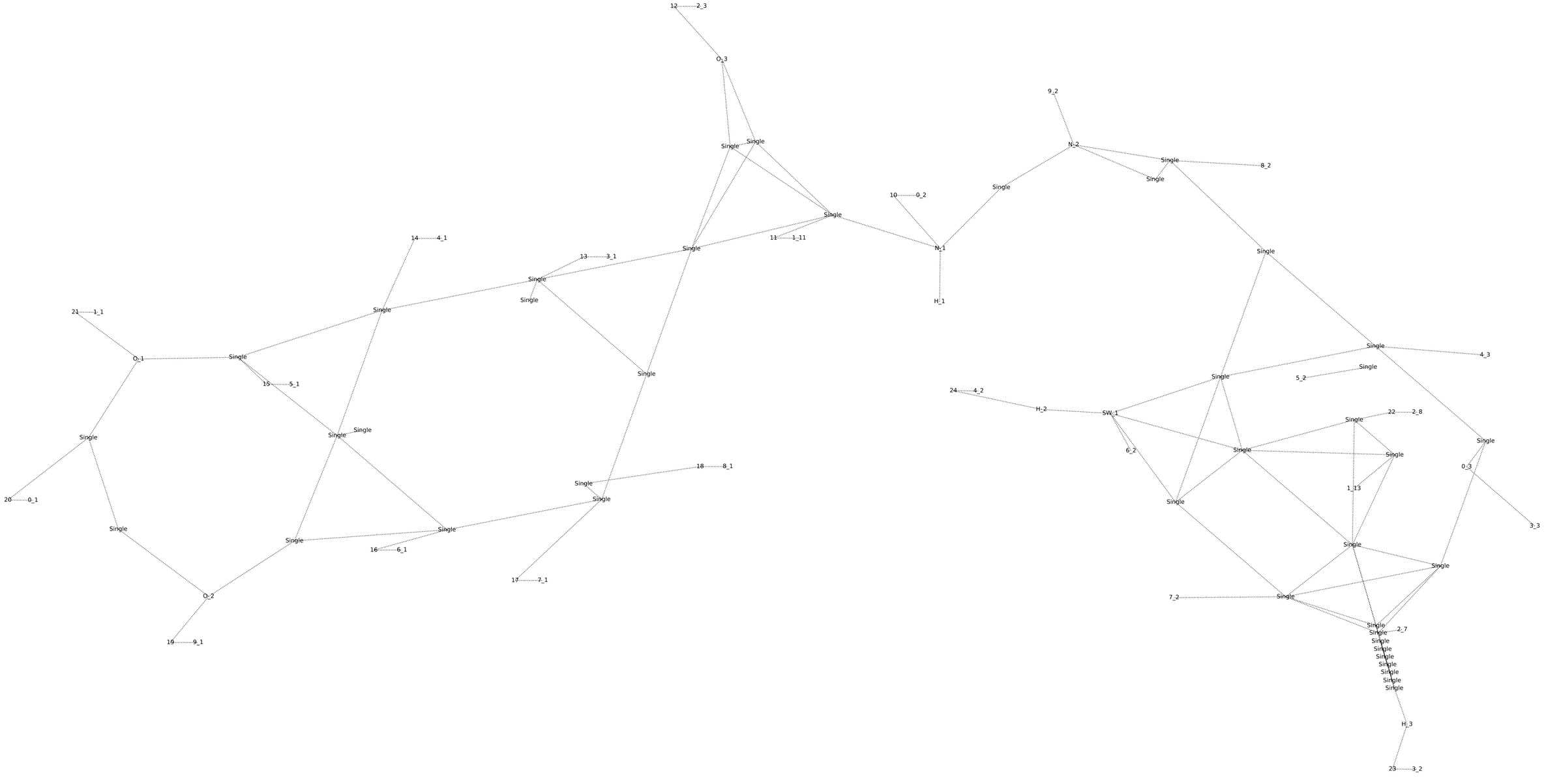7427445_rdkit