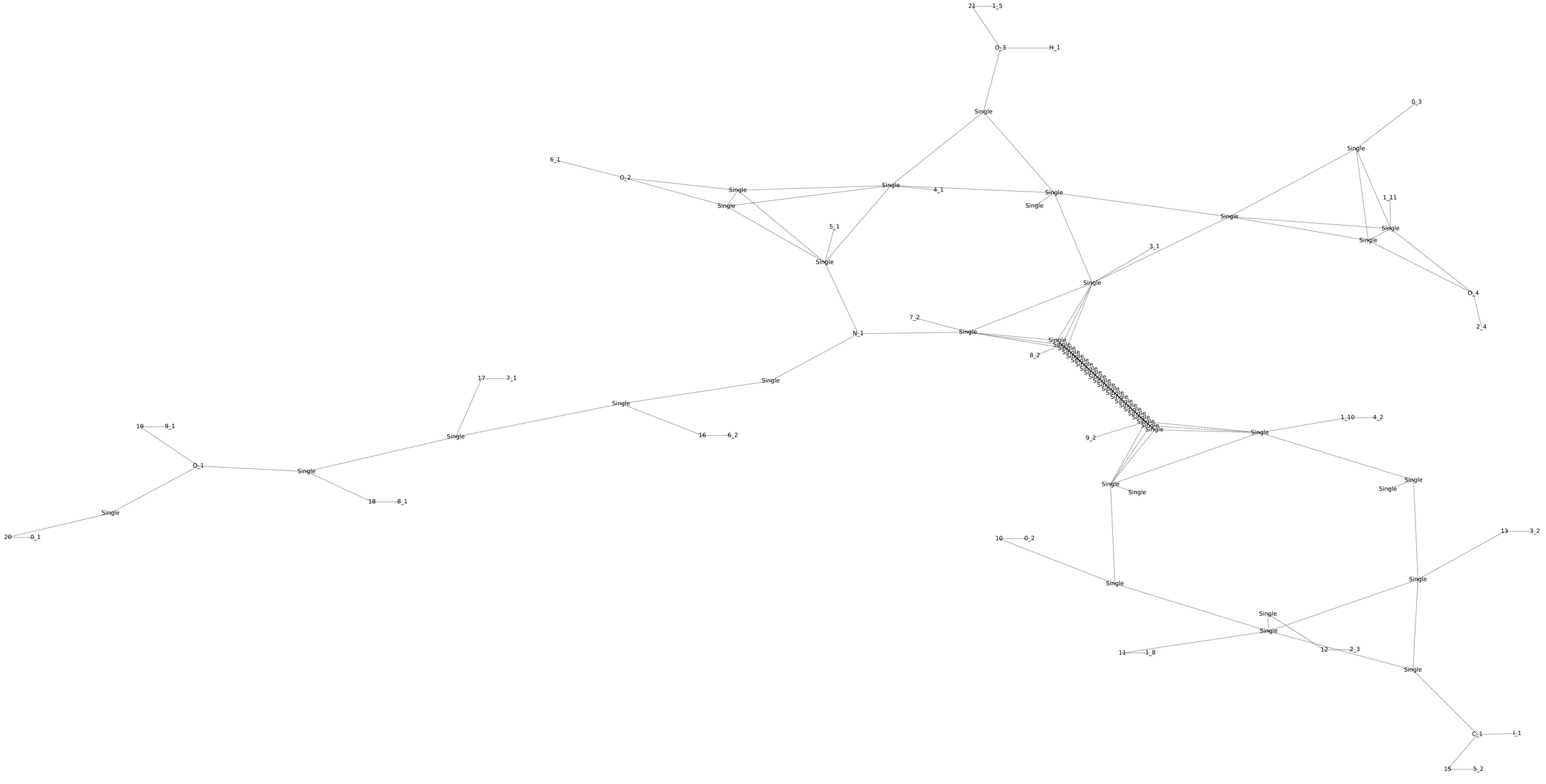7274463_rdkit