# Paths of analysis*

OP_Exp

Synthia

February 13, 2024

## 1 Analysis parameters

**Analysis type:** Automatic Retrosynthesis

**Rules:** Expert-Coded Rules

**Published Reactions:** none selected

**Filters:** Exclude Diastereoselecitve reactions, Tunnels, FGI, FGI with protections

**Max. paths returned:** 50

**Max. iterations:** 2000

**Commercial:**

1. Max. molecular weight - 1000 g/mol
2. Max. price - 1500 $/g

**Published:**

1. Max. molecular weight - 1000 g/mol
2. Popularity - 5

**My Stockroom:**

1. Max. molecular weight - 1000 g/mol

**Shorter paths:** no

**Pathway linearity:** COMBO

**Protecting groups:** BALANCED

**Reaction scoring formula:** TUNNEL_COEF*FGI_COEF*STEP*20+1000000*(FILTERS+CONFLICT+NON_SELECTIVITY)+40*PROTECT

**Chemical scoring formula:** SMALLER^ 3,SMALLER^ 1.5

**Min. search width:** 400

**Max. reactions per product:** 60

**Strategies:** none selected

**FGI Coeff:** 1

**Tunnels Coeff:** 1

**JSON Parameters:** {}

# 2 Paths

1 path found. *Paths are sorted by score. Reactions are sorted in appearance order for each path.*

## 2.1 Path 1

**Score:** `141.07`

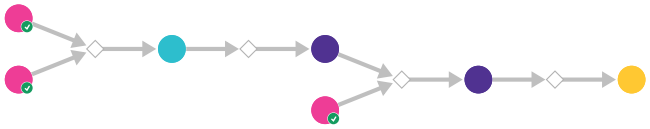
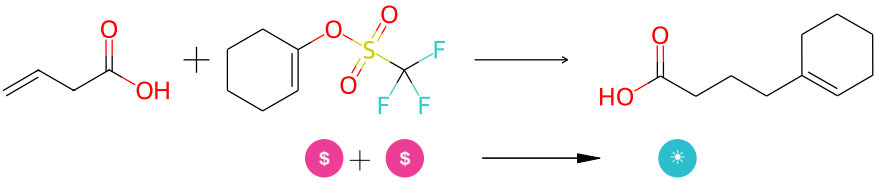


Figure 1: Outline of path 1

### 2.1.1 Suzuki alkyl-vinyl coupling




**Substrates:**

1. 3-Butenoic acid - *available at Sigma-Aldrich*
2. 1-Cyclohexenyl trifluoromethanesulfonate - *available at Sigma-Aldrich*

**Products:**

1. 4-Cyclohex-1-enyl-butyric acid

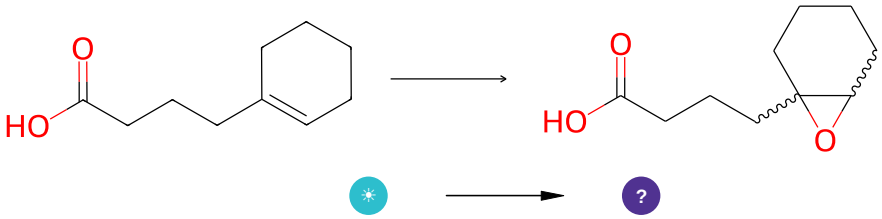
**Typical conditions:** 1. 9BBN-H. or. PinB-Bpin. Cu. 2. [Pd]. Ligand. Base

**Protections:** none

**Reference:** *10.1002/1521-3773(20011217)40:24<4544::AID-ANIE4544>3.0.CO;2-N* and *10.1021/jo00060a041* and *10.1021/ol300575d*

**Retrosynthesis ID:** 10034485

### 2.1.2 Shi epoxidation




**Substrates:**

1. 4-Cyclohex-1-enyl-butyric acid

**Products:**

1. O=C(O)CCCC12CCCCC1O2

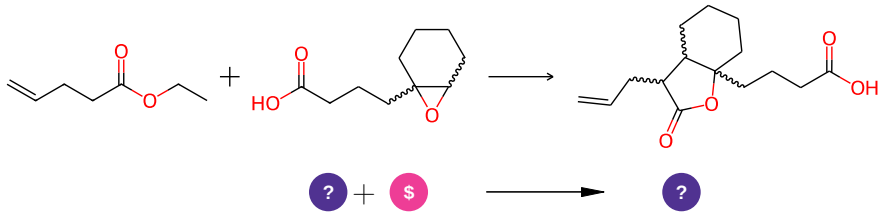
**Typical conditions:** sugar.based.catalyst.KHSO5.K2CO3.H2O.ACN.0C

**Protections:** none

**Reference:** *10.1055/s-0028-1083545* and *10.1021/ja972272g* and *10.1021/ja003049d* and *10.1021/jo972106r*

**Retrosynthesis ID:** 7430

### 2.1.3 Synthesis of lactones from epoxides




**Substrates:**

1. O=C(O)CCCC12CCCCC1O2

2. Ethyl 4-pentenoate - *available at Sigma-Aldrich*

**Products:**

1. C=CCC1C(=O)OC2(CCCC(=O)O)CCCCC12

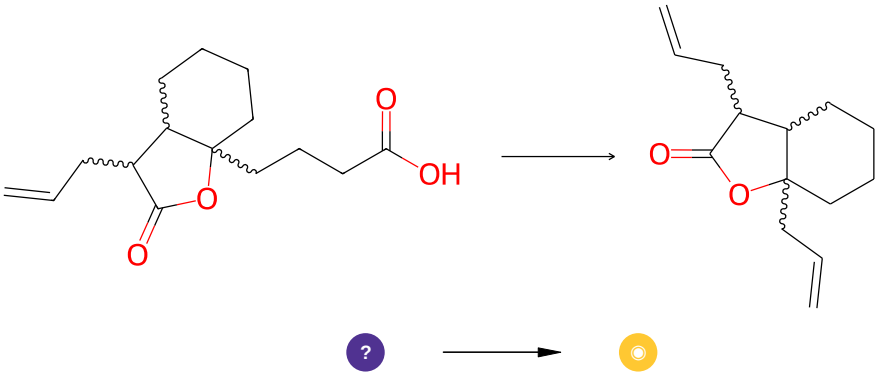
**Typical conditions:** EtONa.EtOH.rt

**Protections:** none

**Reference:** *10.1021/ja9049959* and *10.1016/j.tetlet.2014.12.024* and *10.1021/jo00077a012* and *10.1016/0040-4039(96)00494-7* and *10.1002/chem.201403294*

**Retrosynthesis ID:** 21259

### 2.1.4 Catalytic dehydrogenative decarboxyolefination of carboxylic acids




**Substrates:**

1. C=CCC1C(=O)OC2(CCCC(=O)O)CCCCC12

**Products:**

1. C=CCC1C(=O)OC2(CC=C)CCCCC12

**Typical conditions:** [Ir]-photocatalyst.[Co]-catalyst.Cs2CO3.DME/H2O.blue.light.rt

**Protections:** none

**Reference:** *10.1038/s41557-018-0142-4* and *10.1021/acscatal.8b03282* and *10.1021/acs.joc.9b00167*

**Retrosynthesis ID:** 10032311