

Slide 2: Gavestinel (GV-150,526)

Initial Task: BBBP

SMILES: C1=CC=C(C=C1)NC(=O)/C=C/C2=C(C(=O)O)NC3=C2C(=CC(=C3)Cl)Cl

✖ Optimization Failed for Gavestinel (GV-150,526)

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

Initial Molecule Scores

Input SMILES: C1=CC=C(C=C1)NC(=O)/C=C/C2=C(C(=O)O)NC3=C2C(=CC(=C3)Cl)Cl

- **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