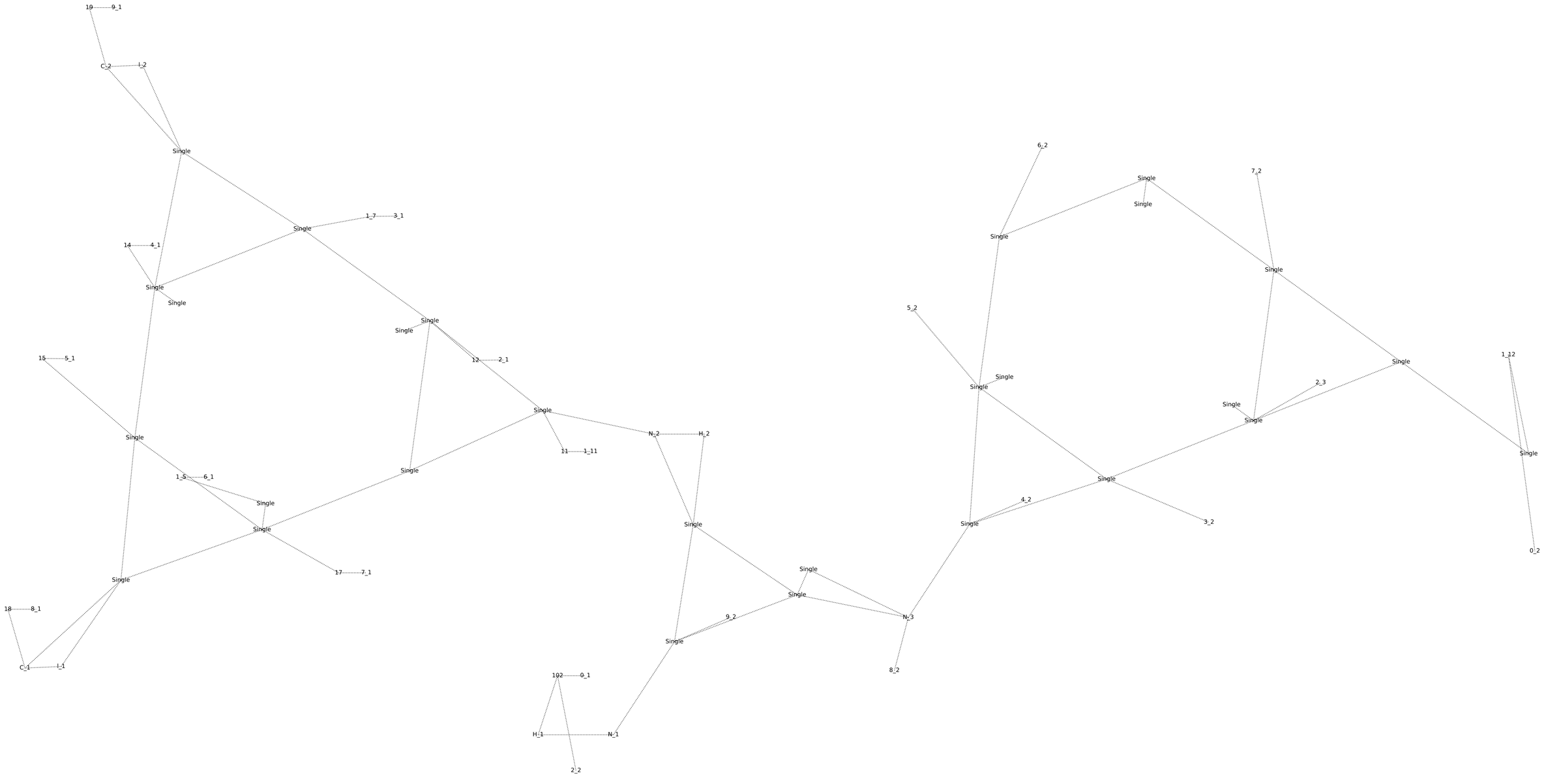10638488_rdkit