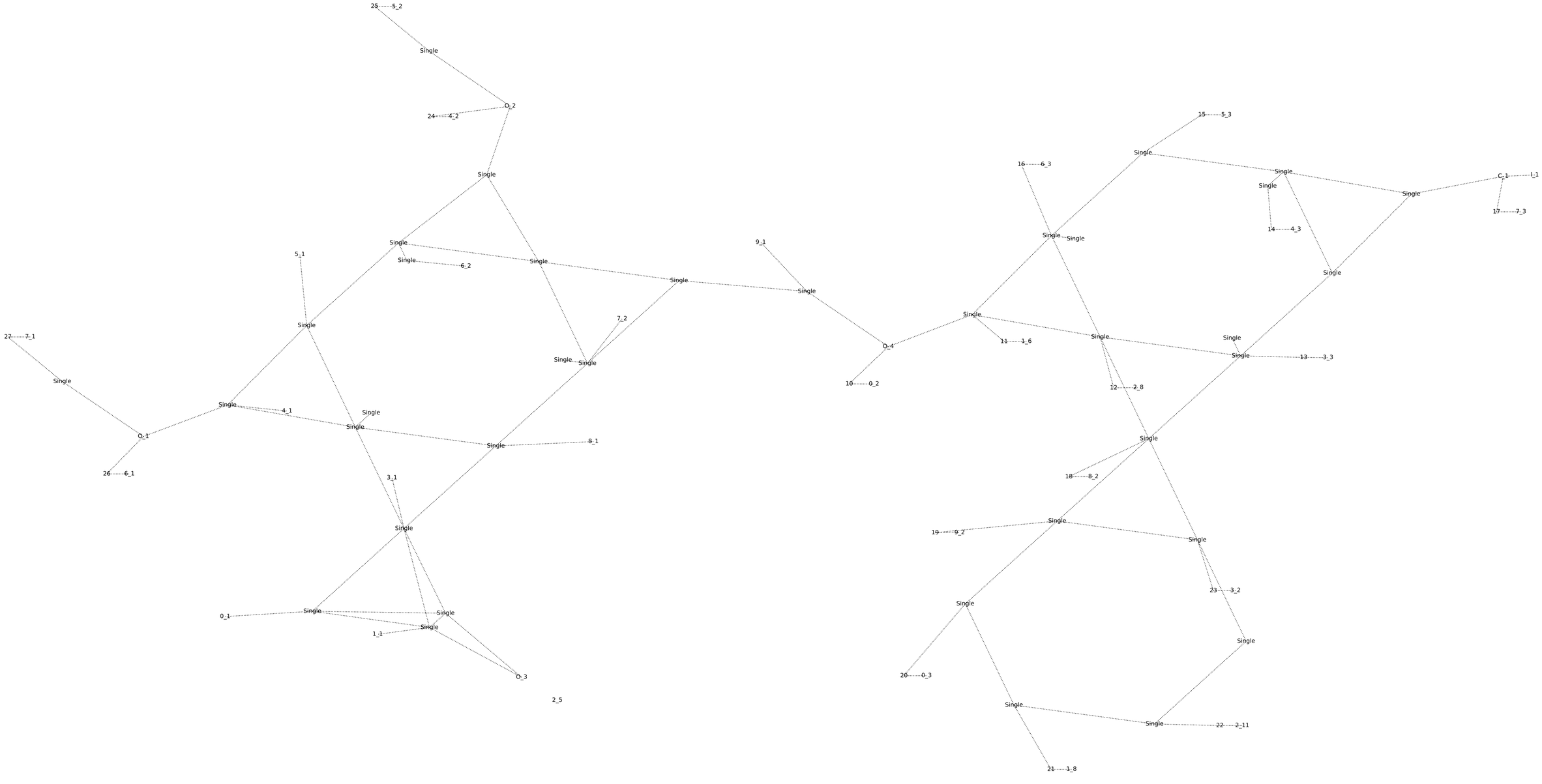8025814_rdkit