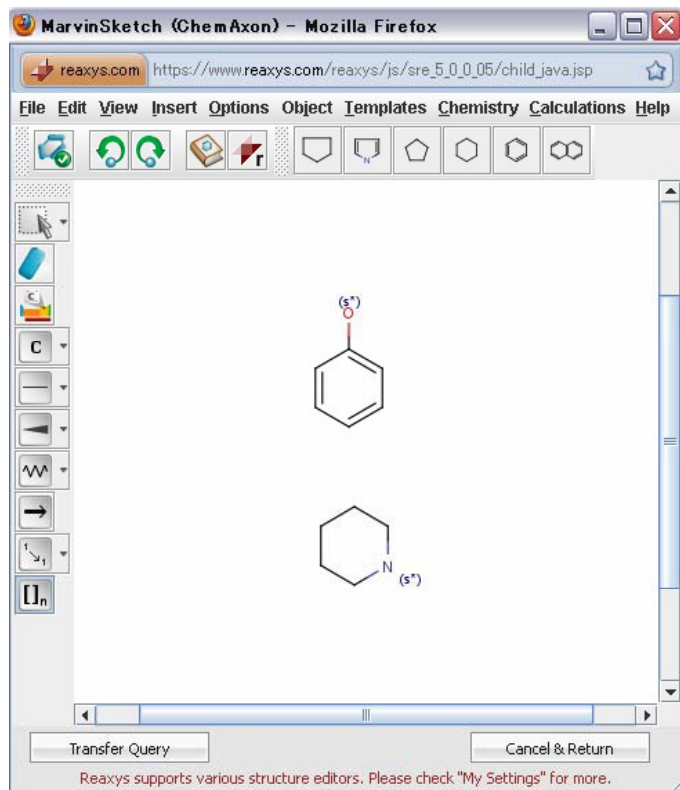


<検索1 (Query 1)>

Step 1.

構造を描き、必要に応じて置換基の発生を制御 → Transfer Query



Step 2.

検索の条件設定

- 1) Starting material
 - 2) Substructure
 - 3) Keep Fragments – together
- 検索 (3954hits)

Reactions Substances and Properties Literature

Generate structure from name

Double click this frame and draw reaction query STRUCTURE EDITOR

Search as / by

- Product
- Starting material
- Any role
- Reagent/ Catalyst
- As drawn
- Substructure:
 - on heteroatoms
 - on all atoms
- Similarity

Include tautomers
Ignore stereo
No isotopes
No charges
No radicals
No additional rings
 Keep Fragments ...

- separate
- together

 Ignore Atom Mappings

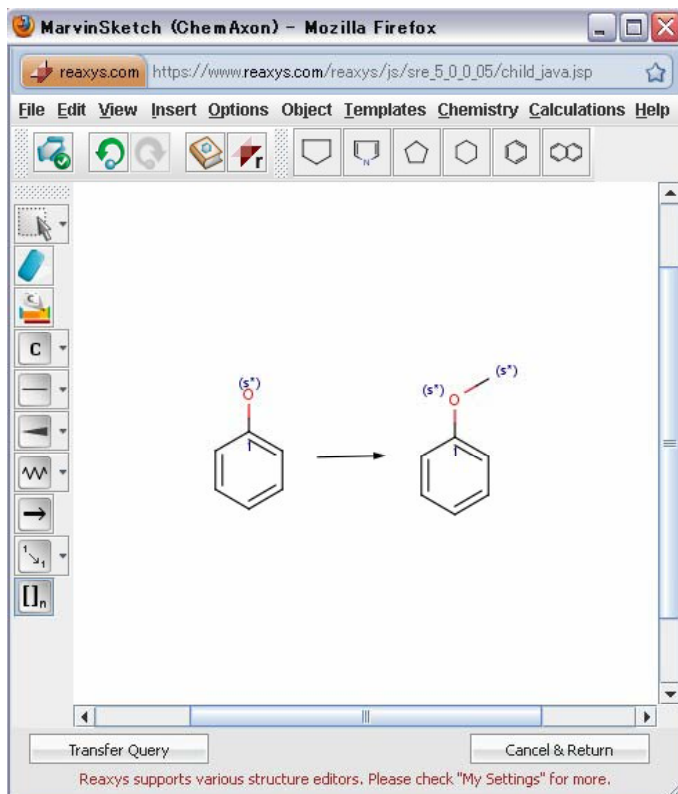
Conditions (Form-based) Conditions (Advanced)

Search

<検索2 (Query 2)>

Step 3.

反応式を描き、マッピングをする(必要に応じて置換基の発生を制御) → Transfer Query



Step 4.

検索の条件設定

1) Substructure

→ 検索(46912hits)

<掛け合わせ (Combine hitsets)>

Step 5.

Historyから検索1&2の結果を掛け合わせ、共通項を選択

Query Results Synthesis Plans History My Alerts My Settings Help

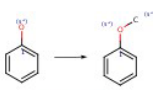

Reaxys PubChem

Select how you want to combine the hitsets

Merge 4 with 2 **Overlap 4 with 2** Exclude 4 from 2 Exclude 2 from 4

Cancel

Combine hitsets Select at least two hitsets for combining

Query	Temporary result description
<input checked="" type="checkbox"/> 4 <input type="checkbox"/> 3	 46912 reactions Reactions: Substructure: on all atoms 17510 citations Edit Create Alert Reactions: Substructure: on all atoms
<input checked="" type="checkbox"/> 2 <input type="checkbox"/> 1	 3954 reactions Reactions: Starting material, Substructure: on all atoms, Keep Fragments together 945 citations Edit Create Alert Reactions: Starting material, Substructure: on all atoms, Keep Fragments together

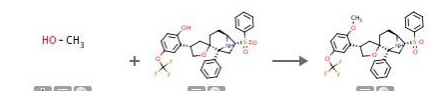
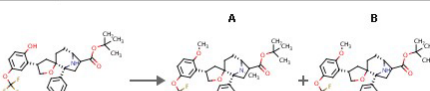
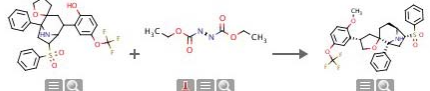
<検索結果>

134hits

134 reactions out of 71 citations

Reactions Citations go to Page Page 1 of 15

Limit to Exclude Output Print Zoom in Zoom out Hide Sort by Reaxys-Ranking

Yield	Conditions	References
<input type="checkbox"/> 1	 Synthesize Synthesize Synthesize Rx-ID: 23064890 Find similar reactions	MERCK SHARP and DOHME LIMITED Patent: WO2004/31191 A1, 2004 ; Location in patent: Page 50 ; Title/Abstract Full Text Show Details
84%	Stage #1: With triphenylphosphine; diethylazodicarboxylate in tetrahydrofuran T=20°C; 12 h; Stage #2: With sodium hydroxide in tetrahydrofuran; methanol T=20°C; 24 h; Alkaline aqueous solution; Show Experimental Procedure	
<input type="checkbox"/> 2	 Synthesize Synthesize Synthesize Rx-ID: 23064867 Find similar reactions	MERCK SHARP and DOHME LIMITED Patent: WO2004/31191 A1, 2004 ; Location in patent: Page 50 ; Title/Abstract Full Text Show Details
	Stage #1: With methanol; triphenylphosphine; diethylazodicarboxylate in tetrahydrofuran T=20°C; 2 h; Stage #2: With water in tetrahydrofuran Show Experimental Procedure	
<input type="checkbox"/> 3	 Synthesize Synthesize Synthesize Rx-ID: 24134568 Find similar reactions	Huscroft, Ian Thomas; Kulagowski, Janusz Jozef; Raubo, Piotr Antoni Patent: US2002/147207 A1, 2002 ; Title/Abstract Full Text Show Details
	With sodium hydroxide; triphenylphosphine in tetrahydrofuran; methanol Show Experimental Procedure	