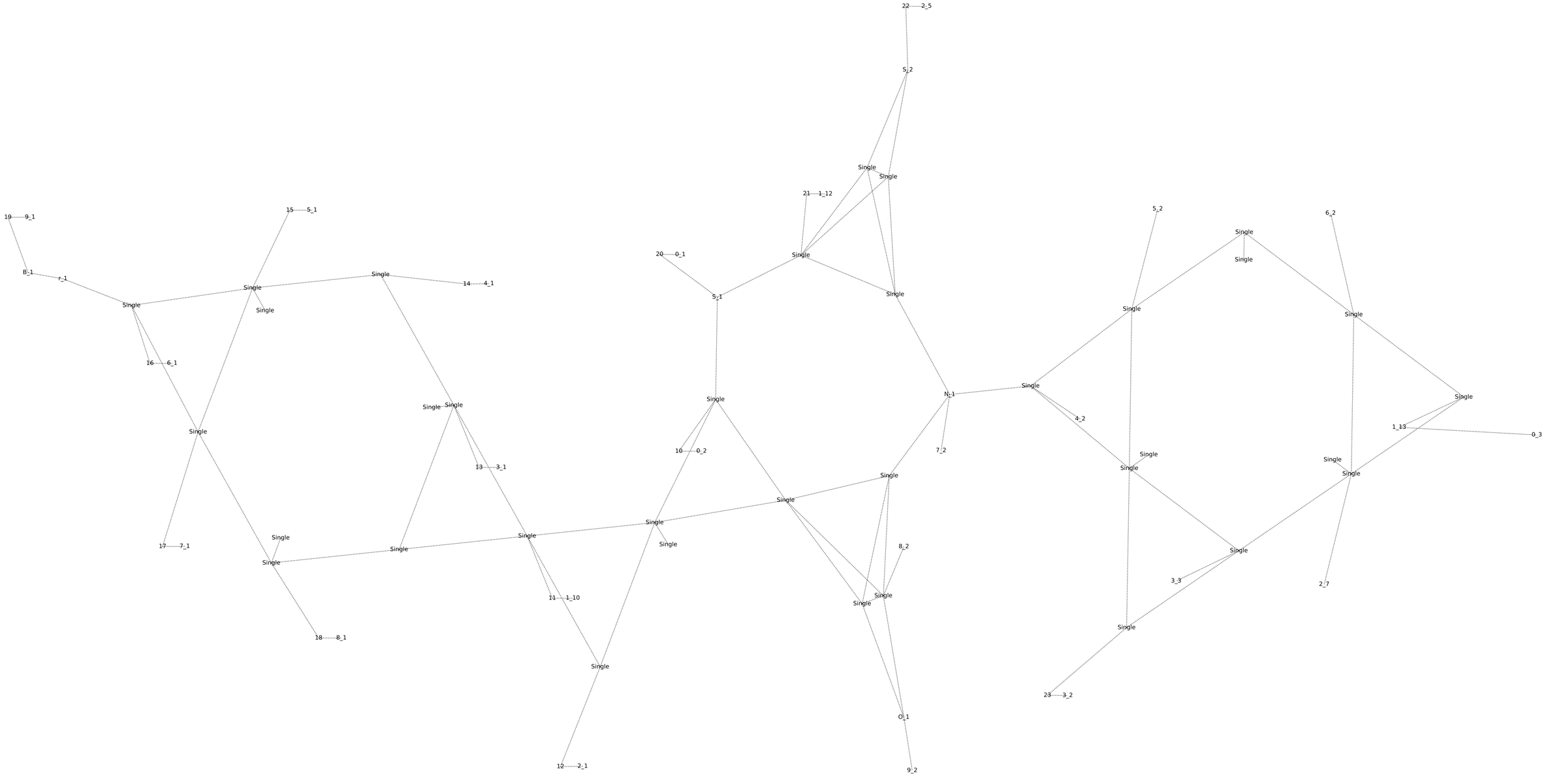2142141_rdkit