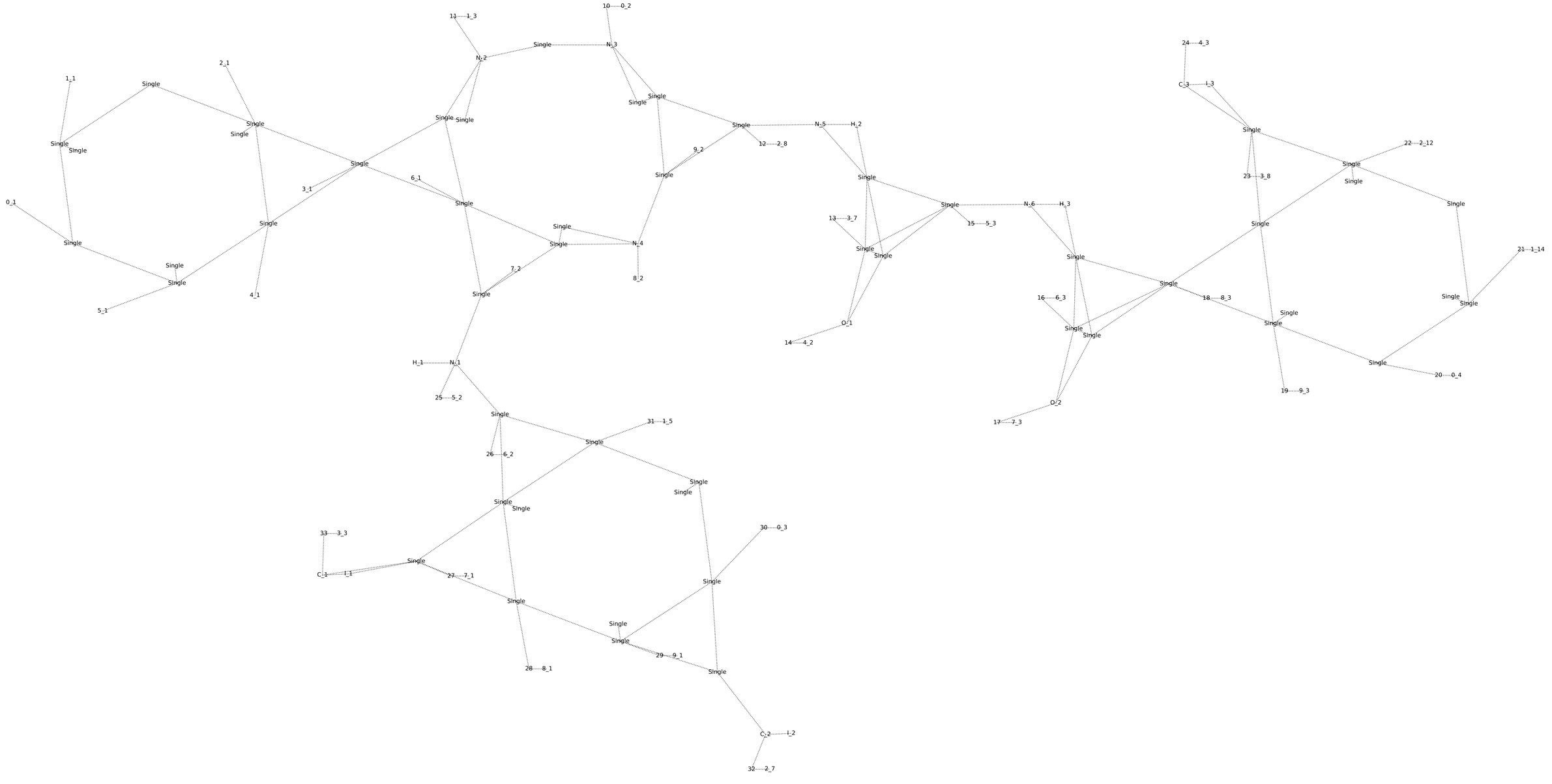10791903_rdkit