

Slide 6: EPI-506 (ralaniten acetate / prodrug of EPI-002)

Initial Task: HIA

SMILES: CC(=O)OC[C@H](COC1=CC=C(C=C1)C(C)(C)C2=CC=C(C=C2)OC[C@H](CC1)OC(=O)C)OC(=O)C

✖ Optimization Failed for EPI-506 (ralaniten acetate / prodrug of EPI-002)

No valid paths found. The optimization could not generate any improved molecules.

Initial Molecule Scores

Input SMILES: CC(=O)OC[C@H](COC1=CC=C(C=C1)C(C)(C)C2=CC=C(C=C2)OC[C@H](CC1)OC(=O)C)OC(=O)C

- Molecules Generated: 85
- Valid Paths: 0

Reason: All generated molecules had worse scores than the initial molecule.

Recommendations

1. **Increase beams:** Try `num_beams=7` or `num_beams=10` for more diversity
2. **Change initial task:** Try a different task as the starting point
3. **Reduce depth:** Start with `depth=1` to see if single-step improvements work
4. **Check initial molecule:** It may already be highly optimized