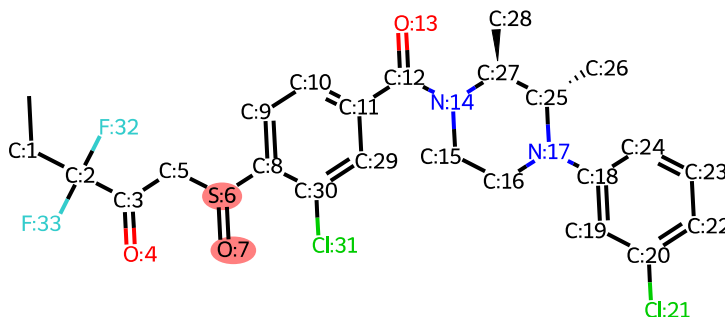


Reaction Report for *LEI_515*, Priority 7

Selected Position: S:6 0:7

Selected Forward Reaction: Sulfanyl to sulfinyl_H2O2

Product



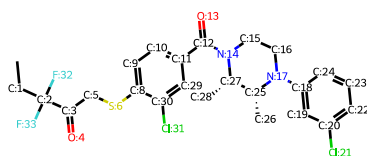
Reaction site highlighted at position S:6 0:7

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:** Sulfanyl to sulfinyl_H2O2
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This is a valid retrosynthetic step. The reactant, an aryl alkyl sulfide, is a stable molecule. The forward reaction, the oxidation of a sulfide to a sulfoxide using hydrogen peroxide, is a classic, highly plausible, and widely employed transformation in organic synthesis. While the substrate contains other potentially oxidizable sites, such as the piperazine nitrogen, selective oxidation at the electron-rich sulfur atom is a common and chemoselective process that can be controlled by reaction conditions (e.g., stoichiometry, temperature). The reaction is electronically favorable and poses no significant steric issues.
- **Is Smiles Valid:** True
- **Reactant 1:** C[CH2:1][C:2]([F:32])([F:33])[C:3](=[O:4])[CH2:5][S:6][c:8]1[cH:9][cH:10][c:11]([C:12](=[O:13])[N:14]2[C@@H:27]([CH3:28])[C@@H:25]([CH3:26])[N:17]([c:18]3[cH:19][c:20]([Cl:21])[cH:22][cH:23][cH:24]3)[CH2:16][CH2:15]2)[cH:29][c:30]1[Cl:31]



R1

Reactants for Transition 1