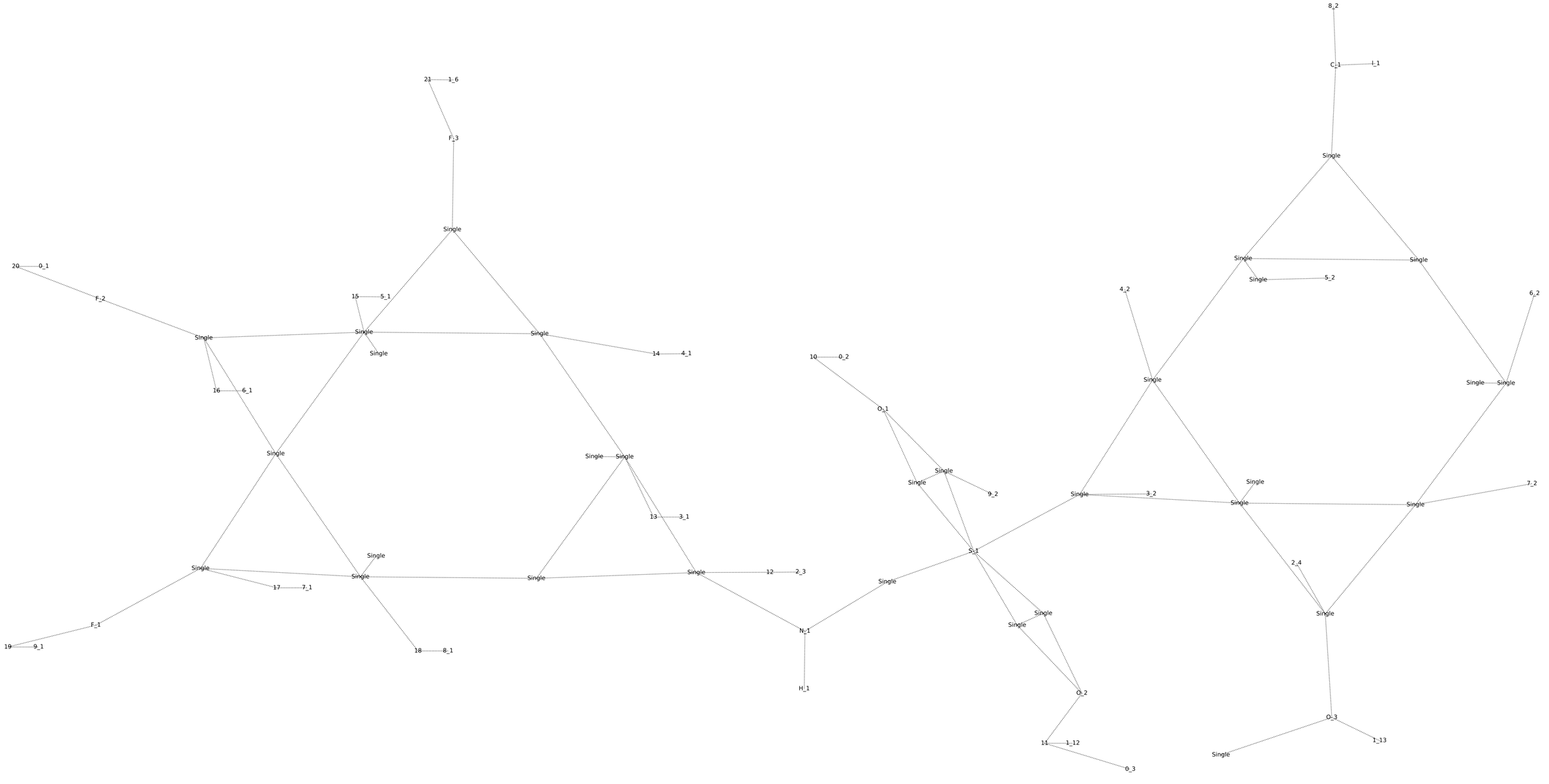3291676_rdkit