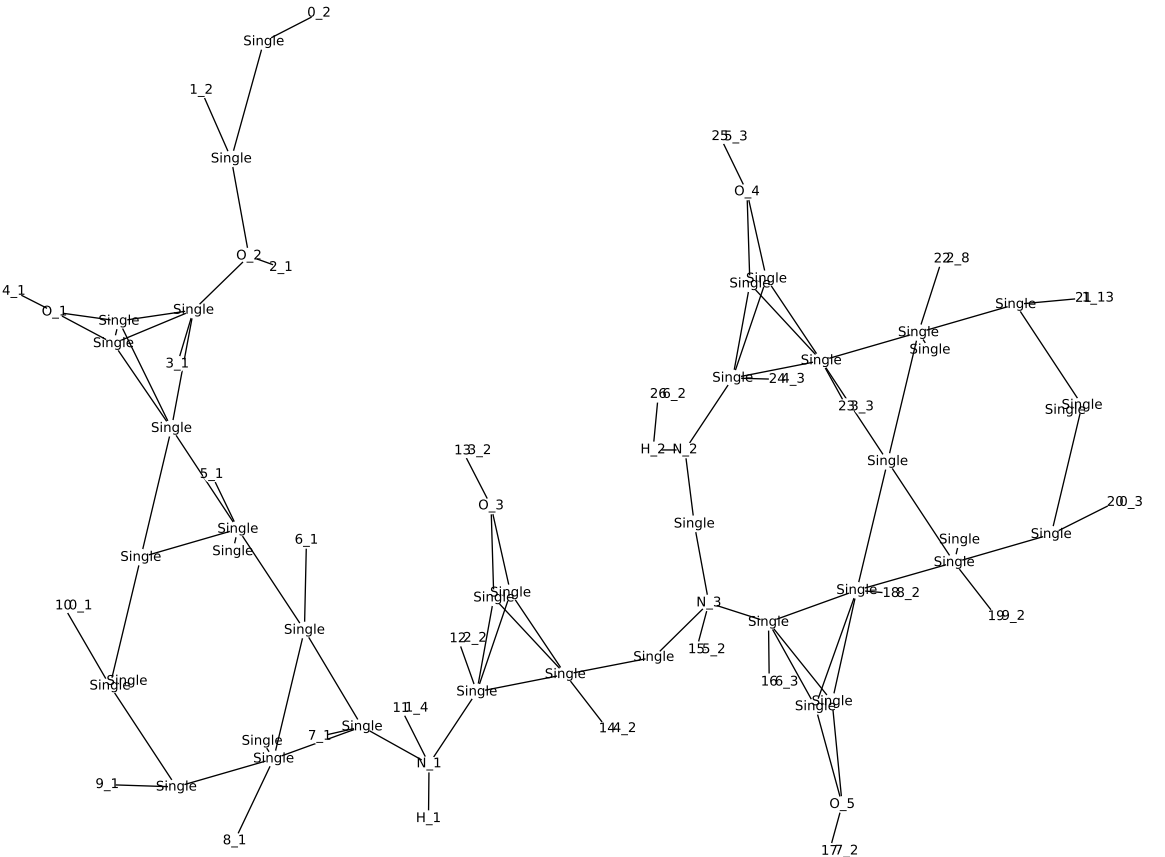9228145_rdkit