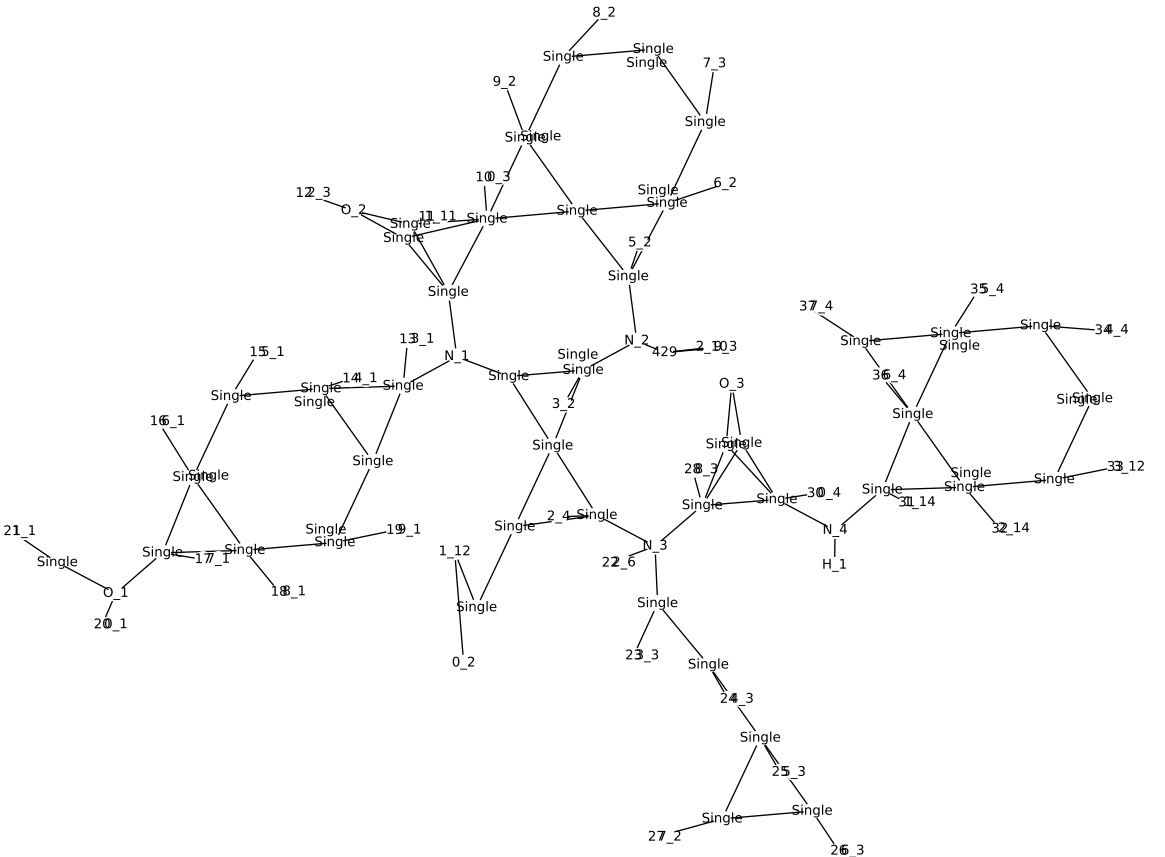3436755_rdkit