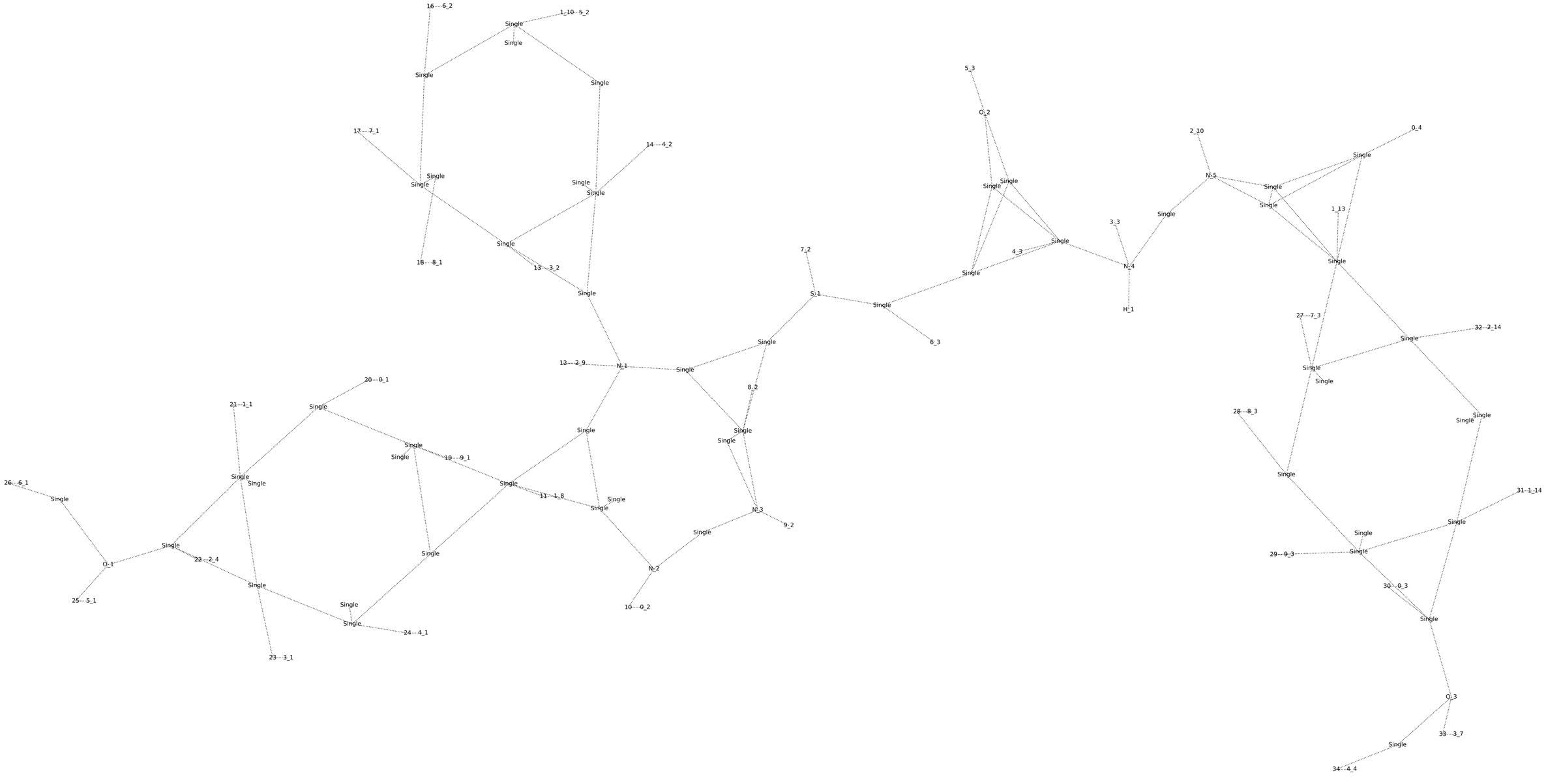6344398_rdkit