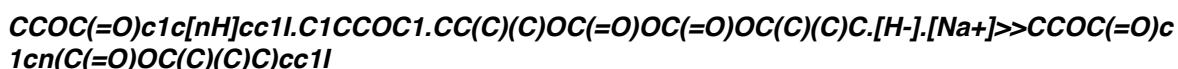


## Step 12

*Type: Amino to iodo, Confidence: 0.975*
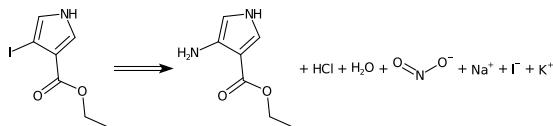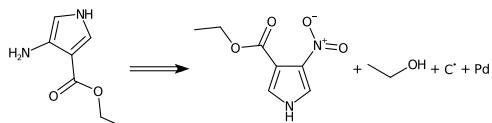
*CCOC(=O)c1c[nH]cc1N.Cl.O.O=N[O-].[Na+].[I-].[K+]>>CCOC(=O)c1c[nH]cc1I*



## Step 13

*Type: Nitro to amino, Confidence: 0.983*

*CCOC(=O)c1c[nH]cc1[N+](=O)[O-].CCO.[C].[Pd]>>CCOC(=O)c1c[nH]cc1N*

## Step 14

*Type: Fischer-Speier esterification, Confidence: 0.987*

*O=C(O)c1c[nH]cc1[N+](=O)[O-].CCO.O=S(=O)(O)O>>CCOC(=O)c1c[nH]cc1[N+](=O)[O-]*



## Step 15

*Type: CO2H-Me deprotection, Confidence: 0.963*

*COC(=O)c1c[nH]cc1[N+](=O)[O-].C1CCOC1.O.[Li+].[OH-]>>O=C(O)c1c[nH]cc1[N+](=O)[O-]*
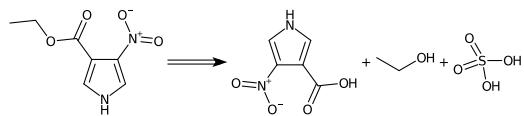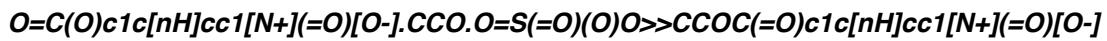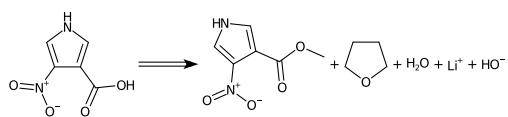
# Information about the retrosynthesis

Created On: 2019-09-26T19:44:27.917000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
C1(CC(C)(C)NC(C)(C)C1)N(C)C1C=CC(C2C=CC(C(CNC(C3CC3)=O)O)=CC=2OC)=NN=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
C1(CC(C)(C)NC(C)(C)C1)N(C)C1C=CC(C2C=CC(C(CNC(C3CC3)=O)O)=CC=2OC)=NN=1
Exclude substructures:

## Sequence 0, Confidence: 0.87

### Step 1

*Type: Chloro Suzuki-type coupling, Confidence: 0.959*
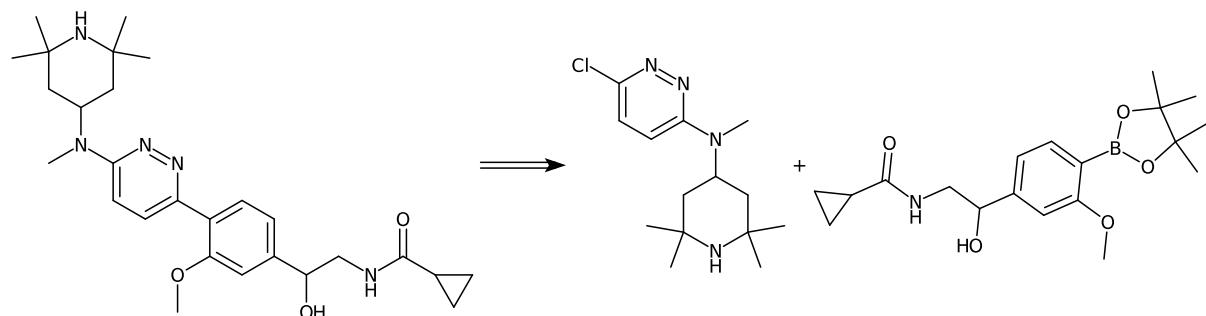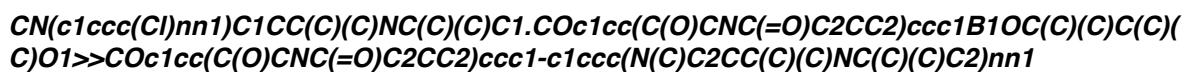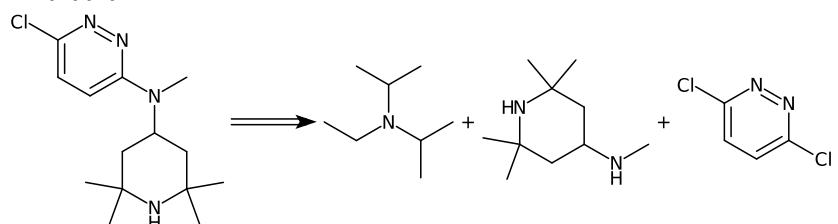
*CN(c1ccc(Cl)nn1)C1CC(C)(C)NC(C)(C)C1.COc1cc(C(O)CNC(=O)C2CC2)ccc1B1OC(C)(C)C(C)(C)O1>>COc1cc(C(O)CNC(=O)C2CC2)ccc1-c1ccc(N(C)C2CC(C)(C)NC(C)(C)C2)nn1*



### Step 2

*Type: Chloro N-arylation, Confidence: 0.972*

*CCN(C(C)C)C(C)C.CNC1CC(C)(C)NC(C)(C)C1.Clc1ccc(Cl)nn1>>CN(c1ccc(Cl)nn1)C1CC(C)(C)NC(C)(C)C1*



*Type: Bromo Miyaura boration, Confidence: 0.967*

*COc1cc(C(O)CNC(=O)C2CC2)ccc1Br.CC(=O)[O-].[K+].CC1(C)OB(B2OC(C)(C)C(C)(C)O2)OC1(C)C>>COc1cc(C(O)CNC(=O)C2CC2)ccc1B1OC(C)(C)C(C)(C)O1*



### Step 3

*Type: Amide Schotten-Baumann, Confidence: 0.965*

C1CCOC1.CCN(C(C)C)C(C)C.COc1cc(C(O)CN)ccc1Br.O=C(Cl)C1CC1>>COc1cc(C(O)CNC(=O)C2CC2)ccc1Br
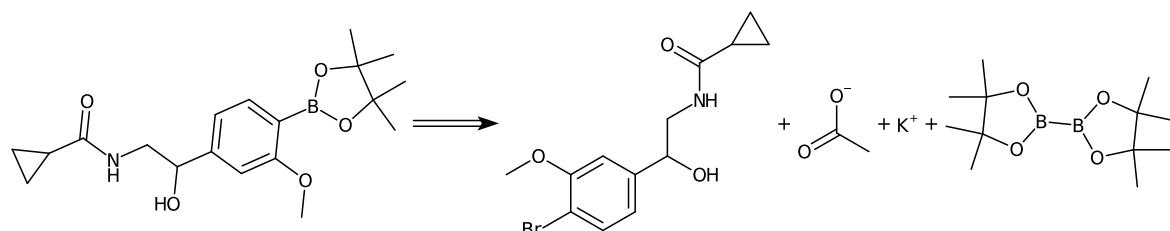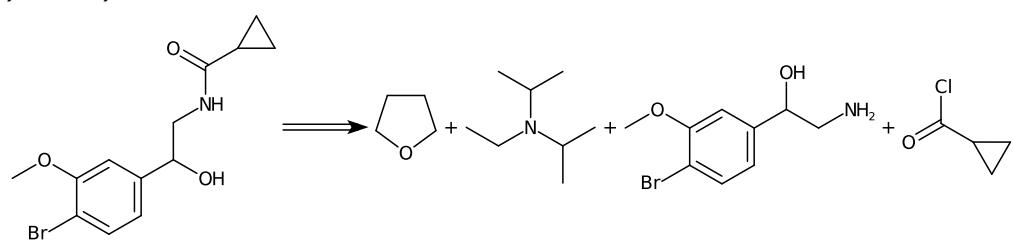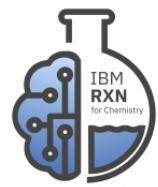
# Information about the retrosynthesis

Created On: 2019-09-30T15:45:28.894000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product: COC1C=CC(CN(C(C)C)C(N2N=C(S(C3CC4CC3CC4)(=O)=O)N=C2)=O)=CC=1
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles: COC1C=CC(CN(C(C)C)C(N2N=C(S(C3CC4CC3CC4)(=O)=O)N=C2)=O)=CC=1
Exclude substructures:

# Sequence 0, Confidence: 0.81

## Step 1

*Type: Amide Schotten-Baumann, Confidence: 0.949*
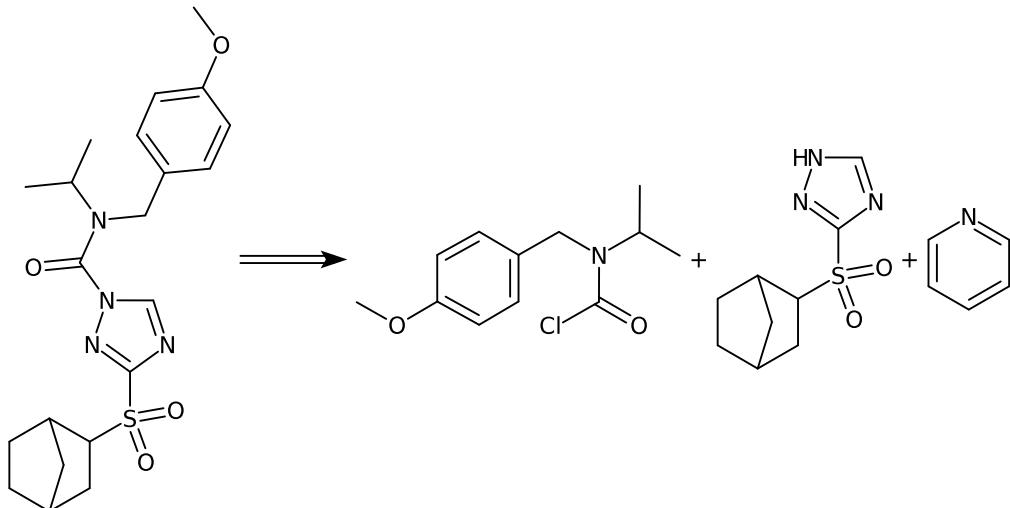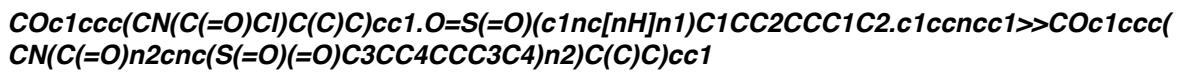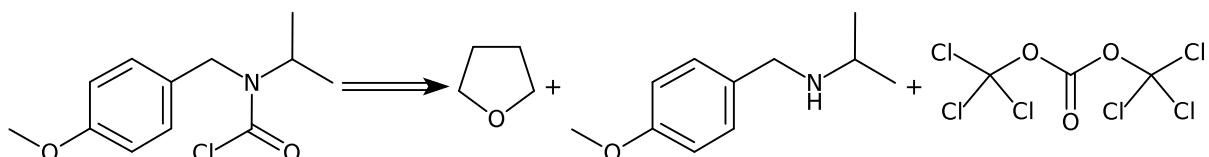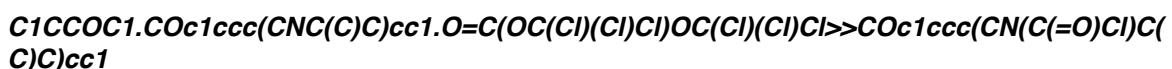
*COc1ccc(CN(C(=O)Cl)C(C)C)cc1.O=S(=O)(c1nc[nH]n1)C1CC2CCC1C2.c1ccncc1>>COc1ccc(CN(C(=O)n2cnc(S(=O)(=O)C3CC4CCC3C4)n2)C(C)C)cc1*



## Step 2

*Type: Unrecognized, Confidence: 0.964*

*C1CCOC1.COc1ccc(CNC(C)C)cc1.O=C(OC(Cl)(Cl)Cl)OC(Cl)(Cl)Cl>>COc1ccc(CN(C(=O)Cl)C(C)C)cc1*



*Type: Sulfanyl to sulfonyl, Confidence: 0.954*

*c1nc(SC2CC3CCC2C3)n[nH]1.CO.O.O=S([O-])OO.[K+]>>O=S(=O)(c1nc[nH]n1)C1CC2CCC1C2*

## Step 3

*Type: Unrecognized, Confidence: 0.93*

*Cc1ccc(S(=O)(=O)OC2CC3CCC2C3)cc1.Sc1nc[nH]n1>>c1nc(SC2CC3CCC2C3)n[nH]1*



## Step 4

*Type: Sulfonic ester Schotten-Baumann, Confidence: 0.998*

*Cc1ccc(S(=O)(=O)Cl)cc1.OC1CC2CCC1C2>>Cc1ccc(S(=O)(=O)OC2CC3CCC2C3)cc1*
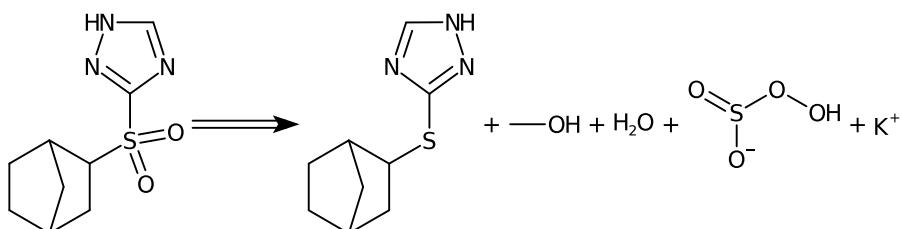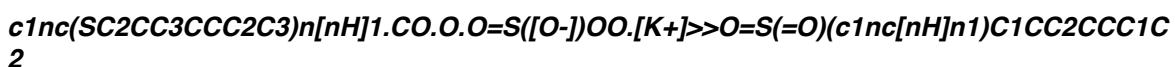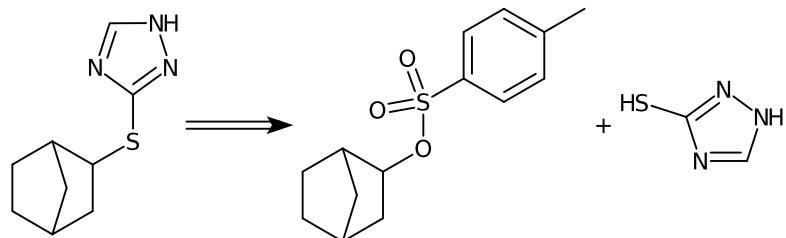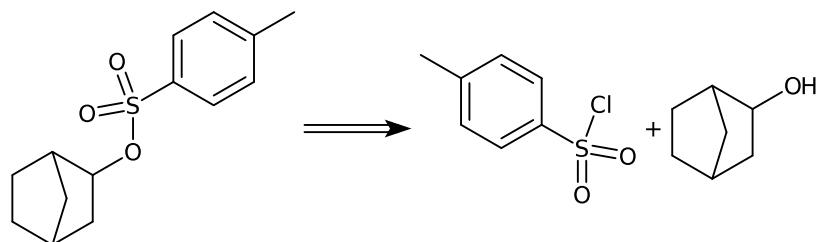
# Information about the retrosynthesis

Created On: 2019-09-26T19:44:51.971000
Model: MolecularTransformer_v2.0_R-Inchi-MolecularTransformer_v2.0_F
Product:
N1C2=C(CCC2)C(NC2=NNC(C3CCCC3)=C2)=NC=1N1CCCC1C(N1CCN(C(CC)=O)CC1)=O
MSSR: 15
FAP: 0.75
MRP: 20
SbP: 2
Available smiles:
Exclude smiles:
N1C2=C(CCC2)C(NC2=NNC(C3CCCC3)=C2)=NC=1N1CCCC1C(N1CCN(C(CC)=O)CC1)=O
Exclude substructures:

# Sequence 0, Confidence: 0.703

Metadata:
Warnings: 'ERROR MESSAGE'

## *Step 1*

*Type: Alkene hydrogenation, Confidence: 0.902*

*CCC(=O)N1CCN(C(=O)C2CCCN2c2nc3c(c(Nc4cc(C5=CCCC5)[nH]n4)n2)CCC3)CC1.CCO.[Pd]
>>CCC(=O)N1CCN(C(=O)C2CCCN2c2nc3c(c(Nc4cc(C5CCCC5)[nH]n4)n2)CCC3)CC1*
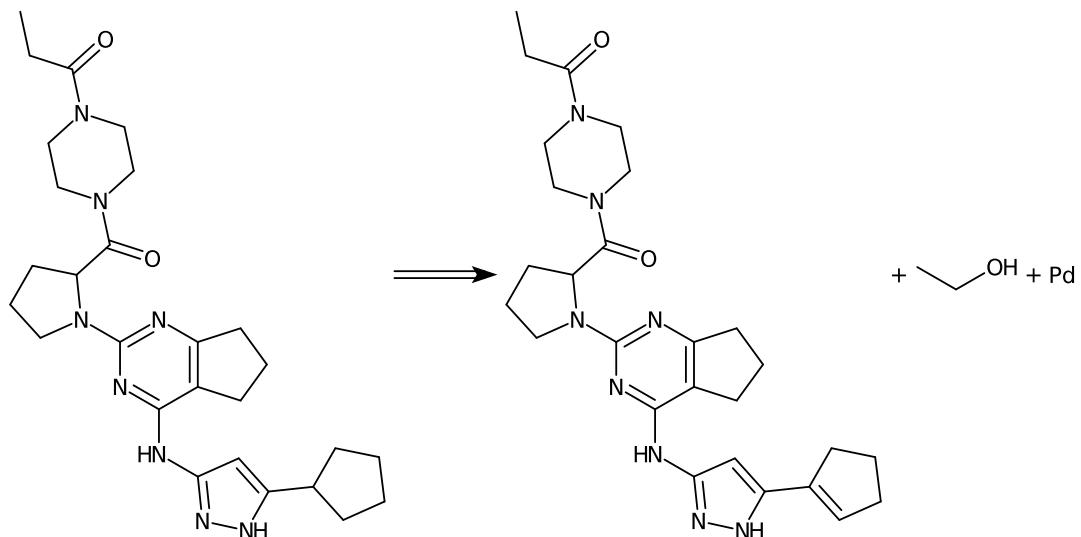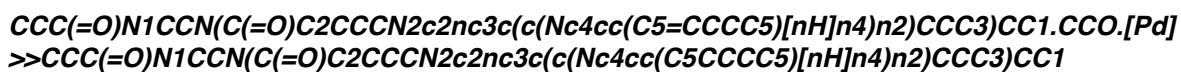


## *Step 2*

*Type: N-SEM deprotection, Confidence: 0.779*

*CCC(=O)N1CCN(C(=O)C2CCCN2c2nc3c(c(Nc4cc(C5=CCCC5)n(COCC[Si](C)(C)C)n4)n2)CCC
3)CC1.ClCCl.O=C(O)C(F)(F)F>>CCC(=O)N1CCN(C(=O)C2CCCN2c2nc3c(c(Nc4cc(C5=CCCC5)
[nH]n4)n2)CCC3)CC1*

## Step 3

*Type: Undefined, Confidence: 0.0*

*CCC(=O)N1CCN(C(=O)C2CCCN2c2nc3c(c(Nc4cc(C5=CCCC5)n(COCC[Si](C)(C)C)n4)n2)CCC3)CC1>>CCC(=O)N1CCN(C(=O)C2CCCN2c2nc3c(c(Nc4cc(C5=CCCC5)n(COCC[Si](C)(C)C)n4)n2)CCC3)CC1*
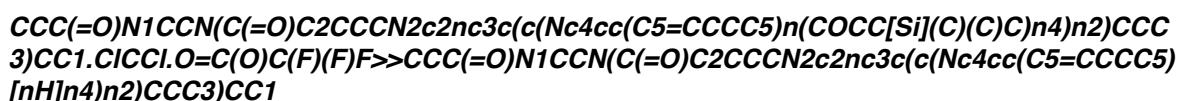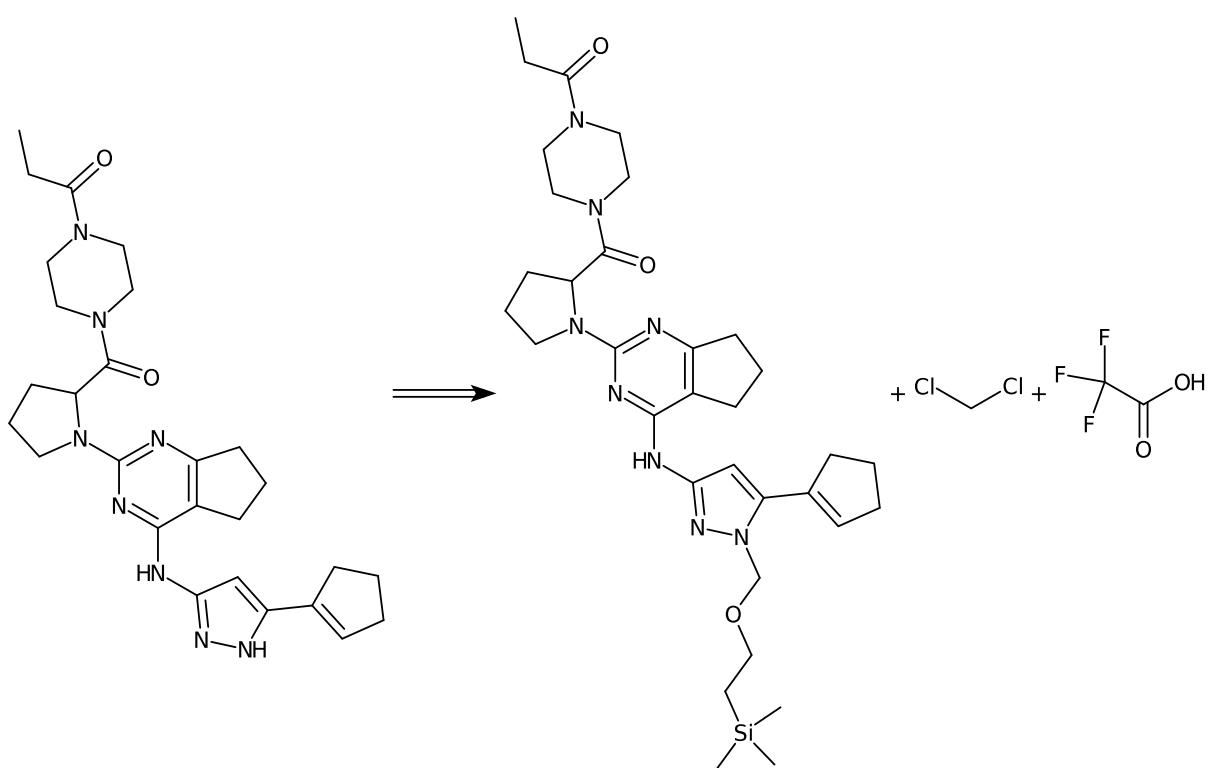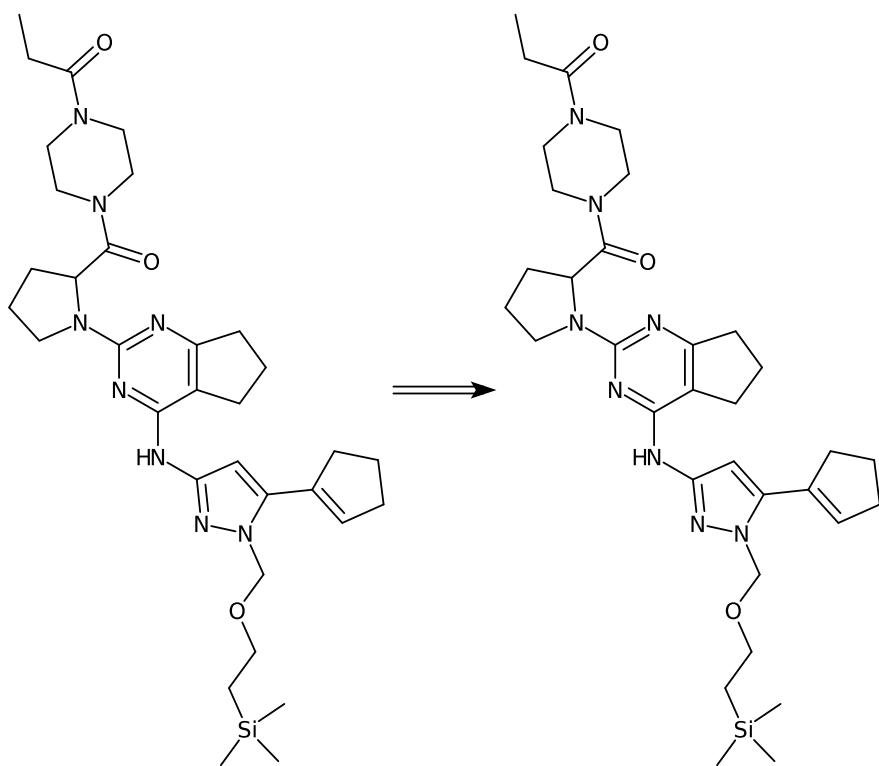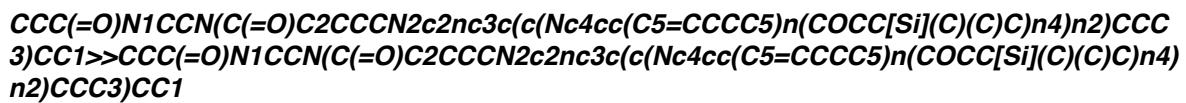
# Sequence 0, Confidence: 0.583

Metadata:
Warnings: The retrosynthesis could not be finished: try increasing the number of steps or start a new one for the missing molecules.

## *Step 1*

*Type: Unrecognized, Confidence: 0.976*

*FC(F)(F)c1c(-c2cc(Cl)nc(N3CCOCC3)n2)c[nH]c2nccc1-2.C1COCCN1>>FC(F)(F)c1c(-c2cc(N3CCOCC3)nc(N3CCOCC3)n2)c[nH]c2nccc1-2*
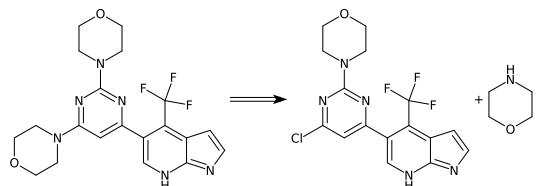


## *Step 2*

*Type: Chloride salt formation, Confidence: 0.96*

*Oc1cc(-c2c[nH]c3nccc-3c2C(F)(F)F)nc(N2CCOCC2)n1.CC#N.O=P(Cl)(Cl)Cl.[Na+].[OH-]>>FC(F)(F)c1c(-c2cc(Cl)nc(N3CCOCC3)n2)c[nH]c2nccc1-2*
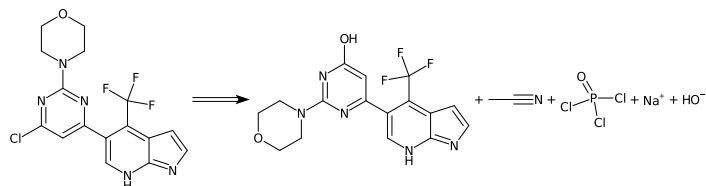


## *Step 3*

*Type: Unrecognized, Confidence: 0.973*

*Oc1cc(-c2c[nH]c3nccc-3c2C(F)(F)F)nc(Cl)n1.C1COCCN1>>Oc1cc(-c2c[nH]c3nccc-3c2C(F)(F)F)nc(N2CCOCC2)n1*
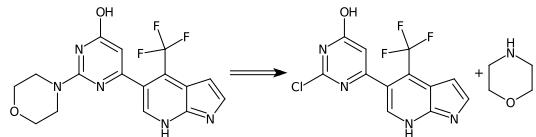


## *Step 4*

*Type: Methoxy to hydroxy, Confidence: 0.958*

*COc1cc(-c2c[nH]c3nccc-3c2C(F)(F)F)nc(Cl)n1.BrB(Br)Br.ClCCl>>Oc1cc(-c2c[nH]c3nccc-3c2C(F)(F)F)nc(Cl)n1*
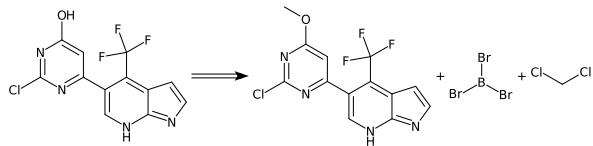
## Step 5

*Type: Unrecognized, Confidence: 0.944*

*COc1cc(-c2cn([Si](C(C)C)(C(C)C)C(C)C)c3nccc-3c2C(F)(F)F)nc(Cl)n1.C1CCOC1.CCCC[N+](CCCC)(CCCC)CCCC.[F-]>>COc1cc(-c2c[nH]c3nccc-3c2C(F)(F)F)nc(Cl)n1*



## Step 6

*Type: Iodo Suzuki coupling, Confidence: 0.862*

*CC(C)[Si](C(C)C)(C(C)C)n1cc(I)c(C(F)(F)F)c2ccnc1-2.COc1cc(B2OC(C)(C)C(C)(C)O2)nc(Cl)n1.C1COCCO1.O.O=C([O-])[O-].[Na+].[Na+].[Cl-].[Cl-].[Pd+2].c1ccc(P(c2ccccc2)c2ccccc2)cc1.c1ccc(P(c2ccccc2)c2ccccc2)cc1>>COc1cc(-c2cn([Si](C(C)C)(C(C)C)C(C)C)c3nccc-3c2C(F)(F)F)nc(Cl)n1*
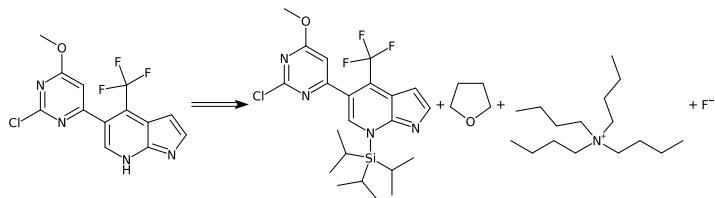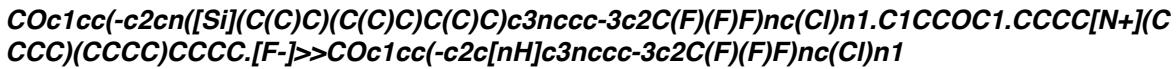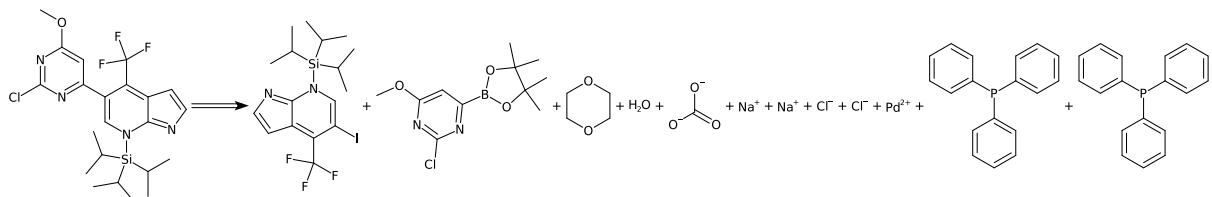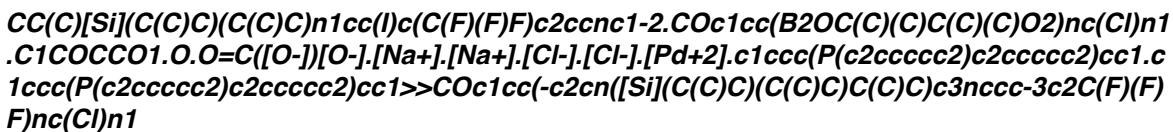


## Step 7

*Type: Chloro Miyaura boration, Confidence: 0.82*

*C1COCCO1.CC(=O)[O-].[K+].CC1(C)OB(B2OC(C)(C)C(C)(C)O2)OC1(C)C.COc1cc(Cl)nc(Cl)n1.ClCCl.CC(=O)[O-].[K+]>>COc1cc(B2OC(C)(C)C(C)(C)O2)nc(Cl)n1*
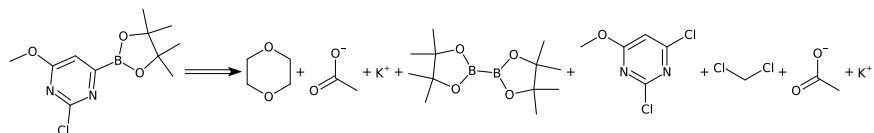
# Sequence 0, Confidence: 0.255

Metadata:
Warnings: The retrosynthesis could not be finished: try increasing the number of steps or start a new one for the missing molecules.

## *Step 1*

*Type: Unrecognized, Confidence: 0.875*
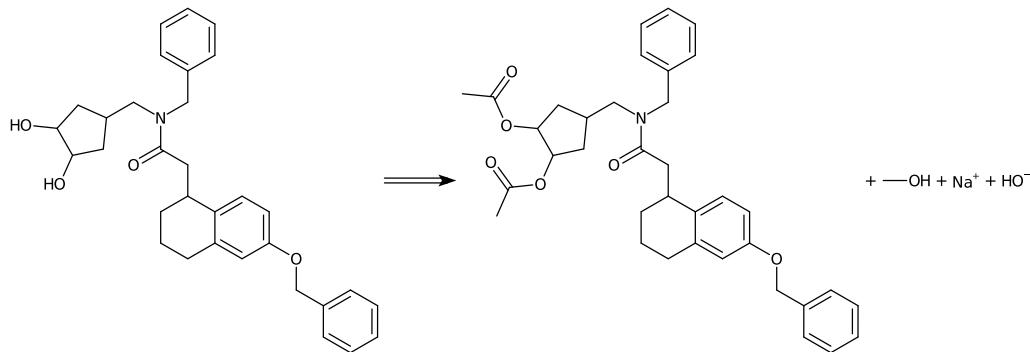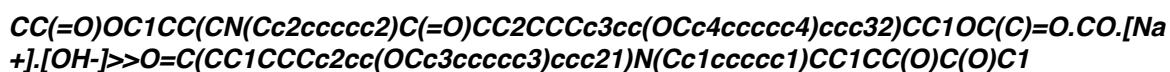
*CC(=O)OC1CC(CN(Cc2ccccc2)C(=O)CC2CCCc3cc(OCc4ccccc4)ccc32)CC1OC(C)=O.CO.[Na+].[OH-]>>O=C(CC1CCCc2cc(OCc3ccccc3)ccc21)N(Cc1ccccc1)CC1CC(O)C(O)C1*

## *Step 2*

*Type: Unrecognized, Confidence: 0.762*

*CC(=O)OC1CC(CNCc2ccccc2)CC1OC(C)=O.O=C(O)CC1CCCc2cc(OCc3ccccc3)ccc21>>CC(=O)OC1CC(CN(Cc2ccccc2)C(=O)CC2CCCc3cc(OCc4ccccc4)ccc32)CC1OC(C)=O*

## *Step 3*

*Type: Unrecognized, Confidence: 0.771*

*CC(=O)OC1CC(C=O)CC1OC(C)=O.CC(=O)O[BH-](OC(C)=O)OC(C)=O.[Na+].CC(=O)O[BH-](OC(C)=O)OC(C)=O.[Na+].ClCCl.NCc1ccccc1>>CC(=O)OC1CC(CNCc2ccccc2)CC1OC(C)=O*
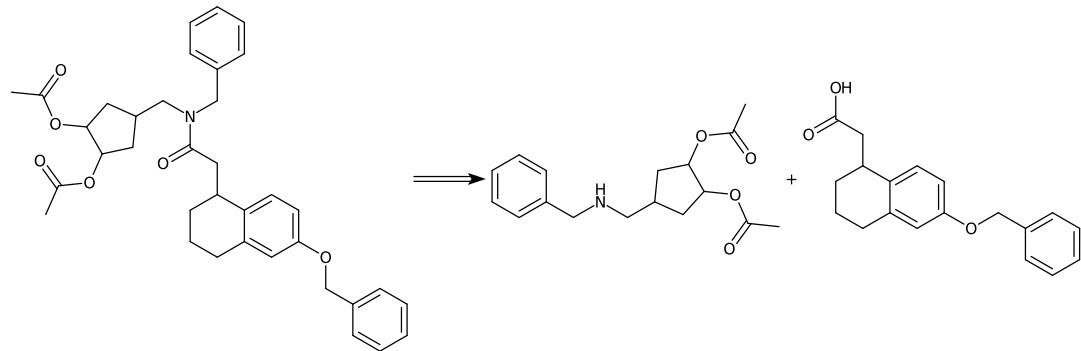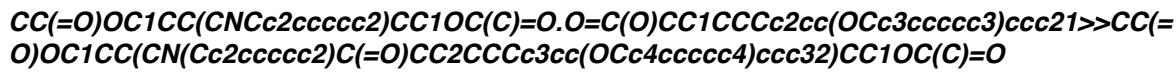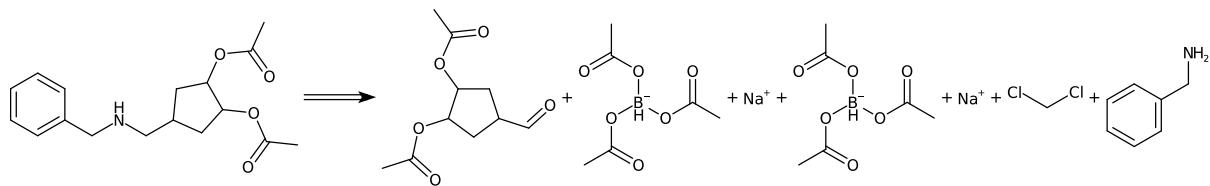
*Type: Unrecognized, Confidence: 0.948*

*N#CCC1CCCc2cc(OCc3ccccc3)ccc21.CCO.[Na+].[OH-]>>O=C(O)CC1CCCc2cc(OCc3ccccc3)ccc21*
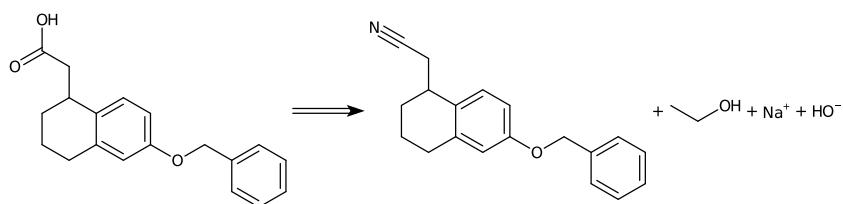


## Step 4

*Type: Separation, Confidence: 0.917*

*CC(=O)OC1CC(CO)CC1OC(C)=O.ClCCl.Cl.[Cr+].[O-].[O].[O].c1ccncc1>>CC(=O)OC1CC(C=O)CC1OC(C)=O*
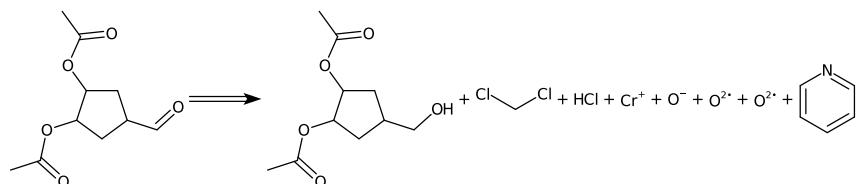


*Type: Williamson ether synthesis, Confidence: 0.978*

*N#CCC1CCCc2cc(O)ccc21.BrCc1ccccc1.CC(C)=O.O=C([O-])[O-].[K+].[K+]>>N#CCC1CCCc2cc(OCc3ccccc3)ccc21*
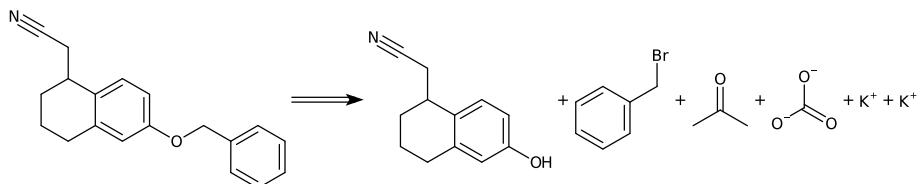


## Step 5

*Type: Unrecognized, Confidence: 0.894*

*CC(=O)OC1CC(C(=O)O)CC1OC(C)=O.B.C1CCOC1.C1CCOC1>>CC(=O)OC1CC(CO)CC1OC(C)=O*
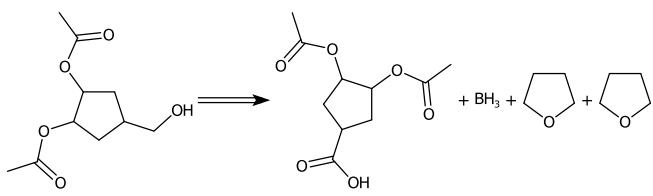
*Type: Methoxy to hydroxy, Confidence: 0.98*

*COc1ccc2c(c1)CCCC2CC#N.BrB(Br)Br.ClCCl.O>>N#CCC1CCCc2cc(O)ccc21*
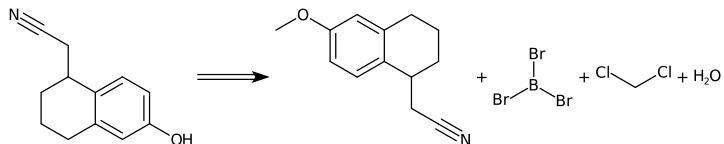


## Step 6

*Type: O-Ac protection, Confidence: 0.88*

*O=C(O)C1CC(O)C(O)C1.CC(=O)OC(C)=O.O=S(=O)(O)O>>CC(=O)OC1CC(C(=O)O)CC1OC(C)=O*
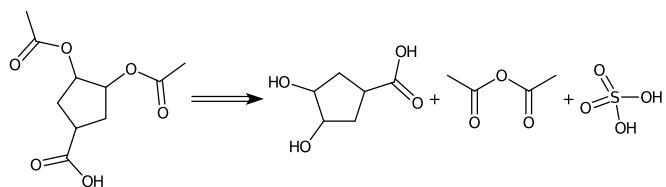


*Type: Chloro Kolbe nitrile synthesis, Confidence: 0.977*

*COc1ccc2c(c1)CCCC2CCl.CN(C)C=O.[C-]#N.[K+]>>COc1ccc2c(c1)CCCC2CC#N*
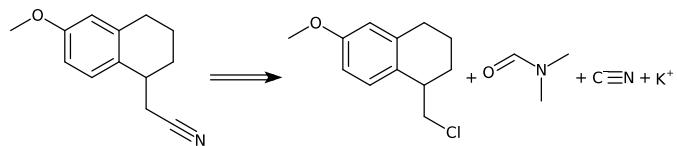


## Step 7

*Type: Unrecognized, Confidence: 0.952*

*O=C1OC2CC1CC2O.O.[Na+].[OH-]>>O=C(O)C1CC(O)C(O)C1*



*Type: Hydroxy to chloro, Confidence: 0.986*

*COc1ccc2c(c1)CCCC2CO.O=S(Cl)Cl>>COc1ccc2c(c1)CCCC2CCl*
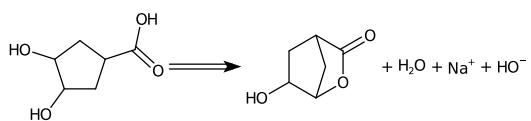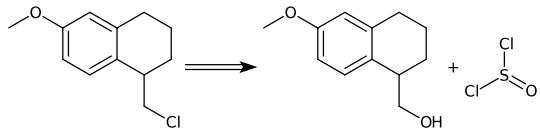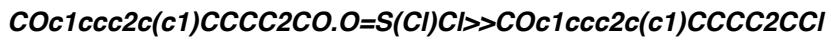


## Step 8

*Type: O-Bn deprotection, Confidence: 0.837*

*O=C1OC2CC1CC2OCc1ccccc1.CO.[HH].[Pd]>>O=C1OC2CC1CC2O*



*Type: Methoxy to hydroxy, Confidence: 0.986*

*B.C1CCOC1.COc1ccc2c(c1)CCCC2C(=O)O>>COc1ccc2c(c1)CCCC2CO*
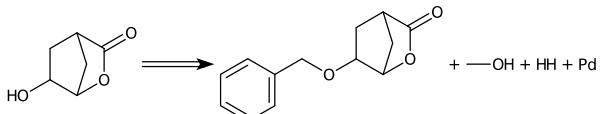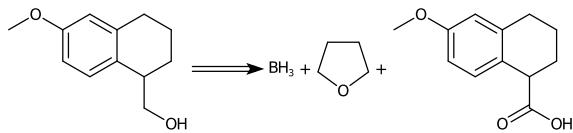
# Sequence 0, Confidence: 0.609

Metadata:
Warnings: The retrosynthesis could not be finished: try increasing the number of steps or start a new one for the missing molecules.

## *Step 1*

*Type: Unrecognized, Confidence: 0.798*

*CC(=O)C[C@@H](c1ccccc1)c1c(OCc2ccccc2)c2ccccc2oc1=O.CCOC(C)=O.[Pd]>>CC(=O)C[C@@H](c1ccccc1)c1c(O)c2ccccc2oc1=O*



## *Step 2*

*Type: Unrecognized, Confidence: 0.962*

*CON(C)C(=O)C[C@@H](c1ccccc1)c1c(OCc2ccccc2)c2ccccc2oc1=O.[CH3].[Cl-].[Mg+].C1CCOC1.[CH3].[Cl-].[Mg+]>>CC(=O)C[C@@H](c1ccccc1)c1c(OCc2ccccc2)c2ccccc2oc1=O*



## *Step 3*

*Type: Unrecognized, Confidence: 0.921*

*O=C(O)C[C@@H](c1ccccc1)c1c(OCc2ccccc2)c2ccccc2oc1=O.CCN(CC)CC.CCN=C=NCCCN(C)C.Cl.CNOC.Cl.ClCCl.On1nnc2ccccc21>>CON(C)C(=O)C[C@@H](c1ccccc1)c1c(OCc2ccccc2)c2ccccc2oc1=O*



## *Step 4*

*Type: Unrecognized, Confidence: 0.948*

*CC(C)(C)OC(=O)C[C@@H](c1ccccc1)c1c(OCc2ccccc2)c2ccccc2oc1=O.ClCCl.O=C(O)C(F)(F)F>>O=C(O)C[C@@H](c1ccccc1)c1c(OCc2ccccc2)c2ccccc2oc1=O*



## Step 5

*Type: Unrecognized, Confidence: 0.908*

*CC(C)(C)OC(=O)C[C@@H](c1ccccc1)c1c(O)c2ccccc2oc1=O.BrCc1ccccc1.CC(C)=O.O=C([O-])[O-].[K+].[K+]>>CC(C)(C)OC(=O)C[C@@H](c1ccccc1)c1c(OCc2ccccc2)c2ccccc2oc1=O*