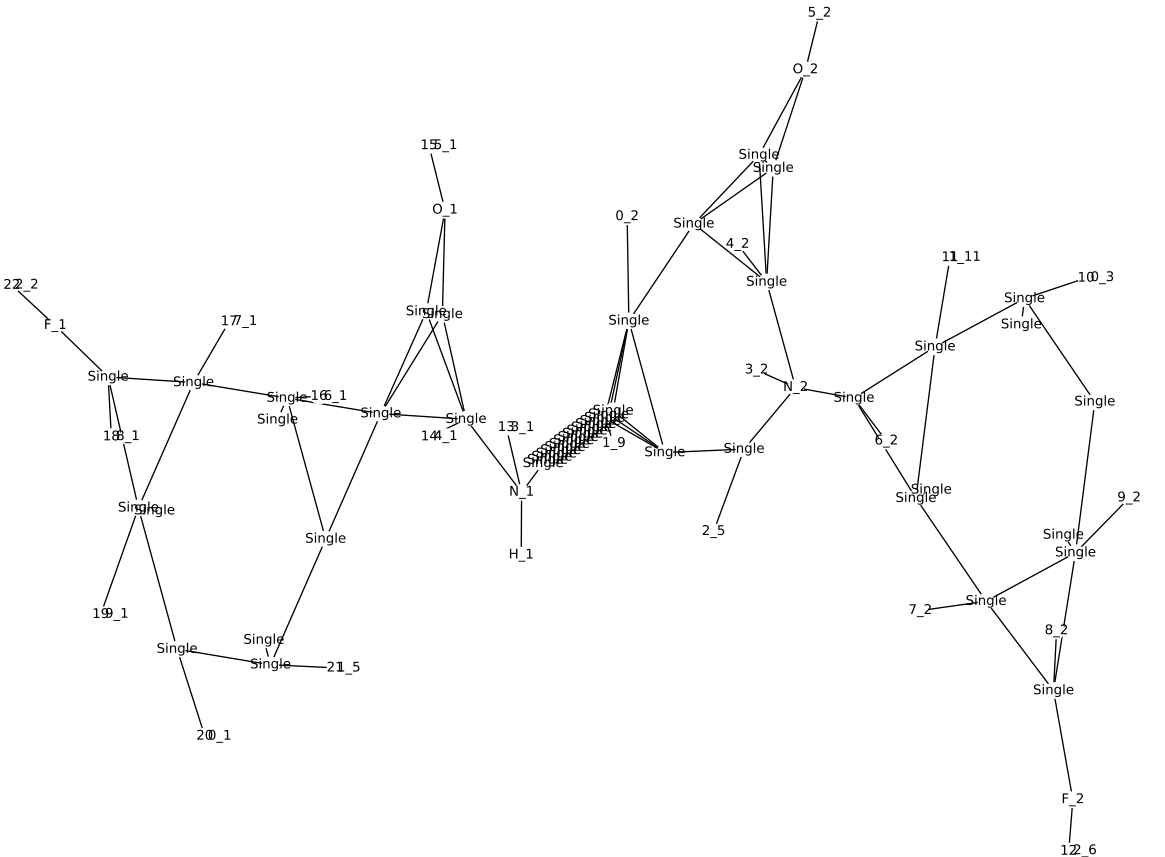7563399_rdkit