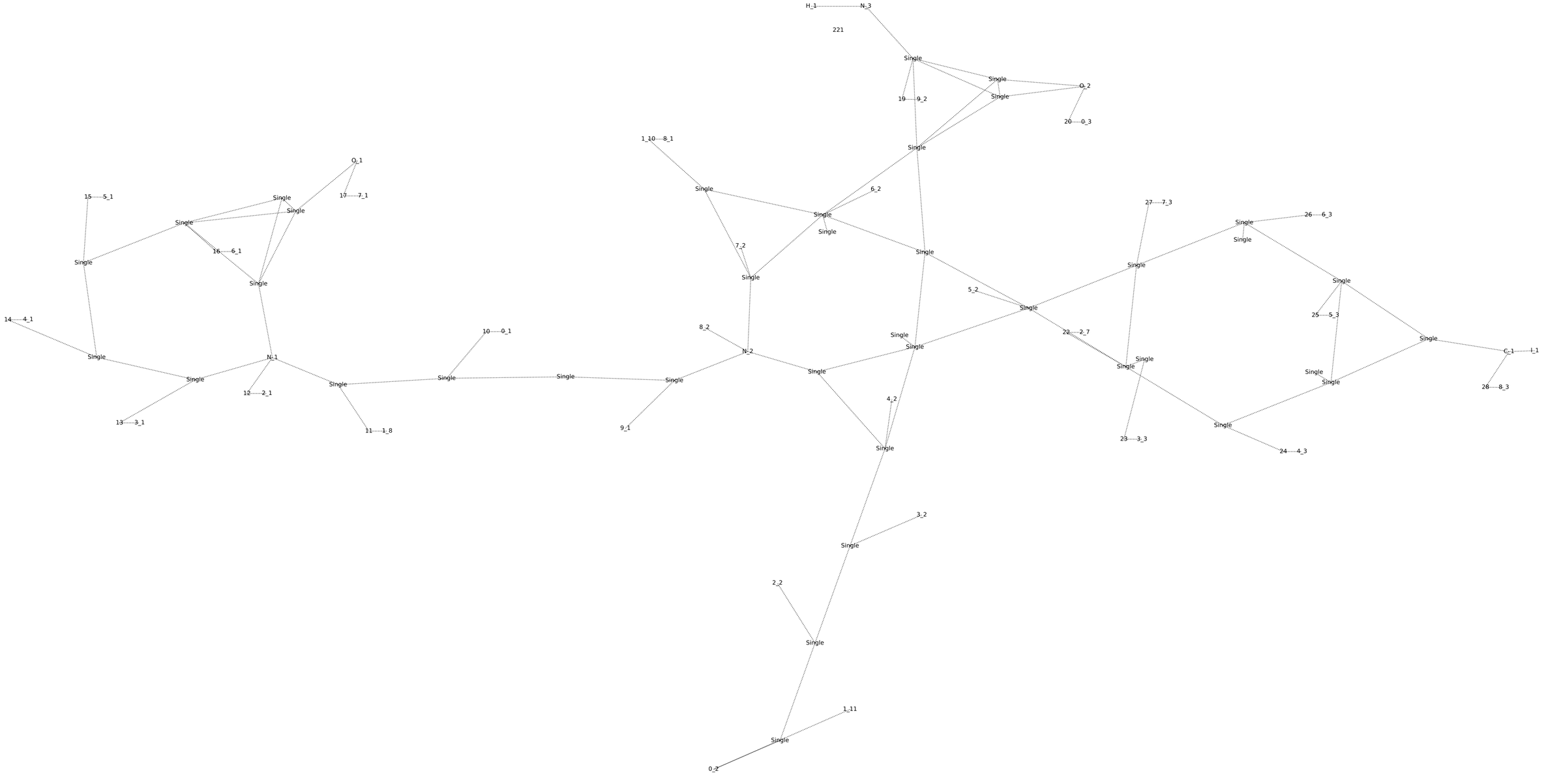3742850_rdkit