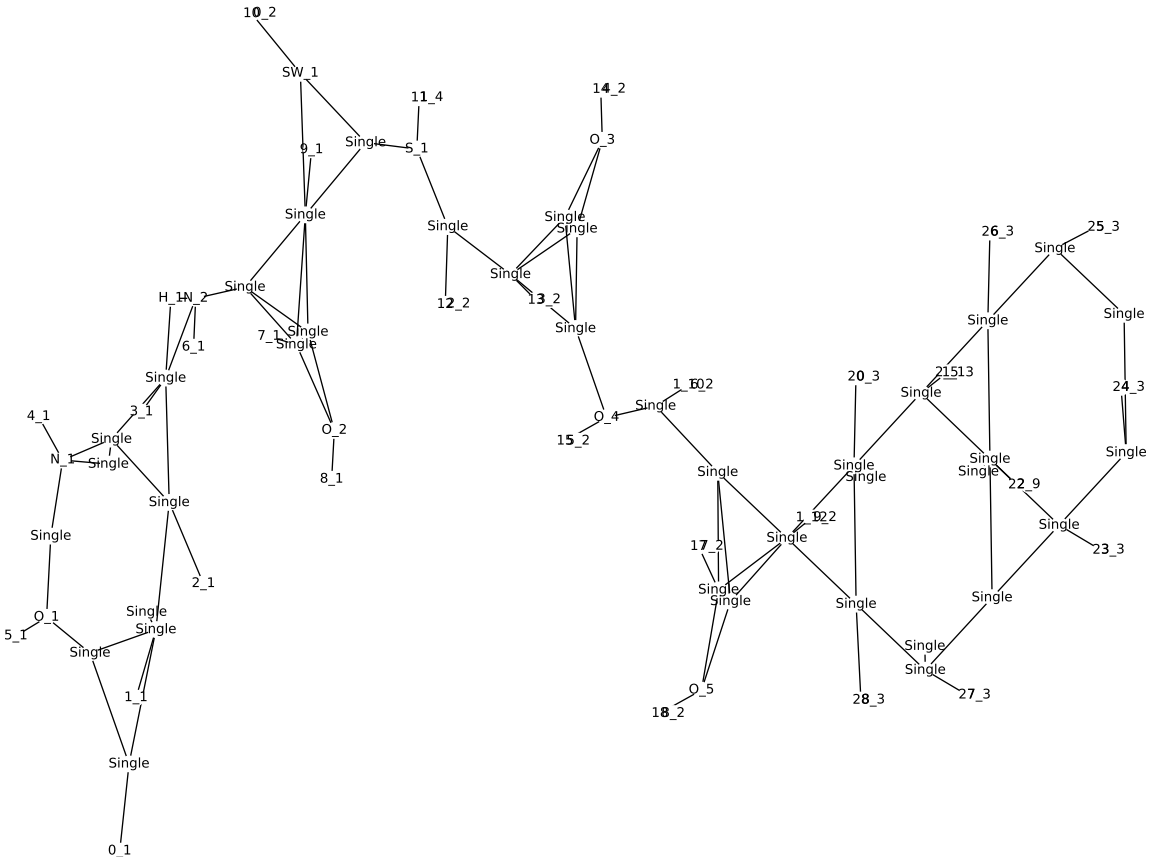7952521_rdkit