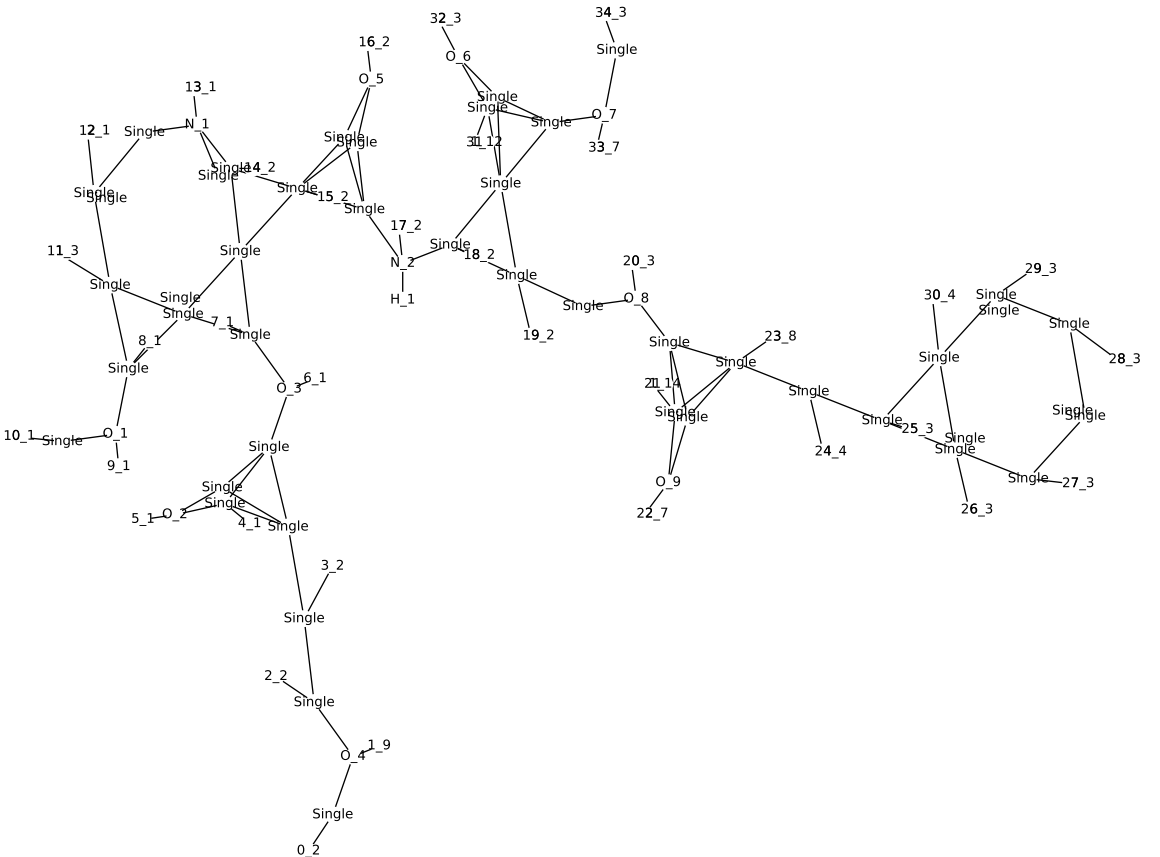USRE039991-20080101-C00476_rdkit