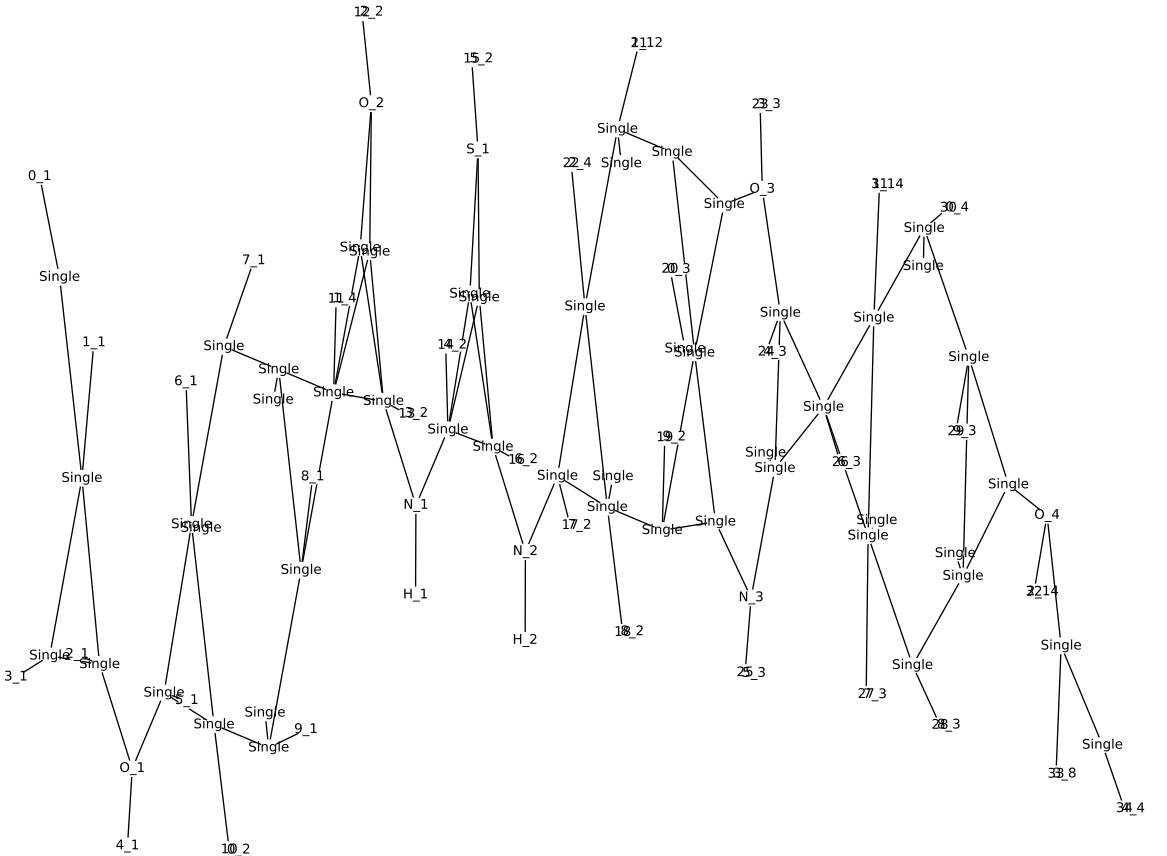4506129_rdkit