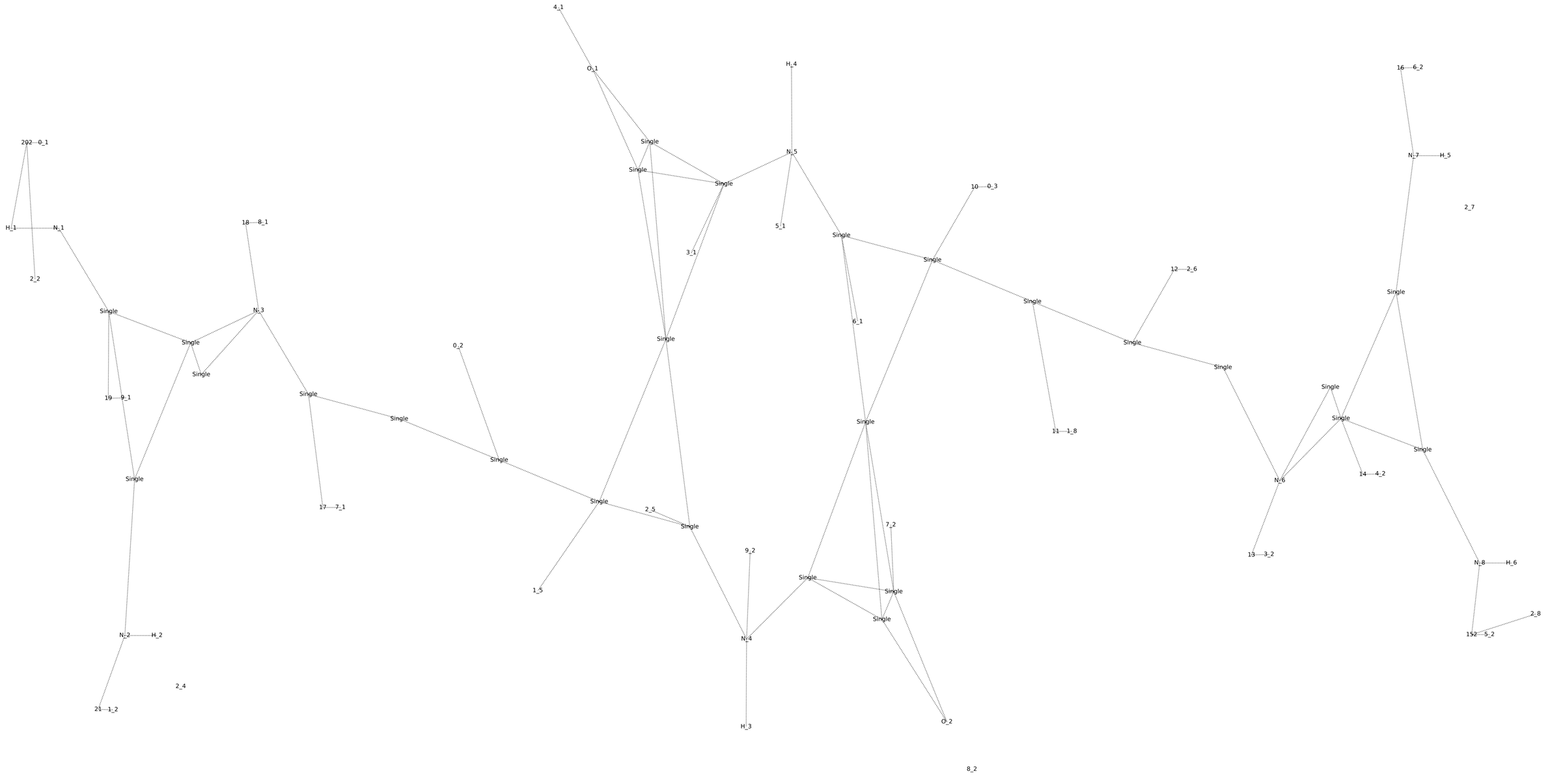10018406_rdkit