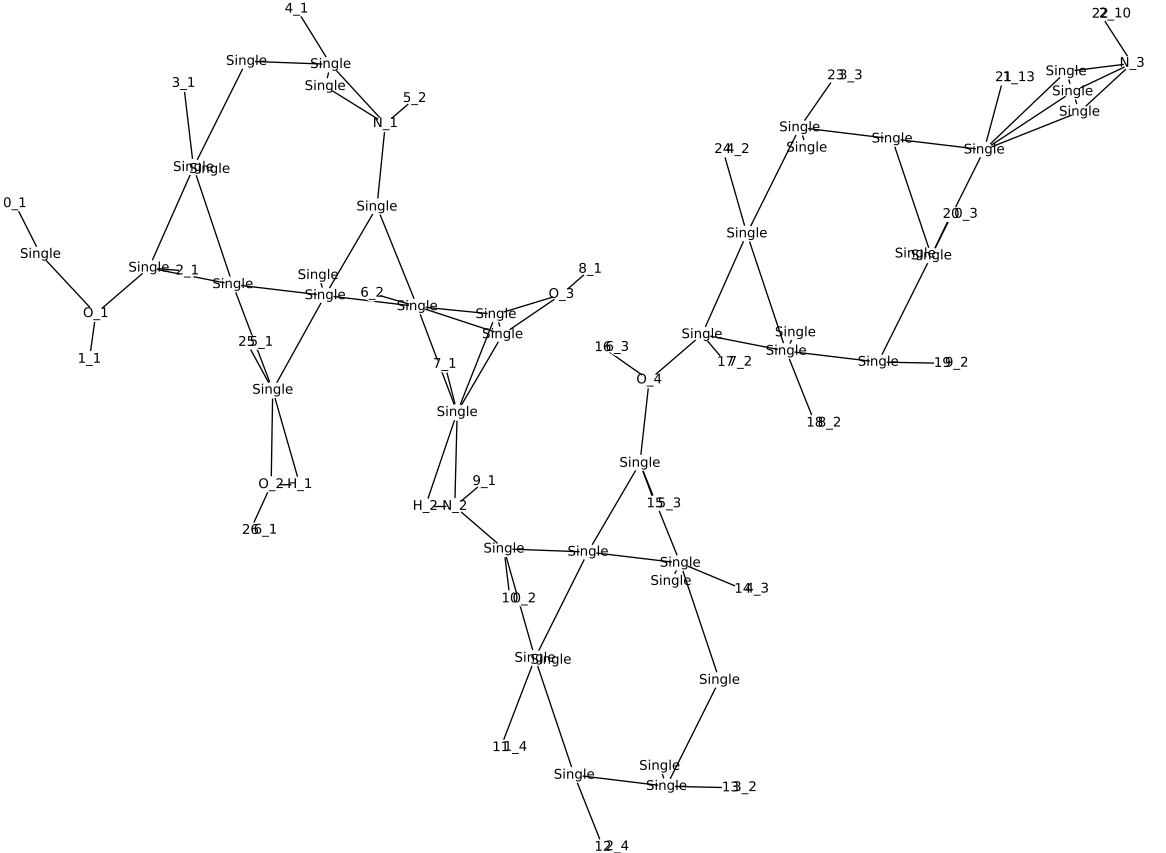USRE039991-20080101-C00312_rdkit