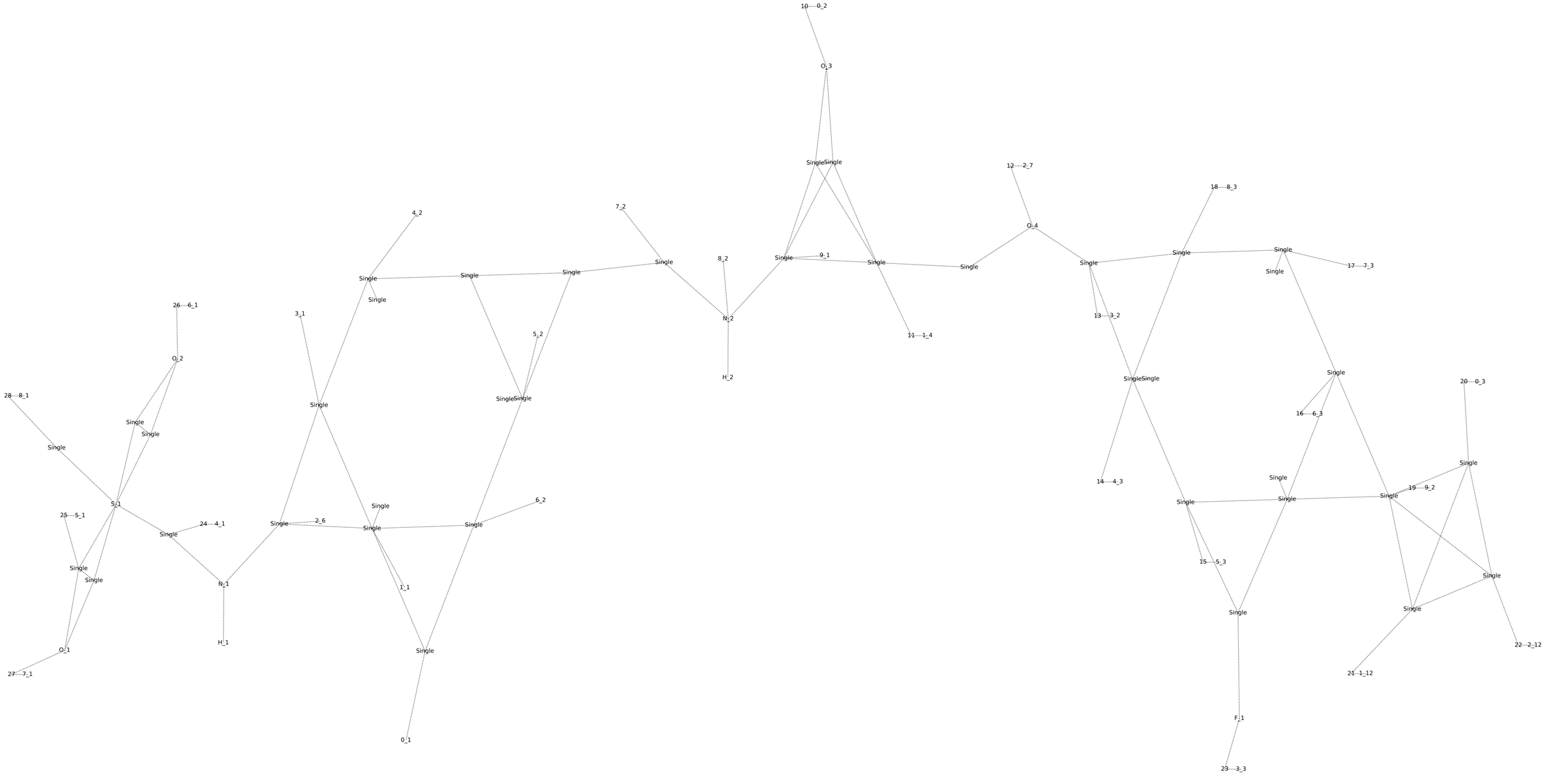11510067_rdkit