

# Paths of analysis\*

C63

Synthia

March 3, 2022

## 1 Analysis parameters

**Analysis type:** Automatic Retrosynthesis

**Rules:** none selected

**Filters:** FGI, FGI with protections

**Max. paths returned:** 5

**Max. iterations:** 300

**Commercial:**

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

**Published:**

1. Max. molecular weight - 1000 g/mol
2. Popularity - 10

**My Stockroom:**

1. Max. molecular weight - 1000 g/mol

**Reaction scoring formula:**  $\text{TUNNEL\_COEF} * \text{FGI\_COEF} * \text{STEP} * 20 + 1000000 * (\text{CONFLICT} + \text{NON\_SELECTIVITY} + \text{FILTERS} + \text{PROTECT})$

**Chemical scoring formula:**  $\text{SMALLER}^3, \text{SMALLER}^{1.5}$

**Min. search width:** 400

**Max. reactions per product:** 60

**Strategies:** none selected

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\*The results stated herein were generated using the proprietary platform owned and maintained by Grzybowski Scientific Inventions, Inc., a subsidiary of Merck KGaA, Darmstadt Germany. The results are provided on an as is basis, and shall be used solely in connection with the rights afforded in the license agreement and for no other purpose.

FGI Coeff: 0

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: 140.92

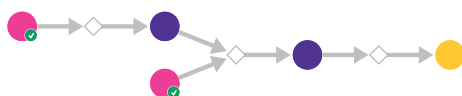
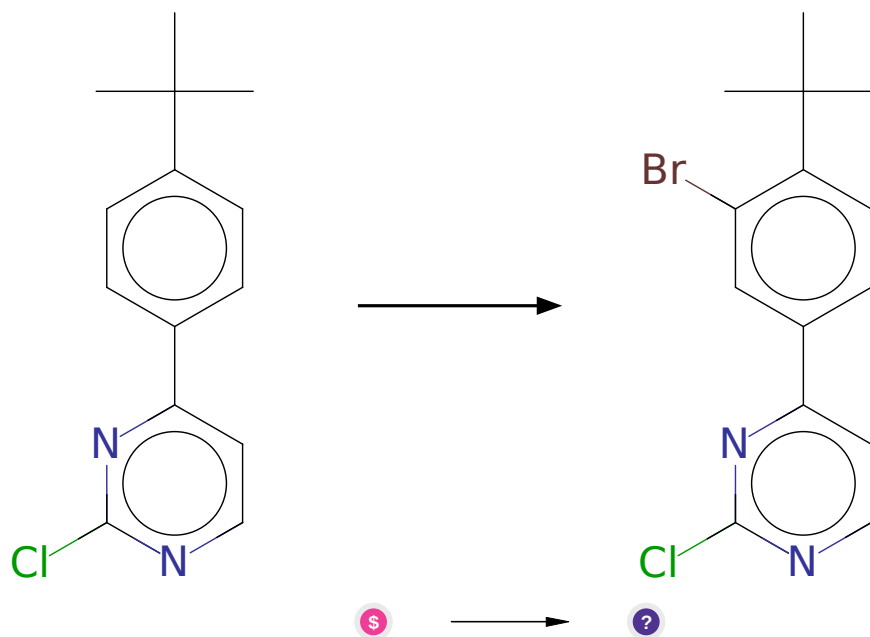


Figure 1: Outline of path 1

#### 2.1.1 Bromination of aromatic compounds



Substrates:

1. 2-Chloro-4-(4-tert-butylphenyl)pyrimidine - *available at Sigma-Aldrich*

**Products:**

1. CC(C)(C)c1ccc(-c2ccnc(Cl)n2)cc1Br

**Typical conditions:** Br<sub>2</sub>.Fe

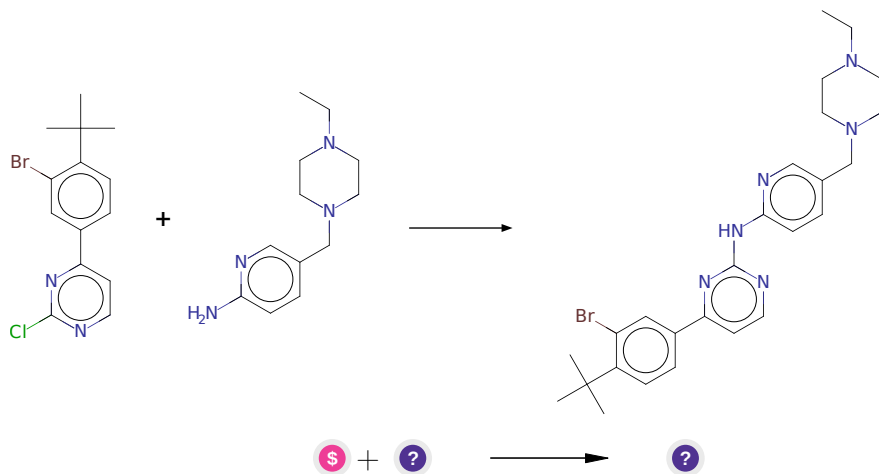
**Protections:** none

**Yield:** good

**Reference:** [10.1021/acs.accounts.6b00120](#)

**Retrosynthesis ID:** 7777000

**2.1.2 Nucleophilic aromatic substitution**



**Substrates:**

1. 5-((4-Ethylpiperazin-1-yl)methyl)pyridin-2-amine - *available at Sigma-Aldrich*
2. CC(C)(C)c1ccc(-c2ccnc(Cl)n2)cc1Br

**Products:**

1. CCN1CCN(Cc2ccc(Nc3cccc(-c4ccc(C(C)(C)C)c(Br)c4)n3)nc2)CC1

**Typical conditions:** solvent. Heating or pressure

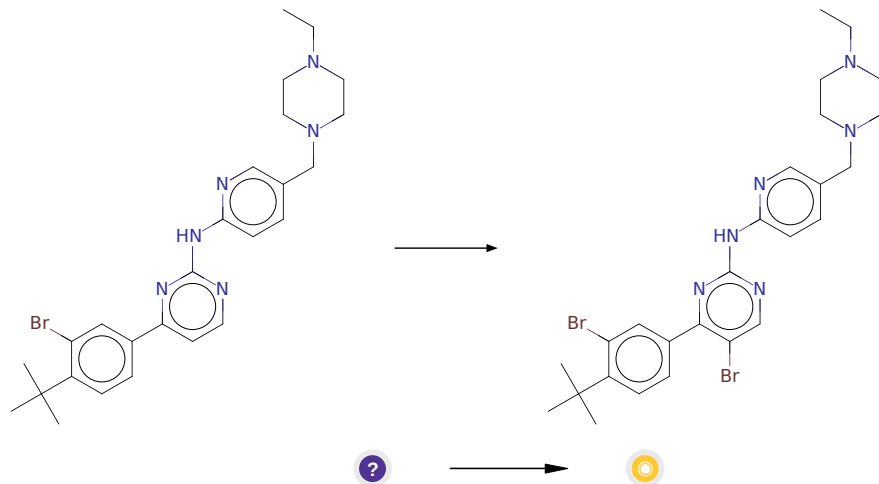
**Protections:** none

**Yield:** good

**Reference:** [10.1021/jm00040a009](#) or [10.1111/bph.12233](#) or [10.1246/cl.1987.1187](#)

**Retrosynthesis ID:** 5003

### 2.1.3 Bromination of aromatic compounds



#### Substrates:

1. CCN1CCN(Cc2ccc(Nc3nccc(-c4ccc(C(C)(C)C)c(Br)c4)n3)nc2)CC1

#### Products:

1. CCN1CCN(Cc2ccc(Nc3ncc(Br)c(-c4ccc(C(C)(C)C)c(Br)c4)n3)nc2)CC1

**Typical conditions:** Br<sub>2</sub>.Fe

**Protections:** none

**Yield:** good

**Reference:** [10.1021/acs.accounts.6b00120](#)

**Retrosynthesis ID:** 7777000