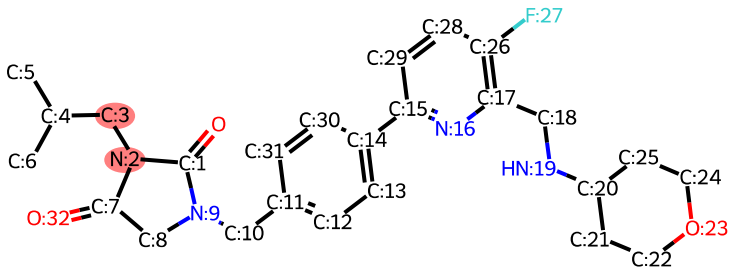
Reaction Report for *LEI_102*, Priority 13

Selected Position: `N:2 C:3`

Selected Forward Reaction: N-alkylation of secondary amines with alkyl halides

Product



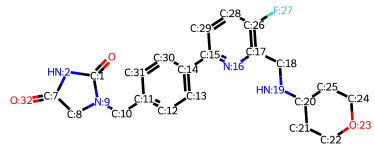
Reaction site highlighted at position `N:2 C:3`

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:** N-alkylation of secondary amines with alkyl halides
- **Is Chemically Valid:** True
- **Is Template-based:** True
- **Reasoning:** This is a general template for N-alkylation. The wildcard atom [*] represents a suitable leaving group attached to the isobutyl electrophile.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]1[NH:2][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`
- **Reactant 2:** `[*][CH2:3][CH:4]([CH3:5])[CH3:6]`



R1

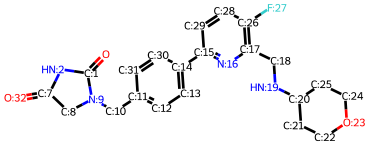
R2

Reactants for Transition 1

Transition 2

- **Forward Reaction:** N-alkylation of secondary amines with alkyl halides
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. Triflate is an excellent leaving group, making the isobutyl triflate highly electrophilic and suitable for this SN2 reaction. However, the reaction may face chemoselectivity challenges from the secondary amine ([NH:19]) in the side chain, which could also act as a nucleophile. Additionally, the β-branched isobutyl electrophile is susceptible to E2 elimination as a competing pathway.
- **Is Smiles Valid:** True

- **Reactant 1:** `O=[C:1]1[NH:2][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`
- **Reactant 2:** `O(S(=O)(=O)C(F)(F)F)[CH2:3][CH:4]([CH3:5])[CH3:6]`



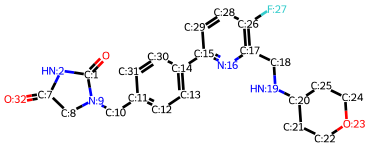
R1

R2

Reactants for Transition 2

Transition 3

- **Forward Reaction:** N-alkylation of secondary amines with alkyl halides
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. Iodide is an excellent leaving group, making isobutyl iodide a suitable electrophile for this SN2 reaction. However, the reaction may face chemoselectivity challenges from the secondary amine ([NH:19]) in the side chain, which could also act as a nucleophile. Additionally, the β-branched isobutyl electrophile is susceptible to E2 elimination as a competing pathway.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]1[NH:2][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`
- **Reactant 2:** `I[CH2:3][CH:4]([CH3:5])[CH3:6]`



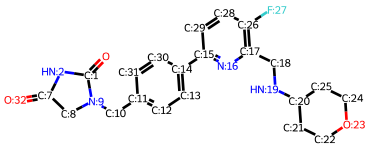
R1

R2

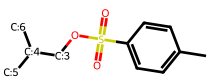
Reactants for Transition 3

Transition 4

- **Forward Reaction:** N-alkylation of secondary amines with alkyl halides
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. Tosylate is an excellent leaving group, making isobutyl tosylate a suitable electrophile for this SN2 reaction. However, the reaction may face chemoselectivity challenges from the secondary amine ([NH:19]) in the side chain, which could also act as a nucleophile. Additionally, the β-branched isobutyl electrophile is susceptible to E2 elimination as a competing pathway.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]1[NH:2][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`
- **Reactant 2:** `Cc1ccc(S(=O)(=O)O[CH2:3][CH:4]([CH3:5])[CH3:6])cc1`



R1

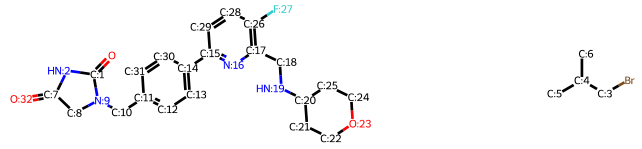


R2

Reactants for Transition 4

Transition 5

- **Forward Reaction:** N-alkylation of secondary amines with alkyl halides
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. Bromide is a very good leaving group, making isobutyl bromide a common and suitable electrophile for this SN2 reaction. However, the reaction may face chemoselectivity challenges from the secondary amine ([NH:19]) in the side chain, which could also act as a nucleophile. Additionally, the β-branched isobutyl electrophile is susceptible to E2 elimination as a competing pathway.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]1[NH:2][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`
- **Reactant 2:** `Br[CH2:3][CH:4]([CH3:5])[CH3:6]`



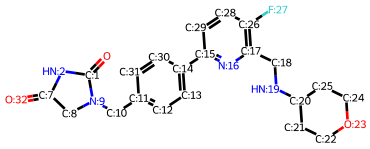
R1 R2

Reactants for Transition 5

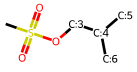
Transition 6

- **Forward Reaction:** N-alkylation of secondary amines with alkyl halides
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. Mesylate is a very good leaving group, making isobutyl mesylate a suitable electrophile for this SN2 reaction. However, the reaction may face chemoselectivity challenges from the secondary amine ([NH:19]) in the side chain, which could also act as a nucleophile. Additionally, the β-branched isobutyl electrophile is susceptible to E2 elimination as a competing pathway.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]1[NH:2][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`

- **Reactant 2:** `CS(=O)(=O)O[CH2:3][CH:4]([CH3:5])[CH3:6]`



R1

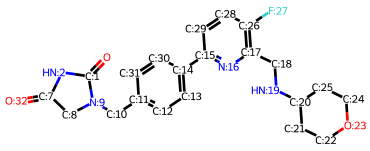


R2

Reactants for Transition 6

Transition 7

- **Forward Reaction:** N-alkylation of secondary amines with alkyl halides
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is valid. Chloride is a moderate leaving group, less reactive than bromide or iodide. The reaction is plausible but may require harsher conditions, which could increase side reactions. The reaction may face chemoselectivity challenges from the secondary amine ([NH:19]) in the side chain, which could also act as a nucleophile. Additionally, the β-branched isobutyl electrophile is susceptible to E2 elimination as a competing pathway.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]1[NH:2][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`
- **Reactant 2:** `Cl[CH2:3][CH:4]([CH3:5])[CH3:6]`



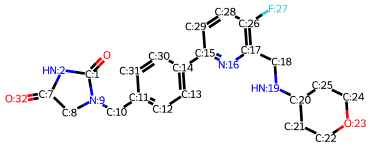
R1

R2

Reactants for Transition 7

Transition 8

- **Forward Reaction:** N-alkylation of secondary amines with alkyl halides
- **Is Chemically Valid:** False
- **Is Template-based:** False
- **Reasoning:** This permutation is invalid. Fluoride is a very poor leaving group for SN2-type nucleophilic substitution reactions due to the high strength of the C-F bond, making this transformation synthetically unfeasible under standard N-alkylation conditions.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]1[NH:2][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`
- **Reactant 2:** `F[CH2:3][CH:4]([CH3:5])[CH3:6]`



R1

R2

Reactants for Transition 8