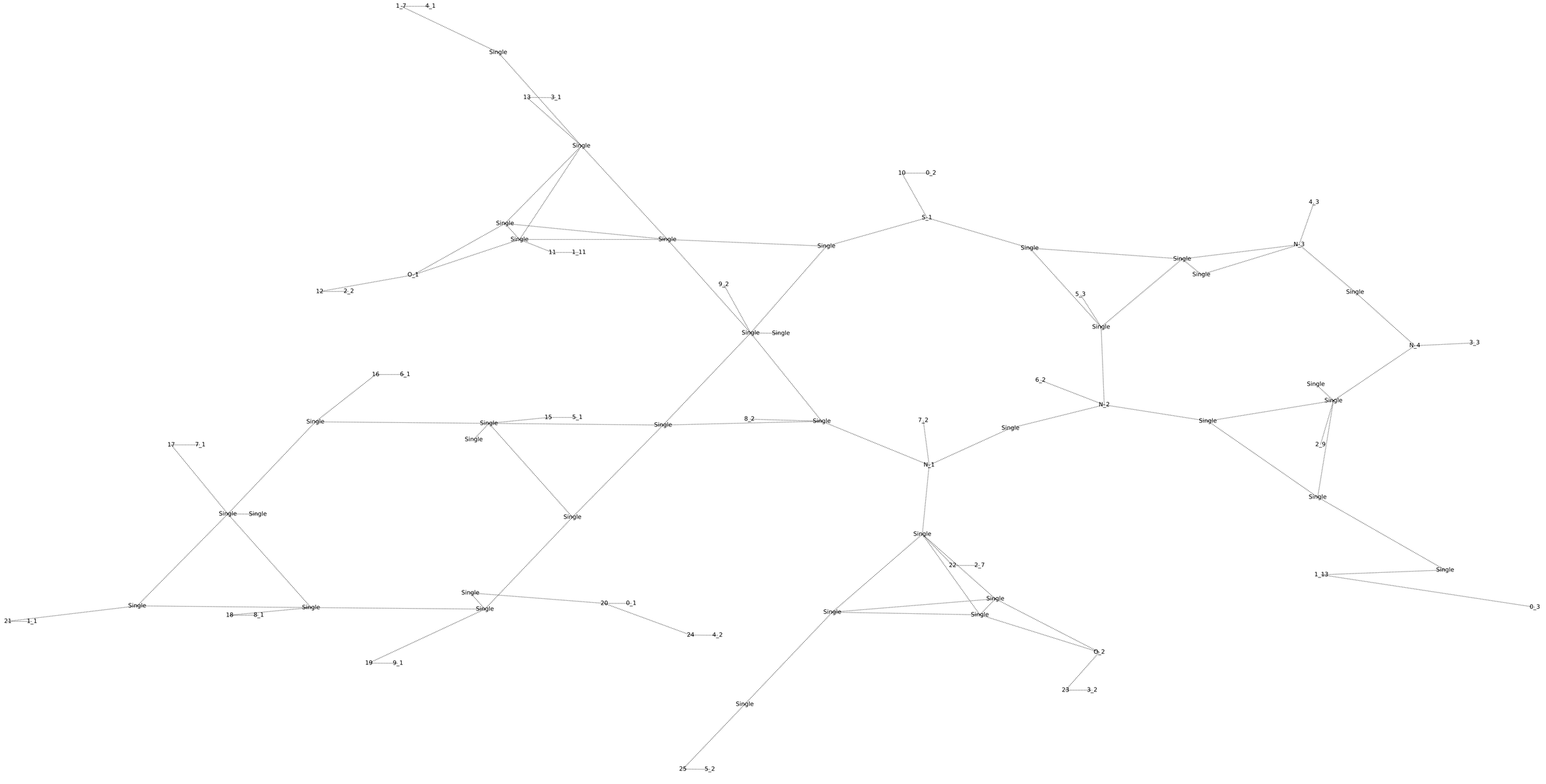7267428_rdkit