Slide 21: Taranabant (MK-0364)

Initial Task: DILI

SMILES: `C[C@@H]([C@@H](CC1=CC=C(C=C1)Cl)C2=CC=CC(=C2)C#N)NC(=O)C(C)(C)OC3=NC=C(C=C3)C(F)(F)F`

❌ Optimization Failed for Taranabant (MK-0364)

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

📊 Initial Molecule Scores

Input SMILES: `C[C@@H]([C@@H](CC1=CC=C(C=C1)Cl)C2=CC=CC(=C2)C#N)NC(=O)C(C)(C)OC3=NC=C(C=C3)C(F)(F)F`

- **Molecules Generated:** 1
- **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