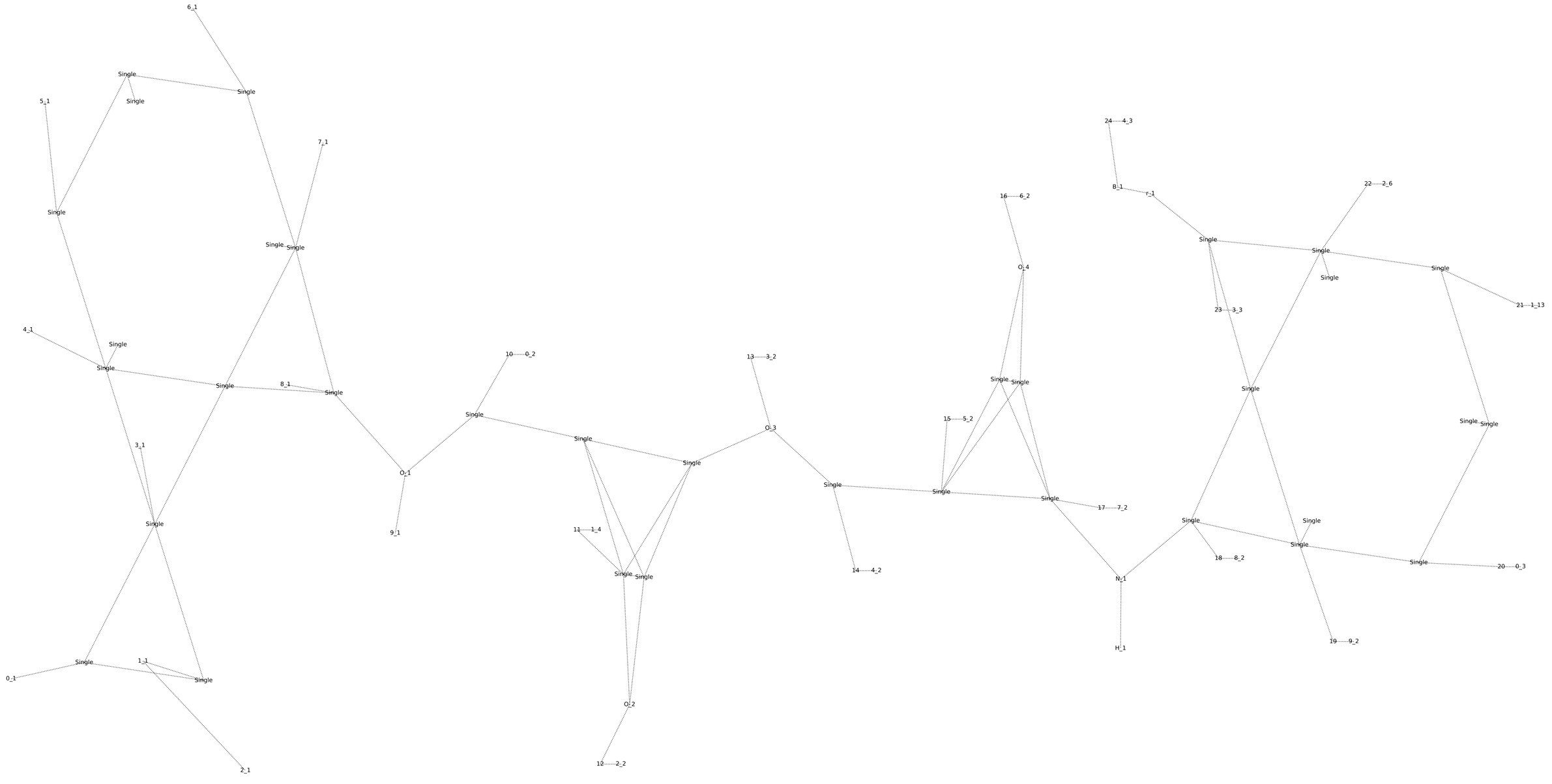7903943_rdkit