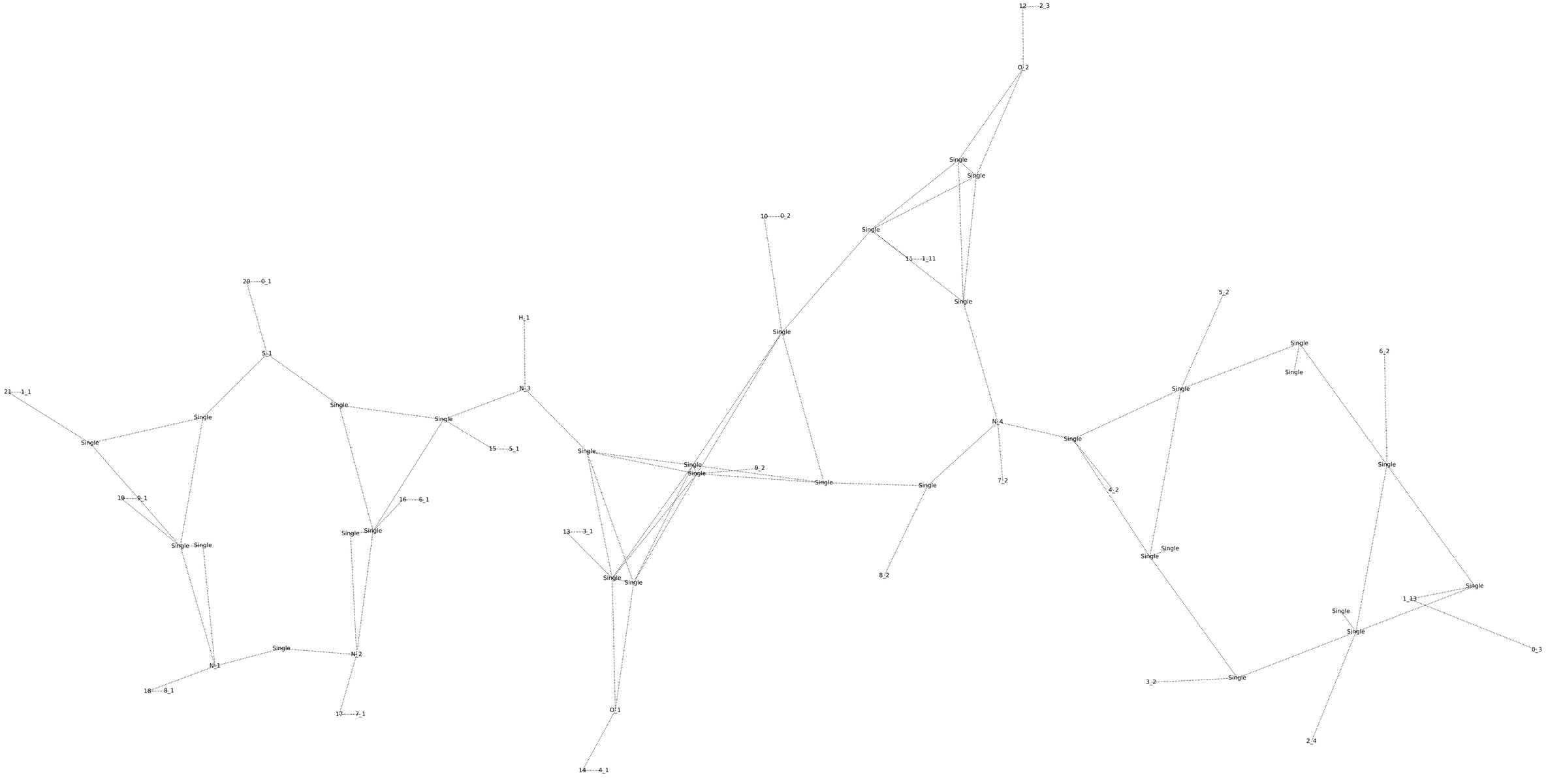1094143_rdkit