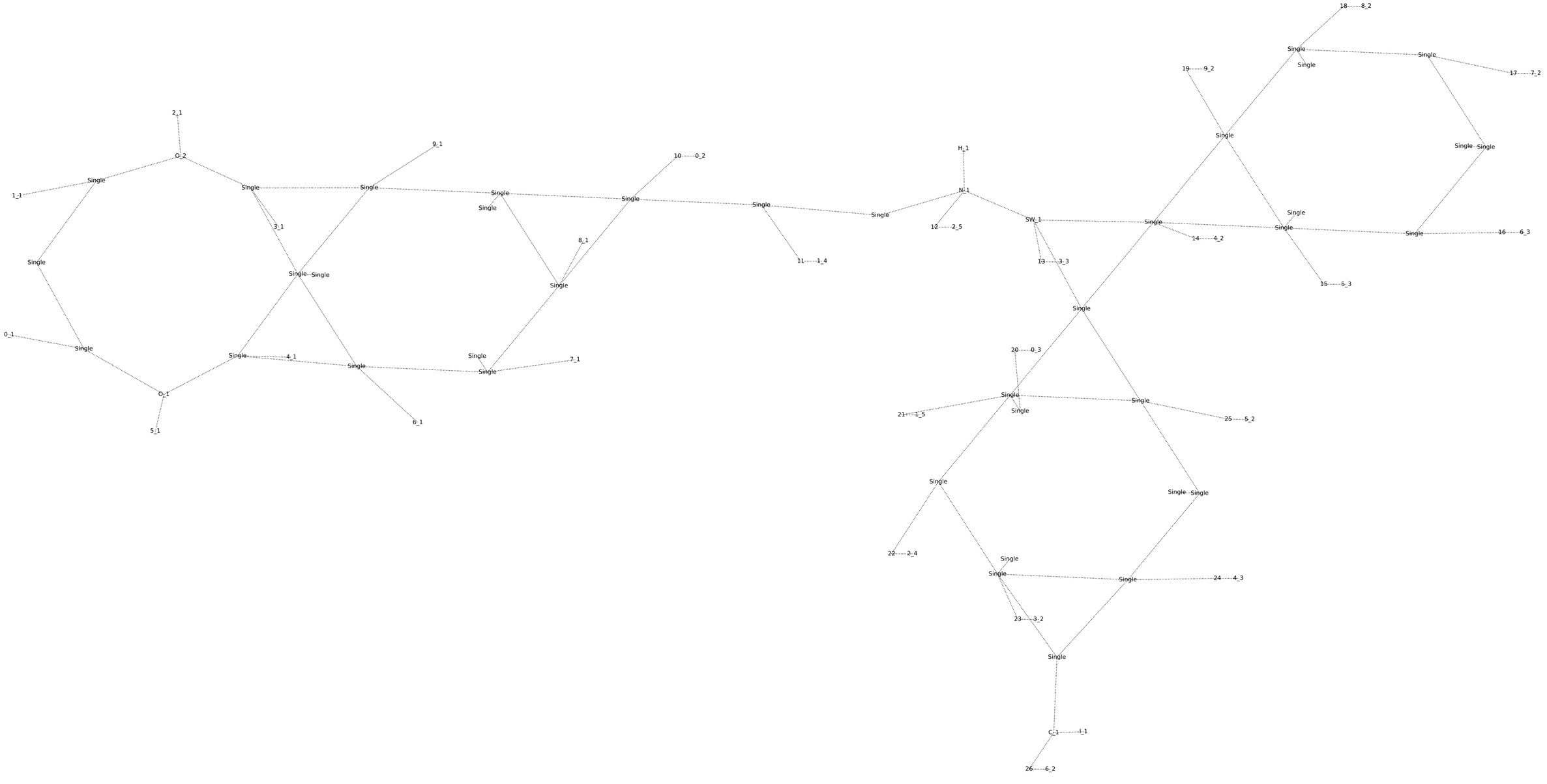2546483_rdkit