Slide 3: NXY-059 (Cerovive)

Initial Task: BBBP

SMILES: `CC(C)(C)/[N+](=C/C1=CC=C(C=C1S(=O)(=O)OC)S(=O)(=O)OC)/[O-]`

❌ Optimization Failed for NXY-059 (Cerovive)

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

📊 Initial Molecule Scores

Input SMILES: `CC(C)(C)/[N+](=C/C1=CC=C(C=C1S(=O)(=O)OC)S(=O)(=O)OC)/[O-]`

- **Molecules Generated:** 73
- **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