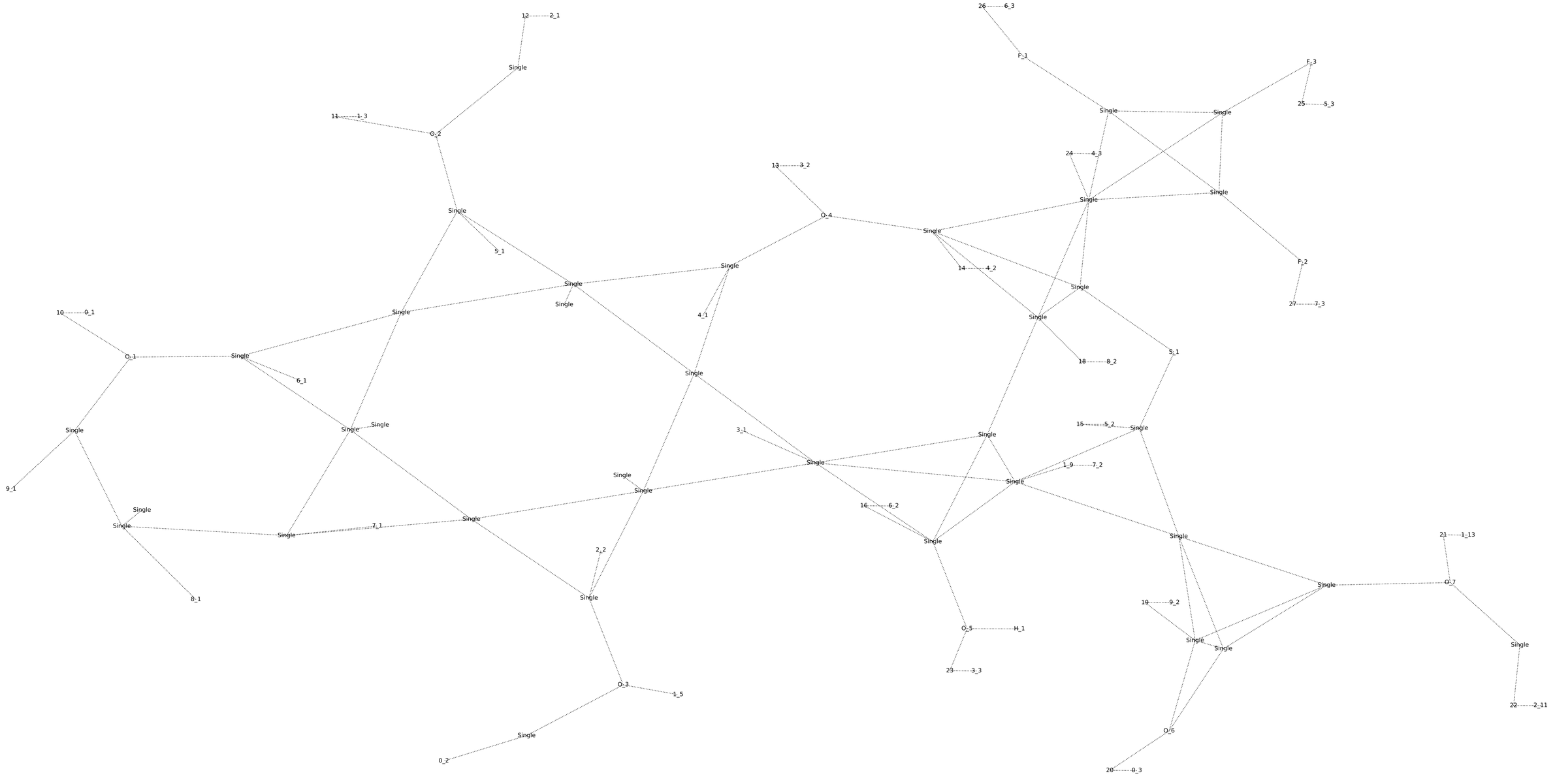5096231_rdkit