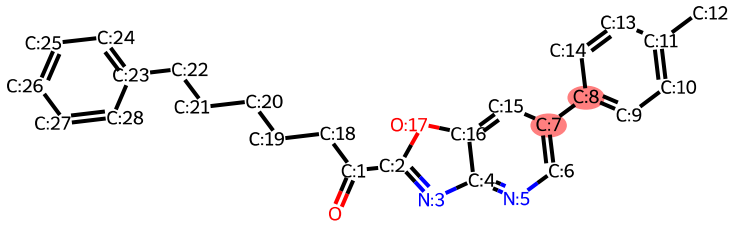
Reaction Report for *LEI_105*, Priority 2

Selected Position: `C:7 C:8`

Selected Forward Reaction: Suzuki coupling with boronic acids

Product



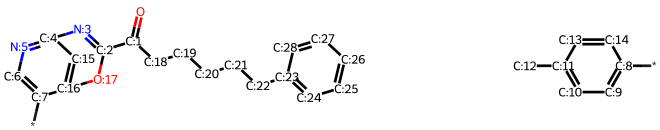
Reaction site highlighted at position `C:7 C:8`

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

Proposed Transitions

Transition 1

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** True
- **Reasoning:** This is the general template for a Suzuki coupling. One wildcard [*] represents a group (-B(O)O), and the other represents a suitable leaving group, typically a halide (I, Br, Cl) or a triflate (-OS(O)2CF3).
- **Is Smiles Valid:** True
- **Reactant 1:** `*[c:7]1[cH:6][n:5][c:4]2[n:3][c:2]([C:1](=O)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]3[cH:24][cH:25][cH:26][cH:27][cH:28]3)[o:17][c:16]1[cH:15]2`
- **Reactant 2:** `*[c:8]1[cH:9][cH:10][c:11]([CH3:12])[cH:13][cH:14]1`



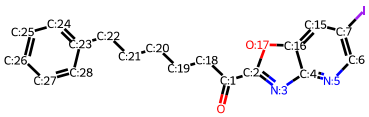
R1 R2

Reactants for Transition 1

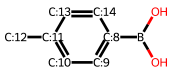
Transition 2

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This is a highly plausible permutation. The reactants are stable. The coupling involves an electron-deficient heteroaryl iodide and an electron-neutral arylboronic acid, which is electronically favorable for the catalytic cycle. Chemoselectivity is expected to be high, with no other functional groups likely to interfere under standard Suzuki conditions.
- **Is Smiles Valid:** True

- **Reactant 1:** `O=[C:1]([c:2]1[n:3][c:4]2[n:5][cH:6][c:7](I)[cH:15][c:16]2[o:17]1)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]1[cH:24][cH:25][cH:26][cH:27][cH:28]1`
- **Reactant 2:** `OB(O)[c:8]1[cH:9][cH:10][c:11]([CH3:12])[cH:13][cH:14]1`



R1

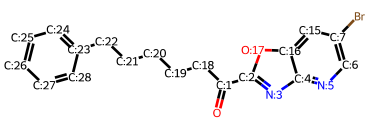


R2

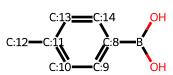
Reactants for Transition 2

Transition 3

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This is a highly plausible permutation. The reactants are stable. The coupling involves an electron-deficient heteroaryl bromide and an electron-neutral arylboronic acid, which is electronically favorable for the catalytic cycle. This is a very common and reliable variant of the Suzuki coupling.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]([c:2]1[n:3][c:4]2[n:5][cH:6][c:7](Br)[cH:15][c:16]2[o:17]1)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]1[cH:24][cH:25][cH:26][cH:27][cH:28]1`
- **Reactant 2:** `OB(O)[c:8]1[cH:9][cH:10][c:11]([CH3:12])[cH:13][cH:14]1`



R1

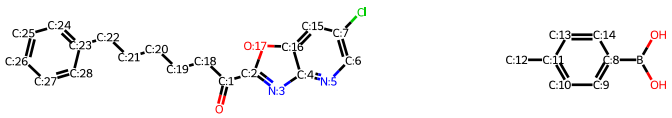


R2

Reactants for Transition 3

Transition 4

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This is a plausible permutation. Reactants are stable. Coupling of electron-deficient heteroaryl chlorides requires more active catalysts (e.g., bulky phosphine ligands) than bromides or iodides but is a well-established transformation. The electronic pairing is favorable.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]([c:2]1[n:3][c:4]2[n:5][cH:6][c:7](Cl)[cH:15][c:16]2[o:17]1)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]1[cH:24][cH:25][cH:26][cH:27][cH:28]1`
- **Reactant 2:** `OB(O)[c:8]1[cH:9][cH:10][c:11]([CH3:12])[cH:13][cH:14]1`

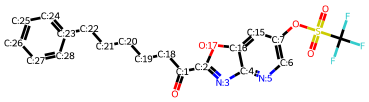


R1 R2

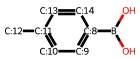
Reactants for Transition 4

Transition 5

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This is a highly plausible permutation. The reactants are stable. Aryl triflates are excellent electrophiles for Suzuki coupling, with reactivity often comparable to aryl iodides. The electronic pairing is favorable for this reaction.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]([c:2]1[n:3][c:4]2[n:5][cH:6][c:7](OS(=O)(=O)C(F)(F)F)[cH:15][c:16]2[o:17]1)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]1[cH:24][cH:25][cH:26][cH:27][cH:28]1`
- **Reactant 2:** `OB(O)[c:8]1[cH:9][cH:10][c:11]([CH3:12])[cH:13][cH:14]1`



R1

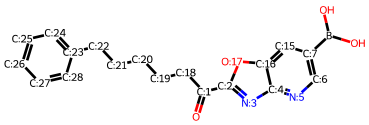


R2

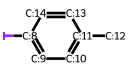
Reactants for Transition 5

Transition 6

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is chemically valid. The reactants are stable. The coupling of an electron-neutral aryl iodide with an electron-deficient heteroarylboronic acid is a viable strategy, although it might be less efficient than the alternative electronic pairing. Chemoselectivity is expected to be good.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]([c:2]1[n:3][c:4]2[n:5][cH:6][c:7](B(O)O)[cH:15][c:16]2[o:17]1)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]1[cH:24][cH:25][cH:26][cH:27][cH:28]1`
- **Reactant 2:** `[CH3:12][c:11]1[cH:10][cH:9][c:8](I)[cH:14][cH:13]1`



R1

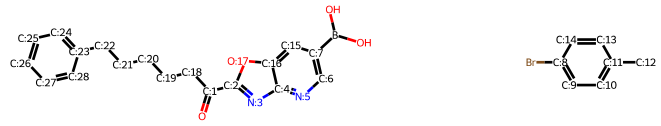


R2

Reactants for Transition 6

Transition 7

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is chemically valid. The reactants are stable. The coupling of an electron-neutral aryl bromide with an electron-deficient heteroarylboronic acid is a viable strategy, though potentially requiring more optimized conditions than the electronically opposite pairing. Chemoselectivity is expected to be good.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]([c:2]1[n:3][c:4]2[n:5][cH:6][c:7](B(O)O)[cH:15][c:16]2[o:17]1)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]1[cH:24][cH:25][cH:26][cH:27][cH:28]1`
- **Reactant 2:** `[CH3:12][c:11]1[cH:10][cH:9][c:8](Br)[cH:14][cH:13]1`

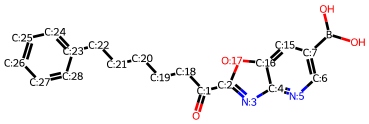


R1 R2

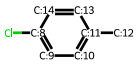
Reactants for Transition 7

Transition 8

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is chemically possible but may be challenging. The reactants are stable. The coupling of an unactivated, electron-neutral aryl chloride is difficult and requires highly specialized, active catalyst systems. While plausible in principle, it would likely be a low-yielding or disfavored synthetic route.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]([c:2]1[n:3][c:4]2[n:5][cH:6][c:7](B(O)O)[cH:15][c:16]2[o:17]1)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]1[cH:24][cH:25][cH:26][cH:27][cH:28]1`
- **Reactant 2:** `[CH3:12][c:11]1[cH:10][cH:9][c:8](Cl)[cH:14][cH:13]1`



R1

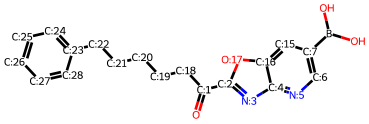


R2

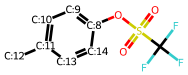
Reactants for Transition 8

Transition 9

- **Forward Reaction:** Suzuki coupling with boronic acids
- **Is Chemically Valid:** True
- **Is Template-based:** False
- **Reasoning:** This permutation is chemically valid and plausible. The reactants are stable. The aryl triflate is a sufficiently reactive electrophile to couple effectively with the electron-deficient heteroarylboronic acid. This represents a good alternative to the corresponding aryl halide.
- **Is Smiles Valid:** True
- **Reactant 1:** `O=[C:1]([c:2]1[n:3][c:4]2[n:5][cH:6][c:7](B(O)O)[cH:15][c:16]2[o:17]1)[CH2:18][CH2:19][CH2:20][CH2:21][CH2:22][c:23]1[cH:24][cH:25][cH:26][cH:27][cH:28]1`
- **Reactant 2:** `[CH3:12][c:11]1[cH:10][cH:9][c:8](OS(=O)(=O)C(F)(F)F)[cH:14][cH:13]1`



R1



R2

Reactants for Transition 9