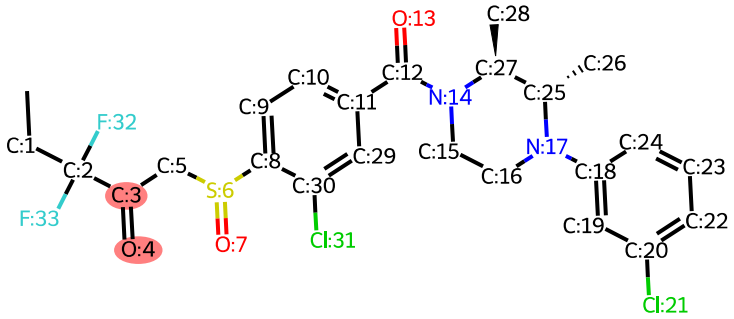
Reaction Report for *LEI_515*, Priority 11

Selected Position: `C:3 0:4`

Selected Forward Reaction: Oxidation or Dehydrogenation of Alcohols to Aldehydes and Ketones

Product



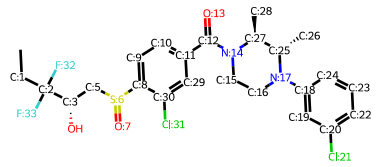
Reaction site highlighted at position `C:3 0:4`

Product SMILES: `C[CH2:1][C:2]([C:3](=[O:4])[CH2:5][S:6](=[O:7])[c:8]1[cH:9][cH:10][c:11]([C:12](=[O:13])[N:14]2[CH2:15][CH2:16][N:17]([c:18]3[cH:19][c:20]([Cl:21])[cH:22][cH:23][cH:24]3)[C@@H:25]([CH3:26])[C@@H:27]2[CH3:28])[cH:29][c:30]1[Cl:31])([F:32])[F:33]`

Proposed Transitions

Transition 1

- **Forward Reaction:** Oxidation or Dehydrogenation of Alcohols to Aldehydes and Ketones
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. The reactant, a secondary alcohol, is chemically stable. The transformation to the ketone product is a standard oxidation reaction. Common reagents for this transformation (e.g., Dess-Martin periodinane, Swern oxidation) are highly chemoselective and would not interfere with the amide, sulfoxide, or aromatic halides present in the molecule. The oxidation of this specific enantiomer correctly yields the achiral ketone product by removing the stereocenter at C:3.
- **Is Smiles Valid:** True
- **Reactant 1:** `C[CH2:1][C:2]([C@@H:3](O)[CH2:5][S:6](=[O:7])[c:8]1[cH:9][cH:10][c:11]([C:12](=[O:13])[N:14]2[CH2:15][CH2:16][N:17]([c:18]3[cH:19][c:20]([Cl:21])[cH:22][cH:23][cH:24]3)[C@@H:25]([CH3:26])[C@@H:27]2[CH3:28])[cH:29][c:30]1[Cl:31])([F:32])[F:33]`



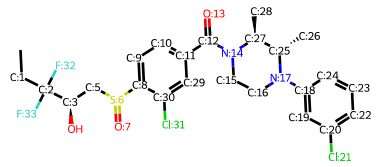
R1

Reactants for Transition 1

Transition 2

- **Forward Reaction:** Oxidation or Dehydrogenation of Alcohols to Aldehydes and Ketones
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. Similar to its enantiomer, this secondary alcohol is a stable and suitable precursor. The chemoselectivity and stereochemical consistency arguments hold true; the oxidation is a highly plausible transformation that selectively targets the alcohol and produces the desired achiral ketone.
- **Is Smiles Valid:** True

- **Reactant 1:** `C[CH2:1][C:2]([C@H:3](O)[CH2:5][S:6](=[O:7])[c:8]1[cH:9][cH:10][c:11]([C:12](=[O:13])[N:14]2[CH2:15][CH2:16][N:17]([c:18]3[cH:19][c:20]([Cl:21])[cH:22][cH:23][cH:24]3)[C@@H:25]([CH3:26])[C@@H:27]2[CH3:28])[cH:29][c:30]1[Cl:31])([F:32])[F:33]`

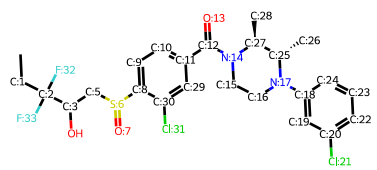


R1

Reactants for Transition 2

Transition 3

- **Forward Reaction:** Oxidation or Dehydrogenation of Alcohols to Aldehydes and Ketones
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. It represents the use of a racemic mixture of the alcohol precursor. In many synthetic contexts, controlling the stereochemistry at this position may not be necessary, making the racemic precursor a practical and efficient starting material. Oxidation of the racemate will yield the single desired achiral ketone product, making this a chemically sound and plausible option.
- **Is Smiles Valid:** True
- **Reactant 1:** `C[CH2:1][C:2]([CH:3](O)[CH2:5][S:6](=[O:7])[c:8]1[cH:9][cH:10][c:11]([C:12](=[O:13])[N:14]2[CH2:15][CH2:16][N:17]([c:18]3[cH:19][c:20]([Cl:21])[cH:22][cH:23][cH:24]3)[C@@H:25]([CH3:26])[C@@H:27]2[CH3:28])[cH:29][c:30]1[Cl:31])([F:32])[F:33]`



R1

Reactants for Transition 3