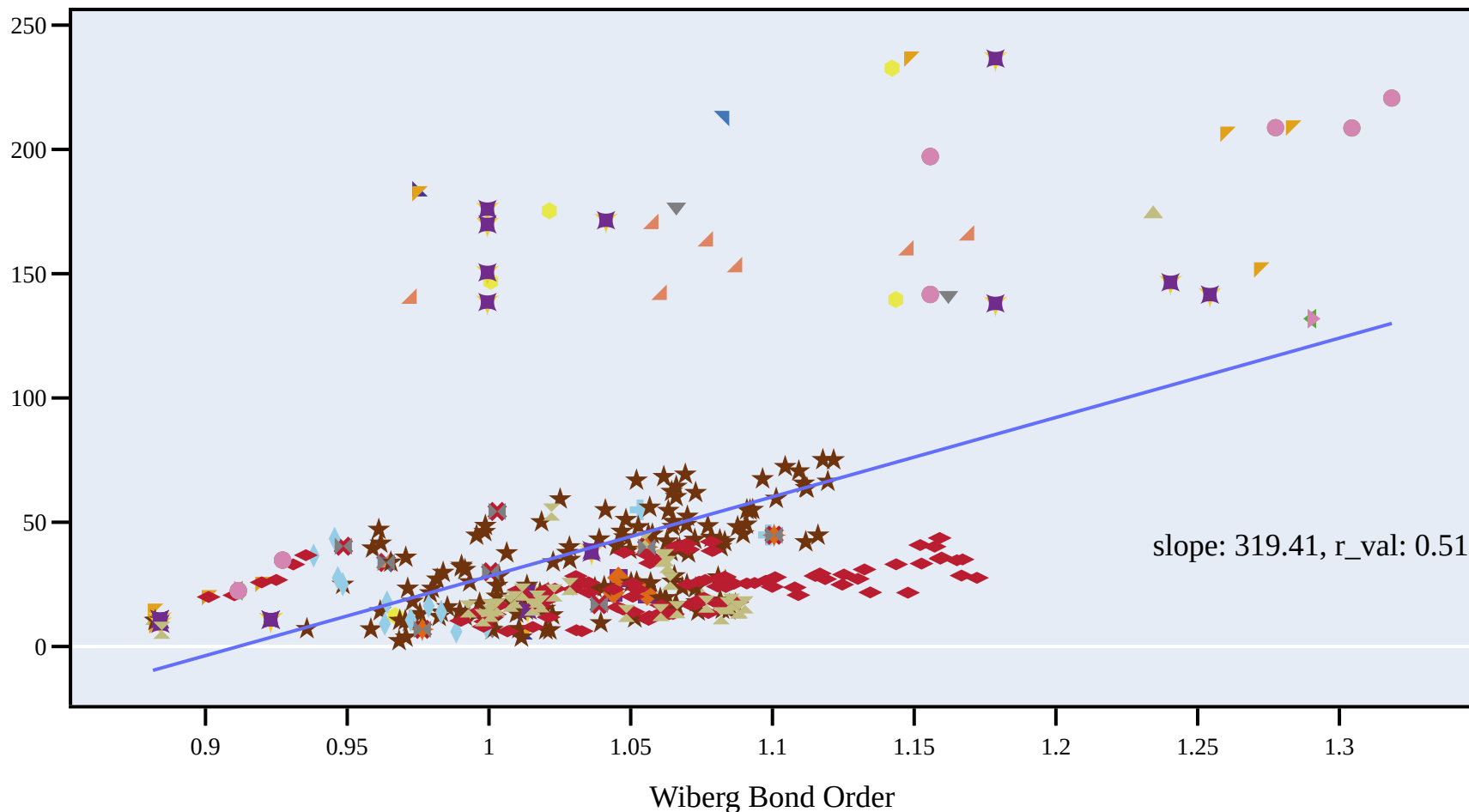


Torsion barrier in KJ/mol

TIG6



Wiberg Bond Order

- | | |
|---|---|
| ● Fragment Stability Benchmark.oeb | ■ Fragment Stability Benchmark.oeb |
| ◆ Fragment Stability Benchmark.oeb | + OpenFF Fragmenter Validation 1.0.oeb |
| ✕ OpenFF Full TorsionDrive Benchmark 1.oeb | ▲ OpenFF Gen 2 Torsion Set 1 Roche.oeb |
| ▼ OpenFF Gen 2 Torsion Set 1 Roche 2.oeb | ▼ OpenFF Gen 2 Torsion Set 2 Coverage.oeb |
| ▶ OpenFF Gen 2 Torsion Set 2 Coverage 2.oeb | ▶ OpenFF Gen 2 Torsion Set 3 Pfizer Discrepancy.oeb |
| ▲ OpenFF Gen 2 Torsion Set 3 Pfizer Discrepancy 2.oeb | ▶ OpenFF Gen 2 Torsion Set 4 eMolecules Discrepancy.oeb |
| ▶ OpenFF Gen 2 Torsion Set 4 eMolecules Discrepancy 2.oeb | ● OpenFF Gen 2 Torsion Set 5 Bayer 2.oeb |
| ★ OpenFF Group1 Torsions.oeb | ▼ OpenFF Primary Benchmark 1 Torsion Set.oeb |
| ■ OpenFF Primary Benchmark 1 Torsion Set.oeb | ◆ OpenFF Primary TorsionDrive Benchmark 1.oeb |
| ◆ OpenFF Rowley Biaryl v1.0.oeb | ◆ OpenFF Substituted Phenyl Set 1.oeb |
| ✕ OpenFF-benchmark-ligand-fragments-v1.0.oeb | ✕ Pfizer Discrepancy Torsion Dataset 1.oeb |
| ● SMIRNOFF Coverage Torsion Set 1.oeb | ● SMIRNOFF Coverage Torsion Set 1.oeb |