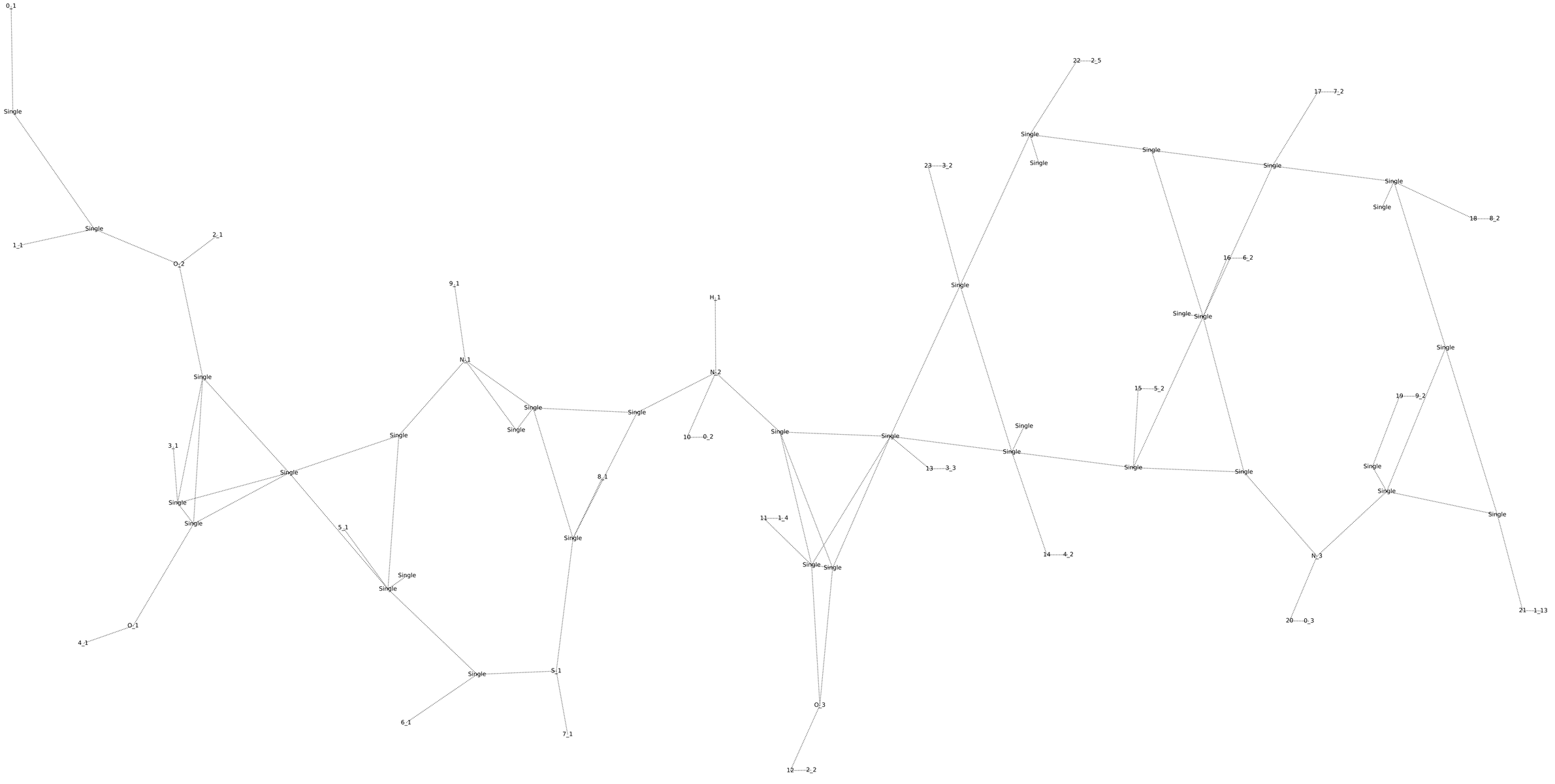4559002_rdkit