

IV - 1) 結合次数の指定

❖ Types機能を使い、任意の結合や、一重または二重結合といった結合次数を指定

1 結合を指定したいボンドの上で右クリック

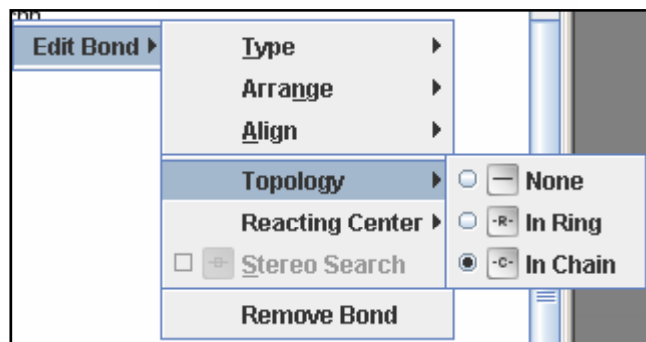
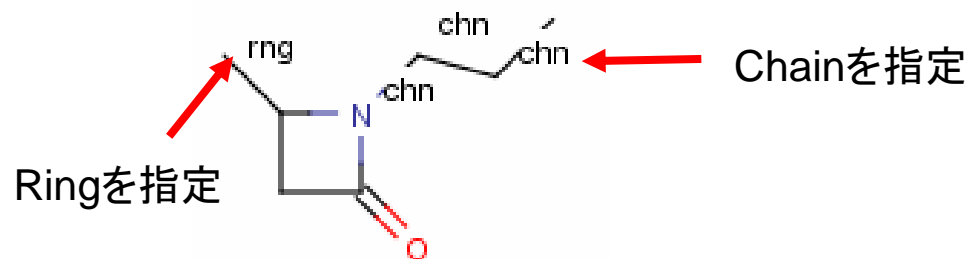
2 [Edit Bond]-[Type]から、項目を選択

3 結合の種類を選択

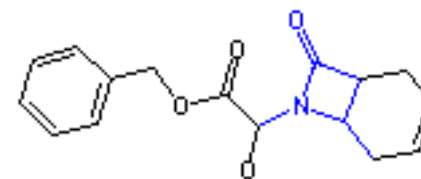
The screenshot shows a chemical structure editor with a toolbar at the top and a vertical toolbar on the left. The main canvas displays a skeletal structure of a 1-butanol molecule. A context menu is open over the C-O bond, with the 'Edit Bond' option selected. The 'Edit Bond' submenu is also open, showing the 'Type' option selected. The 'Type' submenu lists various bond types with radio buttons: Single (selected), Double, Triple, Aromatic, Single Up, Single Down, Single Up or Down, Double Cis or Trans, Double C/T or Unspec, Single or Double (highlighted), Single or Aromatic, Double or Aromatic, Any, and Coordinate.

IV - 2) 環状・鎖状結合の指定

❖ Topology機能を使って鎖状か環状結合を指定



検索結果例



Reaxysの検索オプション指定:

- Substructureを指定
- No additional rings (チェックせず)

- 1 反応位置を指定したいボンドの上で右クリック
- 2 [Edit Bond]-[Topology]から、項目を選択
 - None 指定なし
 - In Ring 環状
 - In Chain 鎖状