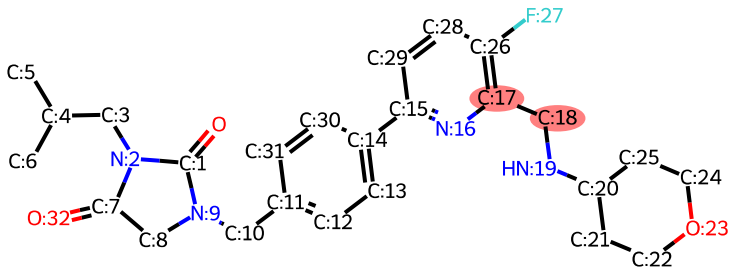
Reaction Report for *LEI_102*, Priority 9

Selected Position: `C:17 C:18`

Selected Forward Reaction: Reductive amination with aldehyde

Product

Reaction site highlighted at position `C:17 C:18`

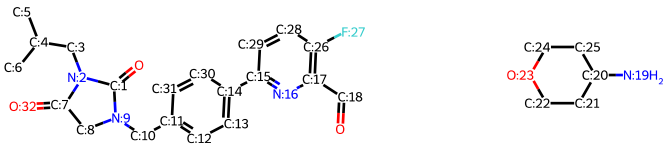


Product SMILES: `O=[C:1]1[N:2]([CH2:3][CH:4]([CH3:5])[CH3:6])[C:7](=[O:32])[CH2:8][N:9]1[CH2:10][c:11]1[cH:12][cH:13][c:14](-[c:15]2[n:16][c:17]([CH2:18][NH:19][CH:20]3[CH2:21][CH2:22][O:23][CH2:24][CH2:25]3)[c:26]([F:27])[cH:28][cH:29]2)[cH:30][cH:31]1`

Proposed Transitions

Transition 1

- **Forward Reaction:** Reductive amination with aldehyde
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This is a standard and highly plausible reductive amination. The aldehyde and primary amine reactants are stable. The reaction is chemoselective as the aldehyde is the most electrophilic carbonyl and the primary amine is the most nucleophilic nitrogen. Other functional groups (amides, imidazole) are unreactive under these conditions. The transformation is stereochemically consistent, preserving the existing stereocenter at C:4 and any stereochemistry at C:20.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]1[N:2]([CH2:3][CH:4]([CH3:5])[CH3:6])[C:7](=[O:32])[CH2:8][N:9]1[CH2:10][c:11]1[cH:12][cH:13][c:14](-[c:15]2[n:16][c:17]([CH:18]=O)[c:26]([F:27])[cH:28][cH:29]2)[cH:30][cH:31]1`
- **Reactant 2:** `[NH2:19][CH:20]1[CH2:21][CH2:22][O:23][CH2:24][CH2:25]1`



R1

R2

Reactants for Transition 1