

Slide 1: Tarenflurbil (Flurizan)

Initial Task: BBBP

SMILES: C[C@H](C1=CC(=C(C=C1)C2=CC=CC=C2)F)C(=O)O

✖ Optimization Failed for Tarenflurbil (Flurizan)

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

Initial Molecule Scores

Input SMILES: C[C@H](C1=CC(=C(C=C1)C2=CC=CC=C2)F)C(=O)O

- Molecules Generated: 7
- 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