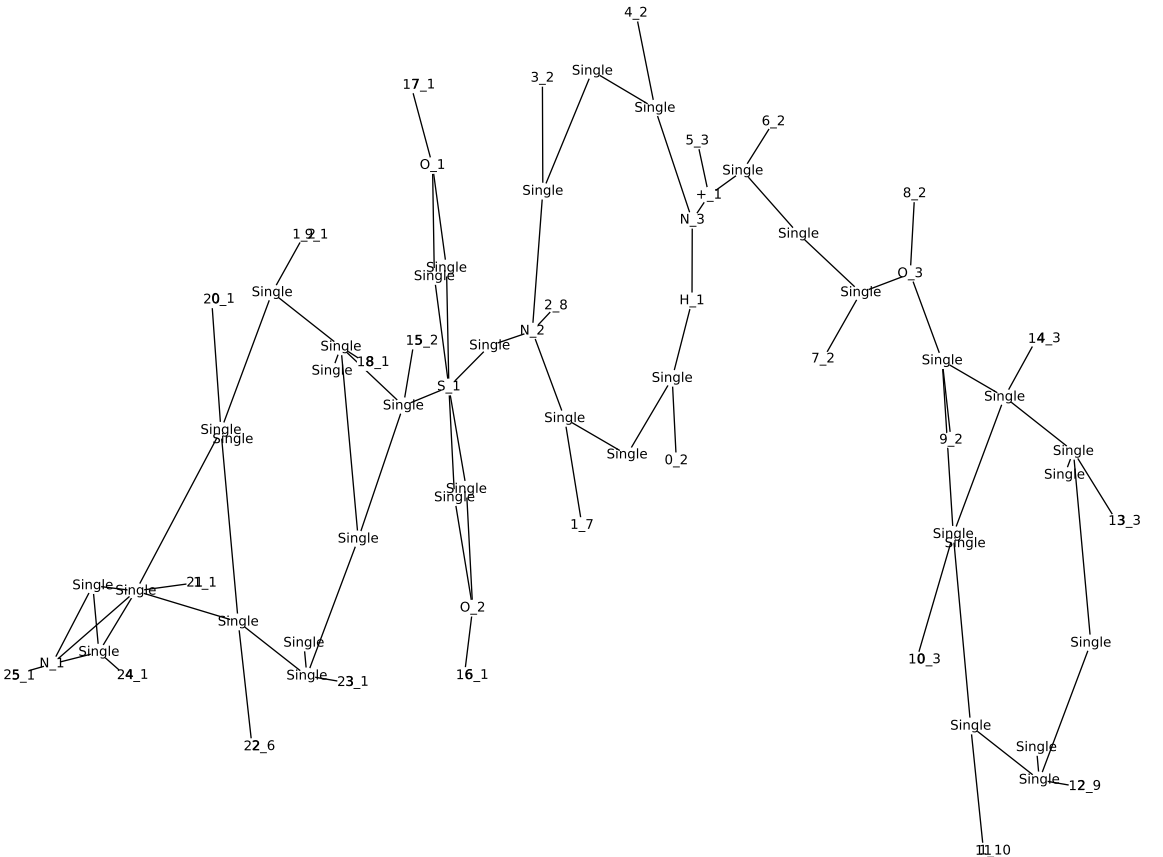9301115_rdkit