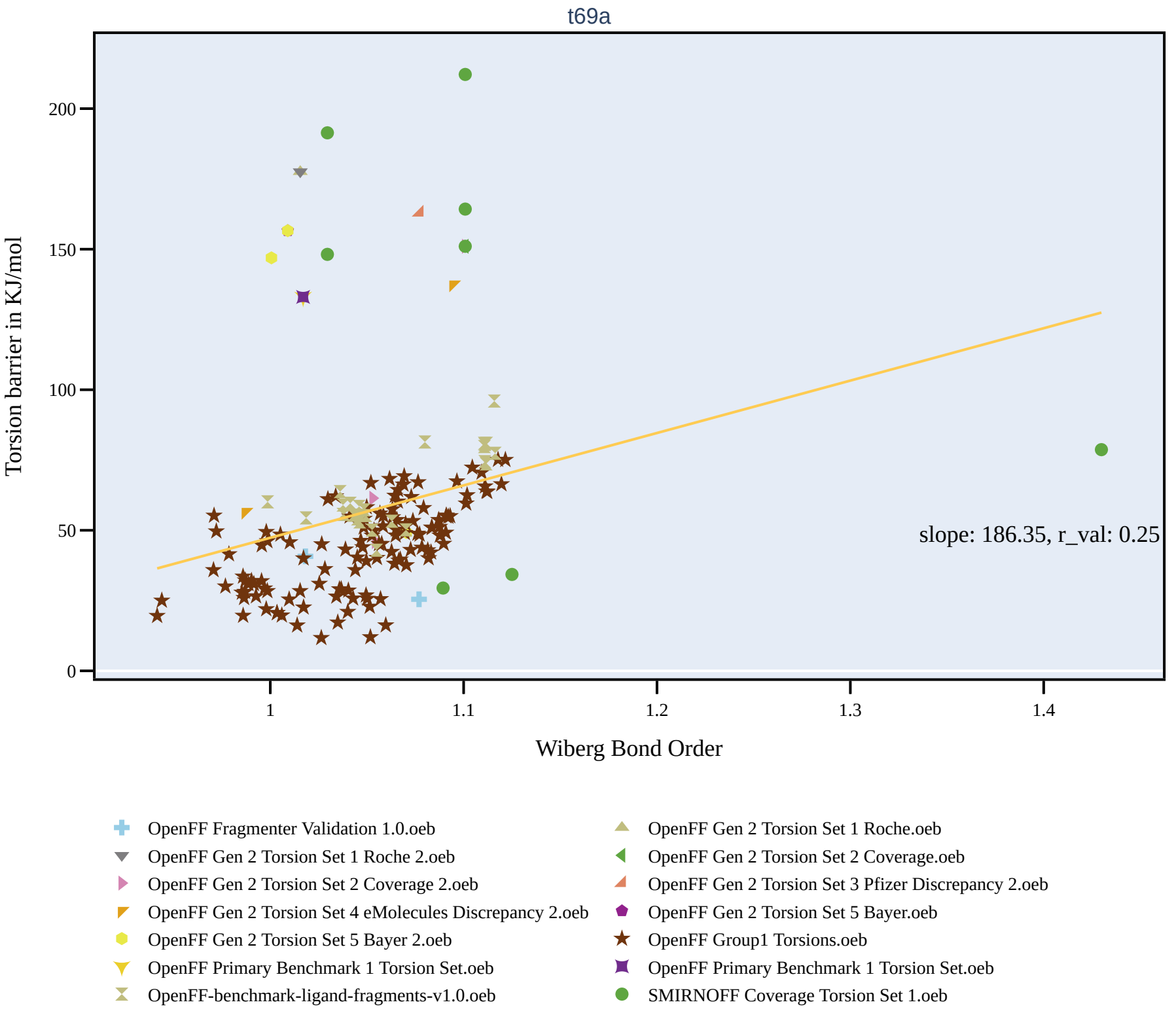
t69a
Torsion barrier in KJ/mol
Wiberg Bond Order
slope: 186.35, r_val: 0.25
0
50
100
150
200
1
1.1
1.2
1.3
1.4
OpenFF Fragmenter Validation 1.0.oeb
OpenFF Gen 2 Torsion Set 1 Roche 2.oeb
OpenFF Gen 2 Torsion Set 2 Coverage 2.oeb
OpenFF Gen 2 Torsion Set 4 eMolecules Discrepancy 2.oeb
OpenFF Gen 2 Torsion Set 5 Bayer 2.oeb
OpenFF Primary Benchmark 1 Torsion Set.oeb
OpenFF-benchmark-ligand-fragments-v1.0.oeb
OpenFF Gen 2 Torsion Set 1 Roche.oeb
OpenFF Gen 2 Torsion Set 2 Coverage.oeb
OpenFF Gen 2 Torsion Set 3 Pfizer Discrepancy 2.oeb
OpenFF Gen 2 Torsion Set 5 Bayer.oeb
OpenFF Group1 Torsions.oeb
OpenFF Primary Benchmark 1 Torsion Set.oeb
SMIRNOFF Coverage Torsion Set 1.oeb